



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 04:36 PM UTC

PDB ID : 7A5G / pdb_00007a5g
EMDB ID : EMD-11642
Title : Structure of the elongating human mitoribosome bound to mtEF-Tu.GMPPCP and A/T mt-tRNA
Authors : Desai, N.; Yang, H.; Chandrasekaran, V.; Kazi, R.; Minczuk, M.; Ramakrishnan, V.
Deposited on : 2020-08-21
Resolution : 4.33 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:

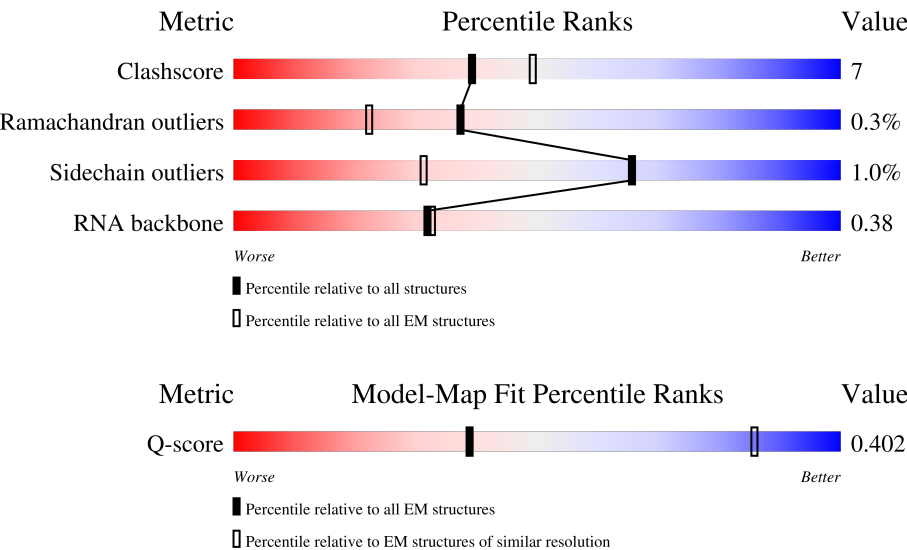
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 4.33 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	3854 (3.83 - 4.83)

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	
2	A3	1559	
3	B3	69	

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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	13	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	

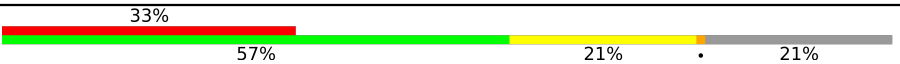
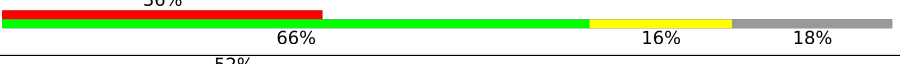
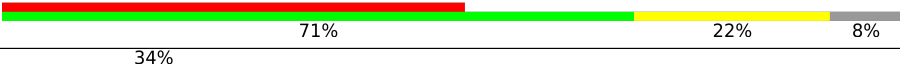
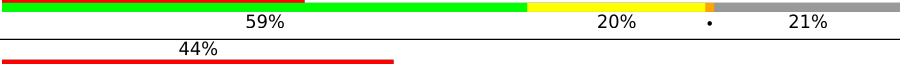
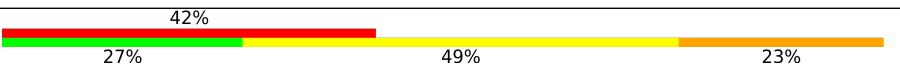
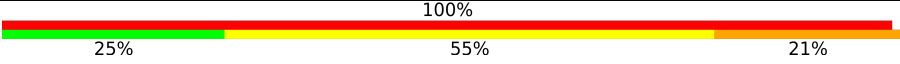
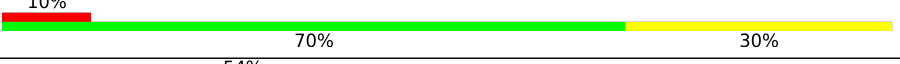
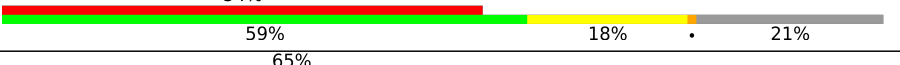
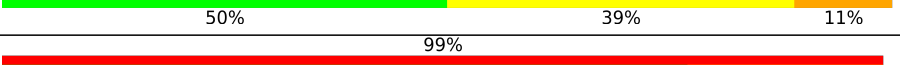
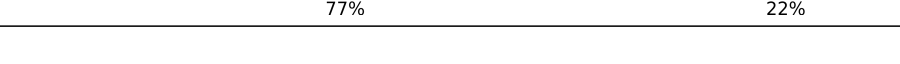
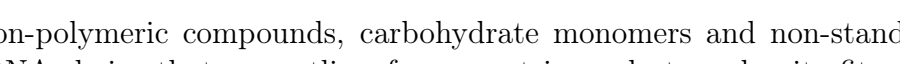
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Mol	Chain	Length	Quality of chain
52	t3	467	
53	u3	2	
54	A5	28	
55	B6	296	
56	C6	167	
57	D6	430	
58	E6	125	
59	F6	242	
60	G6	396	
61	H6	201	
62	I6	194	
63	J6	138	
64	K6	128	
65	L6	257	
66	M6	137	
67	N6	130	
68	O6	258	
69	P6	142	
70	Q6	87	
71	R6	360	
72	S6	190	
73	T6	173	
74	U6	205	
75	V6	414	
76	W6	187	

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Mol	Chain	Length	Quality of chain
77	X6	398	
78	Y6	395	
79	Z6	106	
80	a6	218	
81	b6	323	
82	c6	118	
83	d6	199	
84	e6	689	
85	A6	954	
86	24	73	
86	C	73	
87	i4	10	
88	A	206	
89	Z	452	
90	j	76	
91	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
100	CL	n	307	-	-	X	-

2 Entry composition

There are 101 unique types of molecules in this entry. The entry contains 170507 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-tRNAVal.

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, 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 RNA chain called RNA (5'-R(P*CP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
53	u3	2	Total	C	N	O	P	0	0
			42	19	8	13	2		

- Molecule 54 is a protein called Oxa1L tail.

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

- Molecule 55 is a protein called 28S ribosomal protein S2, mitochondrial.

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

- Molecule 56 is a protein called 28S ribosomal protein S24, mitochondrial.

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

- Molecule 57 is a protein called 28S ribosomal protein S5, mitochondrial.

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

- Molecule 58 is a protein called 28S ribosomal protein S6, mitochondrial.

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

- Molecule 59 is a protein called 28S ribosomal protein S7, mitochondrial.

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

- Molecule 60 is a protein called 28S ribosomal protein S9, mitochondrial.

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

- Molecule 61 is a protein called 28S ribosomal protein S10, mitochondrial.

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

- Molecule 62 is a protein called 28S ribosomal protein S11, mitochondrial.

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

- Molecule 63 is a protein called 28S ribosomal protein S12, mitochondrial.

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

- Molecule 64 is a protein called 28S ribosomal protein S14, mitochondrial.

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

- Molecule 65 is a protein called 28S ribosomal protein S15, mitochondrial.

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

- Molecule 66 is a protein called 28S ribosomal protein S16, mitochondrial.

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

- Molecule 67 is a protein called 28S ribosomal protein S17, mitochondrial.

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

- Molecule 68 is a protein called 28S ribosomal protein S18b, mitochondrial.

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

- Molecule 69 is a protein called 28S ribosomal protein S18c, mitochondrial.

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

- Molecule 70 is a protein called 28S ribosomal protein S21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	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 71 is a protein called 28S ribosomal protein S22, mitochondrial.

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

- Molecule 72 is a protein called 28S ribosomal protein S23, mitochondrial.

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

- Molecule 73 is a protein called 28S ribosomal protein S25, mitochondrial.

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

- Molecule 74 is a protein called 28S ribosomal protein S26, mitochondrial.

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

- Molecule 75 is a protein called 28S ribosomal protein S27, mitochondrial.

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

- Molecule 76 is a protein called 28S ribosomal protein S28, mitochondrial.

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

- Molecule 77 is a protein called 28S ribosomal protein S29, mitochondrial.

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

- Molecule 78 is a protein called 28S ribosomal protein S31, mitochondrial.

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

- Molecule 79 is a protein called 28S ribosomal protein S33, mitochondrial.

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

- Molecule 80 is a protein called 28S ribosomal protein S34, mitochondrial.

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

- Molecule 81 is a protein called 28S ribosomal protein S35, mitochondrial.

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

- Molecule 82 is a protein called Coiled-coil-helix-coiled-coil-helix domain-containing protein 1.

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

- Molecule 83 is a protein called Aurora kinase A-interacting protein.

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

- Molecule 84 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

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

- Molecule 85 is a RNA chain called 12S rRNA.

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

- Molecule 86 is a RNA chain called P tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	24	73	Total	C	N	O	P	0	0
			1547	696	280	499	72		
86	C	73	Total	C	N	O	P	0	0
			1547	696	280	499	72		

- Molecule 87 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	i4	10	Total	C	N	O	P	0	0
			216	97	41	68	10		

- Molecule 88 is a protein called 39S ribosomal protein L40, mitochondrial.

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

- Molecule 89 is a protein called Elongation factor Tu, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
89	Z	394	Total	C	N	O	S	0	0
			3042	1923	538	566	15		

- Molecule 90 is a RNA chain called E tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
90	j	76	Total	C	N	O	P	0	0
			1616	723	291	527	75		

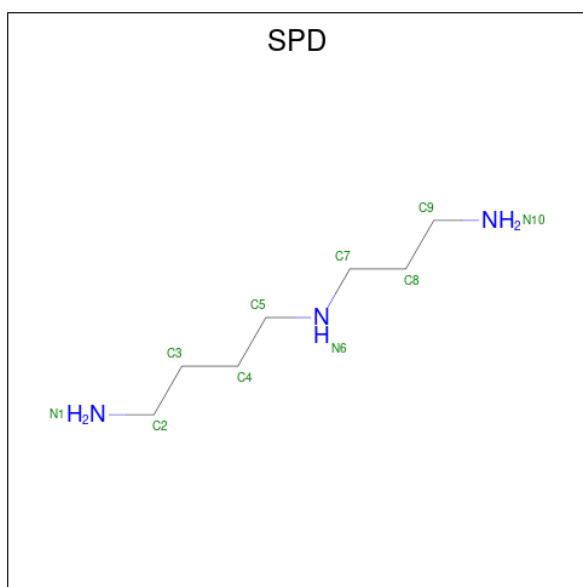
- Molecule 91 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
91	n	228	Total	C	N	O	S	4	0
			1767	1121	321	322	3		

- Molecule 92 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
92	A3	95	Total	Mg	0
			95	95	
92	D3	1	Total	Mg	0
			1	1	
92	M3	1	Total	Mg	0
			1	1	
92	g3	1	Total	Mg	0
			1	1	
92	o3	1	Total	Mg	0
			1	1	
92	A6	28	Total	Mg	0
			28	28	
92	n	1	Total	Mg	0
			1	1	

- Molecule 93 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃).

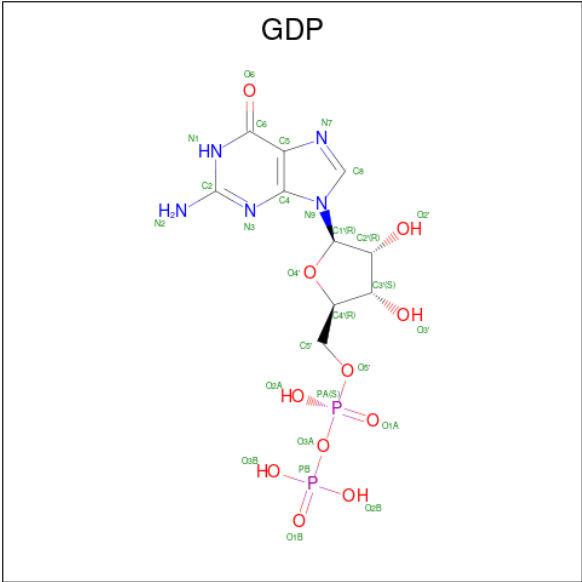


Mol	Chain	Residues	Atoms			AltConf
93	A3	1	Total	C	N	0
			10	7	3	

- Molecule 94 is ZINC ION (CCD ID: ZN) (formula: Zn).

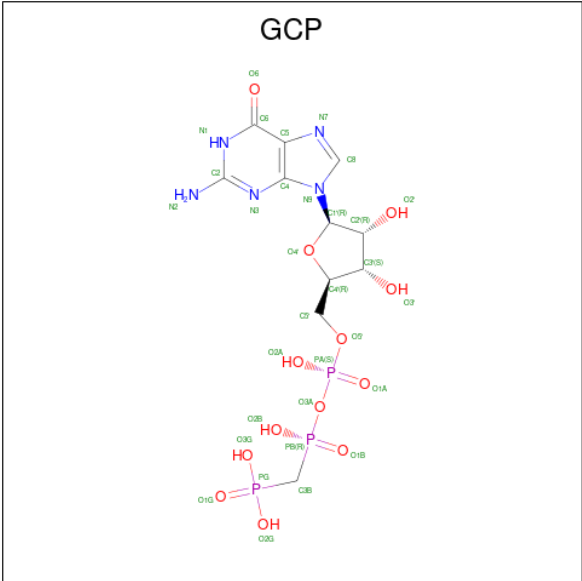
Mol	Chain	Residues	Atoms		AltConf
94	03	1	Total	Zn	0
			1	1	
94	43	1	Total	Zn	0
			1	1	
94	r3	1	Total	Zn	0
			1	1	
94	B6	1	Total	Zn	0
			1	1	
94	O6	1	Total	Zn	0
			1	1	
94	P6	1	Total	Zn	0
			1	1	
94	T6	1	Total	Zn	0
			1	1	

- Molecule 95 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					AltConf
95	X6	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 96 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: C₁₁H₁₈N₅O₁₃P₃).

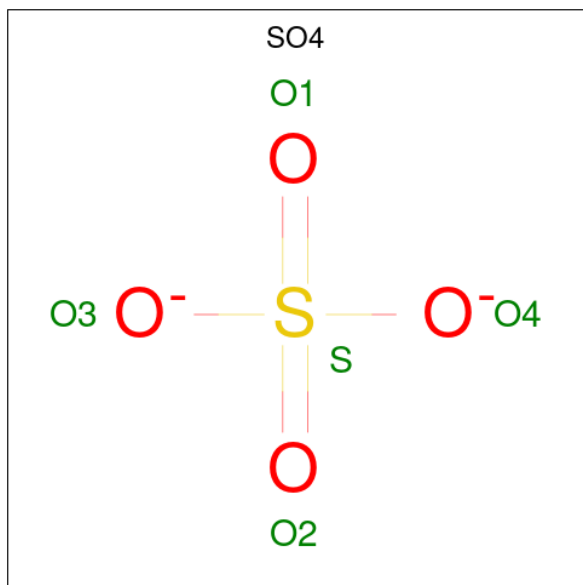


Mol	Chain	Residues	Atoms					AltConf
96	Z	1	Total	C	N	O	P	0
			32	11	5	13	3	

- Molecule 97 is SODIUM ION (CCD ID: NA) (formula: Na).

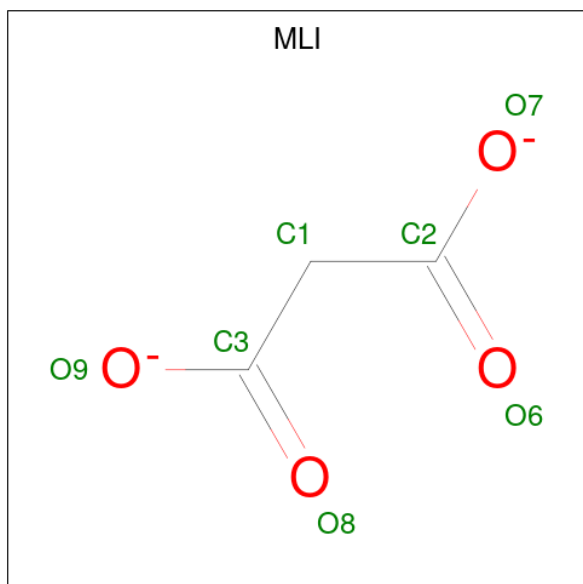
Mol	Chain	Residues	Atoms		AltConf
97	D	2	Total	Na	0
			2	2	
97	n	2	Total	Na	0
			2	2	

- Molecule 98 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

- Molecule 99 is MALONATE ION (CCD ID: MLI) (formula: $C_3H_2O_4$).



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

- Molecule 100 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

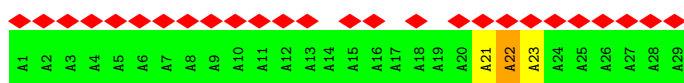
- Molecule 101 is water.

Mol	Chain	Residues	Atoms		AltConf
101	A3	3	Total	O	0
			3	3	
101	D	9	Total	O	0
			9	9	
101	n	67	Total	O	0
			67	67	

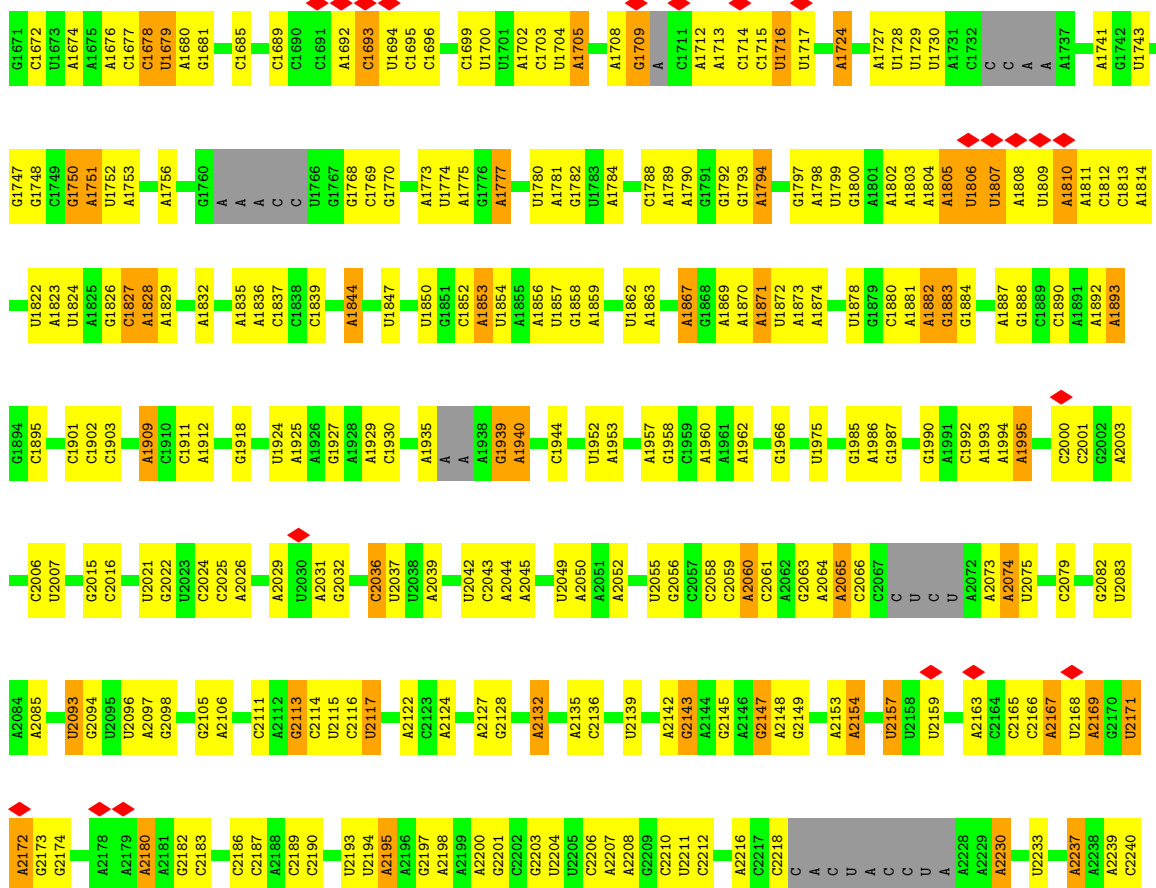
3 Residue-property plots

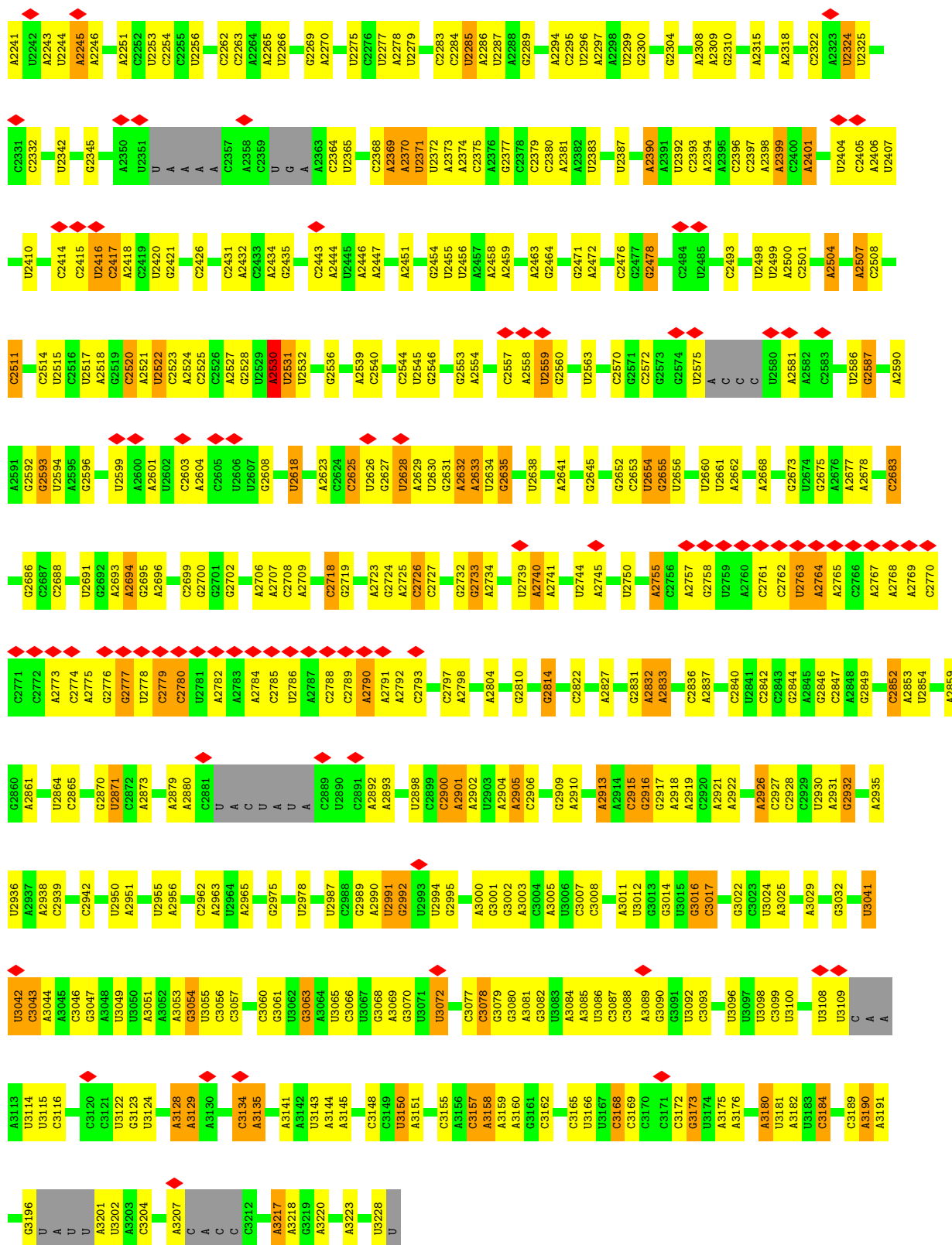
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

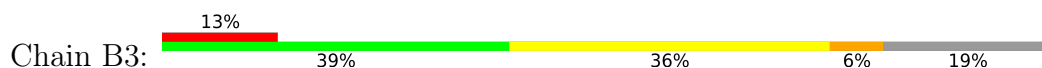


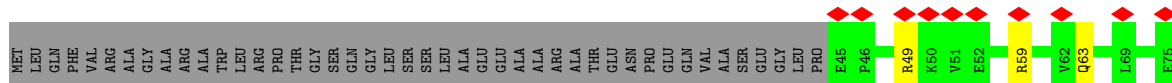
- Molecule 2: 16S rRNA



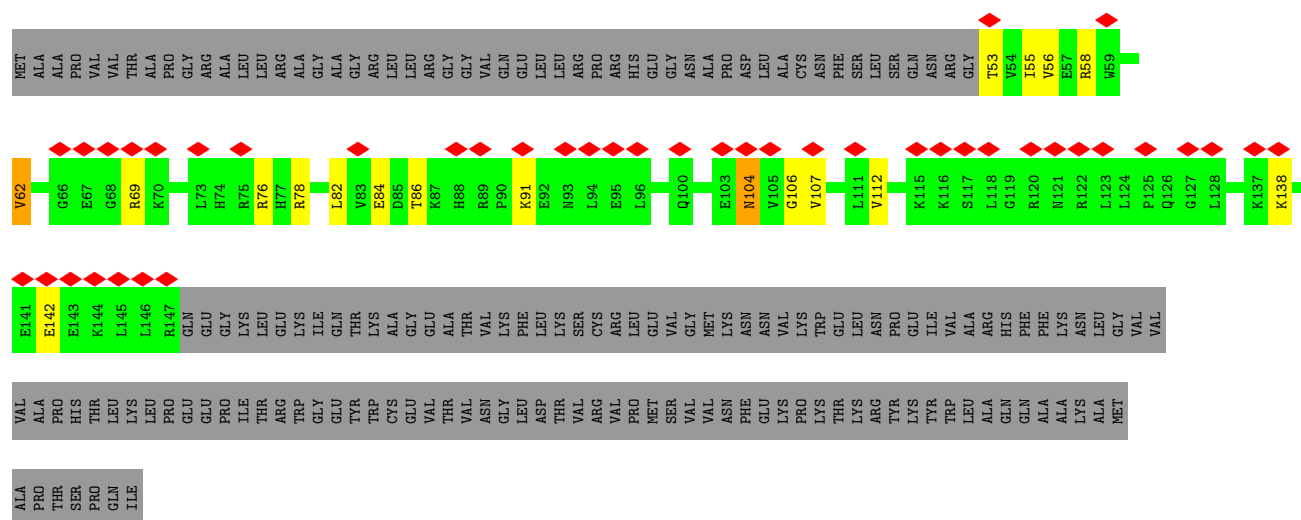


• Molecule 3: mt-tRNA^{Val}

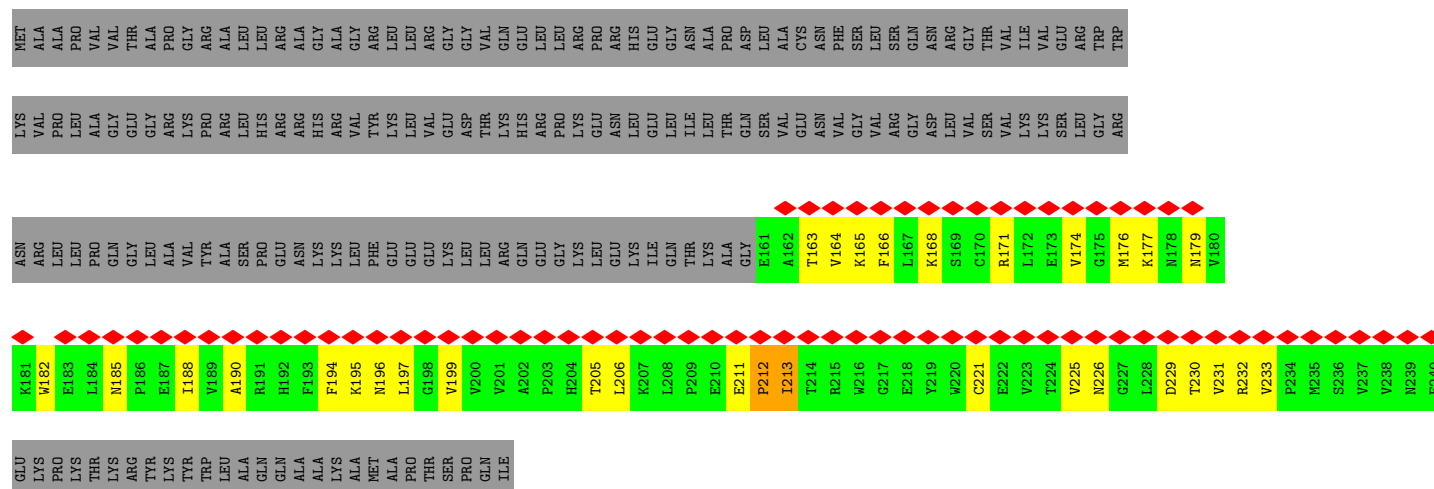




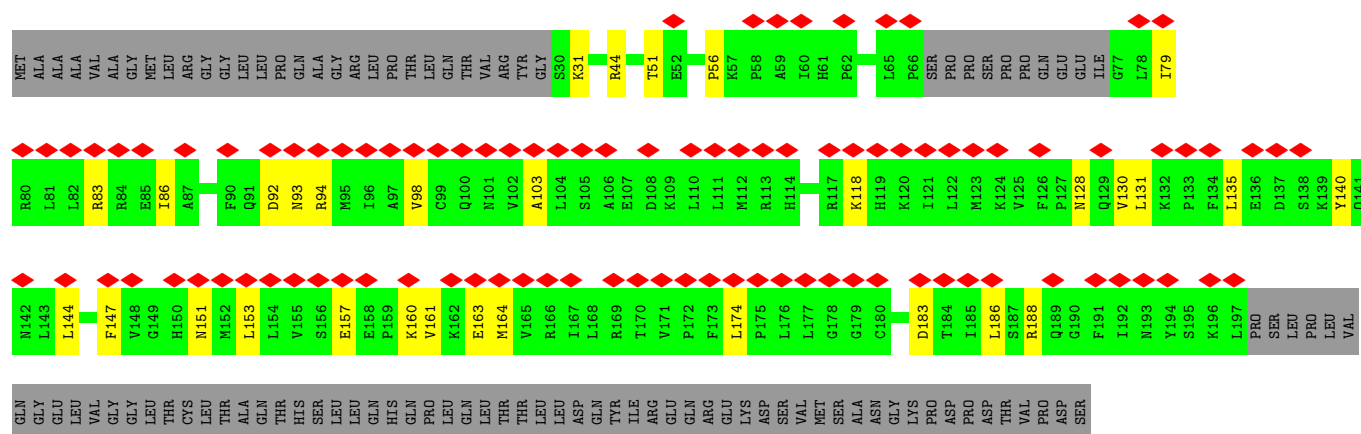
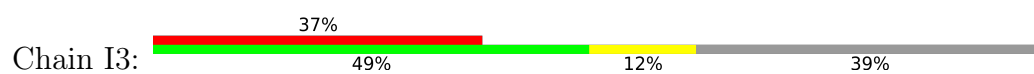
- Molecule 7: 39S ribosomal protein L9, mitochondrial



- Molecule 7: 39S ribosomal protein L9, mitochondrial



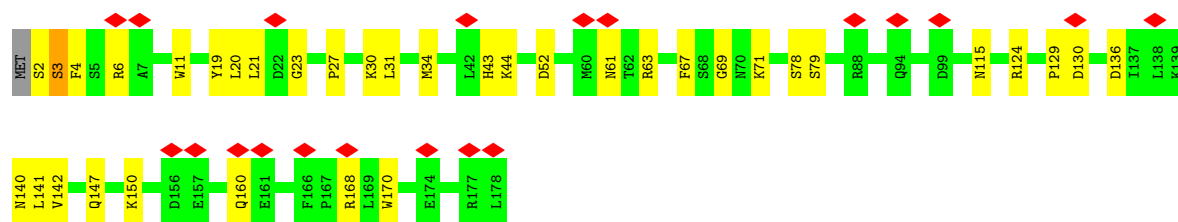
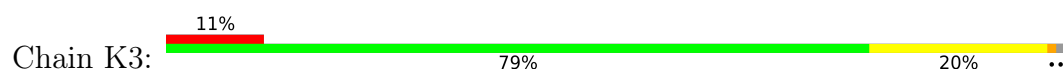
- Molecule 8: 39S ribosomal protein L10, mitochondrial



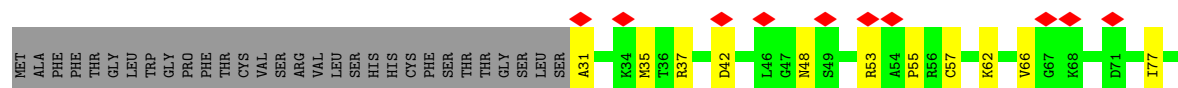
• Molecule 9: 39S ribosomal protein L11, mitochondrial

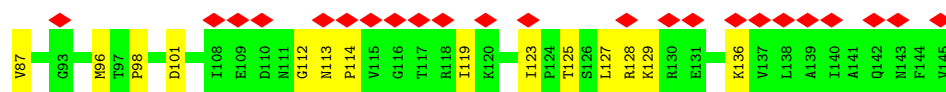


• Molecule 10: 39S ribosomal protein L13, mitochondrial

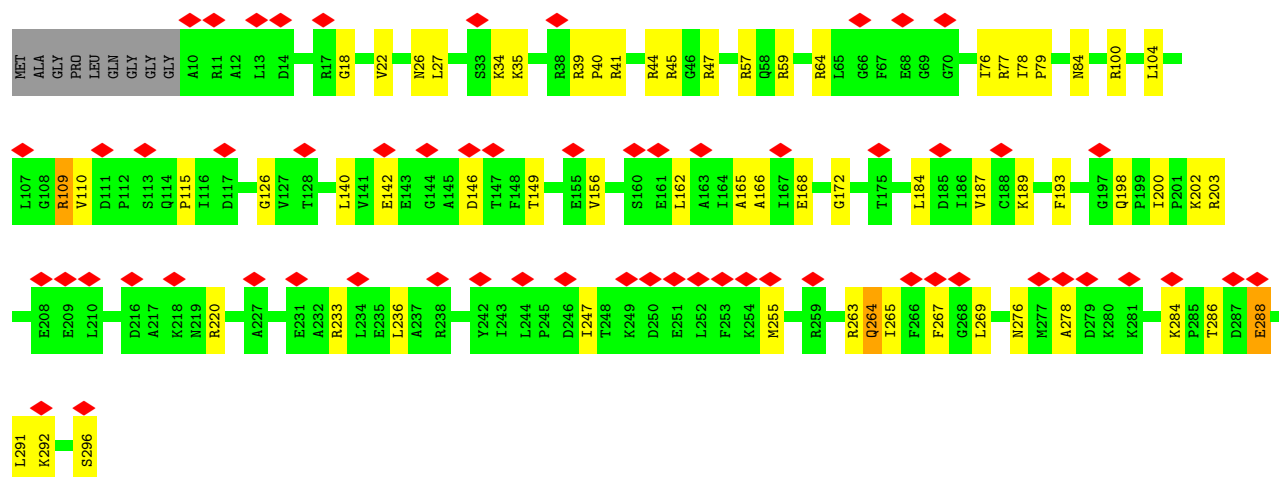
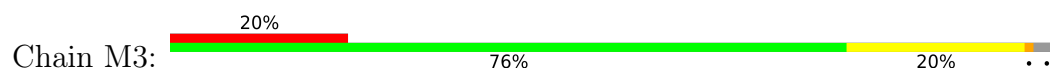


• Molecule 11: 39S ribosomal protein L14, mitochondrial

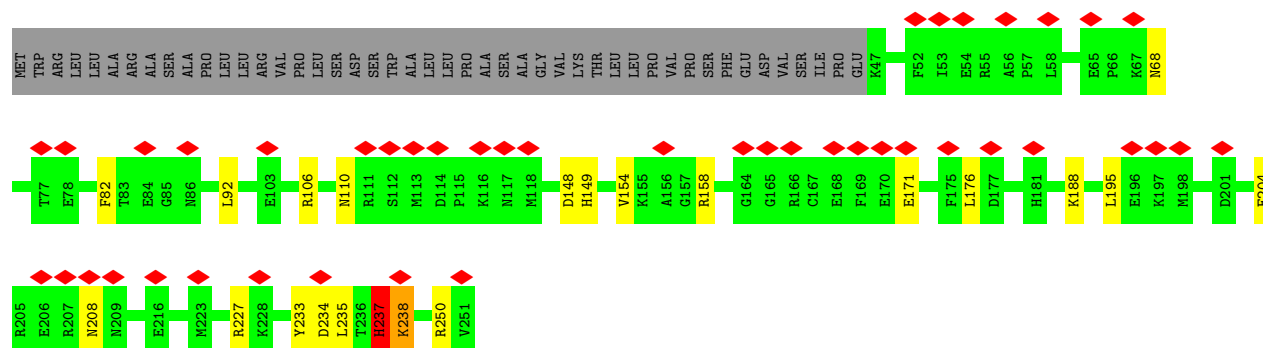
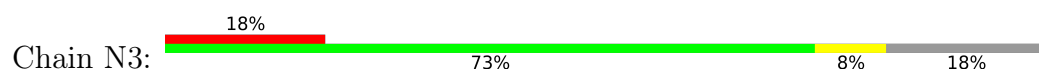




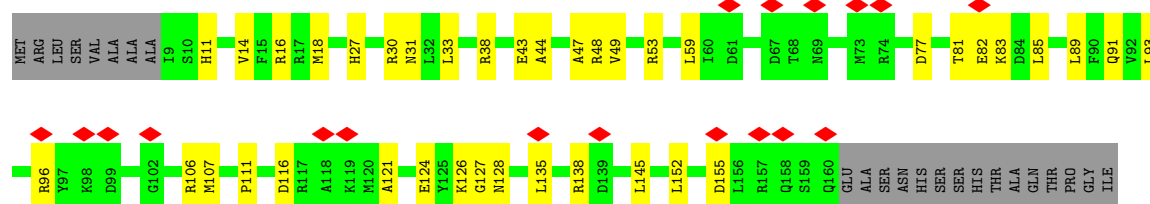
- Molecule 12: 39S ribosomal protein L15, mitochondrial



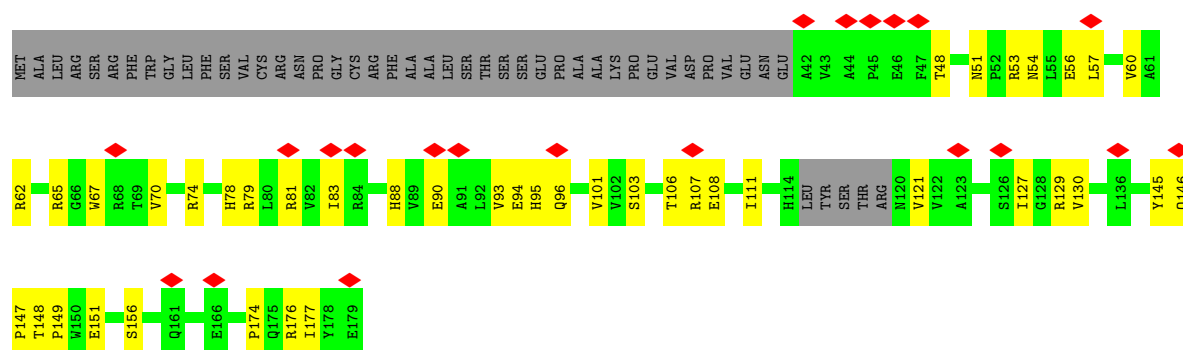
- Molecule 13: 39S ribosomal protein L16, mitochondrial



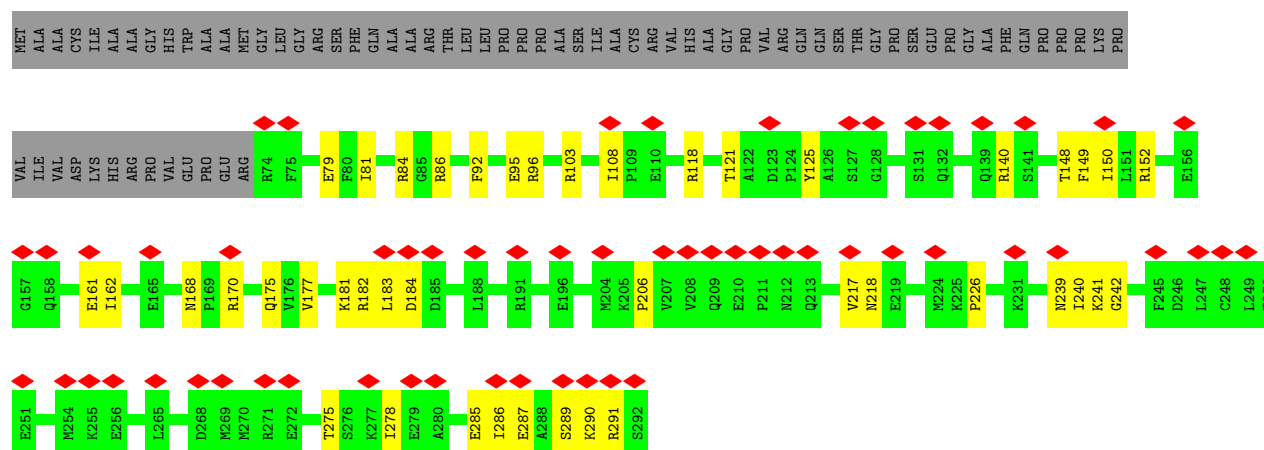
- Molecule 14: 39S ribosomal protein L17, mitochondrial



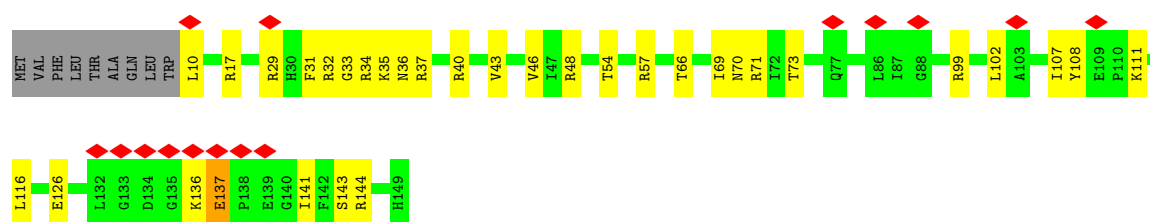
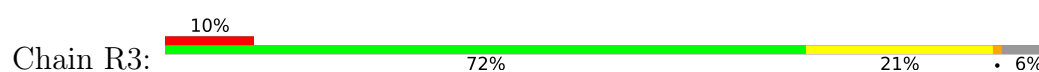
- Molecule 15: 39S ribosomal protein L18, mitochondrial



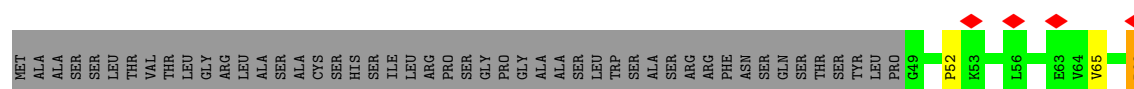
• Molecule 16: 39S ribosomal protein L19, mitochondrial

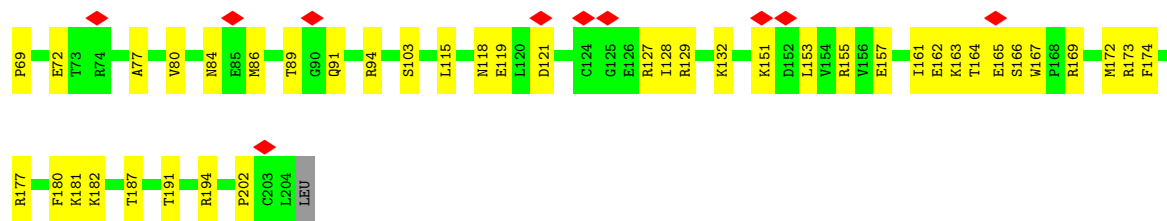


• Molecule 17: 39S ribosomal protein L20, mitochondrial

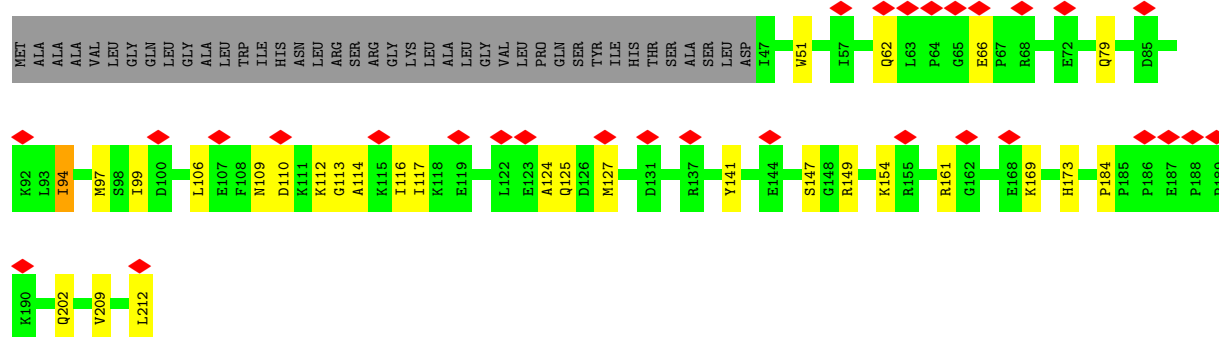


• Molecule 18: 39S ribosomal protein L21, mitochondrial

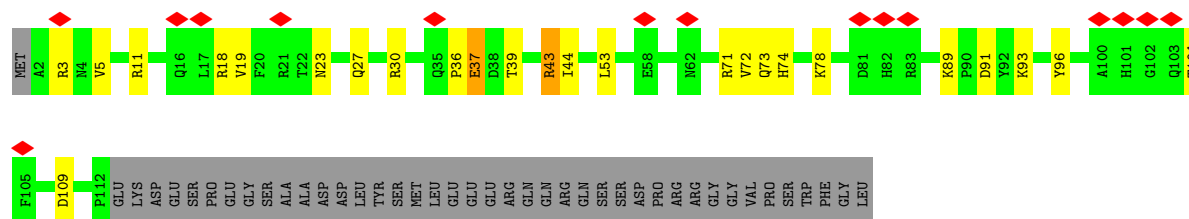




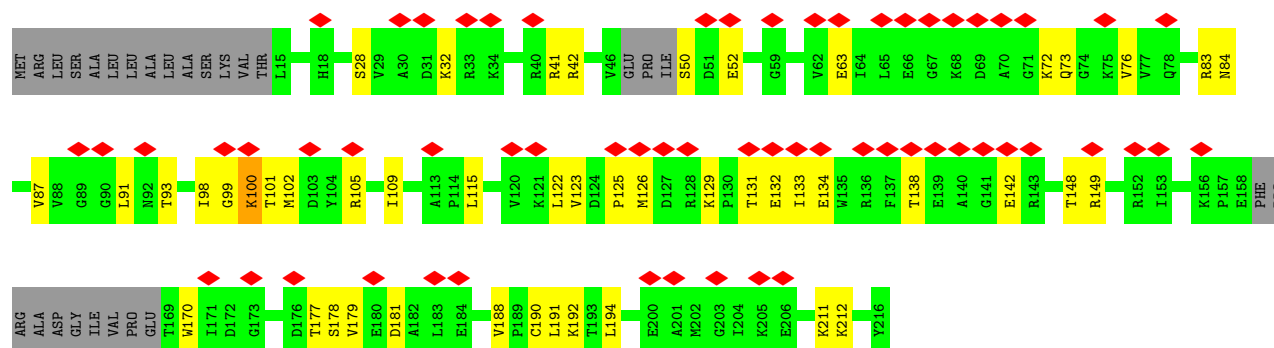
- Molecule 19: 39S ribosomal protein L22, mitochondrial



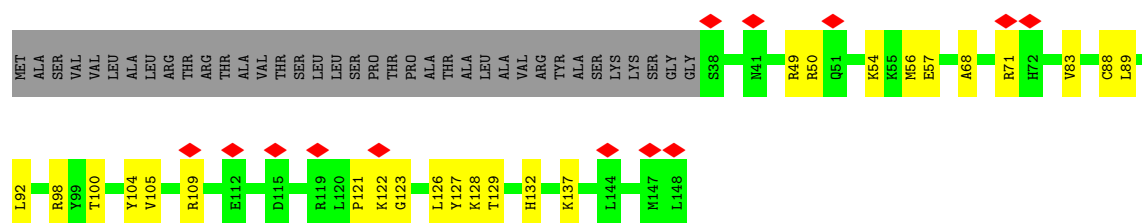
- Molecule 20: 39S ribosomal protein L23, mitochondrial



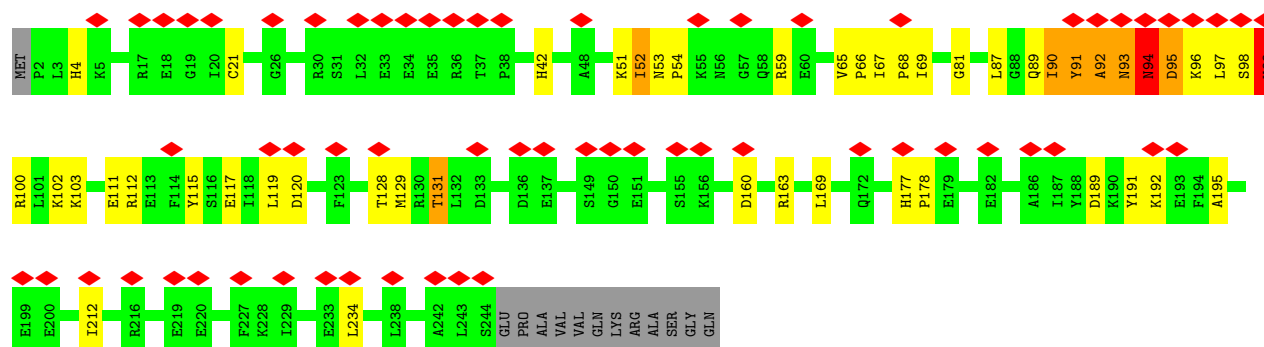
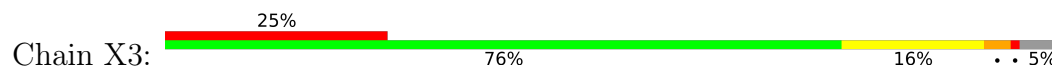
- Molecule 21: 39S ribosomal protein L24, mitochondrial



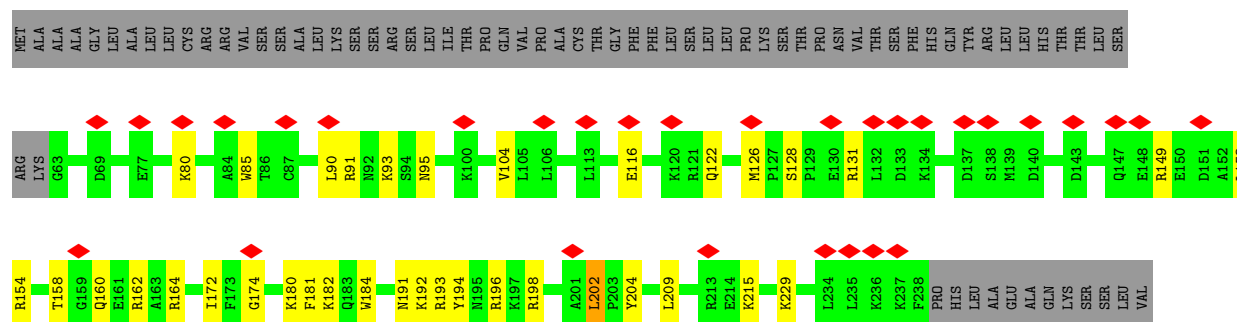
- Molecule 22: 39S ribosomal protein L27, mitochondrial



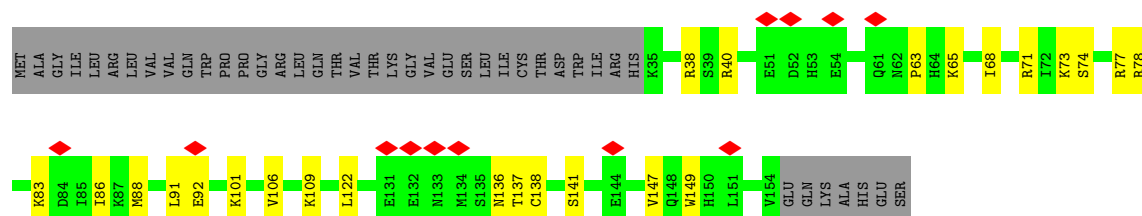
- Molecule 23: 39S ribosomal protein L28, mitochondrial



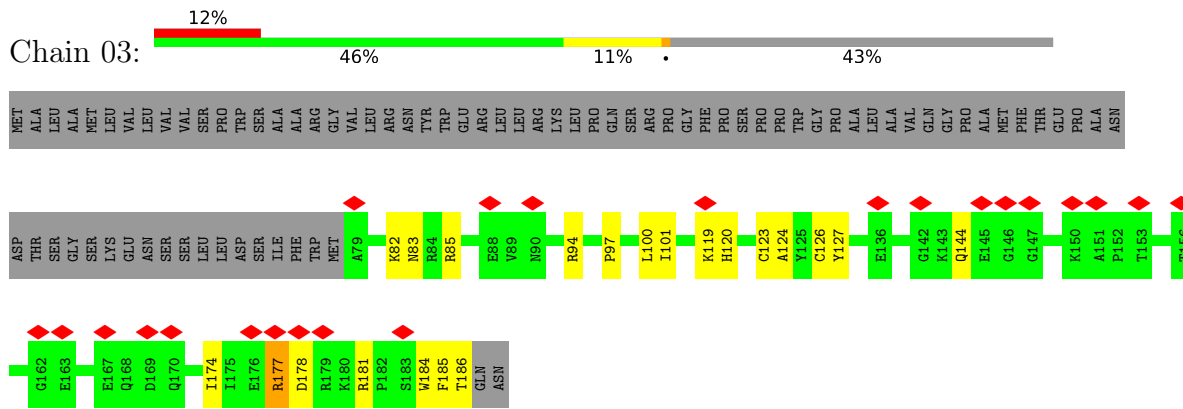
- Molecule 24: 39S ribosomal protein L47, mitochondrial



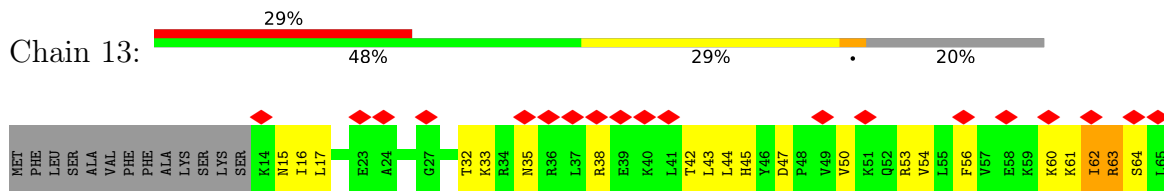
- Molecule 25: 39S ribosomal protein L30, mitochondrial



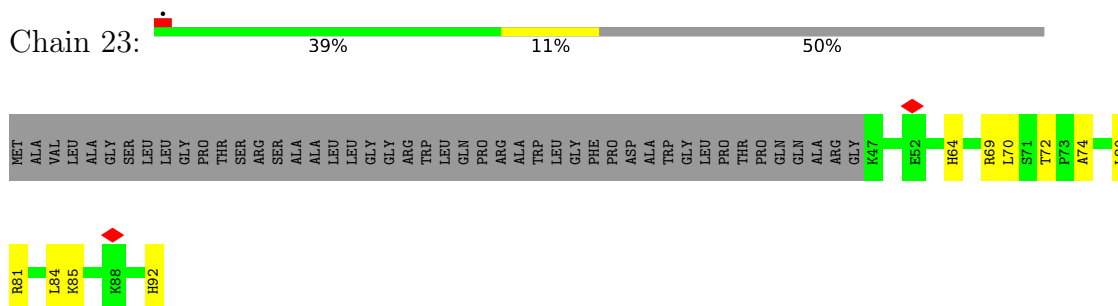
- Molecule 26: 39S ribosomal protein L32, mitochondrial



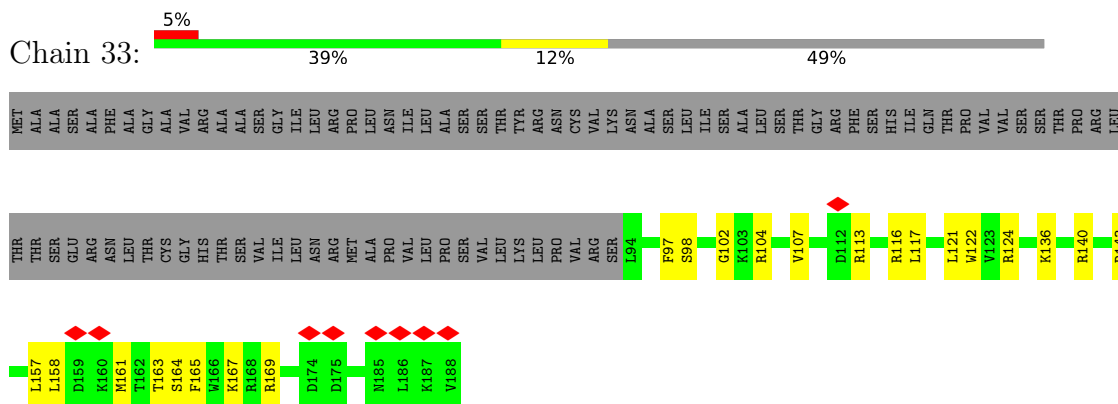
- Molecule 27: 39S ribosomal protein L33, mitochondrial



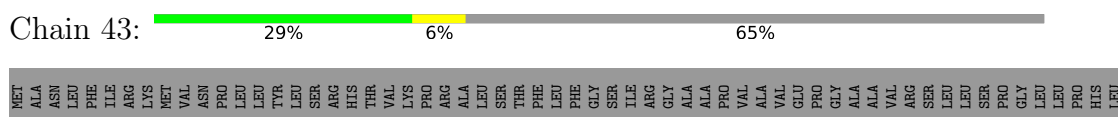
- Molecule 28: 39S ribosomal protein L34, mitochondrial



- Molecule 29: 39S ribosomal protein L35, mitochondrial

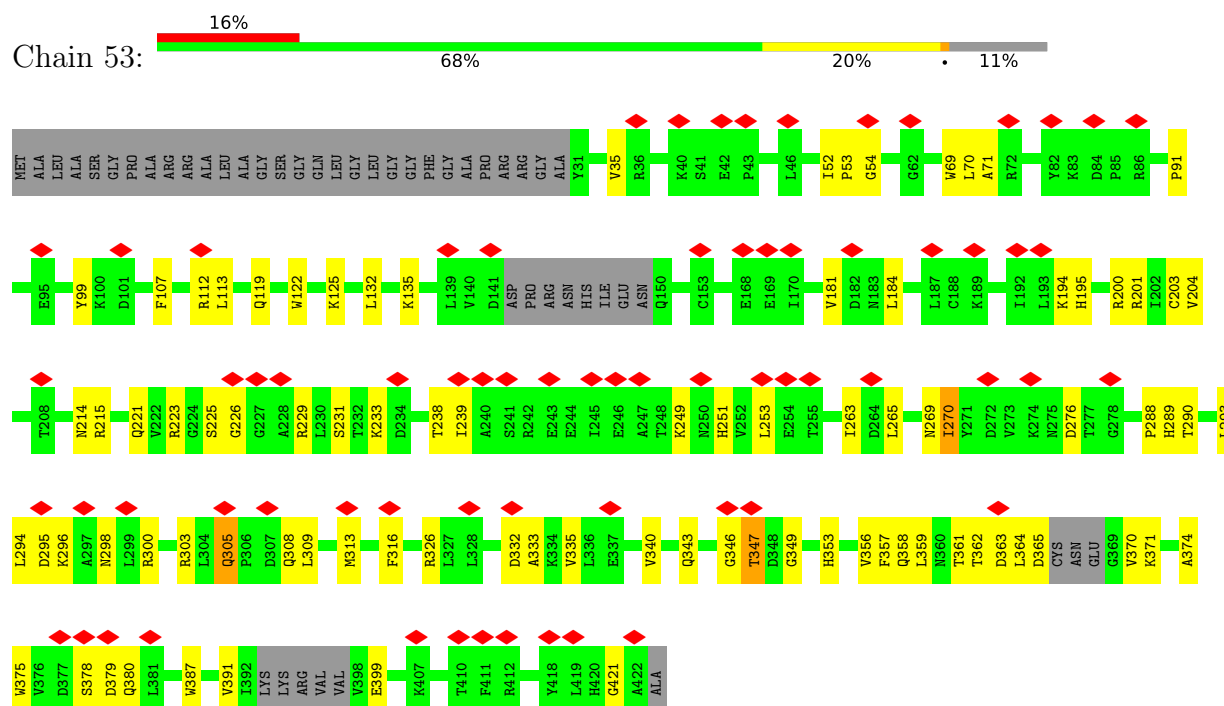


- Molecule 30: 39S ribosomal protein L36, mitochondrial

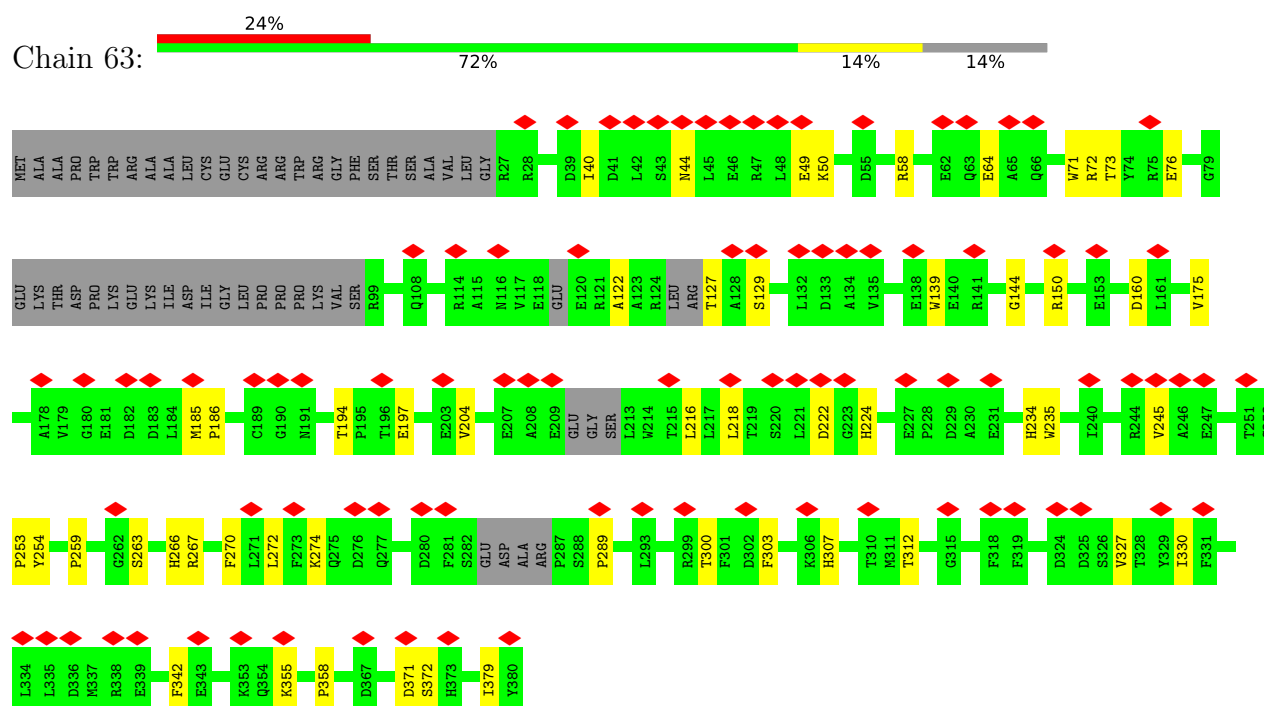




- Molecule 31: 39S ribosomal protein L37, mitochondrial

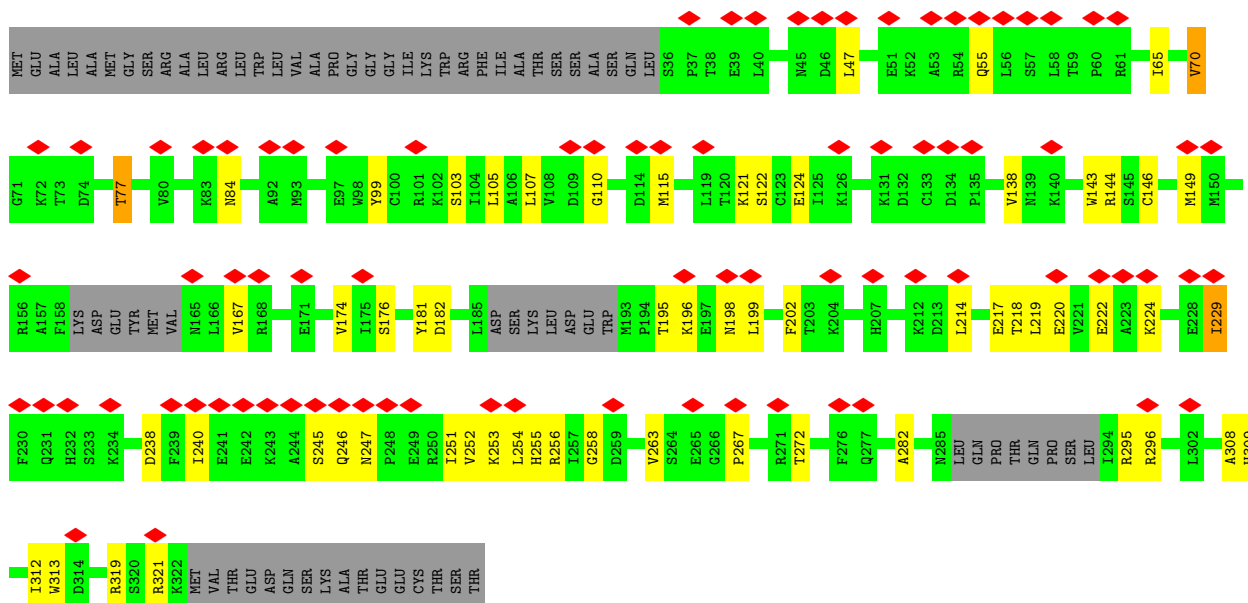


- Molecule 32: 39S ribosomal protein L38, mitochondrial

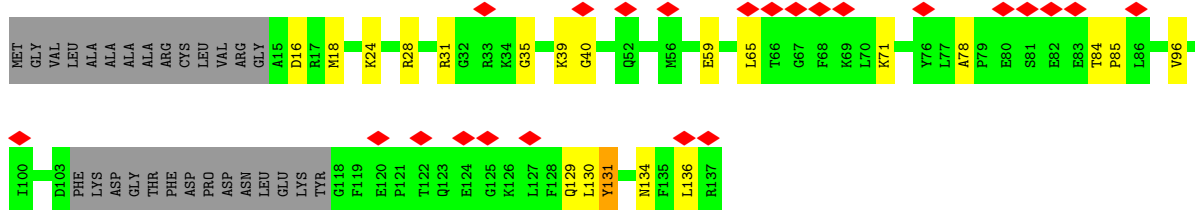


- Molecule 33: 39S ribosomal protein L39, mitochondrial

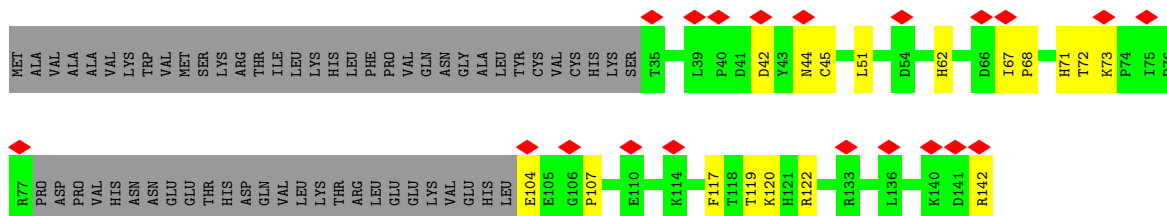




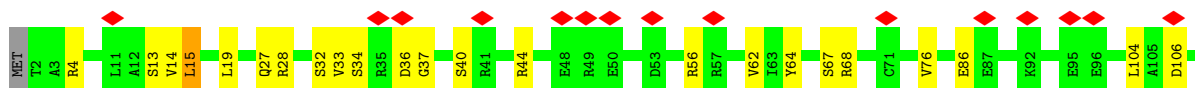
- Molecule 34: 39S ribosomal protein L41, mitochondrial

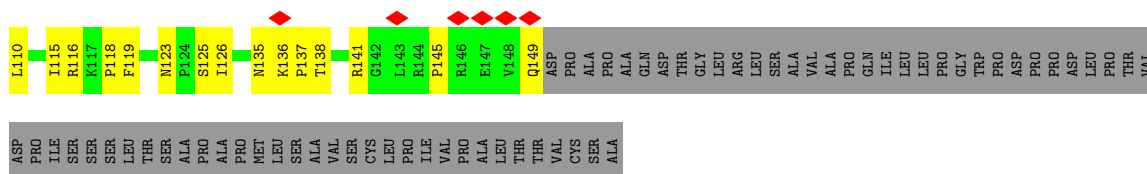


- Molecule 35: 39S ribosomal protein L42, mitochondrial

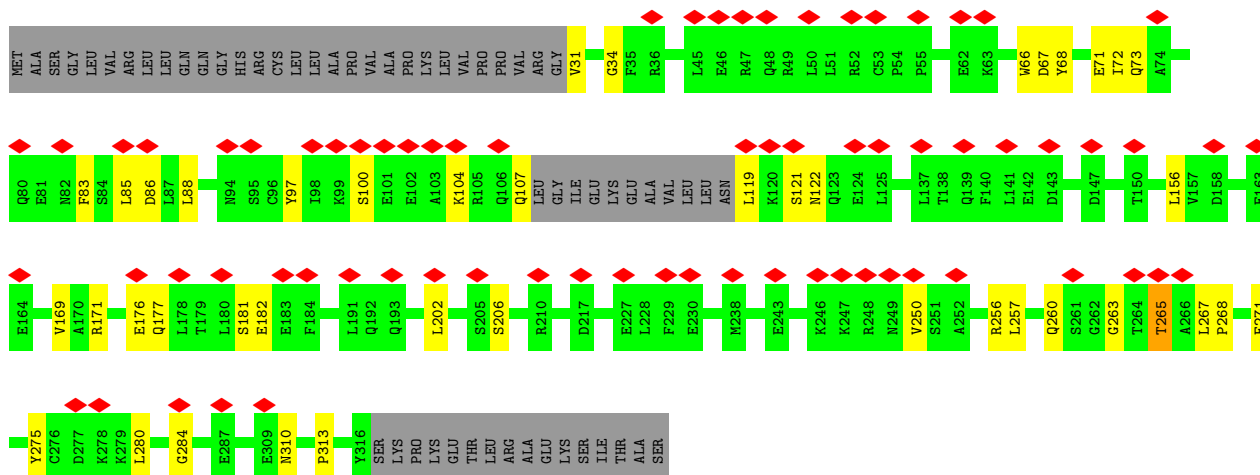


- Molecule 36: 39S ribosomal protein L43, mitochondrial

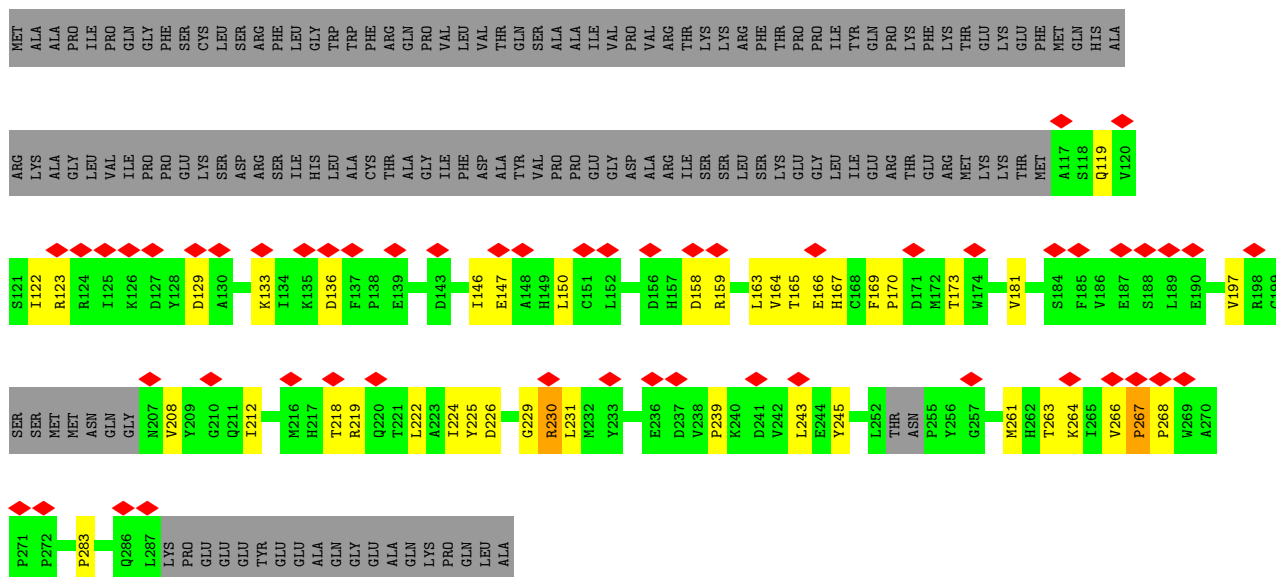
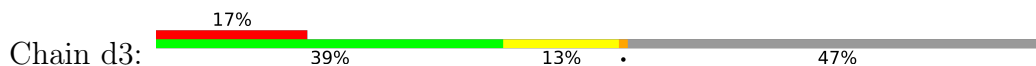




• Molecule 37: 39S ribosomal protein L44, mitochondrial

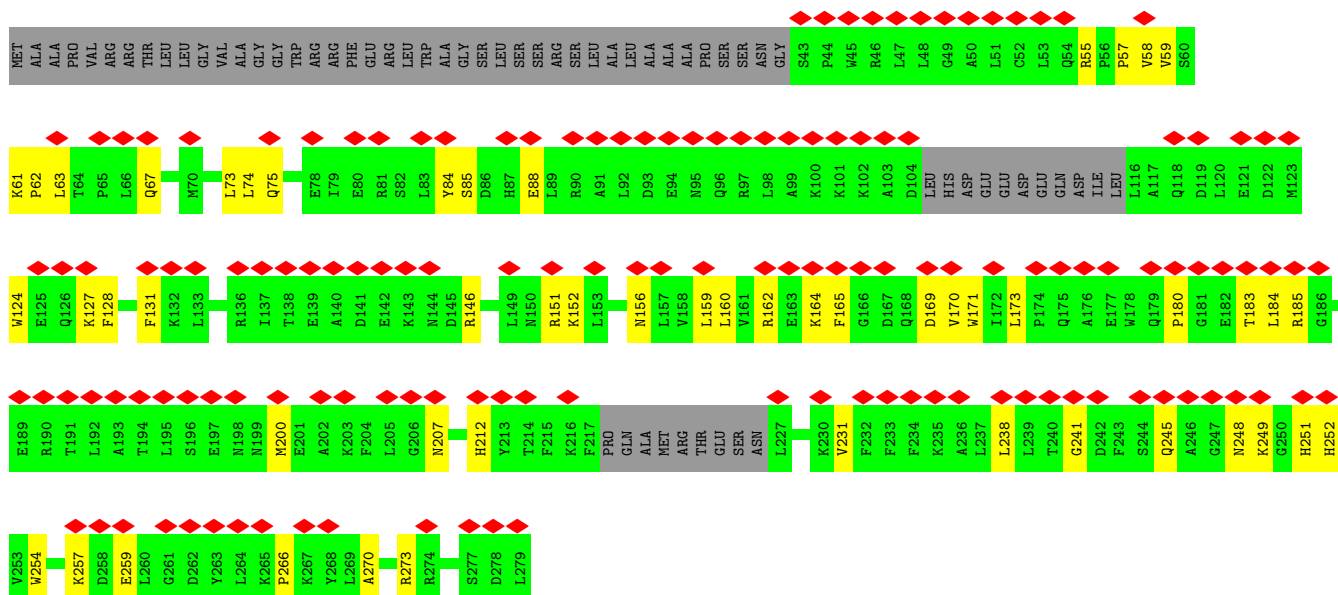


• Molecule 38: 39S ribosomal protein L45, mitochondrial

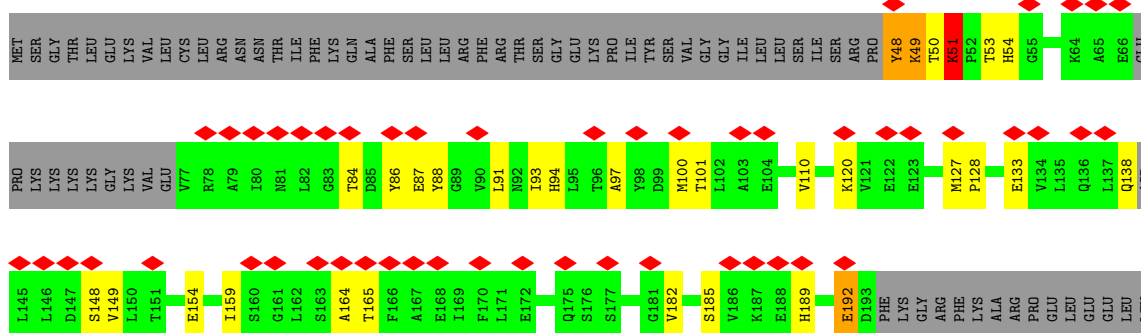


• Molecule 39: 39S ribosomal protein L46, mitochondrial

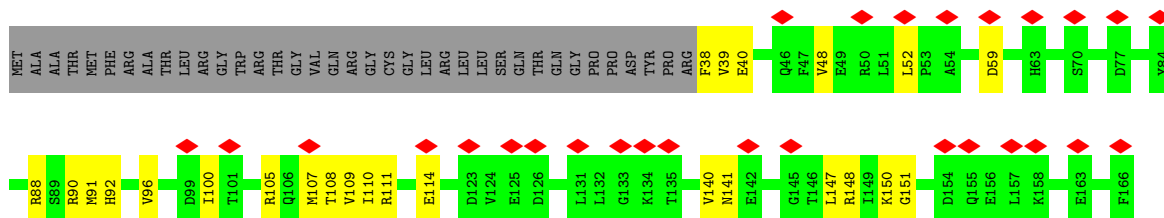




- Molecule 40: 39S ribosomal protein L48, mitochondrial

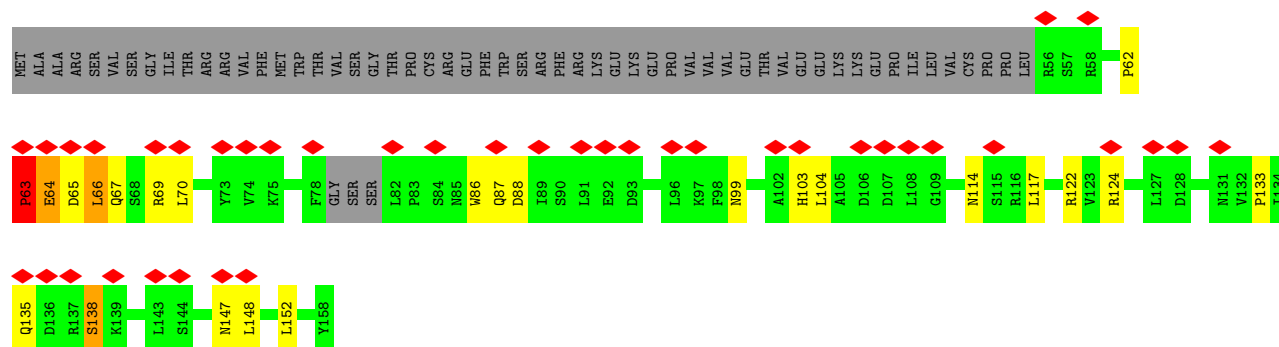


- Molecule 41: 39S ribosomal protein L49, mitochondrial

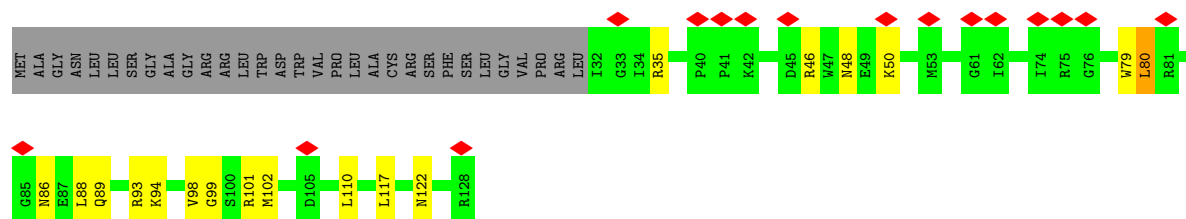


- Molecule 42: 39S ribosomal protein L50, mitochondrial

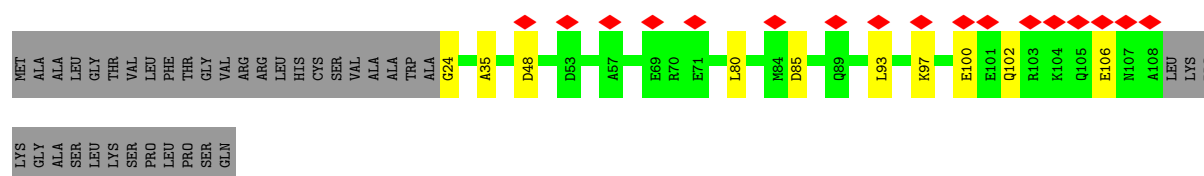




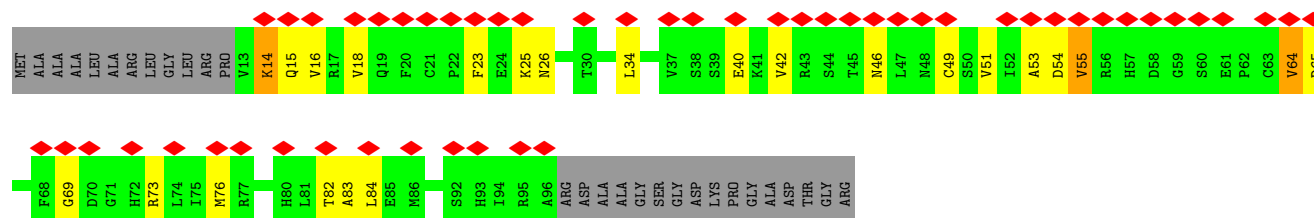
- Molecule 43: 39S ribosomal protein L51, mitochondrial



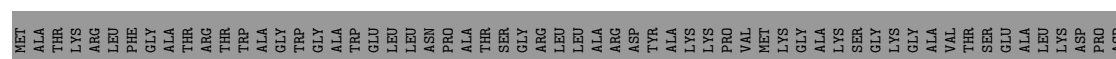
- Molecule 44: 39S ribosomal protein L52, mitochondrial

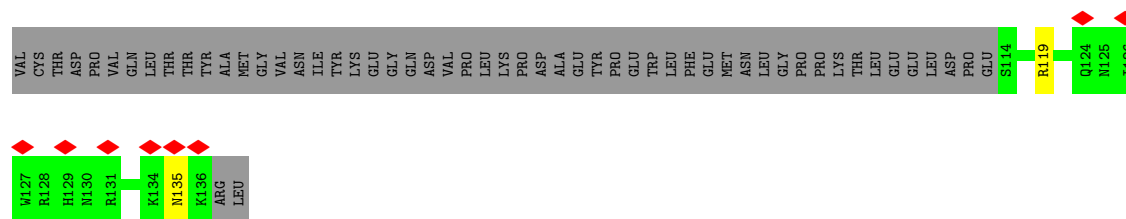


- Molecule 45: 39S ribosomal protein L53, mitochondrial

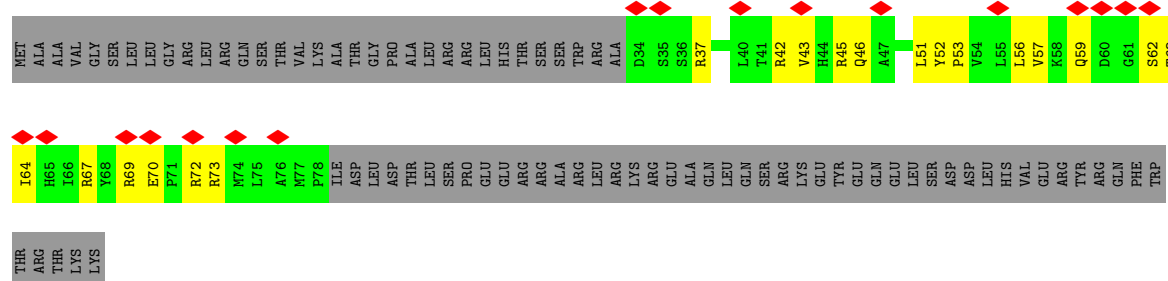


- Molecule 46: 39S ribosomal protein L54, mitochondrial

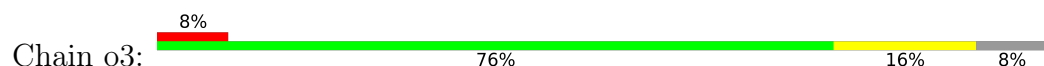




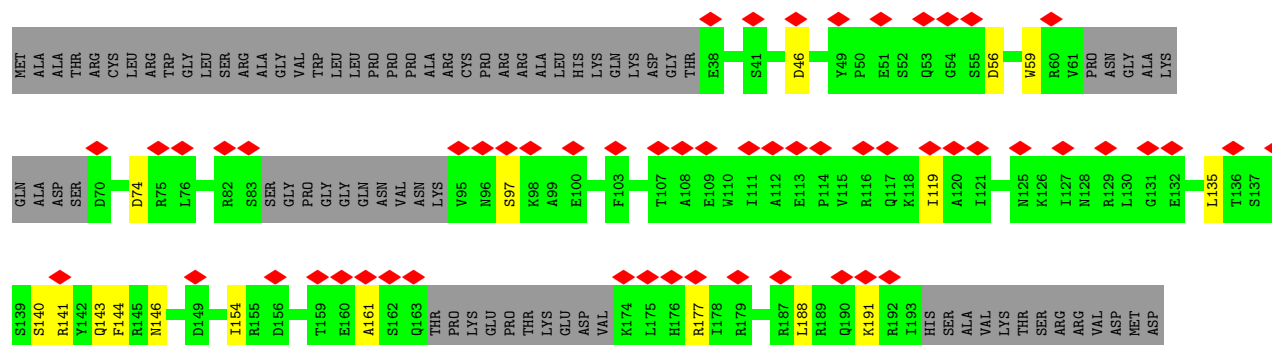
- Molecule 47: 39S ribosomal protein L55, mitochondrial



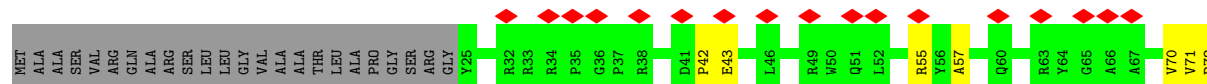
- Molecule 48: Ribosomal protein 63, mitochondrial



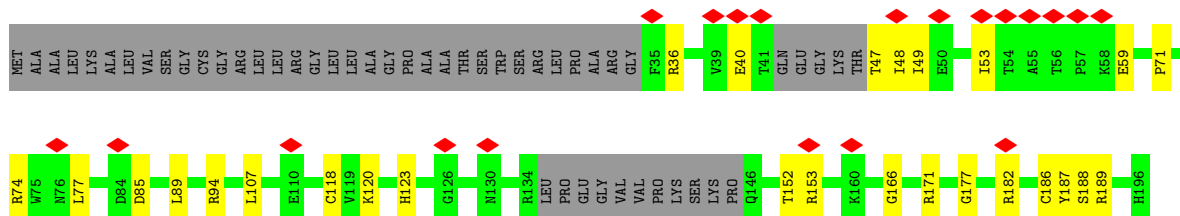
- Molecule 49: Peptidyl-tRNA hydrolase ICT1, mitochondrial



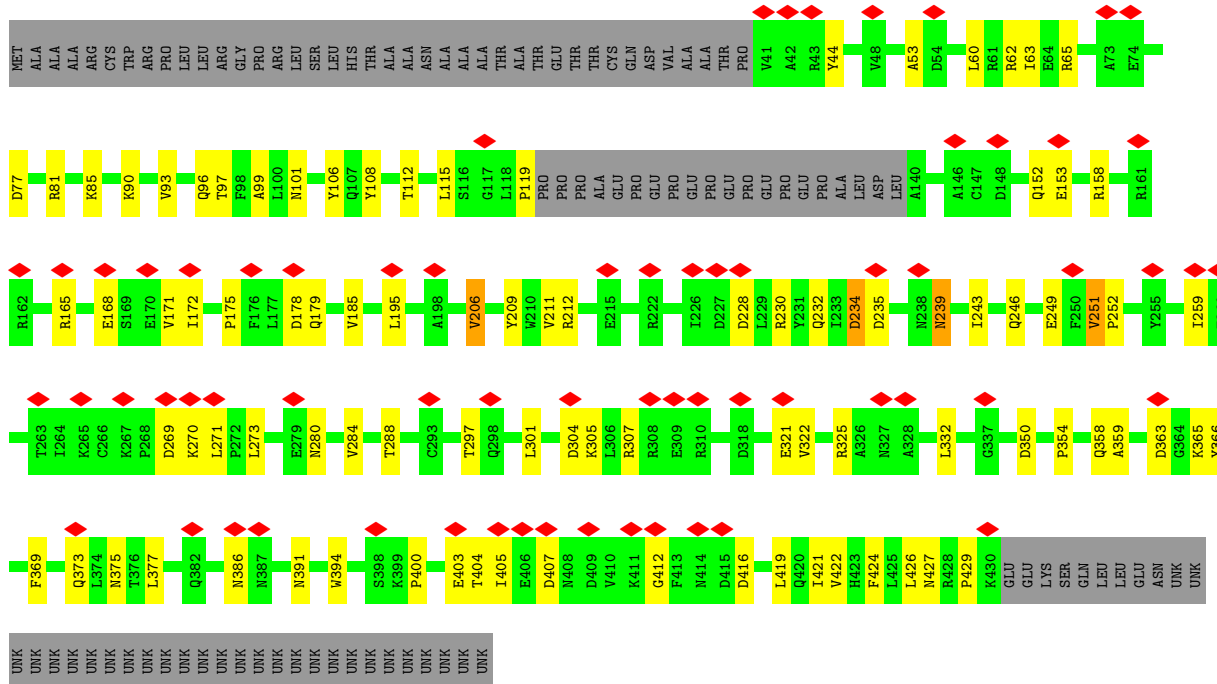
- Molecule 50: Growth arrest and DNA damage-inducible proteins-interacting protein 1



- Molecule 51: 39S ribosomal protein S18a, mitochondrial



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

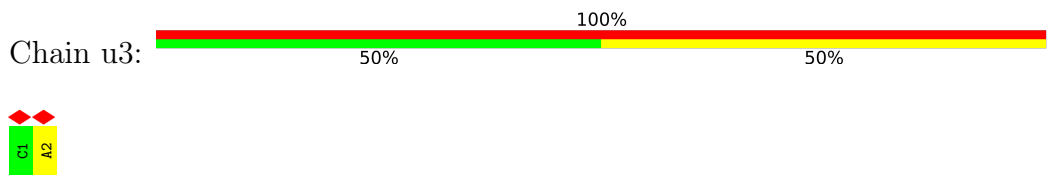


- Molecule 52: 39S ribosomal protein S30, mitochondrial,39S ribosomal protein S30, mitochondrial,mL65

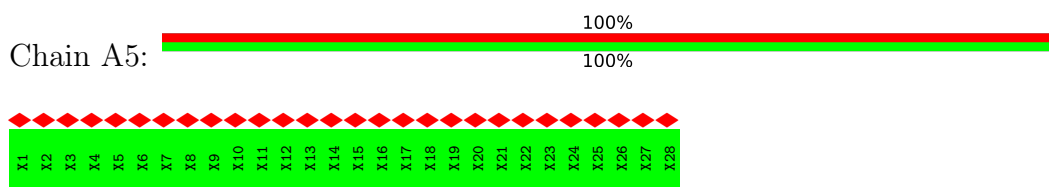


TLE	VAL	HIS	PHE	LEU	LEU	ASN	ARG	PRO	LYS	GLU	GLY	LYS	SER	GLN	LEU	LEU	GLU	ASN	X1	X2	X3	X4	X5	X6	X7	X8	X9	X10	X11	X12	X13	X14	X15		X18	X19	X20	X21	X22	X23	X24	X25	X26	X27	X28
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	----	----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	--	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 53: RNA (5'-R(P*CP*A)-3')



- Molecule 54: Oxa1L tail

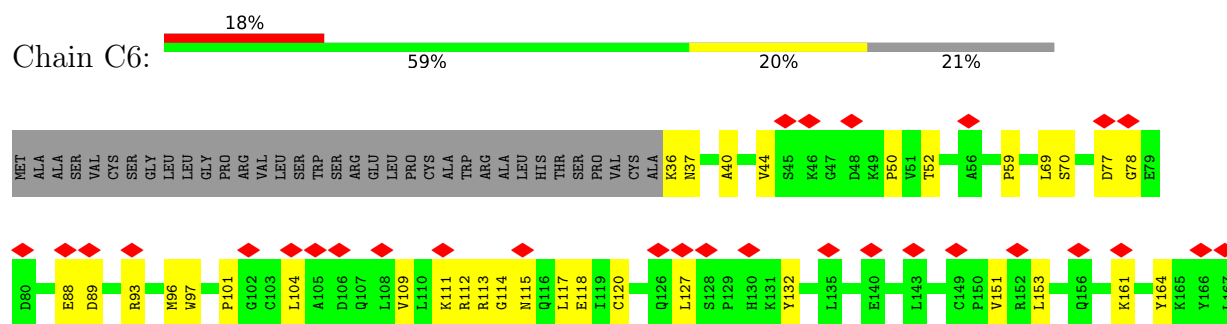


- Molecule 55: 28S ribosomal protein S2, mitochondrial

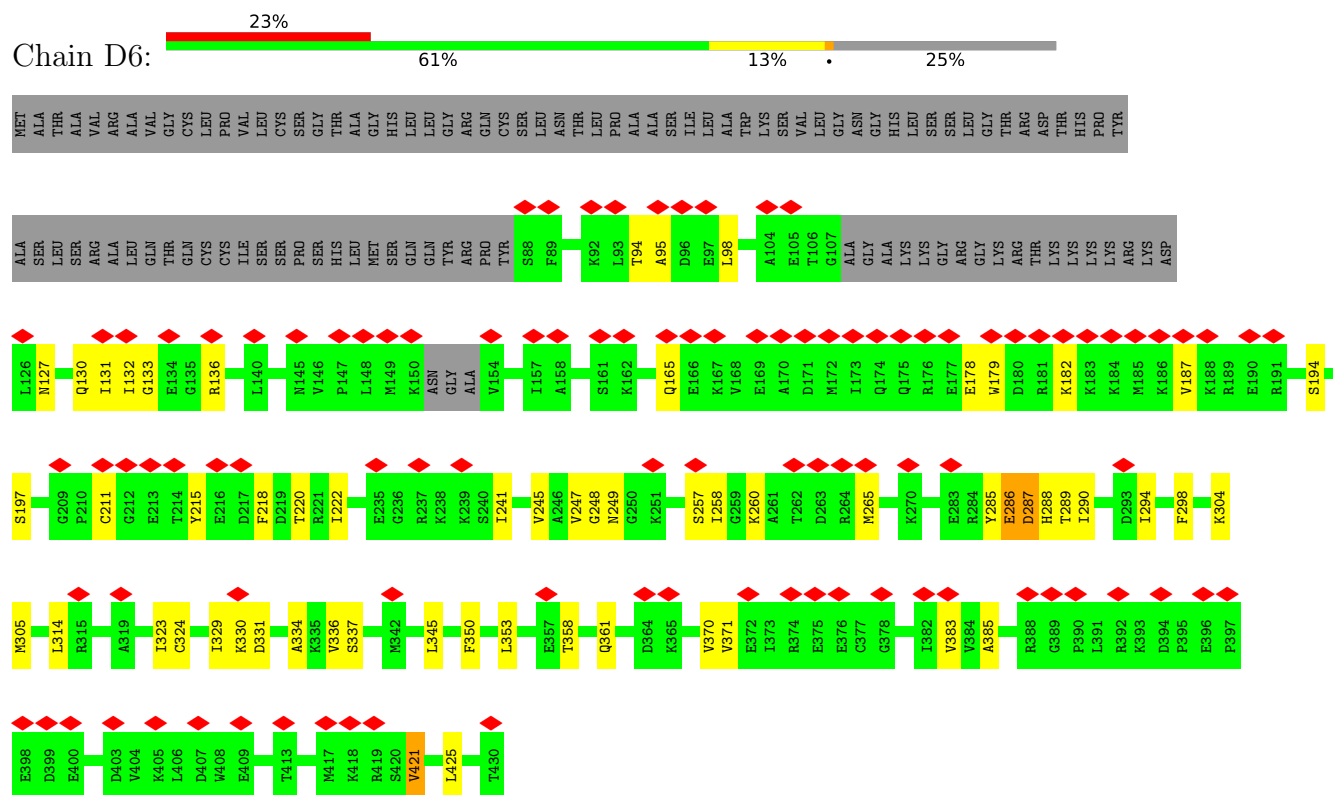


L189	P190	D191	L192	H197	N201	D211	N228	N239	D240	D241	S242	P243	H247	C250	K261	E268	Y271	R272	L273	Q274	GLY	GLN	LYS	GLU	PRO	GLY	ASP	GLN	GLY	PRO	ALA	HIS	PRO	PRO	GLY	ALA	ASP	ASP	GLU	SER	SER	HIS	LEU
D71	V75	R76	R82	D86	R87	R88	L91	K94	C97	H98	H99	R100	F101	M102	I106	D114	D117	L118	E119	Q120	M130	F131	R138	I142	R147	N148	R149	N157	M158	A159	R160	D161	C162	G163	E164	G174	R180	F183	V187	R188			
MET	THR	SER	SER	ALA	ALA	LEU	PRO	ARG	LEU	GLY	ALA	GLY	ALA	ALA	ARG	ARG	LYS	THR	PRO	ARG	PRO	ALA	ARG	SER	ARG	THR	LEU	GLY	SER	SER	ILE	ARG	GLU	SER	GLU	ASP	SER	THR	ASP	F59	S70		

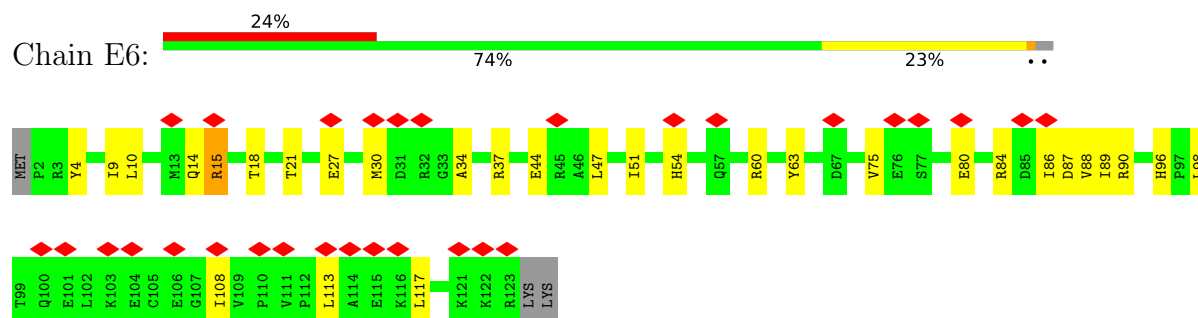
- Molecule 56: 28S ribosomal protein S24, mitochondrial



- Molecule 57: 28S ribosomal protein S5, mitochondrial

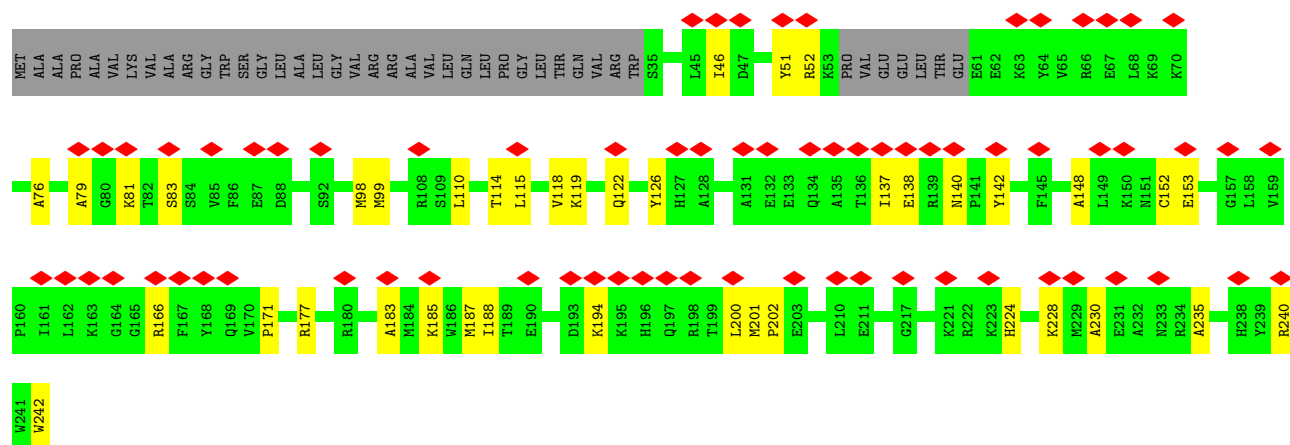


- Molecule 58: 28S ribosomal protein S6, mitochondrial

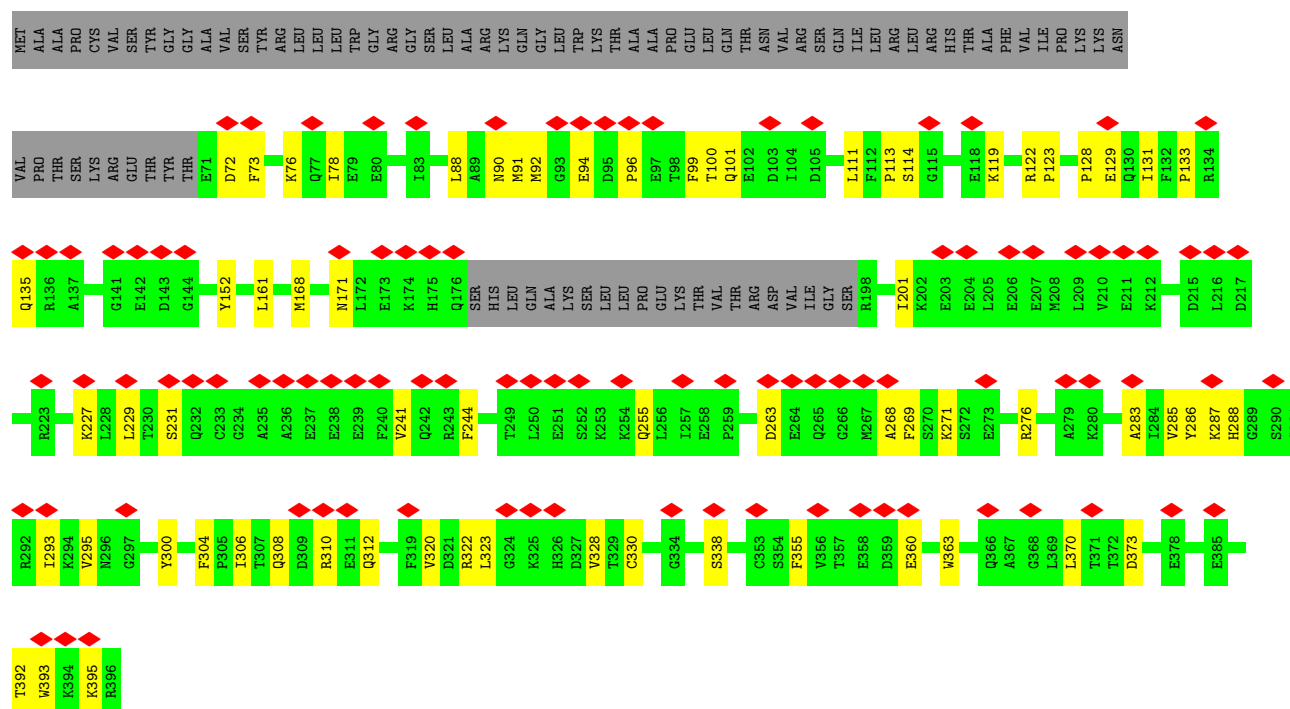


- Molecule 59: 28S ribosomal protein S7, mitochondrial

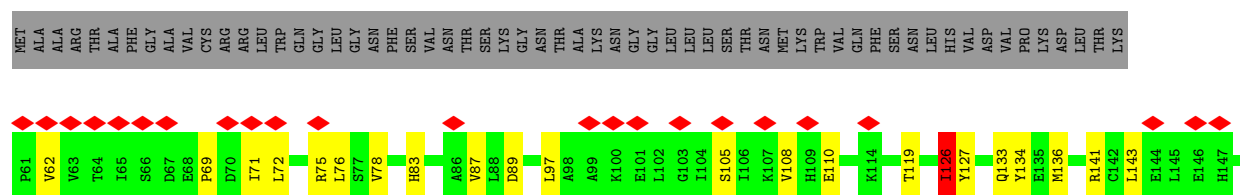


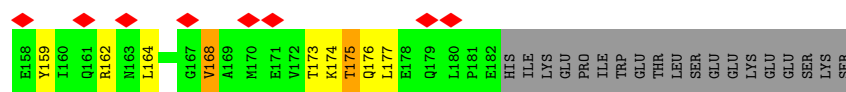


- Molecule 60: 28S ribosomal protein S9, mitochondrial

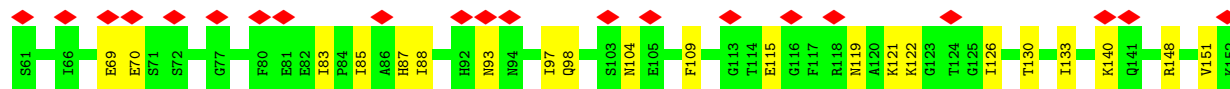
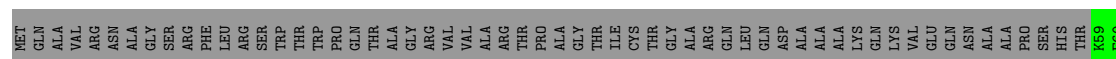


- Molecule 61: 28S ribosomal protein S10, mitochondrial

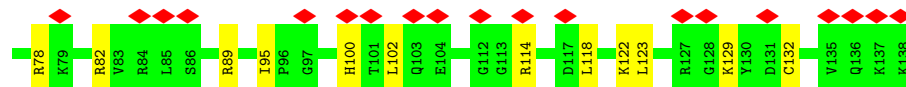
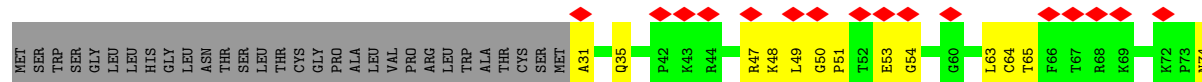




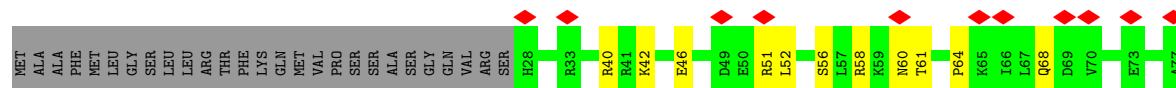
- Molecule 62: 28S ribosomal protein S11, mitochondrial



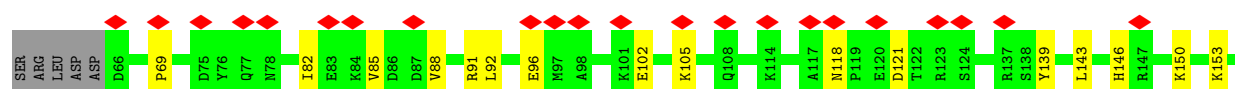
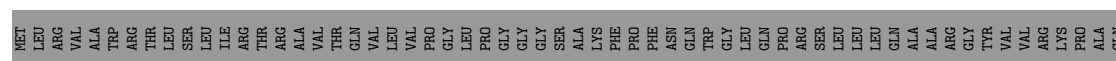
- Molecule 63: 28S ribosomal protein S12, mitochondrial

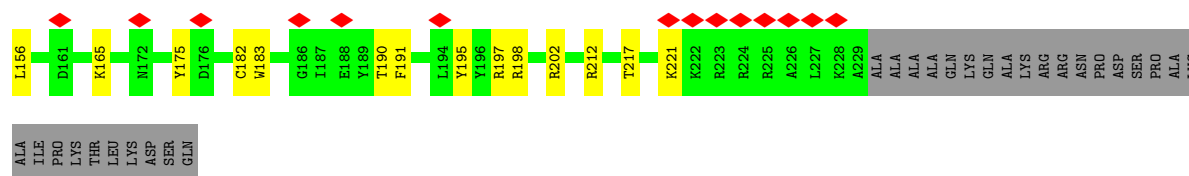


- Molecule 64: 28S ribosomal protein S14, mitochondrial

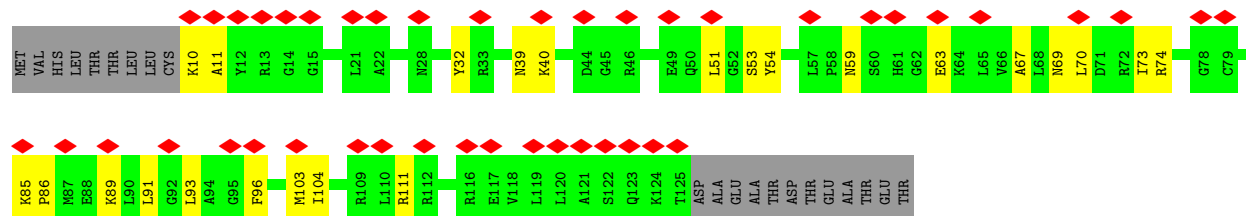


- Molecule 65: 28S ribosomal protein S15, mitochondrial

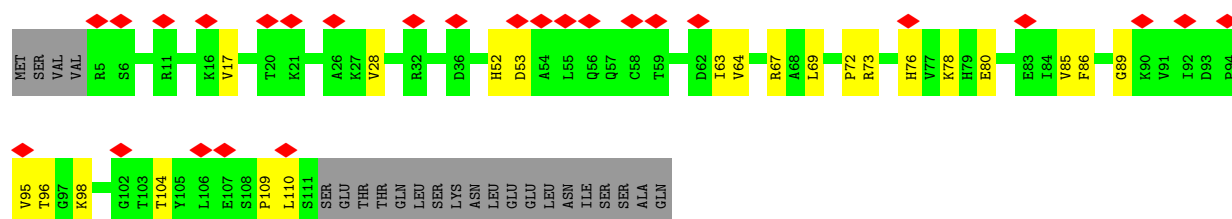




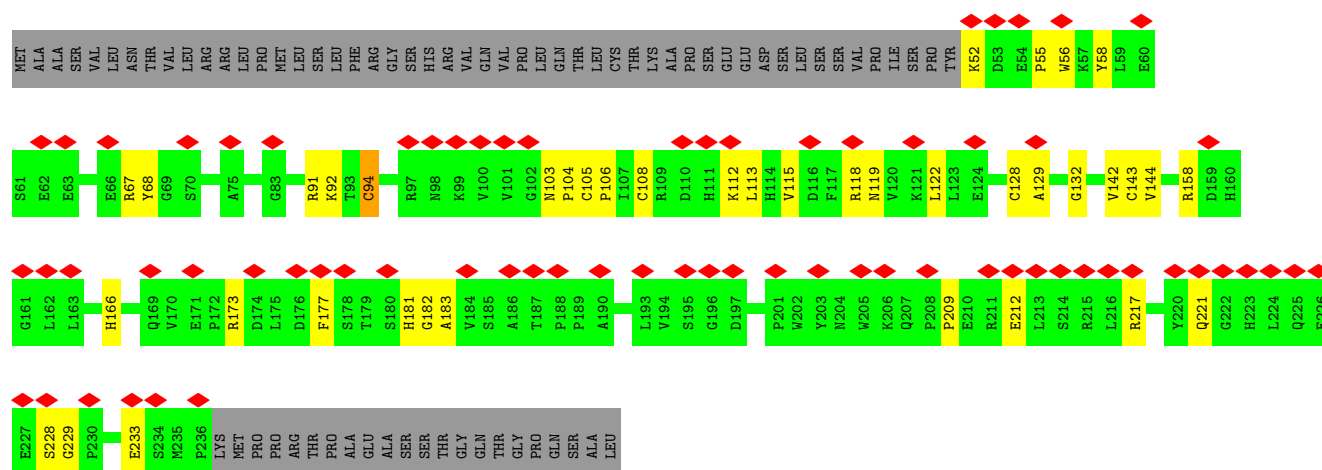
- Molecule 66: 28S ribosomal protein S16, mitochondrial



- Molecule 67: 28S ribosomal protein S17, mitochondrial

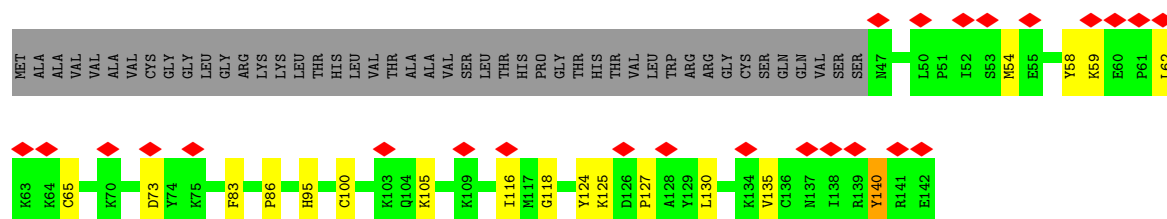


- Molecule 68: 28S ribosomal protein S18b, mitochondrial

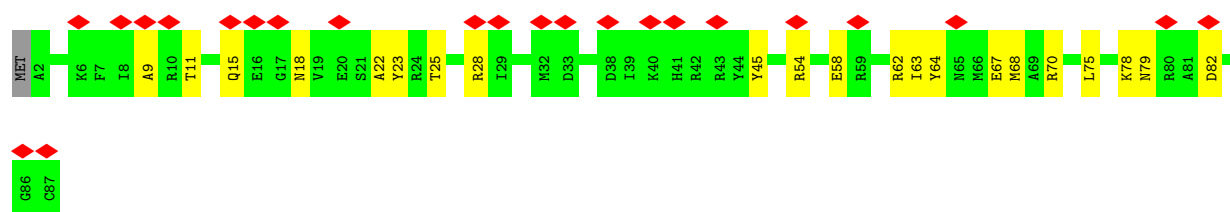
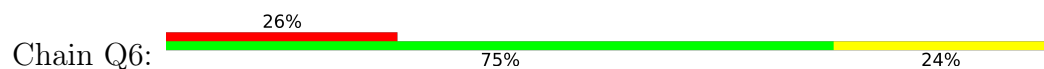


- Molecule 69: 28S ribosomal protein S18c, mitochondrial

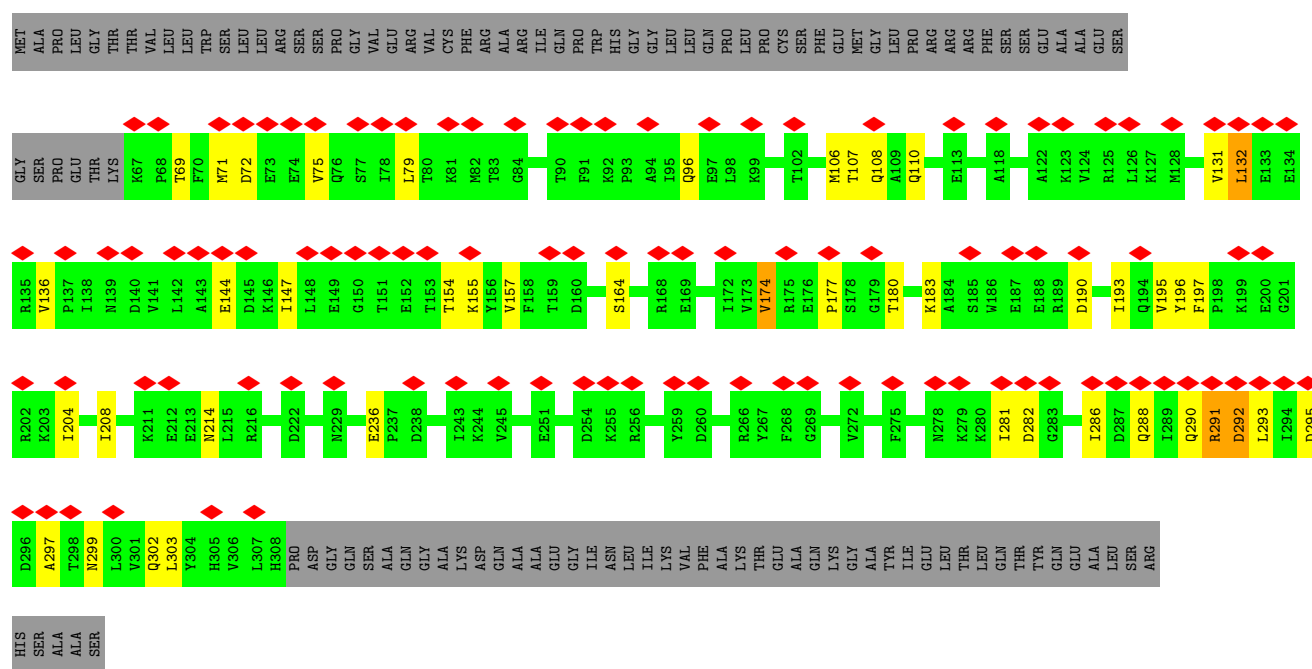




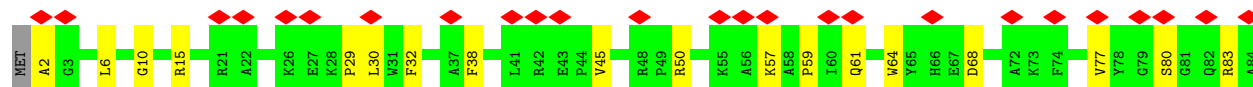
- Molecule 70: 28S ribosomal protein S21, mitochondrial

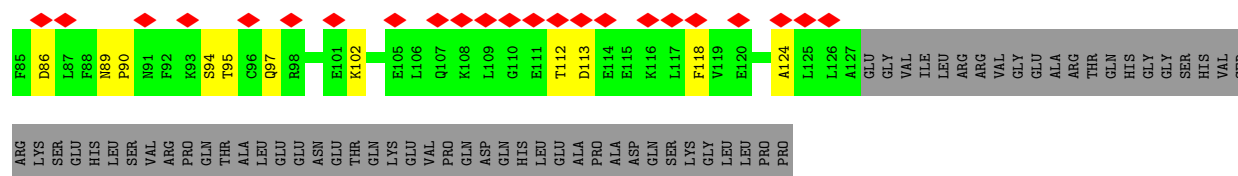


- Molecule 71: 28S ribosomal protein S22, mitochondrial

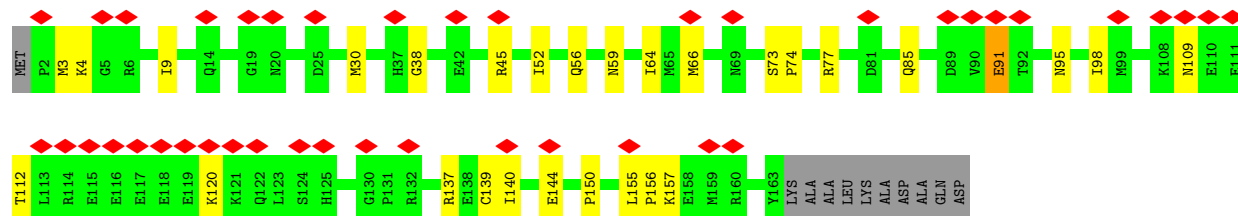
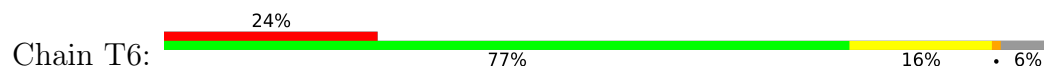


- Molecule 72: 28S ribosomal protein S23, mitochondrial

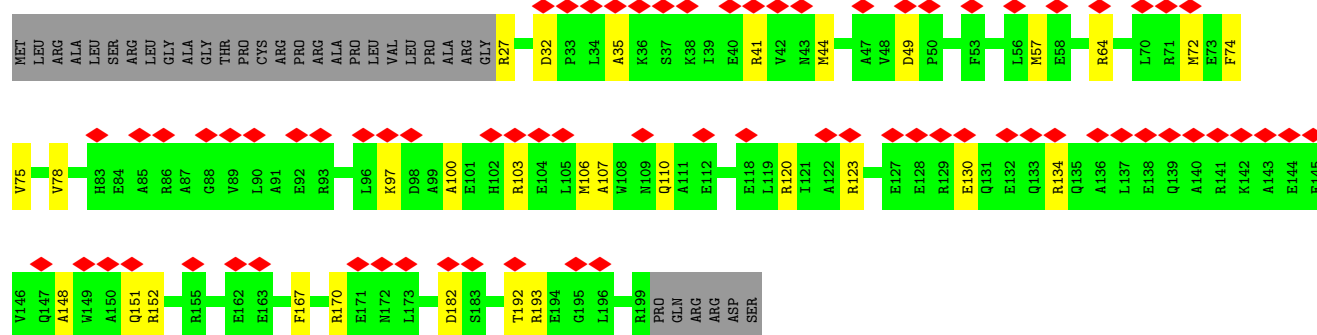




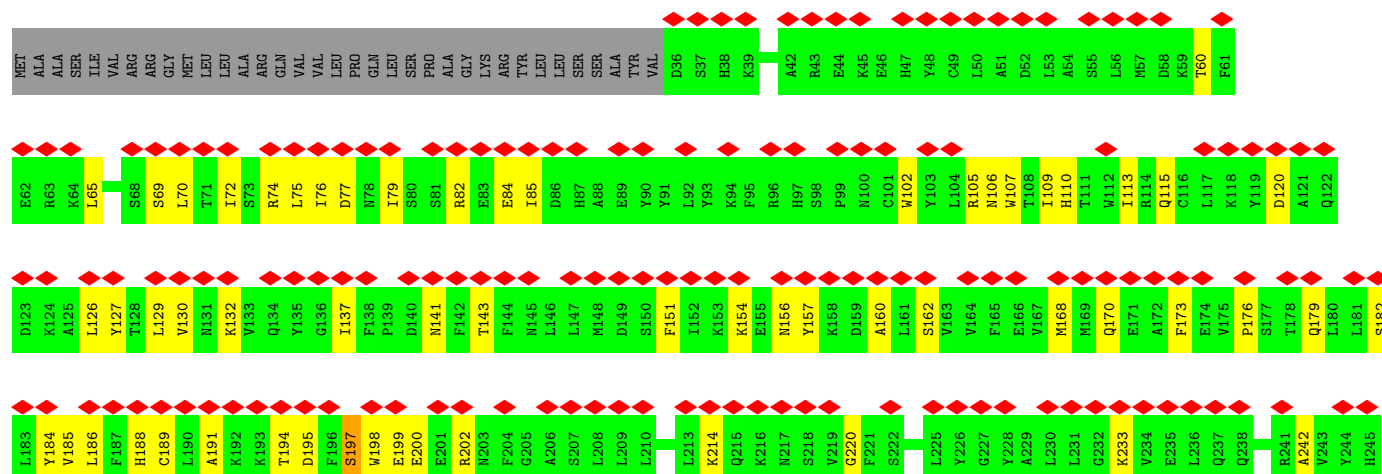
- Molecule 73: 28S ribosomal protein S25, mitochondrial



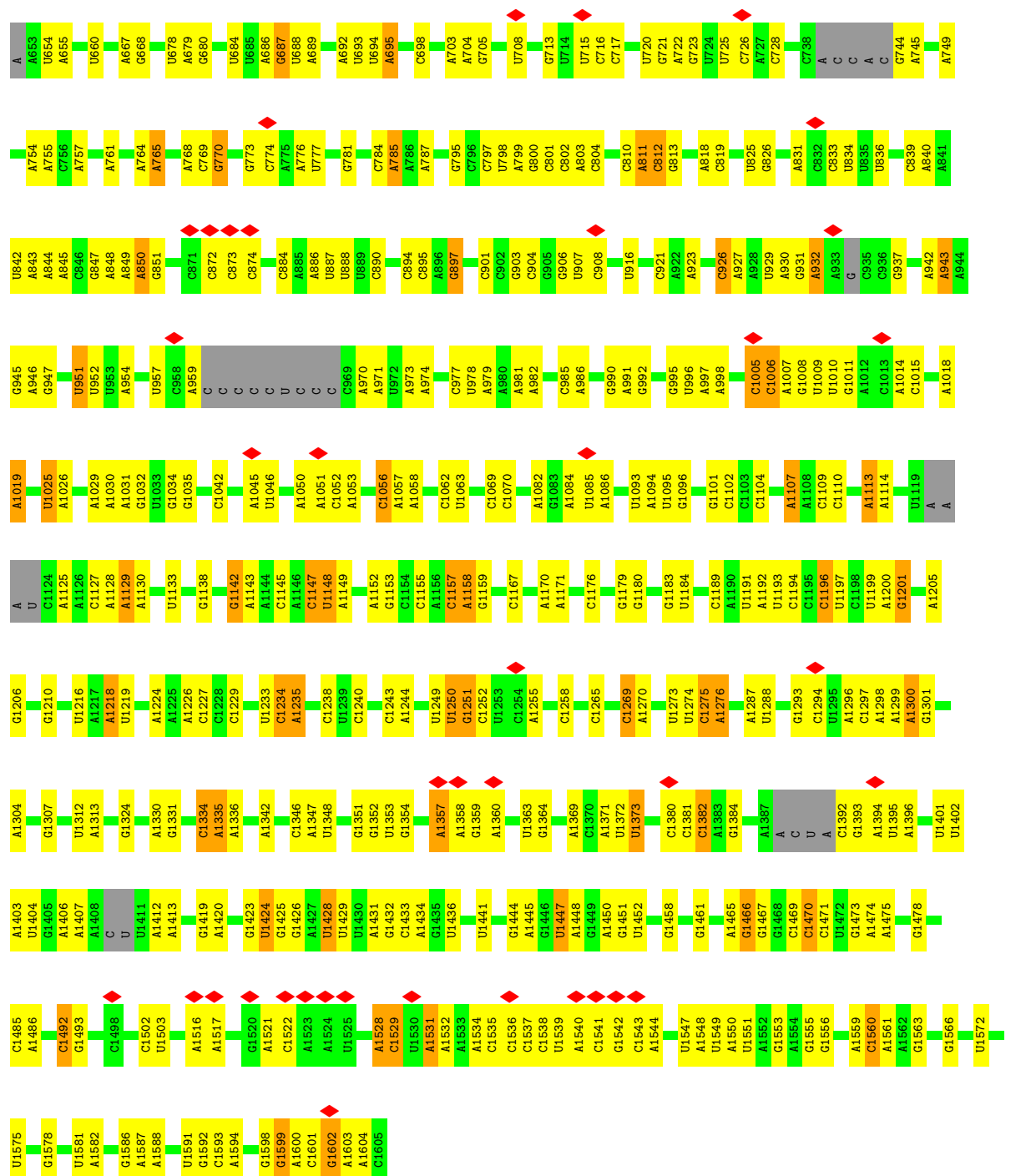
- Molecule 74: 28S ribosomal protein S26, mitochondrial



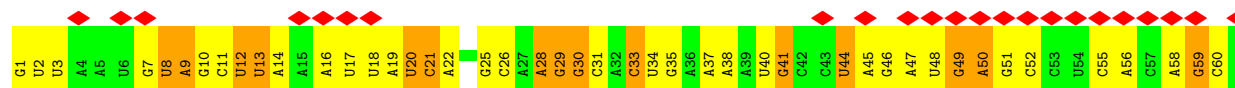
- Molecule 75: 28S ribosomal protein S27, mitochondrial







• Molecule 86: P tRNA

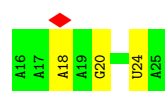




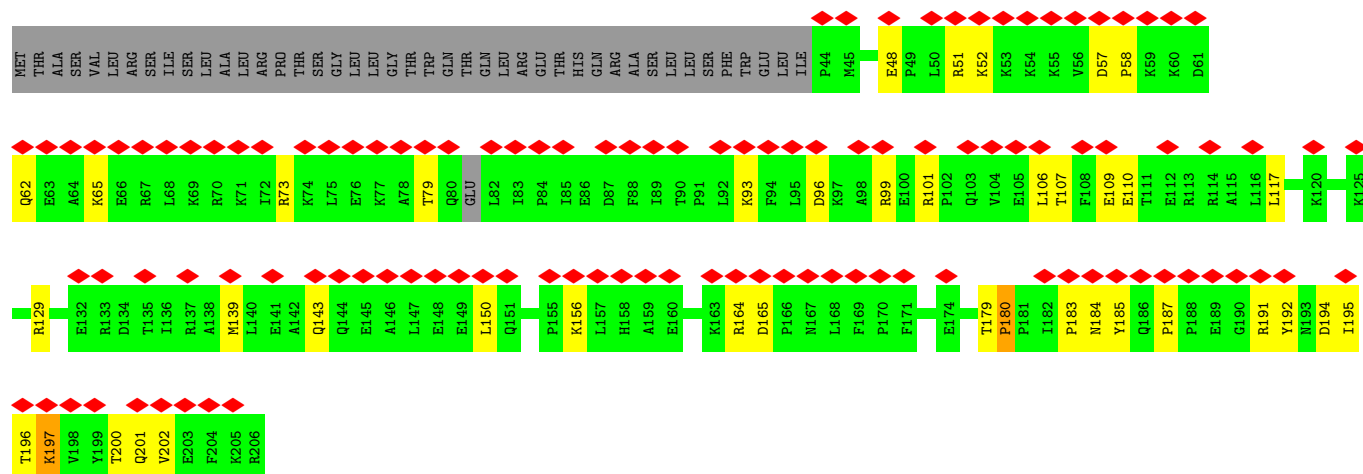
• Molecule 86: P tRNA



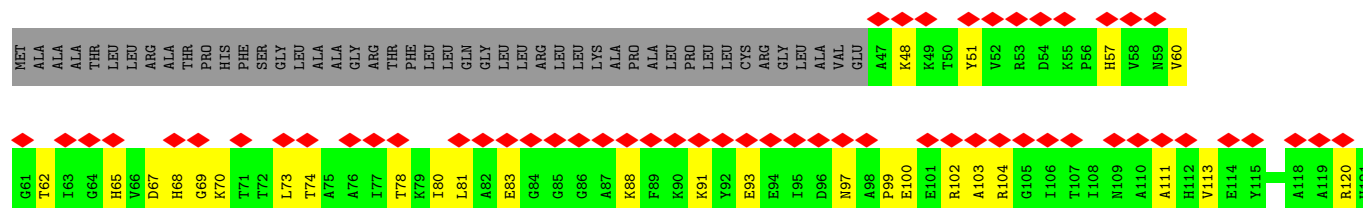
• Molecule 87: mRNA

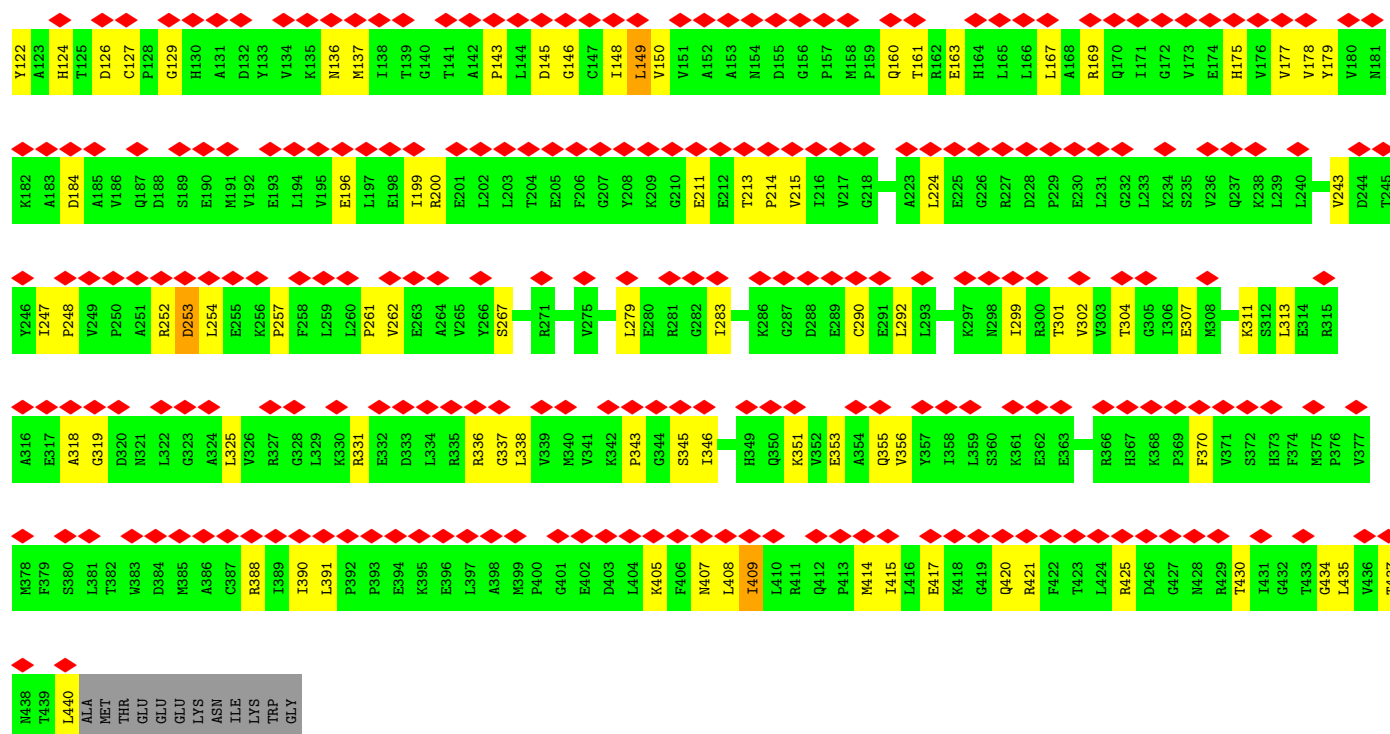


• Molecule 88: 39S ribosomal protein L40, mitochondrial

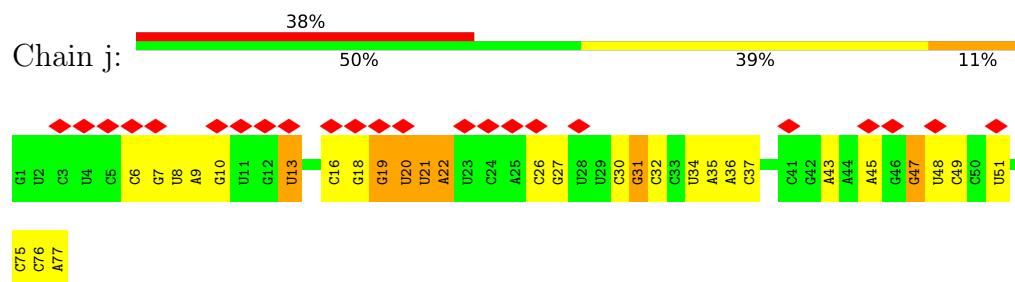


• Molecule 89: Elongation factor Tu, mitochondrial

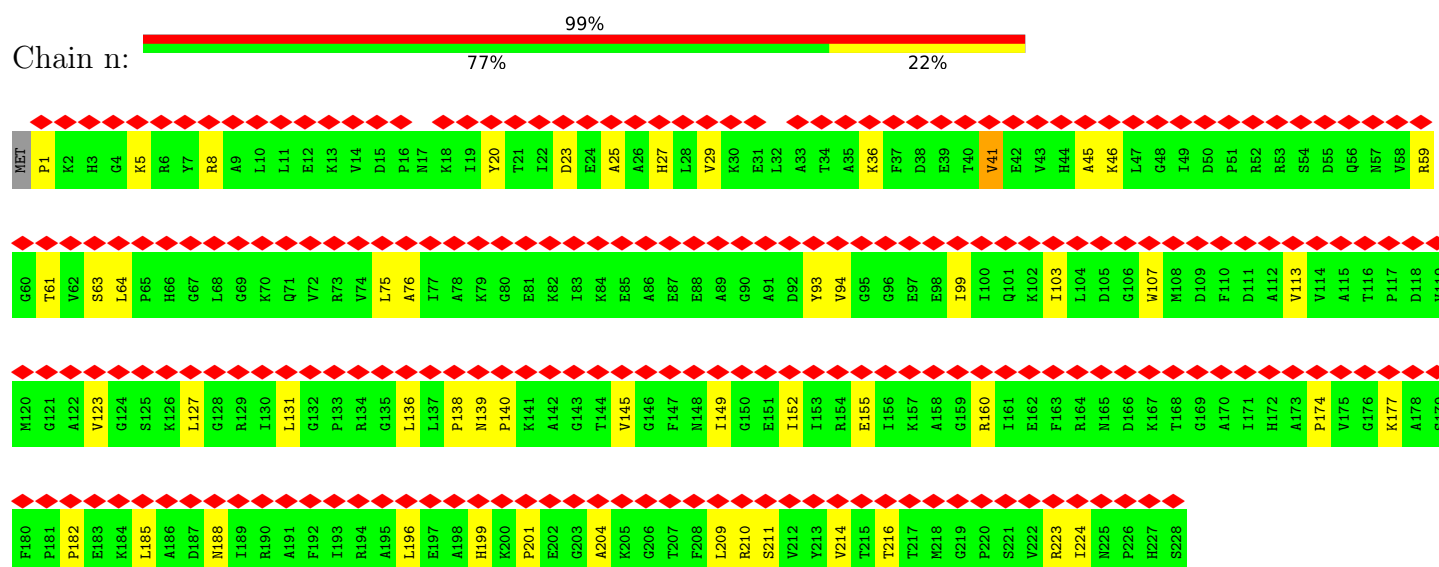




• Molecule 90: E tRNA



• Molecule 91: 50S ribosomal protein L1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	18188	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	0.227	Depositor
Minimum map value	-0.130	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: CL, SO4, SPD, GDP, GCP, MG, MLI, NA, ZN

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	0.32	0/144	0.97	1/200 (0.5%)
2	A3	0.46	0/35697	0.53	5/55544 (0.0%)
3	B3	0.32	0/1328	0.48	0/2056
4	D3	0.45	0/1879	0.70	0/2527
5	E3	0.47	1/2433 (0.0%)	0.71	2/3299 (0.1%)
6	F3	0.44	0/2071	0.77	0/2817
7	D	0.36	0/665	0.94	4/905 (0.4%)
7	H3	0.36	0/798	0.72	0/1073
8	I3	0.33	0/1308	0.63	0/1761
9	J3	0.34	0/1077	0.73	0/1452
10	K3	0.45	0/1495	0.72	0/2029
11	L3	0.42	0/904	0.73	2/1218 (0.2%)
12	M3	0.46	0/2359	0.78	1/3185 (0.0%)
13	N3	0.43	0/1697	0.69	2/2281 (0.1%)
14	O3	0.45	0/1269	0.72	0/1708
15	P3	0.42	0/1103	0.72	1/1491 (0.1%)
16	Q3	0.39	0/1863	0.66	0/2509
17	R3	0.48	0/1174	0.70	0/1572
18	S3	0.47	0/1276	0.69	0/1729
19	T3	0.43	0/1402	0.69	0/1886
20	U3	0.49	1/946 (0.1%)	0.73	2/1283 (0.2%)
21	V3	0.38	0/1590	0.79	2/2151 (0.1%)
22	W3	0.45	0/893	0.67	0/1204
23	X3	0.47	0/2081	0.84	8/2812 (0.3%)
24	Y3	0.40	0/1552	0.64	0/2079
25	Z3	0.46	0/1003	0.66	0/1354
26	O3	0.40	0/895	0.81	3/1201 (0.2%)
27	13	0.38	0/438	0.78	0/583
28	23	0.48	0/382	0.64	0/507
29	33	0.45	0/852	0.63	0/1136
30	43	0.46	0/329	0.60	0/435
31	53	0.44	1/3154 (0.0%)	0.76	0/4295

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	63	0.37	0/2722	0.66	0/3709
33	73	0.37	0/2207	0.70	0/2978
34	93	0.41	0/896	0.69	2/1205 (0.2%)
35	a3	0.36	0/709	0.63	0/963
36	b3	0.44	0/1202	0.66	0/1626
37	c3	0.37	0/2264	0.67	1/3059 (0.0%)
38	d3	0.37	0/1385	0.83	7/1877 (0.4%)
39	e3	0.34	0/1797	0.70	0/2422
40	f3	0.45	0/1055	1.01	3/1427 (0.2%)
41	g3	0.44	0/1102	0.71	1/1503 (0.1%)
42	h3	0.40	0/847	0.83	4/1150 (0.3%)
43	i3	0.45	0/849	0.70	0/1135
44	j3	0.40	0/698	0.68	0/940
45	k3	0.32	0/665	0.82	2/897 (0.2%)
46	l3	0.34	0/226	0.57	0/299
47	m3	0.35	0/379	0.65	0/510
48	o3	0.46	0/818	0.70	0/1097
49	p3	0.31	0/1071	0.61	0/1433
50	q3	0.37	0/1107	0.66	0/1498
51	r3	0.42	0/1238	0.64	0/1676
52	s3	0.41	0/3114	0.69	3/4225 (0.1%)
53	u3	0.25	0/46	0.36	0/69
55	B6	0.45	0/1811	0.69	0/2451
56	C6	0.44	0/1112	0.68	0/1505
57	D6	0.40	0/2607	0.72	3/3498 (0.1%)
58	E6	0.38	0/989	0.70	2/1335 (0.1%)
59	F6	0.40	0/1708	0.73	0/2291
60	G6	0.38	0/2570	0.67	0/3443
61	H6	0.50	0/1019	0.79	1/1379 (0.1%)
62	I6	0.37	0/1031	0.62	0/1390
63	J6	0.43	0/854	0.72	0/1148
64	K6	0.45	0/879	0.68	0/1182
65	L6	0.37	0/1406	0.65	0/1878
66	M6	0.35	0/941	0.69	0/1265
67	N6	0.39	0/864	0.67	1/1169 (0.1%)
68	O6	0.34	0/1580	0.66	0/2150
69	P6	0.41	0/791	0.67	2/1062 (0.2%)
70	Q6	0.42	0/752	0.70	0/1001
71	R6	0.35	0/2050	0.73	2/2770 (0.1%)
72	S6	0.37	0/1069	0.66	0/1441
73	T6	0.38	0/1361	0.74	2/1829 (0.1%)
74	U6	0.32	0/1482	0.68	2/1987 (0.1%)
75	V6	0.29	0/2758	0.73	5/3724 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	W6	0.38	0/778	0.72	0/1048
77	X6	0.37	0/2596	0.75	5/3519 (0.1%)
78	Y6	0.37	0/943	0.70	0/1274
79	Z6	0.37	0/757	0.75	2/1011 (0.2%)
80	a6	0.32	0/1727	0.66	0/2338
81	b6	0.35	0/2121	0.74	2/2873 (0.1%)
82	c6	0.37	0/939	0.68	0/1256
83	d6	0.41	0/621	0.79	0/820
84	e6	0.37	0/2859	0.80	4/3864 (0.1%)
85	A6	0.42	0/22053	0.50	1/34324 (0.0%)
86	24	0.30	0/1731	0.61	2/2693 (0.1%)
86	C	0.30	0/1731	0.61	2/2693 (0.1%)
87	i4	0.44	0/242	0.62	0/375
88	A	0.39	0/1403	0.89	5/1880 (0.3%)
89	Z	0.37	0/3097	0.79	3/4190 (0.1%)
90	j	0.30	0/1805	0.53	0/2809
91	n	0.30	0/1813	0.69	0/2443
All	All	0.41	3/179304 (0.0%)	0.65	102/255288 (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	2
4	D3	0	1
5	E3	0	7
6	F3	0	1
9	J3	0	1
10	K3	0	1
12	M3	0	2
13	N3	0	1
15	P3	0	2
16	Q3	0	2
17	R3	0	1
19	T3	0	1
21	V3	0	3
23	X3	0	6
24	Y3	0	1
25	Z3	0	1
26	O3	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
27	l3	0	1
31	53	0	4
38	d3	0	3
40	f3	0	6
42	h3	0	2
45	k3	0	2
50	q3	0	1
52	s3	0	2
57	D6	0	2
63	J6	0	1
64	K6	0	1
67	N6	0	1
68	O6	0	1
69	P6	0	1
71	R6	0	3
75	V6	0	1
82	c6	0	2
84	e6	0	1
88	A	0	6
89	Z	0	1
All	All	0	76

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E3	284	TYR	CA-CB	-6.16	1.44	1.53
20	U3	43	ARG	CA-CB	-6.15	1.44	1.53
31	53	91	PRO	CA-C	5.55	1.54	1.51

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	A	202	VAL	N-CA-C	-10.08	102.89	111.56
23	X3	92	ALA	N-CA-C	9.43	128.97	114.64
42	h3	64	GLU	CA-C-N	8.24	137.29	121.54
42	h3	64	GLU	C-N-CA	8.24	137.29	121.54
57	D6	421	VAL	N-CA-C	-8.17	104.74	112.83
52	s3	284	VAL	N-CA-C	-7.42	101.96	110.05
41	g3	48	VAL	N-CA-C	-7.07	107.00	113.71
1	Y2	23	ALA	N-CA-C	6.74	119.44	111.02
75	V6	195	ASP	CA-C-N	6.71	134.37	121.54
75	V6	195	ASP	C-N-CA	6.71	134.37	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	d3	129	ASP	CA-C-N	6.51	133.42	121.70
38	d3	129	ASP	C-N-CA	6.51	133.42	121.70
40	f3	88	TYR	N-CA-C	6.38	118.53	110.24
77	X6	342	PRO	CA-C-N	6.33	133.37	121.97
77	X6	342	PRO	C-N-CA	6.33	133.37	121.97
7	D	232	ARG	CA-C-N	-6.31	116.49	123.43
7	D	232	ARG	C-N-CA	-6.31	116.49	123.43
79	Z6	90	GLY	CA-C-N	6.29	133.02	121.70
79	Z6	90	GLY	C-N-CA	6.29	133.02	121.70
11	L3	112	GLY	CA-C-N	6.27	132.99	121.70
11	L3	112	GLY	C-N-CA	6.27	132.99	121.70
23	X3	99	LYS	CA-C-N	6.24	130.99	122.19
23	X3	99	LYS	C-N-CA	6.24	130.99	122.19
42	h3	63	PRO	CA-C-N	6.24	132.93	121.70
42	h3	63	PRO	C-N-CA	6.24	132.93	121.70
12	M3	76	ILE	N-CA-C	-6.22	106.86	111.90
84	e6	147	PRO	N-CA-CB	6.11	110.28	103.44
5	E3	323	GLY	CA-C-N	6.10	132.68	121.70
5	E3	323	GLY	C-N-CA	6.10	132.68	121.70
21	V3	99	GLY	CA-C-N	6.07	133.14	121.54
21	V3	99	GLY	C-N-CA	6.07	133.14	121.54
75	V6	154	LYS	CA-C-N	6.03	133.05	121.54
75	V6	154	LYS	C-N-CA	6.03	133.05	121.54
45	k3	23	PHE	N-CA-C	-6.02	106.58	114.04
45	k3	55	VAL	N-CA-C	-5.98	108.03	113.71
2	A3	2900	C	OP1-P-O3'	5.91	125.74	108.00
23	X3	92	ALA	N-CA-CB	-5.87	101.72	111.06
86	C	30	G	C4'-C3'-O3'	5.87	121.81	113.00
89	Z	129	GLY	N-CA-C	5.87	115.55	110.21
86	24	30	G	P-O3'-C3'	5.85	128.98	120.20
86	24	30	G	C4'-C3'-O3'	5.85	121.78	113.00
86	C	30	G	P-O3'-C3'	5.83	128.95	120.20
77	X6	96	GLU	CA-C-N	5.83	132.67	121.54
77	X6	96	GLU	C-N-CA	5.83	132.67	121.54
40	f3	51	LYS	CA-CB-CG	-5.80	102.49	114.10
37	c3	265	THR	N-CA-C	-5.80	107.45	114.75
23	X3	94	ASN	CA-C-N	5.76	132.55	121.54
23	X3	94	ASN	C-N-CA	5.76	132.55	121.54
73	T6	91	GLU	CA-C-N	5.75	132.52	121.54
73	T6	91	GLU	C-N-CA	5.75	132.52	121.54
74	U6	35	ALA	CA-C-N	5.73	128.23	120.38
74	U6	35	ALA	C-N-CA	5.73	128.23	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	f3	51	LYS	CB-CA-C	5.66	121.32	110.17
75	V6	372	ILE	N-CA-C	-5.63	106.29	113.22
23	X3	91	TYR	CA-C-N	-5.61	111.14	121.41
23	X3	91	TYR	C-N-CA	-5.61	111.14	121.41
38	d3	267	PRO	CA-C-N	5.50	140.19	127.00
38	d3	267	PRO	C-N-CA	5.50	140.19	127.00
20	U3	37	GLU	CA-C-N	5.47	131.98	121.54
20	U3	37	GLU	C-N-CA	5.47	131.98	121.54
88	A	180	PRO	CA-C-N	5.45	140.08	127.00
88	A	180	PRO	C-N-CA	5.45	140.08	127.00
34	93	131	TYR	CA-C-N	-5.42	113.07	119.84
34	93	131	TYR	C-N-CA	-5.42	113.07	119.84
38	d3	230	ARG	CA-C-N	5.39	131.84	121.54
38	d3	230	ARG	C-N-CA	5.39	131.84	121.54
13	N3	237	HIS	CA-C-N	5.39	131.83	121.54
13	N3	237	HIS	C-N-CA	5.39	131.83	121.54
15	P3	60	VAL	N-CA-C	-5.38	108.26	113.53
67	N6	110	LEU	CA-CB-CG	5.38	135.11	116.30
89	Z	99	PRO	CA-C-N	5.31	131.68	121.54
89	Z	99	PRO	C-N-CA	5.31	131.68	121.54
84	e6	68	VAL	N-CA-C	5.30	120.37	109.34
38	d3	267	PRO	C-N-CD	-5.25	109.06	120.60
88	A	183	PRO	CA-C-N	5.24	131.13	121.70
88	A	183	PRO	C-N-CA	5.24	131.13	121.70
2	A3	1807	U	P-O3'-C3'	5.22	128.04	120.20
26	03	184	TRP	N-CA-C	-5.22	108.17	114.75
26	03	177	ARG	CA-C-N	5.19	131.44	121.54
26	03	177	ARG	C-N-CA	5.19	131.44	121.54
84	e6	91	ASP	CA-C-N	5.18	134.45	121.80
84	e6	91	ASP	C-N-CA	5.18	134.45	121.80
2	A3	2530	A	P-O3'-C3'	5.18	127.97	120.20
2	A3	1806	U	P-O3'-C3'	5.17	127.96	120.20
81	b6	243	LYS	CA-C-N	5.15	131.37	121.54
81	b6	243	LYS	C-N-CA	5.15	131.37	121.54
85	A6	1560	C	C2'-C3'-O3'	5.14	117.22	109.50
71	R6	292	ASP	CA-C-N	5.13	131.34	121.54
71	R6	292	ASP	C-N-CA	5.13	131.34	121.54
58	E6	14	GLN	CA-C-N	5.09	134.23	121.80
58	E6	14	GLN	C-N-CA	5.09	134.23	121.80
77	X6	343	ILE	N-CA-C	-5.08	98.77	109.34
2	A3	2507	A	C2'-C3'-O3'	5.08	121.32	113.70
61	H6	168	VAL	N-CA-C	-5.08	104.52	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	s3	249	GLU	CA-C-N	5.07	131.22	121.54
52	s3	249	GLU	C-N-CA	5.07	131.22	121.54
57	D6	298	PHE	CA-C-N	5.06	131.20	121.54
57	D6	298	PHE	C-N-CA	5.06	131.20	121.54
7	D	176	MET	CA-C-N	5.04	128.01	120.90
7	D	176	MET	C-N-CA	5.04	128.01	120.90
69	P6	140	TYR	CA-C-N	5.04	131.17	121.54
69	P6	140	TYR	C-N-CA	5.04	131.17	121.54

There are no chirality outliers.

All (76) 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
31	53	305	GLN	Peptide
31	53	347	THR	Peptide
31	53	71	ALA	Peptide
88	A	184	ASN	Peptide
88	A	185	TYR	Peptide
88	A	187	PRO	Peptide
88	A	192	TYR	Peptide
88	A	197	LYS	Peptide
88	A	57	ASP	Peptide
4	D3	206	TYR	Peptide
57	D6	285	TYR	Peptide
57	D6	286	GLU	Peptide
5	E3	126	ASP	Peptide
5	E3	169	GLY	Peptide
5	E3	203	TYR	Peptide
5	E3	244	ALA	Peptide
5	E3	250	ARG	Peptide
5	E3	315	PRO	Peptide
5	E3	85	TRP	Peptide
6	F3	129	PRO	Peptide
9	J3	33	PRO	Peptide
63	J6	129	LYS	Peptide
10	K3	3	SER	Peptide
64	K6	64	PRO	Peptide
12	M3	18	GLY	Peptide
12	M3	264	GLN	Peptide

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Mol	Chain	Res	Type	Group
13	N3	237	HIS	Peptide
67	N6	109	PRO	Peptide
68	O6	55	PRO	Peptide
15	P3	174	PRO	Peptide
15	P3	176	ARG	Peptide
69	P6	65	CYS	Peptide
16	Q3	182	ARG	Peptide
16	Q3	226	PRO	Peptide
17	R3	137	GLU	Peptide
71	R6	132	LEU	Peptide
71	R6	154	THR	Peptide
71	R6	291	ARG	Peptide
19	T3	94	ILE	Peptide
21	V3	100	LYS	Peptide
21	V3	170	TRP	Peptide
21	V3	192	LYS	Peptide
75	V6	173	PHE	Peptide
23	X3	51	LYS	Peptide
23	X3	90	ILE	Peptide
23	X3	93	ASN	Peptide
23	X3	95	ASP	Peptide
23	X3	98	SER	Peptide
23	X3	99	LYS	Peptide
1	Y2	21	ALA	Peptide
1	Y2	22	ALA	Peptide
24	Y3	202	LEU	Peptide
89	Z	143	PRO	Peptide
25	Z3	141	SER	Peptide
82	c6	38	ARG	Peptide
82	c6	60	GLU	Peptide
38	d3	163	LEU	Peptide
38	d3	230	ARG	Peptide
38	d3	268	PRO	Peptide
84	e6	67	LYS	Peptide
40	f3	189	HIS	Peptide
40	f3	48	TYR	Peptide
40	f3	49	LYS	Peptide
40	f3	50	THR	Peptide
40	f3	84	THR	Peptide
40	f3	87	GLU	Peptide
42	h3	138	SER	Peptide
42	h3	63	PRO	Peptide

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Mol	Chain	Res	Type	Group
45	k3	14	LYS	Peptide
45	k3	55	VAL	Peptide
50	q3	78	SER	Peptide
52	s3	259	ILE	Peptide
52	s3	270	LYS	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	16214	315	0
3	B3	1191	0	607	14	0
4	D3	1842	0	1895	33	0
5	E3	2365	0	2378	51	0
6	F3	2013	0	2044	37	0
7	D	648	0	657	18	0
7	H3	784	0	832	13	0
8	I3	1283	0	1369	22	0
9	J3	1061	0	1141	14	0
10	K3	1451	0	1448	25	0
11	L3	889	0	941	17	0
12	M3	2305	0	2378	48	0
13	N3	1654	0	1681	14	0
14	O3	1245	0	1283	28	0
15	P3	1080	0	1081	26	0
16	Q3	1822	0	1859	30	0
17	R3	1153	0	1214	25	0
18	S3	1251	0	1322	34	0
19	T3	1368	0	1410	21	0
20	U3	922	0	935	21	0
21	V3	1551	0	1558	30	0
22	W3	871	0	898	20	0
23	X3	2027	0	2040	38	0
24	Y3	1517	0	1561	30	0
25	Z3	978	0	1030	18	0
26	O3	880	0	904	13	0
27	I3	433	0	475	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	23	376	0	406	8	0
29	33	831	0	883	15	0
30	43	322	0	344	5	0
31	53	3064	0	3059	55	0
32	63	2636	0	2450	34	0
33	73	2158	0	2173	41	0
34	93	873	0	878	19	0
35	a3	686	0	658	15	0
36	b3	1178	0	1180	34	0
37	c3	2217	0	2220	29	0
38	d3	1347	0	1343	21	0
39	e3	1762	0	1767	44	0
40	f3	1039	0	1044	20	0
41	g3	1067	0	1056	24	0
42	h3	827	0	806	18	0
43	i3	827	0	857	13	0
44	j3	684	0	673	6	0
45	k3	655	0	656	14	0
46	l3	221	0	227	3	0
47	m3	372	0	387	17	0
48	o3	797	0	804	13	0
49	p3	1058	0	1083	14	0
50	q3	1076	0	1049	16	0
51	r3	1203	0	1220	21	0
52	s3	3036	0	3022	56	0
52	t3	140	0	31	0	0
53	u3	42	0	23	0	0
54	A5	140	0	34	0	0
55	B6	1768	0	1765	25	0
56	C6	1082	0	1088	23	0
57	D6	2557	0	2596	40	0
58	E6	972	0	1000	20	0
59	F6	1668	0	1716	37	0
60	G6	2516	0	2503	46	0
61	H6	999	0	1024	22	0
62	I6	1011	0	1052	26	0
63	J6	838	0	887	16	0
64	K6	861	0	885	16	0
65	L6	1382	0	1472	20	0
66	M6	920	0	951	17	0
67	N6	846	0	908	14	0
68	O6	1528	0	1487	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	P6	774	0	802	15	0
70	Q6	740	0	754	19	0
71	R6	2008	0	2031	32	0
72	S6	1042	0	1037	20	0
73	T6	1330	0	1344	20	0
74	U6	1461	0	1471	24	0
75	V6	2702	0	2690	54	0
76	W6	766	0	785	21	0
77	X6	2531	0	2520	60	0
78	Y6	914	0	859	8	0
79	Z6	740	0	747	16	0
80	a6	1684	0	1685	34	0
81	b6	2076	0	2097	51	0
82	c6	925	0	962	16	0
83	d6	610	0	682	11	0
84	e6	2838	0	2416	33	0
85	A6	19716	0	10015	173	0
86	24	1547	0	787	22	0
86	C	1547	0	788	28	0
87	i4	216	0	108	1	0
88	A	1375	0	1426	32	0
89	Z	3042	0	3112	66	0
90	j	1616	0	824	14	0
91	n	1767	0	1829	36	0
92	A3	95	0	0	0	0
92	A6	28	0	0	0	0
92	D3	1	0	0	0	0
92	M3	1	0	0	0	0
92	g3	1	0	0	0	0
92	n	1	0	0	0	0
92	o3	1	0	0	0	0
93	A3	10	0	19	1	0
94	03	1	0	0	0	0
94	43	1	0	0	0	0
94	B6	1	0	0	0	0
94	O6	1	0	0	0	0
94	P6	1	0	0	0	0
94	T6	1	0	0	0	0
94	r3	1	0	0	0	0
95	X6	28	0	12	1	0
96	Z	32	0	13	3	0
97	D	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
97	n	2	0	0	0	0
98	n	5	0	0	0	0
99	n	21	0	6	0	0
100	n	2	0	0	2	0
101	A3	3	0	0	0	0
101	D	9	0	0	0	0
101	n	67	0	0	2	0
All	All	170507	0	142790	2200	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 (2200) 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)
96:Z:501:GCP:O4'	96:Z:501:GCP:C4'	1.64	1.22
3:B3:1607:U:H3	3:B3:1664:G:H1	1.00	0.97
90:j:51:U:H3	90:j:65:G:H1	0.87	0.84
32:63:303:PHE:O	32:63:307:HIS:HB3	1.82	0.79
86:C:13:U:H3	86:C:21:C:N4	1.82	0.78
86:24:13:U:H3	86:24:21:C:N4	1.81	0.77
39:e3:151:ARG:HH22	39:e3:259:GLU:HG3	1.49	0.77
67:N6:95:VAL:HG22	74:U6:120:ARG:HH22	1.51	0.76
86:24:29:G:H1	86:24:37:A:H61	1.34	0.76
85:A6:1201:G:H1	85:A6:1429:U:H3	1.34	0.76
85:A6:728:C:H42	85:A6:754:A:H61	1.35	0.75
2:A3:2064:A:N7	40:f3:48:TYR:N	2.35	0.74
23:X3:96:LYS:HA	86:C:73:A:H2'	1.69	0.73
86:C:29:G:H1	86:C:37:A:H61	1.34	0.73
2:A3:2390:A:H62	2:A3:2399:A:H61	1.36	0.72
33:73:99:TYR:O	33:73:103:SER:HB2	1.89	0.71
75:V6:70:LEU:HB2	75:V6:74:ARG:HH21	1.56	0.71
71:R6:193:ILE:O	71:R6:197:PHE:HB2	1.91	0.71
7:D:190:ALA:O	7:D:194:PHE:HB2	1.90	0.71
2:A3:2545:U:H5''	2:A3:2546:G:H5'	1.73	0.70
31:53:119:GLN:HE22	31:53:263:ILE:HG22	1.55	0.70
80:a6:30:ASP:O	80:a6:34:TYR:HB2	1.90	0.70
77:X6:123:ARG:HE	77:X6:338:ASP:H	1.37	0.70
29:33:163:THR:HG23	29:33:165:PHE:H	1.55	0.70
39:e3:160:LEU:O	39:e3:252:HIS:HA	1.91	0.70
33:73:247:ASN:ND2	33:73:251:ILE:O	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:C:13:U:N3	86:C:21:C:N4	2.39	0.69
75:V6:263:MET:HB3	75:V6:337:LEU:HD11	1.74	0.69
32:63:186:PRO:HG3	49:p3:191:LYS:HD3	1.75	0.69
60:G6:90:ASN:HD21	81:b6:64:GLN:H	1.38	0.69
39:e3:245:GLN:HG3	39:e3:248:ASN:HB3	1.74	0.69
58:E6:96:HIS:HD2	58:E6:98:LEU:H	1.39	0.69
86:24:28:A:H61	86:24:38:A:H61	1.41	0.69
86:C:28:A:H61	86:C:38:A:H61	1.41	0.68
91:n:45:ALA:HA	91:n:211:SER:O	1.93	0.68
81:b6:149:ILE:HD11	81:b6:173:LEU:HG	1.74	0.67
86:24:13:U:N3	86:24:21:C:N4	2.39	0.67
57:D6:127:ASN:HD21	79:Z6:72:ARG:HD3	1.58	0.67
60:G6:119:LYS:HA	60:G6:122:ARG:HD2	1.77	0.67
2:A3:3072:U:H5'	86:24:73:A:H5'	1.75	0.67
17:R3:57:ARG:HE	18:S3:169:ARG:HH21	1.42	0.67
82:c6:11:ALA:HB2	82:c6:19:PRO:HB3	1.76	0.67
2:A3:3011:A:O2'	2:A3:3173:G:N2	2.27	0.67
2:A3:2106:A:N7	8:I3:31:LYS:NZ	2.42	0.67
23:X3:90:ILE:O	23:X3:100:ARG:HA	1.94	0.67
61:H6:72:LEU:HD12	84:e6:59:ILE:HD13	1.77	0.67
14:O3:38:ARG:HE	14:O3:85:LEU:HD21	1.60	0.66
52:s3:403:GLU:HG3	52:s3:404:THR:HG22	1.76	0.66
88:A:96:ASP:O	88:A:99:ARG:NH1	2.28	0.66
2:A3:1883:G:OP2	12:M3:100:ARG:NH2	2.28	0.66
12:M3:284:LYS:HB3	41:g3:40:GLU:HB2	1.77	0.66
23:X3:160:ASP:OD1	23:X3:163:ARG:NH1	2.28	0.66
11:L3:96:MET:SD	16:Q3:168:ASN:ND2	2.67	0.66
39:e3:212:HIS:HE1	88:A:150:LEU:HB2	1.60	0.66
57:D6:324:CYS:HB3	57:D6:329:ILE:HB	1.78	0.66
55:B6:180:ARG:NH1	57:D6:211:CYS:SG	2.69	0.66
31:53:229:ARG:HE	31:53:288:PRO:HB3	1.61	0.66
89:Z:292:LEU:HB3	89:Z:299:ILE:HB	1.77	0.66
56:C6:109:VAL:HB	56:C6:120:CYS:HB2	1.77	0.66
88:A:48:GLU:O	88:A:52:LYS:HB2	1.95	0.66
80:a6:63:ARG:H	80:a6:66:GLN:HE21	1.44	0.65
74:U6:41:ARG:H	80:a6:49:ARG:HH22	1.43	0.65
51:r3:85:ASP:OD1	51:r3:85:ASP:N	2.29	0.65
52:s3:77:ASP:HB3	52:s3:288:THR:HG21	1.78	0.65
8:I3:188:ARG:NH2	45:k3:54:ASP:O	2.29	0.65
15:P3:51:ASN:HB3	15:P3:54:ASN:HB2	1.78	0.65
2:A3:1800:G:H22	2:A3:1803:A:H5'	1.59	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:h3:64:GLU:O	42:h3:69:ARG:NH2	2.30	0.65
61:H6:78:VAL:HB	61:H6:143:LEU:HB3	1.76	0.65
89:Z:175:HIS:HB3	89:Z:247:ILE:HG12	1.77	0.65
2:A3:2390:A:H62	2:A3:2399:A:N6	1.95	0.65
10:K3:27:PRO:HG2	10:K3:30:LYS:HB2	1.76	0.65
77:X6:348:TYR:HB2	77:X6:386:ALA:HB1	1.77	0.65
23:X3:96:LYS:HA	86:C:73:A:H8	1.61	0.65
33:73:65:ILE:HB	33:73:122:SER:HB2	1.79	0.65
81:b6:174:ARG:HG2	81:b6:206:THR:HG22	1.80	0.64
24:Y3:164:ARG:NH1	24:Y3:181:PHE:O	2.30	0.64
36:b3:126:ILE:O	37:c3:310:ASN:ND2	2.30	0.64
51:r3:89:LEU:HD21	51:r3:118:CYS:HB3	1.78	0.64
10:K3:6:ARG:HH12	35:a3:142:ARG:HG2	1.63	0.64
55:B6:157:ASN:OD1	55:B6:160:ARG:NH2	2.30	0.64
91:n:103:ILE:HA	91:n:107:TRP:HB2	1.79	0.64
5:E3:80:LEU:HD12	5:E3:322:ASP:HB2	1.80	0.64
75:V6:198:TRP:HD1	75:V6:199:GLU:HB3	1.62	0.64
31:53:113:LEU:O	31:53:308:GLN:NE2	2.29	0.64
33:73:240:ILE:HD11	33:73:263:VAL:HG11	1.79	0.64
2:A3:2256:U:O2'	18:S3:118:ASN:ND2	2.31	0.64
29:33:107:VAL:HG21	29:33:161:MET:HE2	1.80	0.64
6:F3:49:ARG:HD3	6:F3:263:LEU:HD12	1.79	0.64
7:H3:78:ARG:NH1	23:X3:87:LEU:O	2.29	0.63
52:s3:209:TYR:HB2	52:s3:232:GLN:HG3	1.80	0.63
80:a6:12:ALA:HB2	85:A6:810:C:H1'	1.81	0.63
2:A3:1777:A:N6	2:A3:1780:U:OP2	2.32	0.63
75:V6:106:ASN:HA	75:V6:109:ILE:HD12	1.81	0.63
80:a6:67:LEU:HD21	80:a6:141:LEU:HB2	1.79	0.63
74:U6:152:ARG:NH2	74:U6:152:ARG:O	2.31	0.63
2:A3:1881:A:OP2	41:g3:111:ARG:NH2	2.31	0.63
77:X6:337:LEU:O	81:b6:260:ARG:NH1	2.31	0.63
19:T3:212:LEU:O	35:a3:142:ARG:NH2	2.31	0.63
4:D3:121:PRO:HB3	4:D3:166:SER:HA	1.80	0.63
22:W3:68:ALA:HB3	22:W3:89:LEU:HD12	1.80	0.63
2:A3:2417:C:O2'	52:s3:305:LYS:NZ	2.31	0.63
80:a6:48:ARG:NH2	85:A6:705:G:O6	2.32	0.63
86:24:29:G:N2	86:24:37:A:N1	2.45	0.63
91:n:127:LEU:HB3	91:n:131:LEU:HG	1.81	0.63
2:A3:2849:G:OP2	27:13:15:ASN:ND2	2.32	0.63
52:s3:90:LYS:NZ	52:s3:280:ASN:OD1	2.31	0.63
14:O3:18:MET:HE3	14:O3:48:ARG:HG2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:g3:110:ILE:HD12	41:g3:147:LEU:HD23	1.80	0.62
84:e6:534:LEU:HD23	84:e6:537:ARG:HE	1.63	0.62
89:Z:177:VAL:HG13	89:Z:214:PRO:HG2	1.79	0.62
90:j:13:U:H3	90:j:22:A:H61	1.47	0.62
74:U6:130:GLU:OE2	74:U6:134:ARG:NH1	2.32	0.62
2:A3:1867:A:H62	2:A3:2295:C:H5	1.47	0.62
89:Z:150:VAL:HG12	89:Z:179:TYR:HB3	1.80	0.62
89:Z:390:ILE:HB	89:Z:407:ASN:HB3	1.82	0.62
11:L3:128:ARG:HB2	16:Q3:125:TYR:HB3	1.82	0.62
83:d6:160:GLY:HA2	83:d6:163:ARG:HD2	1.82	0.62
3:B3:1607:U:O2	3:B3:1664:G:N2	2.28	0.62
6:F3:282:PRO:O	6:F3:290:TYR:OH	2.17	0.62
12:M3:104:LEU:HD11	12:M3:126:GLY:HA3	1.82	0.62
12:M3:264:GLN:NE2	12:M3:269:LEU:O	2.33	0.62
20:U3:44:ILE:HD11	20:U3:53:LEU:HD22	1.81	0.62
31:53:200:ARG:HB3	31:53:233:LYS:HB2	1.80	0.62
61:H6:83:HIS:H	61:H6:168:VAL:HG13	1.64	0.62
81:b6:251:TYR:HB3	81:b6:297:VAL:HG12	1.80	0.62
89:Z:331:ARG:NH2	90:j:75:C:N3	2.47	0.62
7:D:196:ASN:ND2	91:n:20:TYR:OH	2.32	0.62
4:D3:194:ASN:ND2	4:D3:245:GLY:O	2.32	0.61
16:Q3:103:ARG:HG2	16:Q3:108:ILE:HD12	1.82	0.61
21:V3:178:SER:HG	21:V3:181:ASP:H	1.48	0.61
39:e3:162:ARG:NH1	39:e3:169:ASP:O	2.33	0.61
50:q3:148:ALA:O	50:q3:152:ARG:NH1	2.33	0.61
73:T6:95:ASN:HA	73:T6:98:ILE:HD12	1.81	0.61
76:W6:159:ASP:OD1	76:W6:159:ASP:N	2.28	0.61
7:H3:107:VAL:HG22	7:D:165:LYS:HD2	1.82	0.61
33:73:195:THR:OG1	33:73:198:ASN:ND2	2.33	0.61
39:e3:85:SER:H	88:A:101:ARG:HH22	1.45	0.61
13:N3:171:GLU:O	46:l3:135:ASN:ND2	2.34	0.61
15:P3:57:LEU:HD23	49:p3:177:ARG:HH21	1.64	0.61
18:S3:132:LYS:HE3	44:j3:48:ASP:HA	1.81	0.61
33:73:196:LYS:HA	33:73:199:LEU:HD12	1.82	0.61
2:A3:1802:A:N7	2:A3:1805:A:N6	2.48	0.61
23:X3:93:ASN:ND2	23:X3:95:ASP:O	2.30	0.61
52:s3:365:LYS:NZ	52:s3:403:GLU:O	2.30	0.61
2:A3:1724:A:OP2	12:M3:64:ARG:NH2	2.33	0.61
2:A3:2157:U:OP1	51:r3:182:ARG:NH1	2.33	0.61
16:Q3:287:GLU:HA	16:Q3:290:LYS:HG2	1.81	0.61
52:s3:165:ARG:O	52:s3:307:ARG:NH2	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:L6:202:ARG:NH1	85:A6:765:A:OP1	2.33	0.61
2:A3:3157:C:H1'	16:Q3:84:ARG:HB3	1.82	0.61
26:03:97:PRO:HA	26:03:100:LEU:HB2	1.81	0.61
31:53:290:THR:HG22	31:53:343:GLN:HB2	1.81	0.61
75:V6:384:LEU:O	75:V6:388:GLN:NE2	2.33	0.61
47:m3:69:ARG:NH2	47:m3:70:GLU:OE1	2.34	0.61
52:s3:234:ASP:OD2	52:s3:234:ASP:N	2.33	0.61
82:c6:62:ARG:HH22	82:c6:64:ASP:HB2	1.66	0.61
36:b3:56:ARG:NH2	42:h3:147:ASN:O	2.34	0.61
66:M6:111:ARG:NH2	68:O6:233:GLU:O	2.34	0.61
91:n:61:THR:OG1	100:n:307:CL:CL	2.54	0.61
2:A3:1839:C:H5''	10:K3:115:ASN:HB2	1.82	0.61
16:Q3:96:ARG:NH1	16:Q3:285:GLU:OE2	2.34	0.61
52:s3:97:THR:HG22	52:s3:99:ALA:H	1.65	0.61
52:s3:228:ASP:O	52:s3:230:ARG:NH1	2.34	0.61
68:O6:105:CYS:HB3	68:O6:143:CYS:H	1.66	0.61
71:R6:195:VAL:O	73:T6:137:ARG:NH1	2.34	0.61
91:n:76:ALA:HB3	91:n:94:VAL:HG22	1.83	0.61
39:e3:266:PRO:O	39:e3:270:ALA:HB2	2.01	0.61
67:N6:76:HIS:O	67:N6:78:LYS:NZ	2.34	0.61
70:Q6:78:LYS:NZ	76:W6:162:VAL:O	2.34	0.61
72:S6:97:GLN:OE1	76:W6:91:GLN:NE2	2.33	0.61
75:V6:82:ARG:NH2	75:V6:120:ASP:OD2	2.34	0.61
75:V6:170:GLN:HE21	80:a6:72:PRO:HD3	1.64	0.61
2:A3:1695:C:H5''	24:Y3:162:ARG:HH12	1.65	0.60
9:J3:34:PRO:HG2	9:J3:35:LEU:HD12	1.82	0.60
15:P3:79:ARG:HG3	15:P3:146:GLN:HE21	1.66	0.60
39:e3:63:LEU:HD12	39:e3:67:GLN:HB3	1.82	0.60
61:H6:71:ILE:HD11	61:H6:177:LEU:HG	1.82	0.60
86:C:29:G:N2	86:C:37:A:N1	2.45	0.60
2:A3:2499:U:OP2	2:A3:2504:A:N6	2.31	0.60
20:U3:71:ARG:NH2	20:U3:96:TYR:OH	2.34	0.60
59:F6:119:LYS:NZ	77:X6:365:TRP:O	2.33	0.60
59:F6:240:ARG:HG2	59:F6:242:TRP:H	1.66	0.60
63:J6:114:ARG:HD3	63:J6:122:LYS:HE3	1.81	0.60
20:U3:18:ARG:NH1	34:93:59:GLU:OE2	2.34	0.60
33:73:105:LEU:HD23	33:73:138:VAL:HG13	1.83	0.60
86:24:33:C:H42	87:i4:20:G:H1	1.46	0.60
89:Z:145:ASP:OD2	89:Z:252:ARG:NH2	2.33	0.60
41:g3:107:MET:SD	41:g3:148:ARG:NH1	2.74	0.60
63:J6:47:ARG:NH2	85:A6:1167:C:OP2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:J6:64:CYS:SG	63:J6:65:THR:N	2.75	0.60
84:e6:492:THR:OG1	84:e6:493:MET:SD	2.60	0.60
89:Z:91:LYS:HE3	89:Z:93:GLU:HB2	1.83	0.60
41:g3:100:ILE:HA	41:g3:105:ARG:O	2.01	0.60
85:A6:843:A:H2'	85:A6:844:A:H8	1.65	0.60
24:Y3:95:ASN:OD1	24:Y3:149:ARG:NH1	2.34	0.60
57:D6:131:ILE:HG23	57:D6:133:GLY:H	1.67	0.60
2:A3:2055:U:H2'	2:A3:2056:G:H8	1.67	0.60
12:M3:40:PRO:HA	12:M3:45:ARG:HB3	1.82	0.60
16:Q3:287:GLU:HB2	16:Q3:291:ARG:HH21	1.65	0.60
59:F6:166:ARG:NH1	85:A6:998:A:O2'	2.35	0.60
79:Z6:32:LYS:HZ3	79:Z6:36:LEU:HD13	1.66	0.60
85:A6:847:G:N2	85:A6:850:A:OP2	2.31	0.60
33:73:144:ARG:NH1	33:73:267:PRO:O	2.34	0.60
85:A6:679:A:H2'	85:A6:680:G:H8	1.66	0.60
2:A3:2604:A:N6	2:A3:2628:U:OP1	2.35	0.60
51:r3:186:CYS:SG	51:r3:187:TYR:N	2.73	0.60
59:F6:119:LYS:NZ	77:X6:398:LEU:O	2.32	0.60
82:c6:9:ARG:NH2	85:A6:1025:U:OP2	2.34	0.60
60:G6:322:ARG:NH2	60:G6:355:PHE:O	2.35	0.60
73:T6:150:PRO:HB3	73:T6:155:LEU:HD23	1.84	0.60
2:A3:2530:A:H4'	2:A3:2531:U:H5'	1.84	0.59
20:U3:3:ARG:HG2	20:U3:23:ASN:HB3	1.83	0.59
23:X3:93:ASN:HB3	23:X3:95:ASP:N	2.17	0.59
66:M6:39:ASN:ND2	85:A6:845:A:OP1	2.35	0.59
78:Y6:286:LEU:O	78:Y6:290:ASN:ND2	2.35	0.59
66:M6:104:ILE:HG23	71:R6:147:ILE:HG21	1.84	0.59
75:V6:258:ARG:HH12	75:V6:261:GLN:HG3	1.67	0.59
81:b6:250:GLU:HA	81:b6:301:ASN:HD21	1.68	0.59
83:d6:139:ASN:ND2	85:A6:1145:C:OP1	2.35	0.59
5:E3:248:ILE:HG22	5:E3:250:ARG:H	1.67	0.59
19:T3:79:GLN:OE1	19:T3:173:HIS:NE2	2.35	0.59
23:X3:177:HIS:ND1	23:X3:178:PRO:O	2.35	0.59
84:e6:85:VAL:HG11	84:e6:97:PRO:HG2	1.85	0.59
91:n:23:ASP:O	91:n:27:HIS:ND1	2.34	0.59
6:F3:191:ASP:HA	6:F3:263:LEU:HD23	1.84	0.59
38:d3:164:VAL:HG12	38:d3:261:MET:HB3	1.83	0.59
2:A3:2661:U:OP2	5:E3:238:ARG:NH2	2.35	0.59
31:53:332:ASP:N	31:53:332:ASP:OD1	2.35	0.59
58:E6:18:THR:HA	58:E6:21:THR:HG22	1.84	0.59
60:G6:113:PRO:HG2	81:b6:109:PRO:HG2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:K6:51:ARG:NH2	64:K6:82:SER:OG	2.36	0.59
70:Q6:54:ARG:NH2	70:Q6:58:GLU:OE1	2.36	0.59
52:s3:81:ARG:O	52:s3:85:LYS:HB3	2.03	0.59
71:R6:295:ASP:OD1	71:R6:295:ASP:N	2.34	0.59
2:A3:1853:A:OP2	18:S3:177:ARG:NH2	2.36	0.59
2:A3:2218:C:OP1	8:I3:128:ASN:ND2	2.34	0.59
18:S3:115:LEU:HD13	36:b3:115:ILE:HG12	1.85	0.59
68:O6:182:GLY:O	71:R6:183:LYS:NZ	2.35	0.59
8:I3:118:LYS:NZ	8:I3:163:GLU:OE2	2.35	0.59
13:N3:154:VAL:HG23	13:N3:158:ARG:HD3	1.83	0.59
21:V3:191:LEU:HB2	24:Y3:153:LEU:HD13	1.84	0.59
89:Z:254:LEU:HD12	89:Z:283:ILE:HD11	1.84	0.59
2:A3:2879:A:O3'	27:13:53:ARG:NH2	2.35	0.59
6:F3:291:SER:HB3	41:g3:52:LEU:HB3	1.83	0.59
52:s3:422:VAL:O	52:s3:426:LEU:HB2	2.03	0.59
2:A3:2420:U:OP1	20:U3:93:LYS:NZ	2.34	0.59
5:E3:126:ASP:O	5:E3:128:HIS:ND1	2.35	0.59
40:f3:164:ALA:O	88:A:164:ARG:NH1	2.35	0.59
40:f3:165:THR:O	88:A:143:GLN:NE2	2.36	0.59
88:A:195:ILE:HG22	88:A:197:LYS:HE3	1.83	0.59
8:I3:147:PHE:HA	8:I3:151:ASN:HD21	1.68	0.58
77:X6:275:LYS:HE2	77:X6:279:LYS:HA	1.85	0.58
85:A6:773:G:H21	85:A6:776:A:H2	1.49	0.58
22:W3:121:PRO:HA	32:63:50:LYS:HA	1.85	0.58
24:Y3:104:VAL:HG22	34:93:65:LEU:HD21	1.85	0.58
27:13:35:ASN:HB3	27:13:38:ARG:HG2	1.85	0.58
42:h3:67:GLN:HE21	42:h3:86:TRP:HZ2	1.48	0.58
61:H6:119:THR:HG23	61:H6:133:GLN:HG2	1.85	0.58
75:V6:202:ARG:NH2	75:V6:242:ALA:O	2.36	0.58
20:U3:91:ASP:N	20:U3:91:ASP:OD1	2.36	0.58
31:53:122:TRP:O	31:53:215:ARG:NH1	2.36	0.58
73:T6:91:GLU:OE2	74:U6:123:ARG:NH1	2.36	0.58
85:A6:977:C:O2	85:A6:1035:G:N2	2.33	0.58
91:n:41:VAL:O	91:n:174:PRO:HA	2.03	0.58
15:P3:88:HIS:ND1	15:P3:106:THR:OG1	2.35	0.58
24:Y3:128:SER:HB2	24:Y3:131:ARG:HE	1.68	0.58
57:D6:220:THR:HG22	57:D6:247:VAL:HG12	1.86	0.58
2:A3:1800:G:N7	21:V3:41:ARG:NH2	2.49	0.58
66:M6:10:LYS:NZ	66:M6:11:ALA:O	2.37	0.58
66:M6:85:LYS:HG2	66:M6:89:LYS:HE3	1.85	0.58
88:A:107:THR:H	88:A:110:GLU:HB3	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F3:188:HIS:O	6:F3:260:VAL:HA	2.02	0.58
40:f3:91:LEU:H	40:f3:159:ILE:HG22	1.69	0.58
68:O6:67:ARG:NH1	68:O6:68:TYR:OH	2.37	0.58
2:A3:2416:U:H3	52:s3:165:ARG:HB3	1.68	0.58
2:A3:3190:A:OP2	51:r3:120:LYS:NZ	2.36	0.58
4:D3:213:CYS:HB3	4:D3:246:ARG:HB3	1.84	0.58
25:Z3:65:LYS:NZ	44:j3:85:ASP:OD1	2.37	0.58
25:Z3:68:ILE:HD11	25:Z3:122:LEU:HD13	1.84	0.58
26:O3:123:CYS:SG	26:O3:124:ALA:N	2.76	0.58
38:d3:147:GLU:OE1	38:d3:159:ARG:NH1	2.37	0.58
52:s3:168:GLU:HA	52:s3:172:ILE:HD13	1.84	0.58
56:C6:113:ARG:NH1	61:H6:164:LEU:O	2.36	0.58
68:O6:132:GLY:O	68:O6:158:ARG:NH2	2.37	0.58
71:R6:288:GLN:HB3	71:R6:297:ALA:HB2	1.86	0.58
60:G6:287:LYS:O	60:G6:288:HIS:ND1	2.37	0.58
76:W6:122:CYS:HB2	76:W6:165:ALA:HB3	1.86	0.58
85:A6:1057:A:N1	85:A6:1104:C:O2'	2.34	0.58
2:A3:1730:U:OP1	7:H3:76:ARG:NH2	2.36	0.58
62:I6:85:ILE:HG22	62:I6:148:ARG:HB2	1.85	0.58
86:C:50:A:N6	86:C:59:G:H1	2.02	0.58
5:E3:104:LEU:HB2	5:E3:121:LEU:HB2	1.86	0.58
36:b3:15:LEU:HD11	37:c3:169:VAL:HG23	1.86	0.58
80:a6:129:ARG:NH1	80:a6:204:PRO:O	2.37	0.58
85:A6:1312:U:H2'	85:A6:1313:A:H8	1.68	0.58
89:Z:414:MET:HE3	89:Z:415:ILE:H	1.68	0.58
23:X3:93:ASN:HB3	23:X3:95:ASP:H	1.69	0.57
39:e3:200:MET:HA	39:e3:241:GLY:HA2	1.85	0.57
39:e3:257:LYS:O	39:e3:257:LYS:NZ	2.36	0.57
58:E6:90:ARG:NH2	69:P6:116:ILE:O	2.37	0.57
68:O6:181:HIS:HD2	68:O6:183:ALA:H	1.52	0.57
72:S6:10:GLY:HA2	72:S6:45:VAL:HG12	1.86	0.57
72:S6:94:SER:OG	72:S6:95:THR:N	2.34	0.57
2:A3:1837:C:OP1	36:b3:4:ARG:NH2	2.37	0.57
17:R3:54:THR:HG21	18:S3:172:MET:H	1.69	0.57
86:24:50:A:N6	86:24:59:G:H1	2.02	0.57
14:O3:33:LEU:HD21	14:O3:59:LEU:HD22	1.87	0.57
84:e6:511:LYS:HA	84:e6:514:LYS:HE2	1.86	0.57
85:A6:764:A:N1	85:A6:784:C:O2'	2.36	0.57
2:A3:2139:U:O4	25:Z3:77:ARG:NH1	2.38	0.57
8:I3:51:THR:OG1	13:N3:250:ARG:NH2	2.37	0.57
12:M3:142:GLU:HB2	12:M3:162:LEU:HD22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y3:158:THR:HG21	34:93:131:TYR:HB2	1.87	0.57
29:33:97:PHE:H	43:i3:122:ASN:HD21	1.51	0.57
2:A3:3180:A:O3'	51:r3:94:ARG:NH1	2.37	0.57
17:R3:31:PHE:HB2	17:R3:36:ASN:HB3	1.85	0.57
22:W3:123:GLY:HA3	32:63:40:ILE:HG21	1.85	0.57
32:63:204:VAL:HB	32:63:245:VAL:HG11	1.86	0.57
39:e3:159:LEU:HD11	39:e3:252:HIS:HD2	1.69	0.57
42:h3:88:ASP:HB3	42:h3:122:ARG:HH21	1.69	0.57
48:o3:28:SER:OG	48:o3:29:LEU:N	2.37	0.57
70:Q6:58:GLU:OE2	70:Q6:62:ARG:NH2	2.37	0.57
75:V6:197:SER:HG	75:V6:200:GLU:H	1.51	0.57
77:X6:51:THR:OG1	77:X6:52:ASN:N	2.37	0.57
89:Z:57:HIS:O	89:Z:252:ARG:NH1	2.38	0.57
23:X3:93:ASN:HA	86:C:72:C:H3'	1.87	0.57
41:g3:150:LYS:NZ	48:o3:79:THR:O	2.37	0.57
52:s3:112:THR:HA	52:s3:391:ASN:O	2.03	0.57
63:J6:51:PRO:HD3	63:J6:123:LEU:HD21	1.87	0.57
73:T6:77:ARG:NH2	73:T6:85:GLN:OE1	2.37	0.57
2:A3:2117:U:O2'	2:A3:2836:C:O2'	2.20	0.57
10:K3:136:ASP:O	10:K3:140:ASN:ND2	2.37	0.57
21:V3:105:ARG:HD2	38:d3:170:PRO:HB2	1.85	0.57
37:c3:121:SER:OG	37:c3:122:ASN:N	2.38	0.57
81:b6:197:ARG:HH12	81:b6:208:LYS:HG2	1.69	0.57
88:A:194:ASP:HB3	88:A:196:THR:HG23	1.87	0.57
9:J3:25:ARG:HA	9:J3:65:PRO:HA	1.87	0.57
16:Q3:177:VAL:HG13	16:Q3:206:PRO:HA	1.87	0.57
26:O3:119:LYS:O	26:O3:120:HIS:ND1	2.38	0.57
30:43:90:VAL:HB	30:43:100:GLN:HB2	1.86	0.57
32:63:122:ALA:O	32:63:127:THR:N	2.38	0.57
59:F6:228:LYS:HG3	86:C:39:A:H4'	1.86	0.57
2:A3:2073:A:H62	2:A3:2832:A:H2	1.52	0.56
52:s3:304:ASP:N	52:s3:304:ASP:OD1	2.35	0.56
81:b6:209:THR:O	81:b6:218:ASN:ND2	2.36	0.56
84:e6:111:LYS:O	84:e6:115:ASN:ND2	2.38	0.56
2:A3:2153:A:H2'	48:o3:30:ARG:HH11	1.69	0.56
2:A3:2154:A:OP1	48:o3:25:ARG:NH2	2.38	0.56
2:A3:2195:A:OP2	46:l3:119:ARG:NH2	2.38	0.56
5:E3:129:VAL:HG22	5:E3:147:VAL:HG22	1.87	0.56
45:k3:18:VAL:HG11	45:k3:34:LEU:HB2	1.86	0.56
55:B6:100:ARG:NH1	72:S6:50:ARG:O	2.39	0.56
67:N6:73:ARG:NH2	85:A6:773:G:OP2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:b6:159:SER:OG	81:b6:160:GLY:N	2.37	0.56
10:K3:20:LEU:HD13	10:K3:141:LEU:HD21	1.87	0.56
11:L3:114:PRO:HD2	11:L3:136:LYS:HB3	1.86	0.56
15:P3:79:ARG:NH2	15:P3:94:GLU:OE2	2.37	0.56
17:R3:66:THR:O	17:R3:70:ASN:ND2	2.38	0.56
42:h3:99:ASN:O	42:h3:103:HIS:ND1	2.39	0.56
52:s3:178:ASP:N	52:s3:178:ASP:OD1	2.38	0.56
55:B6:99:HIS:HD2	55:B6:101:PHE:H	1.54	0.56
55:B6:201:ASN:ND2	85:A6:1298:A:OP1	2.37	0.56
56:C6:115:ASN:ND2	78:Y6:309:LYS:O	2.39	0.56
85:A6:1474:A:H2'	85:A6:1475:A:H8	1.71	0.56
23:X3:91:TYR:HA	23:X3:99:LYS:O	2.05	0.56
40:f3:51:LYS:O	40:f3:53:THR:N	2.36	0.56
45:k3:73:ARG:O	51:r3:47:THR:N	2.38	0.56
60:G6:304:PHE:O	60:G6:310:ARG:NH1	2.38	0.56
67:N6:67:ARG:NH2	67:N6:80:GLU:OE1	2.38	0.56
68:O6:91:ARG:NH2	85:A6:921:C:OP2	2.38	0.56
72:S6:80:SER:OG	76:W6:97:ASP:O	2.22	0.56
76:W6:92:MET:HE3	76:W6:98:LYS:HD2	1.88	0.56
77:X6:179:ASP:OD2	77:X6:289:LEU:N	2.37	0.56
80:a6:183:ASP:OD1	80:a6:183:ASP:N	2.39	0.56
85:A6:1363:U:H2'	85:A6:1364:G:H8	1.70	0.56
5:E3:94:SER:OG	5:E3:184:ASN:ND2	2.38	0.56
9:J3:69:LYS:HB2	9:J3:81:LYS:HB2	1.85	0.56
16:Q3:150:ILE:HD11	16:Q3:161:GLU:HB3	1.86	0.56
18:S3:172:MET:HA	18:S3:182:LYS:O	2.05	0.56
57:D6:178:GLU:HG3	57:D6:182:LYS:HE2	1.87	0.56
75:V6:102:TRP:HE1	80:a6:73:LEU:HG	1.69	0.56
85:A6:1006:C:H2'	85:A6:1007:A:H8	1.70	0.56
5:E3:134:SER:OG	5:E3:135:LYS:N	2.38	0.56
2:A3:2016:C:OP2	12:M3:59:ARG:NH1	2.38	0.56
2:A3:3217:A:N3	16:Q3:86:ARG:NH2	2.54	0.56
88:A:58:PRO:O	88:A:62:GLN:NE2	2.38	0.56
2:A3:2143:G:OP1	18:S3:173:ARG:NH2	2.35	0.56
2:A3:2310:G:OP2	26:O3:94:ARG:NH2	2.38	0.56
2:A3:2528:G:OP1	4:D3:135:ARG:NH2	2.39	0.56
72:S6:89:ASN:ND2	72:S6:90:PRO:O	2.39	0.56
79:Z6:89:ARG:NH1	85:A6:1342:A:OP2	2.38	0.56
81:b6:60:MET:SD	84:e6:83:THR:OG1	2.61	0.56
85:A6:1428:U:OP2	86:C:32:A:O2'	2.16	0.56
2:A3:1880:C:OP2	41:g3:111:ARG:NH1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A3:1939:G:H5'	2:A3:1940:A:H5''	1.87	0.56
2:A3:2063:G:N2	22:W3:56:MET:SD	2.79	0.56
3:B3:1622:A:OP1	15:P3:88:HIS:NE2	2.34	0.56
4:D3:228:LEU:HD12	4:D3:232:ARG:HB3	1.87	0.56
20:U3:11:ARG:HD3	21:V3:211:LYS:HE3	1.88	0.56
50:q3:57:ALA:HB1	50:q3:70:VAL:HG11	1.88	0.56
60:G6:268:ALA:O	60:G6:286:TYR:HA	2.06	0.56
64:K6:58:ARG:NH1	85:A6:1407:A:OP1	2.37	0.56
75:V6:283:LEU:O	75:V6:287:LEU:HB2	2.05	0.56
86:C:50:A:N6	86:C:60:C:N3	2.54	0.56
2:A3:2926:A:O2'	2:A3:3087:C:OP1	2.21	0.56
10:K3:23:GLY:O	10:K3:147:GLN:NE2	2.39	0.56
58:E6:27:GLU:OE2	74:U6:170:ARG:NH1	2.39	0.56
58:E6:80:GLU:O	58:E6:84:ARG:NH2	2.39	0.56
7:H3:138:LYS:NZ	7:H3:142:GLU:OE2	2.38	0.55
20:U3:74:HIS:HB2	34:93:24:LYS:HE2	1.88	0.55
33:73:245:SER:OG	33:73:246:GLN:NE2	2.37	0.55
38:d3:146:ILE:O	38:d3:150:LEU:HB2	2.06	0.55
39:e3:212:HIS:HA	39:e3:231:VAL:O	2.05	0.55
2:A3:1827:C:O2'	17:R3:48:ARG:NH1	2.40	0.55
44:j3:102:GLN:NE2	44:j3:106:GLU:OE2	2.38	0.55
57:D6:304:LYS:NZ	57:D6:337:SER:OG	2.34	0.55
66:M6:51:LEU:HA	66:M6:69:ASN:HD21	1.71	0.55
76:W6:83:MET:O	76:W6:87:SER:OG	2.24	0.55
77:X6:152:ILE:HG23	77:X6:259:LEU:HD23	1.87	0.55
80:a6:29:ARG:HB2	80:a6:32:GLN:HE22	1.71	0.55
86:24:50:A:N6	86:24:60:C:N3	2.54	0.55
2:A3:1814:A:N3	2:A3:1862:U:O2'	2.36	0.55
2:A3:2871:U:OP2	29:33:143:ARG:NH2	2.40	0.55
63:J6:35:GLN:NE2	85:A6:1138:G:OP2	2.38	0.55
71:R6:292:ASP:OD1	71:R6:292:ASP:N	2.40	0.55
2:A3:1953:A:O2'	2:A3:2463:A:OP1	2.25	0.55
2:A3:2065:A:H5''	22:W3:129:THR:HG21	1.89	0.55
4:D3:132:ASP:OD2	4:D3:135:ARG:NH1	2.38	0.55
6:F3:262:THR:HG22	6:F3:264:PRO:HD2	1.89	0.55
14:O3:106:ARG:HD2	14:O3:135:LEU:HD21	1.88	0.55
14:O3:155:ASP:OD2	33:73:319:ARG:NH2	2.39	0.55
26:03:181:ARG:HG3	26:03:185:PHE:HD2	1.72	0.55
36:b3:44:ARG:NH1	48:o3:99:LYS:O	2.40	0.55
38:d3:226:ASP:H	38:d3:229:GLY:HA2	1.71	0.55
40:f3:49:LYS:HA	40:f3:51:LYS:HB2	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:h3:133:PRO:HB2	42:h3:135:GLN:HE22	1.71	0.55
59:F6:194:LYS:NZ	85:A6:1424:U:OP2	2.39	0.55
80:a6:29:ARG:NH1	85:A6:1534:A:OP1	2.40	0.55
85:A6:723:G:N2	85:A6:803:A:O2'	2.40	0.55
2:A3:1835:A:OP2	36:b3:116:ARG:NH2	2.39	0.55
14:O3:91:GLN:NE2	52:s3:44:TYR:OH	2.40	0.55
24:Y3:116:GLU:HG2	24:Y3:126:MET:HE1	1.88	0.55
67:N6:69:LEU:HD21	67:N6:80:GLU:HB2	1.89	0.55
77:X6:101:VAL:HG22	77:X6:140:HIS:HE1	1.72	0.55
91:n:36:LYS:NZ	101:n:416:HOH:O	2.40	0.55
64:K6:40:ARG:NH1	85:A6:1238:C:O2'	2.40	0.55
85:A6:1234:C:N4	85:A6:1450:A:O2'	2.39	0.55
15:P3:53:ARG:NH2	15:P3:56:GLU:OE1	2.40	0.55
31:53:200:ARG:HE	31:53:233:LYS:HE3	1.72	0.55
77:X6:108:LEU:HD21	77:X6:307:VAL:HG11	1.88	0.55
77:X6:124:TYR:HB2	77:X6:307:VAL:HG12	1.88	0.55
96:Z:501:GCP:H5'2	96:Z:501:GCP:H8	1.89	0.55
6:F3:81:ASP:OD1	6:F3:81:ASP:N	2.32	0.55
13:N3:204:GLU:OE2	13:N3:208:ASN:ND2	2.40	0.55
39:e3:270:ALA:O	39:e3:273:ARG:NH1	2.40	0.55
49:p3:46:ASP:OD1	49:p3:46:ASP:N	2.38	0.55
59:F6:177:ARG:NH2	85:A6:1465:A:OP2	2.39	0.55
64:K6:78:LEU:HD12	64:K6:79:PRO:HD2	1.89	0.55
75:V6:356:THR:HA	75:V6:359:LEU:HD12	1.88	0.55
85:A6:1148:U:H2'	85:A6:1149:A:H8	1.71	0.55
85:A6:1216:U:O2'	85:A6:1218:A:N7	2.35	0.55
2:A3:3065:U:OP2	5:E3:239:ARG:NH1	2.40	0.55
14:O3:116:ASP:OD1	14:O3:116:ASP:N	2.40	0.55
33:73:256:ARG:NH1	33:73:258:GLY:O	2.39	0.55
59:F6:126:TYR:HB2	59:F6:137:ILE:HG21	1.88	0.55
60:G6:133:PRO:O	60:G6:135:GLN:NE2	2.40	0.55
63:J6:50:GLY:O	63:J6:89:ARG:NH1	2.40	0.55
64:K6:89:ASN:ND2	85:A6:1447:U:OP1	2.40	0.55
2:A3:1752:U:H2'	2:A3:1753:A:H8	1.71	0.55
2:A3:2401:A:OP1	4:D3:262:ARG:NH1	2.39	0.55
5:E3:147:VAL:O	5:E3:176:VAL:HA	2.07	0.55
8:I3:103:ALA:HB1	45:k3:40:GLU:HG2	1.87	0.55
66:M6:32:TYR:O	66:M6:53:SER:OG	2.25	0.55
74:U6:107:ALA:O	74:U6:110:GLN:NE2	2.36	0.55
77:X6:155:ILE:HG12	77:X6:262:VAL:HA	1.87	0.55
80:a6:25:LEU:HD21	85:A6:1535:C:H2'	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E3:275:ARG:O	5:E3:284:TYR:HB2	2.06	0.54
16:Q3:181:LYS:HB3	16:Q3:217:VAL:HG13	1.89	0.54
39:e3:146:ARG:HA	39:e3:151:ARG:HD2	1.89	0.54
41:g3:88:ARG:NH1	41:g3:92:HIS:O	2.39	0.54
81:b6:144:GLU:HG3	81:b6:176:LYS:HE3	1.88	0.54
15:P3:129:ARG:NH1	32:63:129:SER:O	2.40	0.54
24:Y3:193:ARG:HA	24:Y3:196:ARG:HE	1.71	0.54
27:13:42:THR:HA	27:13:56:PHE:O	2.08	0.54
67:N6:72:PRO:HB3	67:N6:78:LYS:HG2	1.87	0.54
71:R6:208:ILE:O	71:R6:214:ASN:ND2	2.39	0.54
73:T6:139:CYS:SG	73:T6:140:ILE:N	2.79	0.54
89:Z:48:LYS:NZ	89:Z:307:GLU:OE2	2.39	0.54
3:B3:1628:C:H2'	3:B3:1629:A:H8	1.72	0.54
17:R3:33:GLY:O	17:R3:37:ARG:NH1	2.40	0.54
19:T3:109:ASN:HD21	26:03:101:ILE:HG21	1.72	0.54
21:V3:131:THR:OG1	21:V3:132:GLU:N	2.39	0.54
31:53:204:VAL:HG23	52:s3:152:GLN:HE21	1.71	0.54
38:d3:225:TYR:HB3	38:d3:229:GLY:HA2	1.89	0.54
68:O6:173:ARG:NH2	71:R6:236:GLU:OE1	2.40	0.54
85:A6:1269:C:H2'	85:A6:1270:A:H8	1.72	0.54
89:Z:200:ARG:NH1	89:Z:213:THR:O	2.39	0.54
2:A3:1822:U:O2	2:A3:2707:A:O2'	2.25	0.54
4:D3:103:ARG:O	4:D3:105:ARG:NH1	2.38	0.54
72:S6:59:PRO:O	72:S6:61:GLN:NE2	2.40	0.54
76:W6:122:CYS:SG	76:W6:123:VAL:N	2.80	0.54
80:a6:9:ARG:HB3	80:a6:12:ALA:HB3	1.90	0.54
85:A6:825:U:H2'	85:A6:826:G:H8	1.73	0.54
2:A3:2755:A:N6	2:A3:2790:A:O2'	2.40	0.54
31:53:69:TRP:HD1	31:53:70:LEU:HD13	1.73	0.54
52:s3:206:VAL:HG13	52:s3:235:ASP:HB3	1.89	0.54
66:M6:63:GLU:HG2	71:R6:155:LYS:HG2	1.88	0.54
89:Z:51:TYR:HA	89:Z:311:LYS:HE2	1.89	0.54
2:A3:1747:G:N2	2:A3:1750:G:O2'	2.41	0.54
2:A3:1844:A:OP2	17:R3:48:ARG:NH2	2.40	0.54
2:A3:2377:G:O2'	34:93:28:ARG:O	2.25	0.54
6:F3:59:ARG:NH2	41:g3:114:GLU:OE2	2.40	0.54
36:b3:37:GLY:O	36:b3:44:ARG:NH2	2.39	0.54
57:D6:358:THR:OG1	57:D6:361:GLN:OE1	2.25	0.54
71:R6:299:ASN:O	71:R6:302:GLN:NE2	2.40	0.54
75:V6:182:SER:HA	75:V6:185:VAL:HG12	1.89	0.54
90:j:21:U:O4	90:j:47:G:O2'	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:230:THR:OG1	7:D:231:VAL:N	2.38	0.54
91:n:210:ARG:O	91:n:223:ARG:NH2	2.41	0.54
2:A3:1882:A:N6	2:A3:1893:A:O4'	2.40	0.54
2:A3:2289:G:OP1	12:M3:34:LYS:NZ	2.40	0.54
6:F3:79:LEU:HD11	42:h3:117:LEU:HD21	1.90	0.54
21:V3:28:SER:O	21:V3:32:LYS:NZ	2.40	0.54
22:W3:104:TYR:HB2	22:W3:128:LYS:HB2	1.90	0.54
24:Y3:91:ARG:NE	34:93:84:THR:O	2.39	0.54
31:53:298:ASN:O	31:53:303:ARG:NH1	2.40	0.54
56:C6:113:ARG:NH2	61:H6:162:ARG:O	2.41	0.54
66:M6:39:ASN:HB3	66:M6:40:LYS:HZ2	1.72	0.54
78:Y6:322:ASP:HA	81:b6:214:LEU:HD21	1.89	0.54
84:e6:513:TRP:HD1	84:e6:531:ILE:HD13	1.73	0.54
90:j:16:C:N4	90:j:61:A:O2'	2.41	0.54
91:n:182:PRO:HA	91:n:185:LEU:HD12	1.90	0.54
2:A3:1990:G:OP1	4:D3:269:ARG:NH2	2.41	0.54
2:A3:2025:C:H2'	2:A3:2026:A:H8	1.73	0.54
12:M3:165:ALA:HB2	12:M3:236:LEU:HD12	1.90	0.54
32:63:327:VAL:HA	32:63:330:ILE:HD12	1.88	0.54
61:H6:173:THR:OG1	81:b6:155:ASP:OD1	2.25	0.54
64:K6:89:ASN:OD1	64:K6:89:ASN:N	2.40	0.54
68:O6:128:CYS:SG	68:O6:129:ALA:N	2.81	0.54
81:b6:173:LEU:O	81:b6:206:THR:HA	2.07	0.54
2:A3:3082:G:N2	2:A3:3085:A:OP2	2.37	0.54
18:S3:127:ARG:NH2	18:S3:157:GLU:OE1	2.40	0.54
25:Z3:78:ARG:O	25:Z3:83:LYS:NZ	2.40	0.54
39:e3:84:TYR:HE2	88:A:93:LYS:HG2	1.73	0.54
57:D6:127:ASN:OD1	79:Z6:72:ARG:NH1	2.40	0.54
74:U6:103:ARG:HA	74:U6:106:MET:HE3	1.89	0.54
15:P3:74:ARG:O	15:P3:96:GLN:NE2	2.32	0.54
19:T3:110:ASP:OD1	19:T3:110:ASP:N	2.35	0.54
52:s3:243:ILE:HG21	52:s3:429:PRO:HG3	1.89	0.54
85:A6:667:A:H2'	85:A6:668:G:C8	2.42	0.54
89:Z:353:GLU:O	89:Z:437:THR:OG1	2.24	0.54
2:A3:2294:A:OP2	12:M3:41:ARG:NH1	2.40	0.53
15:P3:149:PRO:HB3	22:W3:109:ARG:HH11	1.73	0.53
19:T3:212:LEU:H	36:b3:119:PHE:HE2	1.56	0.53
32:63:253:PRO:HD3	32:63:289:PRO:HB3	1.91	0.53
62:I6:130:THR:HA	62:I6:133:ILE:HD12	1.90	0.53
77:X6:133:GLY:HA3	95:X6:500:GDP:HN22	1.73	0.53
80:a6:171:ARG:NH2	80:a6:189:PRO:O	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:179:ASN:HB3	7:D:182:TRP:HD1	1.72	0.53
12:M3:140:LEU:HG	12:M3:156:VAL:HG21	1.90	0.53
16:Q3:118:ARG:NH1	16:Q3:175:GLN:OE1	2.39	0.53
49:p3:97:SER:O	49:p3:146:ASN:ND2	2.41	0.53
69:P6:73:ASP:OD2	69:P6:73:ASP:N	2.41	0.53
80:a6:194:GLN:O	80:a6:197:ARG:NH1	2.35	0.53
23:X3:169:LEU:HB3	23:X3:195:ALA:HB2	1.91	0.53
52:s3:269:ASP:OD1	52:s3:269:ASP:N	2.36	0.53
60:G6:392:THR:OG1	60:G6:393:TRP:N	2.41	0.53
89:Z:267:SER:HB2	89:Z:331:ARG:HD2	1.90	0.53
2:A3:2310:G:O2'	2:A3:2675:G:O6	2.24	0.53
2:A3:2455:U:H5''	14:O3:47:ALA:HB3	1.91	0.53
21:V3:98:ILE:HD12	21:V3:109:ILE:HD13	1.90	0.53
21:V3:138:THR:N	21:V3:142:GLU:O	2.42	0.53
31:53:290:THR:HA	31:53:343:GLN:O	2.09	0.53
45:k3:15:GLN:NE2	45:k3:49:CYS:O	2.39	0.53
62:I6:182:PRO:HB2	62:I6:185:GLY:H	1.73	0.53
85:A6:688:U:H2'	85:A6:689:A:H8	1.73	0.53
32:63:222:ASP:OD1	32:63:267:ARG:NH1	2.41	0.53
42:h3:114:ASN:HA	42:h3:117:LEU:HB2	1.90	0.53
56:C6:37:ASN:N	56:C6:37:ASN:OD1	2.40	0.53
60:G6:295:VAL:HG22	60:G6:330:CYS:HB2	1.91	0.53
84:e6:536:ALA:HA	84:e6:582:LEU:HD11	1.90	0.53
2:A3:3143:U:H2'	2:A3:3144:A:H8	1.73	0.53
37:c3:181:SER:OG	37:c3:182:GLU:N	2.42	0.53
66:M6:93:LEU:HD21	66:M6:103:MET:HE3	1.90	0.53
2:A3:2295:C:OP2	17:R3:17:ARG:NH2	2.42	0.53
2:A3:3128:A:O2'	2:A3:3129:A:O4'	2.26	0.53
8:I3:174:LEU:H	45:k3:53:ALA:HB3	1.73	0.53
17:R3:111:LYS:HD2	35:a3:45:CYS:HB3	1.91	0.53
33:73:218:THR:HG22	33:73:255:HIS:HD1	1.74	0.53
40:f3:51:LYS:O	40:f3:54:HIS:N	2.38	0.53
75:V6:392:ARG:NH1	85:A6:1529:C:OP1	2.39	0.53
82:c6:66:CYS:HB2	82:c6:69:GLU:HB2	1.91	0.53
85:A6:704:A:N1	85:A6:713:G:O2'	2.37	0.53
91:n:223:ARG:NH2	101:n:418:HOH:O	2.41	0.53
2:A3:2052:A:H5''	41:g3:150:LYS:HE3	1.91	0.53
2:A3:2761:C:O2'	7:D:171:ARG:NH1	2.42	0.53
2:A3:3168:C:N3	5:E3:303:LYS:NZ	2.57	0.53
12:M3:276:ASN:ND2	12:M3:278:ALA:O	2.41	0.53
15:P3:121:VAL:HG23	15:P3:156:SER:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:b3:34:SER:OG	36:b3:36:ASP:O	2.22	0.53
38:d3:169:PHE:O	38:d3:173:THR:OG1	2.24	0.53
42:h3:62:PRO:HD3	42:h3:133:PRO:HB3	1.90	0.53
52:s3:239:ASN:N	52:s3:239:ASN:OD1	2.42	0.53
2:A3:2688:C:O2	2:A3:2702:G:N2	2.42	0.53
12:M3:286:THR:OG1	41:g3:38:PHE:O	2.27	0.53
55:B6:211:ASP:OD1	85:A6:1300:A:N6	2.42	0.53
59:F6:51:TYR:O	59:F6:52:ARG:NH1	2.41	0.53
75:V6:233:LYS:O	75:V6:288:LYS:NZ	2.36	0.53
85:A6:1205:A:H2'	85:A6:1206:G:C8	2.44	0.53
2:A3:2777:G:OP2	7:D:177:LYS:NZ	2.42	0.53
2:A3:2950:U:H2'	2:A3:2951:A:H8	1.72	0.53
6:F3:140:SER:OG	6:F3:141:ILE:O	2.26	0.53
12:M3:109:ARG:NH2	41:g3:91:MET:SD	2.82	0.53
21:V3:179:VAL:HG13	34:93:78:ALA:HA	1.91	0.53
24:Y3:85:TRP:HB3	24:Y3:90:LEU:HD11	1.90	0.53
57:D6:136:ARG:O	57:D6:165:GLN:NE2	2.42	0.53
63:J6:49:LEU:HG	63:J6:51:PRO:HD2	1.90	0.53
65:L6:165:LYS:NZ	85:A6:951:U:OP1	2.40	0.53
2:A3:2661:U:H2'	2:A3:2662:A:H8	1.74	0.52
16:Q3:239:ASN:O	16:Q3:241:LYS:NZ	2.42	0.52
29:33:117:LEU:HD12	29:33:121:LEU:HB2	1.90	0.52
37:c3:83:PHE:HD2	37:c3:88:LEU:HD22	1.73	0.52
41:g3:96:VAL:HG22	41:g3:110:ILE:HG12	1.90	0.52
56:C6:40:ALA:HB3	56:C6:59:PRO:HD3	1.91	0.52
64:K6:80:ARG:NH1	85:A6:1354:G:OP2	2.43	0.52
91:n:214:VAL:HB	91:n:224:ILE:HD11	1.91	0.52
12:M3:146:ASP:OD1	49:p3:143:GLN:NE2	2.41	0.52
18:S3:52:PRO:HD2	51:r3:77:LEU:HD21	1.89	0.52
36:b3:33:VAL:O	36:b3:67:SER:HA	2.09	0.52
38:d3:243:LEU:HD12	38:d3:245:TYR:HE1	1.74	0.52
76:W6:101:ILE:HG22	76:W6:141:ARG:HG2	1.90	0.52
3:B3:1630:A:OP1	47:m3:42:ARG:NH1	2.43	0.52
31:53:229:ARG:NH1	31:53:231:SER:OG	2.41	0.52
38:d3:219:ARG:HB3	38:d3:239:PRO:HB2	1.90	0.52
39:e3:245:GLN:O	39:e3:248:ASN:ND2	2.38	0.52
71:R6:282:ASP:OD1	71:R6:282:ASP:N	2.37	0.52
74:U6:27:ARG:NH1	85:A6:704:A:OP2	2.41	0.52
76:W6:137:GLY:O	76:W6:139:ARG:NH1	2.42	0.52
80:a6:98:THR:OG1	80:a6:115:TRP:O	2.28	0.52
80:a6:167:PRO:HG2	80:a6:170:LEU:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A3:1792:G:OP2	28:23:85:LYS:NZ	2.42	0.52
2:A3:2846:G:O2'	2:A3:2913:A:N6	2.40	0.52
2:A3:3066:C:O2'	5:E3:233:GLN:NE2	2.42	0.52
4:D3:154:THR:HA	4:D3:247:VAL:HA	1.92	0.52
5:E3:112:LYS:NZ	5:E3:335:GLU:O	2.42	0.52
5:E3:234:THR:OG1	5:E3:235:LYS:N	2.43	0.52
25:Z3:137:THR:HG22	25:Z3:147:VAL:HA	1.92	0.52
32:63:263:SER:HB2	32:63:342:PHE:HD2	1.74	0.52
42:h3:70:LEU:HD13	42:h3:104:LEU:HD11	1.90	0.52
69:P6:86:PRO:HA	69:P6:125:LYS:HB2	1.92	0.52
76:W6:150:THR:HG22	76:W6:161:THR:HA	1.90	0.52
80:a6:19:ARG:NH2	85:A6:812:C:OP1	2.43	0.52
2:A3:1909:A:HO2'	2:A3:2733:G:HO2'	1.58	0.52
6:F3:283:LEU:O	12:M3:189:LYS:NZ	2.42	0.52
31:53:203:CYS:O	52:s3:179:GLN:NE2	2.41	0.52
33:73:99:TYR:O	33:73:103:SER:CB	2.55	0.52
41:g3:108:THR:OG1	41:g3:151:GLY:O	2.26	0.52
51:r3:188:SER:OG	51:r3:189:ARG:N	2.43	0.52
52:s3:424:PHE:O	52:s3:427:ASN:ND2	2.43	0.52
59:F6:122:GLN:NE2	59:F6:138:GLU:O	2.39	0.52
60:G6:373:ASP:OD1	60:G6:373:ASP:N	2.43	0.52
66:M6:53:SER:OG	66:M6:54:TYR:N	2.42	0.52
81:b6:210:ASP:HA	81:b6:218:ASN:HD21	1.74	0.52
85:A6:1093:U:H2'	85:A6:1094:A:H8	1.74	0.52
2:A3:1911:C:H2'	2:A3:1912:A:H8	1.73	0.52
2:A3:2003:A:OP2	2:A3:2734:A:O2'	2.27	0.52
2:A3:2094:G:OP2	12:M3:57:ARG:NH2	2.42	0.52
2:A3:2390:A:N6	2:A3:2399:A:H61	2.06	0.52
2:A3:2454:G:OP1	14:O3:48:ARG:NH2	2.40	0.52
2:A3:3068:G:N2	2:A3:3068:G:OP2	2.41	0.52
8:I3:79:ILE:HD11	8:I3:130:VAL:HG21	1.90	0.52
11:L3:113:ASN:HA	11:L3:136:LYS:HE2	1.92	0.52
16:Q3:218:ASN:OD1	16:Q3:218:ASN:N	2.42	0.52
16:Q3:240:ILE:HG22	16:Q3:242:GLY:H	1.73	0.52
40:f3:127:MET:HB2	40:f3:154:GLU:HG2	1.92	0.52
80:a6:115:TRP:HA	80:a6:131:ILE:HG23	1.91	0.52
91:n:123:VAL:HG11	91:n:138:PRO:HG2	1.92	0.52
2:A3:1705:A:N6	34:93:40:GLY:O	2.36	0.52
2:A3:2145:G:O2'	2:A3:2147:G:OP1	2.24	0.52
5:E3:301:ASP:OD2	5:E3:301:ASP:N	2.43	0.52
23:X3:4:HIS:O	43:i3:101:ARG:NH1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:73:222:GLU:OE1	33:73:224:LYS:NZ	2.43	0.52
51:r3:40:GLU:HA	51:r3:48:ILE:O	2.09	0.52
65:L6:143:LEU:HD11	65:L6:153:LYS:HA	1.92	0.52
89:Z:113:VAL:HG23	89:Z:124:HIS:HB3	1.91	0.52
89:Z:262:VAL:HB	89:Z:337:GLY:H	1.75	0.52
89:Z:353:GLU:HA	89:Z:407:ASN:HA	1.92	0.52
7:D:229:ASP:OD1	7:D:229:ASP:N	2.43	0.52
2:A3:3051:A:OP1	2:A3:3116:C:O2'	2.27	0.52
52:s3:60:LEU:HD23	52:s3:63:ILE:HD11	1.92	0.52
75:V6:76:ILE:O	75:V6:115:GLN:NE2	2.43	0.52
75:V6:214:LYS:HB2	75:V6:220:GLY:HA3	1.90	0.52
77:X6:349:ASN:ND2	77:X6:352:GLU:OE2	2.43	0.52
81:b6:291:GLU:HA	81:b6:294:LYS:HD2	1.92	0.52
85:A6:1157:C:H4'	85:A6:1158:A:H5''	1.91	0.52
89:Z:163:GLU:OE2	89:Z:425:ARG:NH2	2.42	0.52
89:Z:388:ARG:HB2	89:Z:409:ILE:HG23	1.92	0.52
2:A3:1957:A:OP2	19:T3:161:ARG:NH1	2.42	0.52
2:A3:2392:U:H2'	2:A3:2394:A:H62	1.74	0.52
23:X3:92:ALA:H	86:C:73:A:H4'	1.75	0.52
31:53:251:HIS:O	31:53:371:LYS:NZ	2.30	0.52
33:73:182:ASP:HA	33:73:295:ARG:O	2.09	0.52
86:24:9:A:O2'	86:24:10:G:N7	2.43	0.52
41:g3:90:ARG:HB2	41:g3:91:MET:HE2	1.91	0.52
56:C6:89:ASP:OD2	56:C6:112:ARG:NH2	2.40	0.52
58:E6:15:ARG:NH1	74:U6:182:ASP:OD1	2.36	0.52
2:A3:2545:U:O2'	2:A3:2633:A:OP2	2.28	0.51
2:A3:2822:C:O2'	2:A3:2915:C:OP2	2.28	0.51
2:A3:3014:G:H5''	30:43:96:PRO:HB2	1.91	0.51
6:F3:97:HIS:HA	12:M3:27:LEU:HD13	1.92	0.51
31:53:313:MET:HE1	31:53:346:GLY:HA2	1.92	0.51
36:b3:13:SER:OG	36:b3:14:VAL:N	2.41	0.51
50:q3:141:GLU:HG2	50:q3:145:LYS:HE3	1.93	0.51
52:s3:53:ALA:O	52:s3:62:ARG:NH2	2.43	0.51
57:D6:304:LYS:O	57:D6:334:ALA:HA	2.10	0.51
62:I6:151:VAL:O	62:I6:177:ASP:HA	2.10	0.51
64:K6:52:LEU:O	64:K6:56:SER:OG	2.25	0.51
85:A6:1276:A:N1	85:A6:1307:G:O2'	2.41	0.51
89:Z:345:SER:OG	89:Z:346:ILE:N	2.40	0.51
2:A3:1800:G:N1	2:A3:1803:A:OP2	2.40	0.51
2:A3:2296:U:O4	18:S3:181:LYS:NZ	2.43	0.51
2:A3:2779:C:H1'	2:A3:2780:C:H5''	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A3:3024:U:H2'	2:A3:3025:A:H8	1.75	0.51
4:D3:228:LEU:HD11	4:D3:234:MET:HE3	1.93	0.51
6:F3:63:GLN:HG2	6:F3:81:ASP:HB3	1.92	0.51
6:F3:230:ILE:HG23	6:F3:242:LEU:HD11	1.92	0.51
10:K3:78:SER:OG	10:K3:79:SER:N	2.43	0.51
39:e3:200:MET:HB3	39:e3:238:LEU:HD21	1.92	0.51
60:G6:94:GLU:HG3	60:G6:96:PRO:HD2	1.91	0.51
68:O6:92:LYS:HA	68:O6:144:VAL:HG12	1.92	0.51
91:n:59:ARG:HH22	91:n:139:ASN:HD22	1.59	0.51
2:A3:1911:C:H2'	2:A3:1912:A:C8	2.45	0.51
2:A3:2459:A:N6	2:A3:2668:A:O2'	2.43	0.51
6:F3:97:HIS:HB2	12:M3:27:LEU:HB3	1.92	0.51
15:P3:78:HIS:HA	15:P3:94:GLU:O	2.09	0.51
60:G6:128:PRO:HA	60:G6:131:ILE:HG22	1.92	0.51
71:R6:71:MET:N	71:R6:71:MET:SD	2.84	0.51
71:R6:204:ILE:HD13	73:T6:144:GLU:HB3	1.93	0.51
91:n:155:GLU:HB3	91:n:160:ARG:HD3	1.91	0.51
2:A3:2240:C:H4'	10:K3:30:LYS:HG3	1.92	0.51
12:M3:202:LYS:HD2	12:M3:263:ARG:HH21	1.74	0.51
71:R6:107:THR:OG1	71:R6:108:GLN:N	2.44	0.51
71:R6:155:LYS:H	71:R6:177:PRO:HD3	1.75	0.51
77:X6:287:LEU:HB2	77:X6:290:VAL:HG12	1.92	0.51
79:Z6:73:ASP:N	79:Z6:73:ASP:OD1	2.40	0.51
81:b6:68:SER:HB2	84:e6:81:ASP:HB3	1.92	0.51
90:j:20:U:O2'	90:j:22:A:OP1	2.24	0.51
35:a3:119:THR:OG1	35:a3:120:LYS:N	2.43	0.51
85:A6:1205:A:H2'	85:A6:1206:G:H8	1.74	0.51
85:A6:1444:G:H2'	85:A6:1445:A:C8	2.45	0.51
86:C:9:A:O2'	86:C:10:G:N7	2.43	0.51
11:L3:101:ASP:OD2	16:Q3:152:ARG:NH2	2.43	0.51
17:R3:32:ARG:O	17:R3:35:LYS:NZ	2.40	0.51
39:e3:55:ARG:NH2	39:e3:152:LYS:O	2.42	0.51
41:g3:59:ASP:OD1	41:g3:59:ASP:N	2.40	0.51
42:h3:148:LEU:HD22	42:h3:152:LEU:HD22	1.91	0.51
62:I6:177:ASP:OD1	62:I6:177:ASP:N	2.40	0.51
77:X6:104:PRO:HG3	77:X6:345:VAL:HG23	1.92	0.51
81:b6:121:LYS:HZ1	84:e6:78:VAL:HA	1.75	0.51
85:A6:1395:U:H3'	85:A6:1396:A:H8	1.74	0.51
2:A3:2919:A:C4	23:X3:97:LEU:HD13	2.45	0.51
11:L3:129:LYS:NZ	16:Q3:125:TYR:OH	2.38	0.51
18:S3:84:ASN:ND2	18:S3:202:PRO:O	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S3:163:LYS:HG2	18:S3:191:THR:HG22	1.93	0.51
37:c3:104:LYS:O	37:c3:107:GLN:NE2	2.35	0.51
62:I6:187:ARG:O	85:A6:1070:C:O2'	2.28	0.51
77:X6:268:LEU:HD13	77:X6:290:VAL:HG22	1.92	0.51
5:E3:292:HIS:ND1	5:E3:293:LYS:O	2.44	0.51
20:U3:72:VAL:HG22	20:U3:93:LYS:HG2	1.93	0.51
85:A6:1113:A:H2'	85:A6:1114:A:H8	1.76	0.51
2:A3:2522:U:H2'	31:53:35:VAL:HG23	1.93	0.51
5:E3:175:THR:HG22	5:E3:296:LEU:HD23	1.93	0.51
10:K3:2:SER:OG	10:K3:3:SER:N	2.44	0.51
15:P3:103:SER:OG	32:63:150:ARG:NH1	2.44	0.51
59:F6:242:TRP:O	82:c6:84:ARG:NH1	2.44	0.51
61:H6:97:LEU:HB3	81:b6:119:ILE:HG21	1.93	0.51
62:I6:184:ASN:ND2	85:A6:1019:A:O5'	2.44	0.51
63:J6:95:ILE:HG21	63:J6:100:HIS:HB3	1.92	0.51
72:S6:77:VAL:HG11	72:S6:118:PHE:HZ	1.76	0.51
77:X6:325:PRO:O	77:X6:329:LEU:HB2	2.10	0.51
89:Z:178:VAL:HG11	89:Z:199:ILE:HG21	1.93	0.51
89:Z:261:PRO:HA	89:Z:338:LEU:O	2.11	0.51
89:Z:420:GLN:O	89:Z:435:LEU:HA	2.11	0.51
2:A3:3191:A:H4'	51:r3:123:HIS:HB3	1.93	0.51
3:B3:1622:A:H2'	3:B3:1623:G:C8	2.45	0.51
14:O3:124:GLU:OE2	14:O3:128:ASN:ND2	2.44	0.51
21:V3:177:THR:OG1	21:V3:178:SER:N	2.44	0.51
36:b3:62:VAL:HG21	37:c3:71:GLU:HG2	1.92	0.51
41:g3:39:VAL:HG21	50:q3:72:PRO:HB2	1.93	0.51
42:h3:87:GLN:OE1	42:h3:124:ARG:NH2	2.44	0.51
50:q3:107:GLN:NE2	50:q3:110:GLU:OE1	2.43	0.51
51:r3:71:PRO:HD2	51:r3:107:LEU:HD23	1.92	0.51
52:s3:112:THR:HG22	52:s3:391:ASN:HB2	1.93	0.51
58:E6:9:ILE:HG22	58:E6:89:ILE:HD12	1.93	0.51
81:b6:116:PRO:O	81:b6:120:LYS:NZ	2.36	0.51
86:24:50:A:N6	86:24:59:G:N1	2.58	0.51
89:Z:60:VAL:HA	89:Z:146:GLY:O	2.11	0.51
89:Z:111:ALA:HB3	89:Z:126:ASP:HB3	1.93	0.51
2:A3:1784:A:H62	2:A3:1793:G:H21	1.60	0.50
2:A3:2074:A:OP2	25:Z3:40:ARG:NH2	2.44	0.50
2:A3:2093:U:O2	2:A3:2266:U:O2'	2.28	0.50
2:A3:3080:G:H2'	2:A3:3081:A:H8	1.76	0.50
20:U3:30:ARG:NH2	24:Y3:122:GLN:OE1	2.40	0.50
57:D6:215:TYR:HH	72:S6:2:ALA:N	2.08	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:L6:150:LYS:NZ	85:A6:1056:C:OP1	2.44	0.50
65:L6:198:ARG:HH11	85:A6:1053:A:H5'	1.75	0.50
75:V6:393:GLU:OE2	75:V6:397:ARG:NH2	2.44	0.50
85:A6:679:A:H2'	85:A6:680:G:C8	2.45	0.50
85:A6:1293:G:O2'	85:A6:1301:G:OP2	2.25	0.50
85:A6:1431:A:H2'	85:A6:1432:G:C8	2.46	0.50
2:A3:1802:A:OP1	21:V3:83:ARG:NH1	2.40	0.50
2:A3:2082:G:O6	48:o3:67:ARG:NH2	2.36	0.50
2:A3:2632:A:O2'	2:A3:2635:G:N3	2.38	0.50
39:e3:88:GLU:OE1	88:A:101:ARG:NH1	2.43	0.50
40:f3:94:HIS:HB2	40:f3:185:SER:HB3	1.93	0.50
60:G6:100:THR:OG1	60:G6:101:GLN:N	2.44	0.50
62:I6:104:ASN:OD1	85:A6:1009:U:O2'	2.26	0.50
64:K6:90:ARG:NH1	64:K6:95:SER:O	2.44	0.50
77:X6:354:GLU:HA	77:X6:357:ILE:HG12	1.91	0.50
32:63:160:ASP:OD2	32:63:267:ARG:NH2	2.44	0.50
35:a3:44:ASN:ND2	36:b3:135:ASN:OD1	2.44	0.50
40:f3:133:GLU:HA	40:f3:149:VAL:HA	1.93	0.50
50:q3:94:PRO:HG2	50:q3:99:MET:HE2	1.93	0.50
68:O6:105:CYS:O	68:O6:108:CYS:N	2.44	0.50
68:O6:228:SER:OG	68:O6:229:GLY:N	2.44	0.50
77:X6:111:TYR:HD2	77:X6:124:TYR:HE2	1.60	0.50
2:A3:2406:A:N1	31:53:112:ARG:NH2	2.60	0.50
2:A3:2572:C:O2'	86:24:12:U:OP1	2.28	0.50
7:H3:58:ARG:NH2	23:X3:66:PRO:O	2.39	0.50
17:R3:99:ARG:HA	17:R3:102:LEU:HB2	1.93	0.50
31:53:340:VAL:HG23	31:53:359:LEU:HB3	1.94	0.50
32:63:73:THR:OG1	32:63:76:GLU:N	2.41	0.50
32:63:218:LEU:HB3	32:63:234:HIS:HB2	1.93	0.50
45:k3:76:MET:HG2	51:r3:49:ILE:HD12	1.94	0.50
68:O6:181:HIS:CE1	80:a6:180:LYS:HD2	2.47	0.50
70:Q6:15:GLN:O	70:Q6:18:ASN:ND2	2.44	0.50
74:U6:192:THR:OG1	74:U6:193:ARG:N	2.43	0.50
2:A3:2145:G:N2	18:S3:103:SER:OG	2.44	0.50
18:S3:161:ILE:HD11	18:S3:194:ARG:HB2	1.92	0.50
21:V3:181:ASP:O	24:Y3:93:LYS:NZ	2.42	0.50
28:23:64:HIS:HB2	28:23:92:HIS:HD2	1.77	0.50
36:b3:64:TYR:OH	37:c3:67:ASP:N	2.45	0.50
46:l3:135:ASN:OD1	46:l3:135:ASN:N	2.43	0.50
75:V6:156:ASN:O	75:V6:160:ALA:CB	2.59	0.50
80:a6:31:SER:OG	80:a6:32:GLN:NE2	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:b6:56:ARG:NH2	84:e6:91:ASP:OD1	2.45	0.50
2:A3:2726:C:O2'	86:24:73:A:N3	2.38	0.50
12:M3:292:LYS:O	12:M3:296:SER:OG	2.24	0.50
15:P3:108:GLU:HB3	15:P3:111:ILE:HG22	1.93	0.50
60:G6:111:LEU:HD22	81:b6:112:LEU:HD23	1.92	0.50
62:I6:88:ILE:HG13	62:I6:97:ILE:HD13	1.93	0.50
68:O6:106:PRO:HD2	68:O6:142:VAL:HA	1.93	0.50
18:S3:174:PHE:HA	18:S3:180:PHE:O	2.12	0.50
23:X3:234:LEU:HD13	34:93:96:VAL:HG21	1.94	0.50
31:53:99:TYR:HA	31:53:270:ILE:HG22	1.93	0.50
41:g3:140:VAL:HG12	41:g3:147:LEU:HD13	1.94	0.50
57:D6:194:SER:HB2	57:D6:197:SER:HB3	1.94	0.50
77:X6:349:ASN:OD1	77:X6:352:GLU:N	2.44	0.50
81:b6:65:ASP:O	81:b6:68:SER:OG	2.29	0.50
89:Z:65:HIS:HB3	89:Z:68:HIS:CD2	2.47	0.50
90:j:19:G:O4'	90:j:58:G:N2	2.45	0.50
2:A3:1775:A:HO2'	17:R3:10:LEU:N	2.08	0.50
5:E3:109:LEU:HD21	5:E3:337:VAL:HG22	1.94	0.50
19:T3:113:GLY:HA2	19:T3:116:ILE:HD12	1.93	0.50
23:X3:111:GLU:O	23:X3:112:ARG:NH1	2.42	0.50
32:63:303:PHE:O	32:63:307:HIS:CB	2.57	0.50
56:C6:120:CYS:HB3	81:b6:106:LEU:HD13	1.93	0.50
77:X6:366:LEU:HD12	77:X6:371:ALA:HB1	1.94	0.50
86:C:50:A:N6	86:C:59:G:N1	2.58	0.50
2:A3:2718:C:OP1	26:03:82:LYS:NZ	2.37	0.50
11:L3:35:MET:N	11:L3:57:CYS:O	2.44	0.50
22:W3:122:LYS:HB2	32:63:49:GLU:HB3	1.93	0.50
40:f3:148:SER:OG	47:m3:72:ARG:NH2	2.43	0.50
49:p3:56:ASP:OD1	49:p3:56:ASP:N	2.32	0.50
52:s3:332:LEU:HD21	52:s3:359:ALA:HB2	1.94	0.50
59:F6:171:PRO:HB3	59:F6:230:ALA:HB1	1.93	0.50
2:A3:1750:G:OP2	29:33:113:ARG:NH2	2.45	0.49
74:U6:32:ASP:OD2	85:A6:703:A:N6	2.45	0.49
2:A3:1672:C:O2'	19:T3:149:ARG:O	2.30	0.49
42:h3:63:PRO:HB2	42:h3:66:LEU:HA	1.95	0.49
57:D6:95:ALA:HB2	79:Z6:74:GLU:HB3	1.93	0.49
60:G6:227:LYS:O	60:G6:231:SER:OG	2.28	0.49
69:P6:58:TYR:OH	72:S6:68:ASP:OD1	2.24	0.49
80:a6:43:ARG:HH21	80:a6:50:LEU:HD11	1.77	0.49
81:b6:257:SER:O	81:b6:261:ASN:ND2	2.45	0.49
2:A3:2852:C:O2'	27:13:45:HIS:ND1	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A3:2987:U:O2'	2:A3:2991:U:OP1	2.29	0.49
4:D3:221:ASN:N	4:D3:221:ASN:OD1	2.43	0.49
9:J3:86:THR:O	9:J3:90:PHE:HB2	2.11	0.49
10:K3:63:ARG:HH21	10:K3:129:PRO:HB2	1.77	0.49
16:Q3:148:THR:OG1	16:Q3:149:PHE:N	2.45	0.49
55:B6:149:ARG:NH1	70:Q6:82:ASP:OD1	2.43	0.49
58:E6:113:LEU:HD11	76:W6:154:LEU:HA	1.95	0.49
65:L6:82:ILE:HD12	65:L6:85:VAL:HG11	1.94	0.49
72:S6:29:PRO:HG2	72:S6:32:PHE:HB2	1.93	0.49
2:A3:2122:A:O2'	2:A3:2136:C:OP2	2.26	0.49
2:A3:2898:U:H5''	12:M3:79:PRO:HB3	1.94	0.49
12:M3:288:GLU:HA	12:M3:291:LEU:HD13	1.94	0.49
18:S3:68:ASP:OD1	18:S3:68:ASP:N	2.46	0.49
20:U3:109:ASP:OD1	20:U3:109:ASP:N	2.34	0.49
31:53:112:ARG:HB2	31:53:308:GLN:NE2	2.27	0.49
52:s3:211:VAL:HG12	52:s3:230:ARG:HG3	1.95	0.49
80:a6:97:LEU:HD21	80:a6:100:VAL:HG23	1.95	0.49
83:d6:165:LYS:NZ	85:A6:1152:A:OP2	2.45	0.49
2:A3:3000:A:H2'	2:A3:3001:G:C8	2.48	0.49
5:E3:318:THR:OG1	5:E3:319:TYR:N	2.43	0.49
13:N3:92:LEU:HD11	13:N3:188:LYS:HE3	1.95	0.49
14:O3:96:ARG:HD3	14:O3:127:GLY:HA3	1.94	0.49
20:U3:19:VAL:HG23	34:93:136:LEU:HD22	1.95	0.49
39:e3:185:ARG:HD2	39:e3:207:ASN:HB2	1.94	0.49
2:A3:2096:U:O4	12:M3:57:ARG:NH1	2.45	0.49
33:73:55:GLN:O	33:73:84:ASN:ND2	2.45	0.49
52:s3:108:TYR:O	52:s3:212:ARG:NE	2.35	0.49
71:R6:286:ILE:O	71:R6:290:GLN:HB2	2.13	0.49
75:V6:197:SER:OG	75:V6:199:GLU:N	2.45	0.49
81:b6:290:GLU:HG3	81:b6:294:LYS:HE3	1.95	0.49
89:Z:120:ARG:NH1	89:Z:247:ILE:O	2.40	0.49
2:A3:2180:A:O2'	2:A3:2206:C:O3'	2.30	0.49
2:A3:3016:G:N7	30:43:97:ARG:NH2	2.51	0.49
22:W3:57:GLU:HG3	22:W3:98:ARG:HA	1.94	0.49
24:Y3:154:ARG:HG3	34:93:130:LEU:HB3	1.95	0.49
33:73:217:GLU:O	33:73:255:HIS:HA	2.12	0.49
84:e6:462:PHE:HD1	84:e6:481:LEU:HD12	1.77	0.49
7:D:195:LYS:HE2	7:D:197:LEU:HD13	1.95	0.49
2:A3:1890:C:O2'	2:A3:1895:C:OP1	2.31	0.49
35:a3:72:THR:OG1	35:a3:73:LYS:N	2.45	0.49
36:b3:28:ARG:HG2	36:b3:62:VAL:HB	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:C6:50:PRO:O	56:C6:161:LYS:NZ	2.35	0.49
56:C6:97:TRP:HD1	56:C6:104:LEU:HD22	1.78	0.49
58:E6:63:TYR:OH	69:P6:118:GLY:O	2.28	0.49
81:b6:155:ASP:OD1	81:b6:155:ASP:N	2.43	0.49
85:A6:843:A:H2'	85:A6:844:A:C8	2.48	0.49
2:A3:2237:A:OP1	51:r3:171:ARG:NH1	2.45	0.49
2:A3:2294:A:N7	12:M3:39:ARG:NH2	2.61	0.49
2:A3:2365:U:OP2	20:U3:78:LYS:NZ	2.40	0.49
2:A3:2661:U:H2'	2:A3:2662:A:C8	2.47	0.49
47:m3:57:VAL:HA	47:m3:62:SER:O	2.13	0.49
55:B6:142:ILE:HG12	55:B6:192:LEU:HD23	1.94	0.49
56:C6:111:LYS:HB2	56:C6:118:GLU:HG3	1.95	0.49
60:G6:263:ASP:HB3	60:G6:269:PHE:HE1	1.76	0.49
83:d6:132:LYS:NZ	85:A6:943:A:OP1	2.45	0.49
89:Z:100:GLU:HA	89:Z:103:ALA:HB3	1.94	0.49
2:A3:1798:A:N3	21:V3:42:ARG:NH2	2.61	0.49
2:A3:2036:C:N4	2:A3:2918:A:N7	2.61	0.49
6:F3:63:GLN:HB2	42:h3:117:LEU:HD22	1.95	0.49
21:V3:134:GLU:OE1	21:V3:148:THR:OG1	2.30	0.49
31:53:125:LYS:HA	31:53:253:LEU:HD11	1.95	0.49
32:63:355:LYS:HD2	32:63:358:PRO:HA	1.95	0.49
75:V6:396:GLN:HE21	85:A6:1528:A:H62	1.60	0.49
77:X6:273:THR:HG23	77:X6:316:LEU:HD13	1.95	0.49
85:A6:744:G:H2'	85:A6:745:A:H8	1.78	0.49
89:Z:200:ARG:HD3	89:Z:211:GLU:HA	1.93	0.49
91:n:149:ILE:HA	91:n:152:ILE:HD12	1.94	0.49
2:A3:2149:G:OP1	44:j3:24:GLY:N	2.46	0.48
2:A3:2371:U:H2'	20:U3:71:ARG:HD2	1.95	0.48
15:P3:127:ILE:HA	15:P3:130:VAL:HG12	1.94	0.48
16:Q3:92:PHE:HA	16:Q3:95:GLU:HG2	1.94	0.48
39:e3:165:PHE:HB2	39:e3:170:VAL:HG22	1.95	0.48
65:L6:197:ARG:NH2	85:A6:784:C:N3	2.61	0.48
5:E3:103:LYS:NZ	5:E3:291:GLY:O	2.38	0.48
18:S3:161:ILE:HG22	18:S3:162:GLU:HG3	1.94	0.48
32:63:259:PRO:HB3	32:63:266:HIS:CD2	2.48	0.48
39:e3:207:ASN:HB3	88:A:164:ARG:HA	1.95	0.48
61:H6:159:TYR:HH	81:b6:122:HIS:HD1	1.61	0.48
63:J6:54:GLY:O	85:A6:929:U:O2'	2.31	0.48
2:A3:2599:U:OP2	2:A3:2625:C:N4	2.46	0.48
2:A3:3181:U:OP2	2:A3:3182:A:O2'	2.27	0.48
7:H3:106:GLY:HA2	7:H3:112:VAL:HG11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:T3:94:ILE:HA	19:T3:97:MET:HE2	1.94	0.48
20:U3:27:GLN:HG3	20:U3:43:ARG:HB2	1.94	0.48
25:Z3:136:ASN:OD1	25:Z3:136:ASN:N	2.46	0.48
32:63:185:MET:HE3	49:p3:188:LEU:HD11	1.95	0.48
57:D6:257:SER:OG	57:D6:258:ILE:N	2.43	0.48
62:I6:176:THR:HG22	70:Q6:11:THR:HG23	1.95	0.48
65:L6:102:GLU:OE1	65:L6:105:LYS:NZ	2.41	0.48
85:A6:1357:A:H4'	85:A6:1358:A:C8	2.48	0.48
89:Z:65:HIS:O	89:Z:70:LYS:NZ	2.45	0.48
2:A3:1790:A:O3'	28:23:81:ARG:NH2	2.46	0.48
5:E3:100:ILE:HD11	5:E3:177:LYS:HB2	1.95	0.48
5:E3:208:ALA:HB2	5:E3:297:VAL:HG12	1.95	0.48
6:F3:94:ASP:OD1	6:F3:94:ASP:N	2.45	0.48
24:Y3:91:ARG:HH11	34:93:85:PRO:HA	1.78	0.48
24:Y3:158:THR:HG23	24:Y3:160:GLN:H	1.79	0.48
45:k3:14:LYS:HD2	45:k3:69:GLY:HA2	1.94	0.48
56:C6:164:TYR:OH	81:b6:89:TYR:O	2.24	0.48
59:F6:110:LEU:HD11	85:A6:1373:U:H5'	1.95	0.48
62:I6:188:PRO:HD2	70:Q6:45:TYR:HB2	1.95	0.48
65:L6:69:PRO:HB2	65:L6:96:GLU:HB3	1.96	0.48
70:Q6:79:ASN:HD22	82:c6:107:LEU:HD12	1.77	0.48
2:A3:2308:A:H5''	26:03:85:ARG:HH21	1.78	0.48
2:A3:3016:G:H5''	2:A3:3017:C:H5''	1.96	0.48
7:H3:55:ILE:HB	7:H3:84:GLU:HG3	1.94	0.48
19:T3:147:SER:O	19:T3:147:SER:OG	2.32	0.48
26:03:123:CYS:HB3	26:03:126:CYS:HB2	1.95	0.48
35:a3:104:GLU:HG3	35:a3:107:PRO:HD2	1.94	0.48
71:R6:72:ASP:HB3	71:R6:75:VAL:HG12	1.95	0.48
83:d6:152:PHE:HD1	83:d6:155:ARG:HH21	1.60	0.48
86:C:48:U:N3	86:C:49:G:O6	2.46	0.48
16:Q3:79:GLU:OE2	16:Q3:140:ARG:NH2	2.46	0.48
27:13:54:VAL:HG13	50:q3:128:MET:HE3	1.95	0.48
52:s3:246:GLN:NE2	52:s3:354:PRO:O	2.47	0.48
59:F6:224:HIS:HB3	59:F6:228:LYS:HZ1	1.78	0.48
68:O6:56:TRP:HB3	68:O6:119:ASN:HD22	1.78	0.48
74:U6:64:ARG:NH1	85:A6:848:A:O2'	2.46	0.48
85:A6:842:U:H2'	85:A6:843:A:H8	1.78	0.48
85:A6:1351:G:H2'	85:A6:1352:G:H8	1.79	0.48
24:Y3:174:GLY:HA3	24:Y3:209:LEU:HD11	1.94	0.48
33:73:121:LYS:HB3	33:73:121:LYS:HE2	1.68	0.48
40:f3:86:TYR:HD2	88:A:164:ARG:HH21	1.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:F6:240:ARG:NH2	82:c6:44:THR:O	2.47	0.48
60:G6:96:PRO:HG2	60:G6:99:PHE:HB3	1.96	0.48
68:O6:221:GLN:NE2	75:V6:314:VAL:O	2.40	0.48
71:R6:157:VAL:HG13	71:R6:174:VAL:HG12	1.95	0.48
75:V6:129:LEU:HA	75:V6:137:ILE:HD11	1.96	0.48
78:Y6:361:ASN:ND2	79:Z6:38:SER:O	2.47	0.48
82:c6:12:ARG:NH1	85:A6:1129:A:O4'	2.47	0.48
86:24:48:U:N3	86:24:49:G:O6	2.46	0.48
5:E3:307:TYR:HD1	5:E3:310:LEU:HD13	1.78	0.48
12:M3:78:ILE:HD13	29:33:124:ARG:HD2	1.96	0.48
13:N3:148:ASP:OD1	13:N3:149:HIS:ND1	2.35	0.48
22:W3:122:LYS:HD2	32:63:49:GLU:HG2	1.96	0.48
39:e3:185:ARG:HB3	39:e3:207:ASN:HD22	1.78	0.48
57:D6:218:PHE:HA	57:D6:248:GLY:O	2.13	0.48
58:E6:108:ILE:HG12	69:P6:100:CYS:HB3	1.95	0.48
72:S6:6:LEU:O	72:S6:15:ARG:NH1	2.47	0.48
85:A6:1593:C:H2'	85:A6:1594:A:C8	2.48	0.48
2:A3:1789:A:H2'	2:A3:1790:A:C8	2.49	0.48
2:A3:2279:U:OP2	43:i3:46:ARG:NH2	2.45	0.48
2:A3:3046:C:H2'	2:A3:3047:G:H8	1.79	0.48
2:A3:3181:U:H3'	2:A3:3182:A:H2'	1.95	0.48
4:D3:162:THR:O	4:D3:177:ARG:NH2	2.41	0.48
6:F3:133:THR:HG22	6:F3:135:ARG:H	1.79	0.48
17:R3:143:SER:OG	17:R3:144:ARG:N	2.43	0.48
22:W3:50:ARG:O	22:W3:54:LYS:NZ	2.47	0.48
26:O3:144:GLN:NE2	26:O3:174:ILE:O	2.44	0.48
27:13:47:ASP:HB3	27:13:50:VAL:HG22	1.95	0.48
40:f3:93:ILE:HD11	40:f3:110:VAL:HG11	1.96	0.48
57:D6:371:VAL:HG12	57:D6:383:VAL:HA	1.95	0.48
84:e6:515:ASP:HA	84:e6:518:GLU:HG2	1.95	0.48
85:A6:1466:G:H2'	85:A6:1467:G:C8	2.49	0.48
89:Z:253:ASP:N	89:Z:253:ASP:OD2	2.45	0.48
7:D:185:ASN:HB2	7:D:188:ILE:HG12	1.94	0.48
91:n:201:PRO:HG2	91:n:204:ALA:HB2	1.96	0.48
2:A3:1826:G:H4'	2:A3:1828:A:H2	1.79	0.48
2:A3:1883:G:H2'	2:A3:1884:G:H8	1.79	0.48
2:A3:1960:A:OP1	2:A3:2431:C:N4	2.45	0.48
2:A3:2169:A:O2'	9:J3:130:PHE:O	2.32	0.48
5:E3:309:ASP:OD1	5:E3:309:ASP:N	2.44	0.48
6:F3:188:HIS:HB2	6:F3:260:VAL:HG22	1.96	0.48
13:N3:238:LYS:HD2	13:N3:238:LYS:HA	1.70	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:73:107:LEU:HD22	33:73:110:GLY:HA2	1.95	0.48
47:m3:56:LEU:O	47:m3:63:THR:HA	2.13	0.48
52:s3:403:GLU:HB3	52:s3:412:GLY:H	1.77	0.48
62:I6:115:GLU:HG2	62:I6:130:THR:HB	1.96	0.48
81:b6:184:ASP:OD1	81:b6:184:ASP:N	2.47	0.48
85:A6:1581:U:H2'	85:A6:1582:A:C8	2.48	0.48
89:Z:356:VAL:HG22	89:Z:434:GLY:HA3	1.95	0.48
2:A3:1709:G:H5'	24:Y3:192:LYS:HE3	1.96	0.47
6:F3:138:HIS:CE1	6:F3:146:TRP:HE1	2.32	0.47
14:O3:152:LEU:HD13	33:73:319:ARG:HD2	1.95	0.47
21:V3:73:GLN:HG3	21:V3:123:VAL:HG21	1.95	0.47
38:d3:266:VAL:HG23	38:d3:267:PRO:HD3	1.96	0.47
65:L6:88:VAL:HA	65:L6:91:ARG:HB2	1.96	0.47
80:a6:93:CYS:HB2	80:a6:121:LYS:H	1.79	0.47
91:n:64:LEU:HD11	91:n:188:ASN:HB3	1.96	0.47
2:A3:3043:C:H3'	2:A3:3044:A:H8	1.80	0.47
10:K3:19:TYR:OH	36:b3:136:LYS:NZ	2.46	0.47
18:S3:164:THR:OG1	18:S3:165:GLU:N	2.47	0.47
19:T3:106:LEU:HD12	19:T3:114:ALA:HA	1.96	0.47
37:c3:100:SER:OG	37:c3:182:GLU:OE1	2.31	0.47
43:i3:86:ASN:H	43:i3:89:GLN:HB2	1.77	0.47
56:C6:114:GLY:HA2	81:b6:159:SER:HA	1.96	0.47
73:T6:38:GLY:O	73:T6:45:ARG:NH1	2.38	0.47
75:V6:69:SER:OG	75:V6:105:ARG:NH2	2.47	0.47
77:X6:129:GLU:HA	77:X6:323:TYR:HB2	1.96	0.47
85:A6:1549:U:H2'	85:A6:1550:A:H8	1.79	0.47
2:A3:1871:A:N3	29:33:104:ARG:NH2	2.54	0.47
2:A3:2075:U:O2'	2:A3:2833:A:N7	2.39	0.47
2:A3:2919:A:N1	23:X3:97:LEU:HB3	2.30	0.47
5:E3:50:ASP:OD2	14:O3:138:ARG:NH1	2.47	0.47
14:O3:43:GLU:OE1	26:O3:127:TYR:OH	2.25	0.47
43:i3:48:ASN:HD22	43:i3:50:LYS:H	1.61	0.47
50:q3:78:SER:O	50:q3:80:GLU:N	2.47	0.47
81:b6:317:LYS:HE2	81:b6:323:THR:HA	1.96	0.47
88:A:197:LYS:NZ	88:A:201:GLN:O	2.40	0.47
89:Z:69:GLY:O	89:Z:73:LEU:HB2	2.13	0.47
90:j:59:A:O2'	90:j:61:A:OP2	2.27	0.47
91:n:140:PRO:HG3	91:n:145:VAL:HB	1.95	0.47
2:A3:1862:U:H2'	2:A3:1863:A:H8	1.78	0.47
2:A3:1962:A:OP2	2:A3:2501:C:N4	2.47	0.47
2:A3:3024:U:H2'	2:A3:3025:A:C8	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P3:81:ARG:NH2	15:P3:94:GLU:OE1	2.38	0.47
58:E6:54:HIS:CE1	58:E6:86:ILE:HG13	2.48	0.47
2:A3:1799:U:OP1	21:V3:41:ARG:NE	2.48	0.47
2:A3:2275:U:H5''	37:c3:34:GLY:HA2	1.96	0.47
2:A3:2285:U:H2'	2:A3:2286:A:H8	1.79	0.47
2:A3:2930:U:H2'	2:A3:2931:A:C8	2.49	0.47
2:A3:3002:G:H2'	2:A3:3003:A:H8	1.78	0.47
10:K3:140:ASN:OD1	37:c3:265:THR:OG1	2.31	0.47
14:O3:96:ARG:NH1	14:O3:126:LYS:O	2.47	0.47
20:U3:36:PRO:O	20:U3:39:THR:OG1	2.29	0.47
21:V3:190:CYS:SG	21:V3:191:LEU:N	2.88	0.47
23:X3:21:CYS:HB3	23:X3:212:ILE:HD13	1.96	0.47
28:23:72:THR:HG22	28:23:74:ALA:H	1.80	0.47
37:c3:97:TYR:HB2	37:c3:181:SER:HA	1.97	0.47
40:f3:100:MET:SD	47:m3:45:ARG:NH1	2.88	0.47
62:I6:189:ARG:HH12	62:I6:192:ARG:HB3	1.80	0.47
71:R6:144:GLU:HA	71:R6:180:THR:HA	1.96	0.47
85:A6:825:U:H2'	85:A6:826:G:C8	2.49	0.47
2:A3:1924:U:H2'	2:A3:1925:A:C8	2.49	0.47
2:A3:2531:U:O2	4:D3:253:ASN:N	2.46	0.47
2:A3:2618:U:O4	2:A3:3043:C:N4	2.38	0.47
23:X3:53:ASN:ND2	23:X3:54:PRO:O	2.48	0.47
24:Y3:182:LYS:HB3	24:Y3:184:TRP:HE1	1.79	0.47
25:Z3:138:CYS:HG	25:Z3:149:TRP:CG	2.32	0.47
31:53:333:ALA:HB1	31:53:363:ASP:HA	1.95	0.47
38:d3:197:VAL:HG12	38:d3:212:ILE:HG12	1.97	0.47
59:F6:114:THR:HG22	59:F6:202:PRO:HA	1.95	0.47
63:J6:102:LEU:HD21	63:J6:132:CYS:HB3	1.96	0.47
69:P6:124:TYR:HB3	70:Q6:9:ALA:HB2	1.97	0.47
70:Q6:67:GLU:HG3	76:W6:154:LEU:HB2	1.96	0.47
2:A3:2269:G:H2'	2:A3:2270:A:H8	1.80	0.47
2:A3:2420:U:H2'	2:A3:2421:G:H8	1.80	0.47
2:A3:2520:C:O2	2:A3:2528:G:N2	2.47	0.47
3:B3:1613:U:H2'	3:B3:1615:A:H5''	1.97	0.47
5:E3:102:LEU:HD12	5:E3:294:ASN:HA	1.97	0.47
12:M3:184:LEU:HA	12:M3:187:VAL:HG12	1.96	0.47
19:T3:62:GLN:NE2	19:T3:66:GLU:OE1	2.47	0.47
22:W3:83:VAL:HA	22:W3:88:CYS:O	2.15	0.47
23:X3:94:ASN:HA	86:C:73:A:C5	2.50	0.47
32:63:216:LEU:HD21	32:63:270:PHE:HD2	1.79	0.47
47:m3:51:LEU:HB3	47:m3:67:ARG:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:B6:158:MET:HG2	55:B6:250:CYS:HB2	1.96	0.47
55:B6:239:ASN:OD1	55:B6:241:ASP:N	2.39	0.47
60:G6:293:ILE:HG12	60:G6:328:VAL:HB	1.97	0.47
68:O6:177:PHE:HB3	71:R6:132:LEU:HD21	1.96	0.47
68:O6:209:PRO:HG2	68:O6:212:GLU:HG2	1.97	0.47
75:V6:381:GLN:HA	75:V6:384:LEU:HD12	1.97	0.47
85:A6:811:A:H8	85:A6:812:C:H5	1.61	0.47
88:A:165:ASP:N	88:A:165:ASP:OD1	2.48	0.47
91:n:113:VAL:HG23	91:n:136:LEU:HD22	1.97	0.47
2:A3:1768:G:N7	24:Y3:229:LYS:NZ	2.62	0.47
12:M3:35:LYS:HE2	12:M3:35:LYS:HB3	1.74	0.47
15:P3:62:ARG:NH1	22:W3:137:LYS:O	2.44	0.47
49:p3:74:ASP:N	49:p3:74:ASP:OD1	2.45	0.47
52:s3:386:ASN:N	52:s3:386:ASN:OD1	2.48	0.47
59:F6:110:LEU:HD13	59:F6:201:MET:HG2	1.96	0.47
75:V6:72:ILE:HD12	75:V6:75:LEU:HD23	1.95	0.47
2:A3:2025:C:H2'	2:A3:2026:A:C8	2.50	0.47
2:A3:3063:G:O2'	2:A3:3066:C:OP2	2.30	0.47
4:D3:220:VAL:HB	4:D3:223:THR:HB	1.96	0.47
11:L3:62:LYS:NZ	11:L3:66:VAL:O	2.41	0.47
16:Q3:275:THR:HG22	16:Q3:278:ILE:HD12	1.97	0.47
57:D6:323:ILE:HD13	57:D6:350:PHE:HE1	1.80	0.47
75:V6:60:THR:O	75:V6:65:LEU:N	2.43	0.47
2:A3:2049:U:H2'	2:A3:2050:A:C8	2.50	0.47
2:A3:2060:A:O2'	2:A3:2061:C:O2	2.25	0.47
2:A3:2472:A:O2'	2:A3:2478:G:N7	2.39	0.47
2:A3:2511:C:H4'	4:D3:257:ILE:HB	1.97	0.47
5:E3:296:LEU:HD12	5:E3:296:LEU:HA	1.82	0.47
12:M3:44:ARG:HG3	12:M3:45:ARG:HD2	1.97	0.47
31:53:238:THR:OG1	31:53:358:GLN:NE2	2.48	0.47
55:B6:138:ARG:NH1	72:S6:30:LEU:O	2.47	0.47
59:F6:79:ALA:O	60:G6:312:GLN:NE2	2.48	0.47
59:F6:110:LEU:O	59:F6:114:THR:HG23	2.15	0.47
59:F6:142:TYR:HE2	77:X6:398:LEU:HD13	1.80	0.47
81:b6:184:ASP:O	81:b6:188:LYS:NZ	2.41	0.47
84:e6:552:ALA:HA	84:e6:555:ILE:HG22	1.97	0.47
4:D3:88:THR:HG23	4:D3:90:ARG:H	1.80	0.46
5:E3:76:LYS:HE3	5:E3:170:LEU:HG	1.97	0.46
9:J3:39:LEU:HD23	9:J3:44:VAL:HG21	1.96	0.46
35:a3:71:HIS:ND1	36:b3:138:THR:OG1	2.48	0.46
52:s3:373:GLN:NE2	52:s3:375:ASN:OD1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:C6:115:ASN:HB2	78:Y6:311:TRP:CE2	2.50	0.46
76:W6:152:ARG:NH1	76:W6:157:THR:O	2.48	0.46
85:A6:1423:G:H5''	85:A6:1425:G:H21	1.79	0.46
85:A6:1502:C:H2'	85:A6:1503:U:H6	1.79	0.46
2:A3:2265:A:OP1	12:M3:47:ARG:NH2	2.48	0.46
5:E3:114:GLY:HA3	16:Q3:170:ARG:HD3	1.96	0.46
12:M3:168:GLU:HA	12:M3:172:GLY:H	1.80	0.46
17:R3:136:LYS:HA	17:R3:137:GLU:HA	1.82	0.46
31:53:357:PHE:HD1	31:53:374:ALA:HB2	1.79	0.46
33:73:254:LEU:HA	33:73:263:VAL:HA	1.97	0.46
56:C6:70:SER:OG	56:C6:93:ARG:NH2	2.47	0.46
69:P6:54:MET:HE3	72:S6:64:TRP:HB3	1.97	0.46
70:Q6:64:TYR:HE1	82:c6:29:LEU:HA	1.80	0.46
77:X6:96:GLU:HG3	77:X6:97:ALA:H	1.79	0.46
78:Y6:316:ASN:O	81:b6:215:ARG:NH1	2.48	0.46
2:A3:2586:U:H2'	2:A3:2587:G:C8	2.50	0.46
5:E3:201:GLY:HA2	5:E3:272:LYS:HE2	1.98	0.46
39:e3:212:HIS:CE1	88:A:150:LEU:HB2	2.45	0.46
55:B6:188:ARG:O	60:G6:152:TYR:OH	2.32	0.46
56:C6:77:ASP:HA	56:C6:78:GLY:HA2	1.69	0.46
60:G6:72:ASP:N	60:G6:72:ASP:OD1	2.47	0.46
75:V6:157:TYR:O	75:V6:184:TYR:OH	2.33	0.46
80:a6:101:ARG:HH11	85:A6:1532:A:H5'	1.80	0.46
2:A3:1990:G:C2	2:A3:1995:A:N6	2.83	0.46
2:A3:2514:C:H2'	2:A3:2515:U:H6	1.80	0.46
5:E3:124:VAL:HB	5:E3:281:ASN:HB3	1.96	0.46
9:J3:99:LYS:HA	9:J3:99:LYS:HD3	1.72	0.46
22:W3:49:ARG:HH21	22:W3:71:ARG:HD3	1.79	0.46
27:13:32:THR:OG1	27:13:33:LYS:N	2.49	0.46
32:63:235:TRP:HD1	32:63:254:TYR:HA	1.80	0.46
39:e3:73:LEU:HD22	88:A:117:LEU:HD23	1.95	0.46
55:B6:106:ILE:HD12	55:B6:114:ASP:HB3	1.97	0.46
77:X6:90:GLN:NE2	77:X6:360:TYR:OH	2.46	0.46
85:A6:1566:G:H1'	85:A6:1587:A:H2	1.80	0.46
4:D3:111:ARG:HH11	4:D3:165:ASN:HD21	1.63	0.46
8:I3:160:LYS:HE3	8:I3:163:GLU:HB3	1.97	0.46
18:S3:69:PRO:HA	18:S3:72:GLU:HB2	1.98	0.46
18:S3:129:ARG:NH2	18:S3:151:LYS:O	2.49	0.46
18:S3:163:LYS:HB2	36:b3:106:ASP:HB3	1.96	0.46
33:73:309:HIS:O	33:73:313:TRP:HB2	2.15	0.46
61:H6:126:ILE:HG22	61:H6:127:TYR:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:L6:217:THR:HG21	83:d6:180:ALA:HB1	1.98	0.46
85:A6:1243:C:H2'	85:A6:1244:A:H8	1.79	0.46
85:A6:1492:C:H2'	85:A6:1493:G:C8	2.51	0.46
7:D:168:LYS:HE3	7:D:231:VAL:HA	1.97	0.46
2:A3:2471:G:N2	2:A3:2655:G:OP2	2.46	0.46
4:D3:113:ARG:O	4:D3:147:ARG:NH1	2.48	0.46
12:M3:168:GLU:OE1	12:M3:220:ARG:NH2	2.48	0.46
30:43:72:LEU:HD13	30:43:90:VAL:HG23	1.96	0.46
35:a3:42:ASP:HB3	36:b3:137:PRO:HB3	1.98	0.46
56:C6:36:LYS:N	85:A6:1270:A:OP2	2.48	0.46
60:G6:73:PHE:HA	60:G6:76:LYS:HD3	1.98	0.46
67:N6:53:ASP:N	67:N6:53:ASP:OD1	2.49	0.46
76:W6:92:MET:O	76:W6:98:LYS:NZ	2.49	0.46
84:e6:462:PHE:HA	84:e6:465:ILE:HB	1.98	0.46
84:e6:493:MET:HA	84:e6:496:LEU:HG	1.97	0.46
85:A6:773:G:N2	85:A6:776:A:OP2	2.29	0.46
89:Z:279:LEU:O	89:Z:319:GLY:N	2.44	0.46
89:Z:304:THR:HB	89:Z:325:LEU:HB3	1.97	0.46
91:n:1:PRO:HG3	91:n:46:LYS:HB3	1.97	0.46
2:A3:2116:C:O2'	2:A3:2837:A:N3	2.44	0.46
2:A3:2559:U:OP2	85:A6:1005:C:N4	2.48	0.46
11:L3:87:VAL:HG12	11:L3:127:LEU:HD11	1.98	0.46
18:S3:89:THR:OG1	18:S3:91:GLN:NE2	2.49	0.46
18:S3:167:TRP:HE1	18:S3:169:ARG:HH11	1.62	0.46
39:e3:131:PHE:HA	88:A:191:ARG:HH21	1.81	0.46
40:f3:120:LYS:HA	40:f3:120:LYS:HD2	1.70	0.46
57:D6:289:THR:HG22	57:D6:290:ILE:H	1.80	0.46
58:E6:44:GLU:HG2	58:E6:60:ARG:HH21	1.81	0.46
65:L6:175:TYR:HB2	67:N6:89:GLY:HA3	1.97	0.46
77:X6:116:SER:OG	77:X6:117:PHE:N	2.49	0.46
77:X6:123:ARG:NH2	77:X6:338:ASP:OD1	2.49	0.46
77:X6:150:TRP:CG	77:X6:257:HIS:HB3	2.50	0.46
85:A6:1142:G:H2'	85:A6:1143:A:H8	1.81	0.46
2:A3:2230:A:H61	2:A3:2950:U:H1'	1.81	0.46
12:M3:166:ALA:HA	49:p3:144:PHE:HE2	1.80	0.46
15:P3:148:THR:HB	15:P3:151:GLU:HG2	1.96	0.46
18:S3:166:SER:OG	18:S3:167:TRP:N	2.48	0.46
32:63:274:LYS:HB2	32:63:312:THR:HG23	1.96	0.46
38:d3:165:THR:HG23	38:d3:167:HIS:H	1.81	0.46
57:D6:130:GLN:O	79:Z6:72:ARG:NH2	2.48	0.46
58:E6:10:LEU:HD21	58:E6:88:VAL:HG12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:G6:123:PRO:HD3	81:b6:87:MET:HE3	1.97	0.46
77:X6:164:ASN:HD21	85:A6:1384:G:H21	1.64	0.46
85:A6:842:U:H2'	85:A6:843:A:C8	2.50	0.46
88:A:106:LEU:HD23	88:A:110:GLU:HG3	1.97	0.46
6:F3:141:ILE:HG12	6:F3:142:ARG:HH11	1.80	0.46
12:M3:109:ARG:HB3	12:M3:110:VAL:H	1.59	0.46
13:N3:106:ARG:O	13:N3:110:ASN:ND2	2.49	0.46
20:U3:5:VAL:O	34:93:39:LYS:NZ	2.46	0.46
23:X3:94:ASN:HA	86:C:73:A:C6	2.51	0.46
31:53:107:PHE:HB2	31:53:265:LEU:HD22	1.98	0.46
49:p3:119:ILE:HG13	49:p3:161:ALA:HB2	1.98	0.46
52:s3:366:TYR:HA	52:s3:400:PRO:HA	1.96	0.46
63:J6:78:ARG:HG3	63:J6:118:LEU:HD21	1.98	0.46
65:L6:92:LEU:HD23	65:L6:92:LEU:HA	1.83	0.46
75:V6:287:LEU:HA	75:V6:290:LEU:HG	1.97	0.46
78:Y6:325:GLY:HA2	81:b6:216:ARG:HH22	1.81	0.46
89:Z:196:GLU:HG3	89:Z:215:VAL:HG21	1.98	0.46
2:A3:1952:U:H2'	2:A3:1953:A:H8	1.80	0.46
2:A3:2421:G:H5''	34:93:24:LYS:HG2	1.98	0.46
2:A3:3175:A:OP2	30:43:91:TYR:OH	2.29	0.46
17:R3:126:GLU:OE2	17:R3:141:ILE:N	2.43	0.46
21:V3:178:SER:OG	21:V3:181:ASP:N	2.38	0.46
33:73:146:CYS:HA	33:73:149:MET:HE3	1.98	0.46
39:e3:57:PRO:HD3	39:e3:156:ASN:HB2	1.98	0.46
75:V6:327:LEU:HD13	75:V6:330:TYR:HB2	1.98	0.46
77:X6:260:VAL:HG11	77:X6:296:MET:HE2	1.97	0.46
81:b6:292:TYR:HB2	81:b6:319:LEU:HD11	1.98	0.46
84:e6:462:PHE:HE1	84:e6:478:TYR:HA	1.80	0.46
85:A6:844:A:H2'	85:A6:845:A:H8	1.81	0.46
85:A6:929:U:H2'	85:A6:930:A:C8	2.50	0.46
85:A6:1107:A:N7	85:A6:1578:G:O2'	2.44	0.46
89:Z:351:LYS:HA	89:Z:408:LEU:O	2.15	0.46
91:n:61:THR:N	100:n:307:CL:CL	2.86	0.46
2:A3:3184:C:H5'	45:k3:84:LEU:HD21	1.98	0.45
7:H3:56:VAL:HG12	7:H3:82:LEU:HA	1.98	0.45
13:N3:68:ASN:N	13:N3:68:ASN:OD1	2.43	0.45
23:X3:189:ASP:HA	23:X3:192:LYS:HB3	1.97	0.45
31:53:313:MET:HB3	31:53:313:MET:HE2	1.75	0.45
52:s3:77:ASP:OD1	52:s3:77:ASP:N	2.49	0.45
52:s3:404:THR:OG1	52:s3:405:ILE:N	2.48	0.45
55:B6:82:ARG:HH21	55:B6:86:ASP:HB3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:D6:287:ASP:N	57:D6:287:ASP:OD1	2.48	0.45
70:Q6:22:ALA:HA	70:Q6:25:THR:HG22	1.98	0.45
75:V6:151:PHE:HD1	75:V6:156:ASN:HD22	1.64	0.45
76:W6:96:LYS:HE3	76:W6:96:LYS:HB3	1.74	0.45
81:b6:128:ASP:OD1	81:b6:128:ASP:N	2.43	0.45
89:Z:136:ASN:HA	89:Z:336:ARG:HH22	1.81	0.45
90:j:18:G:H1	90:j:56:U:H1'	1.81	0.45
12:M3:26:ASN:HD22	48:o3:95:LEU:HA	1.81	0.45
16:Q3:121:THR:OG1	16:Q3:170:ARG:O	2.27	0.45
27:13:16:ILE:HG21	27:13:61:LYS:HD2	1.97	0.45
36:b3:141:ARG:NH2	36:b3:149:GLN:O	2.48	0.45
47:m3:56:LEU:HD23	47:m3:64:ILE:HD11	1.97	0.45
62:I6:93:ASN:ND2	85:A6:995:G:N7	2.64	0.45
64:K6:91:CYS:SG	64:K6:94:THR:OG1	2.63	0.45
71:R6:106:MET:HB3	71:R6:110:GLN:HB3	1.98	0.45
85:A6:1549:U:H2'	85:A6:1550:A:C8	2.51	0.45
85:A6:1591:U:H2'	85:A6:1592:G:H8	1.80	0.45
89:Z:100:GLU:O	89:Z:104:ARG:HB2	2.16	0.45
89:Z:290:CYS:HA	89:Z:343:PRO:HD3	1.99	0.45
7:D:212:PRO:HA	7:D:213:ILE:HA	1.72	0.45
2:A3:2139:U:H3'	25:Z3:74:SER:HB2	1.97	0.45
2:A3:2517:U:H2'	2:A3:2518:A:C8	2.52	0.45
2:A3:3150:U:O2	5:E3:116:LYS:NZ	2.50	0.45
4:D3:140:ALA:HB2	4:D3:153:ALA:HB2	1.97	0.45
5:E3:295:CYS:SG	5:E3:296:LEU:N	2.90	0.45
9:J3:104:THR:HA	9:J3:105:GLY:HA2	1.68	0.45
32:63:194:THR:OG1	32:63:197:GLU:OE1	2.30	0.45
68:O6:181:HIS:HE1	80:a6:180:LYS:HD2	1.82	0.45
70:Q6:70:ARG:HG2	76:W6:153:PHE:HE1	1.80	0.45
75:V6:106:ASN:OD1	75:V6:106:ASN:N	2.48	0.45
77:X6:265:ILE:HG23	77:X6:329:LEU:HD21	1.98	0.45
77:X6:297:MET:HE1	77:X6:306:ILE:HD12	1.97	0.45
85:A6:1599:G:H2'	85:A6:1600:A:C8	2.51	0.45
86:C:26:C:O2	86:C:41:G:N2	2.49	0.45
33:73:70:VAL:HG12	33:73:124:GLU:HB2	1.99	0.45
37:c3:86:ASP:OD1	37:c3:86:ASP:N	2.37	0.45
38:d3:181:VAL:HG22	38:d3:224:ILE:HG12	1.97	0.45
42:h3:66:LEU:HD12	42:h3:67:GLN:HB2	1.98	0.45
2:A3:2593:G:O2'	2:A3:2631:G:O6	2.34	0.45
2:A3:2673:G:H5''	19:T3:112:LYS:HB2	1.97	0.45
2:A3:2763:U:H3'	2:A3:2764:A:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H3:91:LYS:HD3	7:H3:91:LYS:HA	1.77	0.45
33:73:309:HIS:HB3	33:73:312:ILE:HG22	1.99	0.45
39:e3:162:ARG:HB3	39:e3:251:HIS:HB2	1.99	0.45
55:B6:91:LEU:HD11	76:W6:89:LEU:HD13	1.99	0.45
56:C6:127:LEU:HB2	56:C6:132:TYR:CZ	2.51	0.45
59:F6:98:MET:HG2	59:F6:188:ILE:HD13	1.98	0.45
62:I6:151:VAL:HB	62:I6:177:ASP:HB3	1.98	0.45
66:M6:86:PRO:HA	66:M6:89:LYS:HD2	1.97	0.45
68:O6:113:LEU:HD21	68:O6:122:LEU:HD21	1.98	0.45
77:X6:55:ASP:OD1	77:X6:55:ASP:N	2.49	0.45
77:X6:316:LEU:HD23	77:X6:316:LEU:HA	1.69	0.45
85:A6:973:A:H2'	85:A6:974:A:H8	1.81	0.45
88:A:197:LYS:HD3	88:A:200:THR:HA	1.98	0.45
89:Z:67:ASP:H	96:Z:501:GCP:H3B2	1.82	0.45
2:A3:1773:A:OP2	37:c3:31:VAL:N	2.49	0.45
2:A3:2694:A:N3	2:A3:2942:C:O2'	2.40	0.45
4:D3:187:LEU:O	4:D3:219:LYS:NZ	2.45	0.45
5:E3:148:GLY:HA3	5:E3:173:LYS:HG3	1.98	0.45
17:R3:116:LEU:HD23	17:R3:116:LEU:HA	1.79	0.45
26:O3:181:ARG:NH1	26:O3:186:THR:O	2.49	0.45
27:13:17:LEU:HB2	27:13:63:ARG:HG2	1.99	0.45
31:53:309:LEU:HD11	31:53:347:THR:HG21	1.98	0.45
32:63:272:LEU:HD23	32:63:272:LEU:HA	1.84	0.45
45:k3:82:THR:OG1	45:k3:83:ALA:N	2.49	0.45
56:C6:101:PRO:HG3	57:D6:132:ILE:HD13	1.99	0.45
57:D6:241:ILE:O	57:D6:260:LYS:HA	2.17	0.45
60:G6:114:SER:HB3	60:G6:123:PRO:HD2	1.99	0.45
62:I6:158:ARG:NH1	70:Q6:23:TYR:OH	2.44	0.45
64:K6:120:LEU:HB3	64:K6:123:ILE:HD12	1.99	0.45
66:M6:67:ALA:HB2	71:R6:196:TYR:CZ	2.51	0.45
68:O6:118:ARG:HE	68:O6:118:ARG:HB2	1.57	0.45
85:A6:1006:C:H2'	85:A6:1007:A:C8	2.50	0.45
89:Z:127:CYS:HB2	89:Z:137:MET:HG2	1.99	0.45
2:A3:2683:C:OP2	17:R3:34:ARG:NH1	2.50	0.45
2:A3:3041:U:H2'	2:A3:3042:U:H6	1.81	0.45
5:E3:150:LYS:O	5:E3:174:GLN:N	2.49	0.45
33:73:309:HIS:O	33:73:313:TRP:CB	2.65	0.45
41:g3:109:VAL:HA	41:g3:147:LEU:O	2.17	0.45
56:C6:117:LEU:O	56:C6:151:VAL:HA	2.16	0.45
58:E6:117:LEU:HD13	82:c6:10:LEU:HD12	1.99	0.45
73:T6:155:LEU:HD13	73:T6:156:PRO:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:V6:392:ARG:HH22	85:A6:1528:A:H5''	1.80	0.45
84:e6:617:SER:HA	84:e6:620:VAL:HG12	1.98	0.45
86:C:50:A:N1	86:C:59:G:N2	2.59	0.45
2:A3:1847:U:OP1	12:M3:47:ARG:NE	2.37	0.45
3:B3:1605:A:H2'	3:B3:1606:G:C8	2.52	0.45
7:H3:53:THR:OG1	7:H3:86:THR:OG1	2.28	0.45
10:K3:168:ARG:HE	10:K3:170:TRP:CD1	2.35	0.45
11:L3:98:PRO:HA	16:Q3:162:ILE:HG12	1.99	0.45
14:O3:145:LEU:HD11	33:73:308:ALA:HB2	1.99	0.45
17:R3:29:ARG:HA	17:R3:29:ARG:HD3	1.65	0.45
31:53:276:ASP:OD1	52:s3:158:ARG:NH2	2.50	0.45
39:e3:61:LYS:HD3	39:e3:62:PRO:HD2	1.99	0.45
55:B6:102:MET:HE3	55:B6:102:MET:HB3	1.70	0.45
56:C6:37:ASN:HA	85:A6:1269:C:H5''	1.99	0.45
59:F6:153:GLU:HA	59:F6:183:ALA:HB2	1.98	0.45
74:U6:72:MET:HA	74:U6:75:VAL:HG12	1.97	0.45
75:V6:82:ARG:HG3	75:V6:85:ILE:HD12	1.98	0.45
77:X6:67:HIS:HB2	77:X6:100:MET:HA	1.98	0.45
77:X6:272:THR:OG1	77:X6:282:ILE:O	2.29	0.45
89:Z:62:THR:HA	89:Z:148:ILE:O	2.17	0.45
7:D:163:THR:HA	7:D:166:PHE:HB2	1.99	0.45
2:A3:2683:C:N4	26:03:83:ASN:OD1	2.39	0.45
6:F3:96:LEU:HD12	6:F3:96:LEU:HA	1.86	0.45
11:L3:125:THR:OG1	16:Q3:125:TYR:O	2.35	0.45
12:M3:255:MET:SD	12:M3:255:MET:N	2.89	0.45
14:O3:77:ASP:OD1	14:O3:83:LYS:NZ	2.39	0.45
43:i3:79:TRP:O	43:i3:93:ARG:NH1	2.44	0.45
52:s3:101:ASN:HA	52:s3:322:VAL:HG11	1.99	0.45
57:D6:179:TRP:HA	57:D6:182:LYS:HE3	1.99	0.45
57:D6:370:VAL:HB	57:D6:385:ALA:HB3	1.98	0.45
59:F6:200:LEU:HB3	59:F6:202:PRO:HD2	1.98	0.45
61:H6:78:VAL:HG22	61:H6:173:THR:HG22	1.99	0.45
64:K6:60:ASN:O	64:K6:68:GLN:NE2	2.35	0.45
75:V6:156:ASN:O	75:V6:160:ALA:HB3	2.17	0.45
85:A6:929:U:H2'	85:A6:930:A:H8	1.80	0.45
7:D:205:THR:OG1	7:D:206:LEU:N	2.44	0.45
2:A3:2114:C:H2'	2:A3:2115:U:H6	1.82	0.45
2:A3:2203:G:N2	2:A3:2208:A:H62	2.14	0.45
5:E3:159:THR:O	5:E3:163:GLU:HB2	2.16	0.45
9:J3:115:LYS:HA	9:J3:115:LYS:HD3	1.79	0.45
15:P3:90:GLU:OE2	15:P3:107:ARG:NH2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:V3:177:THR:HG22	34:93:71:LYS:H	1.82	0.45
50:q3:101:GLU:HA	50:q3:104:ARG:HG2	1.99	0.45
71:R6:164:SER:O	71:R6:164:SER:OG	2.31	0.45
75:V6:126:LEU:HD11	75:V6:162:SER:HB2	1.99	0.45
77:X6:393:ARG:HH22	85:A6:1382:C:H1'	1.81	0.45
83:d6:140:HIS:HB2	85:A6:1147:C:H5	1.81	0.45
85:A6:1196:C:H42	85:A6:1466:G:H1	1.64	0.45
86:C:25:G:H1	86:C:41:G:H1	1.65	0.45
91:n:209:LEU:HD23	91:n:209:LEU:HA	1.81	0.45
2:A3:2082:G:OP1	25:Z3:101:LYS:NZ	2.37	0.44
2:A3:2677:A:H2'	2:A3:2678:A:C8	2.52	0.44
2:A3:2740:A:N3	2:A3:2921:A:O2'	2.44	0.44
10:K3:21:LEU:HD11	10:K3:34:MET:HE3	1.98	0.44
25:Z3:101:LYS:HG3	44:j3:80:LEU:HD22	1.99	0.44
29:33:157:LEU:HD23	29:33:158:LEU:HD23	1.99	0.44
42:h3:88:ASP:O	42:h3:122:ARG:NH2	2.50	0.44
51:r3:153:ARG:NE	51:r3:177:GLY:O	2.49	0.44
64:K6:61:THR:HG21	79:Z6:27:ASN:HD21	1.82	0.44
69:P6:127:PRO:HA	69:P6:130:LEU:HG	1.98	0.44
71:R6:79:LEU:HD23	71:R6:79:LEU:HA	1.80	0.44
75:V6:186:LEU:HA	75:V6:189:CYS:HB3	1.99	0.44
77:X6:240:VAL:HA	77:X6:243:VAL:HB	1.99	0.44
77:X6:312:GLN:NE2	77:X6:319:PRO:O	2.49	0.44
86:24:25:G:H1	86:24:41:G:H1	1.65	0.44
2:A3:2127:A:H2'	2:A3:2128:G:H8	1.82	0.44
2:A3:2699:C:H2'	2:A3:2700:G:H8	1.82	0.44
4:D3:193:ILE:HD11	4:D3:226:ILE:HD13	2.00	0.44
5:E3:206:VAL:HG21	5:E3:289:VAL:HG23	2.00	0.44
19:T3:169:LYS:HA	19:T3:169:LYS:HD2	1.79	0.44
21:V3:122:LEU:HD13	21:V3:133:ILE:HG13	2.00	0.44
72:S6:83:ARG:HH12	72:S6:94:SER:HA	1.81	0.44
80:a6:96:ARG:HB2	80:a6:117:ILE:HB	1.99	0.44
85:A6:990:G:H2'	85:A6:991:A:H8	1.83	0.44
85:A6:1432:G:HO2'	85:A6:1436:U:HO2'	1.64	0.44
4:D3:143:ALA:HB2	4:D3:148:LYS:HB3	2.00	0.44
15:P3:145:TYR:CZ	15:P3:147:PRO:HB3	2.53	0.44
19:T3:124:ALA:HA	19:T3:127:MET:HG2	1.99	0.44
31:53:289:HIS:HE1	31:53:421:GLY:HA3	1.82	0.44
36:b3:32:SER:OG	36:b3:68:ARG:NH1	2.51	0.44
37:c3:83:PHE:HE1	37:c3:202:LEU:HD13	1.82	0.44
38:d3:119:GLN:HA	38:d3:122:ILE:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:e3:160:LEU:HD13	39:e3:171:TRP:HE1	1.82	0.44
39:e3:249:LYS:HA	39:e3:249:LYS:HD3	1.89	0.44
39:e3:266:PRO:O	39:e3:270:ALA:CB	2.65	0.44
52:s3:115:LEU:O	52:s3:394:TRP:HA	2.18	0.44
57:D6:288:HIS:ND1	57:D6:289:THR:OG1	2.34	0.44
57:D6:294:ILE:HG13	57:D6:305:MET:HB2	1.99	0.44
60:G6:276:ARG:NH1	60:G6:373:ASP:OD2	2.46	0.44
60:G6:306:ILE:HG22	60:G6:308:GLN:H	1.82	0.44
60:G6:395:LYS:NZ	85:A6:1431:A:OP1	2.51	0.44
61:H6:75:ARG:HG3	61:H6:176:GLN:HG3	1.98	0.44
63:J6:63:LEU:N	63:J6:82:ARG:O	2.43	0.44
73:T6:30:MET:O	73:T6:64:ILE:HA	2.17	0.44
89:Z:370:PHE:HE2	89:Z:391:LEU:HD21	1.82	0.44
2:A3:2064:A:H61	2:A3:2075:U:H3	1.64	0.44
2:A3:2269:G:H2'	2:A3:2270:A:C8	2.52	0.44
2:A3:2662:A:OP1	2:A3:3159:A:O2'	2.35	0.44
2:A3:2901:A:H2'	2:A3:2902:A:H8	1.81	0.44
2:A3:3144:A:H2'	2:A3:3145:A:H8	1.83	0.44
14:O3:85:LEU:O	14:O3:89:LEU:N	2.51	0.44
15:P3:93:VAL:HG23	15:P3:101:VAL:HG13	1.98	0.44
37:c3:171:ARG:NH1	37:c3:176:GLU:OE2	2.49	0.44
40:f3:192:GLU:HB2	88:A:79:THR:HG22	1.99	0.44
51:r3:71:PRO:HA	51:r3:74:ARG:HB2	2.00	0.44
55:B6:94:LYS:HB2	55:B6:94:LYS:HE2	1.82	0.44
58:E6:80:GLU:OE2	58:E6:84:ARG:NH2	2.50	0.44
74:U6:193:ARG:HE	74:U6:193:ARG:HB2	1.70	0.44
77:X6:348:TYR:HE2	77:X6:388:PRO:HG3	1.82	0.44
80:a6:64:LEU:HD23	80:a6:134:VAL:HG13	1.99	0.44
81:b6:77:LYS:HD3	84:e6:91:ASP:HB2	1.99	0.44
89:Z:149:LEU:HD11	89:Z:178:VAL:HG22	1.97	0.44
2:A3:1678:C:H1'	2:A3:1679:U:H5'	2.00	0.44
2:A3:1693:C:H6	24:Y3:162:ARG:HD3	1.83	0.44
2:A3:1699:C:H5	24:Y3:198:ARG:HG2	1.83	0.44
2:A3:2623:A:HO2'	85:A6:1553:G:HO2'	1.57	0.44
3:B3:1607:U:O4	3:B3:1664:G:O6	2.34	0.44
4:D3:95:GLY:HA2	4:D3:269:ARG:HB2	2.00	0.44
5:E3:94:SER:HA	5:E3:182:THR:HG21	2.00	0.44
52:s3:185:VAL:HG23	52:s3:195:LEU:HD22	2.00	0.44
58:E6:47:LEU:HD13	58:E6:51:ILE:HG22	2.00	0.44
60:G6:338:SER:OG	85:A6:1461:G:OP2	2.35	0.44
77:X6:105:ALA:HB1	77:X6:140:HIS:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
84:e6:482:ILE:HG23	84:e6:483:PRO:HD3	1.99	0.44
85:A6:1555:G:H2'	85:A6:1556:G:H8	1.83	0.44
89:Z:355:GLN:HA	89:Z:405:LYS:HA	1.99	0.44
2:A3:2031:A:N6	2:A3:2045:A:O4'	2.51	0.44
2:A3:2904:A:H2'	2:A3:2905:A:C8	2.52	0.44
4:D3:197:GLU:HB2	4:D3:240:CYS:HB2	1.99	0.44
14:O3:53:ARG:HH11	14:O3:107:MET:HE2	1.83	0.44
15:P3:65:ARG:HH21	22:W3:92:LEU:HD22	1.82	0.44
19:T3:202:GLN:OE1	35:a3:122:ARG:NH1	2.51	0.44
24:Y3:172:ILE:HG12	24:Y3:198:ARG:HG3	2.00	0.44
33:73:219:LEU:HD23	33:73:219:LEU:HA	1.79	0.44
40:f3:97:ALA:HB2	40:f3:182:VAL:HG22	2.00	0.44
42:h3:114:ASN:N	42:h3:114:ASN:OD1	2.39	0.44
52:s3:93:VAL:HG13	52:s3:106:TYR:CZ	2.52	0.44
56:C6:88:GLU:OE2	56:C6:112:ARG:NH2	2.45	0.44
59:F6:115:LEU:HA	59:F6:118:VAL:HG12	1.99	0.44
66:M6:70:LEU:HA	66:M6:73:ILE:HD12	1.98	0.44
85:A6:926:C:H2'	85:A6:927:A:C8	2.52	0.44
89:Z:351:LYS:HB2	89:Z:440:LEU:HB3	2.00	0.44
7:D:197:LEU:HB2	7:D:199:VAL:HG22	1.99	0.44
2:A3:2318:A:N3	14:O3:31:ASN:ND2	2.65	0.44
5:E3:97:VAL:HG11	5:E3:145:LEU:HD12	2.00	0.44
16:Q3:286:ILE:O	16:Q3:289:SER:OG	2.34	0.44
20:U3:89:LYS:H	20:U3:89:LYS:HG3	1.61	0.44
52:s3:350:ASP:OD1	52:s3:377:LEU:N	2.48	0.44
57:D6:425:LEU:HA	57:D6:425:LEU:HD23	1.81	0.44
59:F6:148:ALA:O	59:F6:152:CYS:HB2	2.17	0.44
75:V6:255:TYR:HA	75:V6:258:ARG:HG2	2.00	0.44
89:Z:355:GLN:O	89:Z:434:GLY:HA2	2.17	0.44
2:A3:2016:C:HO2'	2:A3:2932:G:HO2'	1.61	0.44
2:A3:2420:U:O2'	34:93:31:ARG:O	2.30	0.44
2:A3:2930:U:H2'	2:A3:2931:A:H8	1.81	0.44
8:I3:92:ASP:OD1	8:I3:93:ASN:N	2.51	0.44
11:L3:35:MET:O	11:L3:37:ARG:NH2	2.51	0.44
13:N3:82:PHE:HE1	13:N3:195:LEU:HD22	1.83	0.44
22:W3:105:VAL:HG11	32:63:58:ARG:HG3	1.99	0.44
23:X3:81:GLY:HA2	23:X3:131:THR:HG23	1.99	0.44
23:X3:89:GLN:HA	23:X3:102:LYS:HA	1.99	0.44
24:Y3:126:MET:HG2	24:Y3:128:SER:H	1.83	0.44
31:53:298:ASN:OD1	31:53:298:ASN:N	2.51	0.44
35:a3:51:LEU:HD23	35:a3:51:LEU:HA	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:e3:164:LYS:HD3	39:e3:164:LYS:HA	1.76	0.44
49:p3:140:SER:OG	49:p3:141:ARG:N	2.51	0.44
57:D6:127:ASN:ND2	79:Z6:74:GLU:OE2	2.50	0.44
61:H6:69:PRO:HA	84:e6:61:LYS:HA	1.99	0.44
65:L6:190:THR:OG1	65:L6:191:PHE:N	2.50	0.44
67:N6:96:THR:O	67:N6:98:LYS:N	2.49	0.44
68:O6:52:LYS:HG3	68:O6:58:TYR:HB2	1.99	0.44
72:S6:57:LYS:HD2	72:S6:57:LYS:HA	1.76	0.44
85:A6:978:U:O2'	85:A6:979:A:N7	2.48	0.44
85:A6:1243:C:H2'	85:A6:1244:A:C8	2.53	0.44
85:A6:1404:U:O2'	85:A6:1448:A:N3	2.44	0.44
86:24:26:C:O2	86:24:41:G:N2	2.49	0.44
86:C:9:A:O2'	86:C:43:C:O2	2.31	0.44
2:A3:2740:A:H2'	2:A3:2741:A:C8	2.53	0.44
6:F3:284:TYR:O	6:F3:290:TYR:OH	2.36	0.44
8:I3:44:ARG:NH2	13:N3:234:ASP:OD1	2.49	0.44
10:K3:11:TRP:HH2	37:c3:267:LEU:HD22	1.83	0.44
10:K3:69:GLY:HA2	51:r3:152:THR:HA	2.00	0.44
15:P3:78:HIS:CE1	15:P3:95:HIS:HD2	2.36	0.44
21:V3:115:LEU:HD13	21:V3:115:LEU:HA	1.83	0.44
31:53:135:LYS:HD2	31:53:135:LYS:HA	1.76	0.44
31:53:251:HIS:CE1	31:53:371:LYS:HD2	2.52	0.44
31:53:378:SER:O	31:53:380:GLN:NE2	2.51	0.44
62:I6:69:GLU:HA	62:I6:70:GLU:HA	1.73	0.44
65:L6:195:TYR:OH	85:A6:785:A:OP2	2.28	0.44
68:O6:94:CYS:N	68:O6:143:CYS:SG	2.91	0.44
81:b6:93:LYS:HD3	81:b6:93:LYS:HA	1.91	0.44
84:e6:528:ARG:HA	84:e6:531:ILE:HD12	1.99	0.44
85:A6:1062:C:H2'	85:A6:1063:U:H6	1.83	0.44
85:A6:1581:U:H2'	85:A6:1582:A:H8	1.83	0.44
91:n:99:ILE:HD12	91:n:107:TRP:HZ3	1.82	0.44
2:A3:3008:C:C2	2:A3:3032:G:N2	2.86	0.43
4:D3:257:ILE:HG22	4:D3:262:ARG:HB3	2.00	0.43
10:K3:52:ASP:OD2	10:K3:124:ARG:NH2	2.50	0.43
24:Y3:80:LYS:HD2	24:Y3:80:LYS:HA	1.75	0.43
52:s3:96:GLN:NE2	52:s3:301:LEU:O	2.50	0.43
57:D6:249:ASN:N	57:D6:249:ASN:OD1	2.51	0.43
62:I6:153:GLY:H	62:I6:179:THR:HB	1.83	0.43
69:P6:83:PHE:HE1	69:P6:135:VAL:HG11	1.83	0.43
77:X6:168:LEU:HA	77:X6:180:GLN:HB3	2.00	0.43
91:n:196:LEU:HB3	91:n:209:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J3:127:ASP:HB2	9:J3:130:PHE:HB2	2.00	0.43
11:L3:42:ASP:O	11:L3:48:ASN:ND2	2.50	0.43
22:W3:126:LEU:HD23	22:W3:126:LEU:HA	1.87	0.43
36:b3:27:GLN:OE1	37:c3:177:GLN:NE2	2.51	0.43
85:A6:1199:U:H2'	85:A6:1200:A:C8	2.54	0.43
91:n:59:ARG:H	91:n:199:HIS:CE1	2.35	0.43
2:A3:2167:A:N6	2:A3:2212:C:OP2	2.35	0.43
2:A3:2995:G:O2'	2:A3:3041:U:O2'	2.36	0.43
8:I3:56:PRO:HD3	13:N3:208:ASN:HB3	1.99	0.43
13:N3:227:ARG:HH22	13:N3:235:LEU:HD21	1.82	0.43
23:X3:90:ILE:HD12	23:X3:103:LYS:HD3	2.00	0.43
39:e3:180:PRO:O	88:A:156:LYS:NZ	2.51	0.43
57:D6:265:MET:N	57:D6:265:MET:SD	2.91	0.43
61:H6:136:MET:HE3	61:H6:136:MET:HB2	1.80	0.43
64:K6:86:ARG:HH21	85:A6:1238:C:H4'	1.82	0.43
66:M6:59:ASN:OD1	66:M6:63:GLU:N	2.45	0.43
76:W6:161:THR:HG22	76:W6:163:LEU:H	1.83	0.43
2:A3:2132:A:N6	48:o3:16:GLN:OE1	2.52	0.43
2:A3:3000:A:H2'	2:A3:3001:G:H8	1.83	0.43
10:K3:21:LEU:HD21	10:K3:31:LEU:HD22	2.00	0.43
12:M3:198:GLN:OE1	50:q3:55:ARG:NH1	2.51	0.43
14:O3:30:ARG:HE	14:O3:81:THR:HG22	1.82	0.43
31:53:53:PRO:HA	31:53:54:GLY:HA2	1.64	0.43
31:53:300:ARG:O	31:53:305:GLN:NE2	2.51	0.43
33:73:282:ALA:HB2	33:73:321:ARG:HG2	2.01	0.43
37:c3:31:VAL:HG13	43:i3:35:ARG:HH21	1.83	0.43
67:N6:63:ILE:HB	67:N6:86:PHE:HB2	1.99	0.43
81:b6:112:LEU:HD23	81:b6:112:LEU:HA	1.74	0.43
85:A6:1547:U:H2'	85:A6:1548:A:C8	2.53	0.43
90:j:6:C:H2'	90:j:7:G:C8	2.54	0.43
91:n:177:LYS:HD3	91:n:177:LYS:HA	1.85	0.43
91:n:211:SER:O	91:n:211:SER:OG	2.35	0.43
2:A3:1892:A:OP2	29:33:169:ARG:NE	2.41	0.43
2:A3:2691:U:OP2	48:o3:11:ARG:NH1	2.52	0.43
18:S3:94:ARG:CZ	36:b3:123:ASN:HD21	2.31	0.43
19:T3:141:TYR:CD2	19:T3:184:PRO:HD3	2.54	0.43
22:W3:100:THR:OG1	22:W3:132:HIS:NE2	2.47	0.43
32:63:222:ASP:HB2	32:63:224:HIS:HE1	1.83	0.43
37:c3:263:GLY:H	37:c3:268:PRO:HB3	1.83	0.43
40:f3:138:GLN:NE2	88:A:194:ASP:O	2.51	0.43
50:q3:79:PRO:HA	50:q3:82:LEU:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:Q6:63:ILE:HG12	82:c6:4:PRO:HG2	2.00	0.43
71:R6:75:VAL:HG23	71:R6:303:LEU:HD11	2.00	0.43
72:S6:102:LYS:NZ	72:S6:124:ALA:O	2.50	0.43
75:V6:168:MET:HE2	75:V6:168:MET:HB3	1.80	0.43
79:Z6:46:LYS:HB3	79:Z6:46:LYS:HE3	1.84	0.43
85:A6:667:A:H2'	85:A6:668:G:H8	1.84	0.43
85:A6:1010:U:H2'	85:A6:1011:G:H8	1.83	0.43
89:Z:74:THR:O	89:Z:78:THR:OG1	2.26	0.43
86:C:63:C:H2'	86:C:64:A:H8	1.84	0.43
91:n:25:ALA:HB1	91:n:214:VAL:HG11	1.99	0.43
2:A3:1939:G:OP2	4:D3:259:LYS:NZ	2.38	0.43
2:A3:2016:C:O2'	2:A3:2932:G:O2'	2.34	0.43
2:A3:2446:A:OP1	52:s3:65:ARG:NH2	2.50	0.43
3:B3:1605:A:H2'	3:B3:1606:G:H8	1.84	0.43
3:B3:1640:A:OP1	15:P3:156:SER:N	2.45	0.43
4:D3:141:LEU:HD11	4:D3:148:LYS:HB2	2.00	0.43
5:E3:106:MET:HG2	5:E3:120:THR:HG22	2.00	0.43
7:H3:104:ASN:N	7:H3:104:ASN:OD1	2.49	0.43
17:R3:70:ASN:HA	17:R3:73:THR:HG22	2.00	0.43
21:V3:100:LYS:O	21:V3:102:MET:N	2.51	0.43
37:c3:72:ILE:HG23	37:c3:88:LEU:HD23	2.00	0.43
40:f3:101:THR:HG21	47:m3:43:VAL:HG22	2.01	0.43
55:B6:183:PHE:HB2	55:B6:187:VAL:HG21	2.00	0.43
56:C6:96:MET:HE3	56:C6:96:MET:HB3	1.75	0.43
59:F6:110:LEU:HD23	59:F6:110:LEU:HA	1.85	0.43
61:H6:76:LEU:HA	61:H6:174:LYS:O	2.18	0.43
65:L6:139:TYR:OH	85:A6:1042:C:OP1	2.29	0.43
81:b6:189:LYS:HD2	81:b6:233:SER:HA	2.00	0.43
85:A6:978:U:O4	85:A6:1035:G:N1	2.52	0.43
2:A3:2777:G:N2	2:A3:2778:U:O4	2.39	0.43
5:E3:113:ASP:OD2	5:E3:113:ASP:N	2.51	0.43
10:K3:63:ARG:NH2	10:K3:130:ASP:OD1	2.52	0.43
29:33:98:SER:OG	29:33:102:GLY:N	2.44	0.43
31:53:353:HIS:CD2	31:53:379:ASP:H	2.37	0.43
32:63:71:TRP:CD1	32:63:72:ARG:H	2.37	0.43
32:63:175:VAL:HG22	32:63:204:VAL:HG22	1.99	0.43
39:e3:152:LYS:HA	39:e3:152:LYS:HD3	1.89	0.43
41:g3:141:ASN:HD22	48:o3:86:ARG:HD3	1.84	0.43
52:s3:153:GLU:HG3	52:s3:175:PRO:HB2	2.01	0.43
55:B6:70:SER:HA	72:S6:38:PHE:HZ	1.82	0.43
55:B6:147:ARG:NH1	85:A6:1298:A:OP1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:I6:119:ASN:OD1	85:A6:995:G:N2	2.49	0.43
65:L6:182:CYS:SG	65:L6:183:TRP:N	2.92	0.43
73:T6:120:LYS:HE3	73:T6:120:LYS:HB3	1.88	0.43
77:X6:86:ARG:CZ	77:X6:393:ARG:HE	2.31	0.43
77:X6:153:LEU:HB3	77:X6:260:VAL:HA	1.99	0.43
90:j:68:G:H2'	90:j:69:G:H8	1.84	0.43
91:n:64:LEU:HD12	91:n:64:LEU:HA	1.80	0.43
2:A3:1952:U:H2'	2:A3:1953:A:C8	2.54	0.43
2:A3:3144:A:H2'	2:A3:3145:A:C8	2.53	0.43
15:P3:67:TRP:HB3	15:P3:70:VAL:HG22	2.00	0.43
24:Y3:164:ARG:HD3	24:Y3:180:LYS:HB3	2.00	0.43
25:Z3:86:ILE:HG23	25:Z3:91:LEU:HB2	2.00	0.43
38:d3:123:ARG:HE	38:d3:123:ARG:HB3	1.69	0.43
47:m3:52:TYR:HD1	47:m3:69:ARG:HA	1.82	0.43
59:F6:140:ASN:HB2	77:X6:367:GLN:HE21	1.84	0.43
61:H6:89:ASP:HA	61:H6:141:ARG:HH12	1.83	0.43
70:Q6:68:MET:HE1	82:c6:108:LEU:HD11	2.00	0.43
71:R6:291:ARG:HB2	71:R6:293:LEU:HD23	2.01	0.43
83:d6:153:LEU:HD13	83:d6:156:LYS:HE2	2.00	0.43
85:A6:1351:G:H2'	85:A6:1352:G:C8	2.54	0.43
86:24:63:C:H2'	86:24:64:A:H8	1.84	0.43
2:A3:2294:A:OP1	12:M3:41:ARG:NH2	2.52	0.43
2:A3:3078:C:H2'	2:A3:3079:G:C8	2.53	0.43
4:D3:207:ILE:H	4:D3:207:ILE:HG13	1.43	0.43
5:E3:48:TRP:CD1	5:E3:50:ASP:H	2.37	0.43
5:E3:175:THR:OG1	5:E3:176:VAL:N	2.52	0.43
9:J3:85:PRO:O	9:J3:124:LYS:NZ	2.52	0.43
10:K3:124:ARG:NH1	35:a3:117:PHE:O	2.52	0.43
13:N3:233:TYR:HB3	13:N3:237:HIS:CD2	2.54	0.43
31:53:225:SER:OG	31:53:226:GLY:N	2.51	0.43
31:53:333:ALA:HA	31:53:362:THR:HG23	2.01	0.43
37:c3:66:TRP:HE1	37:c3:68:TYR:HB2	1.83	0.43
57:D6:98:LEU:HD11	79:Z6:75:HIS:HD2	1.83	0.43
62:I6:87:HIS:O	62:I6:97:ILE:HA	2.18	0.43
70:Q6:75:LEU:HD23	70:Q6:75:LEU:HA	1.89	0.43
81:b6:149:ILE:HD13	81:b6:175:VAL:HB	2.00	0.43
85:A6:1128:A:H2'	85:A6:1129:A:H2'	2.01	0.43
85:A6:1474:A:H2'	85:A6:1475:A:C8	2.52	0.43
2:A3:1794:A:OP1	6:F3:142:ARG:NH2	2.52	0.43
2:A3:2253:U:H2'	2:A3:2254:C:C6	2.54	0.43
2:A3:2950:U:H2'	2:A3:2951:A:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A3:3115:U:H2'	2:A3:3116:C:C6	2.54	0.43
4:D3:199:GLU:HB2	4:D3:202:ARG:HD2	2.00	0.43
8:I3:135:LEU:HD11	8:I3:144:LEU:HD13	2.00	0.43
10:K3:43:HIS:CD2	10:K3:44:LYS:HG3	2.54	0.43
17:R3:108:TYR:HD1	36:b3:125:SER:HB2	1.83	0.43
23:X3:52:ILE:HG23	23:X3:59:ARG:HB3	2.01	0.43
32:63:300:THR:HA	32:63:303:PHE:HB3	2.01	0.43
33:73:77:THR:HG23	38:d3:283:PRO:HA	2.01	0.43
35:a3:62:HIS:O	35:a3:62:HIS:ND1	2.50	0.43
41:g3:107:MET:HB3	41:g3:107:MET:HE2	1.77	0.43
47:m3:70:GLU:O	47:m3:72:ARG:N	2.46	0.43
52:s3:271:LEU:O	52:s3:273:LEU:N	2.52	0.43
57:D6:421:VAL:HG21	85:A6:932:A:N3	2.33	0.43
60:G6:287:LYS:HG3	60:G6:355:PHE:CG	2.54	0.43
68:O6:166:HIS:CE1	71:R6:96:GLN:HE21	2.37	0.43
73:T6:52:ILE:HD11	73:T6:66:MET:HE3	2.00	0.43
75:V6:132:LYS:HZ3	75:V6:137:ILE:HG13	1.84	0.43
83:d6:130:VAL:HG13	83:d6:134:ARG:HG3	2.01	0.43
2:A3:1924:U:H2'	2:A3:1925:A:H8	1.83	0.42
2:A3:2052:A:H5'	41:g3:105:ARG:HG2	2.01	0.42
2:A3:2926:A:H5'	2:A3:2926:A:H8	1.83	0.42
2:A3:3157:C:C2	16:Q3:84:ARG:HG2	2.54	0.42
7:H3:62:VAL:HG21	23:X3:65:VAL:HG21	2.01	0.42
11:L3:31:ALA:HA	11:L3:66:VAL:HG13	2.01	0.42
60:G6:201:ILE:HD12	60:G6:201:ILE:HA	1.88	0.42
60:G6:360:GLU:HA	60:G6:363:TRP:CD1	2.53	0.42
73:T6:3:MET:HE2	73:T6:3:MET:HB3	1.92	0.42
73:T6:73:SER:HA	73:T6:74:PRO:HD3	1.91	0.42
74:U6:152:ARG:HA	74:U6:152:ARG:HD2	1.88	0.42
85:A6:803:A:H2'	85:A6:804:C:C6	2.53	0.42
85:A6:985:C:H2'	85:A6:986:A:H8	1.84	0.42
85:A6:1250:U:H4'	85:A6:1251:G:H5'	2.01	0.42
2:A3:1729:U:O2'	2:A3:1751:A:N1	2.42	0.42
2:A3:2456:U:OP1	14:O3:16:ARG:NH1	2.44	0.42
6:F3:63:GLN:HA	6:F3:81:ASP:HA	2.00	0.42
6:F3:176:VAL:O	6:F3:179:THR:OG1	2.30	0.42
39:e3:160:LEU:HD22	39:e3:171:TRP:CD1	2.54	0.42
59:F6:235:ALA:HA	62:I6:126:ILE:HG21	2.01	0.42
66:M6:91:LEU:HD22	66:M6:96:PHE:HB3	2.01	0.42
69:P6:95:HIS:H	69:P6:95:HIS:CD2	2.36	0.42
81:b6:113:HIS:CD2	81:b6:114:LEU:HG	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
89:Z:279:LEU:HB3	89:Z:318:ALA:HA	2.01	0.42
86:C:25:G:H22	86:C:41:G:H1	1.66	0.42
91:n:75:LEU:HD21	91:n:103:ILE:HG12	2.00	0.42
2:A3:1769:C:C4	6:F3:108:ARG:HD2	2.55	0.42
5:E3:145:LEU:HD23	5:E3:145:LEU:HA	1.84	0.42
8:I3:93:ASN:ND2	8:I3:157:GLU:OE2	2.52	0.42
38:d3:133:LYS:HD2	38:d3:136:ASP:HB2	2.01	0.42
38:d3:222:LEU:HD23	38:d3:222:LEU:HA	1.92	0.42
59:F6:114:THR:OG1	59:F6:115:LEU:N	2.52	0.42
60:G6:88:LEU:HA	60:G6:91:MET:HG2	2.01	0.42
63:J6:48:LYS:HE2	63:J6:53:GLU:HA	2.00	0.42
71:R6:69:THR:HG23	71:R6:72:ASP:HB2	2.01	0.42
77:X6:163:LYS:HE3	77:X6:316:LEU:HD11	2.00	0.42
85:A6:695:A:N7	85:A6:720:U:O2'	2.52	0.42
2:A3:2525:C:OP1	4:D3:82:SER:OG	2.37	0.42
6:F3:200:PRO:HB3	6:F3:237:LEU:HG	2.01	0.42
31:53:335:VAL:HG22	31:53:361:THR:HG22	2.01	0.42
33:73:181:TYR:O	33:73:296:ARG:HA	2.19	0.42
39:e3:183:THR:OG1	39:e3:184:LEU:N	2.53	0.42
55:B6:88:ARG:HB3	55:B6:91:LEU:HD23	2.00	0.42
57:D6:222:ILE:HD13	57:D6:245:VAL:HG12	2.00	0.42
59:F6:83:SER:O	59:F6:83:SER:OG	2.34	0.42
62:I6:98:GLN:HB2	62:I6:109:PHE:HD1	1.85	0.42
75:V6:129:LEU:HA	75:V6:132:LYS:HE2	2.02	0.42
79:Z6:71:TYR:CE2	79:Z6:73:ASP:HB3	2.54	0.42
85:A6:774:C:H6	85:A6:774:C:H2'	1.70	0.42
85:A6:1402:U:H2'	85:A6:1403:A:H8	1.83	0.42
89:Z:120:ARG:HD2	89:Z:122:TYR:CZ	2.55	0.42
89:Z:184:ASP:OD1	89:Z:184:ASP:N	2.41	0.42
89:Z:243:VAL:HG23	89:Z:247:ILE:HD12	2.00	0.42
12:M3:203:ARG:HG2	12:M3:263:ARG:HA	2.00	0.42
15:P3:83:ILE:HB	15:P3:90:GLU:HB2	2.01	0.42
21:V3:63:GLU:HB2	21:V3:123:VAL:HG22	2.01	0.42
39:e3:128:PHE:HB2	47:m3:73:ARG:HB2	2.02	0.42
57:D6:336:VAL:HG21	57:D6:345:LEU:HD12	2.01	0.42
60:G6:323:LEU:HD23	77:X6:378:LYS:HB3	2.02	0.42
65:L6:118:ASN:ND2	65:L6:121:ASP:OD2	2.53	0.42
74:U6:148:ALA:HA	74:U6:151:GLN:HG2	2.01	0.42
84:e6:497:LEU:HD23	84:e6:534:LEU:HD13	2.01	0.42
84:e6:532:LEU:HD21	84:e6:555:ILE:HG21	2.01	0.42
85:A6:1152:A:H2'	85:A6:1153:G:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A3:2006:C:H2'	2:A3:2007:U:C6	2.55	0.42
2:A3:2286:A:H2'	2:A3:2287:U:C6	2.54	0.42
2:A3:2304:G:OP1	19:T3:154:LYS:NZ	2.53	0.42
2:A3:3148:C:H5'	5:E3:290:PRO:HA	2.00	0.42
6:F3:215:SER:OG	6:F3:257:GLN:N	2.49	0.42
8:I3:94:ARG:HB3	8:I3:157:GLU:HA	2.02	0.42
18:S3:119:GLU:OE2	18:S3:121:ASP:N	2.51	0.42
21:V3:125:PRO:HG2	21:V3:126:MET:HE2	2.01	0.42
21:V3:129:LYS:HB2	21:V3:149:ARG:HH22	1.83	0.42
23:X3:117:GLU:OE1	23:X3:191:TYR:OH	2.36	0.42
23:X3:119:LEU:HD21	31:53:52:ILE:HG23	2.01	0.42
27:13:44:LEU:HA	27:13:44:LEU:HD23	1.79	0.42
31:53:296:LYS:HE2	31:53:296:LYS:HB2	1.95	0.42
31:53:364:LEU:HD13	31:53:364:LEU:HA	1.89	0.42
36:b3:76:VAL:HG22	36:b3:86:GLU:HG3	2.02	0.42
47:m3:59:GLN:HE22	88:A:195:ILE:HG13	1.85	0.42
59:F6:76:ALA:HB3	60:G6:373:ASP:HB3	2.01	0.42
61:H6:105:SER:O	61:H6:105:SER:OG	2.35	0.42
61:H6:141:ARG:HD3	61:H6:141:ARG:HA	1.87	0.42
68:O6:52:LYS:HG2	68:O6:112:LYS:HD2	2.02	0.42
77:X6:92:LYS:HG3	77:X6:93:THR:HG23	2.02	0.42
85:A6:1179:G:H2'	85:A6:1180:G:C8	2.55	0.42
85:A6:1470:C:H2'	85:A6:1471:C:H6	1.85	0.42
86:24:50:A:N1	86:24:59:G:N2	2.59	0.42
2:A3:2575:U:H2'	2:A3:2581:A:H62	1.85	0.42
2:A3:3054:G:H2'	2:A3:3055:U:C6	2.55	0.42
8:I3:140:TYR:OH	8:I3:183:ASP:OD1	2.38	0.42
12:M3:115:PRO:HB2	12:M3:267:PHE:CZ	2.55	0.42
18:S3:77:ALA:HA	18:S3:80:VAL:HG12	2.02	0.42
18:S3:155:ARG:NH1	18:S3:157:GLU:OE2	2.52	0.42
18:S3:187:THR:O	18:S3:187:THR:OG1	2.36	0.42
36:b3:40:SER:O	36:b3:44:ARG:HB2	2.19	0.42
40:f3:127:MET:HE3	40:f3:128:PRO:HD2	2.00	0.42
43:i3:102:MET:HE1	43:i3:110:LEU:HD22	2.02	0.42
45:k3:18:VAL:HA	45:k3:64:VAL:HG12	2.01	0.42
52:s3:251:VAL:HG22	52:s3:252:PRO:HD2	2.01	0.42
57:D6:314:LEU:HD23	57:D6:314:LEU:HA	1.89	0.42
72:S6:112:THR:OG1	72:S6:113:ASP:N	2.53	0.42
73:T6:9:ILE:HD12	73:T6:9:ILE:HA	1.90	0.42
73:T6:56:GLN:NE2	73:T6:59:ASN:O	2.52	0.42
75:V6:110:HIS:HA	75:V6:113:ILE:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:V6:176:PRO:O	75:V6:179:GLN:NE2	2.52	0.42
80:a6:169:LEU:HD23	80:a6:169:LEU:HA	1.85	0.42
85:A6:1029:A:H2'	85:A6:1030:A:C8	2.55	0.42
88:A:73:ARG:HA	88:A:73:ARG:HD3	1.76	0.42
89:Z:65:HIS:HB2	89:Z:161:THR:OG1	2.20	0.42
89:Z:80:ILE:HD12	89:Z:83:GLU:HB2	2.01	0.42
7:D:226:ASN:ND2	7:D:229:ASP:OD1	2.38	0.42
2:A3:1862:U:H2'	2:A3:1863:A:C8	2.53	0.42
6:F3:226:MET:HE1	6:F3:242:LEU:HD22	2.02	0.42
12:M3:247:ILE:HD11	49:p3:59:TRP:CE2	2.55	0.42
23:X3:67:ILE:HA	23:X3:68:PRO:HD3	1.89	0.42
23:X3:96:LYS:HA	86:C:73:A:C8	2.48	0.42
33:73:253:LYS:HG2	33:73:255:HIS:NE2	2.35	0.42
37:c3:156:LEU:HD23	37:c3:156:LEU:HA	1.90	0.42
38:d3:264:LYS:HE3	38:d3:264:LYS:HB2	1.85	0.42
59:F6:235:ALA:HB1	62:I6:121:LYS:HB3	2.01	0.42
60:G6:255:GLN:HG2	60:G6:370:LEU:HD13	2.00	0.42
60:G6:271:LYS:HA	60:G6:283:ALA:O	2.19	0.42
63:J6:31:ALA:O	73:T6:4:LYS:NZ	2.36	0.42
69:P6:105:LYS:HD3	69:P6:105:LYS:HA	1.81	0.42
69:P6:140:TYR:HB3	70:Q6:28:ARG:HG2	2.01	0.42
75:V6:82:ARG:HA	75:V6:85:ILE:HD12	2.02	0.42
81:b6:126:LEU:HD21	84:e6:74:LEU:HD23	2.01	0.42
82:c6:27:LEU:HD23	82:c6:27:LEU:HA	1.88	0.42
85:A6:744:G:H2'	85:A6:745:A:C8	2.55	0.42
85:A6:1095:U:H2'	85:A6:1096:G:C8	2.55	0.42
89:Z:425:ARG:HG2	89:Z:430:THR:HA	2.02	0.42
2:A3:1716:U:C2	23:X3:87:LEU:HD23	2.54	0.42
2:A3:2458:A:O2'	5:E3:215:PHE:O	2.33	0.42
2:A3:3143:U:H2'	2:A3:3144:A:C8	2.53	0.42
6:F3:92:ARG:HB2	6:F3:176:VAL:HG21	2.00	0.42
6:F3:168:LYS:HE2	41:g3:90:ARG:HH22	1.85	0.42
31:53:201:ARG:HA	31:53:231:SER:O	2.20	0.42
34:93:129:GLN:HB2	34:93:134:ASN:HB2	2.02	0.42
36:b3:27:GLN:HE21	36:b3:27:GLN:HB3	1.65	0.42
39:e3:74:LEU:HG	47:m3:42:ARG:HG2	2.02	0.42
47:m3:46:GLN:H	47:m3:46:GLN:HG3	1.76	0.42
50:q3:71:VAL:HA	50:q3:72:PRO:HD3	1.78	0.42
50:q3:96:LEU:HD12	50:q3:96:LEU:HA	1.88	0.42
61:H6:134:TYR:OH	64:K6:116:ASP:OD1	2.36	0.42
67:N6:17:VAL:HA	67:N6:28:VAL:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:X6:329:LEU:HD23	77:X6:329:LEU:HA	1.87	0.42
83:d6:182:LEU:HD11	83:d6:186:PRO:HG3	2.01	0.42
85:A6:973:A:H2'	85:A6:974:A:C8	2.55	0.42
85:A6:1352:G:H2'	85:A6:1353:U:C6	2.55	0.42
86:C:63:C:H2'	86:C:64:A:C8	2.55	0.42
91:n:75:LEU:HA	91:n:93:TYR:O	2.20	0.42
2:A3:1693:C:C6	24:Y3:162:ARG:HD3	2.55	0.42
2:A3:1929:A:H2'	2:A3:1930:C:C6	2.55	0.42
6:F3:217:LEU:HD13	6:F3:256:HIS:CE1	2.54	0.42
14:O3:44:ALA:HB3	14:O3:49:VAL:HG23	2.01	0.42
16:Q3:92:PHE:O	16:Q3:96:ARG:HB2	2.20	0.42
16:Q3:290:LYS:HE2	16:Q3:290:LYS:HB2	1.96	0.42
17:R3:71:ARG:HH11	17:R3:107:ILE:HD11	1.85	0.42
25:Z3:63:PRO:HG2	48:o3:53:TYR:HD1	1.84	0.42
38:d3:166:GLU:H	38:d3:166:GLU:HG3	1.68	0.42
42:h3:65:ASP:O	42:h3:67:GLN:N	2.51	0.42
52:s3:369:PHE:HE1	52:s3:421:ILE:HG13	1.84	0.42
60:G6:229:LEU:HD21	60:G6:241:VAL:HG21	2.02	0.42
64:K6:42:LYS:NZ	64:K6:46:GLU:OE2	2.47	0.42
66:M6:74:ARG:HG2	74:U6:74:PHE:CE1	2.55	0.42
80:a6:64:LEU:HB2	80:a6:139:TRP:CD1	2.55	0.42
85:A6:688:U:H2'	85:A6:689:A:C8	2.53	0.42
86:24:25:G:H22	86:24:41:G:H1	1.66	0.42
91:n:29:VAL:HG12	91:n:216:THR:HG23	2.02	0.42
2:A3:2148:A:H2'	2:A3:2149:G:C8	2.54	0.41
2:A3:2149:G:OP1	17:R3:99:ARG:NH2	2.41	0.41
2:A3:2230:A:H62	2:A3:2975:G:H21	1.67	0.41
2:A3:2797:C:H2'	2:A3:2798:A:H8	1.84	0.41
9:J3:90:PHE:HZ	9:J3:123:ILE:HD11	1.85	0.41
23:X3:128:THR:OG1	23:X3:129:MET:N	2.52	0.41
25:Z3:73:LYS:HE3	25:Z3:73:LYS:HB2	1.86	0.41
29:33:116:ARG:HB2	29:33:122:TRP:CH2	2.55	0.41
31:53:295:ASP:HB2	31:53:347:THR:HB	2.00	0.41
57:D6:94:THR:OG1	57:D6:95:ALA:N	2.53	0.41
57:D6:288:HIS:HA	57:D6:330:LYS:HG2	2.01	0.41
70:Q6:64:TYR:CE1	82:c6:29:LEU:HD23	2.56	0.41
74:U6:97:LYS:HA	74:U6:100:ALA:HB3	2.02	0.41
77:X6:89:MET:HA	77:X6:92:LYS:HG2	2.01	0.41
77:X6:159:HIS:O	77:X6:163:LYS:HB2	2.20	0.41
82:c6:18:LYS:HE2	82:c6:18:LYS:HB3	1.83	0.41
85:A6:1601:C:H4'	85:A6:1602:G:C5	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
91:n:223:ARG:HA	91:n:223:ARG:HD2	1.92	0.41
2:A3:1756:A:OP1	7:H3:69:ARG:NH2	2.52	0.41
5:E3:108:PRO:HB3	5:E3:116:LYS:HD2	2.03	0.41
6:F3:237:LEU:HD23	6:F3:237:LEU:HA	1.73	0.41
18:S3:128:ILE:O	18:S3:157:GLU:HA	2.21	0.41
21:V3:50:SER:N	21:V3:84:ASN:HD21	2.18	0.41
24:Y3:215:LYS:NZ	28:23:84:LEU:O	2.39	0.41
33:73:199:LEU:HA	33:73:202:PHE:HD2	1.84	0.41
43:i3:88:LEU:HD12	43:i3:117:LEU:HB3	2.02	0.41
52:s3:405:ILE:HG22	52:s3:407:ASP:H	1.85	0.41
58:E6:30:MET:HA	58:E6:34:ALA:H	1.85	0.41
59:F6:185:LYS:HA	59:F6:188:ILE:HG22	2.02	0.41
60:G6:92:MET:HE3	60:G6:92:MET:HB3	1.96	0.41
63:J6:74:ASN:HD21	85:A6:904:C:H41	1.67	0.41
69:P6:59:LYS:HD3	69:P6:59:LYS:HA	1.85	0.41
75:V6:79:ILE:HG23	75:V6:84:GLU:HB2	2.01	0.41
80:a6:7:ARG:NE	85:A6:1517:A:N7	2.67	0.41
81:b6:115:THR:HG23	81:b6:118:ALA:H	1.85	0.41
84:e6:475:LEU:HD12	84:e6:475:LEU:HA	1.92	0.41
85:A6:844:A:H2'	85:A6:845:A:C8	2.55	0.41
89:Z:65:HIS:ND1	89:Z:160:GLN:HB2	2.36	0.41
91:n:5:LYS:HG3	91:n:8:ARG:HH12	1.85	0.41
2:A3:2127:A:H4'	2:A3:2251:A:C6	2.55	0.41
9:J3:59:ASP:OD1	9:J3:59:ASP:N	2.37	0.41
18:S3:115:LEU:HB3	36:b3:118:PRO:HB2	2.02	0.41
29:33:163:THR:OG1	29:33:164:SER:N	2.51	0.41
33:73:247:ASN:N	33:73:247:ASN:OD1	2.49	0.41
39:e3:58:VAL:HG13	39:e3:59:VAL:HG23	2.01	0.41
50:q3:148:ALA:HA	50:q3:151:GLU:HG3	2.01	0.41
52:s3:119:PRO:HG3	52:s3:394:TRP:CE2	2.56	0.41
74:U6:75:VAL:HA	74:U6:78:VAL:HG22	2.02	0.41
75:V6:77:ASP:HA	75:V6:115:GLN:HE21	1.85	0.41
81:b6:136:ALA:HA	84:e6:57:VAL:HG11	2.01	0.41
84:e6:376:ILE:HD12	84:e6:415:PHE:HE1	1.84	0.41
86:24:20:U:H5	86:24:44:U:H3	1.68	0.41
86:24:63:C:H2'	86:24:64:A:C8	2.55	0.41
89:Z:301:THR:OG1	89:Z:302:VAL:N	2.54	0.41
2:A3:2049:U:H2'	2:A3:2050:A:H8	1.84	0.41
2:A3:2370:A:N7	20:U3:73:GLN:NE2	2.69	0.41
2:A3:2814:G:N2	2:A3:2840:C:OP1	2.47	0.41
2:A3:3134:C:H3'	2:A3:3135:A:H8	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M3:193:PHE:HE2	12:M3:200:ILE:HG12	1.84	0.41
14:O3:27:HIS:HA	14:O3:30:ARG:HG2	2.02	0.41
21:V3:133:ILE:HD13	21:V3:133:ILE:HA	1.95	0.41
22:W3:127:TYR:OH	32:63:64:GLU:OE1	2.38	0.41
25:Z3:71:ARG:NH1	25:Z3:92:GLU:O	2.53	0.41
27:13:64:SER:O	27:13:64:SER:OG	2.28	0.41
34:93:16:ASP:OD1	34:93:18:MET:N	2.53	0.41
38:d3:158:ASP:OD1	38:d3:159:ARG:N	2.53	0.41
49:p3:135:LEU:HD11	49:p3:154:ILE:HG13	2.02	0.41
51:r3:166:GLY:O	51:r3:171:ARG:NH2	2.53	0.41
63:J6:78:ARG:NH2	85:A6:897:G:N7	2.68	0.41
75:V6:127:TYR:HA	75:V6:130:VAL:HG12	2.03	0.41
76:W6:136:LYS:HE3	76:W6:136:LYS:HB2	1.97	0.41
77:X6:373:THR:OG1	77:X6:374:GLU:OE1	2.38	0.41
85:A6:1007:A:H2'	85:A6:1008:G:H8	1.84	0.41
2:A3:2420:U:H4'	34:93:35:GLY:HA2	2.01	0.41
2:A3:2740:A:H2'	2:A3:2741:A:H8	1.84	0.41
4:D3:111:ARG:HH22	4:D3:163:ILE:HG21	1.86	0.41
5:E3:135:LYS:HB2	5:E3:135:LYS:HE2	1.84	0.41
12:M3:220:ARG:HH21	12:M3:233:ARG:HG2	1.85	0.41
17:R3:43:VAL:HA	17:R3:46:VAL:HG12	2.03	0.41
18:S3:118:ASN:OD1	18:S3:118:ASN:N	2.54	0.41
21:V3:72:LYS:HD2	21:V3:91:LEU:HD11	2.02	0.41
28:23:80:LEU:HD23	28:23:80:LEU:HA	1.82	0.41
33:73:143:TRP:HE1	33:73:174:VAL:HG23	1.85	0.41
37:c3:275:TYR:CZ	37:c3:280:LEU:HD12	2.56	0.41
39:e3:160:LEU:HD21	39:e3:173:LEU:HD22	2.01	0.41
52:s3:363:ASP:O	52:s3:365:LYS:N	2.53	0.41
55:B6:148:ASN:HB2	55:B6:197:HIS:CD2	2.55	0.41
55:B6:243:PRO:O	55:B6:247:HIS:ND1	2.36	0.41
59:F6:46:ILE:HG13	59:F6:81:LYS:HG2	2.03	0.41
60:G6:168:MET:HA	60:G6:171:ASN:HD21	1.84	0.41
62:I6:122:LYS:NZ	85:A6:995:G:O6	2.43	0.41
77:X6:159:HIS:O	77:X6:163:LYS:CB	2.68	0.41
79:Z6:26:THR:HG22	79:Z6:27:ASN:H	1.86	0.41
85:A6:1392:C:H2'	85:A6:1393:G:H8	1.85	0.41
89:Z:417:GLU:HG2	89:Z:420:GLN:HB2	2.01	0.41
86:C:20:U:H5	86:C:44:U:H3	1.68	0.41
2:A3:2324:U:H2'	2:A3:2325:U:C6	2.55	0.41
2:A3:2514:C:H2'	2:A3:2515:U:C6	2.54	0.41
2:A3:2992:G:OP2	93:A3:3396:SPD:N1	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A3:3158:A:O2'	14:O3:11:HIS:O	2.25	0.41
4:D3:187:LEU:HD13	4:D3:187:LEU:HA	1.91	0.41
6:F3:160:SER:HB2	43:I3:80:LEU:HD13	2.03	0.41
10:K3:67:PHE:HB3	10:K3:71:LYS:HB2	2.01	0.41
23:X3:93:ASN:HB2	86:C:73:A:O4'	2.21	0.41
32:63:139:TRP:O	32:63:144:GLY:N	2.51	0.41
84:e6:65:TRP:HE3	84:e6:65:TRP:H	1.67	0.41
85:A6:1473:G:H2'	85:A6:1474:A:H8	1.86	0.41
2:A3:2277:U:H2'	2:A3:2278:A:H8	1.85	0.41
2:A3:2978:U:O2'	2:A3:3057:C:OP1	2.30	0.41
2:A3:3157:C:H6	2:A3:3157:C:H2'	1.70	0.41
8:I3:83:ARG:HA	8:I3:86:ILE:HG22	2.03	0.41
8:I3:131:LEU:HA	8:I3:131:LEU:HD12	1.86	0.41
8:I3:161:VAL:HA	8:I3:164:MET:HB2	2.03	0.41
31:53:132:LEU:HD23	31:53:132:LEU:HA	1.89	0.41
31:53:249:LYS:HG2	31:53:370:VAL:HA	2.03	0.41
31:53:356:VAL:HG22	31:53:375:TRP:HB2	2.02	0.41
37:c3:202:LEU:HD12	37:c3:206:SER:HB3	2.01	0.41
39:e3:75:GLN:HE22	47:m3:53:PRO:HG3	1.85	0.41
48:o3:44:GLU:OE1	48:o3:48:TRP:NE1	2.41	0.41
61:H6:76:LEU:HD13	61:H6:175:THR:HG22	2.01	0.41
69:P6:62:LEU:HD23	69:P6:62:LEU:HA	1.85	0.41
75:V6:141:ASN:HB2	75:V6:143:THR:H	1.86	0.41
75:V6:392:ARG:HH12	85:A6:1528:A:H3'	1.85	0.41
77:X6:125:LEU:HB2	77:X6:342:PRO:HD3	2.03	0.41
79:Z6:66:ARG:HH11	79:Z6:67:PHE:HE1	1.68	0.41
7:D:211:GLU:HA	7:D:212:PRO:HD3	1.82	0.41
2:A3:2042:U:H2'	2:A3:2043:C:C6	2.56	0.41
3:B3:1609:U:O2	3:B3:1616:A:N6	2.53	0.41
8:I3:98:VAL:HG22	8:I3:153:LEU:HD22	2.02	0.41
9:J3:138:SER:HA	9:J3:141:VAL:HG12	2.02	0.41
19:T3:113:GLY:O	19:T3:117:ILE:HG12	2.21	0.41
28:23:69:ARG:HA	28:23:69:ARG:HD3	1.89	0.41
28:23:70:LEU:HD23	28:23:70:LEU:HA	1.89	0.41
31:53:293:LEU:HD22	31:53:316:PHE:HD2	1.86	0.41
35:a3:72:THR:HG23	37:c3:256:ARG:HH11	1.85	0.41
59:F6:99:MET:HB3	59:F6:99:MET:HE2	1.86	0.41
59:F6:137:ILE:HD13	59:F6:137:ILE:HA	1.89	0.41
60:G6:300:TYR:OH	77:X6:382:PHE:O	2.29	0.41
67:N6:76:HIS:NE2	85:A6:770:G:OP2	2.51	0.41
74:U6:44:MET:HE3	74:U6:44:MET:HB3	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:24:8:U:H5'	86:24:47:A:H5'	2.03	0.41
88:A:107:THR:OG1	88:A:109:GLU:OE2	2.36	0.41
90:j:21:U:O2'	90:j:22:A:N7	2.54	0.41
2:A3:2171:U:H4'	2:A3:2172:A:H3'	2.03	0.41
2:A3:2245:A:H2'	51:r3:189:ARG:HD2	2.03	0.41
2:A3:2420:U:H2'	2:A3:2421:G:C8	2.55	0.41
2:A3:2553:G:H2'	2:A3:2554:A:H8	1.86	0.41
2:A3:2916:G:N3	12:M3:77:ARG:NH2	2.67	0.41
2:A3:3084:A:H2'	2:A3:3085:A:C8	2.56	0.41
2:A3:3165:C:H2'	2:A3:3166:U:C6	2.55	0.41
3:B3:1646:U:O2'	3:B3:1648:U:OP1	2.27	0.41
5:E3:252:TRP:O	5:E3:255:THR:OG1	2.36	0.41
8:I3:186:LEU:HD12	8:I3:186:LEU:HA	1.96	0.41
10:K3:142:VAL:HA	36:b3:145:PRO:HD2	2.01	0.41
10:K3:168:ARG:HB3	51:r3:59:GLU:HA	2.02	0.41
11:L3:55:PRO:HB3	11:L3:77:ILE:HD13	2.02	0.41
12:M3:247:ILE:HD11	49:p3:59:TRP:CD2	2.56	0.41
14:O3:93:LEU:HD23	14:O3:93:LEU:HA	1.89	0.41
19:T3:99:ILE:HG12	19:T3:125:GLN:HE21	1.86	0.41
24:Y3:191:ASN:HB3	24:Y3:194:TYR:HB3	2.03	0.41
24:Y3:202:LEU:HG	24:Y3:204:TYR:CE2	2.56	0.41
31:53:184:LEU:HD23	31:53:184:LEU:HA	1.93	0.41
31:53:194:LYS:HD2	31:53:195:HIS:NE2	2.36	0.41
31:53:221:GLN:HE22	31:53:223:ARG:NH1	2.18	0.41
33:73:220:GLU:HA	33:73:252:VAL:O	2.20	0.41
35:a3:67:ILE:HA	35:a3:68:PRO:HD3	1.93	0.41
36:b3:104:LEU:HD23	36:b3:104:LEU:HA	1.86	0.41
37:c3:73:GLN:HG2	37:c3:85:LEU:HD13	2.03	0.41
37:c3:271:PHE:HA	37:c3:284:GLY:O	2.20	0.41
45:k3:42:VAL:O	45:k3:46:ASN:N	2.52	0.41
52:s3:321:GLU:OE1	52:s3:325:ARG:NH2	2.42	0.41
60:G6:131:ILE:HD12	60:G6:131:ILE:HA	1.96	0.41
67:N6:78:LYS:HE2	67:N6:78:LYS:HB2	1.94	0.41
73:T6:150:PRO:O	85:A6:687:G:O2'	2.30	0.41
78:Y6:377:ARG:HA	78:Y6:377:ARG:HD3	1.83	0.41
79:Z6:40:LEU:HD12	79:Z6:41:PRO:HD2	2.03	0.41
80:a6:62:SER:OG	80:a6:63:ARG:N	2.54	0.41
2:A3:2901:A:H2'	2:A3:2902:A:C8	2.55	0.41
12:M3:140:LEU:HD23	12:M3:140:LEU:HA	1.84	0.41
17:R3:69:ILE:HD11	17:R3:99:ARG:HD3	2.03	0.41
25:Z3:38:ARG:HE	25:Z3:38:ARG:HB2	1.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:73:115:MET:HE3	33:73:115:MET:HB2	1.88	0.41
39:e3:151:ARG:NH1	39:e3:254:TRP:O	2.52	0.41
45:k3:16:VAL:HG13	45:k3:51:VAL:HG23	2.02	0.41
50:q3:142:ASN:HA	50:q3:145:LYS:HD2	2.01	0.41
57:D6:353:LEU:HD23	57:D6:353:LEU:HA	1.91	0.41
59:F6:187:MET:HE3	59:F6:187:MET:HB3	1.84	0.41
82:c6:83:ALA:HA	82:c6:86:MET:HG3	2.03	0.41
84:e6:517:LYS:HZ2	84:e6:528:ARG:HD2	1.84	0.41
85:A6:1412:A:H2'	85:A6:1413:A:H8	1.85	0.41
89:Z:81:LEU:HD12	89:Z:88:LYS:HA	2.03	0.41
89:Z:169:ARG:O	89:Z:421:ARG:NH2	2.53	0.41
2:A3:1672:C:OP1	19:T3:51:TRP:N	2.48	0.40
2:A3:1883:G:H2'	2:A3:1884:G:C8	2.57	0.40
2:A3:2024:C:H2'	2:A3:2025:C:C6	2.56	0.40
2:A3:2368:C:H2'	2:A3:2369:A:H8	1.87	0.40
2:A3:2518:A:H2'	2:A3:2530:A:H61	1.85	0.40
10:K3:150:LYS:HD2	10:K3:150:LYS:HA	1.90	0.40
14:O3:38:ARG:NH1	14:O3:82:GLU:OE1	2.53	0.40
14:O3:43:GLU:HA	14:O3:121:ALA:O	2.21	0.40
18:S3:86:MET:HE2	18:S3:86:MET:HB3	1.86	0.40
20:U3:11:ARG:NH2	21:V3:212:LYS:O	2.54	0.40
33:73:214:LEU:O	33:73:272:THR:OG1	2.38	0.40
43:i3:99:GLY:HA2	43:i3:102:MET:HE3	2.02	0.40
47:m3:37:ARG:HH21	88:A:129:ARG:HH21	1.67	0.40
51:r3:36:ARG:HB3	51:r3:53:ILE:HG12	2.03	0.40
55:B6:164:GLU:OE2	55:B6:261:LYS:NZ	2.52	0.40
58:E6:37:ARG:HG3	74:U6:167:PHE:CE1	2.56	0.40
60:G6:78:ILE:HD11	60:G6:129:GLU:HG3	2.04	0.40
60:G6:285:VAL:HG22	60:G6:328:VAL:HG22	2.03	0.40
62:I6:140:LYS:HA	62:I6:140:LYS:HD3	1.78	0.40
71:R6:291:ARG:HB2	71:R6:292:ASP:H	1.81	0.40
74:U6:49:ASP:OD1	74:U6:49:ASP:N	2.38	0.40
75:V6:202:ARG:CZ	75:V6:242:ALA:HB1	2.51	0.40
81:b6:197:ARG:NH1	81:b6:206:THR:O	2.54	0.40
2:A3:2113:G:H1	2:A3:2693:A:P	2.44	0.40
5:E3:320:PHE:HA	5:E3:321:PRO:HD3	1.97	0.40
6:F3:83:HIS:CG	6:F3:274:LEU:HD11	2.56	0.40
16:Q3:184:ASP:OD1	16:Q3:184:ASP:N	2.54	0.40
20:U3:37:GLU:HB2	20:U3:104:THR:HG23	2.02	0.40
23:X3:115:TYR:OH	23:X3:120:ASP:OD1	2.38	0.40
27:13:43:LEU:HD23	27:13:43:LEU:HA	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:33:136:LYS:HG2	29:33:140:ARG:HD3	2.03	0.40
33:73:218:THR:HG22	33:73:255:HIS:ND1	2.36	0.40
36:b3:19:LEU:HD23	36:b3:19:LEU:HA	1.93	0.40
48:o3:42:GLU:OE2	48:o3:46:HIS:NE2	2.54	0.40
52:s3:297:THR:HA	52:s3:358:GLN:O	2.21	0.40
52:s3:416:ASP:HA	52:s3:419:LEU:HB2	2.03	0.40
55:B6:75:VAL:HG11	55:B6:129:LEU:HB3	2.03	0.40
58:E6:47:LEU:HD23	58:E6:47:LEU:HA	1.91	0.40
68:O6:103:ASN:HA	68:O6:104:PRO:HD3	1.95	0.40
75:V6:188:HIS:HA	75:V6:191:ALA:HB3	2.02	0.40
84:e6:418:SER:O	84:e6:421:SER:OG	2.35	0.40
85:A6:1275:C:N4	85:A6:1324:G:O2'	2.55	0.40
88:A:65:LYS:HB3	88:A:65:LYS:HE2	1.84	0.40
2:A3:1835:A:P	36:b3:116:ARG:HH22	2.42	0.40
2:A3:1844:A:H61	2:A3:1859:A:H61	1.70	0.40
2:A3:1857:U:H2'	2:A3:1858:G:C8	2.57	0.40
2:A3:2058:C:O2	25:Z3:109:LYS:NZ	2.42	0.40
2:A3:2082:G:N2	25:Z3:88:MET:SD	2.84	0.40
2:A3:2296:U:H4'	17:R3:40:ARG:HG3	2.02	0.40
2:A3:2471:G:O2'	2:A3:2654:U:O4	2.32	0.40
11:L3:119:ILE:HD13	11:L3:123:ILE:HD11	2.04	0.40
23:X3:42:HIS:HD2	23:X3:69:ILE:HG21	1.86	0.40
29:33:164:SER:HA	29:33:167:LYS:HE2	2.03	0.40
31:53:181:VAL:HG21	31:53:294:LEU:HD11	2.02	0.40
31:53:326:ARG:NH1	31:53:362:THR:OG1	2.54	0.40
43:i3:94:LYS:O	43:i3:98:VAL:HB	2.21	0.40
58:E6:4:TYR:CZ	58:E6:75:VAL:HG11	2.56	0.40
60:G6:161:LEU:HD11	60:G6:244:PHE:HZ	1.85	0.40
60:G6:285:VAL:HG13	60:G6:328:VAL:HG22	2.04	0.40
65:L6:221:LYS:HA	65:L6:221:LYS:HD3	1.85	0.40
71:R6:190:ASP:HA	71:R6:193:ILE:HD12	2.02	0.40
72:S6:86:ASP:HA	76:W6:101:ILE:HG12	2.03	0.40
75:V6:107:TRP:HB3	75:V6:382:TRP:CD2	2.56	0.40
85:A6:801:C:H2'	85:A6:802:C:H6	1.86	0.40
89:Z:224:LEU:HD12	89:Z:224:LEU:HA	1.91	0.40
90:j:30:C:H2'	90:j:31:G:H8	1.85	0.40
2:A3:1810:A:H2'	2:A3:1811:A:C8	2.56	0.40
3:B3:1623:G:H2'	3:B3:1624:C:O4'	2.21	0.40
31:53:387:TRP:NE1	31:53:399:GLU:OE2	2.55	0.40
32:63:371:ASP:HA	32:63:372:SER:HA	1.70	0.40
33:73:176:SER:O	33:73:319:ARG:NH2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:c3:257:LEU:HD21	37:c3:260:GLN:HB3	2.04	0.40
39:e3:124:TRP:HA	39:e3:127:LYS:HG2	2.02	0.40
44:j3:97:LYS:HA	44:j3:100:GLU:HG2	2.04	0.40
50:q3:80:GLU:OE2	50:q3:83:ARG:NH2	2.54	0.40
57:D6:286:GLU:O	57:D6:288:HIS:N	2.55	0.40
61:H6:108:VAL:HG22	61:H6:143:LEU:HD12	2.03	0.40
65:L6:212:ARG:NH1	83:d6:188:GLY:O	2.50	0.40
67:N6:52:HIS:HB3	67:N6:80:GLU:HG3	2.02	0.40
71:R6:71:MET:HE2	71:R6:71:MET:HB2	1.97	0.40
73:T6:109:ASN:O	73:T6:112:THR:OG1	2.35	0.40
77:X6:326:GLN:HB3	81:b6:304:GLU:OE1	2.20	0.40
80:a6:99:ARG:NH2	85:A6:1531:A:O5'	2.54	0.40
84:e6:497:LEU:HD12	84:e6:497:LEU:HA	1.90	0.40
85:A6:849:A:H2'	85:A6:850:A:C8	2.57	0.40
85:A6:1031:A:O2'	85:A6:1058:A:O4'	2.34	0.40
88:A:139:MET:HE3	88:A:139:MET:HB2	1.86	0.40
89:Z:97:ASN:O	89:Z:102:ARG:NH1	2.55	0.40
89:Z:120:ARG:HH22	89:Z:248:PRO:HA	1.85	0.40
7:D:221:CYS:HB3	7:D:233:VAL:HG23	2.03	0.40
2:A3:1880:C:O2'	2:A3:1884:G:OP1	2.39	0.40
2:A3:2043:C:H2'	2:A3:2044:A:H8	1.85	0.40
2:A3:2544:C:O2'	2:A3:2632:A:N1	2.52	0.40
2:A3:2827:A:OP1	22:W3:49:ARG:NH1	2.55	0.40
2:A3:2859:A:N6	2:A3:2873:A:O2'	2.54	0.40
6:F3:277:ASP:OD1	6:F3:277:ASP:N	2.55	0.40
11:L3:53:ARG:HA	11:L3:53:ARG:HD2	1.95	0.40
27:13:60:LYS:HB3	27:13:60:LYS:HE2	1.88	0.40
33:73:47:LEU:HD12	33:73:229:ILE:HG13	2.03	0.40
36:b3:110:LEU:HD23	36:b3:110:LEU:HA	1.91	0.40
43:i3:86:ASN:HB3	43:i3:89:GLN:H	1.87	0.40
45:k3:25:LYS:HD2	45:k3:26:ASN:H	1.85	0.40
62:I6:83:ILE:HD13	62:I6:173:ILE:HG21	2.02	0.40
68:O6:217:ARG:HH12	75:V6:318:ASP:HB2	1.86	0.40
73:T6:157:LYS:HD3	73:T6:157:LYS:HA	1.82	0.40
74:U6:57:MET:HE3	74:U6:57:MET:HB2	1.97	0.40
77:X6:157:ASP:HA	77:X6:263:ASP:HB2	2.03	0.40
81:b6:126:LEU:HD13	81:b6:126:LEU:HA	1.90	0.40
85:A6:1235:A:H1'	85:A6:1240:C:N4	2.37	0.40
85:A6:1334:C:H4'	85:A6:1335:A:H3'	2.04	0.40
88:A:51:ARG:HD2	88:A:51:ARG:HA	1.90	0.40
88:A:179:THR:HA	88:A:180:PRO:HD3	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
90:j:26:C:H2'	90:j:27:G:O4'	2.22	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%)	20 (74%)	6 (22%)	1 (4%)	2	20
4	D3	234/305 (77%)	215 (92%)	18 (8%)	1 (0%)	30	66
5	E3	296/348 (85%)	262 (88%)	32 (11%)	2 (1%)	18	55
6	F3	248/311 (80%)	228 (92%)	20 (8%)	0	100	100
7	D	78/267 (29%)	66 (85%)	11 (14%)	1 (1%)	9	41
7	H3	93/267 (35%)	83 (89%)	9 (10%)	1 (1%)	11	45
8	I3	154/261 (59%)	147 (96%)	7 (4%)	0	100	100
9	J3	138/192 (72%)	127 (92%)	11 (8%)	0	100	100
10	K3	175/178 (98%)	151 (86%)	22 (13%)	2 (1%)	11	45
11	L3	113/145 (78%)	101 (89%)	12 (11%)	0	100	100
12	M3	285/296 (96%)	255 (90%)	27 (10%)	3 (1%)	11	45
13	N3	203/251 (81%)	186 (92%)	16 (8%)	1 (0%)	24	62
14	O3	150/175 (86%)	131 (87%)	18 (12%)	1 (1%)	18	55
15	P3	129/180 (72%)	117 (91%)	11 (8%)	1 (1%)	16	52
16	Q3	217/292 (74%)	193 (89%)	23 (11%)	1 (0%)	24	62
17	R3	138/149 (93%)	133 (96%)	5 (4%)	0	100	100
18	S3	154/205 (75%)	138 (90%)	16 (10%)	0	100	100
19	T3	164/206 (80%)	154 (94%)	10 (6%)	0	100	100
20	U3	109/153 (71%)	97 (89%)	12 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	V3	183/216 (85%)	156 (85%)	24 (13%)	3 (2%)	7	37
22	W3	109/148 (74%)	103 (94%)	6 (6%)	0	100	100
23	X3	241/256 (94%)	210 (87%)	29 (12%)	2 (1%)	16	52
24	Y3	174/250 (70%)	162 (93%)	12 (7%)	0	100	100
25	Z3	118/161 (73%)	109 (92%)	9 (8%)	0	100	100
26	03	106/188 (56%)	91 (86%)	14 (13%)	1 (1%)	14	49
27	13	50/65 (77%)	46 (92%)	3 (6%)	1 (2%)	6	31
28	23	44/92 (48%)	42 (96%)	2 (4%)	0	100	100
29	33	93/188 (50%)	88 (95%)	5 (5%)	0	100	100
30	43	34/103 (33%)	32 (94%)	2 (6%)	0	100	100
31	53	368/423 (87%)	324 (88%)	42 (11%)	2 (0%)	24	62
32	63	313/380 (82%)	273 (87%)	40 (13%)	0	100	100
33	73	258/338 (76%)	234 (91%)	24 (9%)	0	100	100
34	93	105/137 (77%)	90 (86%)	15 (14%)	0	100	100
35	a3	78/142 (55%)	72 (92%)	6 (8%)	0	100	100
36	b3	146/215 (68%)	131 (90%)	15 (10%)	0	100	100
37	c3	271/332 (82%)	249 (92%)	21 (8%)	1 (0%)	30	66
38	d3	156/306 (51%)	142 (91%)	13 (8%)	1 (1%)	21	58
39	e3	211/279 (76%)	191 (90%)	20 (10%)	0	100	100
40	f3	125/212 (59%)	103 (82%)	21 (17%)	1 (1%)	16	52
41	g3	127/166 (76%)	114 (90%)	13 (10%)	0	100	100
42	h3	96/158 (61%)	86 (90%)	8 (8%)	2 (2%)	5	30
43	i3	95/128 (74%)	85 (90%)	10 (10%)	0	100	100
44	j3	83/123 (68%)	78 (94%)	4 (5%)	1 (1%)	10	43
45	k3	82/112 (73%)	67 (82%)	15 (18%)	0	100	100
46	l3	21/138 (15%)	21 (100%)	0	0	100	100
47	m3	43/128 (34%)	37 (86%)	6 (14%)	0	100	100
48	o3	92/102 (90%)	85 (92%)	7 (8%)	0	100	100
49	p3	119/206 (58%)	109 (92%)	10 (8%)	0	100	100
50	q3	126/222 (57%)	117 (93%)	6 (5%)	3 (2%)	4	27
51	r3	140/196 (71%)	126 (90%)	14 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	s3	366/467 (78%)	334 (91%)	32 (9%)	0	100	100
55	B6	215/296 (73%)	198 (92%)	17 (8%)	0	100	100
56	C6	130/167 (78%)	119 (92%)	11 (8%)	0	100	100
57	D6	316/430 (74%)	282 (89%)	33 (10%)	1 (0%)	36	71
58	E6	120/125 (96%)	113 (94%)	6 (5%)	1 (1%)	16	52
59	F6	197/242 (81%)	184 (93%)	13 (7%)	0	100	100
60	G6	301/396 (76%)	281 (93%)	20 (7%)	0	100	100
61	H6	120/201 (60%)	105 (88%)	14 (12%)	1 (1%)	16	52
62	I6	134/194 (69%)	123 (92%)	11 (8%)	0	100	100
63	J6	106/138 (77%)	95 (90%)	11 (10%)	0	100	100
64	K6	99/128 (77%)	97 (98%)	2 (2%)	0	100	100
65	L6	162/257 (63%)	154 (95%)	8 (5%)	0	100	100
66	M6	114/137 (83%)	103 (90%)	11 (10%)	0	100	100
67	N6	105/130 (81%)	98 (93%)	7 (7%)	0	100	100
68	O6	183/258 (71%)	163 (89%)	20 (11%)	0	100	100
69	P6	94/142 (66%)	84 (89%)	10 (11%)	0	100	100
70	Q6	84/87 (97%)	77 (92%)	7 (8%)	0	100	100
71	R6	240/360 (67%)	211 (88%)	29 (12%)	0	100	100
72	S6	124/190 (65%)	115 (93%)	9 (7%)	0	100	100
73	T6	160/173 (92%)	144 (90%)	16 (10%)	0	100	100
74	U6	171/205 (83%)	164 (96%)	7 (4%)	0	100	100
75	V6	320/414 (77%)	283 (88%)	36 (11%)	1 (0%)	36	71
76	W6	95/187 (51%)	85 (90%)	10 (10%)	0	100	100
77	X6	310/398 (78%)	265 (86%)	43 (14%)	2 (1%)	21	58
78	Y6	106/395 (27%)	97 (92%)	9 (8%)	0	100	100
79	Z6	85/106 (80%)	81 (95%)	4 (5%)	0	100	100
80	a6	197/218 (90%)	182 (92%)	15 (8%)	0	100	100
81	b6	252/323 (78%)	224 (89%)	28 (11%)	0	100	100
82	c6	114/118 (97%)	97 (85%)	17 (15%)	0	100	100
83	d6	67/199 (34%)	63 (94%)	4 (6%)	0	100	100
84	e6	362/689 (52%)	328 (91%)	30 (8%)	4 (1%)	11	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
88	A	158/206 (77%)	142 (90%)	16 (10%)	0	100	100
89	Z	392/452 (87%)	352 (90%)	39 (10%)	1 (0%)	36	71
91	n	230/229 (100%)	209 (91%)	21 (9%)	0	100	100
All	All	13541/18977 (71%)	12229 (90%)	1268 (9%)	44 (0%)	37	71

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
40	f3	51	LYS
50	q3	43	GLU
84	e6	68	VAL
10	K3	160	GLN
12	M3	288	GLU
23	X3	52	ILE
31	53	349	GLY
57	D6	287	ASP
77	X6	342	PRO
13	N3	238	LYS
16	Q3	183	LEU
21	V3	194	LEU
23	X3	94	ASN
38	d3	231	LEU
42	h3	66	LEU
21	V3	52	GLU
21	V3	101	THR
31	53	270	ILE
50	q3	42	PRO
50	q3	79	PRO
61	H6	126	ILE
75	V6	197	SER
84	e6	66	ASP
1	Y2	22	ALA
7	H3	104	ASN
10	K3	4	PHE
12	M3	265	ILE
14	O3	111	PRO
42	h3	138	SER
84	e6	317	LEU
7	D	212	PRO
12	M3	109	ARG
26	03	178	ASP

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Mol	Chain	Res	Type
27	13	63	ARG
37	c3	313	PRO
44	j3	35	ALA
77	X6	120	PRO
58	E6	15	ARG
4	D3	207	ILE
84	e6	316	ILE
5	E3	79	PRO
5	E3	246	GLY
15	P3	177	ILE
89	Z	257	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%)	186 (98%)	4 (2%)	47	65
5	E3	255/290 (88%)	252 (99%)	3 (1%)	63	73
6	F3	217/262 (83%)	216 (100%)	1 (0%)	81	81
7	D	73/228 (32%)	69 (94%)	4 (6%)	19	42
7	H3	86/228 (38%)	85 (99%)	1 (1%)	63	73
8	I3	145/232 (62%)	145 (100%)	0	100	100
9	J3	113/150 (75%)	112 (99%)	1 (1%)	70	76
10	K3	155/156 (99%)	154 (99%)	1 (1%)	78	80
11	L3	98/124 (79%)	98 (100%)	0	100	100
12	M3	245/249 (98%)	242 (99%)	3 (1%)	63	73
13	N3	172/211 (82%)	171 (99%)	1 (1%)	78	80
14	O3	133/150 (89%)	132 (99%)	1 (1%)	73	77
15	P3	115/155 (74%)	114 (99%)	1 (1%)	70	76
16	Q3	201/256 (78%)	200 (100%)	1 (0%)	81	81
17	R3	118/126 (94%)	118 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	S3	141/180 (78%)	138 (98%)	3 (2%)	47	65
19	T3	146/176 (83%)	145 (99%)	1 (1%)	76	79
20	U3	99/135 (73%)	99 (100%)	0	100	100
21	V3	169/191 (88%)	165 (98%)	4 (2%)	43	63
22	W3	91/119 (76%)	91 (100%)	0	100	100
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%)	110 (99%)	1 (1%)	70	76
26	03	97/164 (59%)	97 (100%)	0	100	100
27	13	49/60 (82%)	48 (98%)	1 (2%)	48	65
28	23	40/72 (56%)	40 (100%)	0	100	100
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%)	333 (99%)	4 (1%)	63	73
32	63	266/332 (80%)	264 (99%)	2 (1%)	73	77
33	73	242/303 (80%)	237 (98%)	5 (2%)	47	65
34	93	91/112 (81%)	91 (100%)	0	100	100
35	a3	78/133 (59%)	78 (100%)	0	100	100
36	b3	130/186 (70%)	129 (99%)	1 (1%)	73	77
37	c3	241/288 (84%)	239 (99%)	2 (1%)	73	77
38	d3	151/274 (55%)	148 (98%)	3 (2%)	48	65
39	e3	188/236 (80%)	188 (100%)	0	100	100
40	f3	117/188 (62%)	116 (99%)	1 (1%)	70	76
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%)	85 (99%)	1 (1%)	63	73
44	j3	68/97 (70%)	67 (98%)	1 (2%)	57	70
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	133 (100%)	0	100	100
52	s3	326/381 (86%)	321 (98%)	5 (2%)	57	70
55	B6	191/249 (77%)	191 (100%)	0	100	100
56	C6	115/143 (80%)	111 (96%)	4 (4%)	32	53
57	D6	269/357 (75%)	267 (99%)	2 (1%)	76	79
58	E6	104/107 (97%)	103 (99%)	1 (1%)	68	76
59	F6	178/209 (85%)	178 (100%)	0	100	100
60	G6	265/342 (78%)	264 (100%)	1 (0%)	84	82
61	H6	112/180 (62%)	107 (96%)	5 (4%)	24	46
62	I6	104/147 (71%)	103 (99%)	1 (1%)	68	76
63	J6	93/118 (79%)	93 (100%)	0	100	100
64	K6	91/113 (80%)	91 (100%)	0	100	100
65	L6	152/226 (67%)	150 (99%)	2 (1%)	61	72
66	M6	95/113 (84%)	95 (100%)	0	100	100
67	N6	93/115 (81%)	90 (97%)	3 (3%)	34	55
68	O6	166/230 (72%)	164 (99%)	2 (1%)	63	73
69	P6	87/123 (71%)	87 (100%)	0	100	100
70	Q6	78/79 (99%)	78 (100%)	0	100	100
71	R6	224/318 (70%)	220 (98%)	4 (2%)	51	66
72	S6	109/164 (66%)	109 (100%)	0	100	100
73	T6	150/157 (96%)	150 (100%)	0	100	100
74	U6	149/174 (86%)	149 (100%)	0	100	100
75	V6	295/364 (81%)	292 (99%)	3 (1%)	68	76
76	W6	84/158 (53%)	83 (99%)	1 (1%)	63	73
77	X6	275/351 (78%)	273 (99%)	2 (1%)	76	79
78	Y6	99/357 (28%)	97 (98%)	2 (2%)	48	65
79	Z6	80/95 (84%)	80 (100%)	0	100	100
80	a6	176/190 (93%)	175 (99%)	1 (1%)	78	80
81	b6	237/291 (81%)	230 (97%)	7 (3%)	36	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
82	c6	99/101 (98%)	99 (100%)	0	100	100
83	d6	63/166 (38%)	62 (98%)	1 (2%)	55	69
84	e6	226/609 (37%)	221 (98%)	5 (2%)	45	64
88	A	151/190 (80%)	151 (100%)	0	100	100
89	Z	328/371 (88%)	323 (98%)	5 (2%)	57	70
91	n	184/181 (102%)	181 (98%)	3 (2%)	55	69
All	All	11992/16337 (73%)	11877 (99%)	115 (1%)	65	76

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D3	93	VAL
4	D3	192	LEU
4	D3	220	VAL
4	D3	239	THR
5	E3	47	THR
5	E3	151	THR
5	E3	236	THR
6	F3	81	ASP
7	H3	62	VAL
9	J3	156	VAL
10	K3	61	ASN
12	M3	22	VAL
12	M3	84	ASN
12	M3	149	THR
13	N3	176	LEU
14	O3	14	VAL
15	P3	48	THR
16	Q3	81	ILE
18	S3	65	VAL
18	S3	68	ASP
18	S3	153	LEU
19	T3	209	VAL
21	V3	76	VAL
21	V3	87	VAL
21	V3	93	THR
21	V3	188	VAL
23	X3	131	THR
25	Z3	106	VAL
27	13	62	ILE

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Mol	Chain	Res	Type
31	53	214	ASN
31	53	239	ILE
31	53	365	ASP
31	53	391	VAL
32	63	44	ASN
32	63	379	ILE
33	73	70	VAL
33	73	77	THR
33	73	167	VAL
33	73	229	ILE
33	73	238	ASP
36	b3	15	LEU
37	c3	119	LEU
37	c3	250	VAL
38	d3	208	VAL
38	d3	218	THR
38	d3	263	THR
40	f3	192	GLU
43	i3	80	LEU
44	j3	93	LEU
45	k3	64	VAL
45	k3	65	ASP
52	s3	171	VAL
52	s3	206	VAL
52	s3	234	ASP
52	s3	239	ASN
52	s3	251	VAL
56	C6	44	VAL
56	C6	52	THR
56	C6	69	LEU
56	C6	153	LEU
57	D6	187	VAL
57	D6	331	ASP
58	E6	87	ASP
60	G6	320	VAL
61	H6	62	VAL
61	H6	87	VAL
61	H6	110	GLU
61	H6	126	ILE
61	H6	175	THR
62	I6	179	THR
65	L6	146	HIS

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Mol	Chain	Res	Type
65	L6	156	LEU
67	N6	64	VAL
67	N6	85	VAL
67	N6	104	THR
68	O6	94	CYS
68	O6	115	VAL
71	R6	131	VAL
71	R6	136	VAL
71	R6	174	VAL
71	R6	281	ILE
75	V6	194	THR
75	V6	250	ILE
75	V6	337	LEU
76	W6	157	THR
77	X6	262	VAL
77	X6	290	VAL
78	Y6	324	ASP
78	Y6	338	LEU
80	a6	193	VAL
81	b6	65	ASP
81	b6	91	VAL
81	b6	157	VAL
81	b6	172	VAL
81	b6	173	LEU
81	b6	204	VAL
81	b6	322	VAL
83	d6	131	LEU
84	e6	58	VAL
84	e6	108	LEU
84	e6	369	LEU
84	e6	376	ILE
84	e6	546	VAL
89	Z	149	LEU
89	Z	167	LEU
89	Z	253	ASP
89	Z	313	LEU
89	Z	409	ILE
7	D	164	VAL
7	D	174	VAL
7	D	213	ILE
7	D	225	VAL
91	n	41	VAL

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Mol	Chain	Res	Type
91	n	63[A]	SER
91	n	63[B]	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (209) such sidechains are listed below:

Mol	Chain	Res	Type
4	D3	87	HIS
4	D3	165	ASN
4	D3	233	GLN
4	D3	263	ASN
5	E3	57	ASN
5	E3	184	ASN
5	E3	233	GLN
5	E3	286	ASN
6	F3	223	HIS
6	F3	241	ASN
6	F3	249	ASN
6	F3	251	HIS
6	F3	276	GLN
9	J3	103	GLN
10	K3	48	HIS
10	K3	56	HIS
11	L3	33	GLN
11	L3	72	GLN
12	M3	26	ASN
12	M3	84	ASN
12	M3	114	GLN
12	M3	120	GLN
12	M3	153	ASN
12	M3	157	GLN
12	M3	170	ASN
12	M3	264	GLN
13	N3	237	HIS
14	O3	91	GLN
15	P3	78	HIS
15	P3	86	GLN
16	Q3	212	ASN
16	Q3	237	ASN
16	Q3	258	GLN
16	Q3	262	GLN
17	R3	30	HIS
17	R3	70	ASN

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Mol	Chain	Res	Type
17	R3	79	HIS
17	R3	89	ASN
17	R3	125	HIS
18	S3	91	GLN
19	T3	62	GLN
19	T3	105	GLN
19	T3	109	ASN
19	T3	125	GLN
20	U3	41	GLN
20	U3	73	GLN
22	W3	62	HIS
24	Y3	117	GLN
24	Y3	147	GLN
24	Y3	157	GLN
24	Y3	179	HIS
25	Z3	95	HIS
27	13	31	ASN
28	23	92	HIS
30	43	95	HIS
30	43	100	GLN
31	53	65	HIS
31	53	96	HIS
31	53	102	GLN
31	53	119	GLN
31	53	221	GLN
31	53	353	HIS
31	53	358	GLN
32	63	149	GLN
32	63	163	HIS
32	63	292	GLN
32	63	359	HIS
33	73	165	ASN
33	73	198	ASN
33	73	232	HIS
36	b3	16	HIS
36	b3	102	GLN
37	c3	80	GLN
37	c3	123	GLN
37	c3	134	GLN
37	c3	168	HIS
37	c3	193	GLN
38	d3	119	GLN

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Mol	Chain	Res	Type
38	d3	153	ASN
38	d3	211	GLN
39	e3	75	GLN
39	e3	156	ASN
39	e3	212	HIS
39	e3	252	HIS
40	f3	54	HIS
40	f3	153	HIS
40	f3	175	GLN
41	g3	155	GLN
42	h3	67	GLN
42	h3	99	ASN
42	h3	119	GLN
43	i3	48	ASN
43	i3	65	ASN
43	i3	89	GLN
43	i3	122	ASN
44	j3	96	GLN
45	k3	72	HIS
48	o3	21	HIS
48	o3	91	GLN
50	q3	107	GLN
50	q3	120	HIS
50	q3	130	GLN
50	q3	147	GLN
51	r3	65	ASN
51	r3	91	GLN
51	r3	112	HIS
51	r3	148	ASN
52	s3	152	GLN
52	s3	154	HIS
52	s3	296	HIS
52	s3	327	ASN
52	s3	385	GLN
52	s3	427	ASN
55	B6	99	HIS
55	B6	178	ASN
55	B6	197	HIS
55	B6	201	ASN
56	C6	75	ASN
56	C6	81	HIS
56	C6	130	HIS

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Mol	Chain	Res	Type
57	D6	347	GLN
57	D6	356	GLN
57	D6	415	GLN
58	E6	58	HIS
58	E6	96	HIS
59	F6	127	HIS
59	F6	169	GLN
59	F6	233	ASN
60	G6	77	GLN
60	G6	90	ASN
60	G6	156	GLN
60	G6	171	ASN
60	G6	176	GLN
60	G6	220	GLN
60	G6	312	GLN
61	H6	83	HIS
61	H6	125	HIS
61	H6	147	HIS
62	I6	163	HIS
63	J6	35	GLN
63	J6	134	HIS
67	N6	79	HIS
68	O6	204	ASN
69	P6	71	HIS
69	P6	95	HIS
69	P6	104	GLN
69	P6	115	GLN
70	Q6	18	ASN
70	Q6	79	ASN
71	R6	96	GLN
72	S6	61	GLN
72	S6	97	GLN
73	T6	18	GLN
73	T6	54	GLN
73	T6	56	GLN
73	T6	122	GLN
73	T6	128	ASN
74	U6	117	HIS
74	U6	135	GLN
74	U6	161	GLN
74	U6	186	ASN
75	V6	122	GLN

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Mol	Chain	Res	Type
75	V6	156	ASN
75	V6	170	GLN
75	V6	203	ASN
75	V6	215	GLN
75	V6	217	ASN
75	V6	261	GLN
75	V6	342	GLN
75	V6	378	ASN
75	V6	380	GLN
75	V6	388	GLN
75	V6	394	GLN
75	V6	396	GLN
76	W6	91	GLN
76	W6	135	GLN
77	X6	67	HIS
77	X6	69	ASN
77	X6	81	HIS
77	X6	90	GLN
77	X6	140	HIS
77	X6	299	ASN
77	X6	363	ASN
77	X6	367	GLN
78	Y6	290	ASN
78	Y6	331	HIS
80	a6	66	GLN
81	b6	64	GLN
81	b6	110	ASN
81	b6	113	HIS
81	b6	235	ASN
81	b6	261	ASN
81	b6	301	ASN
82	c6	15	ASN
82	c6	109	GLN
83	d6	141	HIS
83	d6	158	GLN
84	e6	79	ASN
84	e6	115	ASN
84	e6	122	ASN
84	e6	129	GLN
84	e6	434	GLN
88	A	80	GLN
89	Z	65	HIS

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Mol	Chain	Res	Type
89	Z	420	GLN
7	D	196	ASN
91	n	139	ASN
91	n	148	ASN
91	n	172	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	A3	1490/1559 (95%)	437 (29%)	31 (2%)
3	B3	52/69 (75%)	16 (30%)	1 (1%)
53	u3	1/2 (50%)	1 (100%)	0
85	A6	921/954 (96%)	233 (25%)	14 (1%)
86	24	73/73 (100%)	42 (57%)	5 (6%)
86	C	73/73 (100%)	43 (58%)	5 (6%)
87	i4	9/10 (90%)	2 (22%)	0
90	j	74/76 (97%)	23 (31%)	0
All	All	2693/2816 (95%)	797 (29%)	56 (2%)

All (797) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	A3	1674	A
2	A3	1676	A
2	A3	1677	C
2	A3	1678	C
2	A3	1679	U
2	A3	1680	A
2	A3	1681	G
2	A3	1685	C
2	A3	1689	C
2	A3	1692	A
2	A3	1693	C
2	A3	1694	U
2	A3	1696	C
2	A3	1700	U
2	A3	1702	A
2	A3	1704	U
2	A3	1705	A
2	A3	1708	A
2	A3	1709	G

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Mol	Chain	Res	Type
2	A3	1712	A
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	1741	A
2	A3	1743	U
2	A3	1748	G
2	A3	1750	G
2	A3	1751	A
2	A3	1770	G
2	A3	1774	U
2	A3	1777	A
2	A3	1781	A
2	A3	1782	G
2	A3	1788	C
2	A3	1794	A
2	A3	1797	G
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	1812	C
2	A3	1813	C
2	A3	1823	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	1850	U
2	A3	1852	C
2	A3	1853	A

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Mol	Chain	Res	Type
2	A3	1854	U
2	A3	1856	A
2	A3	1867	A
2	A3	1869	A
2	A3	1870	A
2	A3	1871	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	1887	A
2	A3	1888	G
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	1927	G
2	A3	1935	A
2	A3	1939	G
2	A3	1940	A
2	A3	1944	C
2	A3	1958	G
2	A3	1966	G
2	A3	1975	U
2	A3	1985	G
2	A3	1986	A
2	A3	1987	G
2	A3	1992	C
2	A3	1993	A
2	A3	1994	A
2	A3	1995	A
2	A3	2000	C
2	A3	2001	C
2	A3	2015	G
2	A3	2021	U
2	A3	2022	G
2	A3	2029	A
2	A3	2032	G

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Mol	Chain	Res	Type
2	A3	2036	C
2	A3	2037	U
2	A3	2039	A
2	A3	2059	C
2	A3	2060	A
2	A3	2065	A
2	A3	2066	C
2	A3	2074	A
2	A3	2079	C
2	A3	2083	U
2	A3	2085	A
2	A3	2093	U
2	A3	2097	A
2	A3	2098	G
2	A3	2105	G
2	A3	2111	C
2	A3	2113	G
2	A3	2117	U
2	A3	2124	A
2	A3	2132	A
2	A3	2135	A
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	2167	A
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	2180	A
2	A3	2182	G
2	A3	2183	C
2	A3	2187	C
2	A3	2189	C

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Mol	Chain	Res	Type
2	A3	2190	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
2	A3	2204	U
2	A3	2207	A
2	A3	2210	C
2	A3	2211	U
2	A3	2216	A
2	A3	2230	A
2	A3	2233	U
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	2297	A
2	A3	2299	U
2	A3	2300	G
2	A3	2309	A
2	A3	2315	A
2	A3	2322	C
2	A3	2324	U
2	A3	2332	C
2	A3	2342	U
2	A3	2345	G
2	A3	2364	C
2	A3	2369	A
2	A3	2370	A
2	A3	2371	U
2	A3	2372	U

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Mol	Chain	Res	Type
2	A3	2373	A
2	A3	2374	A
2	A3	2375	C
2	A3	2379	C
2	A3	2380	C
2	A3	2381	A
2	A3	2383	U
2	A3	2387	U
2	A3	2390	A
2	A3	2393	C
2	A3	2396	C
2	A3	2397	C
2	A3	2398	A
2	A3	2399	A
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	2432	A
2	A3	2434	A
2	A3	2435	G
2	A3	2443	C
2	A3	2444	A
2	A3	2447	A
2	A3	2451	A
2	A3	2464	G
2	A3	2476	C
2	A3	2478	G
2	A3	2493	C
2	A3	2498	U
2	A3	2500	A
2	A3	2504	A
2	A3	2508	C
2	A3	2511	C
2	A3	2520	C

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Mol	Chain	Res	Type
2	A3	2521	A
2	A3	2522	U
2	A3	2523	C
2	A3	2524	A
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	2557	C
2	A3	2558	A
2	A3	2559	U
2	A3	2560	G
2	A3	2563	U
2	A3	2570	C
2	A3	2587	G
2	A3	2590	A
2	A3	2592	G
2	A3	2593	G
2	A3	2594	U
2	A3	2596	G
2	A3	2601	A
2	A3	2603	C
2	A3	2608	G
2	A3	2618	U
2	A3	2625	C
2	A3	2626	U
2	A3	2627	G
2	A3	2628	U
2	A3	2629	A
2	A3	2630	U
2	A3	2632	A
2	A3	2633	A
2	A3	2634	U
2	A3	2635	G
2	A3	2638	U
2	A3	2641	A
2	A3	2645	G
2	A3	2652	G
2	A3	2654	U

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Mol	Chain	Res	Type
2	A3	2655	G
2	A3	2656	U
2	A3	2660	U
2	A3	2683	C
2	A3	2686	G
2	A3	2694	A
2	A3	2695	G
2	A3	2696	A
2	A3	2706	A
2	A3	2708	C
2	A3	2709	A
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	2727	C
2	A3	2732	G
2	A3	2733	G
2	A3	2739	U
2	A3	2740	A
2	A3	2745	A
2	A3	2750	U
2	A3	2755	A
2	A3	2757	A
2	A3	2758	G
2	A3	2762	C
2	A3	2763	U
2	A3	2764	A
2	A3	2765	A
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	2779	C
2	A3	2780	C

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Mol	Chain	Res	Type
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	2793	C
2	A3	2804	A
2	A3	2810	G
2	A3	2814	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	2852	C
2	A3	2853	A
2	A3	2854	U
2	A3	2861	A
2	A3	2864	U
2	A3	2865	C
2	A3	2870	G
2	A3	2871	U
2	A3	2880	A
2	A3	2892	A
2	A3	2893	A
2	A3	2900	C
2	A3	2901	A
2	A3	2906	C
2	A3	2909	G
2	A3	2910	A
2	A3	2913	A
2	A3	2915	C
2	A3	2916	G
2	A3	2917	G
2	A3	2922	A
2	A3	2926	A
2	A3	2927	C
2	A3	2928	C

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Mol	Chain	Res	Type
2	A3	2932	G
2	A3	2935	A
2	A3	2936	U
2	A3	2938	A
2	A3	2939	C
2	A3	2955	U
2	A3	2956	A
2	A3	2962	C
2	A3	2963	A
2	A3	2965	A
2	A3	2989	G
2	A3	2990	A
2	A3	2991	U
2	A3	2992	G
2	A3	2994	U
2	A3	3005	A
2	A3	3007	C
2	A3	3012	U
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	3043	C
2	A3	3049	U
2	A3	3053	A
2	A3	3054	G
2	A3	3056	C
2	A3	3060	C
2	A3	3061	G
2	A3	3063	G
2	A3	3069	A
2	A3	3070	G
2	A3	3072	U
2	A3	3077	C
2	A3	3078	C
2	A3	3086	U
2	A3	3088	C
2	A3	3089	A
2	A3	3090	G
2	A3	3093	C

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Mol	Chain	Res	Type
2	A3	3096	U
2	A3	3098	U
2	A3	3099	C
2	A3	3100	U
2	A3	3108	U
2	A3	3109	U
2	A3	3114	U
2	A3	3122	U
2	A3	3123	G
2	A3	3124	U
2	A3	3128	A
2	A3	3129	A
2	A3	3134	C
2	A3	3135	A
2	A3	3141	A
2	A3	3150	U
2	A3	3151	A
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	3173	G
2	A3	3176	A
2	A3	3180	A
2	A3	3184	C
2	A3	3189	C
2	A3	3190	A
2	A3	3196	G
2	A3	3202	U
2	A3	3204	C
2	A3	3207	A
2	A3	3217	A
2	A3	3218	A
2	A3	3220	A
2	A3	3223	A
2	A3	3228	U
3	B3	1607	U
3	B3	1608	G

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Mol	Chain	Res	Type
3	B3	1609	U
3	B3	1611	G
3	B3	1614	U
3	B3	1615	A
3	B3	1625	A
3	B3	1631	C
3	B3	1632	U
3	B3	1634	A
3	B3	1641	G
3	B3	1644	G
3	B3	1645	A
3	B3	1648	U
3	B3	1649	C
3	B3	1665	C
53	u3	2	A
85	A6	654	U
85	A6	655	A
85	A6	660	U
85	A6	678	U
85	A6	684	U
85	A6	686	A
85	A6	687	G
85	A6	692	A
85	A6	693	U
85	A6	694	U
85	A6	695	A
85	A6	698	C
85	A6	708	U
85	A6	715	U
85	A6	716	C
85	A6	717	C
85	A6	722	A
85	A6	725	U
85	A6	726	C
85	A6	749	A
85	A6	755	A
85	A6	757	A
85	A6	761	A
85	A6	765	A
85	A6	768	A
85	A6	769	C
85	A6	770	G

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Mol	Chain	Res	Type
85	A6	777	U
85	A6	781	G
85	A6	785	A
85	A6	787	A
85	A6	795	G
85	A6	797	C
85	A6	798	U
85	A6	799	A
85	A6	800	G
85	A6	811	A
85	A6	812	C
85	A6	813	G
85	A6	818	A
85	A6	819	C
85	A6	831	A
85	A6	833	C
85	A6	834	U
85	A6	836	U
85	A6	839	C
85	A6	840	A
85	A6	850	A
85	A6	851	G
85	A6	872	C
85	A6	873	C
85	A6	874	C
85	A6	884	C
85	A6	886	A
85	A6	887	U
85	A6	888	U
85	A6	890	C
85	A6	894	C
85	A6	895	C
85	A6	897	G
85	A6	901	C
85	A6	903	G
85	A6	906	G
85	A6	907	U
85	A6	908	C
85	A6	916	U
85	A6	923	A
85	A6	926	C
85	A6	931	G

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Mol	Chain	Res	Type
85	A6	932	A
85	A6	937	G
85	A6	942	A
85	A6	943	A
85	A6	945	G
85	A6	946	A
85	A6	947	G
85	A6	951	U
85	A6	952	U
85	A6	954	A
85	A6	957	U
85	A6	959	A
85	A6	970	A
85	A6	971	A
85	A6	981	A
85	A6	982	A
85	A6	992	G
85	A6	996	U
85	A6	997	A
85	A6	1005	C
85	A6	1006	C
85	A6	1014	A
85	A6	1015	C
85	A6	1018	A
85	A6	1019	A
85	A6	1025	U
85	A6	1026	A
85	A6	1032	G
85	A6	1034	G
85	A6	1046	U
85	A6	1050	A
85	A6	1051	A
85	A6	1052	C
85	A6	1056	C
85	A6	1069	C
85	A6	1082	A
85	A6	1084	A
85	A6	1085	U
85	A6	1086	A
85	A6	1101	G
85	A6	1102	C
85	A6	1107	A

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Mol	Chain	Res	Type
85	A6	1109	C
85	A6	1110	C
85	A6	1113	A
85	A6	1125	A
85	A6	1127	C
85	A6	1129	A
85	A6	1130	A
85	A6	1133	U
85	A6	1142	G
85	A6	1147	C
85	A6	1148	U
85	A6	1155	C
85	A6	1157	C
85	A6	1158	A
85	A6	1159	G
85	A6	1171	A
85	A6	1176	C
85	A6	1183	G
85	A6	1184	U
85	A6	1189	C
85	A6	1191	U
85	A6	1192	A
85	A6	1193	U
85	A6	1194	C
85	A6	1196	C
85	A6	1197	U
85	A6	1201	G
85	A6	1210	G
85	A6	1218	A
85	A6	1219	U
85	A6	1224	A
85	A6	1226	A
85	A6	1227	C
85	A6	1229	C
85	A6	1233	U
85	A6	1234	C
85	A6	1235	A
85	A6	1249	U
85	A6	1250	U
85	A6	1251	G
85	A6	1252	C
85	A6	1255	A

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Mol	Chain	Res	Type
85	A6	1258	C
85	A6	1265	C
85	A6	1269	C
85	A6	1273	U
85	A6	1274	U
85	A6	1275	C
85	A6	1276	A
85	A6	1287	A
85	A6	1288	U
85	A6	1294	C
85	A6	1296	A
85	A6	1297	C
85	A6	1299	A
85	A6	1300	A
85	A6	1304	A
85	A6	1330	A
85	A6	1331	G
85	A6	1334	C
85	A6	1335	A
85	A6	1336	A
85	A6	1346	C
85	A6	1347	A
85	A6	1348	U
85	A6	1357	A
85	A6	1359	G
85	A6	1360	A
85	A6	1369	A
85	A6	1371	A
85	A6	1372	U
85	A6	1373	U
85	A6	1380	C
85	A6	1381	C
85	A6	1382	C
85	A6	1394	A
85	A6	1401	U
85	A6	1406	A
85	A6	1420	A
85	A6	1424	U
85	A6	1426	G
85	A6	1428	U
85	A6	1434	A
85	A6	1441	U

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Mol	Chain	Res	Type
85	A6	1447	U
85	A6	1451	G
85	A6	1452	U
85	A6	1458	G
85	A6	1466	G
85	A6	1469	C
85	A6	1470	C
85	A6	1478	G
85	A6	1485	C
85	A6	1486	A
85	A6	1492	C
85	A6	1516	A
85	A6	1521	A
85	A6	1522	C
85	A6	1528	A
85	A6	1529	C
85	A6	1531	A
85	A6	1536	C
85	A6	1537	C
85	A6	1539	U
85	A6	1540	A
85	A6	1541	C
85	A6	1542	G
85	A6	1543	C
85	A6	1544	A
85	A6	1551	U
85	A6	1559	A
85	A6	1561	A
85	A6	1563	G
85	A6	1572	U
85	A6	1575	U
85	A6	1586	G
85	A6	1588	A
85	A6	1598	G
85	A6	1599	G
85	A6	1602	G
85	A6	1603	A
85	A6	1604	A
86	24	2	U
86	24	3	U
86	24	7	G
86	24	8	U

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Mol	Chain	Res	Type
86	24	9	A
86	24	11	C
86	24	12	U
86	24	13	U
86	24	14	A
86	24	16	A
86	24	17	U
86	24	18	U
86	24	19	A
86	24	20	U
86	24	21	C
86	24	22	A
86	24	28	A
86	24	29	G
86	24	30	G
86	24	31	C
86	24	33	C
86	24	34	U
86	24	35	G
86	24	40	U
86	24	41	G
86	24	44	U
86	24	45	A
86	24	46	G
86	24	50	A
86	24	51	G
86	24	52	C
86	24	55	C
86	24	56	A
86	24	58	A
86	24	59	G
86	24	62	C
86	24	63	C
86	24	67	A
86	24	70	A
86	24	71	C
86	24	72	C
86	24	73	A
87	i4	18	A
87	i4	24	U
90	j	8	U
90	j	9	A

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Mol	Chain	Res	Type
90	j	10	G
90	j	13	U
90	j	19	G
90	j	20	U
90	j	21	U
90	j	22	A
90	j	31	G
90	j	32	C
90	j	34	U
90	j	35	A
90	j	36	A
90	j	37	C
90	j	43	A
90	j	45	A
90	j	47	G
90	j	48	U
90	j	49	C
90	j	60	A
90	j	61	A
90	j	76	C
90	j	77	A
86	C	2	U
86	C	3	U
86	C	7	G
86	C	8	U
86	C	9	A
86	C	11	C
86	C	12	U
86	C	13	U
86	C	14	A
86	C	16	A
86	C	17	U
86	C	18	U
86	C	19	A
86	C	20	U
86	C	21	C
86	C	22	A
86	C	28	A
86	C	29	G
86	C	30	G
86	C	31	C
86	C	33	C

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Mol	Chain	Res	Type
86	C	34	U
86	C	35	G
86	C	40	U
86	C	41	G
86	C	44	U
86	C	45	A
86	C	46	G
86	C	49	G
86	C	50	A
86	C	51	G
86	C	52	C
86	C	55	C
86	C	56	A
86	C	58	A
86	C	59	G
86	C	62	C
86	C	63	C
86	C	67	A
86	C	70	A
86	C	71	C
86	C	72	C
86	C	73	A

All (56) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	A3	1703	C
2	A3	1713	A
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

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Mol	Chain	Res	Type
2	A3	2530	A
2	A3	2531	U
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
2	A3	2900	C
2	A3	2905	A
2	A3	2989	G
2	A3	3041	U
2	A3	3092	U
2	A3	3201	A
3	B3	1607	U
85	A6	721	G
85	A6	797	C
85	A6	886	A
85	A6	1025	U
85	A6	1045	A
85	A6	1170	A
85	A6	1193	U
85	A6	1250	U
85	A6	1335	A
85	A6	1419	G
85	A6	1433	C
85	A6	1538	C
85	A6	1541	C
85	A6	1560	C
86	24	1	G
86	24	30	G
86	24	49	G
86	24	70	A
86	24	71	C
86	C	1	G
86	C	30	G
86	C	49	G
86	C	70	A
86	C	71	C

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 148 ligands modelled in this entry, 141 are monoatomic - leaving 7 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	$\# Z > 2$
99	MLI	n	302	-	6,6,6	1.39	0	7,7,7	1.32	0
99	MLI	n	303	-	6,6,6	1.36	0	7,7,7	1.36	0
93	SPD	A3	3396	-	9,9,9	0.34	0	8,8,8	0.58	0
99	MLI	n	304	-	6,6,6	1.50	0	7,7,7	1.47	1 (14%)
95	GDP	X6	500	-	29,30,30	1.17	3 (10%)	45,47,47	1.98	10 (22%)
96	GCP	Z	501	-	32,34,34	3.79	13 (40%)	49,54,54	1.71	11 (22%)
98	SO4	n	301	-	4,4,4	0.25	0	6,6,6	0.11	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
99	MLI	n	302	-	-	2/4/4/4	-
99	MLI	n	303	-	-	4/4/4/4	-
93	SPD	A3	3396	-	-	4/7/7/7	-
99	MLI	n	304	-	-	2/4/4/4	-
95	GDP	X6	500	-	-	6/16/32/32	0/3/3/3
96	GCP	Z	501	-	-	3/19/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
96	Z	501	GCP	PA-O3A	11.82	1.72	1.59
96	Z	501	GCP	O4'-C4'	8.87	1.64	1.45
96	Z	501	GCP	O6-C6	7.95	1.38	1.23
96	Z	501	GCP	C3'-C4'	-7.81	1.33	1.53
96	Z	501	GCP	O4'-C1'	-4.56	1.31	1.42
96	Z	501	GCP	O2'-C2'	-4.42	1.32	1.43
96	Z	501	GCP	C2-N2	4.13	1.43	1.34
95	X6	500	GDP	C6-N1	-3.18	1.32	1.38
96	Z	501	GCP	C6-N1	-3.00	1.33	1.38
96	Z	501	GCP	C2-N1	-2.91	1.30	1.37
96	Z	501	GCP	PB-O2B	-2.83	1.49	1.56
96	Z	501	GCP	PB-O3A	2.82	1.61	1.58
95	X6	500	GDP	C5-C4	2.67	1.46	1.38
95	X6	500	GDP	C5-N7	-2.45	1.34	1.39
96	Z	501	GCP	PG-O3G	-2.43	1.49	1.55
96	Z	501	GCP	O3'-C3'	2.00	1.47	1.43

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
95	X6	500	GDP	C5-C4-N3	-6.66	117.79	128.39
96	Z	501	GCP	C5-C4-N3	-5.36	119.87	128.39
95	X6	500	GDP	N9-C4-N3	5.35	136.66	125.95
95	X6	500	GDP	C2-N3-C4	5.08	121.05	112.30
96	Z	501	GCP	C2-N3-C4	4.95	120.83	112.30
95	X6	500	GDP	C2'-C1'-N9	-3.82	102.62	113.25
96	Z	501	GCP	N9-C4-N3	3.59	133.13	125.95
96	Z	501	GCP	C6-C5-N7	3.26	136.22	130.29
95	X6	500	GDP	C3'-C2'-C1'	2.87	106.90	101.46
95	X6	500	GDP	O6-C6-C5	-2.83	119.05	126.53
96	Z	501	GCP	C5-C6-N1	2.63	119.94	113.25
95	X6	500	GDP	C6-C5-N7	2.61	135.04	130.29
96	Z	501	GCP	C4-C5-N7	-2.41	106.85	110.67
95	X6	500	GDP	C5-C6-N1	2.34	119.22	113.25
95	X6	500	GDP	C2-N1-C6	-2.32	120.90	125.11
96	Z	501	GCP	C3'-C2'-C1'	2.29	105.80	101.46
99	n	304	MLI	O9-C3-C1	2.28	121.58	114.51
96	Z	501	GCP	O6-C6-C5	-2.13	120.91	126.53
96	Z	501	GCP	C8-N7-C5	2.11	108.02	104.26
96	Z	501	GCP	C2-N1-C6	-2.10	121.30	125.11
95	X6	500	GDP	C4-C5-N7	-2.04	107.44	110.67
96	Z	501	GCP	O2A-PA-O3A	2.01	112.70	107.27

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
95	X6	500	GDP	C5'-O5'-PA-O3A
95	X6	500	GDP	C5'-O5'-PA-O1A
96	Z	501	GCP	PB-C3B-PG-O1G
96	Z	501	GCP	PB-C3B-PG-O2G
96	Z	501	GCP	PB-C3B-PG-O3G
93	A3	3396	SPD	C3-C4-C5-N6
93	A3	3396	SPD	C2-C3-C4-C5
95	X6	500	GDP	C3'-C4'-C5'-O5'
95	X6	500	GDP	O4'-C1'-N9-C4
95	X6	500	GDP	O4'-C1'-N9-C8
93	A3	3396	SPD	C4-C5-N6-C7
93	A3	3396	SPD	N6-C7-C8-C9
95	X6	500	GDP	O4'-C4'-C5'-O5'
99	n	304	MLI	C2-C1-C3-O8
99	n	303	MLI	C2-C1-C3-O8
99	n	303	MLI	C2-C1-C3-O9
99	n	304	MLI	C2-C1-C3-O9
99	n	303	MLI	C3-C1-C2-O6
99	n	303	MLI	C3-C1-C2-O7
99	n	302	MLI	C3-C1-C2-O7
99	n	302	MLI	C3-C1-C2-O6

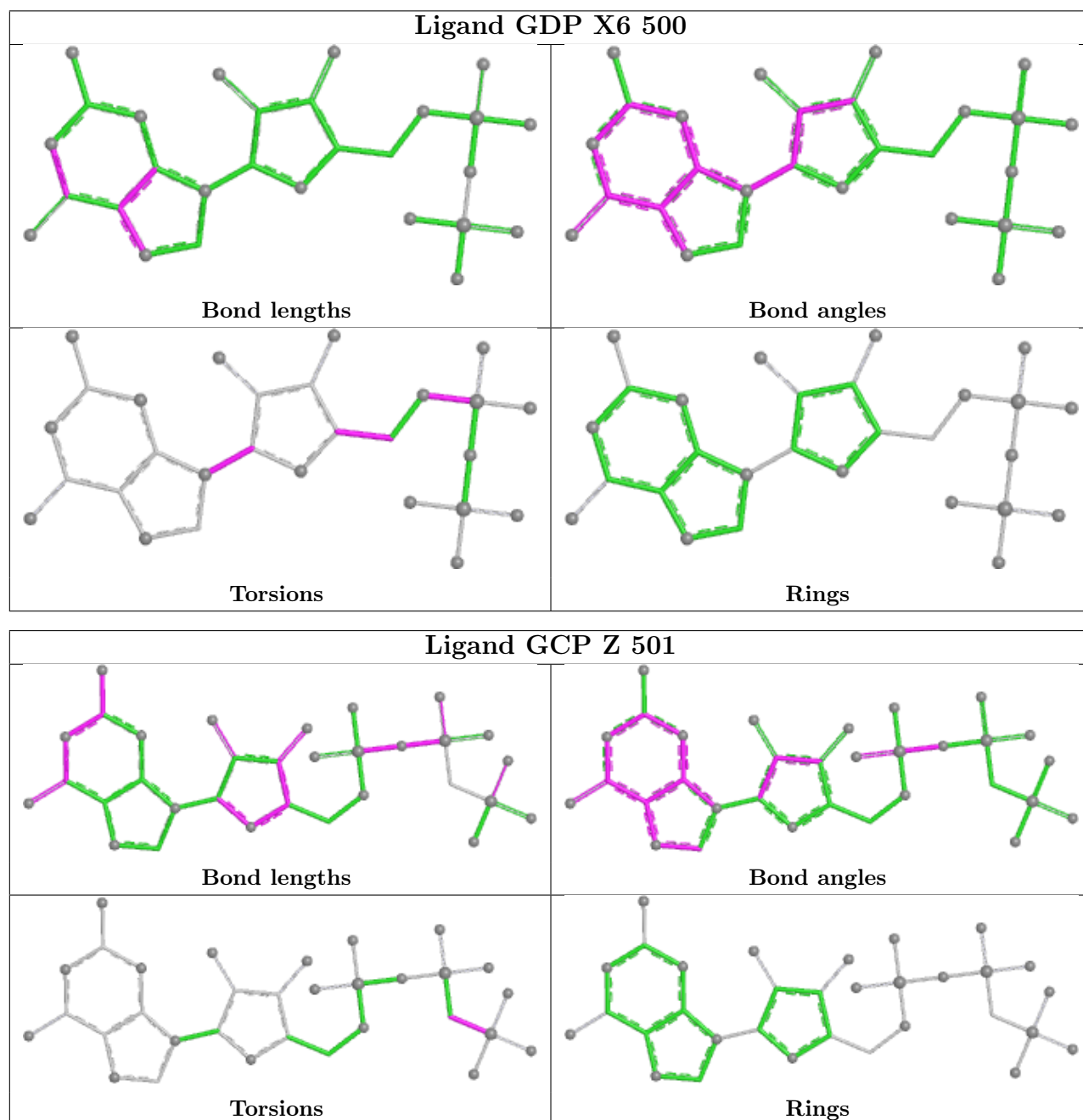
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
93	A3	3396	SPD	1	0
95	X6	500	GDP	1	0
96	Z	501	GCP	3	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
90	j	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	j	16:C	O3'	18:G	P	5.97

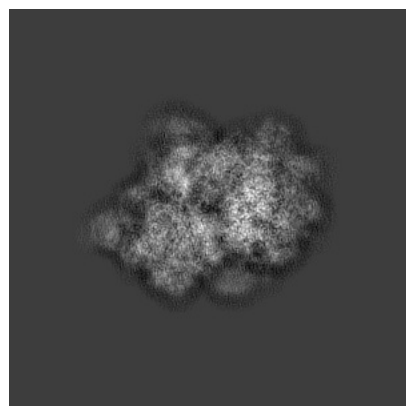
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11642. These allow visual inspection of the internal detail of the map and identification of artifacts.

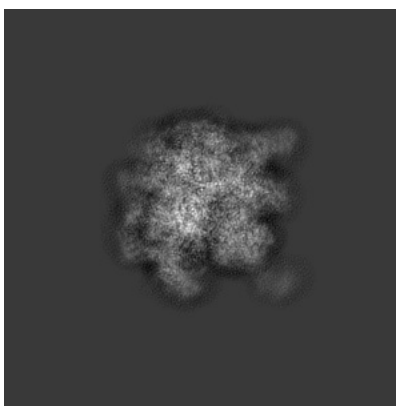
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

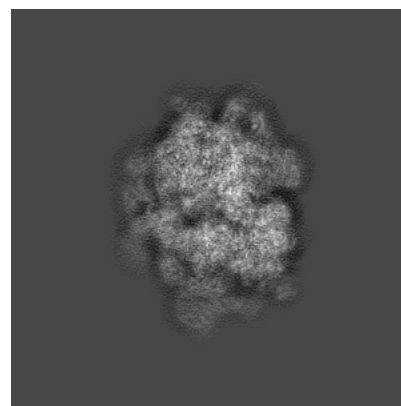
6.1.1 Primary map



X

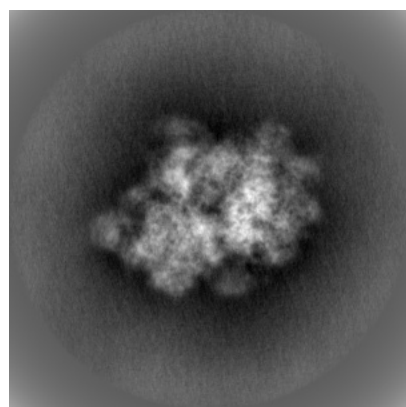


Y

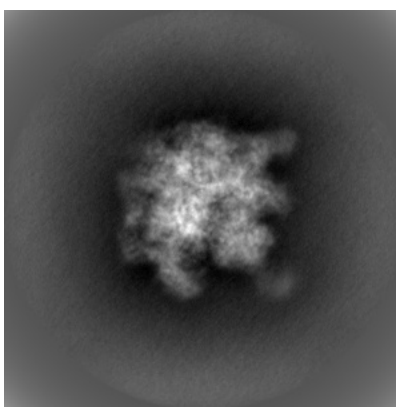


Z

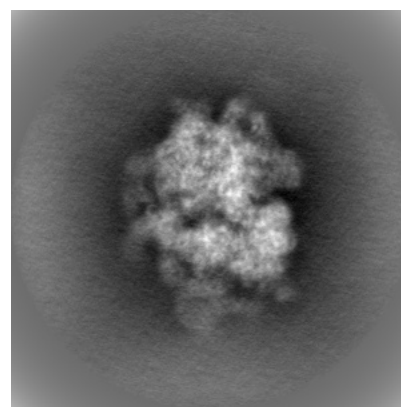
6.1.2 Raw map



X



Y

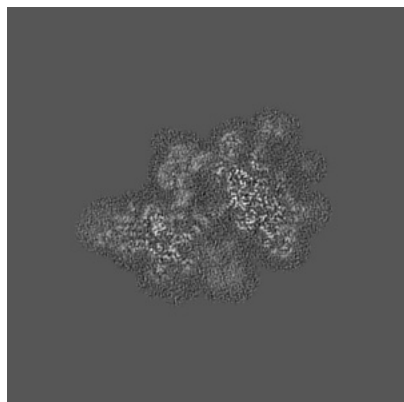


Z

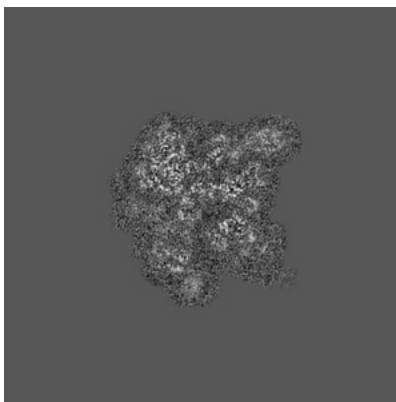
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

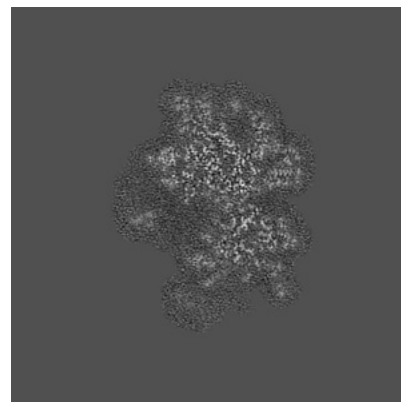
6.2.1 Primary map



X Index: 256

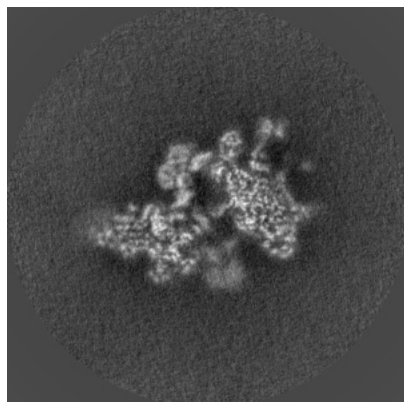


Y Index: 256

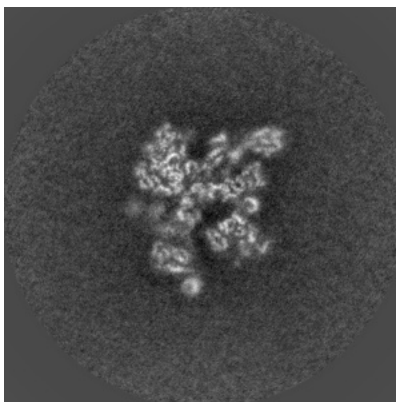


Z Index: 256

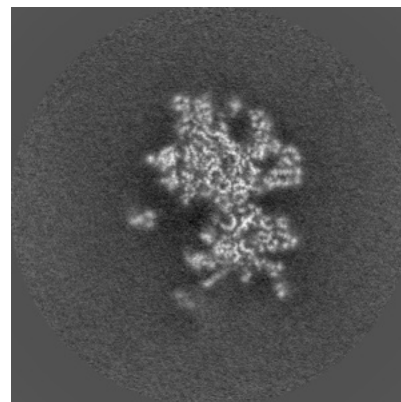
6.2.2 Raw map



X Index: 256



Y Index: 256

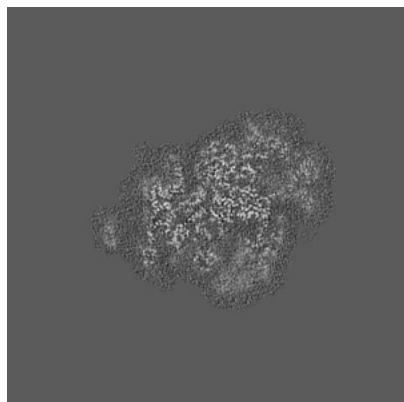


Z Index: 256

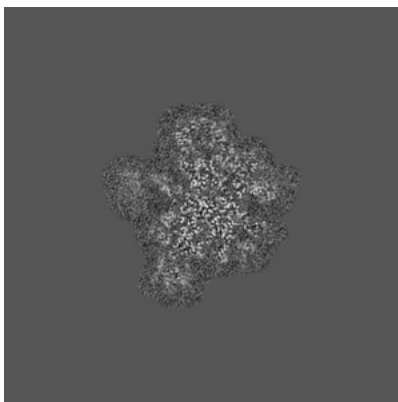
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

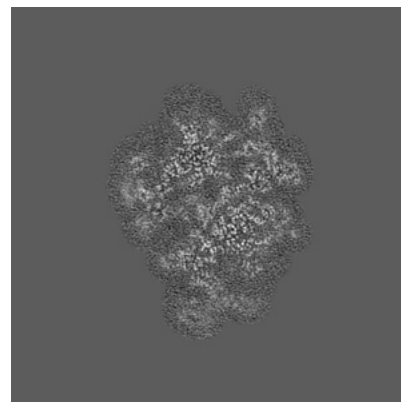
6.3.1 Primary map



X Index: 288

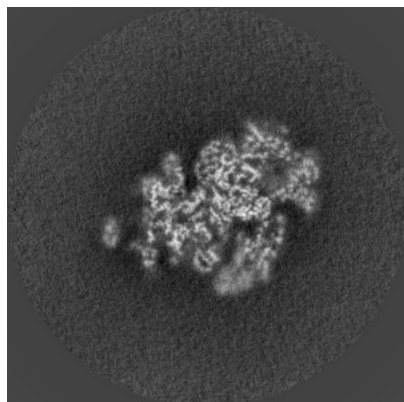


Y Index: 304

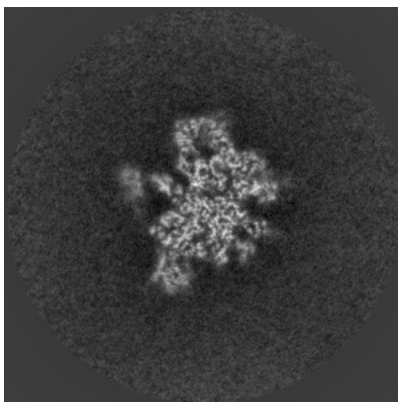


Z Index: 228

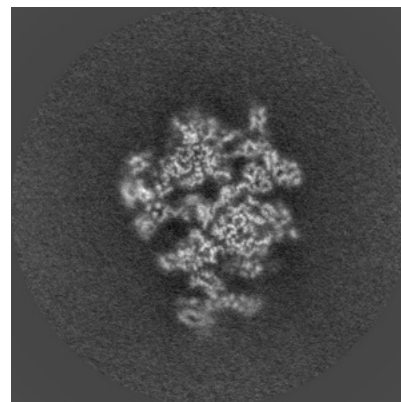
6.3.2 Raw map



X Index: 287



Y Index: 305

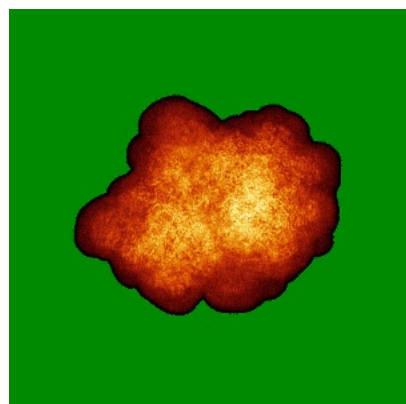


Z Index: 228

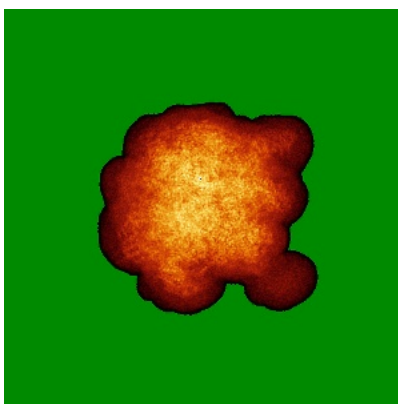
The images above show the largest variance slices of the map in three orthogonal directions.

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

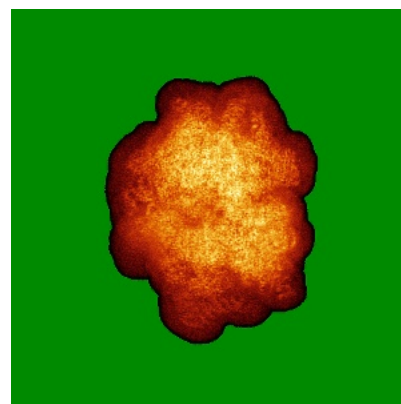
6.4.1 Primary map



X

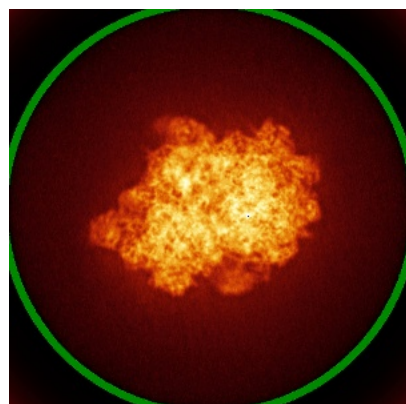


Y

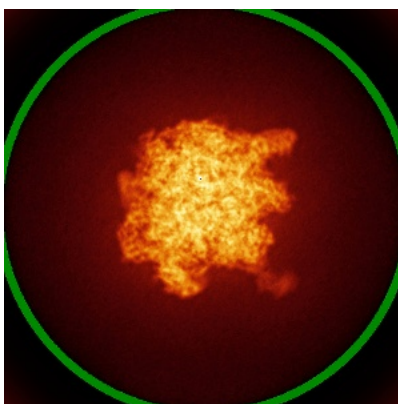


Z

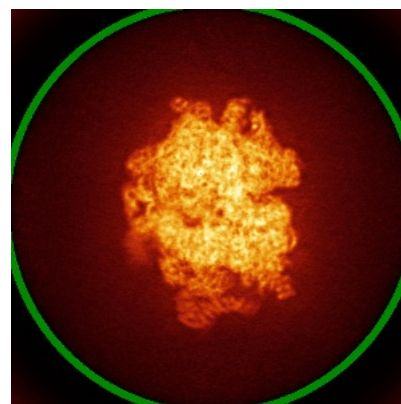
6.4.2 Raw map



X



Y

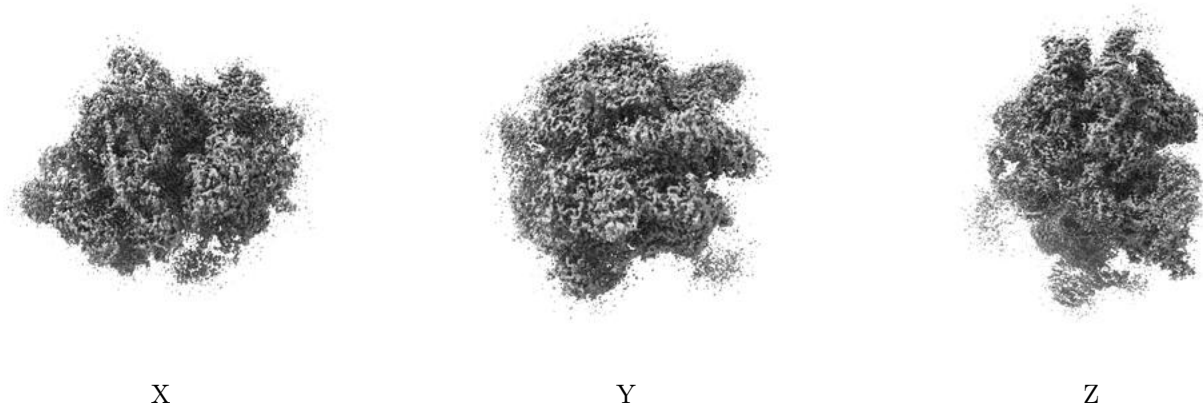


Z

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.

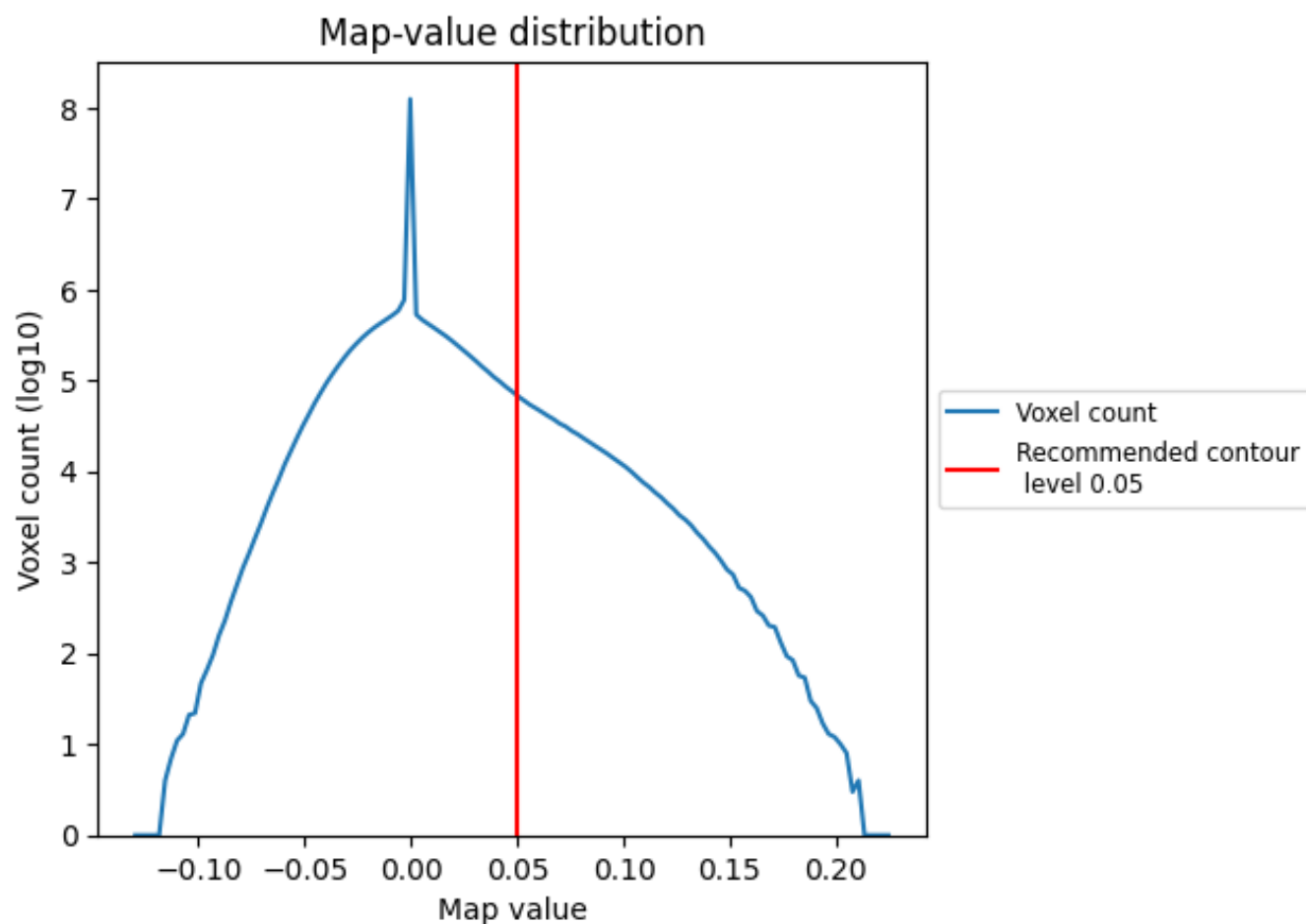
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

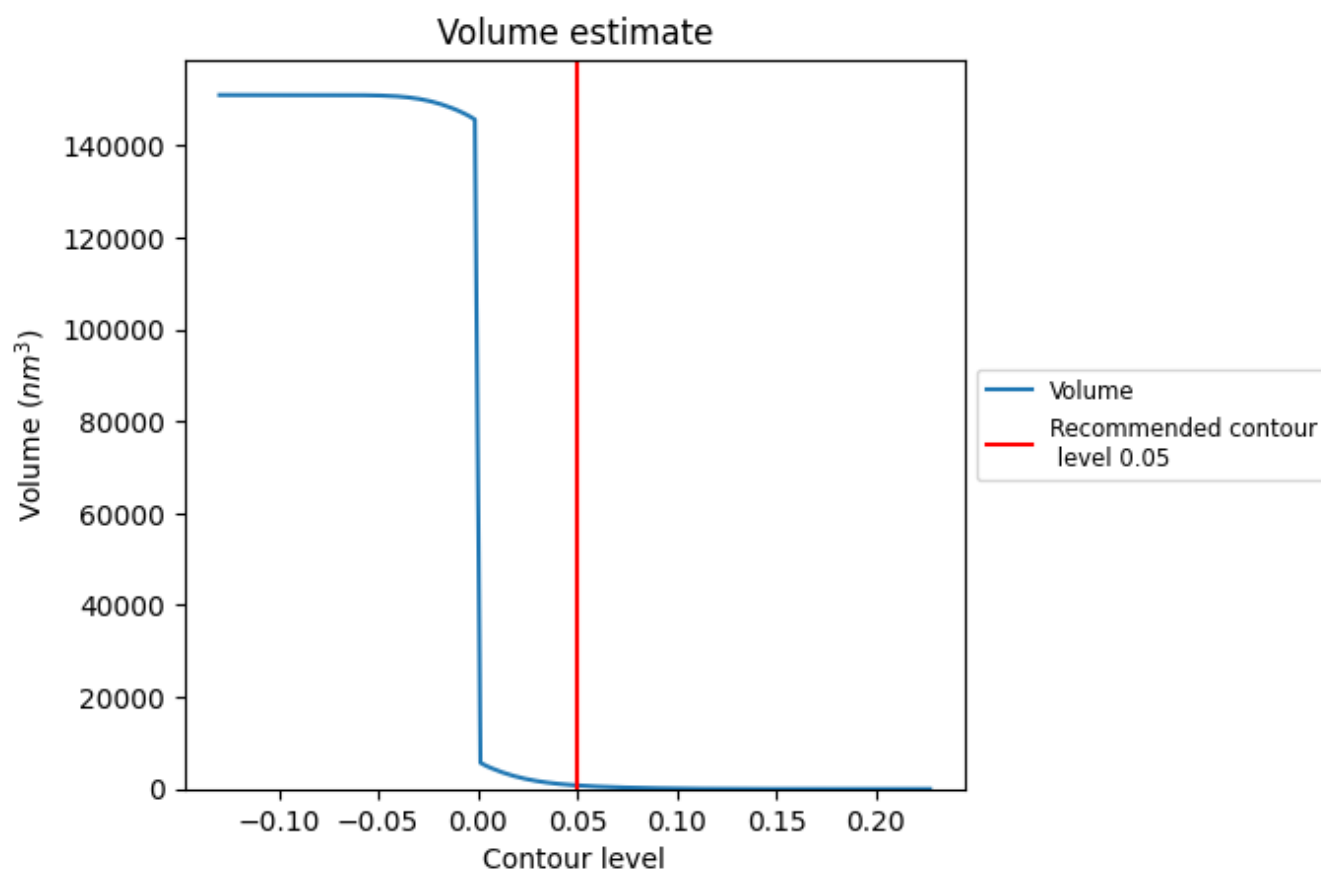
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

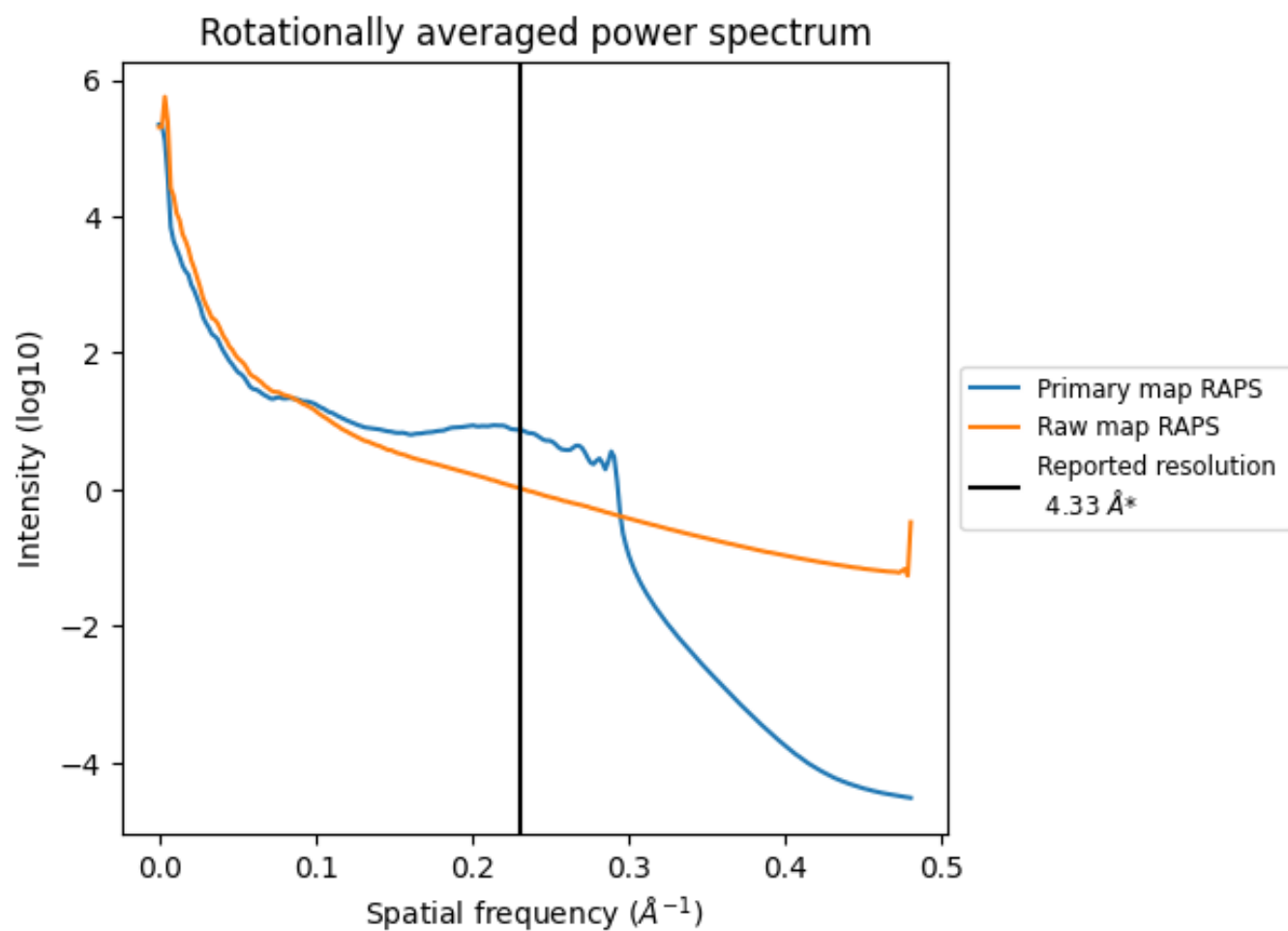
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 775 nm^3 ; this corresponds to an approximate mass of 700 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 ⓘ

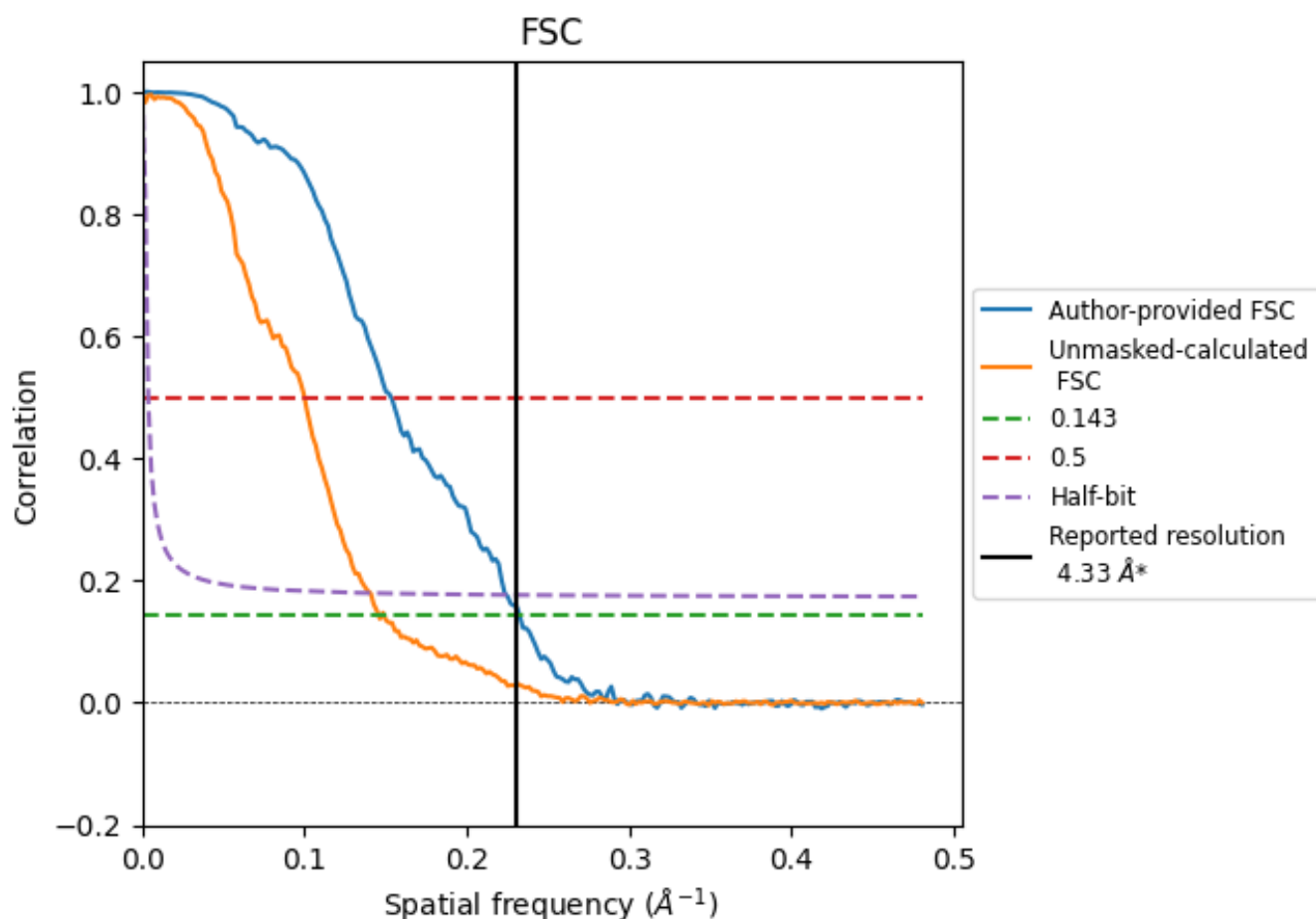


*Reported resolution corresponds to spatial frequency of $0.231 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.231 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

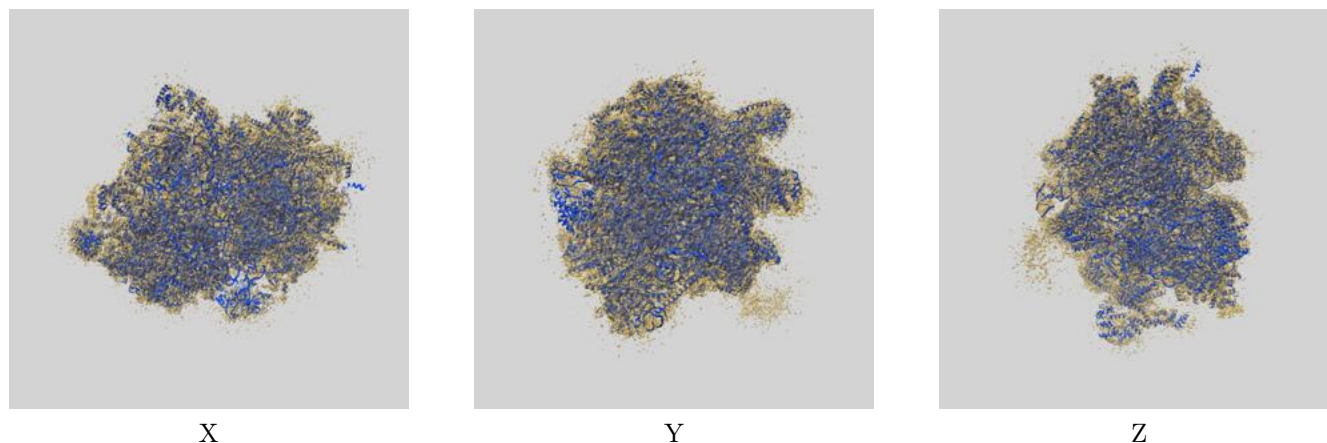
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.33	-	-
Author-provided FSC curve	4.30	6.52	4.46
Unmasked-calculated*	6.86	10.00	7.11

*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 6.86 differs from the reported value 4.33 by more than 10 %

9 Map-model fit [i](#)

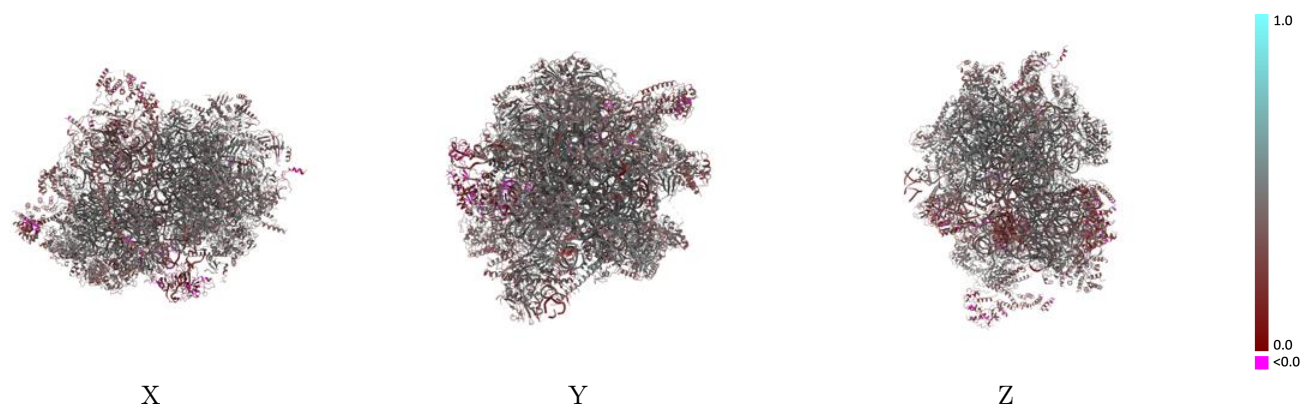
This section contains information regarding the fit between EMDB map EMD-11642 and PDB model 7A5G. Per-residue inclusion information can be found in section 3 on page 25.

9.1 Map-model overlay [i](#)



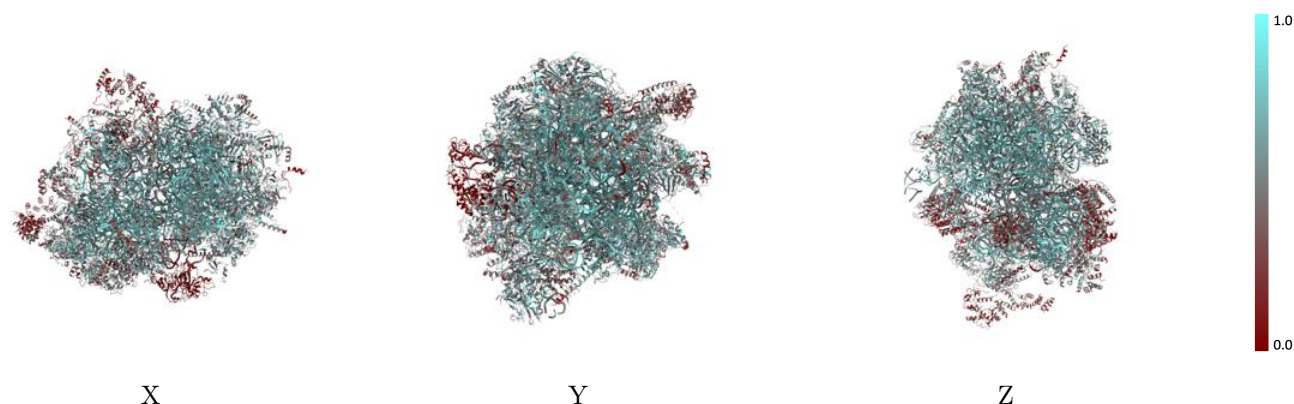
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



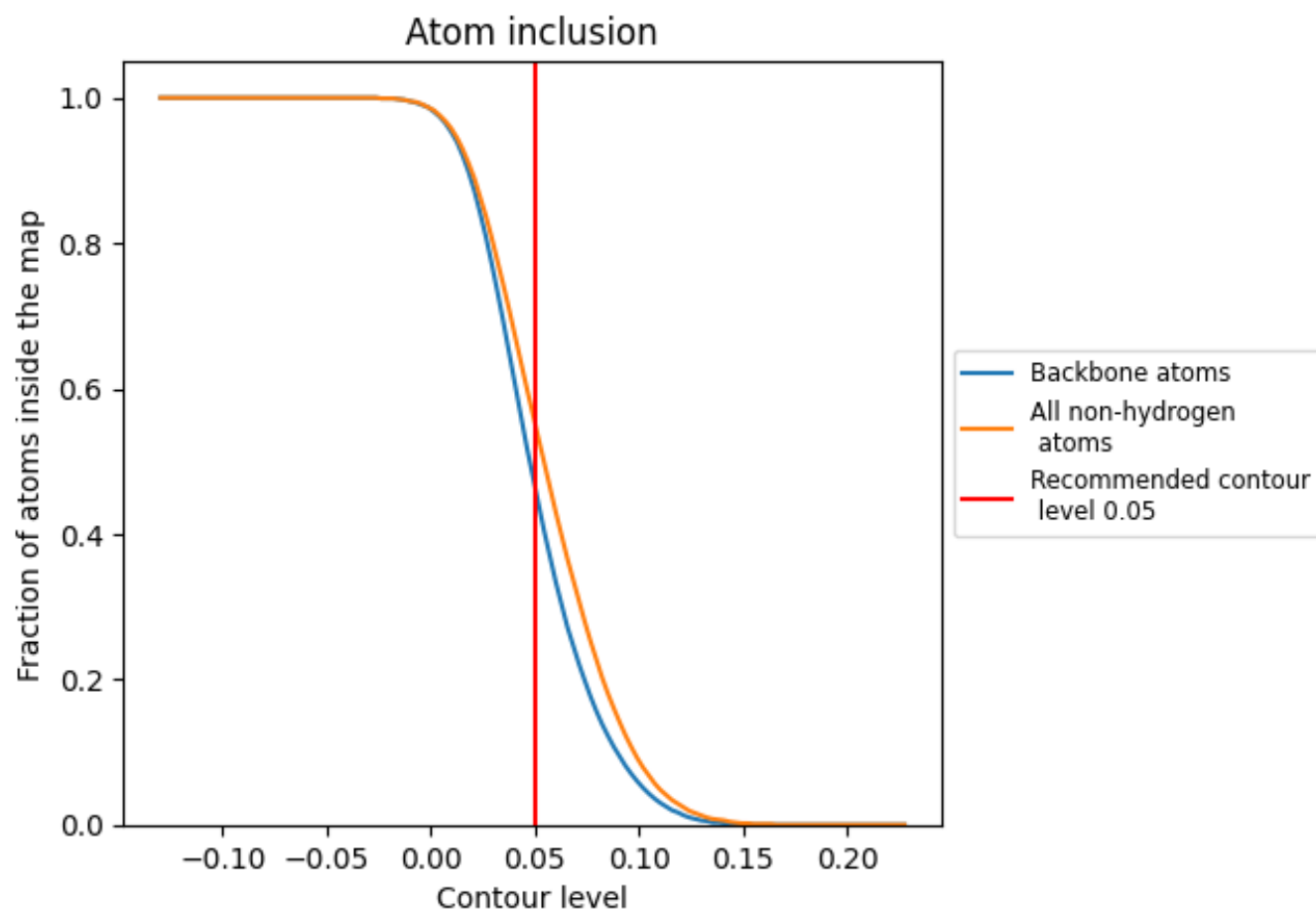
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 46% of all backbone atoms, 55% 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	 0.5530	 0.4020
03	 0.5490	 0.4420
13	 0.4950	 0.4280
23	 0.6640	 0.4860
24	 0.4210	 0.2530
33	 0.6320	 0.4910
43	 0.6680	 0.4910
53	 0.5790	 0.4320
63	 0.5600	 0.4090
73	 0.5000	 0.3880
93	 0.5610	 0.4350
A	 0.2900	 0.2890
A3	 0.7370	 0.4360
A5	 0.0000	 0.1120
A6	 0.7380	 0.4240
B3	 0.6540	 0.3240
B6	 0.6170	 0.4460
C	 0.0410	 0.0670
C6	 0.5480	 0.4550
D	 0.1030	 0.1770
D3	 0.6270	 0.4780
D6	 0.5020	 0.4360
E3	 0.6030	 0.4540
E6	 0.5290	 0.4340
F3	 0.5860	 0.4510
F6	 0.4730	 0.3890
G6	 0.5030	 0.4060
H3	 0.4600	 0.4020
H6	 0.5140	 0.4260
I3	 0.3610	 0.3280
I6	 0.5340	 0.4380
J3	 0.2250	 0.2590
J6	 0.4910	 0.4530
K3	 0.6190	 0.4640
K6	 0.5970	 0.4460



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Chain	Atom inclusion	Q-score
L3	 0.5080	 0.4490
L6	 0.5530	 0.4290
M3	 0.5750	 0.4420
M6	 0.4790	 0.3990
N3	 0.5640	 0.4580
N6	 0.5370	 0.4490
O3	 0.5880	 0.4420
O6	 0.4860	 0.3900
P3	 0.5930	 0.4420
P6	 0.5600	 0.4380
Q3	 0.5100	 0.4330
Q6	 0.5500	 0.4380
R3	 0.6200	 0.4690
R6	 0.4360	 0.3750
S3	 0.6210	 0.4670
S6	 0.4820	 0.3990
T3	 0.5790	 0.4650
T6	 0.5500	 0.4280
U3	 0.6000	 0.4570
U6	 0.4530	 0.3560
V3	 0.5020	 0.4020
V6	 0.2740	 0.2700
W3	 0.6360	 0.4890
W6	 0.5440	 0.4300
X3	 0.5290	 0.4150
X6	 0.4640	 0.3570
Y2	 0.1660	 0.2790
Y3	 0.6020	 0.4440
Y6	 0.4290	 0.3500
Z	 0.2600	 0.2600
Z3	 0.6350	 0.4730
Z6	 0.4680	 0.3970
a3	 0.5910	 0.4530
a6	 0.3910	 0.3510
b3	 0.6020	 0.4580
b6	 0.4350	 0.3700
c3	 0.5340	 0.4080
c6	 0.4140	 0.3970
d3	 0.4950	 0.3930
d6	 0.5450	 0.4520
e3	 0.3240	 0.2840
e6	 0.2880	 0.2730

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Chain	Atom inclusion	Q-score
f3	 0.4560	 0.3670
g3	 0.5770	 0.4400
h3	 0.4740	 0.3670
i3	 0.6100	 0.4690
i4	 0.6710	 0.4480
j	 0.4650	 0.2250
j3	 0.5780	 0.4350
k3	 0.3260	 0.2920
l3	 0.5390	 0.3730
m3	 0.4900	 0.4010
n	 0.0510	 0.1720
o3	 0.6430	 0.4760
p3	 0.4580	 0.3880
q3	 0.4910	 0.3990
r3	 0.6450	 0.4590
s3	 0.5800	 0.4340
t3	 0.2070	 0.2150
u3	 0.1910	 0.3380