



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 10:45 AM UTC

PDB ID : 7A5K / pdb_00007a5k
EMDB ID : EMD-11646
Title : Structure of the human mitoribosome in the post translocation state bound to mtEF-G1
Authors : Desai, N.; Yang, H.; Chandrasekaran, V.; Kazi, R.; Minczuk, M.; Ramakrishnan, V.
Deposited on : 2020-08-21
Resolution : 3.70 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:

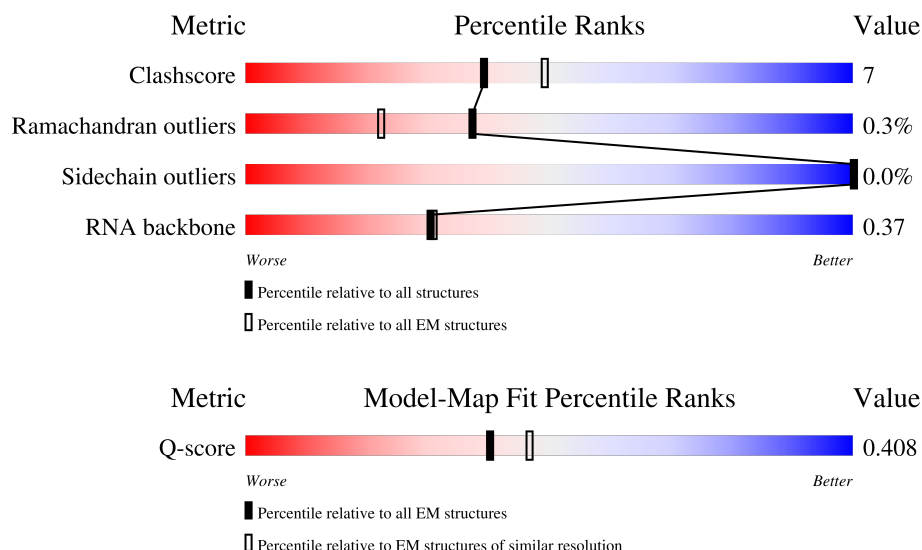
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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.



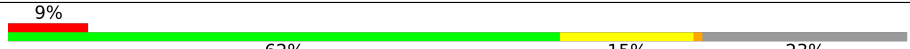
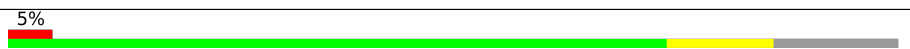
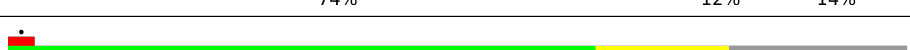
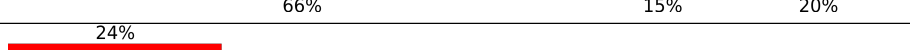
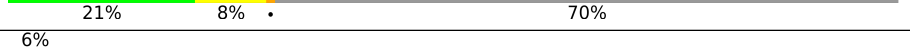
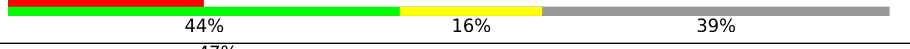
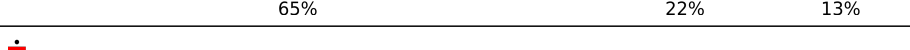
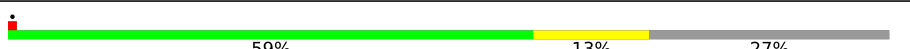
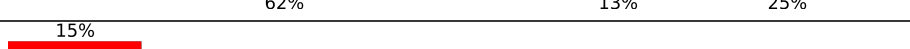
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11569 (3.20 - 4.20)

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	r1	751	38% (red), 63% (green), 27% (yellow), 7% (grey)
2	Y2	29	86% (red), 93% (green), 7% (yellow)
3	8	1559	99% (grey)

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Mol	Chain	Length	Quality of chain
3	A3	1559	
4	B3	73	
5	D3	305	
6	E3	348	
7	F3	311	
8	D	267	
8	H3	267	
9	I3	261	
10	J3	192	
11	K3	178	
12	L3	145	
13	M3	296	
14	N3	251	
15	O3	175	
16	P3	179	
17	Q3	292	
18	R3	149	
19	S3	205	
20	T3	212	
21	U3	153	
22	V3	216	
23	W3	148	
24	X3	256	
25	Y3	250	
26	Z3	161	

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Mol	Chain	Length	Quality of chain
27	03	188	
28	13	65	
29	23	92	
30	33	188	
31	43	103	
32	53	423	
33	63	380	
34	73	338	
35	93	137	
36	a3	142	
37	b3	155	
38	c3	332	
39	d3	306	
40	e3	279	
41	f3	194	
42	g3	166	
43	h3	158	
44	i3	128	
45	j3	123	
46	k3	112	
47	l3	138	
48	m3	128	
49	o3	102	
50	p3	206	
51	q3	222	

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Mol	Chain	Length	Quality of chain
52	r3	196	
53	s3	439	
54	u3	2	
55	A5	435	
56	B6	296	
57	C6	167	
58	D6	430	
59	E6	125	
60	F6	242	
61	G6	396	
62	H6	201	
63	I6	194	
64	J6	138	
65	K6	128	
66	L6	257	
67	M6	137	
68	N6	130	
69	O6	258	
70	P6	142	
71	Q6	87	
72	R6	360	
73	S6	190	
74	T6	173	
75	U6	205	
76	V6	414	

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Mol	Chain	Length	Quality of chain
77	W6	187	
78	X6	398	
79	Y6	395	
80	Z6	106	
81	a6	218	
82	b6	323	
83	c6	118	
84	d6	199	
85	e6	689	
86	A6	954	
87	24	73	
87	FE	73	
88	A	206	
89	n	286	
90	B	28	

2 Entry composition

There are 95 unique types of molecules in this entry. The entry contains 171122 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 Elongation factor G, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	r1	696	Total	C	N	O	S	0	0
			5452	3435	940	1044	33		

- Molecule 2 is a protein called nascent chain.

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

- Molecule 3 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A3	1503	Total	C	N	O	P	0	0
			31913	14319	5761	10330	1503		
3	8	8	Total	C	N	O	P	0	0
			175	79	37	51	8		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A3	3107	U	UNK	conflict	GB 1025814679
8	663	U	UNK	conflict	GB 1025814679

- Molecule 4 is a RNA chain called mt-tRNAVal.

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

- Molecule 5 is a protein called 39S ribosomal protein L2, mitochondrial.

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

- Molecule 6 is a protein called 39S ribosomal protein L3, mitochondrial.

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

- Molecule 7 is a protein called 39S ribosomal protein L4, mitochondrial.

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

- Molecule 8 is a protein called 39S ribosomal protein L9, mitochondrial.

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

- Molecule 9 is a protein called 39S ribosomal protein L10, mitochondrial.

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

- Molecule 10 is a protein called 39S ribosomal protein L11, mitochondrial.

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

- Molecule 11 is a protein called 39S ribosomal protein L13, mitochondrial.

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

- Molecule 12 is a protein called 39S ribosomal protein L14, mitochondrial.

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

- Molecule 13 is a protein called 39S ribosomal protein L15, mitochondrial.

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

- Molecule 14 is a protein called 39S ribosomal protein L16, mitochondrial.

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

- Molecule 15 is a protein called 39S ribosomal protein L17, mitochondrial.

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

- Molecule 16 is a protein called Mitochondrial ribosomal protein L18, isoform CRA_b.

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

- Molecule 17 is a protein called 39S ribosomal protein L19, mitochondrial.

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

- Molecule 18 is a protein called 39S ribosomal protein L20, mitochondrial.

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

- Molecule 19 is a protein called 39S ribosomal protein L21, mitochondrial.

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

- Molecule 20 is a protein called 39S ribosomal protein L22, mitochondrial.

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

- Molecule 21 is a protein called 39S ribosomal protein L23, mitochondrial.

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

- Molecule 22 is a protein called 39S ribosomal protein L24, mitochondrial.

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

- Molecule 23 is a protein called 39S ribosomal protein L27, mitochondrial.

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

- Molecule 24 is a protein called 39S ribosomal protein L28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	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 25 is a protein called 39S ribosomal protein L47, mitochondrial.

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

- Molecule 26 is a protein called 39S ribosomal protein L30, mitochondrial.

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

- Molecule 27 is a protein called 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	03	108	Total	C	N	O	S	0	0
			880	545	172	157	6		

- Molecule 28 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	13	52	Total	C	N	O	S	0	0
			433	278	83	70	2		

- Molecule 29 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	23	46	Total	C	N	O	S	0	0
			376	233	83	59	1		

- Molecule 30 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	33	95	Total	C	N	O	S	0	0
			831	539	162	127	3		

- Molecule 31 is a protein called 39S ribosomal protein L36, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	43	36	Total	C	N	O	S	0	0
			322	203	70	46	3		

- Molecule 32 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	53	376	Total	C	N	O	S	0	0
			3064	1987	529	538	10		

- Molecule 33 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	63	325	Total	C	N	O	S	0	0
			2636	1692	465	470	9		

- Molecule 34 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	73	266	Total	C	N	O	S	0	0
			2158	1383	371	388	16		

- Molecule 35 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	93	109	Total	C	N	O	S	0	0
			873	565	152	154	2		

- Molecule 36 is a protein called 39S ribosomal protein L42, mitochondrial.

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

- Molecule 37 is a protein called 39S ribosomal protein L43, mitochondrial.

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

- Molecule 38 is a protein called 39S ribosomal protein L44, mitochondrial.

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

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

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

- Molecule 40 is a protein called 39S ribosomal protein L46, mitochondrial.

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

- Molecule 41 is a protein called 39S ribosomal protein L48, mitochondrial.

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

- Molecule 42 is a protein called 39S ribosomal protein L49, mitochondrial.

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

- Molecule 43 is a protein called 39S ribosomal protein L50, mitochondrial.

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

- Molecule 44 is a protein called 39S ribosomal protein L51, mitochondrial.

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

- Molecule 45 is a protein called cDNA FLJ76418, highly similar to Homo sapiens mitochondrial ribosomal protein L52 (MRPL52), transcript variant 1, mRNA.

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

- Molecule 46 is a protein called 39S ribosomal protein L53, mitochondrial.

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

- Molecule 47 is a protein called 39S ribosomal protein L54, mitochondrial.

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

- Molecule 48 is a protein called 39S ribosomal protein L55, mitochondrial.

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

- Molecule 49 is a protein called Ribosomal protein 63, mitochondrial.

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

- Molecule 50 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

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

- Molecule 51 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

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

- Molecule 52 is a protein called 39S ribosomal protein S18a, mitochondrial.

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

- Molecule 53 is a protein called 39S ribosomal protein S30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	s3	370	Total	C	N	O	S	0	0
			3036	1946	542	534	14		

- Molecule 54 is a RNA chain called RNA.

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

- Molecule 55 is a protein called Mitochondrial inner membrane protein OXA1L.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	A5	28	Total	C	N	O	0	0
			136	80	28	28		

- Molecule 56 is a protein called 28S ribosomal protein S2, mitochondrial.

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

- Molecule 57 is a protein called 28S ribosomal protein S24, mitochondrial.

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

- Molecule 58 is a protein called 28S ribosomal protein S5, mitochondrial.

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

- Molecule 59 is a protein called 28S ribosomal protein S6, mitochondrial.

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

- Molecule 60 is a protein called 28S ribosomal protein S7, mitochondrial.

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

- Molecule 61 is a protein called 28S ribosomal protein S9, mitochondrial.

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

- Molecule 62 is a protein called 28S ribosomal protein S10, mitochondrial.

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

- Molecule 63 is a protein called 28S ribosomal protein S11, mitochondrial.

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

- Molecule 64 is a protein called 28S ribosomal protein S12, mitochondrial.

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

- Molecule 65 is a protein called 28S ribosomal protein S14, mitochondrial.

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

- Molecule 66 is a protein called 28S ribosomal protein S15, mitochondrial.

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

- Molecule 67 is a protein called 28S ribosomal protein S16, mitochondrial.

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

- Molecule 68 is a protein called 28S ribosomal protein S17, mitochondrial.

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

- Molecule 69 is a protein called 28S ribosomal protein S18b, mitochondrial.

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

- Molecule 70 is a protein called 28S ribosomal protein S18c, mitochondrial.

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

- Molecule 71 is a protein called 28S ribosomal protein S21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	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 72 is a protein called 28S ribosomal protein S22, mitochondrial.

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

- Molecule 73 is a protein called 28S ribosomal protein S23, mitochondrial.

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

- Molecule 74 is a protein called 28S ribosomal protein S25, mitochondrial.

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

- Molecule 75 is a protein called 28S ribosomal protein S26, mitochondrial.

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

- Molecule 76 is a protein called 28S ribosomal protein S27, mitochondrial.

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

- Molecule 77 is a protein called 28S ribosomal protein S28, mitochondrial.

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

- Molecule 78 is a protein called 28S ribosomal protein S29, mitochondrial.

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

- Molecule 79 is a protein called 28S ribosomal protein S31, mitochondrial.

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

- Molecule 80 is a protein called 28S ribosomal protein S33, mitochondrial.

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

- Molecule 81 is a protein called 28S ribosomal protein S34, mitochondrial.

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

- Molecule 82 is a protein called 28S ribosomal protein S35, mitochondrial.

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

- Molecule 83 is a protein called Coiled-coil-helix-coiled-coil-helix domain-containing protein 1.

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

- Molecule 84 is a protein called Aurora kinase A-interacting protein.

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

- Molecule 85 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

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

- Molecule 86 is a RNA chain called 12S rRNA.

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

- Molecule 87 is a RNA chain called mt-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	24	73	Total	C	N	O	P	0	0
			1547	696	280	499	72		
87	FE	73	Total	C	N	O	P	0	0
			1547	696	280	499	72		

- 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		

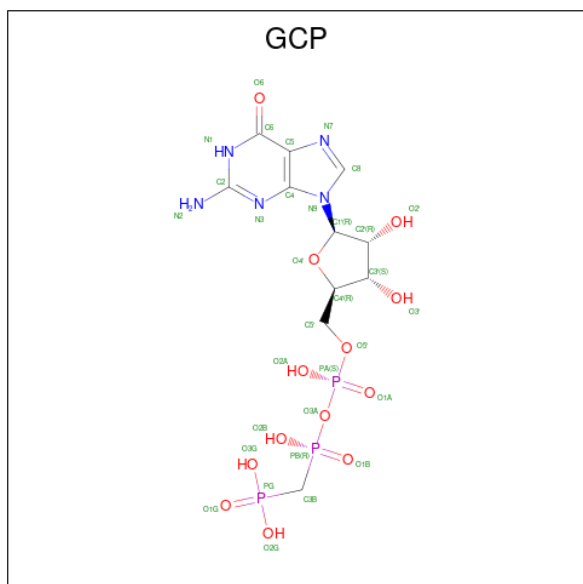
- Molecule 89 is a protein called 39S ribosomal protein L1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
89	n	218	Total	C	N	O	S	0	0
			1744	1121	294	324	5		

- Molecule 90 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
90	B	28	Total	C	N	O	0	0
			140	84	28	28		

- Molecule 91 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).

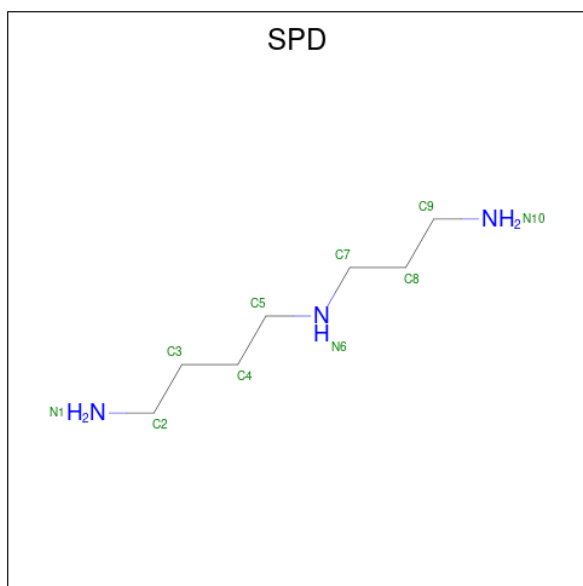


Mol	Chain	Residues	Atoms					AltConf
91	r1	1	Total	C	N	O	P	0
			32	11	5	13	3	

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

Mol	Chain	Residues	Atoms		AltConf
92	r1	1	Total	Mg	0
			1	1	
92	A3	95	Total	Mg	0
			95	95	
92	D3	1	Total	Mg	0
			1	1	
92	E3	1	Total	Mg	0
			1	1	
92	M3	1	Total	Mg	0
			1	1	
92	g3	1	Total	Mg	0
			1	1	
92	A6	28	Total	Mg	0
			28	28	

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

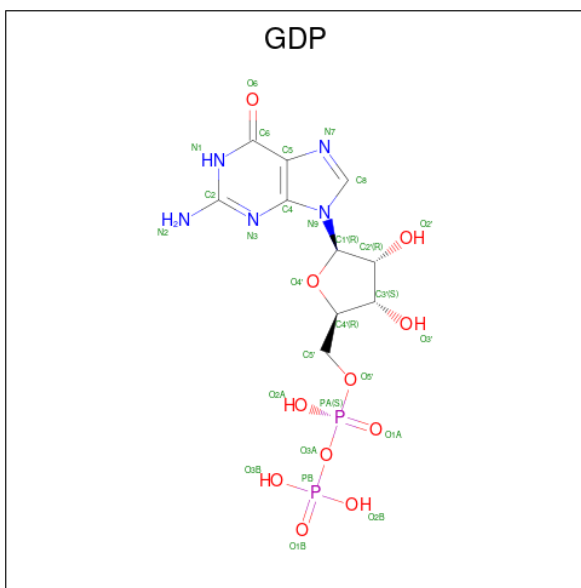


Mol	Chain	Residues	Atoms			AltConf
93	A3	1	Total	C	N	0
			10	7	3	

- 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	

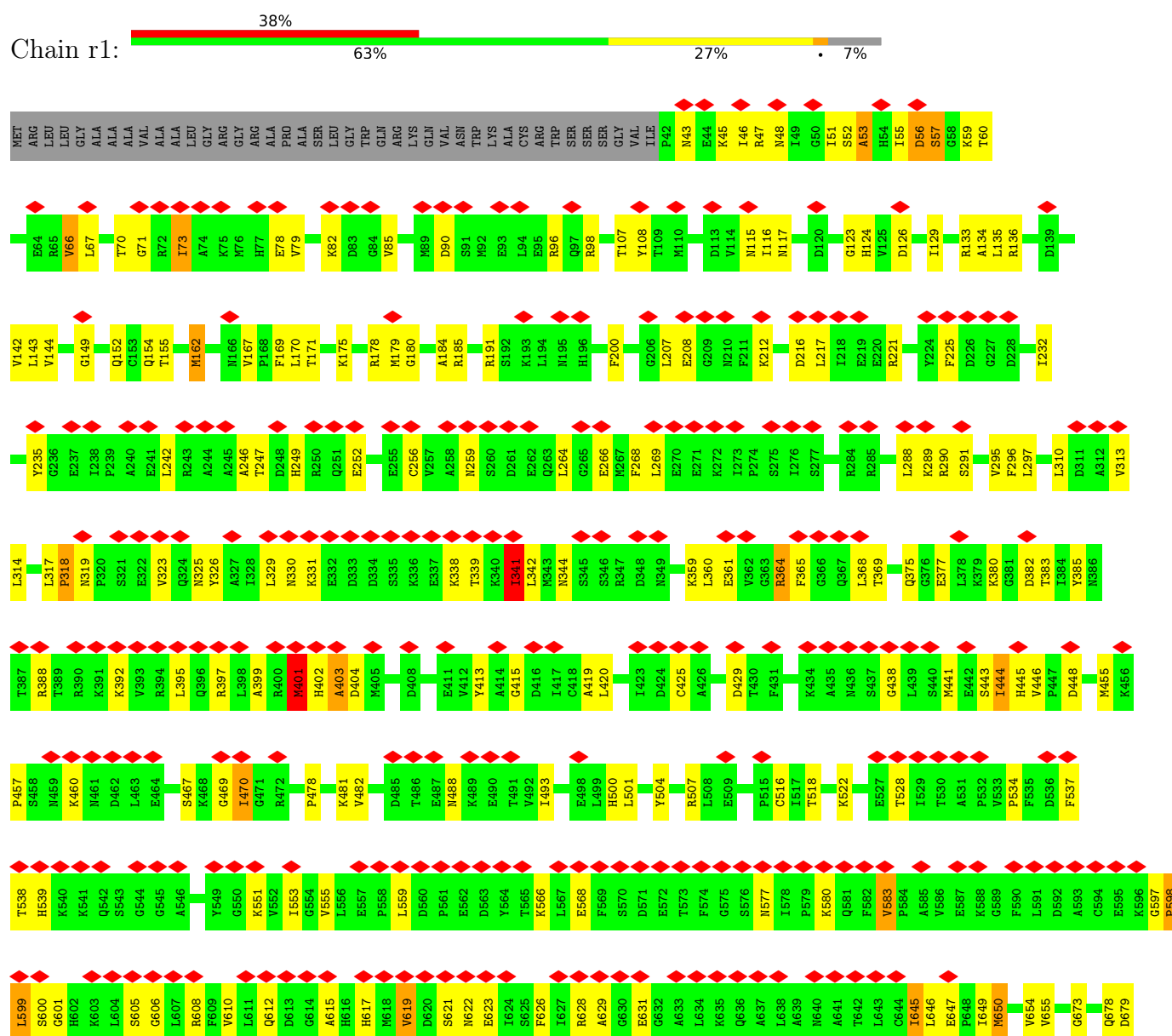
- Molecule 95 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).

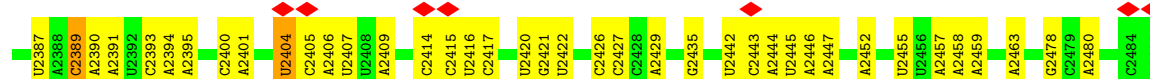


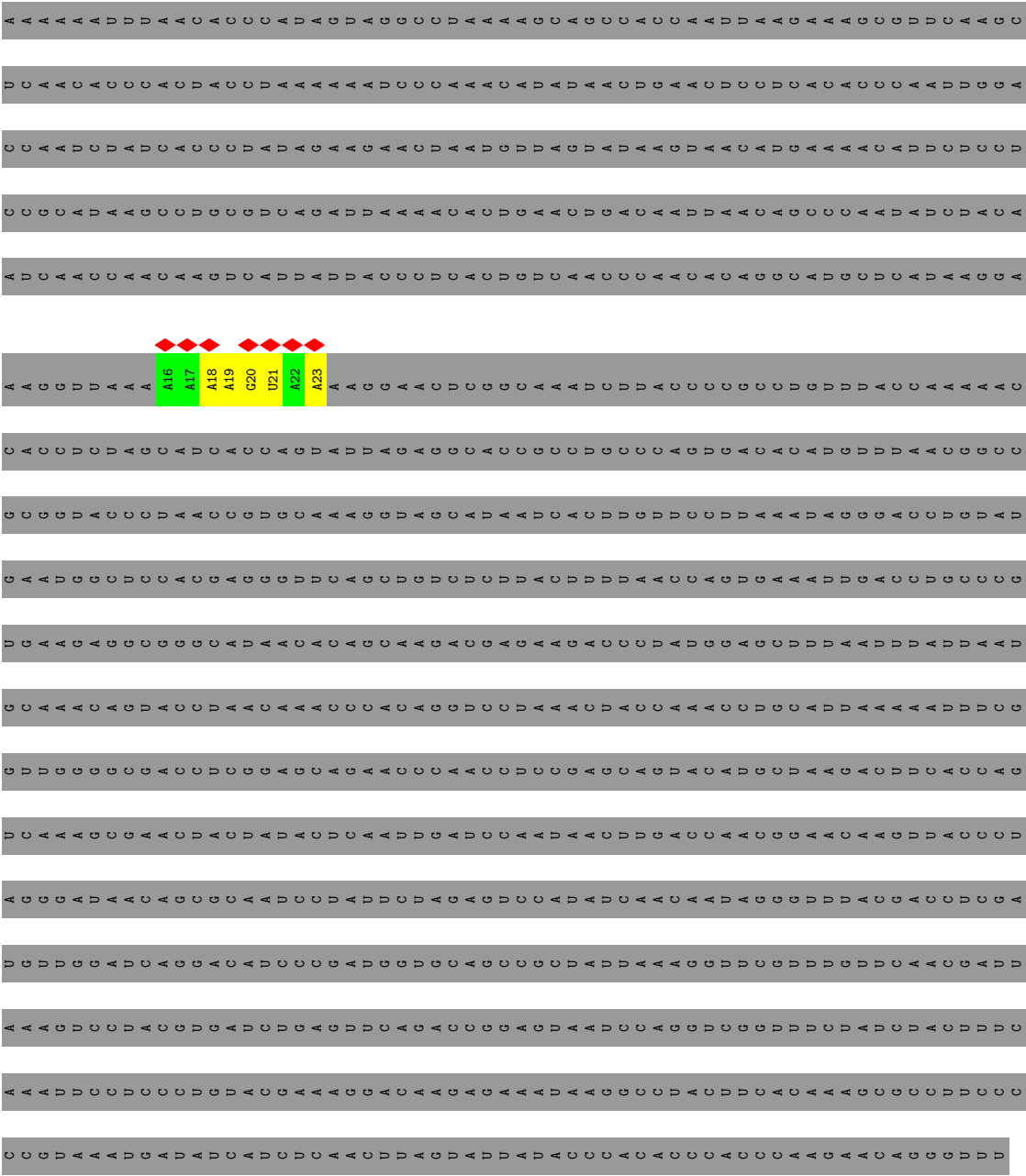
3 Residue-property plots

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.

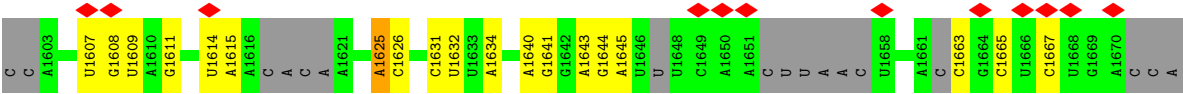
- Molecule 1: Elongation factor G, mitochondrial



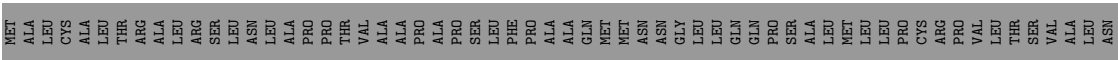


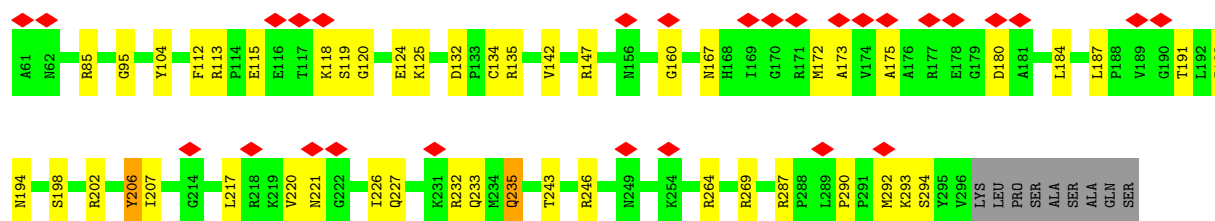


● Molecule 4: mt-tRNAVal

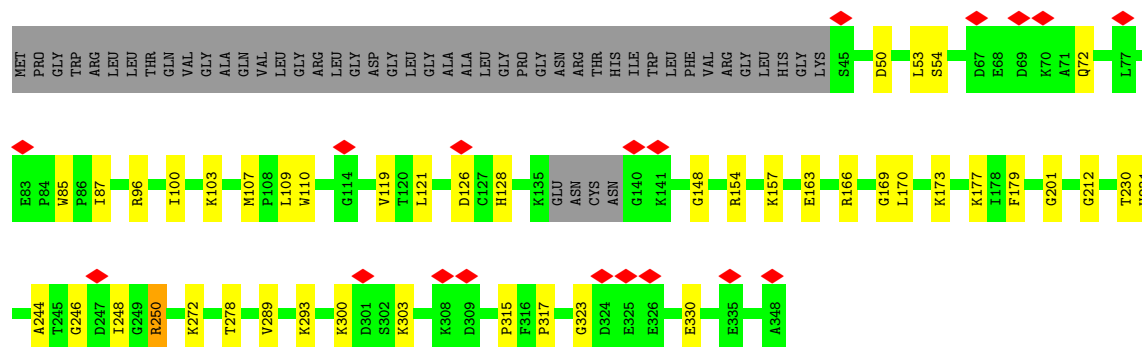
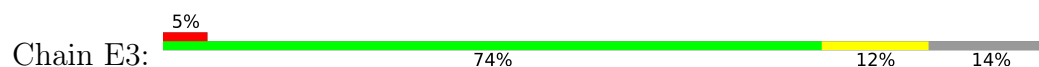


● Molecule 5: 39S ribosomal protein L2, mitochondrial

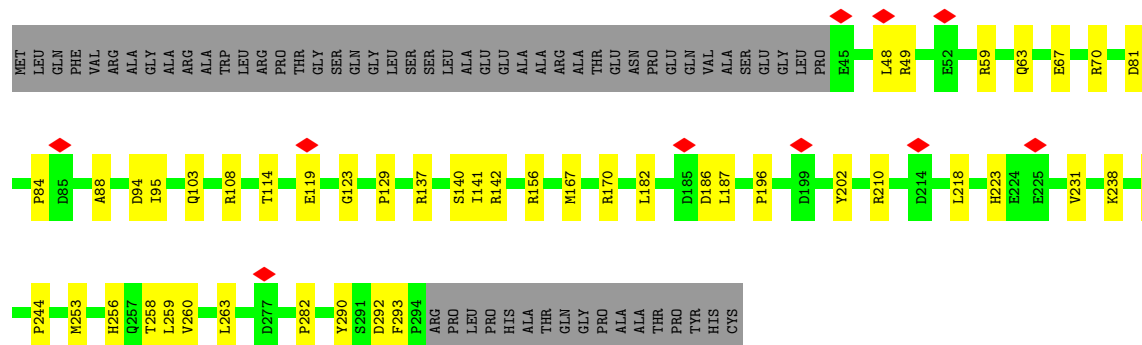




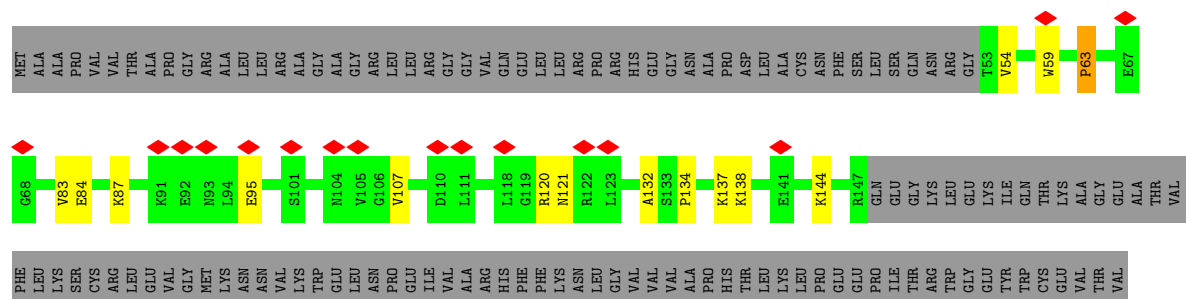
- Molecule 6: 39S ribosomal protein L3, mitochondrial



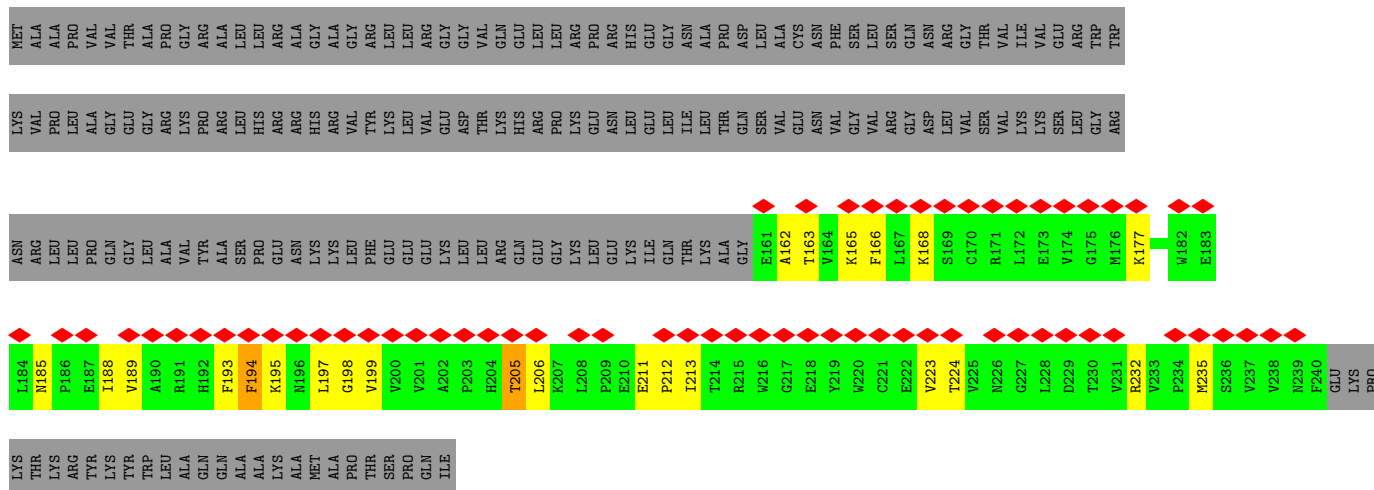
- Molecule 7: 39S ribosomal protein L4, mitochondrial



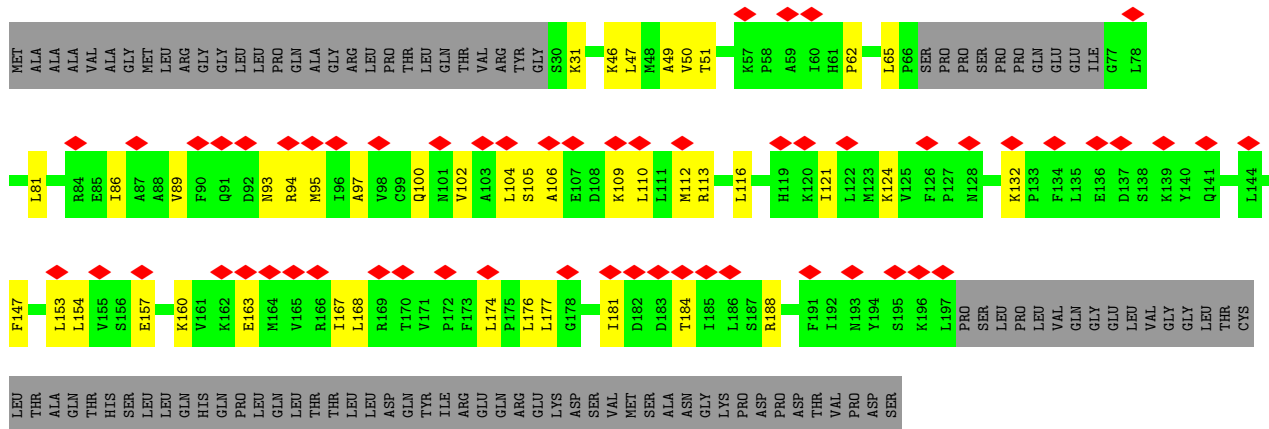
- Molecule 8: 39S ribosomal protein L9, mitochondrial



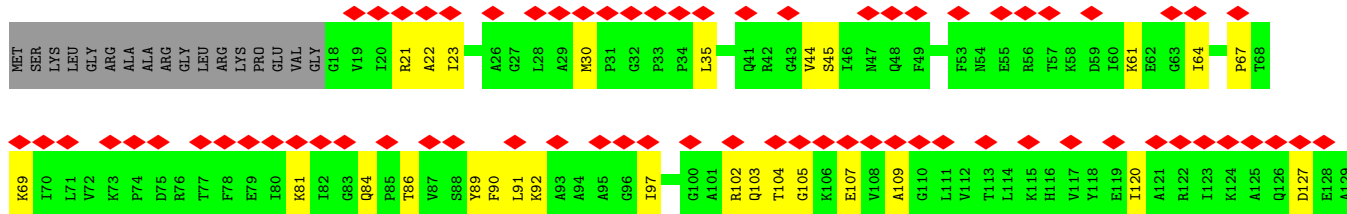
Chain D: 24% 21% 8% 70%

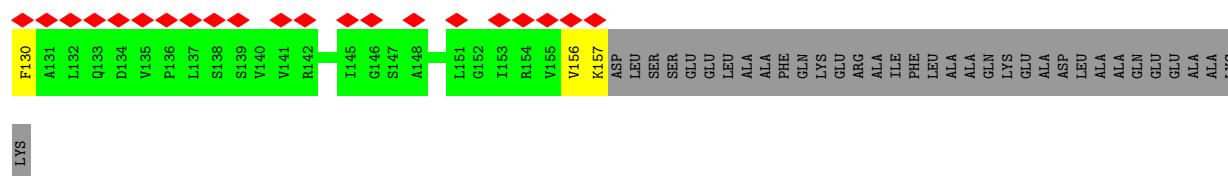


Chain I3:

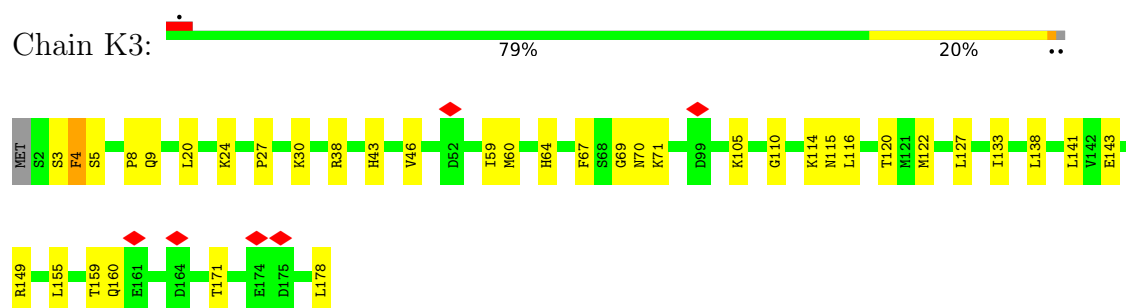


Chain J3:

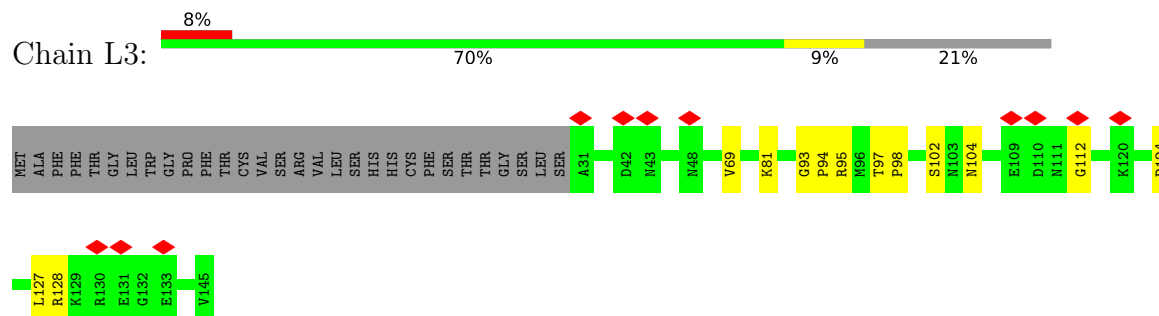




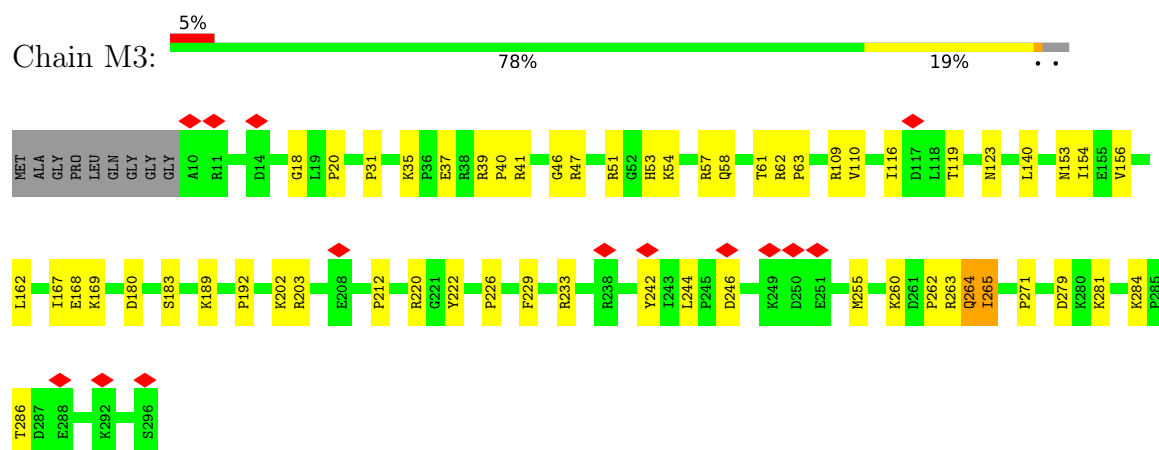
- Molecule 11: 39S ribosomal protein L13, mitochondrial



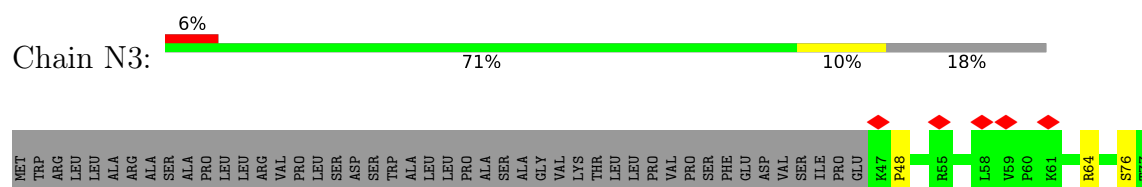
- Molecule 12: 39S ribosomal protein L14, mitochondrial

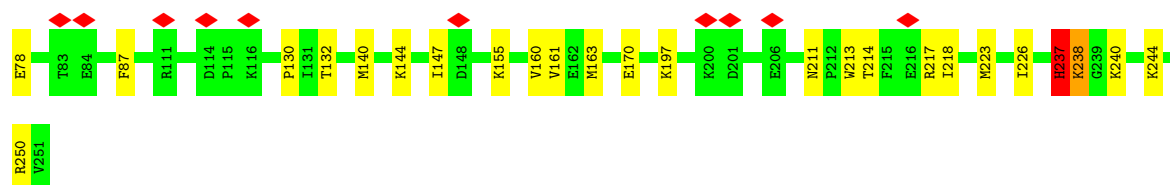


- Molecule 13: 39S ribosomal protein L15, mitochondrial

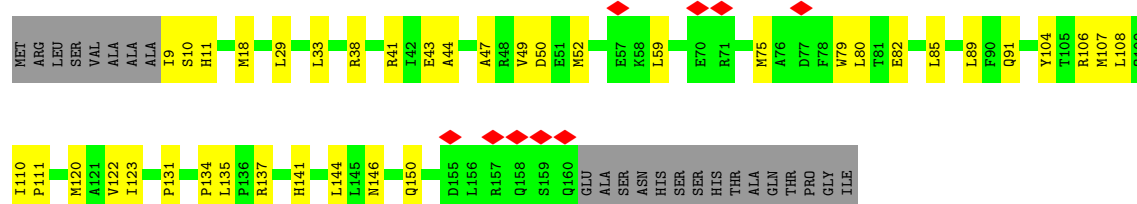


- Molecule 14: 39S ribosomal protein L16, mitochondrial

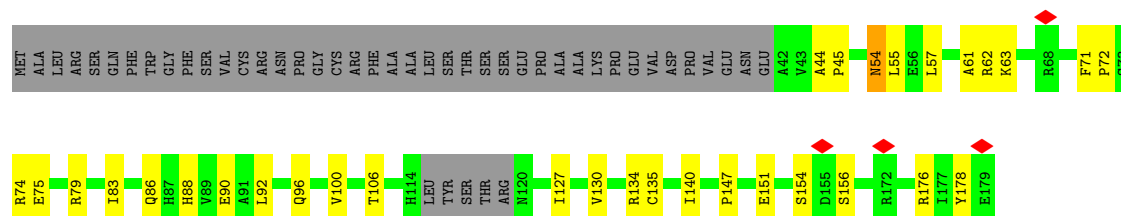




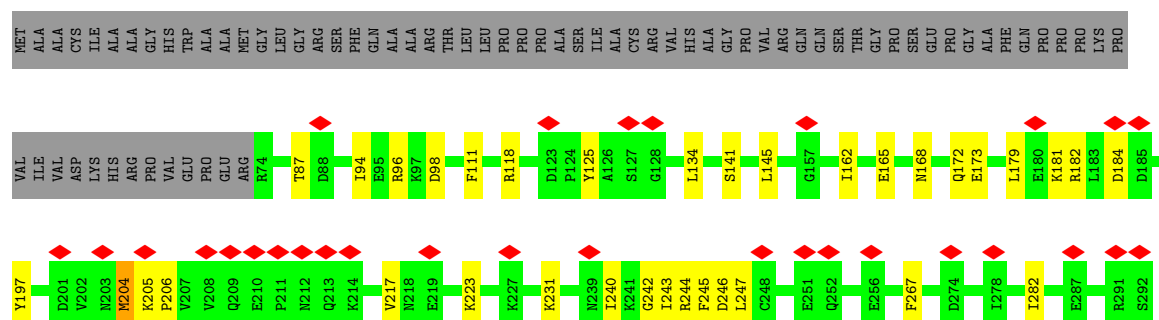
- Molecule 15: 39S ribosomal protein L17, mitochondrial



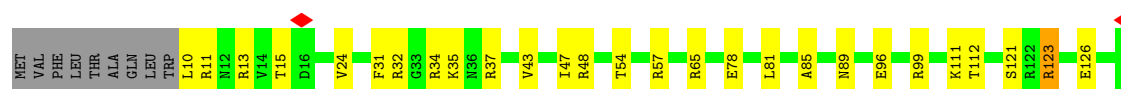
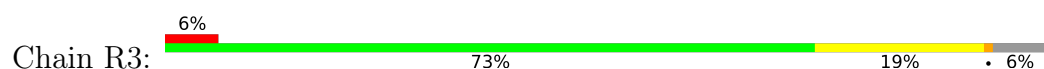
- Molecule 16: Mitochondrial ribosomal protein L18, isoform CRA_b

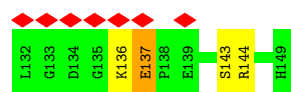


- Molecule 17: 39S ribosomal protein L19, mitochondrial

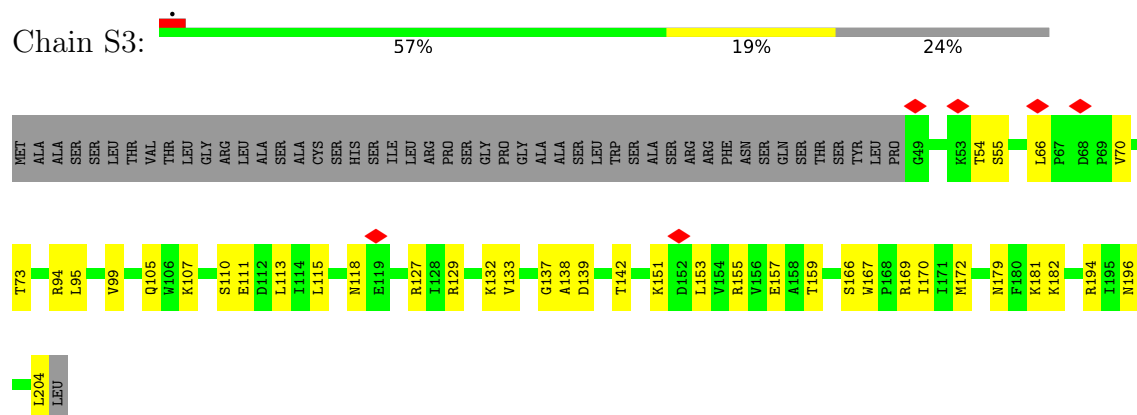


- Molecule 18: 39S ribosomal protein L20, mitochondrial

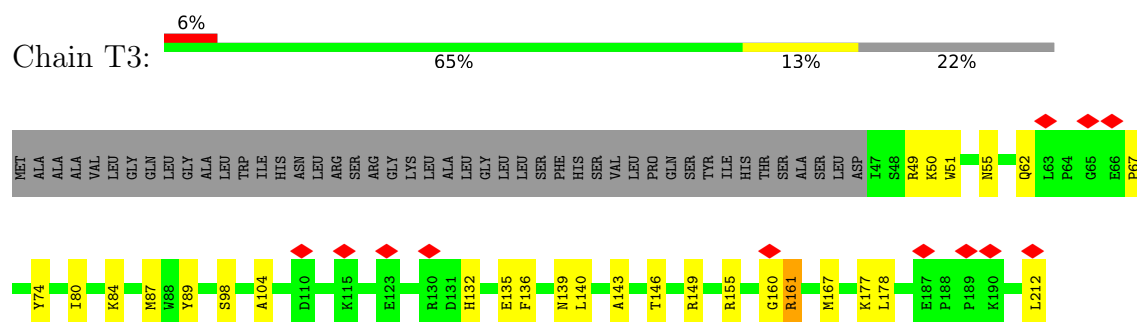




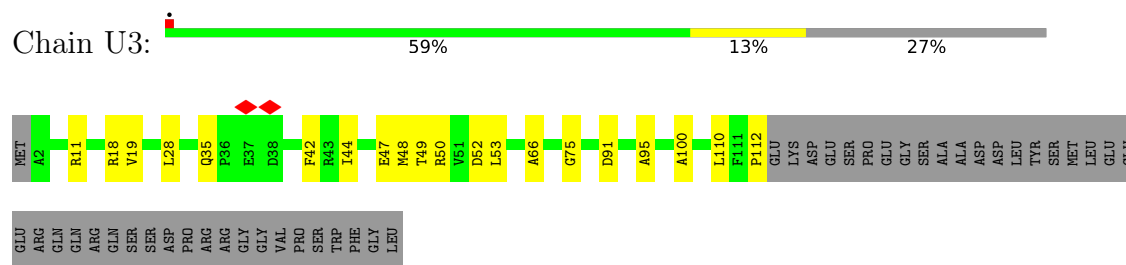
- Molecule 19: 39S ribosomal protein L21, mitochondrial



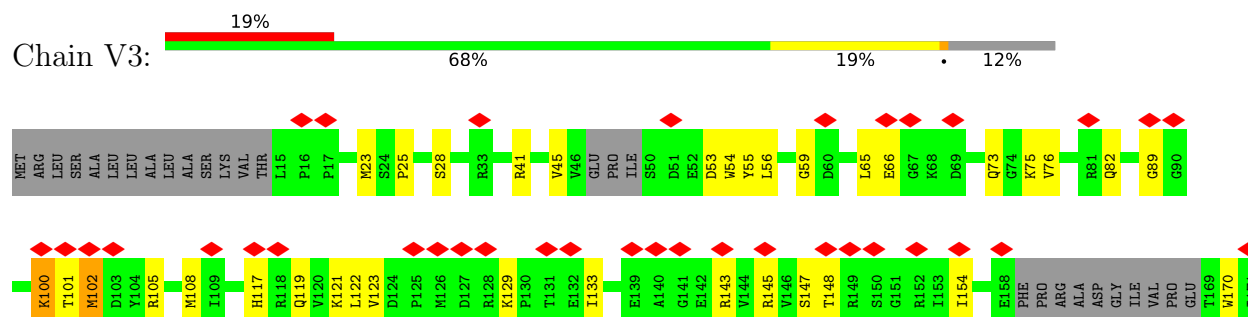
- Molecule 20: 39S ribosomal protein L22, mitochondrial

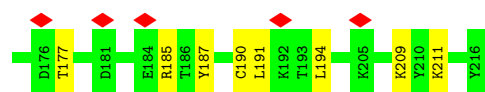


- Molecule 21: 39S ribosomal protein L23, mitochondrial



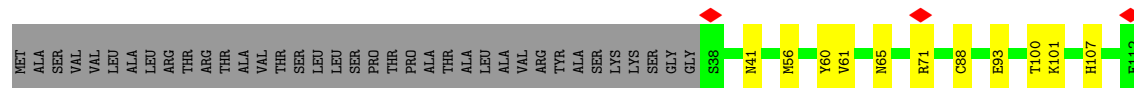
- Molecule 22: 39S ribosomal protein L24, mitochondrial





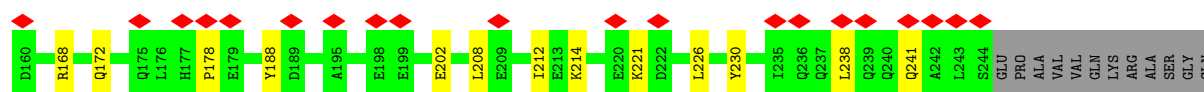
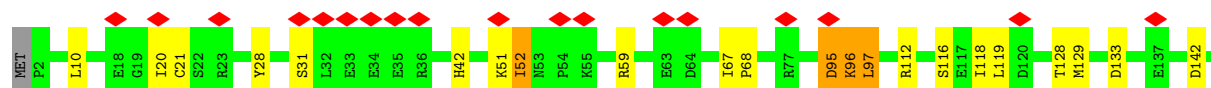
- Molecule 23: 39S ribosomal protein L27, mitochondrial

Chain W3: 62% 13% 25%



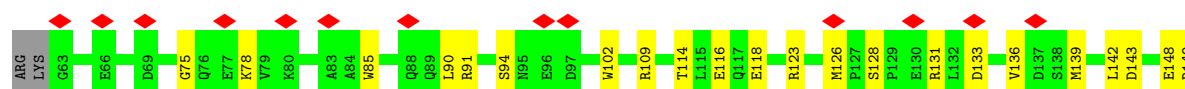
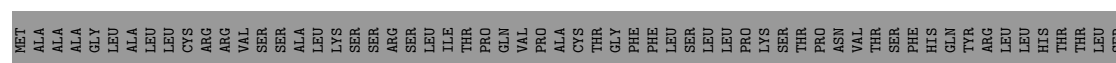
- Molecule 24: 39S ribosomal protein L28, mitochondrial

Chain X3: 15% 81% 12% 5%



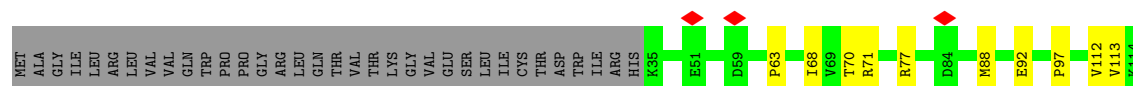
- Molecule 25: 39S ribosomal protein L47, mitochondrial

Chain Y3: 8% 57% 14% 30%

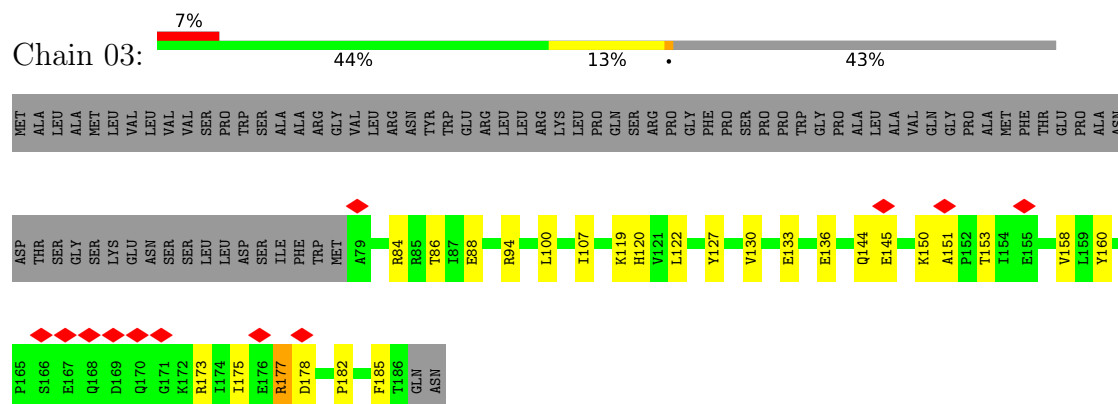


- Molecule 26: 39S ribosomal protein L30, mitochondrial

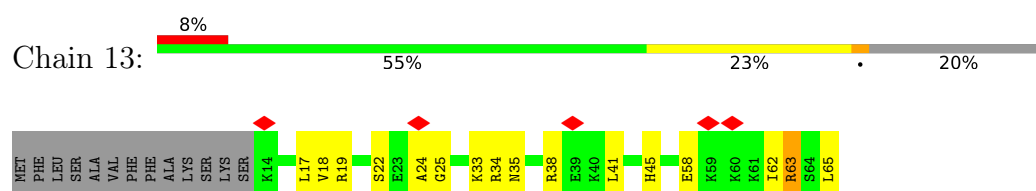
Chain Z3: 63% 11% 25%



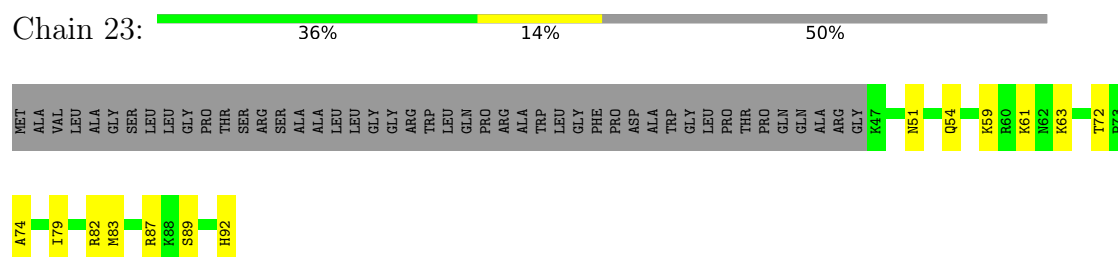
- Molecule 27: 39S ribosomal protein L32, mitochondrial



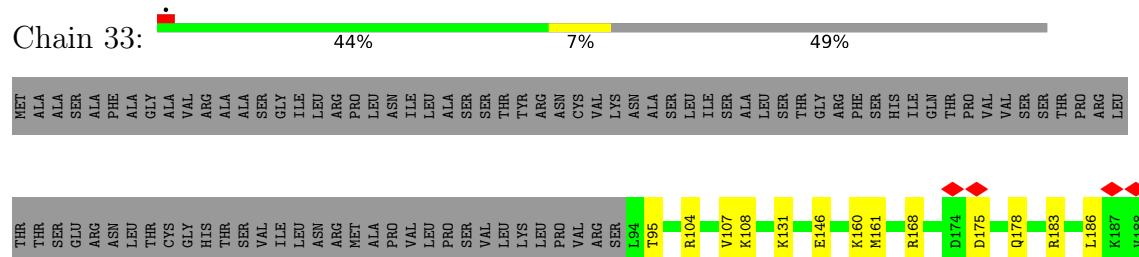
- Molecule 28: 39S ribosomal protein L33, mitochondrial



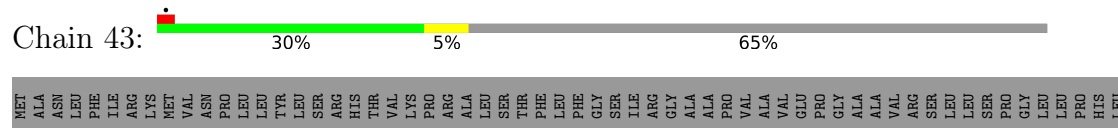
- Molecule 29: 39S ribosomal protein L34, mitochondrial



- Molecule 30: 39S ribosomal protein L35, mitochondrial



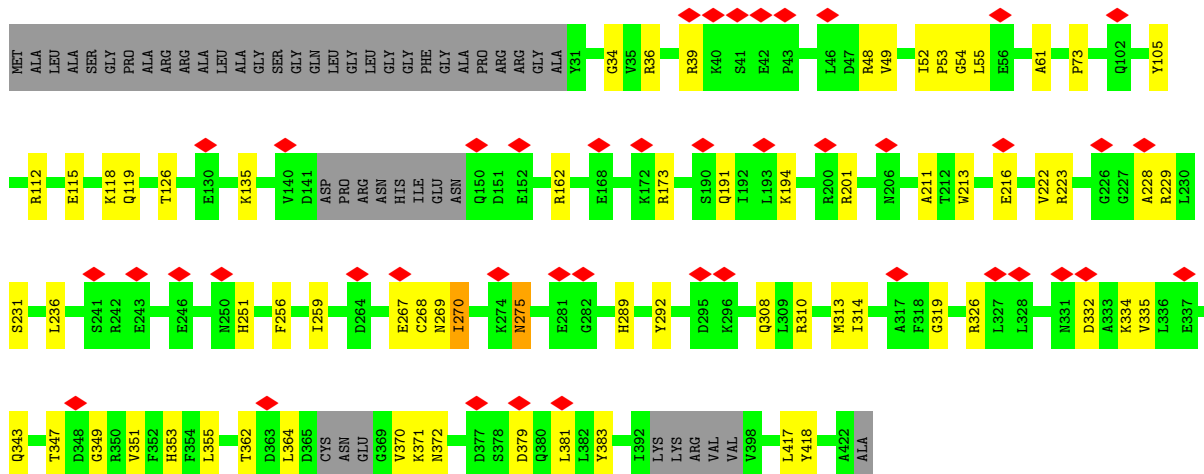
- Molecule 31: 39S ribosomal protein L36, mitochondrial





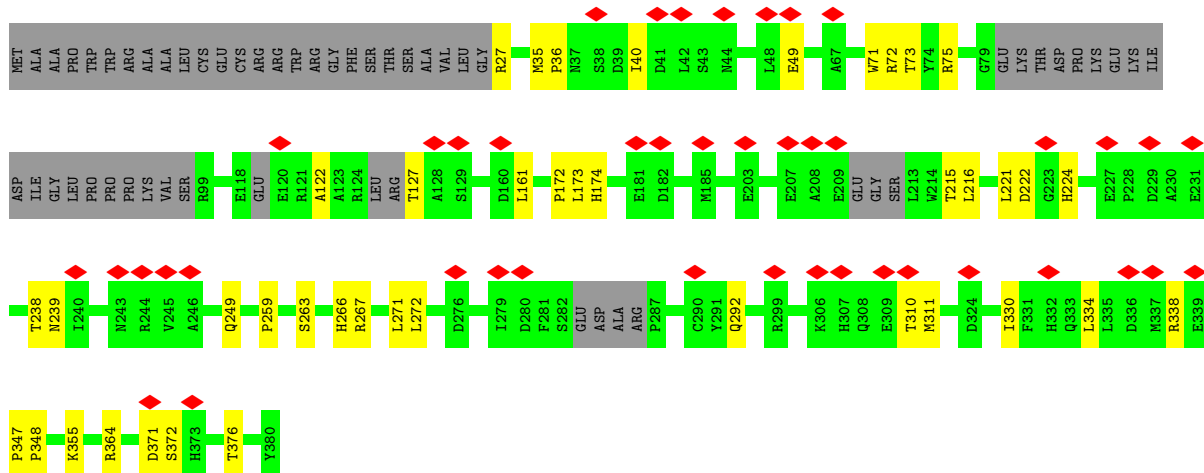
- Molecule 32: 39S ribosomal protein L37, mitochondrial

Chain 53:



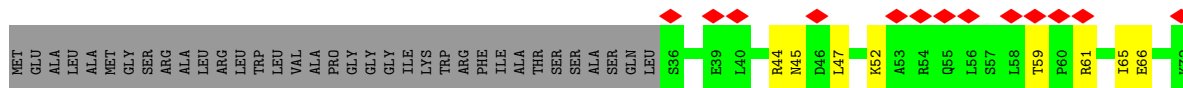
- Molecule 33: 39S ribosomal protein L38, mitochondrial

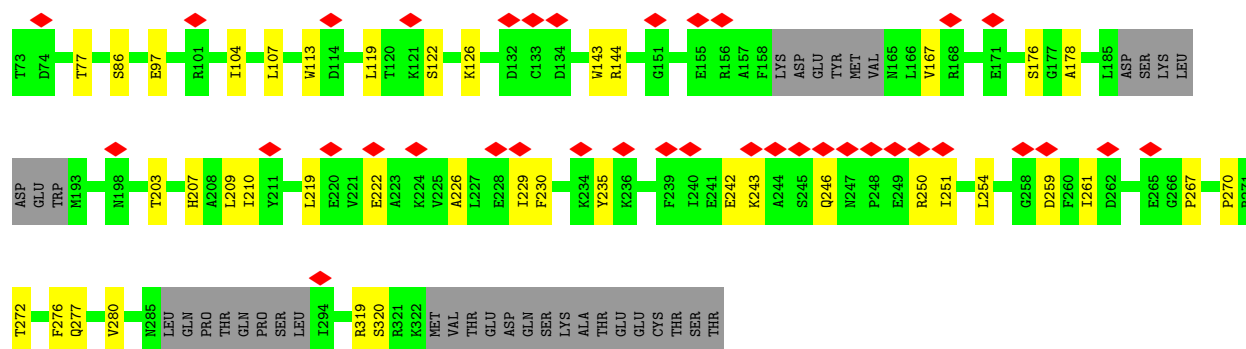
Chain 63:



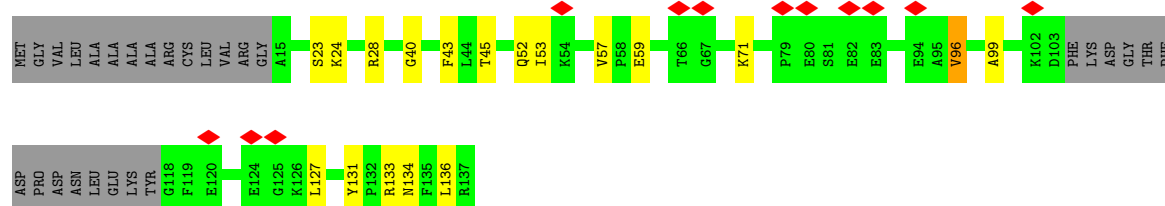
- Molecule 34: 39S ribosomal protein L39, mitochondrial

Chain 73:

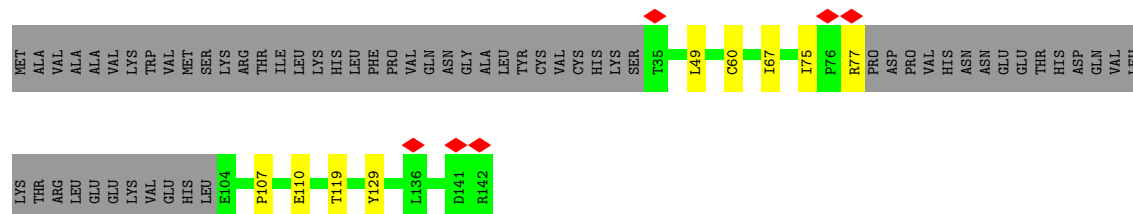




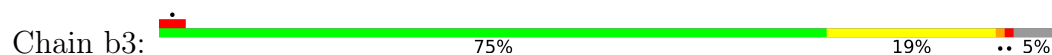
- Molecule 35: 39S ribosomal protein L41, mitochondrial



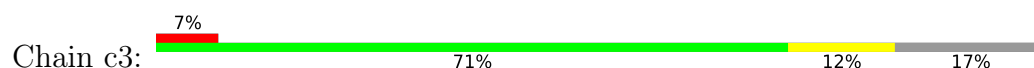
- Molecule 36: 39S ribosomal protein L42, mitochondrial

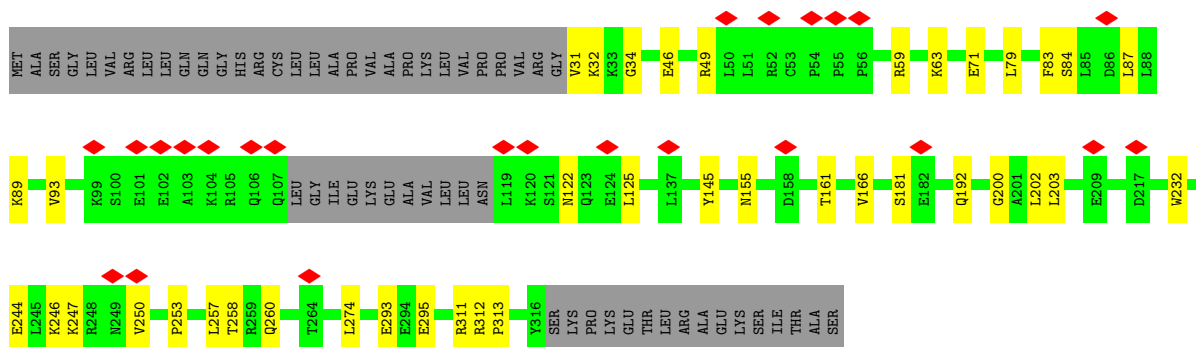


- Molecule 37: 39S ribosomal protein L43, mitochondrial

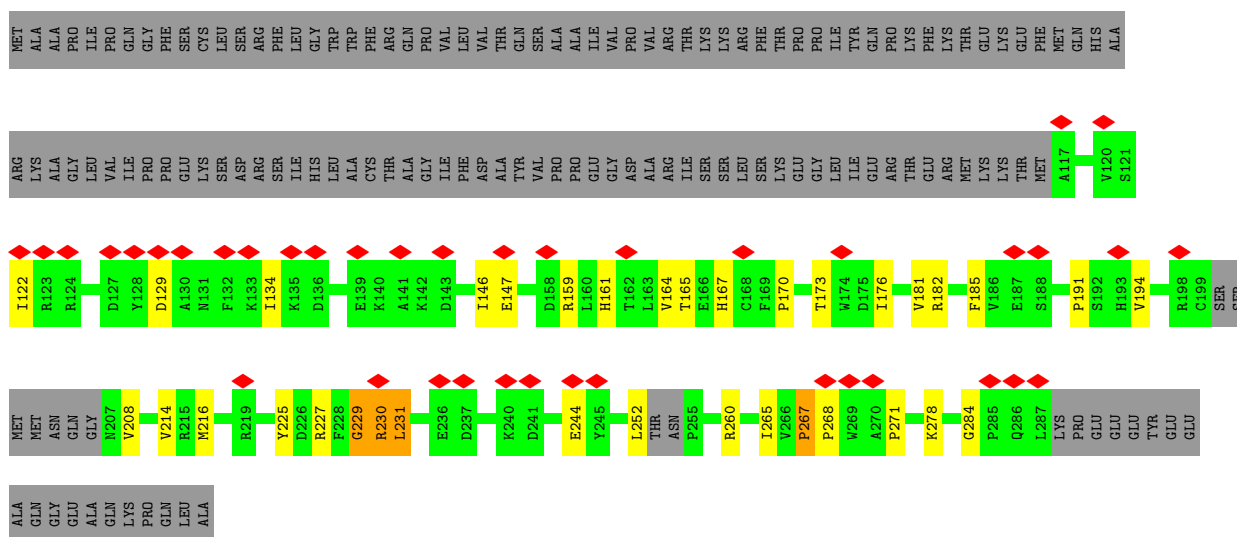


- Molecule 38: 39S ribosomal protein L44, mitochondrial

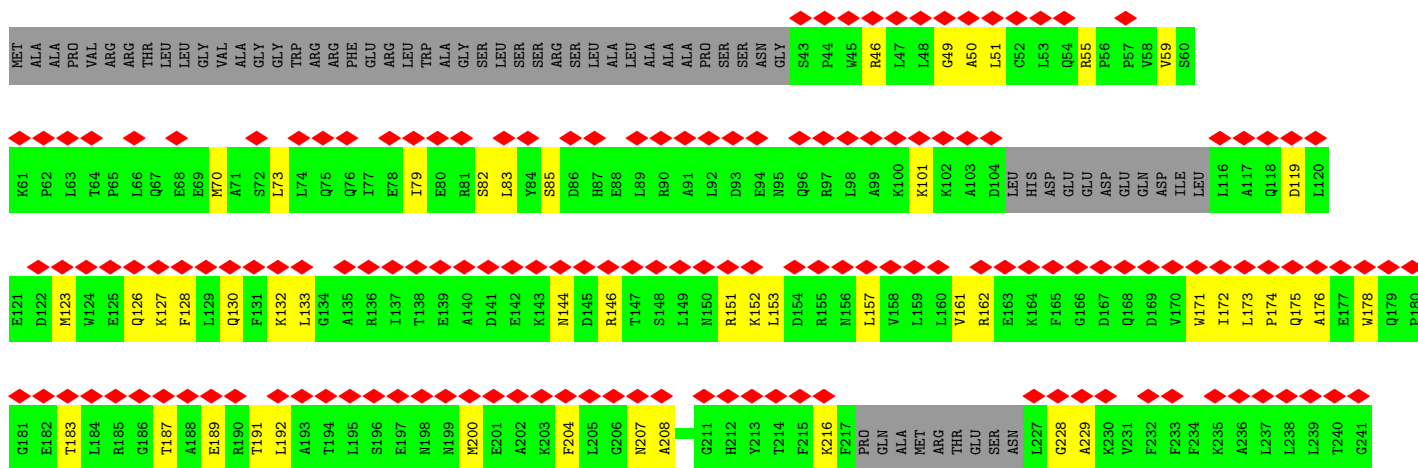


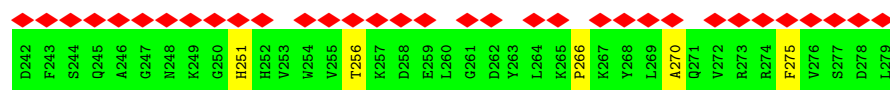


• Molecule 39: 39S ribosomal protein L45, mitochondrial

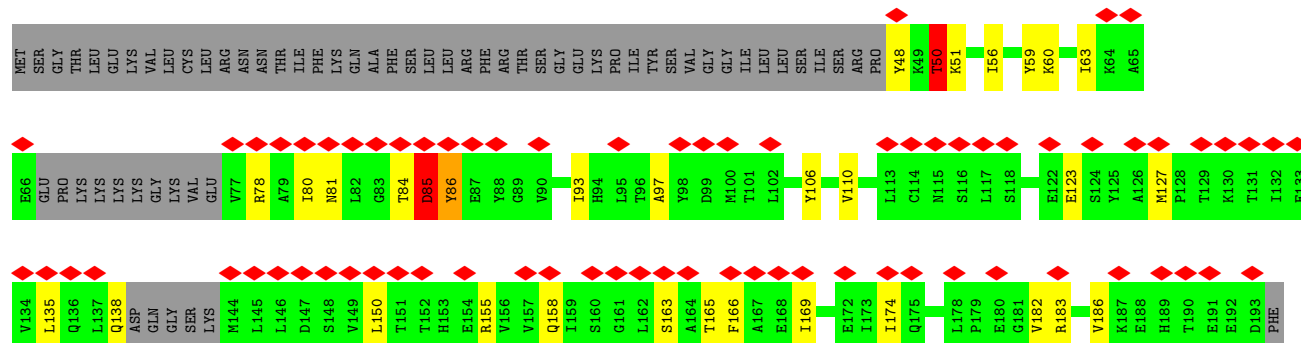
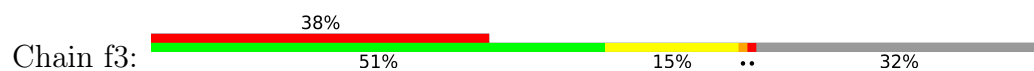


• Molecule 40: 39S ribosomal protein L46, mitochondrial

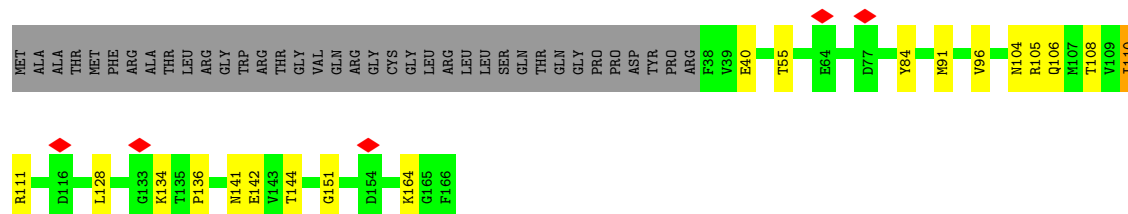




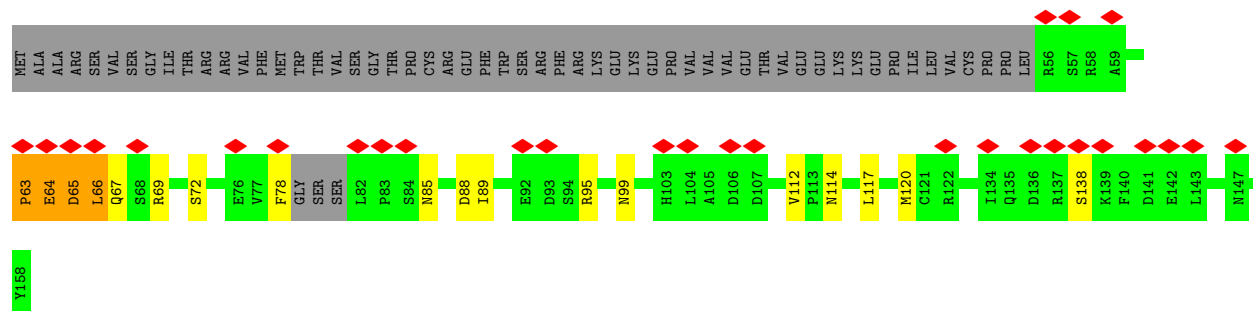
- Molecule 41: 39S ribosomal protein L48, mitochondrial



- Molecule 42: 39S ribosomal protein L49, mitochondrial

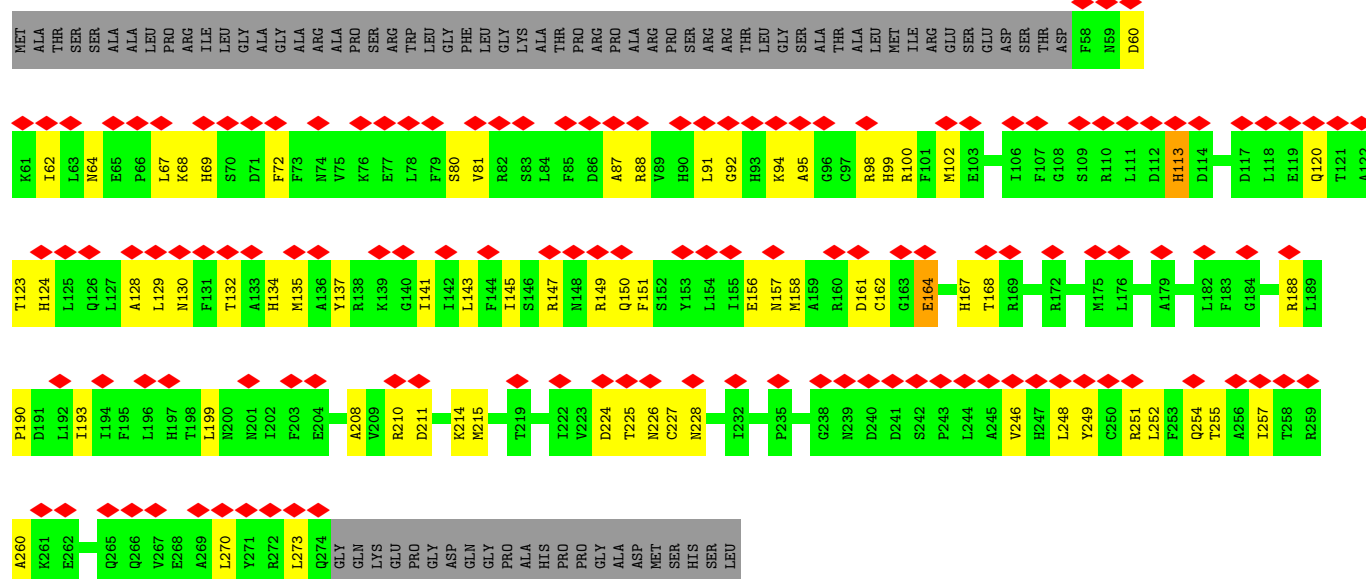


- Molecule 43: 39S ribosomal protein L50, mitochondrial

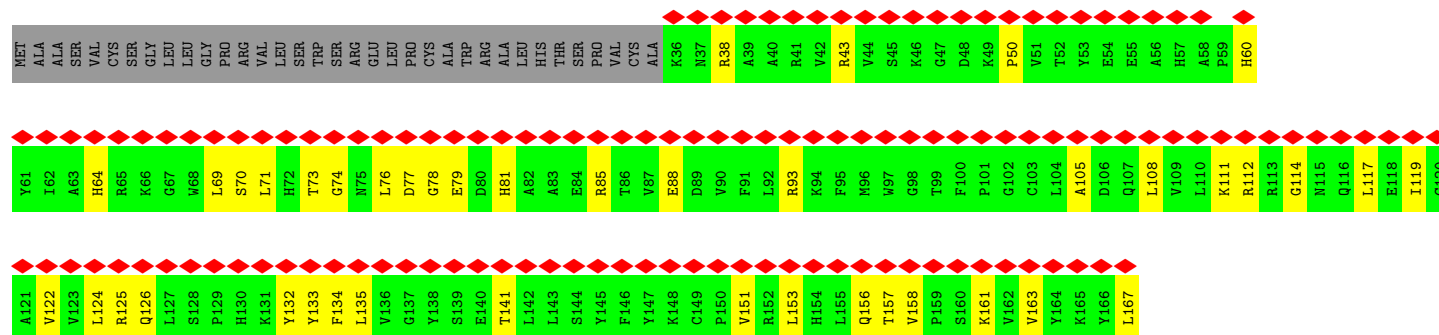
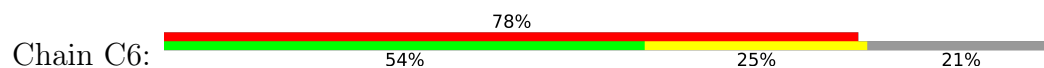


- Molecule 44: 39S ribosomal protein L51, mitochondrial

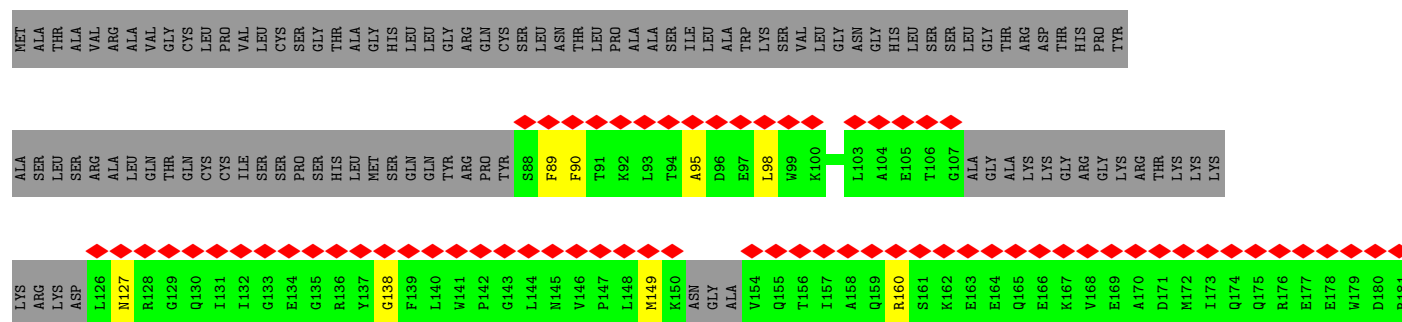
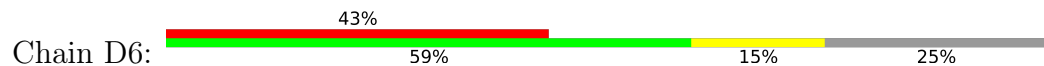


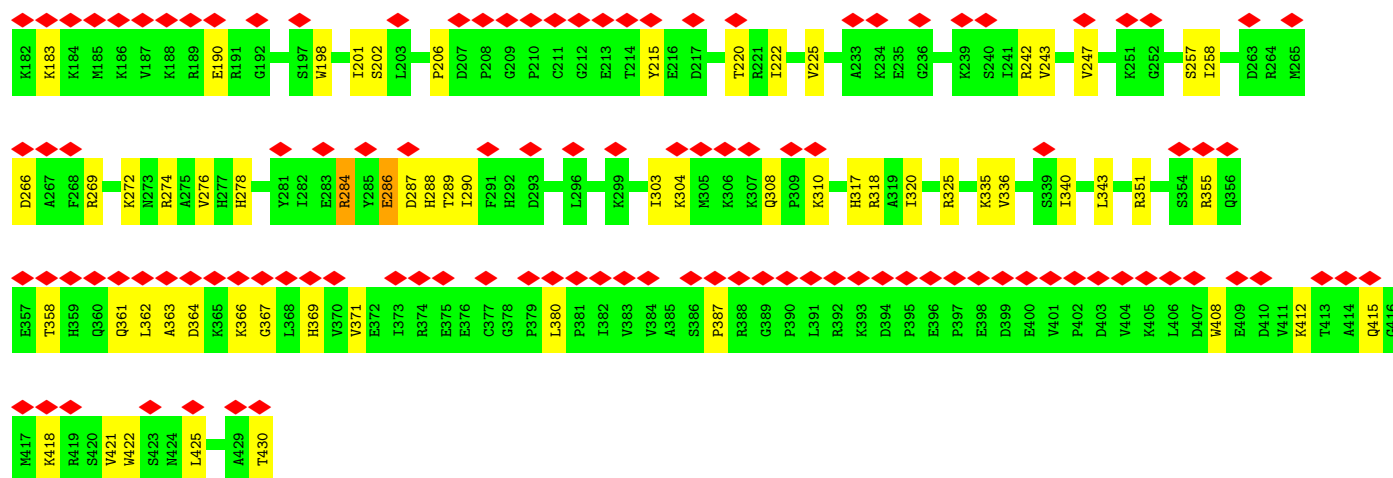


- Molecule 57: 28S ribosomal protein S24, mitochondrial

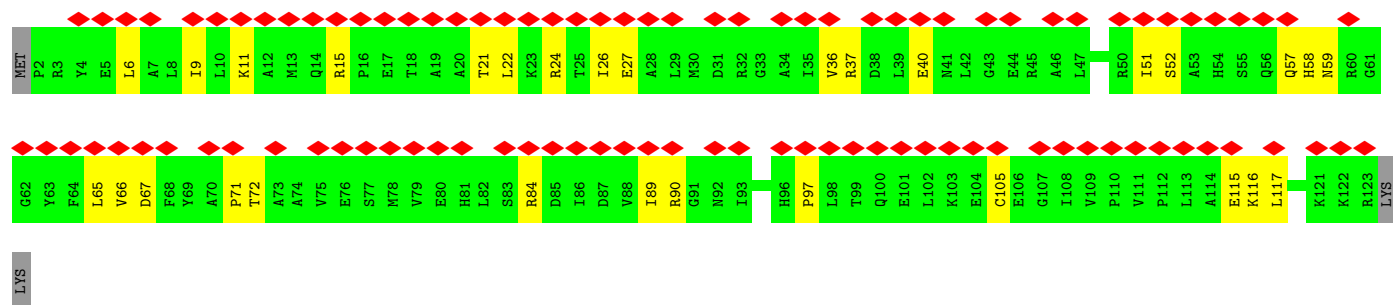
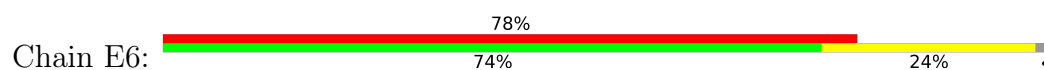


- Molecule 58: 28S ribosomal protein S5, mitochondrial

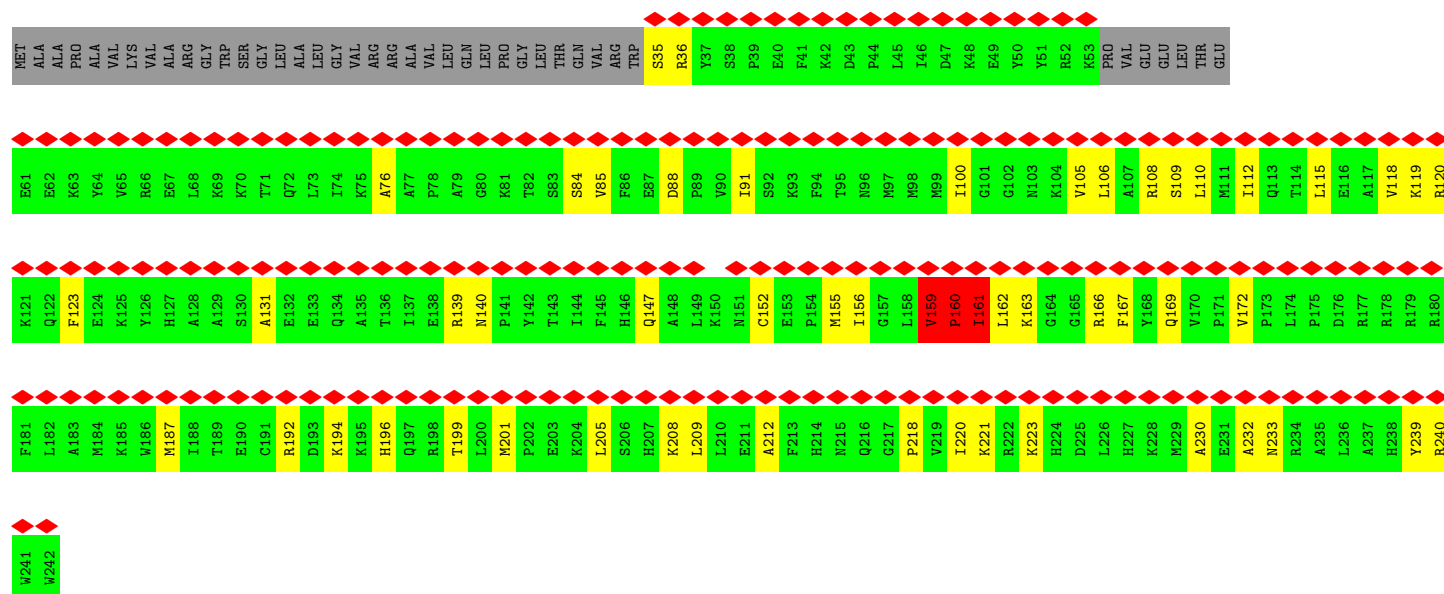
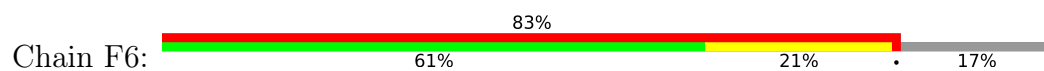




- Molecule 59: 28S ribosomal protein S6, mitochondrial

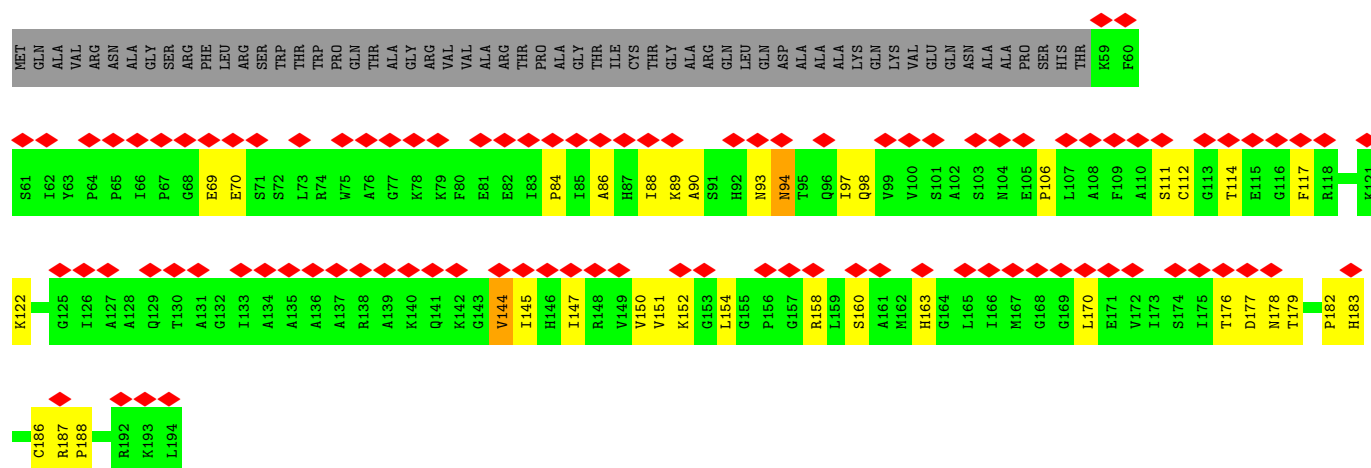


- Molecule 60: 28S ribosomal protein S7, mitochondrial

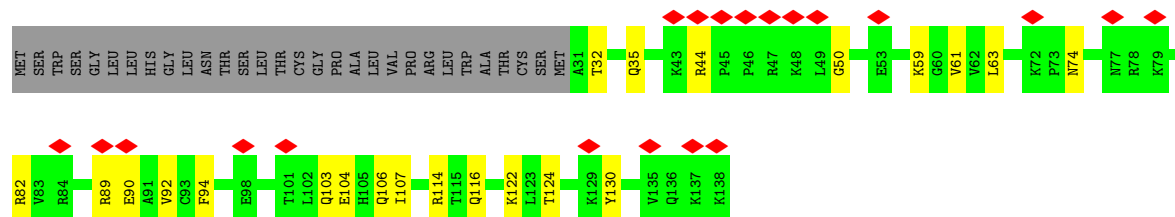


- Chain G6:

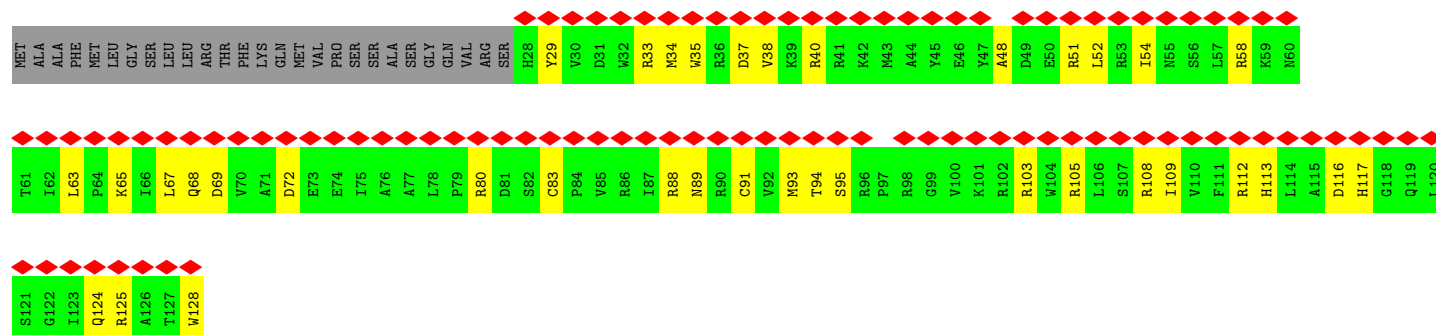
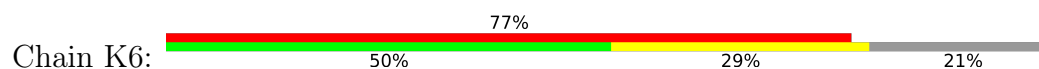




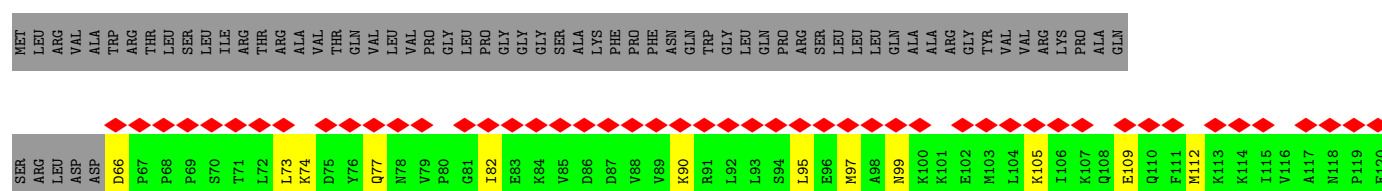
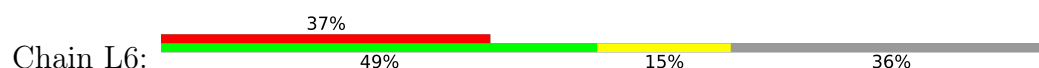
- Molecule 64: 28S ribosomal protein S12, mitochondrial

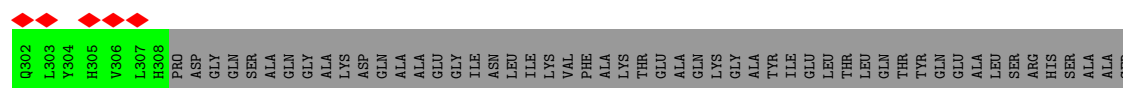


- Molecule 65: 28S ribosomal protein S14, mitochondrial

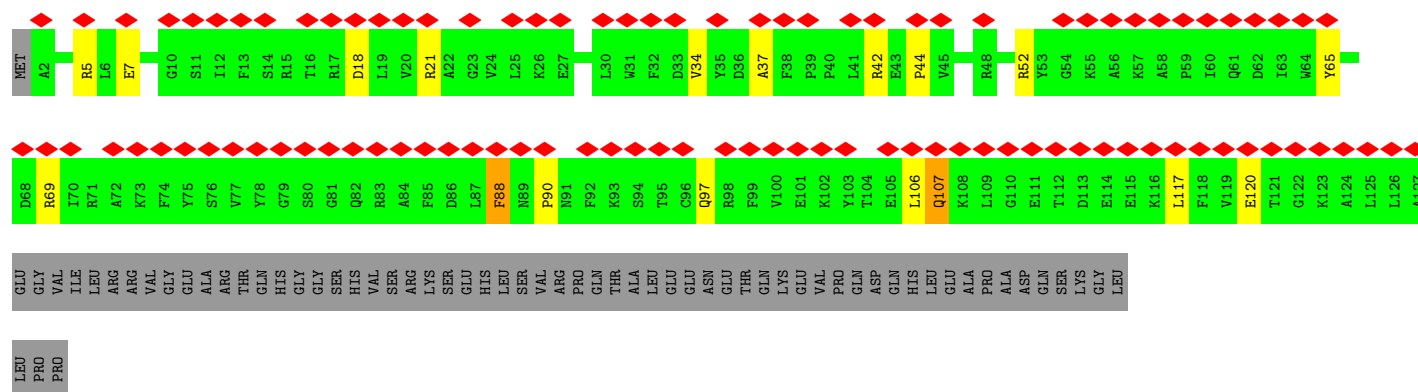


- Molecule 66: 28S ribosomal protein S15, mitochondrial

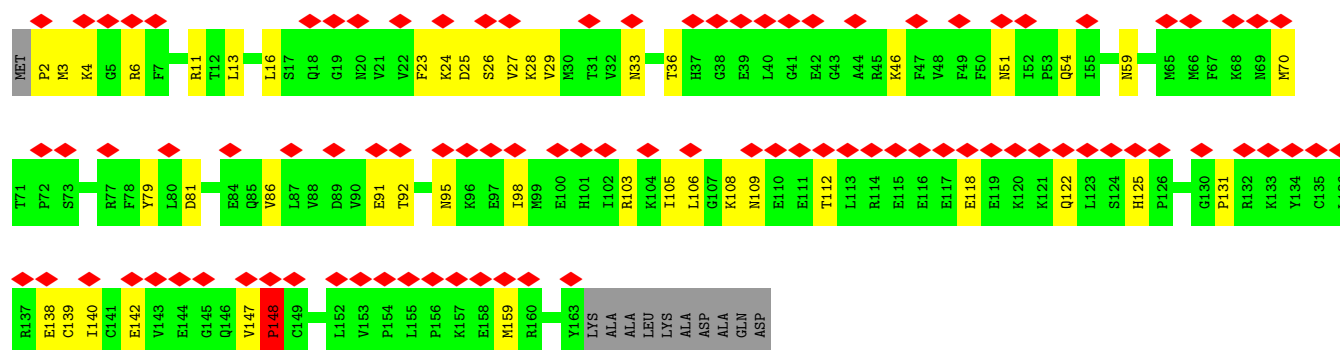




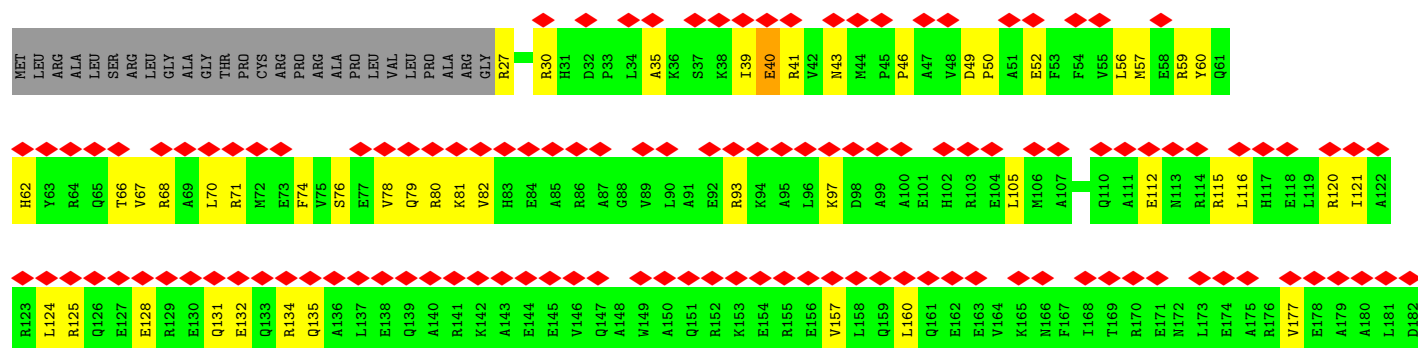
- Molecule 73: 28S ribosomal protein S23, mitochondrial



- Molecule 74: 28S ribosomal protein S25, mitochondrial

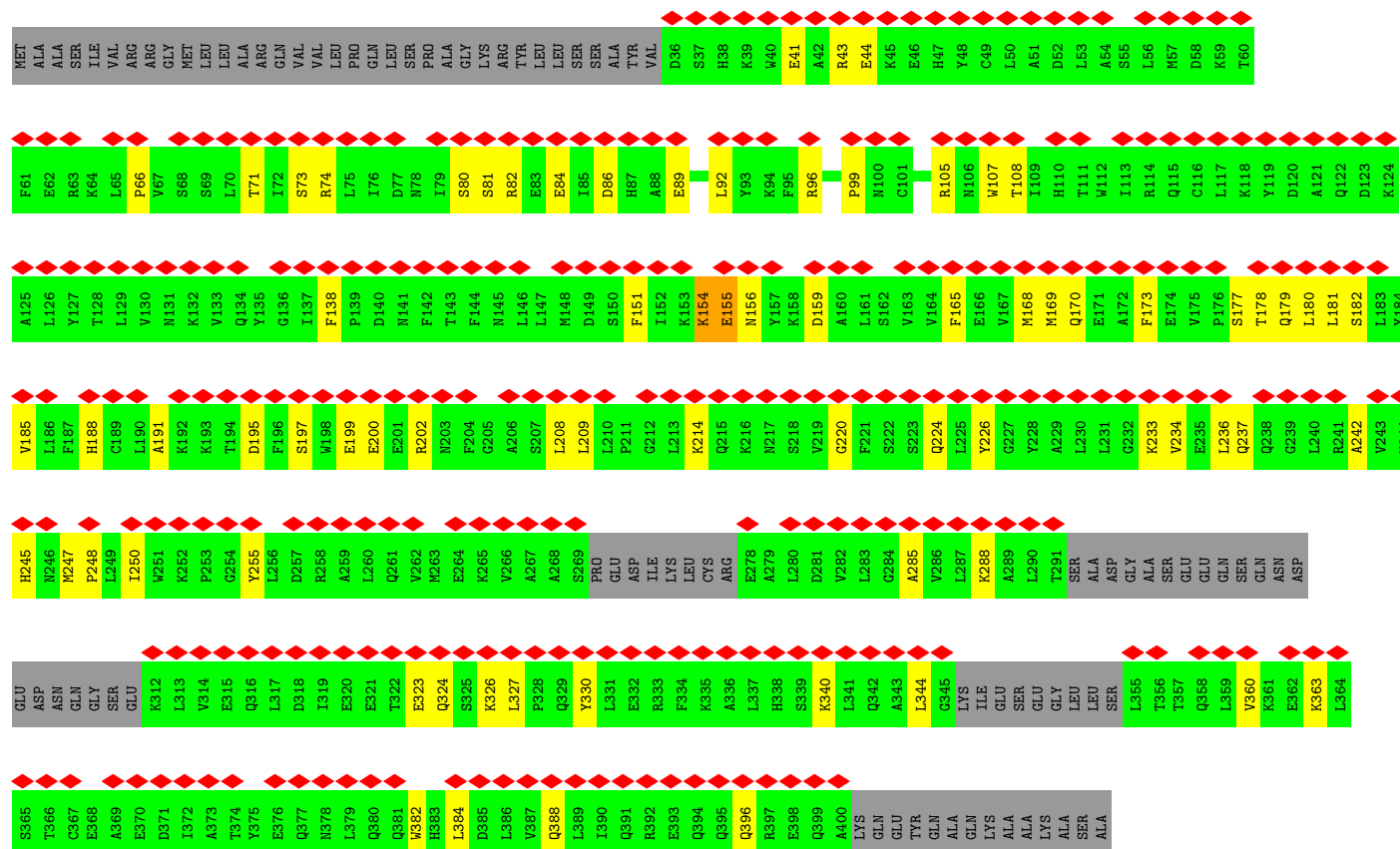
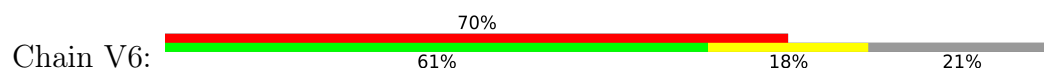


- Molecule 75: 28S ribosomal protein S26, mitochondrial

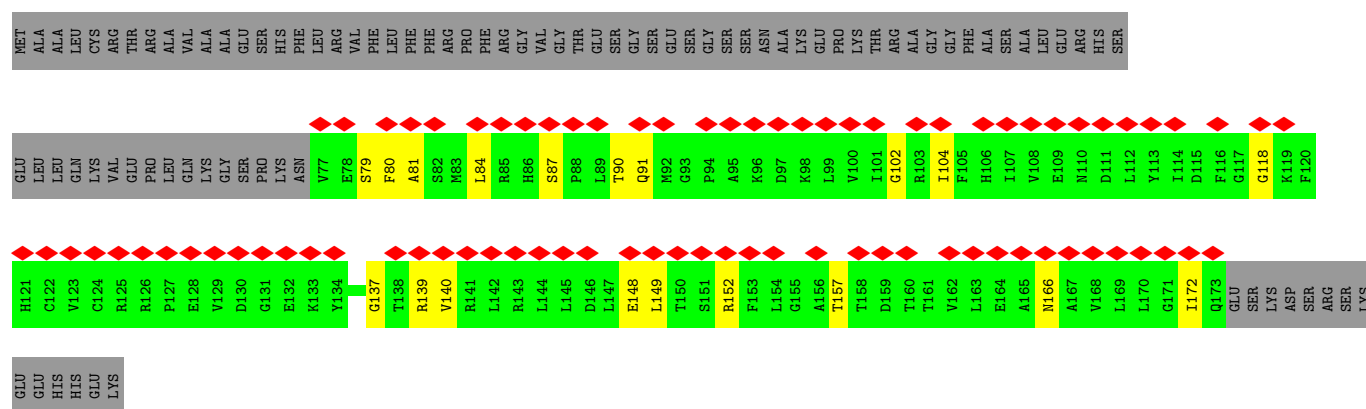
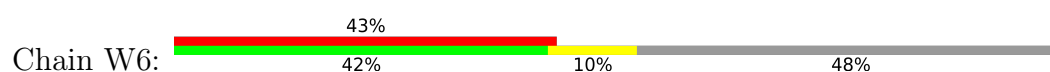




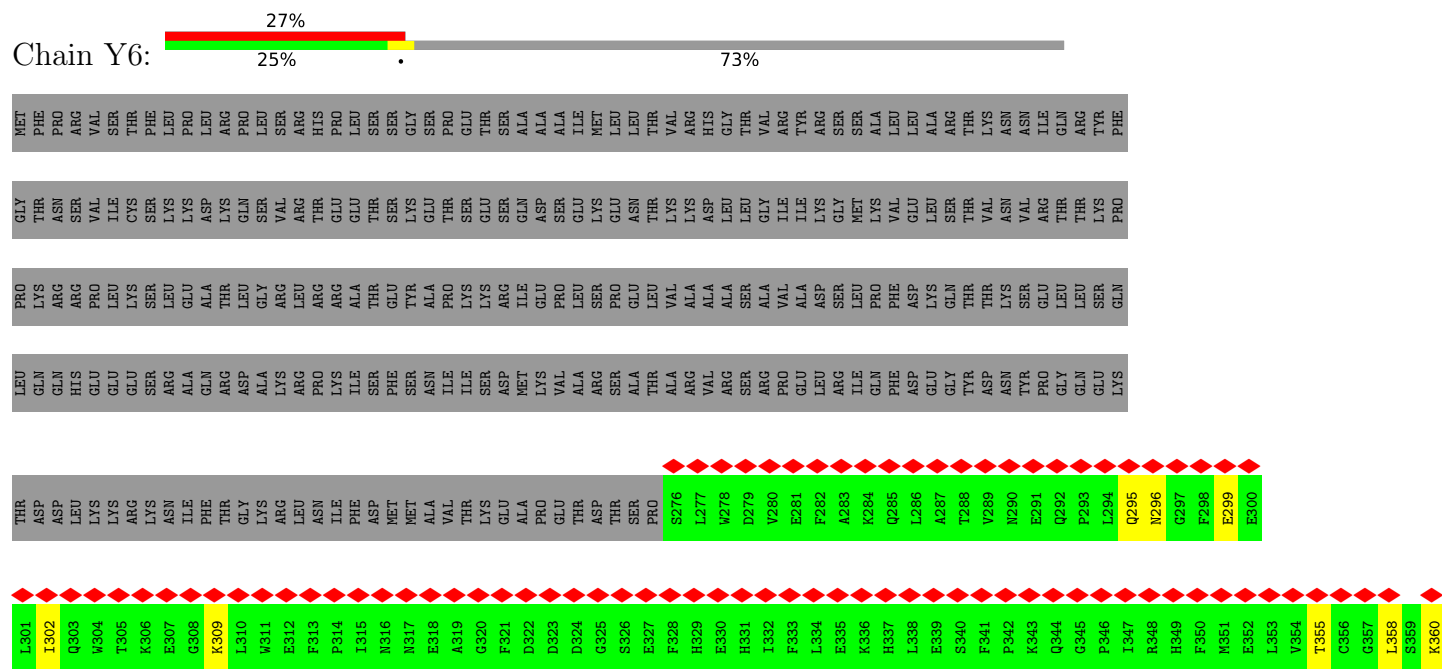
- Molecule 76: 28S ribosomal protein S27, mitochondrial

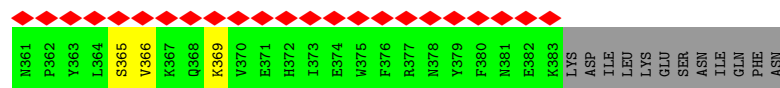


- Molecule 77: 28S ribosomal protein S28, mitochondrial

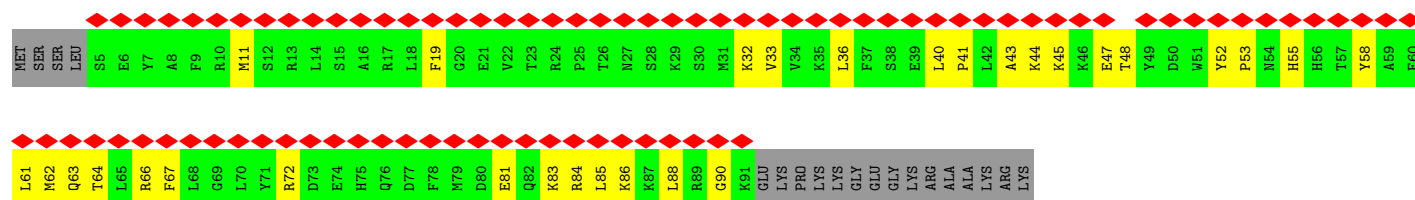
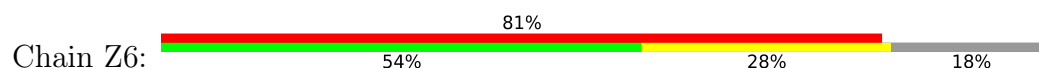


- Molecule 78: 28S ribosomal protein S29, mitochondrial

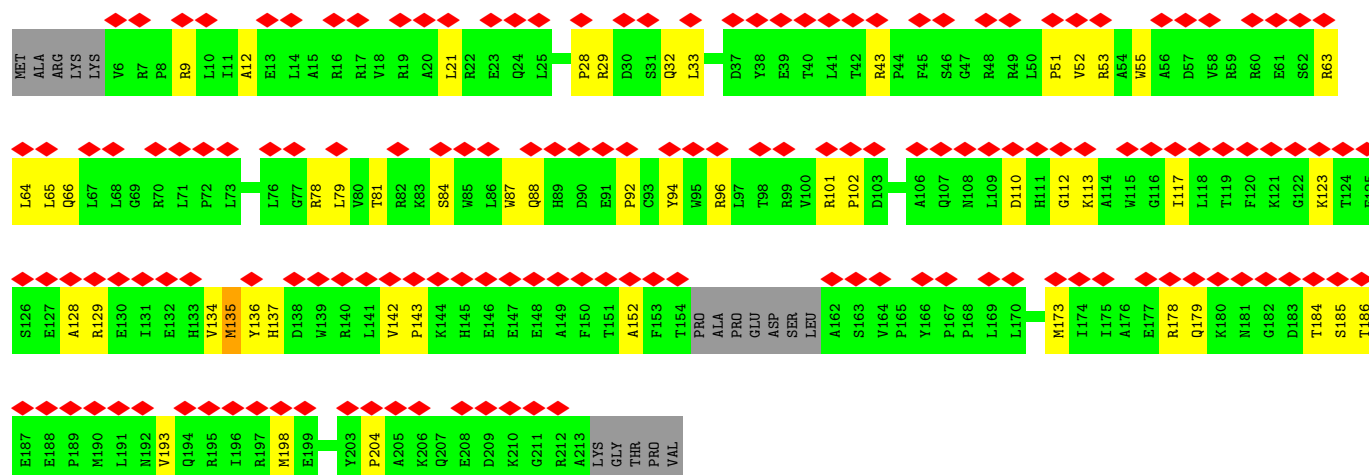
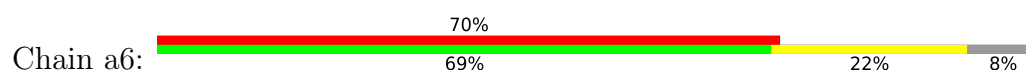




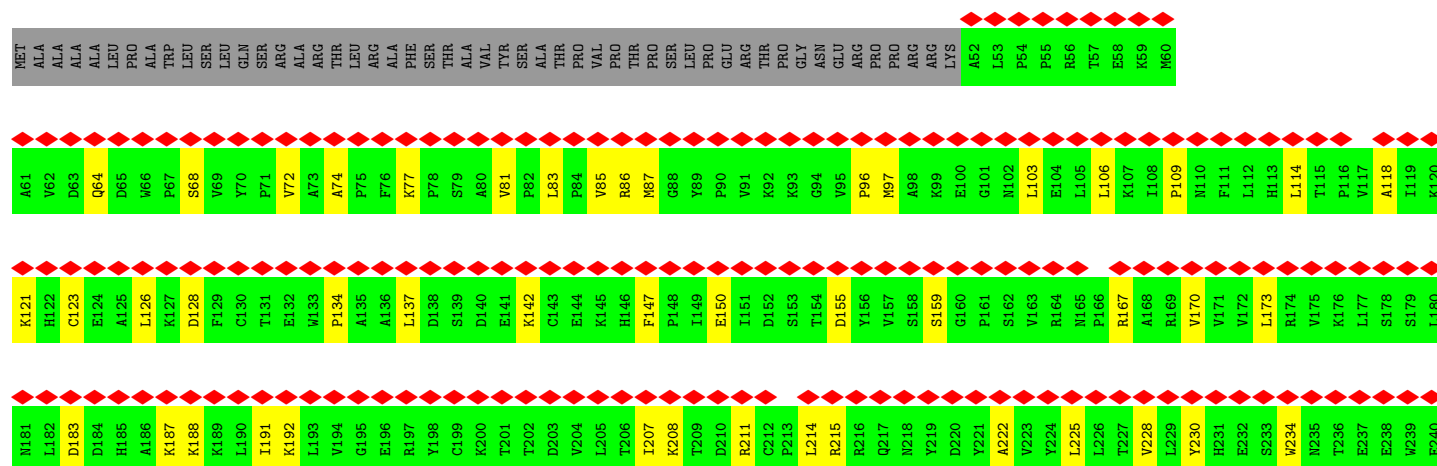
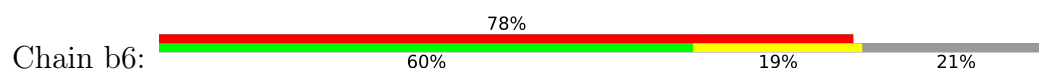
- Molecule 80: 28S ribosomal protein S33, mitochondrial

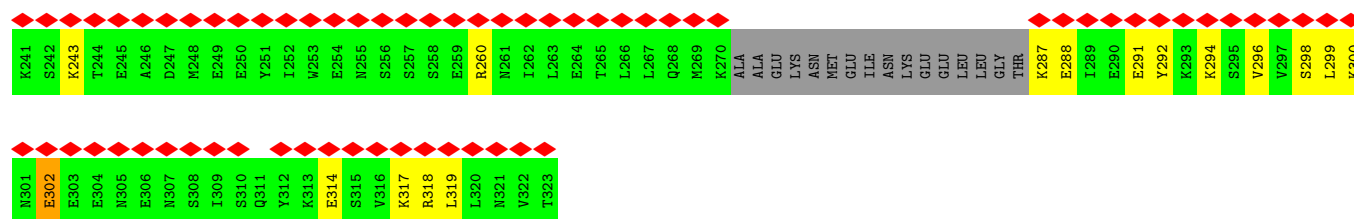


- Molecule 81: 28S ribosomal protein S34, mitochondrial

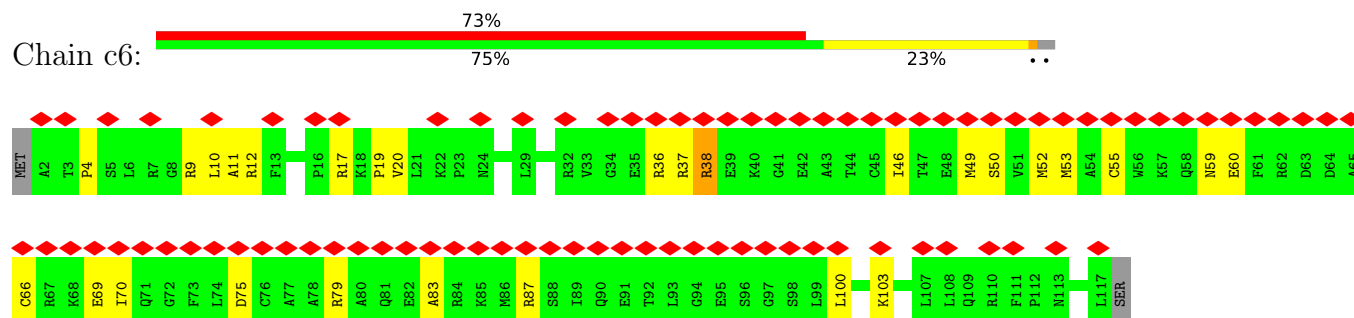


- Molecule 82: 28S ribosomal protein S35, mitochondrial

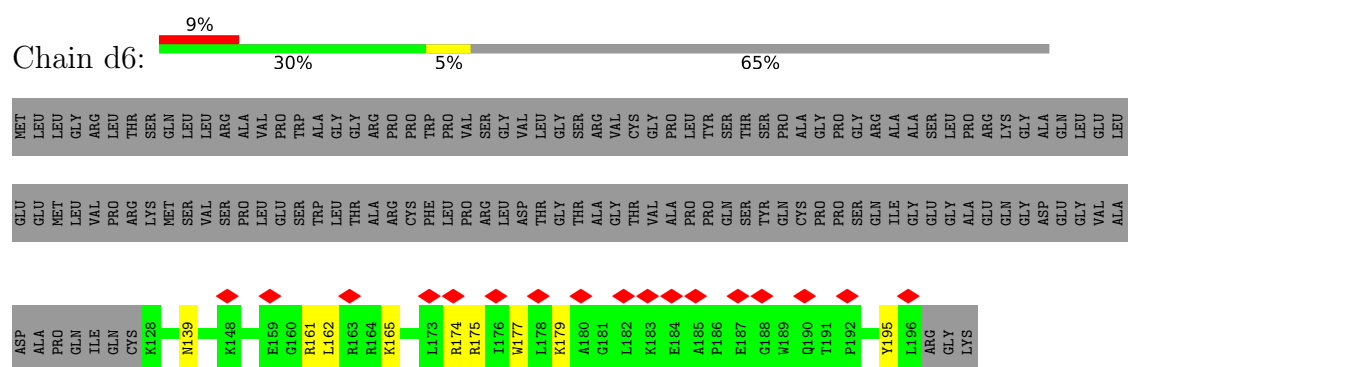




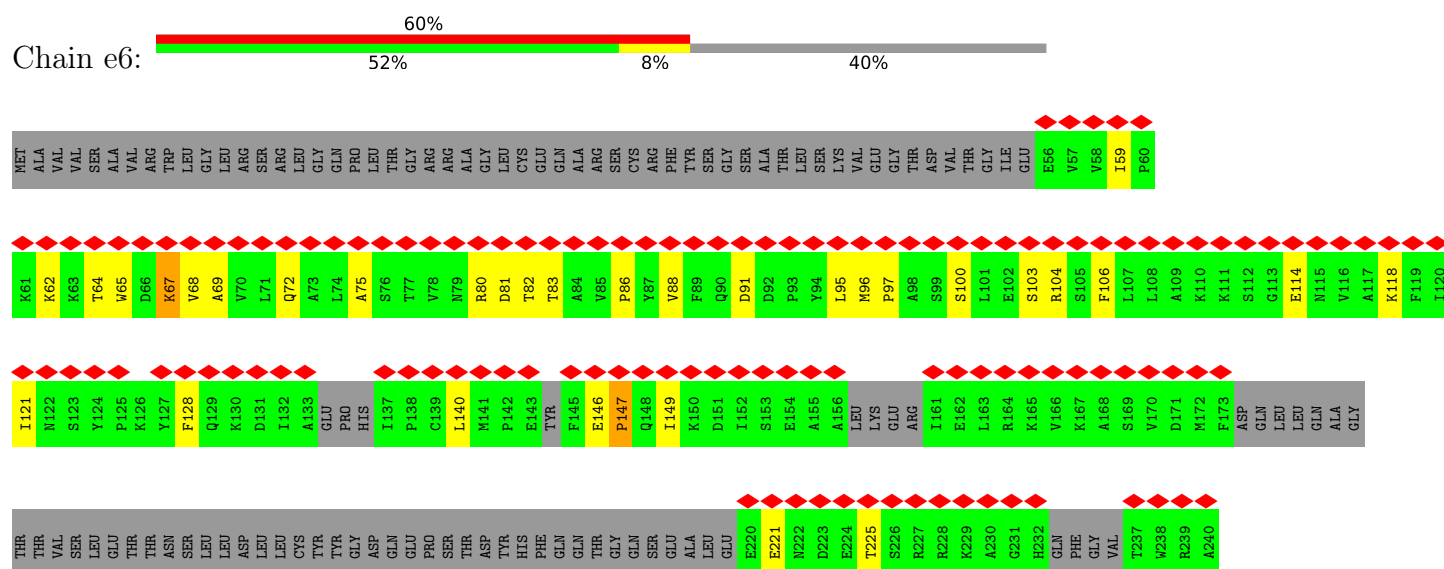
• Molecule 83: Coiled-coil-helix-coiled-coil-helix domain-containing protein 1

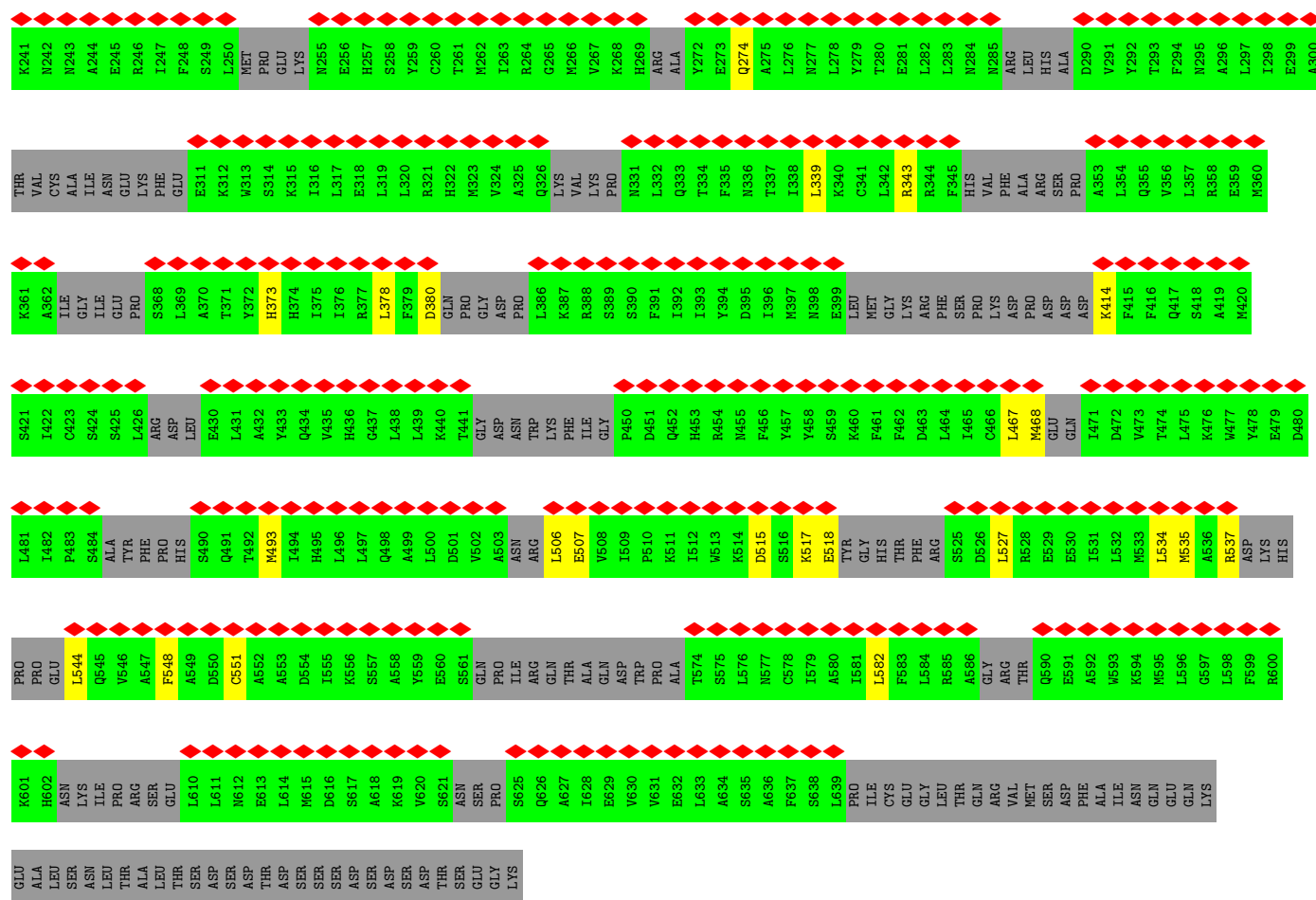


• Molecule 84: Aurora kinase A-interacting protein

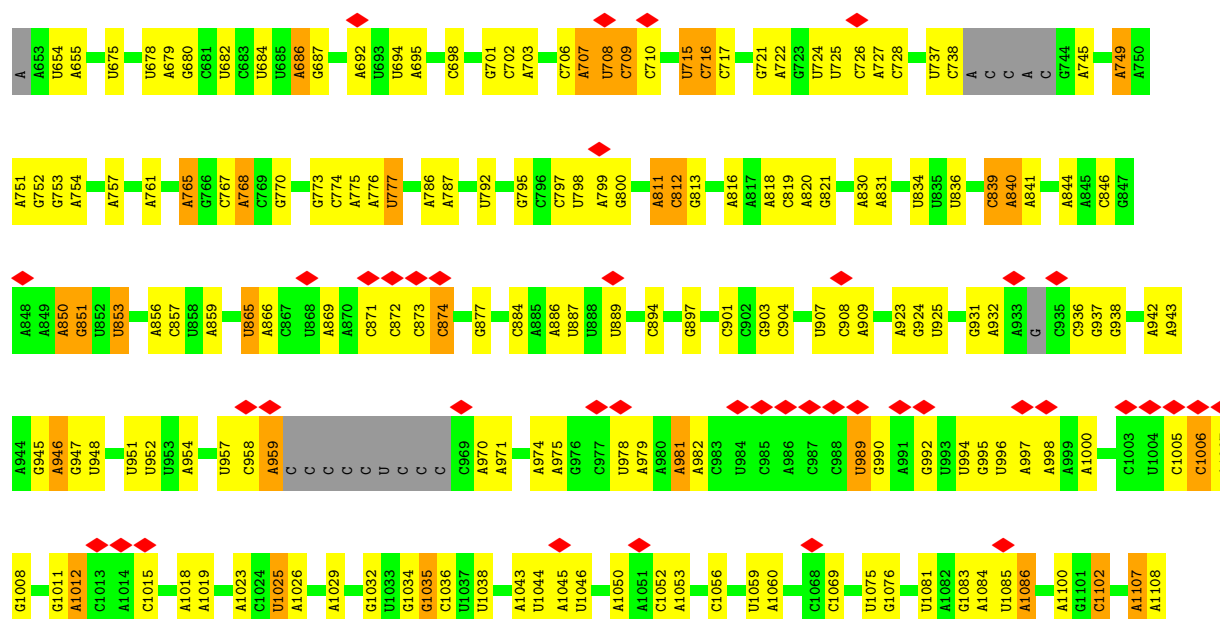


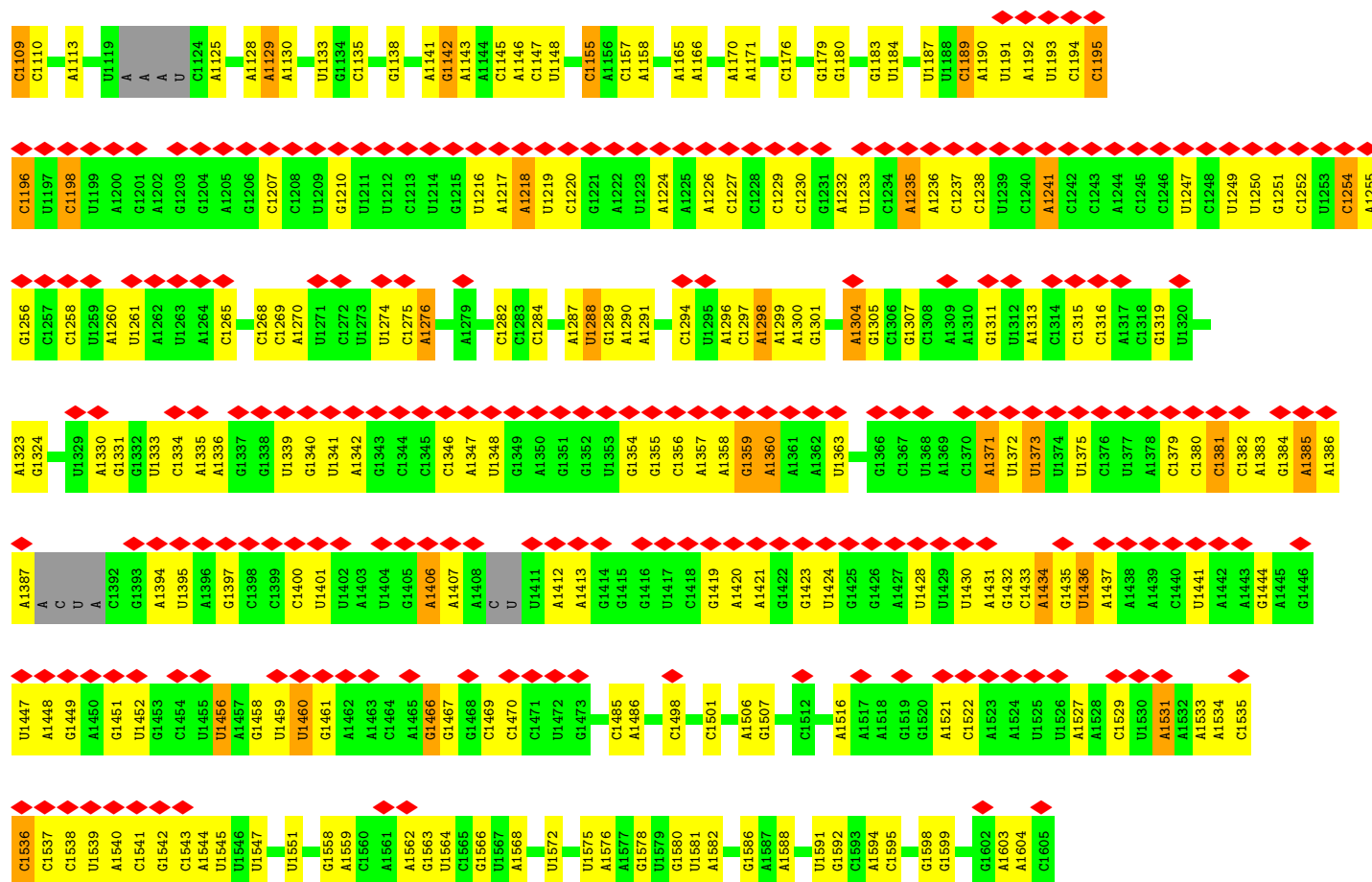
• Molecule 85: Pentatricopeptide repeat domain-containing protein 3, mitochondrial



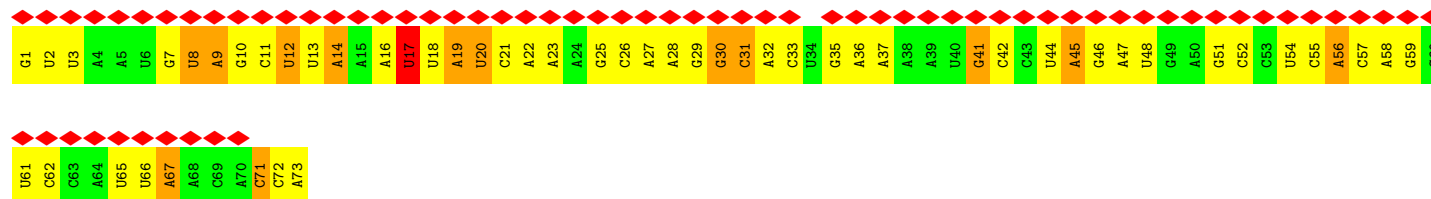


• Molecule 86: 12S rRNA

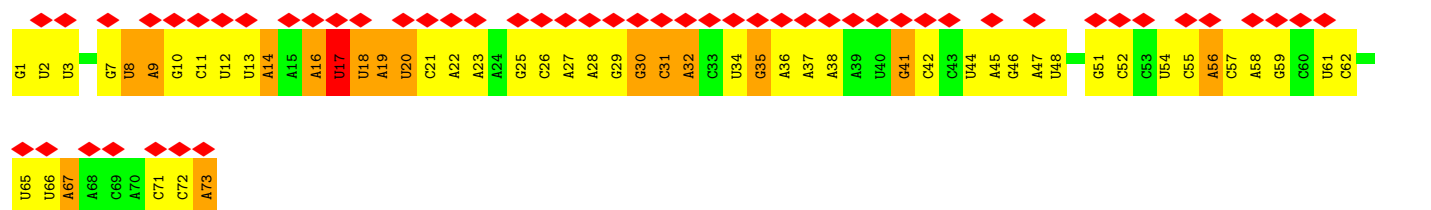
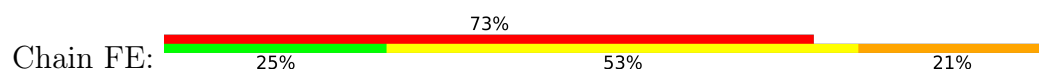




• Molecule 87: mt-tRNA



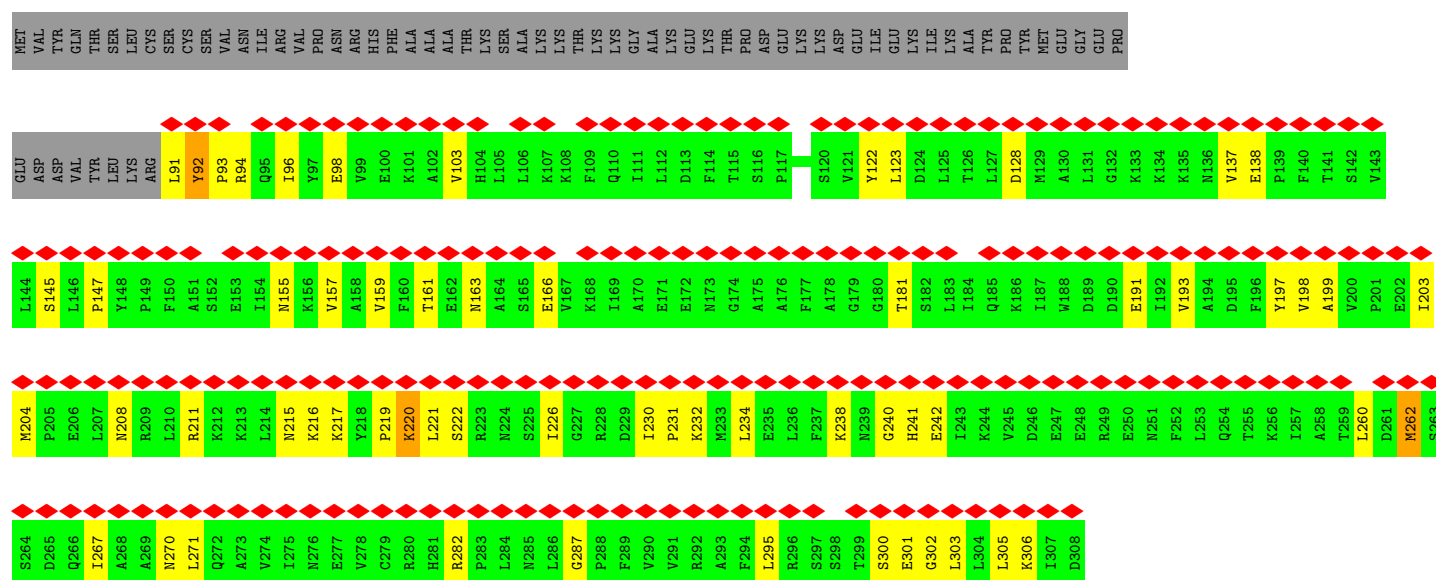
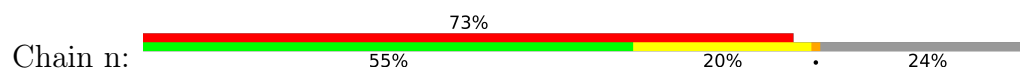
• Molecule 87: mt-tRNA



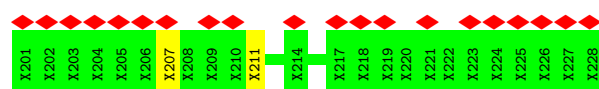
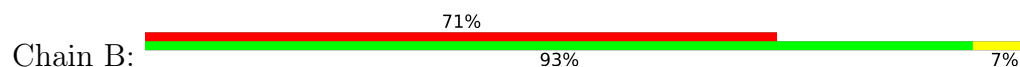
• Molecule 88: 39S ribosomal protein L40, mitochondrial



• Molecule 89: 39S ribosomal protein L1, mitochondrial



• Molecule 90: Unknown protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	19767	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	0.294	Depositor
Minimum map value	-0.153	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: MG, GCP, SPD, ZN, GDP

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	r1	0.49	2/5552 (0.0%)	1.19	36/7490 (0.5%)
3	8	0.29	0/197	0.50	0/305
3	A3	0.50	0/35697	0.50	14/55544 (0.0%)
4	B3	0.29	0/1328	0.39	0/2056
5	D3	0.43	0/1879	0.74	1/2527 (0.0%)
6	E3	0.49	0/2433	0.76	6/3299 (0.2%)
7	F3	0.50	0/2071	0.81	0/2817
8	D	3.49	3/665 (0.5%)	1.20	5/905 (0.6%)
8	H3	0.40	0/798	0.80	0/1073
9	I3	0.39	0/1308	0.82	0/1761
10	J3	0.42	0/1077	0.87	0/1452
11	K3	0.54	0/1495	0.74	1/2029 (0.0%)
12	L3	0.46	0/904	0.75	2/1218 (0.2%)
13	M3	0.52	1/2359 (0.0%)	0.82	2/3185 (0.1%)
14	N3	0.50	0/1697	0.82	3/2281 (0.1%)
15	O3	0.51	0/1269	0.80	0/1708
16	P3	0.47	0/1103	0.82	0/1491
17	Q3	0.43	0/1863	0.76	2/2509 (0.1%)
18	R3	0.57	0/1174	0.73	1/1572 (0.1%)
19	S3	0.52	0/1276	0.76	0/1729
20	T3	0.49	0/1402	0.73	1/1886 (0.1%)
21	U3	0.54	0/946	0.75	0/1283
22	V3	0.40	0/1590	0.83	3/2151 (0.1%)
23	W3	0.54	0/893	0.71	0/1204
24	X3	0.42	0/2081	0.86	11/2812 (0.4%)
25	Y3	0.51	1/1552 (0.1%)	0.71	0/2079
26	Z3	0.50	0/1003	0.69	0/1354
27	03	0.45	0/895	0.79	0/1201
28	13	0.45	0/438	0.94	0/583
29	23	0.56	0/382	0.68	0/507
30	33	0.55	0/852	0.67	0/1136
31	43	0.53	0/329	0.64	0/435

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	53	0.42	1/3154 (0.0%)	0.74	3/4295 (0.1%)
33	63	0.43	0/2722	0.78	0/3709
34	73	0.40	0/2207	0.75	1/2978 (0.0%)
35	93	0.41	0/896	0.82	3/1205 (0.2%)
36	a3	0.43	0/709	0.68	0/963
37	b3	0.48	0/1202	0.75	1/1626 (0.1%)
38	c3	0.42	0/2264	0.72	0/3059
39	d3	0.42	0/1385	0.95	8/1877 (0.4%)
40	e3	0.32	0/1797	0.76	0/2422
41	f3	0.44	0/1055	1.09	7/1427 (0.5%)
42	g3	0.55	0/1102	0.77	0/1503
43	h3	0.38	0/847	0.86	4/1150 (0.3%)
44	i3	0.55	0/849	0.76	0/1135
45	j3	0.42	0/698	0.73	0/940
46	k3	0.34	0/665	0.83	0/897
47	l3	0.43	0/226	0.69	0/299
48	m3	0.37	0/379	0.77	0/510
49	o3	0.53	0/818	0.70	0/1097
50	p3	0.34	0/1071	0.67	2/1433 (0.1%)
51	q3	0.37	0/1107	0.70	0/1498
52	r3	0.51	0/1238	0.77	1/1676 (0.1%)
53	s3	0.47	0/3114	0.94	3/4225 (0.1%)
54	u3	0.43	0/46	0.31	0/69
55	A5	0.34	0/135	0.99	1/185 (0.5%)
56	B6	0.36	0/1811	0.80	0/2451
57	C6	0.28	0/1112	0.65	0/1505
58	D6	0.38	0/2607	0.82	4/3498 (0.1%)
59	E6	0.35	0/989	0.80	0/1335
60	F6	0.40	1/1708 (0.1%)	0.83	7/2291 (0.3%)
61	G6	0.33	0/2570	0.76	0/3443
62	H6	0.30	0/1019	0.80	2/1379 (0.1%)
63	I6	0.33	0/1031	0.84	2/1390 (0.1%)
64	J6	0.58	1/854 (0.1%)	0.87	0/1148
65	K6	0.33	0/879	0.79	0/1182
66	L6	0.31	0/1406	0.76	1/1878 (0.1%)
67	M6	0.41	0/941	0.98	3/1265 (0.2%)
68	N6	0.50	1/864 (0.1%)	0.85	3/1169 (0.3%)
69	O6	0.36	0/1580	0.84	1/2150 (0.0%)
70	P6	0.36	0/791	0.84	0/1062
71	Q6	0.38	0/752	0.87	1/1001 (0.1%)
72	R6	0.33	0/2050	0.84	3/2770 (0.1%)
73	S6	0.59	1/1069 (0.1%)	1.12	8/1441 (0.6%)
74	T6	0.40	0/1361	0.89	1/1829 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	U6	0.33	1/1482 (0.1%)	0.75	2/1987 (0.1%)
76	V6	0.30	0/2758	0.78	6/3724 (0.2%)
77	W6	0.31	0/778	0.82	0/1048
78	X6	0.30	0/2596	0.75	0/3519
79	Y6	0.29	0/943	0.70	0/1274
80	Z6	0.27	0/757	0.75	2/1011 (0.2%)
81	a6	0.39	1/1727 (0.1%)	0.85	2/2338 (0.1%)
82	b6	0.31	0/2121	0.83	4/2873 (0.1%)
83	c6	0.32	0/939	0.74	0/1256
84	d6	0.40	0/621	0.78	0/820
85	e6	0.28	0/2859	0.81	3/3864 (0.1%)
86	A6	0.32	0/22053	0.44	0/34324
87	24	0.52	6/1731 (0.3%)	0.51	1/2693 (0.0%)
87	FE	0.52	6/1731 (0.3%)	0.51	1/2693 (0.0%)
88	A	0.34	0/1403	0.91	6/1880 (0.3%)
89	n	3.25	9/1776 (0.5%)	0.90	3/2397 (0.1%)
All	All	0.58	35/179863 (0.0%)	0.71	188/255648 (0.1%)

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	r1	0	23
2	Y2	0	2
5	D3	0	1
6	E3	0	5
7	F3	0	2
8	D	0	2
8	H3	0	1
9	I3	0	1
10	J3	0	2
11	K3	0	2
13	M3	0	4
14	N3	0	2
15	O3	0	1
17	Q3	0	1
18	R3	0	1
20	T3	0	1
22	V3	0	2
24	X3	0	1

Continued on next page...

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Mol	Chain	#Chirality outliers	#Planarity outliers
26	Z3	0	1
27	03	0	2
28	13	0	2
32	53	0	4
33	63	0	2
35	93	0	1
38	c3	0	1
39	d3	0	5
41	f3	0	4
42	g3	0	1
43	h3	0	2
44	i3	0	1
45	j3	0	1
49	o3	0	1
51	q3	0	1
53	s3	0	2
56	B6	0	1
58	D6	0	4
60	F6	0	4
61	G6	0	1
63	I6	0	2
64	J6	0	1
68	N6	0	1
69	O6	0	3
70	P6	0	3
72	R6	0	3
73	S6	0	1
75	U6	0	2
76	V6	0	2
81	a6	0	1
82	b6	0	1
83	c6	0	1
85	e6	0	2
88	A	0	6
89	n	0	1
All	All	0	125

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
89	n	220	LYS	CE-NZ	104.36	4.62	1.49
8	D	194	PHE	CB-CG	88.76	3.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
89	n	92	TYR	CD1-CE1	44.49	2.72	1.38
89	n	92	TYR	CD2-CE2	42.39	2.65	1.38
89	n	92	TYR	CE2-CZ	32.60	2.16	1.38
89	n	92	TYR	CE1-CZ	32.46	2.16	1.38
89	n	92	TYR	CG-CD2	29.02	2.00	1.39
89	n	92	TYR	CG-CD1	28.80	1.99	1.39
73	S6	90	PRO	CG-CD	-14.37	1.01	1.50
64	J6	104	GLU	CA-C	9.88	1.66	1.52
68	N6	70	PRO	CG-CD	-9.32	1.19	1.50
1	r1	583	VAL	C-N	9.02	1.41	1.33
87	FE	17	U	C2-N3	8.57	1.54	1.37
87	24	17	U	C2-N3	8.57	1.54	1.37
87	FE	17	U	N3-C4	8.30	1.55	1.38
87	24	17	U	N3-C4	8.28	1.55	1.38
25	Y3	123	ARG	C-N	-8.08	1.19	1.33
87	FE	17	U	N1-C2	7.98	1.54	1.38
87	24	17	U	N1-C2	7.94	1.54	1.38
8	D	194	PHE	CG-CD2	7.86	1.55	1.38
1	r1	683	ASP	CA-C	7.58	1.62	1.52
87	24	17	U	N1-C6	7.56	1.53	1.38
8	D	194	PHE	CG-CD1	7.55	1.54	1.38
87	FE	17	U	N1-C6	7.54	1.53	1.38
60	F6	159	VAL	C-N	7.50	1.51	1.33
13	M3	61	THR	C-N	-6.81	1.19	1.33
89	n	230	ILE	C-N	6.45	1.39	1.33
87	24	17	U	C4-C5	6.30	1.56	1.43
87	FE	17	U	C4-C5	6.30	1.56	1.43
87	24	17	U	C5-C6	5.64	1.45	1.34
89	n	204	MET	C-N	5.64	1.40	1.33
87	FE	17	U	C5-C6	5.61	1.45	1.34
75	U6	40	GLU	CA-CB	5.59	1.62	1.53
32	53	48	ARG	CA-C	-5.52	1.45	1.52
81	a6	186	THR	CA-C	5.07	1.59	1.52

All (188) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	s3	427	ASN	CA-C-N	27.57	159.64	120.49
53	s3	427	ASN	C-N-CA	27.57	159.64	120.49
73	S6	90	PRO	N-CD-CG	-18.72	75.12	103.20
3	A3	2790	A	OP1-P-OP2	-14.48	76.15	119.60
8	D	194	PHE	CA-CB-CG	13.85	127.64	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	194	PHE	CD1-CG-CD2	-13.13	98.91	118.60
73	S6	90	PRO	CA-CB-CG	-11.27	83.08	104.50
63	I6	186	CYS	CA-C-N	-10.99	107.83	122.56
63	I6	186	CYS	C-N-CA	-10.99	107.83	122.56
3	A3	2790	A	O5'-P-OP2	-10.52	76.44	108.00
68	N6	70	PRO	N-CD-CG	-10.43	87.56	103.20
3	A3	2789	C	OP1-P-O3'	-10.12	77.63	108.00
73	S6	88	PHE	CA-C-N	9.80	139.56	120.94
73	S6	88	PHE	C-N-CA	9.80	139.56	120.94
1	r1	66	VAL	N-CA-C	-9.74	102.81	113.43
3	A3	2789	C	OP2-P-O3'	9.54	136.62	108.00
68	N6	70	PRO	CA-N-CD	-9.53	98.66	112.00
88	A	202	VAL	N-CA-C	-9.50	104.21	111.90
73	S6	90	PRO	CB-CG-CD	8.97	134.80	106.10
24	X3	97	LEU	CA-CB-CG	8.66	146.61	116.30
1	r1	645	ILE	CG1-CB-CG2	-8.46	85.31	110.70
1	r1	73	ILE	N-CA-C	-8.41	103.02	111.77
1	r1	415	GLY	CA-C-N	-7.99	112.05	121.64
1	r1	415	GLY	C-N-CA	-7.99	112.05	121.64
39	d3	230	ARG	CA-C-N	7.98	136.79	121.54
39	d3	230	ARG	C-N-CA	7.98	136.79	121.54
41	f3	85	ASP	CA-C-N	-7.87	110.15	122.67
41	f3	85	ASP	C-N-CA	-7.87	110.15	122.67
1	r1	107	THR	N-CA-C	7.84	118.30	108.19
14	N3	237	HIS	CA-C-N	7.83	136.50	121.54
14	N3	237	HIS	C-N-CA	7.83	136.50	121.54
13	M3	46	GLY	CA-C-N	7.70	136.25	121.54
13	M3	46	GLY	C-N-CA	7.70	136.25	121.54
1	r1	134	ALA	N-CA-C	-7.66	105.88	114.62
1	r1	401	MET	N-CA-C	-7.66	100.66	112.99
43	h3	63	PRO	CA-C-N	7.40	135.02	121.70
43	h3	63	PRO	C-N-CA	7.40	135.02	121.70
88	A	183	PRO	CA-C-N	7.31	134.86	121.70
88	A	183	PRO	C-N-CA	7.31	134.86	121.70
3	A3	2790	A	O5'-P-OP1	7.28	129.84	108.00
1	r1	318	PRO	N-CA-C	7.26	122.63	111.15
85	e6	91	ASP	CA-C-N	7.20	131.61	121.61
85	e6	91	ASP	C-N-CA	7.20	131.61	121.61
1	r1	297	LEU	N-CA-C	7.13	119.93	111.02
43	h3	64	GLU	CA-C-N	7.12	135.14	121.54
43	h3	64	GLU	C-N-CA	7.12	135.14	121.54
60	F6	160	PRO	N-CA-C	7.12	127.13	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	r1	600	SER	N-CA-C	-7.11	106.52	114.62
55	A5	28	PRO	N-CA-CB	7.07	110.78	103.00
24	X3	96	LYS	CA-C-N	-6.88	112.34	122.86
24	X3	96	LYS	C-N-CA	-6.88	112.34	122.86
1	r1	155	THR	N-CA-C	-6.87	105.83	114.56
75	U6	35	ALA	CA-C-N	6.84	130.13	120.28
75	U6	35	ALA	C-N-CA	6.84	130.13	120.28
76	V6	154	LYS	CA-C-N	6.81	134.55	121.54
76	V6	154	LYS	C-N-CA	6.81	134.55	121.54
3	A3	2779	C	P-O3'-C3'	6.79	130.39	120.20
1	r1	725	PRO	CA-C-N	6.68	134.22	123.93
1	r1	725	PRO	C-N-CA	6.68	134.22	123.93
24	X3	97	LEU	CB-CG-CD2	6.66	130.67	110.70
82	b6	243	LYS	CA-C-N	6.62	134.19	121.54
82	b6	243	LYS	C-N-CA	6.62	134.19	121.54
1	r1	184	ALA	N-CA-C	-6.62	106.16	114.56
39	d3	129	ASP	CA-C-N	6.52	133.44	121.70
39	d3	129	ASP	C-N-CA	6.52	133.44	121.70
85	e6	147	PRO	N-CA-CB	6.50	110.08	103.25
80	Z6	90	GLY	CA-C-N	6.37	133.16	121.70
80	Z6	90	GLY	C-N-CA	6.37	133.16	121.70
20	T3	161	ARG	N-CA-C	-6.35	97.28	110.80
1	r1	364	ARG	CA-C-N	6.32	133.62	121.54
1	r1	364	ARG	C-N-CA	6.32	133.62	121.54
81	a6	173	MET	CB-CG-SD	6.29	131.57	112.70
1	r1	577	ASN	N-CA-C	-6.29	104.82	113.18
58	D6	367	GLY	CA-C-N	6.27	130.65	121.31
58	D6	367	GLY	C-N-CA	6.27	130.65	121.31
24	X3	95	ASP	CA-C-N	-6.21	111.88	122.56
24	X3	95	ASP	C-N-CA	-6.21	111.88	122.56
12	L3	112	GLY	CA-C-N	6.17	132.80	121.70
12	L3	112	GLY	C-N-CA	6.17	132.80	121.70
6	E3	231	HIS	CB-CA-C	-6.15	103.62	111.86
76	V6	195	ASP	CA-C-N	6.14	133.27	121.54
76	V6	195	ASP	C-N-CA	6.14	133.27	121.54
6	E3	323	GLY	CA-C-N	6.11	132.69	121.70
6	E3	323	GLY	C-N-CA	6.11	132.69	121.70
32	53	216	GLU	N-CA-C	6.04	117.54	110.41
67	M6	62	GLY	N-CA-C	5.99	122.22	113.48
8	D	194	PHE	CB-CG-CD2	5.99	130.88	120.70
1	r1	622	ASN	CA-C-N	5.98	132.97	121.54
1	r1	622	ASN	C-N-CA	5.98	132.97	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	F6	160	PRO	CA-C-N	5.90	132.59	121.97
60	F6	160	PRO	C-N-CA	5.90	132.59	121.97
88	A	180	PRO	CA-C-N	5.89	141.14	127.00
88	A	180	PRO	C-N-CA	5.89	141.14	127.00
17	Q3	204	MET	CA-C-N	5.88	129.62	120.68
17	Q3	204	MET	C-N-CA	5.88	129.62	120.68
1	r1	619	VAL	CA-C-N	5.86	132.96	123.93
1	r1	619	VAL	C-N-CA	5.86	132.96	123.93
3	A3	2789	C	O3'-P-O5'	-5.85	95.22	104.00
68	N6	70	PRO	CA-CB-CG	-5.85	93.39	104.50
1	r1	52	SER	N-CA-C	5.82	116.92	107.32
3	A3	2779	C	C2'-C3'-O3'	5.81	118.22	109.50
1	r1	288	LEU	CA-C-N	-5.80	114.59	121.90
1	r1	288	LEU	C-N-CA	-5.80	114.59	121.90
1	r1	470	ILE	N-CA-C	-5.79	104.53	113.16
67	M6	21	LEU	CB-CG-CD2	5.76	127.99	110.70
73	S6	90	PRO	CA-C-N	5.74	132.51	121.54
73	S6	90	PRO	C-N-CA	5.74	132.51	121.54
67	M6	21	LEU	CA-CB-CG	5.68	136.18	116.30
73	S6	90	PRO	CA-N-CD	-5.68	104.05	112.00
3	A3	2757	A	P-O3'-C3'	5.65	128.67	120.20
76	V6	155	GLU	CA-C-N	5.64	132.32	121.54
76	V6	155	GLU	C-N-CA	5.64	132.32	121.54
1	r1	341	ILE	CA-C-N	5.60	132.23	121.54
1	r1	341	ILE	C-N-CA	5.60	132.23	121.54
8	D	194	PHE	CB-CG-CD1	5.57	130.17	120.70
87	FE	31	C	O4'-C1'-N1	5.57	116.85	108.50
66	L6	77	GLN	N-CA-C	-5.56	107.75	114.75
6	E3	246	GLY	N-CA-C	5.55	126.33	113.18
87	24	31	C	O4'-C1'-N1	5.55	116.82	108.50
41	f3	127	MET	N-CA-C	-5.53	103.07	109.93
1	r1	325	ASN	N-CA-C	-5.53	105.53	114.09
24	X3	178	PRO	CA-C-N	5.51	132.07	121.54
24	X3	178	PRO	C-N-CA	5.51	132.07	121.54
60	F6	161	ILE	N-CA-C	5.50	120.78	109.34
6	E3	231	HIS	CA-C-N	5.50	131.60	121.70
6	E3	231	HIS	C-N-CA	5.50	131.60	121.70
1	r1	56	ASP	N-CA-C	-5.50	99.09	110.80
41	f3	50	THR	CA-C-N	5.46	135.12	121.80
41	f3	50	THR	C-N-CA	5.46	135.12	121.80
35	93	131	TYR	CA-C-N	-5.46	113.02	119.84
35	93	131	TYR	C-N-CA	-5.46	113.02	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	b3	117	LYS	CA-CB-CG	5.45	125.00	114.10
72	R6	292	ASP	CA-C-N	5.44	131.93	121.54
72	R6	292	ASP	C-N-CA	5.44	131.93	121.54
22	V3	102	MET	CA-CB-CG	5.43	124.97	114.10
1	r1	718	SER	N-CA-C	5.35	115.09	108.19
35	93	96	VAL	N-CA-C	-5.34	108.29	113.53
1	r1	60	THR	N-CA-C	-5.33	106.66	114.39
60	F6	131	ALA	N-CA-C	5.32	117.20	110.33
5	D3	235	GLN	CA-CB-CG	5.31	124.72	114.10
1	r1	725	PRO	N-CA-C	5.31	123.41	112.47
3	A3	2182	G	C2'-C3'-O3'	5.31	121.66	113.70
32	53	216	GLU	CA-C-N	5.29	131.23	121.70
32	53	216	GLU	C-N-CA	5.29	131.23	121.70
3	A3	2182	G	P-O3'-C3'	5.24	128.06	120.20
82	b6	302	GLU	CA-C-N	5.23	129.11	121.31
82	b6	302	GLU	C-N-CA	5.23	129.11	121.31
3	A3	3201	A	P-O3'-C3'	5.23	128.04	120.20
74	T6	148	PRO	N-CA-C	5.22	123.22	112.47
14	N3	48	PRO	CA-N-CD	-5.21	104.70	112.00
24	X3	52	ILE	CA-C-N	5.20	130.90	122.48
24	X3	52	ILE	C-N-CA	5.20	130.90	122.48
39	d3	229	GLY	CA-C-N	5.19	131.45	121.54
39	d3	229	GLY	C-N-CA	5.19	131.45	121.54
3	A3	1806	U	P-O3'-C3'	5.18	127.97	120.20
1	r1	444	ILE	CA-C-N	5.17	131.42	121.54
1	r1	444	ILE	C-N-CA	5.17	131.42	121.54
39	d3	267	PRO	CA-C-N	5.17	139.41	127.00
39	d3	267	PRO	C-N-CA	5.17	139.41	127.00
8	D	198	GLY	N-CA-C	-5.16	107.41	114.64
22	V3	117	HIS	CA-C-N	5.16	134.10	125.02
22	V3	117	HIS	C-N-CA	5.16	134.10	125.02
72	R6	293	LEU	CA-CB-CG	5.15	134.33	116.30
81	a6	135	MET	CB-CG-SD	-5.15	97.25	112.70
58	D6	421	VAL	N-CA-C	-5.14	107.74	112.83
89	n	262	MET	N-CA-C	5.12	116.60	108.96
60	F6	159	VAL	CA-C-N	5.12	126.24	119.84
60	F6	159	VAL	C-N-CA	5.12	126.24	119.84
1	r1	650	MET	CA-CB-CG	5.12	124.34	114.10
62	H6	126	ILE	CA-C-N	5.11	131.31	121.54
62	H6	126	ILE	C-N-CA	5.11	131.31	121.54
3	A3	2507	A	C2'-C3'-O3'	5.11	121.37	113.70
71	Q6	50	ARG	CB-CG-CD	5.11	123.05	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	D6	286	GLU	N-CA-C	5.10	117.49	110.35
69	O6	108	CYS	CA-CB-SG	5.10	126.13	114.40
89	n	300	SER	CA-C-N	5.09	130.87	121.70
89	n	300	SER	C-N-CA	5.09	130.87	121.70
18	R3	123	ARG	CB-CG-CD	5.09	123.00	111.30
24	X3	96	LYS	CA-CB-CG	5.08	124.27	114.10
11	K3	46	VAL	N-CA-CB	-5.06	106.47	112.39
53	s3	284	VAL	N-CA-C	-5.05	104.50	110.21
41	f3	135	LEU	CA-C-N	5.04	129.27	122.07
41	f3	135	LEU	C-N-CA	5.04	129.27	122.07
88	A	180	PRO	C-N-CD	-5.04	109.52	120.60
50	p3	112	ALA	CA-C-N	5.01	126.36	120.09
50	p3	112	ALA	C-N-CA	5.01	126.36	120.09
34	73	47	LEU	CA-CB-CG	5.01	133.83	116.30
52	r3	59	GLU	CB-CA-C	-5.01	100.45	110.42

There are no chirality outliers.

All (125) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	03	151	ALA	Peptide
27	03	177	ARG	Peptide
28	13	25	GLY	Peptide
28	13	62	ILE	Peptide
32	53	223	ARG	Peptide
32	53	268	CYS	Peptide
32	53	269	ASN	Peptide
32	53	347	THR	Peptide
33	63	221	LEU	Peptide
33	63	49	GLU	Peptide
35	93	45	THR	Peptide
88	A	181	PRO	Peptide
88	A	182	ILE	Peptide
88	A	184	ASN	Peptide
88	A	185	TYR	Peptide
88	A	201	GLN	Peptide
88	A	57	ASP	Peptide
56	B6	164	GLU	Peptide
8	D	193	PHE	Peptide
8	D	205	THR	Peptide
5	D3	206	TYR	Peptide
58	D6	284	ARG	Peptide

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Mol	Chain	Res	Type	Group
58	D6	286	GLU	Peptide
58	D6	422	TRP	Peptide
58	D6	425	LEU	Peptide
6	E3	126	ASP	Peptide
6	E3	169	GLY	Peptide
6	E3	244	ALA	Peptide
6	E3	250	ARG	Peptide
6	E3	85	TRP	Peptide
7	F3	129	PRO	Peptide
7	F3	140	SER	Peptide
60	F6	147	GLN	Peptide
60	F6	159	VAL	Peptide
60	F6	160	PRO	Mainchain
60	F6	161	ILE	Peptide
61	G6	103	ASP	Peptide
8	H3	63	PRO	Peptide
9	I3	102	VAL	Peptide
63	I6	144	VAL	Peptide
63	I6	94	ASN	Peptide
10	J3	44	VAL	Peptide
10	J3	45	SER	Peptide
64	J6	130	TYR	Peptide
11	K3	3	SER	Peptide
11	K3	5	SER	Peptide
13	M3	109	ARG	Peptide
13	M3	18	GLY	Peptide
13	M3	264	GLN	Peptide
13	M3	286	THR	Peptide
14	N3	237	HIS	Peptide
14	N3	78	GLU	Peptide
68	N6	109	PRO	Peptide
15	O3	104	TYR	Peptide
69	O6	53	ASP	Peptide
69	O6	55	PRO	Peptide
69	O6	98	ASN	Peptide
70	P6	139	ARG	Peptide
70	P6	64	LYS	Peptide
70	P6	65	CYS	Peptide
17	Q3	182	ARG	Peptide
18	R3	137	GLU	Peptide
72	R6	132	LEU	Peptide
72	R6	154	THR	Peptide

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Mol	Chain	Res	Type	Group
72	R6	291	ARG	Peptide
73	S6	107	GLN	Peptide
20	T3	160	GLY	Peptide
75	U6	128	GLU	Peptide
75	U6	62	HIS	Peptide
22	V3	100	LYS	Peptide
22	V3	170	TRP	Peptide
76	V6	155	GLU	Peptide
76	V6	44	GLU	Peptide
24	X3	51	LYS	Peptide
2	Y2	21	UNK	Peptide
2	Y2	22	UNK	Peptide
26	Z3	141	SER	Peptide
81	a6	21	LEU	Peptide
82	b6	228	VAL	Peptide
38	c3	63	LYS	Peptide
83	c6	38	ARG	Peptide
39	d3	191	PRO	Peptide
39	d3	230	ARG	Peptide
39	d3	231	LEU	Peptide
39	d3	268	PRO	Peptide
39	d3	271	PRO	Peptide
85	e6	64	THR	Peptide
85	e6	67	LYS	Peptide
41	f3	50	THR	Peptide
41	f3	84	THR	Peptide
41	f3	85	ASP	Peptide
41	f3	86	TYR	Peptide
42	g3	110	ILE	Peptide
43	h3	138	SER	Peptide
43	h3	65	ASP	Peptide
44	i3	57	TYR	Peptide
45	j3	25	GLY	Peptide
89	n	222	SER	Peptide
49	o3	42	GLU	Peptide
51	q3	78	SER	Peptide
1	r1	162	MET	Peptide
1	r1	169	PHE	Peptide
1	r1	207	LEU	Peptide
1	r1	247	THR	Peptide
1	r1	249	HIS	Peptide
1	r1	256	CYS	Peptide

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Mol	Chain	Res	Type	Group
1	r1	296	PHE	Peptide
1	r1	341	ILE	Peptide
1	r1	364	ARG	Peptide
1	r1	401	MET	Peptide
1	r1	402	HIS	Peptide
1	r1	441	MET	Peptide
1	r1	53	ALA	Peptide
1	r1	57	SER	Peptide
1	r1	597	GLY	Peptide
1	r1	678	GLN	Peptide
1	r1	681	VAL	Peptide
1	r1	723	CYS	Peptide
1	r1	724	LEU	Peptide
1	r1	726	SER	Peptide
1	r1	735	TYR	Peptide
1	r1	78	GLU	Peptide
1	r1	98	ARG	Peptide
53	s3	270	LYS	Peptide
53	s3	283	PHE	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	r1	5452	0	5425	125	0
2	Y2	145	0	37	0	0
3	8	175	0	88	2	0
3	A3	31913	0	16215	211	0
4	B3	1191	0	607	3	0
5	D3	1842	0	1895	32	0
6	E3	2365	0	2378	23	0
7	F3	2013	0	2044	32	0
8	D	648	0	657	33	0
8	H3	784	0	832	13	0
9	I3	1283	0	1369	33	0
10	J3	1061	0	1141	17	0
11	K3	1451	0	1448	23	0
12	L3	889	0	941	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	M3	2305	0	2378	42	0
14	N3	1654	0	1681	17	0
15	O3	1245	0	1283	27	0
16	P3	1080	0	1081	20	0
17	Q3	1822	0	1859	25	0
18	R3	1153	0	1214	28	0
19	S3	1251	0	1322	30	0
20	T3	1368	0	1410	19	0
21	U3	922	0	935	16	0
22	V3	1551	0	1558	28	0
23	W3	871	0	898	17	0
24	X3	2027	0	2040	24	0
25	Y3	1517	0	1561	24	0
26	Z3	978	0	1030	12	0
27	03	880	0	902	17	0
28	13	433	0	475	10	0
29	23	376	0	406	7	0
30	33	831	0	883	10	0
31	43	322	0	343	4	0
32	53	3064	0	3059	43	0
33	63	2636	0	2450	27	0
34	73	2158	0	2173	27	0
35	93	873	0	878	13	0
36	a3	686	0	658	9	0
37	b3	1178	0	1180	27	0
38	c3	2217	0	2220	26	0
39	d3	1347	0	1343	18	0
40	e3	1762	0	1767	40	0
41	f3	1039	0	1044	21	0
42	g3	1067	0	1056	15	0
43	h3	827	0	806	11	0
44	i3	827	0	857	11	0
45	j3	684	0	673	10	0
46	k3	655	0	656	15	0
47	l3	221	0	227	4	0
48	m3	372	0	387	12	0
49	o3	797	0	804	15	0
50	p3	1058	0	1083	17	0
51	q3	1076	0	1049	15	0
52	r3	1203	0	1220	21	0
53	s3	3036	0	3021	34	0
54	u3	42	0	23	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	A5	136	0	67	0	0
56	B6	1768	0	1765	51	0
57	C6	1082	0	1088	31	0
58	D6	2557	0	2596	45	0
59	E6	972	0	1000	25	0
60	F6	1668	0	1716	48	0
61	G6	2516	0	2503	54	0
62	H6	999	0	1024	37	0
63	I6	1011	0	1052	33	0
64	J6	838	0	887	16	0
65	K6	861	0	885	33	0
66	L6	1382	0	1472	26	0
67	M6	920	0	951	28	0
68	N6	846	0	908	15	0
69	O6	1528	0	1488	37	0
70	P6	774	0	801	21	0
71	Q6	740	0	754	20	0
72	R6	2008	0	2031	49	0
73	S6	1042	0	1037	15	0
74	T6	1330	0	1342	35	0
75	U6	1461	0	1471	38	0
76	V6	2702	0	2690	45	0
77	W6	766	0	785	16	0
78	X6	2531	0	2520	67	0
79	Y6	914	0	859	10	0
80	Z6	740	0	747	19	0
81	a6	1684	0	1685	40	0
82	b6	2076	0	2097	45	0
83	c6	925	0	962	18	0
84	d6	610	0	682	6	0
85	e6	2838	0	2416	35	0
86	A6	19716	0	10015	155	0
87	24	1547	0	787	20	0
87	FE	1547	0	788	45	0
88	A	1375	0	1426	31	0
89	n	1744	0	1796	74	0
90	B	140	0	32	1	0
91	r1	32	0	14	0	0
92	A3	95	0	0	0	0
92	A6	28	0	0	0	0
92	D3	1	0	0	0	0
92	E3	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
92	M3	1	0	0	0	0
92	g3	1	0	0	0	0
92	r1	1	0	0	0	0
93	A3	10	0	19	0	0
94	O3	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
All	All	171122	0	144140	2127	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 (2127) 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)
89:n:92:TYR:CG	89:n:92:TYR:CD1	1.99	1.49
89:n:92:TYR:CG	89:n:92:TYR:CD2	2.00	1.47
89:n:92:TYR:CE1	89:n:92:TYR:CZ	2.16	1.34
89:n:92:TYR:CZ	89:n:92:TYR:CE2	2.16	1.33
60:F6:161:ILE:HB	87:FE:30:G:H2'	1.54	0.88
59:E6:105:CYS:HB3	70:P6:68:CYS:SG	2.17	0.84
89:n:92:TYR:CD2	89:n:92:TYR:CE2	2.65	0.84
60:F6:169:GLN:HB3	60:F6:233:ASN:HB2	1.63	0.81
87:FE:17:U:C2	89:n:220:LYS:NZ	2.52	0.78
89:n:92:TYR:CD1	89:n:92:TYR:CE1	2.72	0.77
16:P3:54:ASN:C	16:P3:54:ASN:HD22	1.92	0.77
13:M3:47:ARG:HD2	19:S3:179:ASN:HD22	1.51	0.75
87:24:33:C:H42	3:8:20:G:H1	1.34	0.75
70:P6:124:TYR:HB3	71:Q6:9:ALA:HB2	1.69	0.75
5:D3:172:MET:HE3	5:D3:173:ALA:H	1.52	0.74
69:O6:105:CYS:HB2	69:O6:108:CYS:HB3	1.69	0.74
24:X3:95:ASP:HB2	87:FE:73:A:H5'	1.68	0.74
61:G6:149:TYR:HH	61:G6:163:HIS:HD1	1.36	0.73
61:G6:92:MET:HG3	61:G6:94:GLU:H	1.54	0.72
11:K3:143:GLU:OE1	37:b3:136:LYS:NZ	2.23	0.71
58:D6:149:MET:SD	85:e6:104:ARG:NH1	2.64	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:c3:161:THR:O	38:c3:192:GLN:NE2	2.24	0.71
8:D:194:PHE:CG	89:n:92:TYR:CE1	2.78	0.71
19:S3:129:ARG:HE	19:S3:155:ARG:HG3	1.56	0.70
81:a6:65:LEU:HD22	81:a6:112:GLY:H	1.56	0.70
8:D:194:PHE:CG	89:n:92:TYR:CD1	2.79	0.70
6:E3:248:ILE:HG22	6:E3:250:ARG:H	1.57	0.70
78:X6:288:ALA:HA	78:X6:291:HIS:HB3	1.72	0.70
21:U3:28:LEU:H	25:Y3:114:THR:HG22	1.55	0.70
8:D:166:PHE:HB3	8:D:199:VAL:HG12	1.73	0.70
70:P6:109:LYS:HZ3	70:P6:113:ARG:HH12	1.40	0.69
74:T6:29:VAL:HB	74:T6:79:TYR:HB2	1.74	0.69
10:J3:30:MET:HB2	10:J3:35:LEU:HD21	1.75	0.69
58:D6:412:LYS:HE2	58:D6:418:LYS:HB2	1.74	0.69
3:A3:1777:A:N6	3:A3:1780:U:OP2	2.26	0.68
40:e3:161:VAL:HG23	40:e3:172:ILE:HG13	1.73	0.68
1:r1:388:ARG:HH22	1:r1:425:CYS:HB3	1.57	0.68
18:R3:34:ARG:HA	18:R3:37:ARG:HH21	1.57	0.68
60:F6:220:ILE:HG23	60:F6:223:LYS:HE3	1.75	0.68
78:X6:102:ARG:H	78:X6:105:ALA:HB3	1.58	0.68
88:A:50:LEU:HB3	88:A:54:LYS:HE3	1.75	0.68
59:E6:115:GLU:HG3	59:E6:116:LYS:HG3	1.74	0.68
67:M6:21:LEU:HD11	67:M6:54:TYR:HB3	1.76	0.68
1:r1:444:ILE:HG13	1:r1:445:HIS:H	1.59	0.68
8:D:194:PHE:CG	89:n:92:TYR:CD2	2.82	0.68
27:O3:145:GLU:HG3	27:O3:150:LYS:HB2	1.76	0.68
74:T6:3:MET:SD	74:T6:11:ARG:NH1	2.67	0.68
53:s3:201:ASP:OD2	53:s3:242:ARG:NH2	2.27	0.67
83:c6:38:ARG:HH12	86:A6:1187:U:H5''	1.59	0.67
41:f3:93:ILE:HG22	41:f3:186:VAL:HG12	1.75	0.67
25:Y3:85:TRP:HB3	25:Y3:90:LEU:HD11	1.76	0.67
64:J6:61:VAL:HG12	64:J6:107:ILE:HG12	1.75	0.67
69:O6:182:GLY:HA2	69:O6:186:ALA:H	1.60	0.67
59:E6:40:GLU:HB2	59:E6:65:LEU:HB3	1.75	0.67
8:D:194:PHE:CG	89:n:92:TYR:CE2	2.82	0.67
64:J6:114:ARG:HG3	64:J6:122:LYS:HG2	1.76	0.67
8:D:197:LEU:HG	89:n:94:ARG:HB3	1.75	0.67
60:F6:169:GLN:HA	87:FE:30:G:H1'	1.77	0.67
88:A:76:GLU:HG2	88:A:83:ILE:HD11	1.77	0.66
1:r1:142:VAL:HG22	1:r1:170:LEU:HB2	1.77	0.66
3:A3:2906:C:N3	28:13:19:ARG:NH1	2.42	0.66
9:I3:168:LEU:HD21	9:I3:174:LEU:HA	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R3:54:THR:HG21	19:S3:172:MET:H	1.60	0.66
69:O6:123:LEU:HD13	69:O6:154:ILE:HG13	1.78	0.66
7:F3:293:PHE:HB2	42:g3:55:THR:HG21	1.78	0.66
14:N3:132:THR:HG21	14:N3:144:LYS:HG2	1.77	0.66
67:M6:19:ILE:O	67:M6:20:ARG:NH2	2.28	0.66
89:n:161:THR:HB	89:n:166:GLU:HB3	1.77	0.66
43:h3:112:VAL:HG11	43:h3:120:MET:HE1	1.77	0.66
39:d3:265:ILE:HG22	39:d3:267:PRO:HD2	1.78	0.66
63:I6:98:GLN:HE22	86:A6:1008:G:H21	1.44	0.66
8:H3:107:VAL:HG11	8:D:162:ALA:HA	1.78	0.66
35:93:127:LEU:O	35:93:134:ASN:ND2	2.29	0.66
85:e6:121:ILE:HG12	85:e6:128:PHE:HE2	1.61	0.65
8:D:197:LEU:HD12	89:n:94:ARG:HH11	1.61	0.65
68:N6:11:ARG:HA	68:N6:68:ALA:HB2	1.78	0.65
3:A3:2173:G:H1	3:A3:2187:C:H42	1.44	0.65
52:r3:35:PHE:N	52:r3:54:THR:O	2.30	0.65
7:F3:67:GLU:OE1	7:F3:210:ARG:NH1	2.30	0.65
45:j3:104:LYS:O	45:j3:107:ASN:ND2	2.30	0.65
53:s3:152:GLN:HA	53:s3:156:TYR:HB2	1.79	0.65
58:D6:206:PRO:HG2	58:D6:215:TYR:HB3	1.77	0.65
62:H6:71:ILE:HG23	62:H6:150:GLY:HA3	1.78	0.65
20:T3:84:LYS:HD2	20:T3:149:ARG:HB3	1.78	0.65
70:P6:86:PRO:HA	70:P6:125:LYS:HB3	1.78	0.65
9:I3:124:LYS:HB2	9:I3:153:LEU:HB2	1.78	0.65
56:B6:67:LEU:HD23	73:S6:37:ALA:HB2	1.79	0.65
75:U6:41:ARG:NH1	86:A6:706:C:OP1	2.28	0.65
6:E3:293:LYS:HD3	17:Q3:87:THR:HG22	1.79	0.65
28:13:35:ASN:HB3	28:13:38:ARG:HG2	1.79	0.65
1:r1:361:GLU:HB3	1:r1:368:LEU:HB2	1.79	0.64
7:F3:48:LEU:HD11	43:h3:95:ARG:HG2	1.79	0.64
63:I6:98:GLN:HE21	63:I6:106:PRO:HB3	1.62	0.64
79:Y6:360:LYS:HA	82:b6:211:ARG:HG3	1.79	0.64
1:r1:380:LYS:HD2	1:r1:397:ARG:HG2	1.79	0.64
3:A3:2191:A:N6	3:A3:2198:A:OP2	2.30	0.64
5:D3:235:GLN:HB3	5:D3:294:SER:HA	1.79	0.64
86:A6:989:U:H2'	86:A6:990:G:H8	1.62	0.64
3:A3:3168:C:N3	6:E3:303:LYS:NZ	2.44	0.64
75:U6:68:ARG:HD3	75:U6:71:ARG:HE	1.61	0.64
40:e3:55:ARG:HG2	40:e3:157:LEU:HB2	1.79	0.64
58:D6:90:PHE:HB3	65:K6:93:MET:HE2	1.79	0.64
87:FE:17:U:C4	89:n:220:LYS:NZ	2.65	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A3:2171:U:H4'	3:A3:2172:A:H3'	1.80	0.64
61:G6:224:LEU:HD21	71:Q6:86:GLY:HA2	1.78	0.64
76:V6:173:PHE:HB3	76:V6:178:THR:HG22	1.79	0.64
86:A6:728:C:H42	86:A6:754:A:H61	1.44	0.64
72:R6:157:VAL:HG13	72:R6:174:VAL:HG12	1.78	0.64
72:R6:287:ASP:O	72:R6:291:ARG:NH2	2.30	0.64
3:A3:2187:C:O2'	10:J3:103:GLN:NE2	2.31	0.64
40:e3:208:ALA:HB1	88:A:147:LEU:HD21	1.80	0.64
56:B6:227:CYS:SG	56:B6:228:ASN:N	2.71	0.64
33:63:73:THR:HG22	33:63:75:ARG:H	1.63	0.64
87:FE:17:U:N3	89:n:220:LYS:NZ	2.46	0.64
1:r1:47:ARG:NH1	1:r1:319:ASN:OD1	2.30	0.63
86:A6:1591:U:H2'	86:A6:1592:G:H8	1.62	0.63
3:A3:2545:U:H5''	3:A3:2546:G:H5'	1.79	0.63
63:I6:147:ILE:HG13	63:I6:170:LEU:HD13	1.79	0.63
3:A3:1867:A:H62	3:A3:2295:C:H5	1.43	0.63
20:T3:132:HIS:HD2	39:d3:227:ARG:HH11	1.45	0.63
27:03:136:GLU:HB3	27:03:177:ARG:HE	1.64	0.63
63:I6:94:ASN:ND2	86:A6:994:U:OP2	2.32	0.63
88:A:71:LYS:HA	88:A:74:LYS:HB2	1.81	0.63
3:A3:2849:G:H1	3:A3:2889:C:H42	1.46	0.63
50:p3:43:TYR:HA	50:p3:48:LEU:HD21	1.81	0.63
58:D6:289:THR:HG21	58:D6:308:GLN:H	1.63	0.63
67:M6:112:ARG:NH2	75:U6:52:GLU:OE1	2.32	0.63
61:G6:317:PHE:HB3	61:G6:323:LEU:HA	1.81	0.63
21:U3:11:ARG:HH11	22:V3:211:LYS:HB3	1.62	0.63
58:D6:284:ARG:NH1	58:D6:287:ASP:OD1	2.31	0.63
60:F6:166:ARG:HG2	87:FE:34:U:H3	1.62	0.63
85:e6:467:LEU:HG	85:e6:468:MET:HG2	1.78	0.63
1:r1:377:GLU:HG2	1:r1:413:TYR:HA	1.81	0.62
58:D6:361:GLN:HA	58:D6:364:ASP:HB2	1.79	0.62
86:A6:1196:C:H42	86:A6:1466:G:H1	1.46	0.62
3:A3:1886:G:N7	7:F3:170:ARG:NH2	2.43	0.62
7:F3:282:PRO:O	7:F3:290:TYR:OH	2.13	0.62
62:H6:100:LYS:HE2	62:H6:106:ILE:HG12	1.80	0.62
67:M6:21:LEU:H	67:M6:87:MET:HE3	1.63	0.62
82:b6:103:LEU:HD13	82:b6:106:LEU:HD12	1.80	0.62
8:D:194:PHE:CG	89:n:92:TYR:CZ	2.86	0.62
1:r1:617:HIS:ND1	1:r1:619:VAL:O	2.32	0.62
25:Y3:164:ARG:NH1	25:Y3:181:PHE:O	2.32	0.62
63:I6:88:ILE:HB	63:I6:151:VAL:HA	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:K6:37:ASP:HA	65:K6:40:ARG:HB3	1.81	0.62
53:s3:243:ILE:HG22	53:s3:245:LYS:H	1.64	0.62
56:B6:156:GLU:OE2	56:B6:168:THR:OG1	2.16	0.62
58:D6:269:ARG:HA	58:D6:272:LYS:HG3	1.82	0.62
74:T6:103:ARG:NH2	74:T6:103:ARG:O	2.32	0.62
41:f3:155:ARG:HH12	88:A:88:PHE:HZ	1.48	0.62
56:B6:100:ARG:HE	73:S6:52:ARG:HH12	1.47	0.62
65:K6:63:LEU:HB3	65:K6:67:LEU:HD23	1.81	0.62
83:c6:11:ALA:HB2	83:c6:19:PRO:HB3	1.80	0.62
56:B6:94:LYS:HG2	77:W6:148:GLU:HG2	1.81	0.62
86:A6:707:A:H5'	86:A6:851:G:H21	1.64	0.62
42:g3:141:ASN:ND2	42:g3:144:THR:OG1	2.33	0.62
46:k3:32:THR:HA	46:k3:35:GLN:HB2	1.82	0.62
59:E6:57:GLN:NE2	86:A6:1012:A:OP1	2.32	0.62
14:N3:160:VAL:HG12	14:N3:161:VAL:HG23	1.82	0.62
68:N6:18:ILE:HD13	68:N6:29:ARG:HE	1.64	0.62
1:r1:51:ILE:HG22	1:r1:59:LYS:HG3	1.82	0.61
89:n:282:ARG:HG2	89:n:287:GLY:HA2	1.81	0.61
3:A3:2017:U:O2'	3:A3:2723:A:N1	2.32	0.61
78:X6:368:HIS:HB3	78:X6:371:ALA:HB2	1.81	0.61
11:K3:8:PRO:HG2	38:c3:295:GLU:HG3	1.82	0.61
32:53:313:MET:HE1	32:53:353:HIS:HB3	1.82	0.61
33:63:222:ASP:OD1	33:63:267:ARG:NH1	2.33	0.61
67:M6:106:ASN:HA	67:M6:109:ARG:HB2	1.82	0.61
71:Q6:25:THR:OG1	71:Q6:28:ARG:NH2	2.33	0.61
58:D6:220:THR:HG22	58:D6:247:VAL:HG12	1.82	0.61
89:n:145:SER:HA	89:n:240:GLY:HA3	1.81	0.61
40:e3:207:ASN:ND2	88:A:160:GLU:O	2.33	0.61
67:M6:28:ASN:HB3	74:T6:159:MET:HB3	1.83	0.61
84:d6:139:ASN:ND2	86:A6:1145:C:OP1	2.32	0.61
87:24:30:G:H1	87:24:36:A:H61	1.49	0.61
32:53:310:ARG:HA	32:53:313:MET:HE2	1.82	0.61
38:c3:93:VAL:O	38:c3:122:ASN:ND2	2.34	0.61
38:c3:166:VAL:HG11	38:c3:192:GLN:HG3	1.83	0.61
69:O6:204:ASN:O	75:U6:59:ARG:NH2	2.33	0.61
1:r1:317:LEU:HD12	1:r1:318:PRO:HD2	1.81	0.61
3:A3:2521:A:OP2	5:D3:202:ARG:NH2	2.34	0.61
7:F3:231:VAL:HG13	51:q3:26:ARG:HD2	1.82	0.61
59:E6:90:ARG:NH2	70:P6:116:ILE:O	2.34	0.61
87:FE:25:G:N2	87:FE:42:C:O2	2.33	0.61
9:I3:97:ALA:HB3	9:I3:154:LEU:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:G6:323:LEU:HD11	78:X6:378:LYS:HB3	1.83	0.61
65:K6:58:ARG:NH1	65:K6:68:GLN:OE1	2.34	0.61
3:A3:2795:U:O2	8:H3:87:LYS:NZ	2.34	0.60
62:H6:119:THR:HG22	62:H6:133:GLN:HG2	1.82	0.60
72:R6:163:TYR:HB2	74:T6:125:HIS:HE1	1.66	0.60
25:Y3:133:ASP:HA	25:Y3:136:VAL:HG12	1.84	0.60
52:r3:70:CYS:HB3	52:r3:108:CYS:SG	2.41	0.60
77:W6:137:GLY:O	77:W6:139:ARG:NH1	2.34	0.60
87:FE:17:U:C2	89:n:220:LYS:CE	2.84	0.60
29:23:59:LYS:HG2	29:23:63:LYS:HE2	1.84	0.60
51:q3:111:GLU:OE1	51:q3:114:ARG:NH2	2.33	0.60
63:I6:154:LEU:HA	63:I6:158:ARG:HD2	1.82	0.60
78:X6:265:ILE:HG23	78:X6:329:LEU:HD21	1.81	0.60
88:A:47:SER:HA	88:A:50:LEU:HD13	1.82	0.60
75:U6:43:ASN:ND2	86:A6:707:A:OP2	2.34	0.60
87:24:25:G:N2	87:24:42:C:O2	2.33	0.60
76:V6:154:LYS:HG3	76:V6:156:ASN:HB2	1.82	0.60
1:r1:566:LYS:O	1:r1:606:GLY:N	2.32	0.60
14:N3:87:PHE:HB2	14:N3:163:MET:HB2	1.84	0.60
63:I6:117:PHE:HB2	63:I6:122:LYS:HB3	1.84	0.60
78:X6:250:GLN:NE2	78:X6:254:GLY:O	2.34	0.60
86:A6:773:G:N2	86:A6:776:A:OP2	2.34	0.60
24:X3:172:GLN:HA	24:X3:188:TYR:HE2	1.66	0.60
27:03:144:GLN:OE1	27:03:173:ARG:NH2	2.33	0.60
32:53:201:ARG:NH2	32:53:418:TYR:O	2.34	0.60
61:G6:108:ILE:HA	61:G6:111:LEU:HB2	1.84	0.60
69:O6:94:CYS:N	69:O6:143:CYS:SG	2.74	0.60
72:R6:223:ARG:NH1	72:R6:226:ASP:OD2	2.35	0.60
80:Z6:11:MET:HE3	82:b6:192:LYS:HB2	1.84	0.60
86:A6:1359:G:N2	86:A6:1360:A:N1	2.41	0.60
39:d3:165:THR:HG23	39:d3:167:HIS:H	1.66	0.60
72:R6:218:MET:HE3	72:R6:227:VAL:HG22	1.82	0.60
73:S6:18:ASP:OD1	73:S6:21:ARG:NH1	2.34	0.60
74:T6:105:ILE:HG22	74:T6:106:LEU:HG	1.83	0.60
9:I3:132:LYS:NZ	9:I3:147:PHE:O	2.34	0.60
32:53:229:ARG:NH1	32:53:231:SER:OG	2.35	0.60
52:r3:166:GLY:O	52:r3:171:ARG:NH2	2.35	0.60
6:E3:163:GLU:OE1	6:E3:166:ARG:NH1	2.35	0.59
41:f3:165:THR:HA	88:A:164:ARG:HH11	1.65	0.59
65:K6:116:ASP:OD1	65:K6:125:ARG:NH2	2.35	0.59
89:n:98:GLU:HG2	89:n:306:LYS:HD3	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T3:55:ASN:ND2	20:T3:74:TYR:O	2.34	0.59
3:A3:2294:A:OP2	13:M3:39:ARG:NH2	2.36	0.59
5:D3:132:ASP:OD1	5:D3:135:ARG:NH1	2.33	0.59
22:V3:190:CYS:SG	22:V3:191:LEU:N	2.75	0.59
64:J6:50:GLY:O	64:J6:89:ARG:NH1	2.35	0.59
64:J6:82:ARG:NH1	64:J6:90:GLU:OE2	2.34	0.59
65:K6:80:ARG:NH1	86:A6:1354:G:OP2	2.34	0.59
76:V6:209:LEU:HG	76:V6:224:GLN:HG3	1.82	0.59
80:Z6:83:LYS:HA	80:Z6:86:LYS:HB2	1.83	0.59
82:b6:292:TYR:HB2	82:b6:319:LEU:HD11	1.84	0.59
22:V3:73:GLN:HE22	22:V3:123:VAL:HG21	1.67	0.59
56:B6:215:MET:SD	73:S6:5:ARG:NH2	2.76	0.59
70:P6:106:GLU:HA	70:P6:109:LYS:HG2	1.83	0.59
75:U6:68:ARG:NH1	86:A6:738:C:O3'	2.35	0.59
8:D:194:PHE:CG	89:n:92:TYR:CG	2.90	0.59
15:O3:75:MET:HE2	17:Q3:267:PHE:HA	1.85	0.59
56:B6:147:ARG:NH1	86:A6:1298:A:OP1	2.36	0.59
59:E6:22:LEU:HD23	75:U6:177:VAL:HG13	1.85	0.59
86:A6:1371:A:N6	86:A6:1387:A:O2'	2.36	0.59
3:A3:2442:U:OP1	53:s3:81:ARG:NH1	2.36	0.59
6:E3:201:GLY:HA2	6:E3:272:LYS:HE2	1.85	0.59
62:H6:135:GLU:OE2	65:K6:124:GLN:NE2	2.35	0.59
81:a6:81:THR:HG22	81:a6:94:TYR:HB3	1.84	0.59
88:A:160:GLU:HA	88:A:163:LYS:HE2	1.84	0.59
87:FE:30:G:H1	87:FE:36:A:H61	1.49	0.59
8:H3:59:TRP:HE1	24:X3:96:LYS:HG2	1.67	0.59
9:I3:51:THR:OG1	14:N3:250:ARG:NH2	2.36	0.59
30:33:183:ARG:NH1	33:63:355:LYS:O	2.36	0.59
89:n:198:VAL:HG21	89:n:234:LEU:HD21	1.84	0.59
3:A3:3089:A:H2'	87:24:71:C:H5'	1.85	0.59
62:H6:176:GLN:NE2	82:b6:150:GLU:OE2	2.36	0.59
76:V6:248:PRO:HB2	81:a6:143:PRO:HB3	1.85	0.59
3:A3:2517:U:OP1	5:D3:287:ARG:NH2	2.36	0.59
72:R6:271:MET:N	72:R6:271:MET:SD	2.76	0.59
76:V6:66:PRO:HD3	86:A6:1533:A:H1'	1.84	0.59
87:FE:14:A:N1	87:FE:19:A:O2'	2.34	0.59
1:r1:135:LEU:HD13	1:r1:162:MET:HB3	1.84	0.58
3:A3:1881:A:OP2	42:g3:111:ARG:NH2	2.31	0.58
3:A3:2167:A:H5''	9:I3:106:ALA:HB2	1.84	0.58
69:O6:218:ARG:O	69:O6:221:GLN:NE2	2.34	0.58
72:R6:157:VAL:HG11	72:R6:192:MET:HE3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K3:110:GLY:O	11:K3:114:LYS:NZ	2.35	0.58
41:f3:123:GLU:HB2	41:f3:158:GLN:HG3	1.84	0.58
59:E6:9:ILE:HG22	59:E6:89:ILE:HD13	1.86	0.58
68:N6:64:VAL:HG12	68:N6:84:ILE:HA	1.84	0.58
3:A3:2777:G:N7	8:D:177:LYS:NZ	2.46	0.58
13:M3:264:GLN:HA	13:M3:271:PRO:HD3	1.85	0.58
25:Y3:109:ARG:HD2	25:Y3:139:MET:HE1	1.85	0.58
57:C6:88:GLU:OE1	57:C6:112:ARG:NH2	2.37	0.58
60:F6:140:ASN:HB2	78:X6:367:GLN:HE22	1.69	0.58
65:K6:40:ARG:NH2	65:K6:83:CYS:O	2.36	0.58
70:P6:54:MET:HE3	73:S6:69:ARG:HE	1.68	0.58
82:b6:97:MET:N	82:b6:97:MET:SD	2.76	0.58
1:r1:719:ARG:HB3	1:r1:721:GLN:HE22	1.69	0.58
22:V3:65:LEU:HD11	22:V3:121:LYS:HD2	1.85	0.58
66:L6:221:LYS:HG2	66:L6:224:ARG:HH11	1.68	0.58
75:U6:79:GLN:HA	75:U6:82:VAL:HG22	1.85	0.58
82:b6:86:ARG:NH1	82:b6:96:PRO:O	2.37	0.58
89:n:295:LEU:HD12	89:n:303:LEU:H	1.67	0.58
3:A3:1747:G:N2	3:A3:1750:G:O2'	2.36	0.58
3:A3:3126:C:N4	3:A3:3127:G:O6	2.37	0.58
9:I3:188:ARG:NH2	46:k3:54:ASP:O	2.36	0.58
19:S3:127:ARG:NH1	19:S3:157:GLU:OE1	2.36	0.58
82:b6:298:SER:HA	82:b6:302:GLU:HB2	1.84	0.58
8:D:185:ASN:H	8:D:188:ILE:HD12	1.68	0.58
32:53:126:THR:HG22	32:53:372:ASN:HB2	1.85	0.58
39:d3:181:VAL:O	39:d3:182:ARG:NH1	2.36	0.58
58:D6:303:ILE:HG12	58:D6:336:VAL:HG12	1.84	0.58
61:G6:155:LYS:NZ	61:G6:217:ASP:OD2	2.36	0.58
62:H6:124:VAL:HG22	65:K6:109:ILE:HD12	1.84	0.58
78:X6:186:THR:O	78:X6:190:ASN:ND2	2.37	0.58
86:A6:1237:C:OP1	86:A6:1356:C:N4	2.37	0.58
3:A3:2702:G:H5'	11:K3:114:LYS:HE2	1.85	0.58
3:A3:2953:U:H5''	31:43:71:VAL:HG12	1.85	0.58
33:63:122:ALA:O	33:63:127:THR:N	2.37	0.58
56:B6:64:ASN:O	56:B6:68:LYS:NZ	2.37	0.58
69:O6:55:PRO:HA	69:O6:57:LYS:HG2	1.85	0.58
81:a6:78:ARG:NH2	81:a6:142:VAL:O	2.32	0.58
86:A6:1237:C:H1'	86:A6:1406:A:H61	1.65	0.58
56:B6:188:ARG:O	61:G6:152:TYR:OH	2.22	0.58
59:E6:97:PRO:HB2	70:P6:71:HIS:HE1	1.68	0.58
64:J6:63:LEU:HB2	64:J6:82:ARG:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R3:57:ARG:NH2	19:S3:170:ILE:O	2.37	0.58
37:b3:21:ARG:NH1	38:c3:79:LEU:O	2.36	0.58
76:V6:73:SER:HB2	76:V6:108:THR:HG22	1.85	0.58
87:24:48:U:H3	87:24:61:U:H3	1.52	0.58
1:r1:126:ASP:HB3	1:r1:500:HIS:HB2	1.85	0.58
3:A3:2528:G:OP1	5:D3:135:ARG:NH2	2.37	0.58
22:V3:177:THR:HG22	35:93:71:LYS:H	1.68	0.58
22:V3:185:ARG:NH2	22:V3:187:TYR:O	2.37	0.58
59:E6:52:SER:HA	59:E6:57:GLN:HA	1.85	0.58
87:FE:48:U:H3	87:FE:61:U:H3	1.52	0.58
4:B3:1625:A:N6	4:B3:1643:A:N1	2.50	0.57
66:L6:128:ARG:HD3	66:L6:166:MET:HE3	1.85	0.57
69:O6:134:ILE:HD13	69:O6:154:ILE:HG21	1.85	0.57
90:B:207:UNK:O	90:B:211:UNK:N	2.37	0.57
1:r1:628:ARG:HA	1:r1:631:GLU:HG2	1.86	0.57
56:B6:208:ALA:HA	56:B6:211:ASP:HB2	1.86	0.57
59:E6:72:THR:HG21	66:L6:99:ASN:HA	1.86	0.57
76:V6:66:PRO:HB3	76:V6:99:PRO:HB2	1.86	0.57
78:X6:102:ARG:NH1	78:X6:346:SER:O	2.38	0.57
3:A3:1693:C:H6	25:Y3:162:ARG:HH21	1.52	0.57
57:C6:71:LEU:HD12	57:C6:111:LYS:HG2	1.86	0.57
59:E6:24:ARG:HA	59:E6:27:GLU:HB3	1.85	0.57
72:R6:153:THR:HA	72:R6:177:PRO:HB3	1.87	0.57
1:r1:646:LEU:HA	1:r1:722:PRO:HB3	1.85	0.57
3:A3:2284:C:OP2	37:b3:74:ARG:NH2	2.37	0.57
60:F6:88:ASP:HB3	60:F6:91:ILE:HG12	1.86	0.57
60:F6:163:LYS:HE3	60:F6:239:TYR:HB3	1.86	0.57
61:G6:361:VAL:HG13	61:G6:362:GLU:HG3	1.86	0.57
81:a6:63:ARG:HH12	81:a6:135:MET:HA	1.69	0.57
1:r1:143:LEU:HB2	1:r1:171:THR:HG22	1.87	0.57
10:J3:86:THR:O	10:J3:90:PHE:N	2.34	0.57
58:D6:127:ASN:OD1	80:Z6:72:ARG:NH1	2.37	0.57
82:b6:72:VAL:HG23	82:b6:74:ALA:HB2	1.85	0.57
86:A6:1341:U:H2'	86:A6:1342:A:H8	1.69	0.57
3:A3:2293:A:N6	13:M3:37:GLU:OE2	2.38	0.57
32:53:334:LYS:H	32:53:362:THR:HG23	1.69	0.57
37:b3:78:GLU:HG2	37:b3:84:VAL:HG22	1.87	0.57
3:A3:1827:C:O2'	18:R3:48:ARG:NH1	2.37	0.57
3:A3:2422:U:OP2	35:93:24:LYS:NZ	2.37	0.57
17:Q3:197:TYR:OH	17:Q3:223:LYS:NZ	2.34	0.57
41:f3:80:ILE:HG13	41:f3:81:ASN:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:g3:96:VAL:HG22	42:g3:110:ILE:HG12	1.86	0.57
72:R6:136:VAL:O	72:R6:186:TRP:NE1	2.37	0.57
81:a6:63:ARG:HD3	81:a6:66:GLN:HB2	1.86	0.57
1:r1:385:TYR:HD1	1:r1:392:LYS:HB2	1.69	0.57
3:A3:2395:A:OP1	32:53:173:ARG:NH2	2.32	0.57
13:M3:284:LYS:HB2	42:g3:40:GLU:HB2	1.86	0.57
33:63:215:THR:HG22	33:63:239:ASN:H	1.70	0.57
66:L6:175:TYR:HB2	68:N6:89:GLY:HA3	1.87	0.57
1:r1:388:ARG:HH11	1:r1:429:ASP:H	1.52	0.57
3:A3:1775:A:HO2'	18:R3:10:LEU:N	2.01	0.57
3:A3:2073:A:H62	3:A3:2832:A:H2	1.53	0.57
32:53:351:VAL:HA	32:53:381:LEU:HA	1.87	0.57
41:f3:78:ARG:HH21	41:f3:80:ILE:HG22	1.69	0.57
1:r1:47:ARG:HH21	1:r1:314:LEU:HD22	1.70	0.57
8:H3:107:VAL:HG12	8:D:165:LYS:HD2	1.86	0.57
15:O3:38:ARG:HD3	15:O3:85:LEU:HD21	1.87	0.57
32:53:343:GLN:NE2	32:53:417:LEU:O	2.35	0.57
41:f3:97:ALA:HB2	41:f3:182:VAL:HG12	1.86	0.57
60:F6:119:LYS:NZ	78:X6:365:TRP:O	2.34	0.57
64:J6:82:ARG:HD2	64:J6:92:VAL:HG22	1.86	0.57
66:L6:109:GLU:HA	66:L6:112:MET:HB2	1.87	0.57
69:O6:218:ARG:NH1	81:a6:87:TRP:O	2.36	0.57
78:X6:186:THR:HA	78:X6:189:LYS:HE3	1.87	0.57
27:O3:119:LYS:O	27:O3:120:HIS:ND1	2.38	0.56
59:E6:6:LEU:HB2	59:E6:66:VAL:HB	1.87	0.56
60:F6:76:ALA:HB3	61:G6:373:ASP:HB3	1.85	0.56
89:n:197:TYR:HD2	89:n:217:LYS:HG2	1.69	0.56
39:d3:194:VAL:HG12	39:d3:214:VAL:HG22	1.87	0.56
61:G6:120:ARG:NH1	86:A6:1311:G:O2'	2.38	0.56
82:b6:64:GLN:NE2	85:e6:81:ASP:OD1	2.38	0.56
1:r1:57:SER:HA	1:r1:175:LYS:HE3	1.87	0.56
1:r1:167:VAL:O	1:r1:290:ARG:NH1	2.37	0.56
1:r1:559:LEU:HD22	1:r1:608:ARG:HB2	1.88	0.56
8:H3:120:ARG:NH2	24:X3:133:ASP:OD1	2.38	0.56
15:O3:91:GLN:HE21	27:O3:153:THR:HG23	1.71	0.56
17:Q3:244:ARG:HH12	17:Q3:246:ASP:HB2	1.69	0.56
32:53:313:MET:HG3	32:53:355:LEU:HD13	1.86	0.56
58:D6:266:ASP:OD1	58:D6:269:ARG:NH1	2.38	0.56
62:H6:128:LYS:O	62:H6:131:ARG:NH1	2.38	0.56
79:Y6:355:THR:HA	79:Y6:358:LEU:HG	1.87	0.56
82:b6:64:GLN:NE2	82:b6:68:SER:OG	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:b3:37:GLY:O	37:b3:44:ARG:NH2	2.38	0.56
81:a6:137:HIS:HB2	86:A6:709:C:H41	1.70	0.56
88:A:68:LEU:HA	88:A:71:LYS:HB2	1.87	0.56
3:A3:1839:C:H5''	11:K3:115:ASN:HB2	1.88	0.56
5:D3:113:ARG:O	5:D3:147:ARG:NH1	2.38	0.56
22:V3:122:LEU:HD21	22:V3:154:ILE:HG21	1.88	0.56
34:73:44:ARG:HH21	34:73:230:PHE:HA	1.69	0.56
61:G6:276:ARG:HD3	61:G6:277:LYS:HB2	1.87	0.56
74:T6:91:GLU:HG2	74:T6:92:THR:HG23	1.86	0.56
79:Y6:358:LEU:O	79:Y6:369:LYS:NZ	2.33	0.56
85:e6:82:THR:HG23	85:e6:83:THR:HG23	1.87	0.56
1:r1:123:GLY:O	1:r1:154:GLN:NE2	2.38	0.56
1:r1:617:HIS:O	1:r1:621:SER:OG	2.24	0.56
8:H3:134:PRO:HA	8:H3:137:LYS:HE2	1.88	0.56
34:73:176:SER:O	34:73:319:ARG:NH2	2.39	0.56
60:F6:169:GLN:HG2	60:F6:232:ALA:HB3	1.86	0.56
66:L6:125:LEU:HA	66:L6:128:ARG:HD2	1.88	0.56
68:N6:73:ARG:NH1	86:A6:773:G:OP2	2.38	0.56
89:n:260:LEU:HA	89:n:262:MET:HE3	1.88	0.56
3:A3:2136:C:OP2	26:Z3:77:ARG:NH2	2.38	0.56
9:I3:174:LEU:H	46:k3:53:ALA:HB3	1.71	0.56
19:S3:95:LEU:HD23	19:S3:138:ALA:HB2	1.88	0.56
24:X3:118:ILE:O	24:X3:168:ARG:NH1	2.38	0.56
30:33:104:ARG:NH1	30:33:160:LYS:O	2.38	0.56
32:53:162:ARG:NH2	32:53:383:TYR:OH	2.36	0.56
43:h3:78:PHE:HZ	43:h3:89:ILE:HG21	1.69	0.56
53:s3:373:GLN:NE2	53:s3:375:ASN:OD1	2.38	0.56
58:D6:358:THR:OG1	58:D6:361:GLN:OE1	2.23	0.56
8:D:163:THR:HA	8:D:166:PHE:HB2	1.87	0.56
24:X3:97:LEU:HD22	87:FE:73:A:H2'	1.88	0.56
36:a3:67:ILE:HD12	37:b3:138:THR:HG21	1.88	0.56
39:d3:225:TYR:HB3	39:d3:229:GLY:HA2	1.88	0.56
86:A6:1235:A:O3'	86:A6:1238:C:N4	2.38	0.56
88:A:51:ARG:HA	88:A:54:LYS:HB2	1.87	0.56
3:A3:1887:A:N3	13:M3:189:LYS:NZ	2.54	0.56
3:A3:3011:A:O2'	3:A3:3173:G:N2	2.39	0.56
16:P3:130:VAL:HG22	16:P3:134:ARG:HE	1.71	0.56
56:B6:87:ALA:HB2	56:B6:248:LEU:HD13	1.88	0.56
81:a6:64:LEU:HD23	81:a6:134:VAL:HG13	1.87	0.56
86:A6:1217:A:N7	86:A6:1218:A:N6	2.54	0.56
3:A3:2377:G:O2'	35:93:28:ARG:O	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A3:2757:A:OP2	8:H3:121:ASN:ND2	2.39	0.56
7:F3:114:THR:O	7:F3:156:ARG:NH2	2.39	0.56
50:p3:182:ASN:OD1	50:p3:185:ARG:NH1	2.38	0.56
61:G6:384:GLN:NE2	61:G6:386:GLY:O	2.38	0.56
33:63:71:TRP:CD1	33:63:72:ARG:H	2.24	0.55
53:s3:103:ASP:OD2	53:s3:325:ARG:NH2	2.39	0.55
56:B6:246:VAL:HA	56:B6:249:TYR:HD2	1.71	0.55
81:a6:84:SER:O	81:a6:88:GLN:N	2.39	0.55
82:b6:291:GLU:HA	82:b6:294:LYS:HB2	1.88	0.55
87:FE:17:U:C6	89:n:220:LYS:NZ	2.74	0.55
1:r1:313:VAL:HG23	1:r1:317:LEU:HD23	1.87	0.55
3:A3:2073:A:OP2	33:63:27:ARG:N	2.39	0.55
5:D3:232:ARG:HH22	5:D3:293:LYS:HB2	1.71	0.55
40:e3:79:ILE:HG12	48:m3:50:ARG:HD2	1.88	0.55
61:G6:255:GLN:HG3	61:G6:370:LEU:HD13	1.88	0.55
62:H6:70:ASP:HB3	85:e6:62:LYS:HA	1.87	0.55
1:r1:382:ASP:OD1	1:r1:383:THR:N	2.39	0.55
7:F3:63:GLN:HA	7:F3:81:ASP:HA	1.87	0.55
16:P3:127:ILE:HA	16:P3:130:VAL:HG12	1.86	0.55
18:R3:111:LYS:NZ	19:S3:139:ASP:OD1	2.31	0.55
60:F6:218:PRO:HA	60:F6:221:LYS:HB3	1.89	0.55
70:P6:141:ARG:H	71:Q6:28:ARG:HH21	1.54	0.55
78:X6:240:VAL:HA	78:X6:243:VAL:HB	1.88	0.55
3:A3:2140:G:OP2	26:Z3:71:ARG:NH2	2.39	0.55
7:F3:241:ASN:OD1	7:F3:256:HIS:NE2	2.38	0.55
64:J6:35:GLN:NE2	86:A6:1138:G:OP2	2.39	0.55
67:M6:108:GLU:HA	67:M6:111:ARG:HB2	1.88	0.55
8:D:194:PHE:CD1	89:n:92:TYR:CZ	2.93	0.55
15:O3:50:ASP:HB2	15:O3:107:MET:HE1	1.88	0.55
16:P3:74:ARG:O	16:P3:96:GLN:NE2	2.39	0.55
58:D6:201:ILE:HB	58:D6:222:ILE:HD12	1.87	0.55
65:K6:108:ARG:NH2	86:A6:1232:A:OP2	2.39	0.55
67:M6:54:TYR:HD1	67:M6:66:VAL:HG22	1.70	0.55
74:T6:33:ASN:ND2	74:T6:70:MET:SD	2.80	0.55
11:K3:138:LEU:O	37:b3:144:ARG:NH2	2.40	0.55
12:L3:124:PRO:HG2	12:L3:127:LEU:HD13	1.89	0.55
19:S3:99:VAL:HG12	19:S3:133:VAL:HG22	1.88	0.55
48:m3:57:VAL:HG13	88:A:185:TYR:HE1	1.71	0.55
83:c6:55:CYS:SG	83:c6:59:ASN:ND2	2.80	0.55
89:n:91:LEU:HG	89:n:303:LEU:HD12	1.89	0.55
3:A3:2248:U:OP1	18:R3:99:ARG:NH2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D3:232:ARG:HE	5:D3:290:PRO:HB2	1.72	0.55
13:M3:222:TYR:HE2	13:M3:262:PRO:HB3	1.72	0.55
15:O3:141:HIS:NE2	15:O3:150:GLN:OE1	2.34	0.55
17:Q3:118:ARG:HB2	17:Q3:134:LEU:HD12	1.89	0.55
26:Z3:134:MET:HE1	45:j3:78:VAL:HG21	1.88	0.55
39:d3:147:GLU:HG2	39:d3:159:ARG:HH12	1.71	0.55
61:G6:149:TYR:OH	61:G6:163:HIS:ND1	2.27	0.55
66:L6:168:LYS:O	66:L6:172:ASN:ND2	2.40	0.55
67:M6:110:LEU:HA	67:M6:113:LYS:HB2	1.89	0.55
76:V6:384:LEU:O	76:V6:388:GLN:NE2	2.39	0.55
1:r1:268:PHE:HB3	1:r1:269:LEU:HD12	1.88	0.55
1:r1:730:ASP:O	1:r1:734:LYS:N	2.39	0.55
5:D3:194:ASN:OD1	5:D3:243:THR:OG1	2.23	0.55
10:J3:23:ILE:HA	10:J3:67:PRO:HA	1.88	0.55
52:r3:71:PRO:HD2	52:r3:107:LEU:HD23	1.89	0.55
80:Z6:19:PHE:O	82:b6:211:ARG:NH1	2.34	0.55
83:c6:75:ASP:O	83:c6:79:ARG:NH2	2.40	0.55
86:A6:871:C:O2	86:A6:874:C:N4	2.39	0.55
3:A3:2064:A:OP1	23:W3:101:LYS:NZ	2.29	0.55
3:A3:2204:U:O2'	3:A3:2206:C:N4	2.40	0.55
12:L3:93:GLY:O	12:L3:95:ARG:NH1	2.40	0.55
14:N3:238:LYS:HB2	14:N3:240:LYS:HG3	1.89	0.55
15:O3:33:LEU:HD21	15:O3:59:LEU:HD22	1.88	0.55
17:Q3:205:LYS:NZ	17:Q3:206:PRO:O	2.40	0.55
26:Z3:68:ILE:HD11	26:Z3:122:LEU:HD13	1.87	0.55
63:I6:111:SER:O	63:I6:114:THR:OG1	2.24	0.55
82:b6:128:ASP:OD1	82:b6:128:ASP:N	2.40	0.55
30:33:95:THR:HA	44:i3:122:ASN:HD22	1.72	0.55
32:53:228:ALA:HB3	32:53:292:TYR:HB2	1.89	0.55
34:73:65:ILE:HB	34:73:122:SER:HB2	1.88	0.55
52:r3:78:LYS:NZ	52:r3:110:GLU:OE2	2.39	0.55
65:K6:33:ARG:NH2	86:A6:1241:A:OP1	2.39	0.55
72:R6:106:MET:HB2	72:R6:110:GLN:HB2	1.89	0.55
3:A3:1877:U:H5''	49:o3:86:ARG:HH12	1.72	0.54
3:A3:2142:A:O2'	3:A3:2262:C:OP1	2.25	0.54
15:O3:108:LEU:HD23	27:O3:122:LEU:HD21	1.88	0.54
61:G6:276:ARG:NH2	86:A6:1435:G:N7	2.55	0.54
61:G6:336:GLY:H	61:G6:339:ALA:HB3	1.72	0.54
78:X6:133:GLY:HA2	95:X6:500:GDP:H5''	1.89	0.54
3:A3:1705:A:N6	35:93:40:GLY:O	2.37	0.54
3:A3:1868:G:OP2	13:M3:41:ARG:NH1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J3:89:TYR:HD2	10:J3:92:LYS:HD3	1.71	0.54
65:K6:58:ARG:NH2	65:K6:72:ASP:OD2	2.40	0.54
71:Q6:70:ARG:NH2	77:W6:152:ARG:O	2.39	0.54
74:T6:139:CYS:SG	74:T6:140:ILE:N	2.80	0.54
76:V6:105:ARG:O	76:V6:108:THR:OG1	2.23	0.54
78:X6:319:PRO:HA	86:A6:1379:C:H5''	1.89	0.54
3:A3:1883:G:H5'	42:g3:91:MET:HE3	1.89	0.54
3:A3:3063:G:O2'	3:A3:3066:C:OP2	2.22	0.54
9:I3:50:VAL:O	14:N3:211:ASN:ND2	2.39	0.54
9:I3:94:ARG:H	9:I3:157:GLU:HA	1.72	0.54
42:g3:128:LEU:HB2	42:g3:136:PRO:HG3	1.89	0.54
83:c6:83:ALA:O	83:c6:87:ARG:N	2.40	0.54
1:r1:704:ARG:O	3:A3:3128:A:N6	2.40	0.54
3:A3:2537:G:O2'	3:A3:2634:U:OP2	2.25	0.54
34:73:59:THR:O	34:73:61:ARG:NH2	2.41	0.54
40:e3:173:LEU:HD12	40:e3:174:PRO:HD2	1.90	0.54
46:k3:64:VAL:HG13	46:k3:76:MET:HG3	1.89	0.54
82:b6:296:VAL:HG23	82:b6:299:LEU:HD12	1.89	0.54
87:24:14:A:N1	87:24:19:A:O2'	2.34	0.54
9:I3:116:LEU:HD11	9:I3:167:ILE:HG21	1.88	0.54
32:53:251:HIS:O	32:53:371:LYS:NZ	2.41	0.54
53:s3:242:ARG:HA	53:s3:295:GLY:HA2	1.89	0.54
57:C6:78:GLY:O	82:b6:167:ARG:NH1	2.40	0.54
66:L6:135:LYS:NZ	86:A6:1044:U:OP1	2.34	0.54
81:a6:63:ARG:NH2	81:a6:135:MET:O	2.40	0.54
88:A:68:LEU:O	88:A:72:ILE:N	2.35	0.54
8:D:168:LYS:HE2	8:D:232:ARG:H	1.73	0.54
22:V3:54:TRP:NE1	22:V3:56:LEU:O	2.41	0.54
53:s3:177:LEU:HD22	53:s3:238:ASN:HD22	1.72	0.54
56:B6:214:LYS:HZ3	86:A6:1284:C:H5''	1.71	0.54
58:D6:258:ILE:HD12	58:D6:343:LEU:HD11	1.90	0.54
69:O6:110:ASP:OD2	69:O6:111:HIS:N	2.41	0.54
72:R6:138:ILE:HG12	72:R6:186:TRP:HE1	1.73	0.54
75:U6:57:MET:HA	75:U6:60:TYR:HD2	1.71	0.54
83:c6:66:CYS:HB3	83:c6:69:GLU:HB2	1.90	0.54
1:r1:488:ASN:ND2	1:r1:522:LYS:O	2.41	0.54
3:A3:2406:A:H61	32:53:112:ARG:HH11	1.55	0.54
60:F6:115:LEU:HA	60:F6:118:VAL:HG22	1.90	0.54
87:24:8:U:H5'	87:24:47:A:H5'	1.90	0.54
1:r1:46:ILE:HG23	1:r1:115:ASN:HB2	1.90	0.54
57:C6:71:LEU:HB3	62:H6:167:GLY:HA3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:R6:231:CYS:O	72:R6:235:PHE:N	2.34	0.54
87:24:10:G:O6	87:24:23:A:N6	2.41	0.54
3:A3:1812:C:OP1	20:T3:50:LYS:NZ	2.41	0.54
3:A3:1953:A:O2'	3:A3:2463:A:OP1	2.26	0.54
13:M3:180:ASP:N	13:M3:180:ASP:OD1	2.39	0.54
36:a3:67:ILE:HD13	38:c3:258:THR:HG23	1.90	0.54
41:f3:138:GLN:HG2	48:m3:78:PRO:HB3	1.88	0.54
46:k3:41:LYS:O	46:k3:44:SER:OG	2.25	0.54
63:I6:88:ILE:N	63:I6:150:VAL:O	2.40	0.54
70:P6:82:GLN:NE2	75:U6:191:ILE:O	2.33	0.54
89:n:221:LEU:HA	89:n:226:ILE:HD13	1.90	0.54
3:A3:2599:U:OP2	3:A3:2625:C:N4	2.41	0.54
9:I3:104:LEU:HD12	9:I3:112:MET:HE1	1.90	0.54
38:c3:84:SER:HB2	38:c3:87:LEU:HB3	1.90	0.54
40:e3:83:LEU:HG	88:A:98:ALA:HA	1.89	0.54
68:N6:78:LYS:NZ	86:A6:753:G:O3'	2.38	0.54
3:A3:1849:C:OP2	13:M3:53:HIS:NE2	2.38	0.53
7:F3:292:ASP:HB3	42:g3:55:THR:HG22	1.89	0.53
56:B6:129:LEU:HA	56:B6:132:THR:HG22	1.90	0.53
70:P6:139:ARG:HD2	70:P6:142:GLU:HG3	1.90	0.53
75:U6:76:SER:HA	75:U6:79:GLN:HB2	1.89	0.53
77:W6:140:VAL:HA	77:W6:172:ILE:HA	1.88	0.53
87:24:26:C:O2	87:24:41:G:N2	2.42	0.53
19:S3:142:THR:OG1	36:a3:60:CYS:SG	2.66	0.53
29:23:82:ARG:NH1	29:23:89:SER:O	2.41	0.53
30:33:183:ARG:HE	30:33:186:LEU:HD22	1.72	0.53
51:q3:57:ALA:HB1	51:q3:70:VAL:HG11	1.90	0.53
66:L6:170:LEU:HD21	66:L6:177:VAL:HG13	1.90	0.53
80:Z6:53:PRO:O	80:Z6:55:HIS:ND1	2.41	0.53
81:a6:92:PRO:HG3	81:a6:152:ALA:H	1.74	0.53
82:b6:118:ALA:HA	82:b6:121:LYS:HE3	1.89	0.53
86:A6:702:C:H2'	86:A6:703:A:H8	1.73	0.53
13:M3:62:ARG:HB3	44:i3:128:ARG:HH11	1.71	0.53
22:V3:122:LEU:HD23	22:V3:133:ILE:HG13	1.90	0.53
34:73:243:LYS:HA	34:73:246:GLN:HE22	1.73	0.53
52:r3:124:ARG:NH1	52:r3:153:ARG:O	2.36	0.53
58:D6:242:ARG:HD2	58:D6:258:ILE:HD11	1.89	0.53
66:L6:202:ARG:NH1	86:A6:765:A:OP1	2.41	0.53
68:N6:5:ARG:HH22	68:N6:67:ARG:HH12	1.55	0.53
72:R6:82:MET:HE1	72:R6:300:LEU:HB2	1.90	0.53
74:T6:11:ARG:HH22	86:A6:936:C:H41	1.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:A6:773:G:H21	86:A6:776:A:H2	1.57	0.53
3:A3:2003:A:OP2	3:A3:2734:A:O2'	2.26	0.53
22:V3:59:GLY:H	22:V3:76:VAL:HG23	1.71	0.53
56:B6:99:HIS:ND1	56:B6:227:CYS:O	2.40	0.53
56:B6:120:GLN:HA	56:B6:123:THR:HG22	1.89	0.53
76:V6:71:THR:HG22	76:V6:74:ARG:HH22	1.71	0.53
76:V6:396:GLN:NE2	86:A6:1527:A:N7	2.57	0.53
87:FE:10:G:O6	87:FE:23:A:N6	2.41	0.53
87:FE:17:U:N1	89:n:220:LYS:NZ	2.56	0.53
3:A3:3154:U:OP1	17:Q3:231:LYS:NZ	2.35	0.53
20:T3:155:ARG:HB2	20:T3:167:MET:HB3	1.90	0.53
74:T6:122:GLN:O	74:T6:125:HIS:NE2	2.42	0.53
75:U6:49:ASP:HB2	75:U6:52:GLU:HB3	1.90	0.53
84:d6:179:LYS:NZ	86:A6:768:A:OP1	2.34	0.53
23:W3:114:VAL:HA	23:W3:117:ILE:HD12	1.89	0.53
51:q3:149:ASP:OD1	51:q3:152:ARG:NH1	2.42	0.53
72:R6:219:TYR:HE1	72:R6:227:VAL:HG21	1.74	0.53
78:X6:259:LEU:HA	78:X6:306:ILE:HG22	1.91	0.53
82:b6:81:VAL:HG12	82:b6:83:LEU:H	1.73	0.53
9:I3:62:PRO:HA	9:I3:65:LEU:HD12	1.90	0.53
22:V3:25:PRO:HG2	22:V3:28:SER:HB2	1.90	0.53
27:03:133:GLU:HA	27:03:136:GLU:HB2	1.91	0.53
38:c3:253:PRO:HB2	38:c3:274:LEU:HD12	1.89	0.53
58:D6:269:ARG:NH2	86:A6:1282:C:OP1	2.42	0.53
87:FE:8:U:H5'	87:FE:47:A:H5'	1.90	0.53
3:A3:2373:A:OP1	21:U3:50:ARG:NH2	2.37	0.53
22:V3:105:ARG:HD2	39:d3:170:PRO:HB2	1.90	0.53
56:B6:251:ARG:NH1	56:B6:255:THR:OG1	2.42	0.53
57:C6:74:GLY:O	65:K6:103:ARG:NH2	2.41	0.53
63:I6:187:ARG:HE	63:I6:188:PRO:HD2	1.74	0.53
74:T6:118:GLU:O	74:T6:122:GLN:N	2.41	0.53
85:e6:86:PRO:HG2	85:e6:88:VAL:HG22	1.90	0.53
8:D:194:PHE:CD2	89:n:92:TYR:CG	2.97	0.53
1:r1:55:ILE:HG22	1:r1:152:GLN:HE22	1.74	0.53
6:E3:50:ASP:HA	6:E3:53:LEU:HD13	1.91	0.53
28:13:22:SER:OG	28:13:24:ALA:O	2.25	0.53
34:73:203:THR:HG22	34:73:280:VAL:H	1.73	0.53
38:c3:257:LEU:HD21	38:c3:260:GLN:HG2	1.90	0.53
61:G6:101:GLN:HA	61:G6:104:ILE:HD12	1.90	0.53
78:X6:123:ARG:HB2	78:X6:338:ASP:HB3	1.91	0.53
87:FE:26:C:O2	87:FE:41:G:N2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N3:130:PRO:HB2	14:N3:147:ILE:HD12	1.91	0.53
37:b3:27:GLN:OE1	37:b3:28:ARG:NH1	2.42	0.53
43:h3:85:ASN:ND2	43:h3:88:ASP:OD2	2.42	0.53
57:C6:134:PHE:HD2	57:C6:135:LEU:HD12	1.74	0.53
89:n:155:ASN:HB2	89:n:238:LYS:HD3	1.91	0.53
1:r1:467:SER:HA	1:r1:470:ILE:HG22	1.91	0.52
3:A3:2064:A:H62	41:f3:48:TYR:N	2.07	0.52
13:M3:153:ASN:ND2	13:M3:255:MET:O	2.43	0.52
15:O3:43:GLU:OE2	27:O3:127:TYR:OH	2.26	0.52
23:W3:147:MET:HG3	33:63:338:ARG:HG3	1.89	0.52
66:L6:222:LYS:NZ	86:A6:777:U:OP2	2.39	0.52
1:r1:551:LYS:HB3	1:r1:615:ALA:HB3	1.91	0.52
3:A3:1831:G:N7	37:b3:4:ARG:NH1	2.56	0.52
3:A3:2480:A:H1'	6:E3:230:THR:HG21	1.90	0.52
3:A3:2932:G:OP1	7:F3:137:ARG:NH1	2.42	0.52
25:Y3:128:SER:OG	25:Y3:131:ARG:NE	2.42	0.52
56:B6:80:SER:OG	56:B6:81:VAL:N	2.42	0.52
60:F6:196:HIS:HB3	60:F6:199:THR:HG22	1.91	0.52
69:O6:210:GLU:O	69:O6:214:SER:N	2.41	0.52
80:Z6:81:GLU:HA	80:Z6:84:ARG:HB3	1.91	0.52
3:A3:1759:U:OP2	51:q3:55:ARG:NH1	2.43	0.52
3:A3:1788:C:O2	3:A3:1918:G:N2	2.41	0.52
3:A3:1974:A:N3	5:D3:264:ARG:NH1	2.58	0.52
27:O3:158:VAL:HG12	27:O3:175:ILE:HB	1.91	0.52
40:e3:162:ARG:HB3	40:e3:251:HIS:HB2	1.91	0.52
41:f3:169:ILE:HG23	88:A:139:MET:HE2	1.91	0.52
60:F6:201:MET:HE3	60:F6:205:LEU:HB2	1.91	0.52
86:A6:737:U:H3	86:A6:745:A:H61	1.57	0.52
87:24:29:G:H1	87:24:37:A:H61	1.57	0.52
87:FE:29:G:H1	87:FE:37:A:H61	1.57	0.52
3:A3:1826:G:H4'	3:A3:1828:A:H2	1.74	0.52
3:A3:2096:U:O4	13:M3:57:ARG:NH1	2.42	0.52
3:A3:2822:C:O2'	3:A3:2915:C:OP2	2.28	0.52
12:L3:128:ARG:HB2	17:Q3:125:TYR:HB3	1.91	0.52
15:O3:41:ARG:NH2	15:O3:131:PRO:O	2.41	0.52
39:d3:147:GLU:O	39:d3:159:ARG:NH1	2.43	0.52
85:e6:339:LEU:O	85:e6:343:ARG:N	2.42	0.52
1:r1:67:LEU:HB3	1:r1:73:ILE:HB	1.90	0.52
1:r1:566:LYS:HB3	1:r1:605:SER:HB3	1.92	0.52
3:A3:2372:U:O4	21:U3:35:GLN:NE2	2.39	0.52
3:A3:3019:G:O2'	3:A3:3125:A:N1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:e3:133:LEU:HD21	88:A:178:TYR:HE2	1.73	0.52
60:F6:100:ILE:HD13	60:F6:192:ARG:HH21	1.74	0.52
8:D:194:PHE:CB	89:n:92:TYR:CZ	2.92	0.52
1:r1:170:LEU:HG	1:r1:317:LEU:HD22	1.91	0.52
1:r1:482:VAL:HG13	1:r1:493:ILE:HG22	1.91	0.52
3:A3:1822:U:O2	3:A3:2707:A:O2'	2.27	0.52
3:A3:2909:G:OP1	28:13:63:ARG:NH2	2.43	0.52
19:S3:54:THR:OG1	52:r3:85:ASP:OD2	2.24	0.52
69:O6:63:GLU:HA	69:O6:66:GLU:HG3	1.92	0.52
1:r1:344:ASN:HB2	1:r1:375:GLN:HG3	1.90	0.52
3:A3:2909:G:N7	30:33:131:LYS:NZ	2.57	0.52
25:Y3:151:ASP:OD1	25:Y3:154:ARG:NH2	2.43	0.52
32:53:191:GLN:OE1	32:53:194:LYS:NZ	2.42	0.52
40:e3:101:LYS:HE3	78:X6:231:THR:HA	1.92	0.52
48:m3:51:LEU:HB3	48:m3:67:ARG:HB3	1.91	0.52
67:M6:59:ASN:HA	74:T6:147:VAL:HG23	1.92	0.52
75:U6:71:ARG:HA	75:U6:74:PHE:HD2	1.75	0.52
78:X6:86:ARG:NH2	86:A6:1384:G:OP1	2.42	0.52
3:A3:2145:G:OP1	19:S3:169:ARG:NH1	2.43	0.52
3:A3:2632:A:O2'	3:A3:2635:G:N3	2.40	0.52
57:C6:64:HIS:HA	61:G6:117:PHE:HB2	1.92	0.52
64:J6:116:GLN:NE2	86:A6:901:C:OP2	2.43	0.52
68:N6:52:HIS:HB3	68:N6:80:GLU:HG2	1.91	0.52
71:Q6:47:LYS:NZ	86:A6:1594:A:OP2	2.40	0.52
86:A6:1198:C:N4	86:A6:1432:G:O6	2.43	0.52
3:A3:1864:A:O3'	18:R3:13:ARG:NH1	2.43	0.52
58:D6:362:LEU:HB3	72:R6:105:LEU:HD21	1.92	0.52
69:O6:128:CYS:SG	69:O6:129:ALA:N	2.74	0.52
75:U6:121:ILE:HA	75:U6:124:LEU:HB2	1.91	0.52
89:n:96:ILE:HD12	89:n:306:LYS:HE3	1.92	0.52
89:n:199:ALA:H	89:n:219:PRO:HG2	1.74	0.52
23:W3:100:THR:OG1	23:W3:132:HIS:NE2	2.39	0.52
40:e3:49:GLY:O	40:e3:176:ALA:N	2.43	0.52
40:e3:127:LYS:HA	40:e3:130:GLN:HG2	1.91	0.52
56:B6:69:HIS:HB2	56:B6:72:PHE:HB2	1.92	0.52
72:R6:260:ASP:OD1	72:R6:263:ARG:NH1	2.39	0.52
80:Z6:43:ALA:HA	80:Z6:48:THR:HG21	1.92	0.52
7:F3:119:GLU:OE2	7:F3:156:ARG:NH1	2.40	0.51
9:I3:177:LEU:HA	9:I3:188:ARG:HG2	1.91	0.51
38:c3:46:GLU:HA	38:c3:49:ARG:HG3	1.92	0.51
41:f3:150:LEU:HD22	48:m3:56:LEU:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:C6:124:LEU:HB3	57:C6:126:GLN:HG2	1.92	0.51
69:O6:153:ALA:HA	69:O6:156:LYS:HB2	1.92	0.51
3:A3:2200:A:O2'	47:l3:133:SER:O	2.29	0.51
3:A3:2237:A:OP1	52:r3:171:ARG:NH1	2.38	0.51
7:F3:253:MET:HG2	7:F3:259:LEU:HD11	1.93	0.51
10:J3:102:ARG:N	10:J3:107:GLU:OE1	2.37	0.51
12:L3:102:SER:OG	12:L3:104:ASN:OD1	2.28	0.51
17:Q3:118:ARG:NH2	17:Q3:204:MET:O	2.42	0.51
61:G6:336:GLY:HA3	86:A6:1459:U:H4'	1.91	0.51
65:K6:91:CYS:SG	65:K6:95:SER:N	2.83	0.51
79:Y6:295:GLN:HE22	85:e6:80:ARG:HG2	1.75	0.51
86:A6:1107:A:N7	86:A6:1578:G:O2'	2.42	0.51
88:A:73:ARG:NH2	88:A:76:GLU:OE1	2.43	0.51
3:A3:2899:C:N3	54:u3:2:A:O2'	2.44	0.51
29:23:82:ARG:HG2	29:23:87:ARG:HG3	1.91	0.51
37:b3:26:LEU:HD11	37:b3:77:ALA:HB1	1.93	0.51
53:s3:305:LYS:O	53:s3:310:ARG:NE	2.42	0.51
57:C6:71:LEU:HB2	57:C6:111:LYS:HA	1.92	0.51
60:F6:112:ILE:HA	78:X6:397:TYR:HE1	1.76	0.51
74:T6:95:ASN:HA	74:T6:98:ILE:HD12	1.91	0.51
77:W6:152:ARG:NH1	77:W6:157:THR:O	2.44	0.51
86:A6:1102:C:OP1	86:A6:1155:C:N4	2.43	0.51
87:24:19:A:N6	87:24:44:U:O2'	2.43	0.51
1:r1:655:VAL:N	1:r1:712:GLU:O	2.41	0.51
9:I3:121:ILE:HD11	9:I3:154:LEU:HB3	1.92	0.51
13:M3:279:ASP:HB3	13:M3:281:LYS:HE2	1.91	0.51
15:O3:106:ARG:HD3	15:O3:135:LEU:HD11	1.93	0.51
18:R3:47:ILE:HD12	19:S3:172:MET:HE1	1.91	0.51
32:53:335:VAL:HG22	32:53:370:VAL:HG11	1.91	0.51
34:73:144:ARG:NH1	34:73:267:PRO:O	2.44	0.51
34:73:222:GLU:HA	34:73:251:ILE:HA	1.92	0.51
38:c3:145:TYR:OH	38:c3:311:ARG:NH1	2.43	0.51
56:B6:162:CYS:SG	56:B6:254:GLN:NE2	2.77	0.51
57:C6:167:LEU:O	86:A6:1305:G:O2'	2.28	0.51
62:H6:66:SER:OG	62:H6:67:ASP:N	2.42	0.51
74:T6:6:ARG:N	86:A6:1135:C:OP1	2.44	0.51
74:T6:36:THR:HG21	86:A6:959:A:H62	1.75	0.51
8:D:194:PHE:CB	89:n:92:TYR:CE2	2.93	0.51
18:R3:81:LEU:HD11	18:R3:121:SER:HB2	1.92	0.51
27:03:86:THR:HG22	27:03:88:GLU:H	1.75	0.51
30:33:107:VAL:HG21	30:33:161:MET:HE2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:73:242:GLU:O	34:73:246:GLN:NE2	2.44	0.51
45:j3:91:TRP:NE1	49:o3:57:GLU:OE1	2.44	0.51
58:D6:206:PRO:HG3	58:D6:276:VAL:HG11	1.91	0.51
58:D6:225:VAL:HG22	58:D6:243:VAL:HG12	1.93	0.51
58:D6:408:TRP:HE3	74:T6:3:MET:HE1	1.76	0.51
72:R6:260:ASP:OD2	72:R6:291:ARG:NH1	2.44	0.51
82:b6:137:LEU:HD23	82:b6:142:LYS:HG2	1.92	0.51
1:r1:330:ASN:HB2	1:r1:339:THR:HB	1.92	0.51
3:A3:2154:A:OP2	49:o3:30:ARG:NH1	2.43	0.51
7:F3:182:LEU:HD13	7:F3:187:LEU:HD23	1.92	0.51
53:s3:256:SER:OG	53:s3:257:VAL:N	2.44	0.51
56:B6:62:ILE:O	56:B6:137:TYR:OH	2.29	0.51
76:V6:250:ILE:O	76:V6:255:TYR:OH	2.28	0.51
83:c6:36:ARG:HH22	83:c6:37:ARG:HD3	1.76	0.51
8:D:185:ASN:HB2	8:D:188:ILE:HG13	1.93	0.51
87:FE:17:U:C5	89:n:220:LYS:NZ	2.79	0.51
3:A3:2274:A:HO2'	18:R3:15:THR:HG1	1.56	0.51
3:A3:2292:G:O2'	18:R3:11:ARG:O	2.26	0.51
21:U3:42:PHE:HB2	21:U3:95:ALA:HB3	1.92	0.51
21:U3:49:THR:HB	21:U3:52:ASP:HB2	1.93	0.51
22:V3:75:LYS:O	22:V3:89:GLY:N	2.43	0.51
78:X6:262:VAL:HG11	78:X6:265:ILE:HD13	1.92	0.51
81:a6:51:PRO:HG3	86:A6:707:A:H2'	1.91	0.51
81:a6:129:ARG:NH1	81:a6:204:PRO:O	2.44	0.51
85:e6:373:HIS:ND1	85:e6:414:LYS:O	2.44	0.51
1:r1:326:TYR:HB2	1:r1:342:LEU:HA	1.91	0.51
3:A3:2052:A:H5'	42:g3:105:ARG:HG2	1.92	0.51
38:c3:155:ASN:HD22	38:c3:232:TRP:CD1	2.29	0.51
86:A6:1081:U:O2'	86:A6:1083:G:N7	2.42	0.51
7:F3:94:ASP:OD1	7:F3:94:ASP:N	2.43	0.51
36:a3:77:ARG:NH2	38:c3:293:GLU:OE2	2.43	0.51
40:e3:183:THR:O	40:e3:187:THR:OG1	2.29	0.51
52:r3:81:TYR:O	52:r3:184:ASN:ND2	2.39	0.51
74:T6:105:ILE:HG23	75:U6:105:LEU:HD13	1.93	0.51
75:U6:27:ARG:HG2	86:A6:716:C:H42	1.75	0.51
78:X6:166:ARG:NH1	86:A6:1387:A:OP1	2.43	0.51
78:X6:389:SER:OG	78:X6:393:ARG:NH1	2.44	0.51
80:Z6:32:LYS:O	80:Z6:36:LEU:N	2.35	0.51
81:a6:102:PRO:HA	81:a6:112:GLY:HA3	1.93	0.51
86:A6:1385:A:H2'	86:A6:1386:A:H8	1.76	0.51
9:I3:188:ARG:NH1	46:k3:20:PHE:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T3:80:ILE:HG21	20:T3:87:MET:HE1	1.93	0.51
57:C6:76:LEU:O	65:K6:103:ARG:NH2	2.44	0.51
59:E6:26:ILE:HG23	59:E6:36:VAL:HG21	1.93	0.51
59:E6:115:GLU:OE2	77:W6:152:ARG:NH1	2.44	0.51
61:G6:259:PRO:HB2	61:G6:261:GLN:HG2	1.93	0.51
61:G6:302:LEU:HD21	78:X6:321:LYS:HA	1.92	0.51
65:K6:105:ARG:NH2	80:Z6:47:GLU:OE1	2.42	0.51
71:Q6:2:ALA:N	86:A6:981:A:OP2	2.44	0.51
74:T6:109:ASN:O	74:T6:112:THR:OG1	2.25	0.51
75:U6:66:THR:O	75:U6:70:LEU:N	2.41	0.51
3:A3:2758:G:OP2	3:A3:2789:C:N4	2.44	0.50
6:E3:110:TRP:HZ3	17:Q3:145:LEU:HD23	1.76	0.50
13:M3:62:ARG:HG2	13:M3:63:PRO:HD2	1.93	0.50
29:23:61:LYS:NZ	29:23:92:HIS:O	2.45	0.50
40:e3:144:ASN:OD1	40:e3:146:ARG:NH2	2.44	0.50
50:p3:133:LEU:HD21	50:p3:157:MET:HE1	1.94	0.50
56:B6:60:ASP:O	56:B6:64:ASN:ND2	2.43	0.50
60:F6:35:SER:N	86:A6:1434:A:OP1	2.44	0.50
61:G6:91:MET:HG2	61:G6:111:LEU:HD11	1.93	0.50
67:M6:11:ALA:HB2	86:A6:749:A:H4'	1.93	0.50
76:V6:197:SER:OG	76:V6:199:GLU:N	2.44	0.50
87:FE:19:A:N6	87:FE:44:U:O2'	2.43	0.50
1:r1:56:ASP:OD1	1:r1:57:SER:N	2.38	0.50
3:A3:2417:C:N4	53:s3:304:ASP:OD1	2.39	0.50
3:A3:2842:C:OP2	23:W3:41:ASN:ND2	2.39	0.50
11:K3:59:ILE:HB	11:K3:127:LEU:HD23	1.93	0.50
34:73:52:LYS:HD2	34:73:219:LEU:HD21	1.93	0.50
60:F6:152:CYS:HA	60:F6:223:LYS:HE2	1.93	0.50
62:H6:122:GLN:O	86:A6:1268:C:O2'	2.29	0.50
85:e6:100:SER:HA	85:e6:103:SER:HB2	1.91	0.50
3:A3:2582:A:N1	86:A6:1564:U:O2'	2.35	0.50
8:H3:54:VAL:O	24:X3:42:HIS:ND1	2.40	0.50
9:I3:47:LEU:HD22	14:N3:226:ILE:HG12	1.94	0.50
10:J3:156:VAL:HG12	10:J3:157:LYS:HD2	1.92	0.50
32:53:275:ASN:C	32:53:275:ASN:HD22	2.20	0.50
57:C6:132:TYR:HD2	85:e6:95:LEU:HD21	1.76	0.50
8:D:194:PHE:CB	89:n:92:TYR:CD2	2.94	0.50
1:r1:388:ARG:HE	1:r1:429:ASP:HB2	1.76	0.50
10:J3:21:ARG:HE	10:J3:69:LYS:HE2	1.76	0.50
60:F6:169:GLN:HB2	87:FE:30:G:H21	1.77	0.50
86:A6:1276:A:H61	86:A6:1324:G:H1'	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
88:A:54:LYS:HE2	88:A:65:LYS:HE3	1.93	0.50
3:A3:2530:A:H4'	3:A3:2531:U:H5'	1.92	0.50
75:U6:76:SER:O	75:U6:80:ARG:N	2.43	0.50
78:X6:188:LEU:HD21	78:X6:240:VAL:HB	1.92	0.50
81:a6:79:LEU:HD13	81:a6:96:ARG:HG3	1.94	0.50
88:A:123:LEU:O	88:A:127:GLN:NE2	2.44	0.50
1:r1:690:ASP:OD2	1:r1:719:ARG:NH2	2.42	0.50
3:A3:2195:A:OP2	47:l3:119:ARG:NH2	2.45	0.50
7:F3:70:ARG:HA	7:F3:196:PRO:HD3	1.93	0.50
15:O3:38:ARG:NH2	15:O3:82:GLU:OE1	2.41	0.50
17:Q3:98:ASP:HB3	17:Q3:145:LEU:HD11	1.92	0.50
28:l3:34:ARG:HG3	28:l3:41:LEU:HG	1.93	0.50
48:m3:54:VAL:HG21	48:m3:68:TYR:HB3	1.94	0.50
1:r1:216:ASP:OD1	1:r1:217:LEU:N	2.45	0.50
32:53:115:GLU:HB2	32:53:119:GLN:HB2	1.93	0.50
48:m3:70:GLU:O	48:m3:72:ARG:N	2.40	0.50
57:C6:50:PRO:HB2	57:C6:163:VAL:HG11	1.93	0.50
60:F6:139:ARG:HD2	78:X6:367:GLN:HG3	1.93	0.50
72:R6:117:GLN:O	72:R6:121:ALA:N	2.42	0.50
85:e6:534:LEU:HA	85:e6:537:ARG:HD3	1.93	0.50
85:e6:535:MET:HE1	85:e6:551:CYS:HB3	1.94	0.50
1:r1:200:PHE:HA	1:r1:295:VAL:HG22	1.94	0.50
41:f3:183:ARG:NE	88:A:174:GLU:OE1	2.44	0.50
53:s3:112:THR:HG22	53:s3:391:ASN:HB2	1.94	0.50
58:D6:289:THR:HG22	58:D6:290:ILE:H	1.75	0.50
60:F6:187:MET:HG2	60:F6:208:LYS:HZ3	1.77	0.50
67:M6:69:ASN:HB3	72:R6:161:ILE:HB	1.94	0.50
1:r1:66:VAL:HG23	1:r1:310:LEU:HD21	1.93	0.50
1:r1:116:ILE:HD11	1:r1:314:LEU:HD21	1.94	0.50
1:r1:259:ASN:ND2	1:r1:291:SER:O	2.43	0.50
38:c3:83:PHE:HE1	38:c3:202:LEU:HD13	1.76	0.50
1:r1:221:ARG:HD2	1:r1:235:TYR:HB3	1.94	0.49
3:A3:1755:A:O2'	8:H3:63:PRO:O	2.29	0.49
3:A3:2421:G:H5''	35:93:24:LYS:HG2	1.94	0.49
3:A3:2901:A:O5'	87:FE:73:A:N6	2.45	0.49
4:B3:1626:C:N4	16:P3:86:GLN:OE1	2.45	0.49
12:L3:94:PRO:O	12:L3:97:THR:OG1	2.29	0.49
53:s3:228:ASP:OD1	53:s3:230:ARG:NH1	2.44	0.49
56:B6:88:ARG:NE	77:W6:118:GLY:O	2.45	0.49
66:L6:66:ASP:N	66:L6:66:ASP:OD1	2.45	0.49
70:P6:68:CYS:HA	70:P6:103:LYS:HE3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:X6:283:ALA:HB3	78:X6:286:GLU:HB2	1.94	0.49
3:A3:1749:C:OP2	3:A3:2899:C:O2'	2.27	0.49
3:A3:1868:G:H2'	13:M3:40:PRO:HG3	1.94	0.49
3:A3:1939:G:H5'	3:A3:1940:A:H5''	1.94	0.49
7:F3:123:GLY:HA2	7:F3:141:ILE:HG23	1.93	0.49
15:O3:52:MET:HE1	15:O3:123:ILE:HG21	1.94	0.49
43:h3:95:ARG:NH1	43:h3:99:ASN:OD1	2.46	0.49
53:s3:247:LEU:HD11	53:s3:296:HIS:HB2	1.93	0.49
58:D6:138:GLY:HA3	58:D6:160:ARG:HB2	1.94	0.49
61:G6:212:LYS:NZ	86:A6:1304:A:OP1	2.45	0.49
63:I6:89:LYS:NZ	86:A6:1008:G:OP1	2.43	0.49
66:L6:135:LYS:O	66:L6:138:SER:OG	2.29	0.49
9:I3:110:LEU:HA	9:I3:113:ARG:HG3	1.95	0.49
13:M3:220:ARG:HA	13:M3:229:PHE:HE1	1.77	0.49
32:53:332:ASP:HB3	32:53:334:LYS:HD3	1.93	0.49
67:M6:20:ARG:HH12	67:M6:87:MET:HG2	1.76	0.49
78:X6:162:VAL:HG12	78:X6:316:LEU:HD12	1.94	0.49
89:n:295:LEU:HD11	89:n:305:LEU:HD21	1.94	0.49
1:r1:136:ARG:HH21	1:r1:443:SER:H	1.60	0.49
3:A3:2148:A:OP2	18:R3:65:ARG:NH1	2.46	0.49
57:C6:117:LEU:HD11	57:C6:151:VAL:HG13	1.95	0.49
62:H6:79:LEU:HD11	62:H6:140:TYR:HD1	1.77	0.49
63:I6:179:THR:O	71:Q6:10:ARG:NH2	2.33	0.49
74:T6:27:VAL:O	74:T6:28:LYS:NZ	2.37	0.49
75:U6:56:LEU:O	75:U6:60:TYR:N	2.41	0.49
76:V6:242:ALA:HA	76:V6:245:HIS:CD2	2.48	0.49
82:b6:187:LYS:HG3	82:b6:188:LYS:HD3	1.94	0.49
3:A3:2275:U:H5''	38:c3:34:GLY:HA2	1.94	0.49
18:R3:32:ARG:O	18:R3:35:LYS:NZ	2.44	0.49
33:63:172:PRO:HB2	33:63:174:HIS:HE1	1.77	0.49
60:F6:110:LEU:HD11	86:A6:1373:U:H5'	1.94	0.49
81:a6:178:ARG:HD3	81:a6:185:SER:HB2	1.95	0.49
1:r1:178:ARG:HH21	3:A3:3124:U:H5''	1.77	0.49
1:r1:401:MET:H	1:r1:403:ALA:N	2.11	0.49
1:r1:650:MET:HE2	1:r1:715:MET:HG3	1.94	0.49
3:A3:2123:C:O2'	3:A3:2134:A:N3	2.40	0.49
3:A3:2643:G:O2'	3:A3:2645:G:OP2	2.25	0.49
27:O3:133:GLU:OE2	27:O3:160:TYR:OH	2.30	0.49
32:53:105:TYR:HE2	32:53:267:GLU:HG2	1.77	0.49
59:E6:97:PRO:HB2	70:P6:71:HIS:CE1	2.48	0.49
62:H6:133:GLN:OE1	65:K6:128:TRP:NE1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:R6:135:ARG:HD3	72:R6:186:TRP:HB3	1.94	0.49
76:V6:323:GLU:OE1	76:V6:330:TYR:OH	2.31	0.49
86:A6:708:U:OP1	86:A6:850:A:N6	2.41	0.49
19:S3:107:LYS:NZ	37:b3:124:PRO:O	2.45	0.49
24:X3:96:LYS:HG3	87:FE:73:A:O3'	2.13	0.49
32:53:118:LYS:HE3	32:53:256:PHE:HB3	1.95	0.49
36:a3:107:PRO:HA	36:a3:110:GLU:HB3	1.94	0.49
41:f3:93:ILE:HD11	41:f3:110:VAL:HG11	1.94	0.49
45:j3:89:GLN:NE2	45:j3:92:GLN:OE1	2.45	0.49
58:D6:366:LYS:HD2	72:R6:105:LEU:HD22	1.93	0.49
59:E6:21:THR:HA	59:E6:24:ARG:HG2	1.94	0.49
63:I6:151:VAL:O	63:I6:178:ASN:N	2.45	0.49
64:J6:114:ARG:NH2	86:A6:901:C:OP1	2.46	0.49
74:T6:86:VAL:HG21	74:T6:106:LEU:HD11	1.95	0.49
89:n:93:PRO:HB3	89:n:303:LEU:HA	1.95	0.49
89:n:181:THR:HG22	89:n:203:ILE:HD11	1.95	0.49
1:r1:179:MET:HA	1:r1:208:GLU:HG2	1.94	0.49
3:A3:3149:C:N4	3:A3:3161:G:N7	2.60	0.49
13:M3:31:PRO:O	49:o3:86:ARG:NH2	2.39	0.49
53:s3:215:GLU:OE1	53:s3:267:LYS:NZ	2.39	0.49
62:H6:163:ASN:HB3	82:b6:114:LEU:HD21	1.94	0.49
67:M6:34:ILE:HD12	67:M6:51:LEU:HD23	1.94	0.49
81:a6:29:ARG:NH1	86:A6:1534:A:OP1	2.45	0.49
81:a6:52:VAL:HA	81:a6:55:TRP:CD1	2.48	0.49
3:A3:1977:U:H2'	3:A3:1978:A:H8	1.78	0.49
17:Q3:240:ILE:HG22	17:Q3:242:GLY:H	1.78	0.49
34:73:167:VAL:HG23	34:73:235:TYR:HB3	1.95	0.49
37:b3:32:SER:HB2	37:b3:74:ARG:H	1.76	0.49
63:I6:183:HIS:HB2	86:A6:979:A:H2	1.77	0.49
69:O6:105:CYS:HB3	69:O6:143:CYS:H	1.76	0.49
72:R6:187:GLU:OE2	72:R6:240:THR:OG1	2.31	0.49
82:b6:170:VAL:HG13	82:b6:208:LYS:HE3	1.94	0.49
86:A6:1269:C:H2'	86:A6:1270:A:H8	1.77	0.49
1:r1:242:LEU:HB3	1:r1:246:ALA:HB2	1.95	0.49
36:a3:75:ILE:HD13	38:c3:257:LEU:HB2	1.94	0.49
40:e3:151:ARG:HH12	40:e3:256:THR:HG23	1.78	0.49
44:i3:86:ASN:H	44:i3:89:GLN:HB2	1.78	0.49
59:E6:71:PRO:HA	66:L6:97:MET:HA	1.95	0.49
60:F6:172:VAL:HG12	60:F6:240:ARG:HD3	1.95	0.49
61:G6:338:SER:OG	86:A6:1461:G:OP2	2.29	0.49
82:b6:230:TYR:O	82:b6:234:TRP:N	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A3:2204:U:N3	3:A3:2207:A:OP2	2.36	0.48
3:A3:2306:A:O2'	27:03:84:ARG:NH2	2.45	0.48
28:13:17:LEU:HB2	28:13:65:LEU:HD23	1.96	0.48
33:63:216:LEU:HD13	33:63:272:LEU:HD13	1.94	0.48
44:i3:57:TYR:OH	51:q3:28:ARG:O	2.28	0.48
46:k3:16:VAL:HA	46:k3:66:VAL:HA	1.95	0.48
56:B6:158:MET:HA	56:B6:161:ASP:HB2	1.95	0.48
63:I6:179:THR:OG1	71:Q6:10:ARG:NH2	2.46	0.48
72:R6:208:ILE:HG23	72:R6:211:LYS:HE3	1.95	0.48
72:R6:244:LYS:HE3	72:R6:248:LYS:HD3	1.95	0.48
75:U6:93:ARG:HH21	75:U6:97:LYS:HD2	1.77	0.48
76:V6:165:PHE:HA	76:V6:168:MET:HE2	1.95	0.48
78:X6:123:ARG:HG2	78:X6:306:ILE:HD11	1.94	0.48
81:a6:96:ARG:HB2	81:a6:117:ILE:HB	1.94	0.48
3:A3:2112:A:H61	14:N3:140:MET:HE2	1.77	0.48
4:B3:1640:A:OP1	16:P3:156:SER:N	2.45	0.48
9:I3:81:LEU:HD21	47:l3:115:ARG:HG2	1.94	0.48
21:U3:18:ARG:NH1	35:93:59:GLU:OE2	2.46	0.48
22:V3:100:LYS:O	22:V3:102:MET:N	2.45	0.48
27:03:182:PRO:HG2	27:03:185:PHE:HB3	1.95	0.48
32:53:61:ALA:HB2	32:53:73:PRO:HG3	1.95	0.48
33:63:263:SER:OG	33:63:266:HIS:NE2	2.43	0.48
61:G6:125:MET:HB2	82:b6:85:VAL:HG23	1.93	0.48
75:U6:46:PRO:HG3	86:A6:851:G:H4'	1.95	0.48
76:V6:178:THR:OG1	76:V6:214:LYS:NZ	2.43	0.48
78:X6:337:LEU:O	82:b6:260:ARG:NH1	2.40	0.48
80:Z6:66:ARG:HH11	80:Z6:67:PHE:HE1	1.60	0.48
86:A6:1108:A:H5'	86:A6:1109:C:H2'	1.94	0.48
86:A6:1195:C:H42	86:A6:1467:G:H1	1.60	0.48
1:r1:318:PRO:HB3	1:r1:323:VAL:HG11	1.95	0.48
3:A3:2389:C:H42	32:53:308:GLN:HE22	1.60	0.48
9:I3:93:ASN:HA	9:I3:157:GLU:HG3	1.95	0.48
22:V3:55:TYR:O	22:V3:145:ARG:NH2	2.44	0.48
22:V3:66:GLU:HG2	22:V3:119:GLN:HG3	1.95	0.48
53:s3:405:ILE:HG22	53:s3:407:ASP:H	1.78	0.48
56:B6:92:GLY:O	56:B6:113:HIS:HE1	1.96	0.48
67:M6:105:THR:O	67:M6:109:ARG:N	2.42	0.48
74:T6:26:SER:O	74:T6:81:ASP:N	2.46	0.48
83:c6:9:ARG:NH1	86:A6:1025:U:O2	2.42	0.48
86:A6:948:U:O2'	86:A6:1029:A:N3	2.45	0.48
12:L3:98:PRO:HA	17:Q3:162:ILE:HG13	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M3:110:VAL:HG22	13:M3:116:ILE:HD12	1.96	0.48
16:P3:83:ILE:HB	16:P3:90:GLU:HB2	1.95	0.48
56:B6:249:TYR:HA	56:B6:252:LEU:HB2	1.94	0.48
58:D6:317:HIS:HB3	58:D6:320:ILE:HD12	1.95	0.48
66:L6:139:TYR:HB2	66:L6:156:LEU:HD13	1.94	0.48
74:T6:46:LYS:HG2	74:T6:95:ASN:HD22	1.79	0.48
76:V6:197:SER:OG	76:V6:200:GLU:N	2.41	0.48
78:X6:132:THR:HA	78:X6:388:PRO:HD2	1.95	0.48
81:a6:92:PRO:HB2	81:a6:94:TYR:HE1	1.78	0.48
82:b6:173:LEU:HD22	82:b6:222:ALA:HB1	1.95	0.48
1:r1:82:LYS:NZ	1:r1:85:VAL:HG22	2.28	0.48
5:D3:125:LYS:HE2	5:D3:160:GLY:HA2	1.95	0.48
23:W3:60:TYR:OH	23:W3:137:LYS:NZ	2.47	0.48
38:c3:59:ARG:NH1	38:c3:181:SER:O	2.46	0.48
66:L6:148:LYS:NZ	86:A6:1100:A:OP2	2.41	0.48
66:L6:196:TYR:O	86:A6:1052:C:O2'	2.26	0.48
78:X6:360:TYR:HB3	78:X6:365:TRP:HB3	1.94	0.48
1:r1:538:THR:HG22	1:r1:551:LYS:HG3	1.95	0.48
18:R3:10:LEU:HB2	18:R3:13:ARG:HD2	1.94	0.48
32:53:211:ALA:HA	32:53:275:ASN:HB2	1.96	0.48
56:B6:248:LEU:O	56:B6:252:LEU:N	2.43	0.48
58:D6:363:ALA:HB1	58:D6:387:PRO:HD3	1.96	0.48
61:G6:365:ARG:HG3	61:G6:370:LEU:HB2	1.96	0.48
62:H6:110:GLU:HB3	62:H6:141:ARG:HG3	1.96	0.48
67:M6:55:ASP:HB3	67:M6:65:LEU:H	1.78	0.48
76:V6:159:ASP:OD1	76:V6:159:ASP:N	2.46	0.48
89:n:231:PRO:HG2	89:n:232:LYS:HE2	1.95	0.48
3:A3:1892:A:N6	33:63:376:THR:O	2.47	0.48
3:A3:2755:A:O3'	24:X3:112:ARG:NH2	2.46	0.48
6:E3:72:GLN:HE22	6:E3:154:ARG:HH12	1.61	0.48
18:R3:78:GLU:OE1	37:b3:135:ASN:ND2	2.47	0.48
41:f3:60:LYS:HA	41:f3:63:ILE:HG22	1.95	0.48
53:s3:95:PRO:HG2	53:s3:235:ASP:HB2	1.96	0.48
58:D6:274:ARG:O	58:D6:278:HIS:ND1	2.37	0.48
75:U6:78:VAL:HA	75:U6:81:LYS:HB2	1.96	0.48
76:V6:214:LYS:HB2	76:V6:220:GLY:HA3	1.96	0.48
82:b6:173:LEU:HB3	82:b6:207:ILE:HG23	1.94	0.48
3:A3:1728:U:O2'	24:X3:96:LYS:O	2.23	0.48
5:D3:115:GLU:HB2	5:D3:118:LYS:HG3	1.95	0.48
13:M3:168:GLU:OE1	13:M3:233:ARG:NE	2.40	0.48
13:M3:226:PRO:HA	13:M3:229:PHE:CD2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:C6:119:ILE:HB	57:C6:153:LEU:HD13	1.96	0.48
60:F6:105:VAL:HA	61:G6:308:GLN:HE22	1.79	0.48
62:H6:68:GLU:O	85:e6:62:LYS:N	2.47	0.48
89:n:197:TYR:H	89:n:217:LYS:HE3	1.79	0.48
1:r1:149:GLY:O	1:r1:185:ARG:NH1	2.47	0.48
3:A3:2995:G:O2'	3:A3:3041:U:O2'	2.30	0.48
13:M3:189:LYS:HE3	13:M3:192:PRO:HG2	1.94	0.48
22:V3:187:TYR:HD1	25:Y3:94:SER:HA	1.78	0.48
51:q3:40:PRO:HG3	51:q3:51:GLN:HB3	1.96	0.48
57:C6:81:HIS:O	57:C6:85:ARG:NH2	2.47	0.48
59:E6:51:ILE:HG23	59:E6:58:HIS:HB2	1.95	0.48
78:X6:366:LEU:HB3	78:X6:371:ALA:HB1	1.96	0.48
86:A6:1147:C:N4	86:A6:1580:G:OP1	2.46	0.48
3:A3:1849:C:OP1	3:A3:2935:A:N6	2.38	0.48
14:N3:214:THR:HG23	14:N3:217:ARG:H	1.79	0.48
18:R3:143:SER:OG	18:R3:144:ARG:N	2.44	0.48
25:Y3:237:LYS:HB2	25:Y3:237:LYS:HE3	1.69	0.48
32:53:34:GLY:O	32:53:39:ARG:NE	2.36	0.48
32:53:353:HIS:CD2	32:53:379:ASP:H	2.32	0.48
34:73:276:PHE:HD2	34:73:277:GLN:HG3	1.78	0.48
58:D6:95:ALA:HA	58:D6:98:LEU:HD13	1.94	0.48
83:c6:100:LEU:HD22	83:c6:103:LYS:HG3	1.96	0.48
7:F3:290:TYR:O	7:F3:293:PHE:N	2.48	0.47
20:T3:143:ALA:HB3	20:T3:177:LYS:HD3	1.95	0.47
57:C6:105:ALA:HB1	57:C6:161:LYS:HG3	1.96	0.47
72:R6:132:LEU:HD23	72:R6:237:PRO:HG2	1.95	0.47
72:R6:242:TYR:O	72:R6:246:HIS:ND1	2.46	0.47
76:V6:234:VAL:HA	76:V6:237:GLN:HB2	1.96	0.47
86:A6:1260:A:N6	86:A6:1340:G:O6	2.47	0.47
3:A3:2310:G:O2'	3:A3:2675:G:O6	2.25	0.47
23:W3:116:LEU:HD11	41:f3:59:TYR:HD2	1.79	0.47
34:73:45:ASN:HD21	34:73:259:ASP:HB2	1.79	0.47
35:93:96:VAL:HA	35:93:99:ALA:HB3	1.95	0.47
41:f3:106:TYR:OH	41:f3:174:ILE:O	2.32	0.47
58:D6:257:SER:HA	86:A6:1288:U:H5	1.79	0.47
60:F6:160:PRO:HA	87:FE:30:G:H5''	1.95	0.47
64:J6:44:ARG:NH1	86:A6:932:A:OP1	2.47	0.47
67:M6:114:ARG:HG2	69:O6:235:MET:HB2	1.97	0.47
77:W6:81:ALA:HA	77:W6:84:LEU:HB3	1.97	0.47
86:A6:1339:U:H2'	86:A6:1340:G:H8	1.78	0.47
22:V3:45:VAL:HG11	25:Y3:237:LYS:HZ2	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:73:178:ALA:HB2	34:73:320:SER:HB2	1.96	0.47
40:e3:266:PRO:O	40:e3:270:ALA:N	2.48	0.47
63:I6:182:PRO:HG2	71:Q6:42:ARG:HD3	1.95	0.47
69:O6:151:THR:O	69:O6:155:GLN:NE2	2.48	0.47
75:U6:116:LEU:O	75:U6:120:ARG:HD2	2.14	0.47
77:W6:79:SER:OG	77:W6:80:PHE:N	2.44	0.47
77:W6:104:ILE:HB	77:W6:137:GLY:H	1.78	0.47
78:X6:187:TRP:HA	78:X6:190:ASN:HD22	1.80	0.47
86:A6:865:U:H2'	86:A6:866:A:H8	1.79	0.47
86:A6:1436:U:H2'	86:A6:1437:A:H8	1.79	0.47
1:r1:645:ILE:HB	1:r1:724:LEU:HD13	1.95	0.47
1:r1:654:VAL:HG12	1:r1:713:TYR:HB2	1.96	0.47
3:A3:2615:A:H1'	12:L3:81:LYS:HD3	1.95	0.47
3:A3:3082:G:N2	3:A3:3085:A:OP2	2.40	0.47
6:E3:148:GLY:HA3	6:E3:173:LYS:HG3	1.95	0.47
10:J3:84:GLN:HE21	10:J3:90:PHE:HE1	1.62	0.47
13:M3:233:ARG:HB3	13:M3:244:LEU:HD11	1.96	0.47
29:23:79:ILE:HG22	29:23:83:MET:HE2	1.97	0.47
33:63:259:PRO:HB3	33:63:266:HIS:CD2	2.49	0.47
40:e3:51:LEU:HD22	40:e3:204:PHE:HE1	1.79	0.47
56:B6:157:ASN:O	56:B6:161:ASP:N	2.46	0.47
67:M6:111:ARG:NH1	72:R6:147:ILE:O	2.47	0.47
72:R6:135:ARG:HB2	72:R6:240:THR:HG23	1.96	0.47
85:e6:506:LEU:HD13	85:e6:544:LEU:HD21	1.96	0.47
89:n:103:VAL:HG23	89:n:267:ILE:HB	1.96	0.47
89:n:295:LEU:HB2	89:n:302:GLY:HA2	1.96	0.47
1:r1:124:HIS:HE1	3:A3:3130:A:H5'	1.79	0.47
1:r1:553:ILE:HG22	1:r1:612:GLN:HB3	1.96	0.47
6:E3:179:PHE:HE1	6:E3:300:LYS:HB3	1.79	0.47
11:K3:69:GLY:HA3	52:r3:176:VAL:HG22	1.96	0.47
26:Z3:71:ARG:NH1	26:Z3:92:GLU:O	2.47	0.47
39:d3:173:THR:HA	39:d3:176:ILE:HG22	1.96	0.47
64:J6:32:THR:HA	74:T6:4:LYS:HD2	1.96	0.47
75:U6:112:GLU:OE1	75:U6:115:ARG:NH2	2.47	0.47
84:d6:175:ARG:NH2	86:A6:767:C:OP1	2.46	0.47
1:r1:310:LEU:HA	1:r1:313:VAL:HG12	1.96	0.47
1:r1:359:LYS:NZ	1:r1:360:LEU:O	2.48	0.47
1:r1:649:ILE:HD12	1:r1:721:GLN:HB2	1.96	0.47
3:A3:2584:C:H2'	3:A3:2585:G:H8	1.80	0.47
7:F3:238:LYS:NZ	51:q3:25:TYR:OH	2.47	0.47
34:73:66:GLU:O	34:73:122:SER:OG	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:73:86:SER:O	34:73:86:SER:OG	2.30	0.47
34:73:104:ILE:HG23	34:73:270:PRO:HD2	1.96	0.47
61:G6:392:THR:O	86:A6:1430:U:O2'	2.31	0.47
81:a6:28:PRO:HG2	81:a6:33:LEU:HD23	1.96	0.47
1:r1:289:LYS:HG3	1:r1:290:ARG:H	1.79	0.47
3:A3:1742:G:O2'	3:A3:1754:G:O6	2.33	0.47
3:A3:2489:C:O2'	3:A3:2621:G:OP1	2.31	0.47
21:U3:112:PRO:HD2	25:Y3:75:GLY:HA3	1.97	0.47
24:X3:20:ILE:HG23	24:X3:212:ILE:HD12	1.97	0.47
24:X3:119:LEU:HD13	32:53:52:ILE:HG23	1.96	0.47
24:X3:202:GLU:HB3	24:X3:214:LYS:HE2	1.96	0.47
31:43:72:LEU:HD23	31:43:90:VAL:HG23	1.97	0.47
34:73:107:LEU:HB2	34:73:126:LYS:HB3	1.96	0.47
40:e3:59:VAL:HG21	40:e3:153:LEU:HD23	1.96	0.47
45:j3:63:GLN:OE1	45:j3:66:ARG:NH2	2.48	0.47
61:G6:158:TYR:OH	61:G6:217:ASP:O	2.29	0.47
61:G6:250:LEU:HD13	61:G6:253:LYS:HE3	1.96	0.47
67:M6:22:ALA:O	67:M6:33:ARG:N	2.41	0.47
69:O6:81:HIS:ND1	69:O6:82:LYS:O	2.46	0.47
76:V6:177:SER:HA	76:V6:180:LEU:HB3	1.97	0.47
77:W6:140:VAL:HG12	77:W6:172:ILE:HG12	1.95	0.47
78:X6:264:GLY:HA2	78:X6:311:SER:H	1.78	0.47
78:X6:316:LEU:O	78:X6:318:LYS:NZ	2.48	0.47
81:a6:179:GLN:HE21	81:a6:184:THR:HG23	1.79	0.47
82:b6:214:LEU:HD12	82:b6:215:ARG:H	1.80	0.47
1:r1:225:PHE:HB2	1:r1:232:ILE:HB	1.97	0.47
1:r1:478:PRO:O	1:r1:481:LYS:NZ	2.39	0.47
53:s3:211:VAL:HG13	53:s3:380:THR:HG22	1.97	0.47
62:H6:78:VAL:HB	62:H6:143:LEU:HB3	1.97	0.47
62:H6:82:GLY:N	62:H6:139:LEU:O	2.39	0.47
78:X6:155:ILE:HD11	78:X6:263:ASP:H	1.80	0.47
88:A:165:ASP:OD1	88:A:165:ASP:N	2.48	0.47
50:p3:97:SER:O	50:p3:146:ASN:ND2	2.48	0.47
58:D6:351:ARG:HG3	58:D6:355:ARG:HD3	1.96	0.47
67:M6:72:ARG:HB2	67:M6:76:TRP:CD1	2.50	0.47
71:Q6:37:GLU:O	71:Q6:41:HIS:N	2.48	0.47
72:R6:291:ARG:HH21	72:R6:293:LEU:HD11	1.80	0.47
76:V6:202:ARG:HH11	76:V6:247:MET:HE1	1.80	0.47
76:V6:360:VAL:HG22	76:V6:363:LYS:HE3	1.97	0.47
78:X6:240:VAL:HG22	78:X6:244:LEU:HG	1.97	0.47
14:N3:213:TRP:HB3	14:N3:218:ILE:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T3:49:ARG:HA	20:T3:49:ARG:HD3	1.77	0.47
34:73:207:HIS:HA	34:73:210:ILE:HD12	1.97	0.47
43:h3:65:ASP:O	43:h3:67:GLN:N	2.41	0.47
57:C6:141:THR:HG21	85:e6:114:GLU:HA	1.97	0.47
67:M6:29:ARG:HG3	67:M6:57:LEU:HD11	1.97	0.47
1:r1:48:ASN:OD1	1:r1:117:ASN:ND2	2.38	0.46
3:A3:2089:U:O2	42:g3:104:ASN:ND2	2.47	0.46
3:A3:2196:A:O2'	3:A3:2213:A:N1	2.42	0.46
19:S3:115:LEU:HD22	37:b3:115:ILE:HG21	1.97	0.46
34:73:226:ALA:HA	34:73:229:ILE:HD12	1.97	0.46
39:d3:208:VAL:HG13	39:d3:252:LEU:HB2	1.96	0.46
61:G6:202:LYS:HD3	61:G6:218:TYR:HB2	1.96	0.46
81:a6:101:ARG:HH21	81:a6:113:LYS:HD2	1.80	0.46
87:FE:20:U:H5	87:FE:44:U:H3	1.63	0.46
89:n:241:HIS:ND1	89:n:242:GLU:HG3	2.30	0.46
6:E3:87:ILE:HG13	6:E3:317:PRO:HG2	1.96	0.46
6:E3:96:ARG:NH1	6:E3:315:PRO:O	2.48	0.46
16:P3:72:PRO:HG3	16:P3:79:ARG:HH12	1.80	0.46
32:53:222:VAL:HG21	32:53:319:GLY:HA3	1.98	0.46
34:73:209:LEU:HD23	34:73:272:THR:HG21	1.98	0.46
40:e3:119:ASP:OD2	78:X6:232:ARG:NH2	2.47	0.46
67:M6:99:LEU:HD21	67:M6:103:MET:HB2	1.96	0.46
68:N6:74:ALA:HB3	68:N6:77:VAL:HG12	1.96	0.46
73:S6:97:GLN:NE2	77:W6:91:GLN:OE1	2.47	0.46
78:X6:245:LYS:HA	78:X6:248:LYS:HB3	1.96	0.46
86:A6:1527:A:O2'	86:A6:1531:A:N1	2.41	0.46
1:r1:326:TYR:HB3	1:r1:342:LEU:HG	1.98	0.46
3:A3:2127:A:H4'	3:A3:2251:A:C5	2.51	0.46
3:A3:2391:A:O2'	3:A3:2404:U:O4	2.29	0.46
53:s3:271:LEU:O	53:s3:273:LEU:N	2.48	0.46
58:D6:190:GLU:OE2	58:D6:202:SER:N	2.41	0.46
60:F6:106:LEU:HD21	86:A6:1373:U:H4'	1.96	0.46
60:F6:232:ALA:HA	87:FE:38:A:H1'	1.95	0.46
64:J6:103:GLN:HG2	64:J6:106:GLN:HE22	1.79	0.46
70:P6:135:VAL:HA	75:U6:193:ARG:HD3	1.96	0.46
72:R6:258:LYS:HB2	72:R6:261:LEU:HD13	1.97	0.46
76:V6:92:LEU:O	76:V6:96:ARG:N	2.47	0.46
78:X6:138:LEU:HD13	78:X6:307:VAL:HG13	1.96	0.46
8:D:194:PHE:CB	89:n:92:TYR:CG	2.98	0.46
89:n:91:LEU:HD22	89:n:301:GLU:HG3	1.96	0.46
1:r1:455:MET:HG2	1:r1:518:THR:HG22	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A3:2082:G:OP1	49:o3:66:ARG:NH2	2.47	0.46
3:A3:2142:A:H8	3:A3:2261:C:H5'	1.80	0.46
3:A3:2458:A:OP2	15:O3:9:ILE:N	2.48	0.46
8:H3:83:VAL:HG13	8:H3:84:GLU:HG2	1.97	0.46
17:Q3:111:PHE:HA	17:Q3:179:LEU:HD11	1.98	0.46
29:23:51:ASN:O	29:23:54:GLN:NE2	2.48	0.46
38:c3:89:LYS:HE3	38:c3:89:LYS:HB3	1.77	0.46
51:q3:125:MET:HA	51:q3:128:MET:HG3	1.97	0.46
56:B6:102:MET:HG3	56:B6:225:THR:HA	1.97	0.46
58:D6:138:GLY:O	58:D6:160:ARG:N	2.46	0.46
61:G6:277:LYS:NZ	86:A6:1460:U:OP2	2.37	0.46
63:I6:151:VAL:HB	63:I6:177:ASP:HA	1.97	0.46
66:L6:73:LEU:HD12	66:L6:95:LEU:HD22	1.98	0.46
78:X6:284:PRO:HB2	78:X6:294:ARG:HH11	1.81	0.46
89:n:157:VAL:HG21	89:n:234:LEU:HD13	1.96	0.46
3:A3:1773:A:OP2	38:c3:31:VAL:N	2.49	0.46
14:N3:76:SER:HB2	14:N3:155:LYS:HB2	1.97	0.46
36:a3:49:LEU:HD23	36:a3:60:CYS:HB3	1.97	0.46
71:Q6:21:SER:OG	71:Q6:24:ARG:NH2	2.48	0.46
75:U6:67:VAL:O	75:U6:71:ARG:N	2.48	0.46
78:X6:123:ARG:HE	78:X6:338:ASP:H	1.63	0.46
1:r1:329:LEU:HD12	1:r1:338:LYS:HA	1.97	0.46
7:F3:196:PRO:HD2	7:F3:202:TYR:HE2	1.79	0.46
19:S3:70:VAL:HA	19:S3:73:THR:HG22	1.98	0.46
22:V3:147:SER:OG	22:V3:148:THR:N	2.48	0.46
26:Z3:137:THR:HG22	26:Z3:147:VAL:HA	1.98	0.46
40:e3:123:MET:HA	40:e3:126:GLN:HG3	1.98	0.46
58:D6:380:LEU:HD11	72:R6:91:PHE:HB3	1.97	0.46
60:F6:209:LEU:HA	60:F6:212:ALA:HB3	1.98	0.46
76:V6:208:LEU:HD22	76:V6:226:TYR:HB3	1.98	0.46
78:X6:58:LYS:HB3	78:X6:144:PHE:HD1	1.80	0.46
87:FE:17:U:C4	89:n:220:LYS:CE	2.98	0.46
3:A3:3188:U:OP2	31:43:84:ARG:NE	2.44	0.46
53:s3:284:VAL:HG13	53:s3:335:TRP:HE1	1.80	0.46
62:H6:132:VAL:HG11	65:K6:112:ARG:HD3	1.98	0.46
62:H6:151:SER:HA	62:H6:154:ASP:HB2	1.97	0.46
70:P6:114:ALA:HB1	70:P6:119:PHE:HB2	1.96	0.46
72:R6:72:ASP:HB2	72:R6:75:VAL:HB	1.98	0.46
76:V6:80:SER:N	76:V6:84:GLU:OE1	2.44	0.46
78:X6:390:LEU:HA	78:X6:393:ARG:HB2	1.97	0.46
79:Y6:299:GLU:HA	79:Y6:302:ILE:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:a6:78:ARG:NH1	81:a6:79:LEU:O	2.49	0.46
3:A3:2292:G:C8	18:R3:11:ARG:HB3	2.51	0.46
3:A3:2852:C:O2'	28:13:45:HIS:ND1	2.34	0.46
11:K3:178:LEU:HG	52:r3:35:PHE:CD2	2.51	0.46
14:N3:64:ARG:HE	14:N3:144:LYS:HB3	1.79	0.46
26:Z3:70:THR:HG22	26:Z3:97:PRO:HA	1.98	0.46
35:93:52:GLN:HE21	35:93:57:VAL:HG21	1.80	0.46
40:e3:176:ALA:HB2	40:e3:191:THR:HG21	1.97	0.46
48:m3:43:VAL:HG12	48:m3:45:ARG:H	1.80	0.46
62:H6:110:GLU:HA	62:H6:141:ARG:HA	1.97	0.46
63:I6:154:LEU:HB2	71:Q6:43:ARG:HH12	1.81	0.46
69:O6:189:PRO:HB2	69:O6:193:LEU:HD11	1.98	0.46
71:Q6:53:GLN:O	71:Q6:57:TYR:N	2.49	0.46
72:R6:112:GLU:HA	72:R6:115:THR:HG22	1.97	0.46
78:X6:150:TRP:HH2	78:X6:305:ALA:H	1.63	0.46
1:r1:608:ARG:HH11	1:r1:610:VAL:HG11	1.81	0.46
15:O3:134:PRO:HD3	27:O3:130:VAL:HG21	1.98	0.46
19:S3:194:ARG:HH22	37:b3:16:HIS:HA	1.80	0.46
20:T3:212:LEU:O	37:b3:117:LYS:NZ	2.45	0.46
53:s3:251:VAL:HG22	53:s3:252:PRO:HD2	1.98	0.46
58:D6:288:HIS:HB2	58:D6:310:LYS:HE2	1.98	0.46
60:F6:166:ARG:NH2	86:A6:998:A:N3	2.64	0.46
62:H6:120:LEU:HD13	65:K6:108:ARG:HB2	1.98	0.46
81:a6:78:ARG:HH12	81:a6:142:VAL:N	2.14	0.46
86:A6:974:A:H2'	86:A6:975:A:C8	2.51	0.46
87:FE:9:A:O2'	87:FE:10:G:N7	2.40	0.46
1:r1:108:TYR:HE1	1:r1:401:MET:HG2	1.79	0.46
1:r1:264:LEU:O	1:r1:266:GLU:N	2.48	0.46
3:A3:1818:A:O2'	20:T3:146:THR:OG1	2.31	0.46
3:A3:1890:C:OP2	30:33:168:ARG:NH2	2.49	0.46
9:I3:100:GLN:O	46:k3:35:GLN:NE2	2.49	0.46
19:S3:132:LYS:NZ	45:j3:46:LEU:O	2.48	0.46
65:K6:65:LYS:O	65:K6:69:ASP:N	2.49	0.46
69:O6:188:PRO:HA	69:O6:189:PRO:HD3	1.81	0.46
76:V6:285:ALA:HA	76:V6:288:LYS:HE3	1.97	0.46
76:V6:288:LYS:HD2	76:V6:327:LEU:HD22	1.97	0.46
80:Z6:63:GLN:NE2	86:A6:1254:C:OP1	2.48	0.46
8:D:194:PHE:CB	89:n:92:TYR:CE1	2.99	0.46
1:r1:180:GLY:H	1:r1:208:GLU:HG2	1.81	0.45
1:r1:534:PRO:HA	1:r1:555:VAL:HA	1.98	0.45
3:A3:2142:A:C8	3:A3:2261:C:H5'	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D3:180:ASP:OD1	5:D3:180:ASP:N	2.46	0.45
5:D3:198:SER:HB3	5:D3:206:TYR:HE2	1.81	0.45
15:O3:137:ARG:HA	15:O3:137:ARG:HD2	1.73	0.45
48:m3:57:VAL:O	88:A:185:TYR:OH	2.28	0.45
53:s3:352:THR:OG1	53:s3:353:ARG:N	2.47	0.45
56:B6:214:LYS:HG2	73:S6:5:ARG:HB2	1.97	0.45
61:G6:305:PRO:HG2	86:A6:1381:C:H5'	1.98	0.45
66:L6:74:LYS:HD3	66:L6:105:LYS:HG3	1.98	0.45
86:A6:897:G:H1	86:A6:904:C:H42	1.64	0.45
86:A6:1235:A:O2'	86:A6:1237:C:OP2	2.29	0.45
3:A3:1752:U:H2'	3:A3:1753:A:H8	1.80	0.45
3:A3:3127:G:H2'	3:A3:3128:A:H2'	1.98	0.45
13:M3:140:LEU:HB2	13:M3:156:VAL:HG21	1.97	0.45
33:63:222:ASP:H	33:63:224:HIS:CE1	2.34	0.45
38:c3:246:LYS:HG2	38:c3:250:VAL:HG23	1.99	0.45
43:h3:114:ASN:HA	43:h3:117:LEU:HB2	1.97	0.45
57:C6:125:ARG:HE	57:C6:157:THR:HB	1.80	0.45
63:I6:90:ALA:N	63:I6:152:LYS:O	2.45	0.45
63:I6:187:ARG:NE	63:I6:188:PRO:HD2	2.31	0.45
67:M6:70:LEU:HA	67:M6:73:ILE:HG22	1.97	0.45
78:X6:183:GLU:HA	78:X6:186:THR:HG22	1.99	0.45
80:Z6:33:VAL:HA	80:Z6:36:LEU:HB3	1.98	0.45
85:e6:118:LYS:HA	85:e6:121:ILE:HD12	1.97	0.45
1:r1:501:LEU:HD23	1:r1:501:LEU:HA	1.81	0.45
3:A3:1886:G:H1	44:i3:61:GLY:HA3	1.82	0.45
3:A3:2256:U:OP1	45:j3:66:ARG:NH1	2.50	0.45
53:s3:235:ASP:OD1	53:s3:236:LYS:N	2.49	0.45
62:H6:121:LEU:O	65:K6:112:ARG:NH2	2.49	0.45
63:I6:160:SER:HA	63:I6:163:HIS:HB2	1.96	0.45
69:O6:151:THR:HA	69:O6:154:ILE:HG22	1.97	0.45
70:P6:103:LYS:HA	70:P6:106:GLU:HG2	1.99	0.45
79:Y6:358:LEU:HB2	79:Y6:369:LYS:HD3	1.98	0.45
85:e6:96:MET:N	85:e6:96:MET:SD	2.89	0.45
87:24:9:A:O2'	87:24:10:G:N7	2.40	0.45
3:A3:2572:C:O2'	87:24:12:U:OP1	2.27	0.45
7:F3:59:ARG:NH1	7:F3:88:ALA:O	2.49	0.45
22:V3:108:MET:SD	39:d3:170:PRO:HD3	2.56	0.45
50:p3:152:GLN:HA	50:p3:155:ARG:HG2	1.98	0.45
79:Y6:309:LYS:HE2	85:e6:140:LEU:HD11	1.98	0.45
26:Z3:63:PRO:HG2	49:o3:53:TYR:HD2	1.80	0.45
40:e3:162:ARG:HH11	40:e3:171:TRP:HZ3	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:E6:117:LEU:HD23	83:c6:10:LEU:HD22	1.98	0.45
61:G6:114:SER:HB3	61:G6:123:PRO:HD2	1.98	0.45
63:I6:112:CYS:HB2	63:I6:122:LYS:HB2	1.98	0.45
63:I6:151:VAL:N	63:I6:176:THR:O	2.43	0.45
73:S6:106:LEU:HD11	73:S6:120:GLU:HB2	1.97	0.45
81:a6:9:ARG:HG2	81:a6:12:ALA:HB3	1.98	0.45
81:a6:117:ILE:HD13	81:a6:128:ALA:HB2	1.97	0.45
85:e6:343:ARG:HA	85:e6:378:LEU:HD21	1.99	0.45
17:Q3:244:ARG:HG2	17:Q3:247:LEU:HD12	1.99	0.45
53:s3:185:VAL:O	53:s3:189:SER:OG	2.32	0.45
53:s3:215:GLU:HB2	53:s3:229:LEU:HD23	1.98	0.45
65:K6:34:MET:O	65:K6:38:VAL:N	2.50	0.45
75:U6:131:GLN:HA	75:U6:134:ARG:HE	1.82	0.45
79:Y6:295:GLN:NE2	85:e6:80:ARG:HG2	2.32	0.45
85:e6:493:MET:N	85:e6:493:MET:SD	2.89	0.45
1:r1:598:PRO:HA	1:r1:601:GLY:HA2	1.99	0.45
3:A3:1810:A:H2'	3:A3:1811:A:C8	2.52	0.45
3:A3:1882:A:N6	3:A3:1893:A:O4'	2.49	0.45
3:A3:2278:A:OP1	44:i3:51:ARG:NE	2.48	0.45
6:E3:170:LEU:HA	6:E3:170:LEU:HD23	1.74	0.45
7:F3:59:ARG:NH1	7:F3:84:PRO:O	2.50	0.45
23:W3:101:LYS:HD2	41:f3:56:ILE:HG21	1.98	0.45
37:b3:26:LEU:HD22	37:b3:105:ALA:HA	1.99	0.45
58:D6:325:ARG:NH2	58:D6:430:THR:O	2.50	0.45
72:R6:150:GLY:HA2	72:R6:177:PRO:HB2	1.98	0.45
88:A:53:LYS:HB3	88:A:61:ASP:HB3	1.99	0.45
1:r1:331:LYS:N	1:r1:438:GLY:O	2.50	0.45
5:D3:184:LEU:HA	5:D3:187:LEU:HD13	1.97	0.45
13:M3:169:LYS:HD3	13:M3:242:TYR:HB3	1.99	0.45
19:S3:113:LEU:HD21	19:S3:194:ARG:HH21	1.81	0.45
24:X3:59:ARG:NH1	51:q3:93:TYR:OH	2.50	0.45
29:23:72:THR:HG22	29:23:74:ALA:H	1.82	0.45
42:g3:108:THR:OG1	42:g3:151:GLY:O	2.33	0.45
43:h3:63:PRO:HB2	43:h3:66:LEU:HA	1.99	0.45
56:B6:99:HIS:HB3	56:B6:102:MET:HG2	1.99	0.45
56:B6:224:ASP:OD1	56:B6:225:THR:N	2.47	0.45
60:F6:36:ARG:HE	86:A6:1316:C:H41	1.65	0.45
60:F6:123:PHE:HE1	60:F6:139:ARG:HD3	1.82	0.45
76:V6:236:LEU:HD13	76:V6:324:GLN:HG3	1.98	0.45
78:X6:373:THR:HG23	78:X6:376:GLY:H	1.82	0.45
8:D:212:PRO:HA	8:D:213:ILE:HA	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:r1:46:ILE:HD12	1:r1:115:ASN:HB2	1.98	0.45
40:e3:55:ARG:NH1	40:e3:152:LYS:O	2.50	0.45
43:h3:120:MET:SD	43:h3:120:MET:N	2.90	0.45
46:k3:73:ARG:O	52:r3:47:THR:N	2.50	0.45
60:F6:162:LEU:HD13	87:FE:32:A:C8	2.52	0.45
66:L6:207:LYS:NZ	86:A6:767:C:N3	2.49	0.45
71:Q6:63:ILE:HG12	83:c6:4:PRO:HG2	1.98	0.45
78:X6:287:LEU:HB3	78:X6:289:LEU:HD23	1.99	0.45
84:d6:162:LEU:HD23	84:d6:195:TYR:HB3	1.99	0.45
85:e6:65:TRP:CD1	85:e6:65:TRP:H	2.35	0.45
87:FE:17:U:N3	89:n:220:LYS:CE	2.79	0.45
89:n:216:LYS:HB3	89:n:216:LYS:HE2	1.75	0.45
3:A3:3000:A:H2'	3:A3:3001:G:C8	2.52	0.45
15:O3:44:ALA:HB3	15:O3:49:VAL:HG23	1.99	0.45
32:53:105:TYR:CE2	32:53:267:GLU:HG2	2.51	0.45
40:e3:82:SER:OG	40:e3:83:LEU:N	2.46	0.45
62:H6:75:ARG:HA	62:H6:146:GLU:HA	1.99	0.45
67:M6:114:ARG:HA	67:M6:117:GLU:HB2	1.99	0.45
74:T6:2:PRO:O	86:A6:936:C:O2'	2.31	0.45
74:T6:147:VAL:HA	74:T6:148:PRO:HD3	1.78	0.45
87:FE:16:A:O2'	89:n:220:LYS:NZ	2.49	0.45
89:n:159:VAL:HG12	89:n:161:THR:HG23	1.98	0.45
1:r1:537:PHE:HE1	1:r1:539:HIS:HD1	1.64	0.44
3:A3:2521:A:N6	5:D3:202:ARG:O	2.50	0.44
15:O3:79:TRP:NE1	17:Q3:267:PHE:O	2.43	0.44
19:S3:54:THR:OG1	19:S3:55:SER:N	2.50	0.44
33:63:35:MET:HE3	33:63:36:PRO:HD2	1.99	0.44
56:B6:124:HIS:O	56:B6:128:ALA:N	2.49	0.44
56:B6:251:ARG:NH1	56:B6:251:ARG:O	2.50	0.44
61:G6:276:ARG:NH1	61:G6:375:ARG:O	2.50	0.44
68:N6:17:VAL:HA	68:N6:28:VAL:HA	1.99	0.44
70:P6:112:LYS:HE2	86:A6:1035:G:H4'	1.98	0.44
75:U6:132:GLU:O	75:U6:135:GLN:NE2	2.45	0.44
87:24:20:U:H5	87:24:44:U:H3	1.63	0.44
8:D:194:PHE:CB	89:n:92:TYR:CD1	3.00	0.44
3:A3:2409:A:O2'	32:53:270:ILE:O	2.34	0.44
3:A3:2524:A:O2'	5:D3:85:ARG:O	2.29	0.44
5:D3:220:VAL:HG12	5:D3:221:ASN:H	1.81	0.44
11:K3:67:PHE:HB3	11:K3:71:LYS:HB2	1.98	0.44
21:U3:19:VAL:HG22	35:93:136:LEU:HD22	1.98	0.44
21:U3:44:ILE:HG23	21:U3:48:MET:SD	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W3:121:PRO:HG2	33:63:40:ILE:HD12	1.99	0.44
56:B6:145:ILE:HG12	56:B6:167:HIS:HB2	2.00	0.44
65:K6:48:ALA:O	65:K6:52:LEU:N	2.48	0.44
69:O6:220:TYR:HD1	81:a6:53:ARG:HH11	1.64	0.44
71:Q6:49:CYS:HA	71:Q6:52:ARG:HH21	1.81	0.44
81:a6:43:ARG:HH11	81:a6:43:ARG:HD3	1.64	0.44
81:a6:193:VAL:HG12	81:a6:198:MET:HE1	1.99	0.44
87:24:45:A:H62	88:A:48:GLU:HG2	1.82	0.44
1:r1:568:GLU:HG2	1:r1:608:ARG:HG3	1.98	0.44
3:A3:1800:G:O6	22:V3:41:ARG:NH1	2.39	0.44
3:A3:2138:U:O2'	3:A3:2151:A:N3	2.49	0.44
3:A3:2349:G:H2'	3:A3:2350:A:C8	2.52	0.44
11:K3:27:PRO:HG2	11:K3:30:LYS:HB2	1.99	0.44
18:R3:85:ALA:O	18:R3:89:ASN:ND2	2.43	0.44
34:73:222:GLU:HB2	34:73:250:ARG:HB3	1.98	0.44
60:F6:155:MET:HG3	83:c6:70:ILE:HD11	1.98	0.44
60:F6:166:ARG:HH11	87:FE:35:G:H21	1.65	0.44
63:I6:86:ALA:HB1	63:I6:97:ILE:HD11	1.99	0.44
65:K6:29:TYR:CZ	65:K6:38:VAL:HG11	2.52	0.44
76:V6:107:TRP:HB3	76:V6:382:TRP:CE2	2.52	0.44
86:A6:877:G:N3	86:A6:925:U:O2'	2.50	0.44
87:24:9:A:H8	87:24:11:C:H41	1.65	0.44
89:n:147:PRO:HG2	89:n:270:ASN:HA	1.99	0.44
3:A3:3158:A:O2'	15:O3:11:HIS:O	2.24	0.44
5:D3:95:GLY:HA2	5:D3:269:ARG:HB2	1.99	0.44
13:M3:162:LEU:HD13	50:p3:145:ARG:HE	1.81	0.44
13:M3:203:ARG:HB3	13:M3:265:ILE:HG12	1.99	0.44
16:P3:92:LEU:HD22	16:P3:100:VAL:HG21	1.99	0.44
17:Q3:181:LYS:HB2	17:Q3:217:VAL:HA	1.99	0.44
19:S3:159:THR:OG1	19:S3:196:ASN:OD1	2.34	0.44
82:b6:155:ASP:OD1	82:b6:155:ASP:N	2.51	0.44
3:A3:2549:C:H4'	3:A3:2550:A:H5'	1.99	0.44
17:Q3:94:ILE:HD13	17:Q3:94:ILE:HA	1.86	0.44
19:S3:166:SER:OG	19:S3:167:TRP:N	2.51	0.44
25:Y3:163:ALA:HB1	35:93:133:ARG:HD2	2.00	0.44
33:63:173:LEU:HD13	33:63:272:LEU:HD22	1.99	0.44
37:b3:30:SER:HB2	37:b3:76:VAL:HB	2.00	0.44
42:g3:106:GLN:O	42:g3:151:GLY:N	2.41	0.44
42:g3:142:GLU:HG3	49:o3:88:ILE:HG13	1.99	0.44
76:V6:181:LEU:HD12	76:V6:181:LEU:HA	1.85	0.44
82:b6:207:ILE:HG21	82:b6:225:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:c6:17:ARG:HD3	83:c6:17:ARG:HA	1.79	0.44
3:A3:3008:C:O2'	3:A3:3051:A:N3	2.48	0.44
10:J3:97:ILE:HG12	10:J3:109:ALA:HB1	2.00	0.44
13:M3:119:THR:OG1	13:M3:123:ASN:OD1	2.32	0.44
15:O3:80:LEU:HD11	15:O3:89:LEU:HD22	2.00	0.44
15:O3:144:LEU:HD11	34:73:143:TRP:HE1	1.83	0.44
21:U3:50:ARG:HE	21:U3:50:ARG:HB2	1.51	0.44
22:V3:23:MET:HE3	22:V3:23:MET:HB3	1.90	0.44
59:E6:51:ILE:O	59:E6:58:HIS:N	2.41	0.44
60:F6:84:SER:OG	60:F6:85:VAL:N	2.49	0.44
60:F6:109:SER:HA	60:F6:112:ILE:HD12	1.98	0.44
60:F6:120:ARG:NH1	78:X6:89:MET:O	2.50	0.44
60:F6:159:VAL:N	87:FE:30:G:H5'	2.33	0.44
69:O6:72:PRO:HG2	69:O6:75:ALA:HB2	1.99	0.44
76:V6:41:GLU:HG2	76:V6:43:ARG:HH21	1.83	0.44
86:A6:1176:C:O2'	86:A6:1290:A:N1	2.42	0.44
1:r1:55:ILE:HD13	3:A3:3129:A:H4'	1.99	0.44
1:r1:528:THR:HG23	1:r1:646:LEU:HD11	2.00	0.44
1:r1:647:GLU:HG2	1:r1:724:LEU:HG	1.99	0.44
3:A3:1744:A:OP2	30:33:108:LYS:NZ	2.47	0.44
11:K3:24:LYS:HA	11:K3:64:HIS:HB2	2.00	0.44
11:K3:38:ARG:HG3	11:K3:43:HIS:CE1	2.52	0.44
16:P3:88:HIS:ND1	16:P3:106:THR:OG1	2.43	0.44
56:B6:164:GLU:OE2	61:G6:145:ARG:NH1	2.46	0.44
82:b6:74:ALA:HB1	82:b6:77:LYS:HZ1	1.82	0.44
82:b6:74:ALA:HB1	82:b6:77:LYS:NZ	2.33	0.44
86:A6:839:C:O2	86:A6:856:A:N6	2.51	0.44
86:A6:1075:U:H2'	86:A6:1076:G:H8	1.82	0.44
86:A6:1558:G:H2'	86:A6:1559:A:C8	2.52	0.44
87:24:33:C:N4	3:8:20:G:H1	2.08	0.44
89:n:123:LEU:HD22	89:n:271:LEU:HG	1.99	0.44
1:r1:57:SER:O	1:r1:57:SER:OG	2.33	0.44
5:D3:119:SER:OG	5:D3:120:GLY:N	2.50	0.44
18:R3:126:GLU:HG3	19:S3:66:LEU:HD13	2.00	0.44
20:T3:104:ALA:HB1	27:O3:107:ILE:HG21	1.99	0.44
20:T3:136:PHE:HB2	20:T3:139:ASN:HB2	2.00	0.44
22:V3:209:LYS:HD3	22:V3:209:LYS:HA	1.86	0.44
23:W3:61:VAL:HG13	23:W3:65:ASN:HB2	2.00	0.44
25:Y3:148:GLU:O	25:Y3:152:ALA:N	2.49	0.44
30:33:175:ASP:HB3	30:33:178:GLN:HB2	1.99	0.44
37:b3:8:SER:OG	37:b3:116:ARG:NH1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:O6:161:GLY:O	72:R6:223:ARG:NH2	2.43	0.44
72:R6:144:GLU:HA	72:R6:180:THR:HA	1.99	0.44
72:R6:155:LYS:NZ	72:R6:182:ARG:HH21	2.15	0.44
72:R6:163:TYR:HB2	74:T6:125:HIS:CE1	2.49	0.44
82:b6:123:CYS:HA	82:b6:126:LEU:HB2	2.00	0.44
83:c6:50:SER:HA	83:c6:53:MET:HE2	1.99	0.44
8:D:195:LYS:HD3	89:n:94:ARG:HH21	1.82	0.44
87:FE:19:A:OP1	89:n:211:ARG:NH1	2.51	0.44
89:n:163:ASN:HB3	89:n:166:GLU:HB2	1.99	0.44
1:r1:580:LYS:HA	1:r1:583:VAL:HB	2.00	0.44
1:r1:724:LEU:HD23	1:r1:724:LEU:HA	1.61	0.44
3:A3:2612:C:O2'	86:A6:1507:G:O2'	2.28	0.44
3:A3:2901:A:H4'	87:FE:73:A:H61	1.83	0.44
46:k3:40:GLU:HA	46:k3:43:ARG:HB2	2.00	0.44
50:p3:71:ILE:HD11	50:p3:155:ARG:HB3	1.99	0.44
50:p3:98:LYS:HE3	50:p3:136:THR:HG21	2.00	0.44
57:C6:69:LEU:HB3	57:C6:93:ARG:HH12	1.83	0.44
58:D6:318:ARG:HE	58:D6:318:ARG:HB2	1.66	0.44
61:G6:123:PRO:HD3	82:b6:87:MET:HE3	2.00	0.44
73:S6:88:PHE:HE2	77:W6:102:GLY:HA2	1.82	0.44
78:X6:159:HIS:O	78:X6:163:LYS:N	2.46	0.44
1:r1:43:ASN:HB2	1:r1:45:LYS:HE3	1.98	0.43
3:A3:2740:A:N3	3:A3:2921:A:O2'	2.42	0.43
25:Y3:78:LYS:HD2	25:Y3:78:LYS:HA	1.86	0.43
32:53:49:VAL:HG13	32:53:55:LEU:HD11	1.99	0.43
57:C6:77:ASP:HA	57:C6:78:GLY:HA2	1.63	0.43
60:F6:194:LYS:HD3	60:F6:194:LYS:HA	1.81	0.43
76:V6:138:PHE:HD1	76:V6:170:GLN:HE21	1.65	0.43
78:X6:86:ARG:HH22	86:A6:1384:G:P	2.41	0.43
80:Z6:40:LEU:HD12	80:Z6:45:LYS:HA	1.99	0.43
83:c6:46:ILE:HA	83:c6:49:MET:HG2	2.00	0.43
85:e6:67:LYS:O	85:e6:69:ALA:N	2.51	0.43
3:A3:3000:A:H2'	3:A3:3001:G:H8	1.83	0.43
9:I3:49:ALA:HB1	49:o3:32:LYS:HE3	2.01	0.43
11:K3:27:PRO:HD3	11:K3:149:ARG:HD2	1.99	0.43
18:R3:15:THR:HA	38:c3:32:LYS:HD2	1.98	0.43
33:63:161:LEU:HD21	33:63:271:LEU:HD11	2.00	0.43
57:C6:73:THR:HG21	62:H6:170:MET:HB3	1.99	0.43
63:I6:88:ILE:O	63:I6:152:LYS:N	2.52	0.43
68:N6:16:LYS:HG2	68:N6:63:ILE:HG13	2.01	0.43
76:V6:151:PHE:HA	76:V6:154:LYS:HE2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:W6:149:LEU:HD11	77:W6:166:ASN:HB2	2.00	0.43
86:A6:751:A:H2'	86:A6:752:G:H8	1.83	0.43
86:A6:1142:G:H2'	86:A6:1143:A:H8	1.83	0.43
87:FE:9:A:H8	87:FE:11:C:H41	1.65	0.43
1:r1:70:THR:OG1	1:r1:71:GLY:N	2.51	0.43
3:A3:1799:U:OP1	22:V3:41:ARG:NE	2.51	0.43
3:A3:2106:A:H62	9:I3:31:LYS:HE2	1.83	0.43
3:A3:2455:U:H5''	15:O3:47:ALA:HB3	2.00	0.43
3:A3:2599:U:H5	3:A3:2606:U:H3	1.65	0.43
9:I3:160:LYS:NZ	9:I3:163:GLU:H	2.17	0.43
17:Q3:172:GLN:HB3	17:Q3:173:GLU:OE2	2.17	0.43
24:X3:28:TYR:O	24:X3:31:SER:OG	2.35	0.43
31:43:81:LEU:HG	31:43:90:VAL:HG22	2.00	0.43
32:53:213:TRP:HD1	32:53:364:LEU:HG	1.84	0.43
37:b3:85:ARG:HH12	37:b3:107:GLN:NE2	2.16	0.43
40:e3:192:LEU:HD12	40:e3:200:MET:HB2	2.00	0.43
46:k3:77:ARG:HA	46:k3:78:GLY:HA3	1.72	0.43
56:B6:95:ALA:O	56:B6:98:ARG:NH2	2.51	0.43
56:B6:251:ARG:NH1	56:B6:255:THR:HG1	2.16	0.43
56:B6:270:LEU:HA	56:B6:273:LEU:HD12	1.99	0.43
76:V6:182:SER:HA	76:V6:185:VAL:HG12	2.00	0.43
81:a6:78:ARG:HH12	81:a6:142:VAL:H	1.66	0.43
85:e6:515:ASP:HA	85:e6:518:GLU:HB2	1.99	0.43
85:e6:517:LYS:HD3	85:e6:527:LEU:HD11	1.99	0.43
86:A6:1084:A:O2'	86:A6:1086:A:N7	2.40	0.43
88:A:187:PRO:O	88:A:189:GLU:N	2.48	0.43
3:A3:1807:U:H1'	3:A3:1808:A:H5'	1.99	0.43
9:I3:176:LEU:HD23	9:I3:176:LEU:HA	1.87	0.43
21:U3:110:LEU:HD12	25:Y3:118:GLU:HG2	1.99	0.43
25:Y3:139:MET:O	25:Y3:143:ASP:N	2.51	0.43
32:53:213:TRP:CD1	32:53:364:LEU:HG	2.52	0.43
32:53:326:ARG:NH1	32:53:362:THR:OG1	2.47	0.43
34:73:254:LEU:HD21	34:73:261:ILE:HG23	2.01	0.43
58:D6:371:VAL:HG11	72:R6:106:MET:HE1	2.01	0.43
67:M6:105:THR:HB	75:U6:56:LEU:HD11	2.00	0.43
69:O6:67:ARG:HD2	69:O6:68:TYR:CZ	2.54	0.43
78:X6:104:PRO:HG3	78:X6:345:VAL:HA	2.00	0.43
82:b6:287:LYS:HD2	82:b6:287:LYS:HA	1.87	0.43
86:A6:865:U:H2'	86:A6:866:A:C8	2.53	0.43
3:A3:2158:U:OP2	52:r3:195:TYR:OH	2.34	0.43
6:E3:157:LYS:HD3	6:E3:157:LYS:HA	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F3:49:ARG:HD3	7:F3:263:LEU:HD22	2.00	0.43
11:K3:60:MET:HB3	11:K3:133:ILE:HD11	2.00	0.43
14:N3:170:GLU:OE2	14:N3:170:GLU:N	2.50	0.43
41:f3:163:SER:OG	41:f3:166:PHE:N	2.46	0.43
53:s3:89:MET:HG2	53:s3:277:GLN:HB2	2.01	0.43
59:E6:11:LYS:HG2	59:E6:89:ILE:HD11	2.00	0.43
60:F6:109:SER:HA	60:F6:112:ILE:HB	2.00	0.43
62:H6:73:TYR:HB3	62:H6:76:LEU:HD11	2.01	0.43
67:M6:25:GLY:HA3	67:M6:31:PHE:HB3	2.01	0.43
72:R6:167:HIS:HA	72:R6:170:ARG:HD3	2.00	0.43
72:R6:168:ARG:HA	72:R6:189:ARG:HH22	1.83	0.43
74:T6:13:LEU:HA	74:T6:16:LEU:HB2	2.00	0.43
76:V6:233:LYS:HA	76:V6:233:LYS:HD3	1.86	0.43
78:X6:126:LEU:H	78:X6:309:ALA:HA	1.83	0.43
86:A6:1581:U:H2'	86:A6:1582:A:C8	2.53	0.43
3:A3:1769:C:C4	7:F3:108:ARG:HD2	2.53	0.43
12:L3:69:VAL:HG21	12:L3:124:PRO:HG3	2.01	0.43
14:N3:244:LYS:HB3	14:N3:244:LYS:HE3	1.88	0.43
16:P3:151:GLU:HA	16:P3:154:SER:HB3	2.00	0.43
41:f3:85:ASP:HB3	41:f3:86:TYR:HD1	1.83	0.43
42:g3:84:TYR:OH	42:g3:164:LYS:NZ	2.41	0.43
42:g3:134:LYS:HE3	42:g3:134:LYS:HB2	1.85	0.43
44:i3:79:TRP:O	44:i3:93:ARG:NE	2.43	0.43
50:p3:99:ALA:O	50:p3:136:THR:OG1	2.33	0.43
51:q3:95:SER:OG	51:q3:96:LEU:N	2.51	0.43
57:C6:38:ARG:HG3	57:C6:43:ARG:HH21	1.83	0.43
65:K6:88:ARG:NH2	86:A6:1449:G:O6	2.51	0.43
74:T6:24:LYS:HA	74:T6:108:LYS:NZ	2.32	0.43
79:Y6:296:ASN:N	79:Y6:299:GLU:OE2	2.52	0.43
86:A6:1435:G:N2	86:A6:1436:U:O4	2.35	0.43
3:A3:3192:C:O5'	52:r3:132:ARG:NH1	2.50	0.43
6:E3:54:SER:N	15:O3:146:ASN:OD1	2.49	0.43
37:b3:27:GLN:HE21	37:b3:80:LEU:HD23	1.83	0.43
37:b3:123:ASN:O	37:b3:123:ASN:ND2	2.52	0.43
52:r3:56:THR:HA	52:r3:57:PRO:HD3	1.79	0.43
69:O6:116:ASP:OD1	69:O6:116:ASP:N	2.52	0.43
69:O6:224:LEU:HD11	75:U6:50:PRO:HG3	2.00	0.43
73:S6:107:GLN:HG3	73:S6:117:LEU:HD21	2.00	0.43
8:D:194:PHE:HB3	89:n:92:TYR:CD2	2.53	0.43
89:n:217:LYS:HD2	89:n:217:LYS:HA	1.69	0.43
1:r1:446:VAL:HG12	1:r1:448:ASP:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:r1:673:GLY:HA3	1:r1:691:VAL:HG12	2.01	0.43
3:A3:1907:A:N3	3:A3:2930:U:O2'	2.47	0.43
3:A3:2528:G:OP1	5:D3:104:TYR:OH	2.28	0.43
19:S3:137:GLY:HA3	19:S3:142:THR:HG22	2.00	0.43
20:T3:89:TYR:OH	27:O3:94:ARG:O	2.34	0.43
21:U3:75:GLY:H	21:U3:91:ASP:HB3	1.84	0.43
25:Y3:164:ARG:HD3	25:Y3:180:LYS:HB3	2.01	0.43
32:53:53:PRO:HA	32:53:54:GLY:HA2	1.64	0.43
32:53:270:ILE:H	32:53:270:ILE:HD12	1.84	0.43
33:63:330:ILE:HD13	33:63:334:LEU:HD21	2.01	0.43
38:c3:200:GLY:HA2	38:c3:203:LEU:HD12	1.99	0.43
40:e3:216:LYS:HA	40:e3:228:GLY:HA2	2.01	0.43
56:B6:100:ARG:NE	73:S6:52:ARG:HH12	2.14	0.43
56:B6:150:GLN:HG2	56:B6:151:PHE:CE2	2.53	0.43
58:D6:198:TRP:HB3	58:D6:222:ILE:HG21	2.01	0.43
60:F6:167:PHE:N	87:FE:34:U:O4	2.51	0.43
61:G6:198:ARG:HH22	61:G6:201:ILE:HD13	1.83	0.43
64:J6:74:ASN:OD1	86:A6:904:C:N4	2.36	0.43
78:X6:156:PRO:HD3	78:X6:187:TRP:CD1	2.54	0.43
80:Z6:41:PRO:HG2	80:Z6:44:LYS:HB2	2.01	0.43
1:r1:598:PRO:HB2	1:r1:599:LEU:H	1.68	0.43
3:A3:1989:C:N4	3:A3:1990:G:O6	2.52	0.43
3:A3:2182:G:O2'	3:A3:2183:C:OP1	2.36	0.43
5:D3:118:LYS:HB3	5:D3:118:LYS:HE3	1.78	0.43
5:D3:187:LEU:HB3	5:D3:191:THR:HG21	2.00	0.43
9:I3:95:MET:HB3	9:I3:95:MET:HE2	1.71	0.43
11:K3:20:LEU:HB2	11:K3:141:LEU:HD13	2.00	0.43
17:Q3:184:ASP:N	17:Q3:184:ASP:OD1	2.52	0.43
32:53:314:ILE:HG12	32:53:355:LEU:HD11	1.99	0.43
34:73:113:TRP:HZ3	34:73:119:LEU:HA	1.83	0.43
40:e3:161:VAL:HG22	40:e3:174:PRO:HD3	2.00	0.43
40:e3:178:TRP:HB3	40:e3:187:THR:HG21	2.01	0.43
46:k3:18:VAL:HA	46:k3:64:VAL:HG23	2.01	0.43
50:p3:74:ASP:N	50:p3:74:ASP:OD1	2.50	0.43
50:p3:140:SER:OG	50:p3:141:ARG:N	2.52	0.43
56:B6:199:LEU:HD21	56:B6:226:ASN:HB2	2.00	0.43
57:C6:93:ARG:HG2	57:C6:108:LEU:HD22	2.00	0.43
61:G6:229:LEU:HD23	61:G6:229:LEU:HA	1.85	0.43
61:G6:276:ARG:HH11	61:G6:277:LYS:HB2	1.83	0.43
75:U6:157:VAL:HA	75:U6:160:LEU:HD12	2.01	0.43
78:X6:125:LEU:HD23	78:X6:310:LEU:HD23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:194:PHE:HD1	89:n:92:TYR:CZ	2.35	0.43
14:N3:223:MET:O	26:Z3:115:HIS:HB3	2.18	0.43
24:X3:116:SER:OG	24:X3:142:ASP:OD1	2.37	0.43
61:G6:281:ALA:HA	61:G6:332:VAL:HA	2.01	0.43
61:G6:295:VAL:HG12	61:G6:330:CYS:HB2	2.00	0.43
66:L6:156:LEU:O	66:L6:159:SER:OG	2.30	0.43
76:V6:188:HIS:HA	76:V6:191:ALA:HB3	2.01	0.43
77:W6:87:SER:O	77:W6:90:THR:OG1	2.30	0.43
81:a6:79:LEU:HD11	81:a6:94:TYR:CD2	2.53	0.43
82:b6:183:ASP:OD1	82:b6:183:ASP:N	2.52	0.43
85:e6:72:GLN:HA	85:e6:75:ALA:HB3	1.99	0.43
8:D:194:PHE:HD2	89:n:92:TYR:CG	2.37	0.43
3:A3:1961:A:H5'	20:T3:161:ARG:HA	2.01	0.42
3:A3:2230:A:H62	3:A3:2975:G:H21	1.66	0.42
3:A3:2459:A:N6	3:A3:2668:A:O2'	2.52	0.42
19:S3:172:MET:HG3	19:S3:182:LYS:O	2.19	0.42
30:33:146:GLU:OE1	33:63:364:ARG:NH2	2.52	0.42
39:d3:122:ILE:HD13	39:d3:134:ILE:HG13	2.00	0.42
40:e3:152:LYS:HB2	40:e3:157:LEU:HD21	2.00	0.42
47:l3:133:SER:HA	47:l3:136:LYS:HG2	2.00	0.42
61:G6:378:GLU:N	86:A6:1436:U:OP1	2.46	0.42
69:O6:120:VAL:HG22	69:O6:162:LEU:HD12	2.02	0.42
83:c6:52:MET:SD	83:c6:53:MET:N	2.92	0.42
1:r1:457:PRO:HA	1:r1:516:CYS:HA	2.01	0.42
1:r1:469:GLY:O	1:r1:504:TYR:OH	2.30	0.42
3:A3:2180:A:H1'	3:A3:2206:C:H5''	2.01	0.42
5:D3:124:GLU:HB3	5:D3:142:VAL:HG22	2.01	0.42
6:E3:212:GLY:O	15:O3:11:HIS:NE2	2.32	0.42
8:H3:144:LYS:HA	8:H3:144:LYS:HD2	1.82	0.42
10:J3:127:ASP:OD1	10:J3:130:PHE:N	2.46	0.42
16:P3:57:LEU:HD23	50:p3:177:ARG:HH21	1.82	0.42
18:R3:112:THR:OG1	37:b3:127:GLN:NE2	2.48	0.42
50:p3:75:ARG:HD3	50:p3:75:ARG:HA	1.83	0.42
56:B6:130:ASN:O	56:B6:134:HIS:ND1	2.52	0.42
62:H6:127:TYR:CZ	86:A6:1270:A:H1'	2.54	0.42
63:I6:69:GLU:HA	63:I6:70:GLU:HA	1.70	0.42
65:K6:34:MET:HG3	65:K6:95:SER:HB2	2.02	0.42
86:A6:1216:U:O2'	86:A6:1218:A:N7	2.37	0.42
1:r1:504:TYR:HD1	1:r1:507:ARG:HH22	1.67	0.42
1:r1:646:LEU:HB3	1:r1:720:TYR:HE2	1.84	0.42
3:A3:1922:C:O2'	3:A3:1990:G:OP1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P3:135:CYS:HB3	16:P3:140:ILE:HB	2.00	0.42
39:d3:146:ILE:HD11	39:d3:185:PHE:HB2	2.01	0.42
39:d3:216:MET:HB2	39:d3:244:GLU:HB2	2.00	0.42
40:e3:46:ARG:HB3	40:e3:229:ALA:HA	2.01	0.42
53:s3:419:LEU:HA	53:s3:422:VAL:HG12	2.01	0.42
58:D6:183:LYS:HD3	58:D6:183:LYS:HA	1.86	0.42
63:I6:98:GLN:NE2	63:I6:106:PRO:HB3	2.32	0.42
66:L6:152:HIS:HA	66:L6:155:TYR:HD2	1.83	0.42
66:L6:210:CYS:HA	66:L6:213:VAL:HG12	2.02	0.42
69:O6:103:ASN:HA	69:O6:104:PRO:HD3	1.85	0.42
81:a6:65:LEU:HD23	81:a6:110:ASP:HA	2.01	0.42
83:c6:12:ARG:HD3	83:c6:12:ARG:HA	1.84	0.42
88:A:138:ALA:HA	88:A:141:GLU:HG2	2.01	0.42
87:FE:17:U:H4'	87:FE:56:A:N7	2.34	0.42
1:r1:53:ALA:HB3	1:r1:144:VAL:H	1.84	0.42
3:A3:1794:A:OP1	7:F3:142:ARG:NH2	2.37	0.42
3:A3:2457:A:H3'	15:O3:10:SER:HB3	2.00	0.42
3:A3:2993:U:OP2	3:A3:3063:G:N1	2.45	0.42
23:W3:122:LYS:HE3	23:W3:122:LYS:HB3	1.82	0.42
25:Y3:164:ARG:HH11	25:Y3:180:LYS:HB3	1.84	0.42
57:C6:122:VAL:HA	57:C6:156:GLN:HB3	2.00	0.42
60:F6:156:ILE:HG12	60:F6:230:ALA:HB2	2.02	0.42
63:I6:89:LYS:HD2	86:A6:1008:G:H5''	2.00	0.42
68:N6:96:THR:O	68:N6:98:LYS:N	2.51	0.42
71:Q6:13:MET:HE3	71:Q6:14:VAL:H	1.85	0.42
74:T6:25:ASP:O	74:T6:28:LYS:NZ	2.51	0.42
85:e6:380:ASP:N	85:e6:380:ASP:OD1	2.51	0.42
86:A6:844:A:H61	86:A6:853:U:H3	1.67	0.42
86:A6:1165:A:H2'	86:A6:1166:A:C8	2.55	0.42
3:A3:1682:C:O2	3:A3:1770:G:N2	2.38	0.42
3:A3:1851:G:H2'	3:A3:2693:A:N7	2.34	0.42
3:A3:2172:A:H8	10:J3:22:ALA:HA	1.84	0.42
3:A3:3152:C:OP1	17:Q3:141:SER:OG	2.31	0.42
7:F3:218:LEU:HD23	7:F3:260:VAL:HB	2.01	0.42
10:J3:104:THR:HA	10:J3:105:GLY:HA2	1.57	0.42
20:T3:98:SER:OG	34:73:97:GLU:OE2	2.37	0.42
20:T3:140:LEU:HD23	20:T3:178:LEU:HD13	2.00	0.42
32:53:236:LEU:HD11	32:53:289:HIS:HA	2.01	0.42
44:i3:68:LYS:HB3	44:i3:68:LYS:HE3	1.81	0.42
56:B6:94:LYS:HA	56:B6:94:LYS:HD3	1.72	0.42
67:M6:111:ARG:HH12	72:R6:147:ILE:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:U6:78:VAL:O	75:U6:82:VAL:N	2.47	0.42
76:V6:326:LYS:HA	76:V6:326:LYS:HD2	1.88	0.42
78:X6:368:HIS:HB2	78:X6:398:LEU:HB3	2.01	0.42
86:A6:1435:G:O2'	86:A6:1461:G:O6	2.35	0.42
3:A3:2572:C:H42	3:A3:2585:G:H1	1.68	0.42
7:F3:186:ASP:HB3	7:F3:258:THR:HA	2.01	0.42
9:I3:105:SER:OG	9:I3:106:ALA:N	2.53	0.42
10:J3:61:LYS:HE2	10:J3:64:ILE:HG21	2.02	0.42
11:K3:4:PHE:HB3	11:K3:9:GLN:HB2	2.01	0.42
37:b3:28:ARG:NH1	37:b3:78:GLU:OE1	2.38	0.42
50:p3:82:ARG:HH22	50:p3:95:VAL:HB	1.85	0.42
60:F6:160:PRO:HA	87:FE:30:G:H8	1.85	0.42
64:J6:61:VAL:HA	64:J6:107:ILE:HA	2.00	0.42
65:K6:113:HIS:CE1	65:K6:117:HIS:HE1	2.38	0.42
74:T6:51:ASN:O	74:T6:54:GLN:HB3	2.19	0.42
74:T6:131:PRO:HA	74:T6:138:GLU:HB2	2.01	0.42
1:r1:399:ALA:HB3	1:r1:419:ALA:HB3	2.01	0.42
3:A3:2274:A:O2'	18:R3:15:THR:OG1	2.31	0.42
3:A3:2420:U:O2'	35:93:23:SER:OG	2.35	0.42
13:M3:212:PRO:HD3	51:q3:103:LEU:HD13	2.01	0.42
40:e3:128:PHE:HD1	48:m3:74:MET:HE3	1.84	0.42
49:o3:51:MET:HE2	49:o3:51:MET:HB2	1.83	0.42
56:B6:135:MET:HE1	73:S6:34:VAL:HG21	2.01	0.42
57:C6:79:GLU:O	65:K6:103:ARG:NH1	2.44	0.42
57:C6:114:GLY:HA2	82:b6:159:SER:HA	2.01	0.42
61:G6:310:ARG:HA	61:G6:310:ARG:HD2	1.69	0.42
62:H6:77:SER:HA	62:H6:144:GLU:HA	2.01	0.42
69:O6:205:TRP:HE1	69:O6:207:GLN:HB2	1.85	0.42
75:U6:189:TRP:HB3	75:U6:199:ARG:HG3	2.00	0.42
76:V6:81:SER:OG	76:V6:82:ARG:N	2.52	0.42
78:X6:168:LEU:HA	78:X6:180:GLN:HB3	2.01	0.42
81:a6:136:TYR:CZ	86:A6:709:C:H2'	2.55	0.42
3:A3:2152:A:OP1	49:o3:38:ARG:NH2	2.53	0.42
3:A3:2181:A:O2'	3:A3:2208:A:OP2	2.37	0.42
7:F3:167:MET:HE2	7:F3:167:MET:HB3	1.64	0.42
13:M3:51:ARG:HA	13:M3:51:ARG:HD2	1.91	0.42
21:U3:44:ILE:HD11	21:U3:53:LEU:HD22	2.02	0.42
22:V3:129:LYS:HD3	22:V3:129:LYS:HA	1.90	0.42
33:63:292:GLN:HE21	33:63:292:GLN:HB3	1.65	0.42
40:e3:189:GLU:HG2	40:e3:204:PHE:CE2	2.55	0.42
52:r3:40:GLU:HG2	52:r3:49:ILE:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:s3:94:TYR:O	53:s3:106:TYR:OH	2.25	0.42
56:B6:210:ARG:HG3	73:S6:7:GLU:HG2	2.01	0.42
58:D6:415:GLN:HE22	74:T6:13:LEU:HB3	1.84	0.42
59:E6:37:ARG:NE	59:E6:67:ASP:OD2	2.43	0.42
60:F6:108:ARG:O	60:F6:112:ILE:N	2.48	0.42
61:G6:382:PRO:HB2	62:H6:131:ARG:HG3	2.02	0.42
65:K6:89:ASN:ND2	86:A6:1447:U:OP1	2.38	0.42
81:a6:78:ARG:CZ	81:a6:78:ARG:HB3	2.50	0.42
86:A6:840:A:H2'	86:A6:841:A:H8	1.85	0.42
87:24:17:U:H4'	87:24:56:A:N7	2.35	0.42
87:FE:18:U:H1'	89:n:208:ASN:ND2	2.35	0.42
3:A3:1692:A:C6	25:Y3:176:ILE:HD11	2.55	0.42
3:A3:2531:U:O4	5:D3:246:ARG:NH2	2.53	0.42
6:E3:100:ILE:HD11	6:E3:177:LYS:HB2	2.02	0.42
7:F3:223:HIS:HB2	7:F3:244:PRO:HB3	2.02	0.42
17:Q3:96:ARG:HE	17:Q3:282:ILE:HG12	1.85	0.42
63:I6:84:PRO:HG2	63:I6:147:ILE:HD13	2.02	0.42
69:O6:89:ARG:HE	69:O6:89:ARG:HB2	1.72	0.42
69:O6:119:ASN:HD22	69:O6:122:LEU:HD13	1.84	0.42
74:T6:23:PHE:HB2	74:T6:59:ASN:ND2	2.35	0.42
76:V6:86:ASP:HA	76:V6:89:GLU:HG3	2.02	0.42
76:V6:340:LYS:O	76:V6:344:LEU:N	2.50	0.42
78:X6:266:ASN:HA	78:X6:329:LEU:HD23	2.01	0.42
80:Z6:61:LEU:O	80:Z6:64:THR:OG1	2.34	0.42
82:b6:314:GLU:HA	82:b6:317:LYS:HD3	2.02	0.42
89:n:137:VAL:N	89:n:138:GLU:OE2	2.53	0.42
3:A3:2781:U:O2	89:n:122:TYR:OH	2.25	0.42
9:I3:181:ILE:O	9:I3:184:THR:OG1	2.35	0.42
13:M3:202:LYS:HD3	13:M3:263:ARG:NH1	2.35	0.42
19:S3:94:ARG:HH12	19:S3:111:GLU:HG2	1.84	0.42
24:X3:226:LEU:HD23	24:X3:230:TYR:HE2	1.85	0.42
25:Y3:91:ARG:O	25:Y3:149:ARG:NH2	2.53	0.42
40:e3:132:LYS:HE3	88:A:191:ARG:HH12	1.85	0.42
48:m3:57:VAL:HA	48:m3:63:THR:HA	2.02	0.42
49:o3:72:GLU:HA	49:o3:75:LYS:HG2	2.02	0.42
68:N6:65:LEU:HB3	68:N6:82:ALA:HB3	2.02	0.42
69:O6:106:PRO:HD2	69:O6:142:VAL:HG23	2.02	0.42
80:Z6:55:HIS:H	80:Z6:58:TYR:HD2	1.68	0.42
8:D:189:VAL:HG22	8:D:235:MET:HE1	2.01	0.42
1:r1:191:ARG:NH1	1:r1:252:GLU:OE2	2.53	0.41
1:r1:259:ASN:ND2	1:r1:291:SER:OG	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:r1:707:THR:OG1	1:r1:709:GLY:O	2.36	0.41
6:E3:278:THR:HG22	6:E3:330:GLU:HA	2.01	0.41
13:M3:20:PRO:HG3	49:o3:99:LYS:HA	2.00	0.41
15:O3:18:MET:HE1	15:O3:29:LEU:HD21	2.01	0.41
24:X3:10:LEU:HD23	51:q3:45:LEU:HB3	2.02	0.41
32:53:36:ARG:HA	32:53:39:ARG:HG3	2.01	0.41
58:D6:369:HIS:N	72:R6:106:MET:O	2.52	0.41
61:G6:113:PRO:HG2	82:b6:109:PRO:HG2	2.02	0.41
63:I6:145:ILE:HA	63:I6:170:LEU:HD22	2.02	0.41
66:L6:82:ILE:O	66:L6:90:LYS:NZ	2.41	0.41
68:N6:87:LYS:HG2	68:N6:90:LYS:HB2	2.02	0.41
86:A6:1166:A:N3	86:A6:1501:C:O2'	2.44	0.41
1:r1:178:ARG:HH11	1:r1:178:ARG:HD3	1.64	0.41
7:F3:59:ARG:HH11	7:F3:88:ALA:HB3	1.85	0.41
9:I3:100:GLN:OE1	46:k3:35:GLN:NE2	2.53	0.41
28:13:18:VAL:HG11	28:13:58:GLU:HG2	2.02	0.41
56:B6:257:ILE:HA	56:B6:260:ALA:HB3	2.02	0.41
72:R6:285:LEU:HD21	72:R6:301:VAL:HG11	2.03	0.41
84:d6:174:ARG:HA	84:d6:177:TRP:CE3	2.55	0.41
86:A6:1431:A:H2'	86:A6:1432:G:C8	2.55	0.41
8:D:205:THR:HB	8:D:224:THR:H	1.85	0.41
87:FE:66:U:H2'	87:FE:67:A:C8	2.55	0.41
89:n:128:ASP:OD1	89:n:128:ASP:N	2.53	0.41
1:r1:43:ASN:HB2	1:r1:45:LYS:HG2	2.01	0.41
1:r1:460:LYS:HB3	1:r1:460:LYS:HE3	1.72	0.41
3:A3:1782:G:O2'	3:A3:1793:G:O6	2.35	0.41
3:A3:2063:G:O6	41:f3:48:TYR:N	2.53	0.41
6:E3:107:MET:HG2	6:E3:121:LEU:HD21	2.01	0.41
10:J3:81:LYS:HD3	10:J3:81:LYS:HA	1.90	0.41
13:M3:53:HIS:CD2	13:M3:54:LYS:HG2	2.55	0.41
33:63:35:MET:HE1	41:f3:56:ILE:HA	2.02	0.41
40:e3:275:PHE:HA	88:A:139:MET:HG3	2.02	0.41
45:j3:88:LEU:HD12	45:j3:88:LEU:HA	1.82	0.41
50:p3:111:ILE:HD12	50:p3:111:ILE:HA	1.91	0.41
58:D6:284:ARG:HE	58:D6:287:ASP:HA	1.85	0.41
61:G6:151:PHE:HD1	61:G6:156:GLN:HE22	1.67	0.41
75:U6:93:ARG:NH2	75:U6:97:LYS:HD2	2.35	0.41
82:b6:288:GLU:HG2	82:b6:318:ARG:HB3	2.03	0.41
86:A6:1006:C:H2'	86:A6:1007:A:C8	2.55	0.41
86:A6:1128:A:H2'	86:A6:1129:A:H2'	2.01	0.41
1:r1:152:GLN:HG3	1:r1:154:GLN:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:r1:455:MET:SD	1:r1:493:ILE:HD11	2.61	0.41
1:r1:645:ILE:HG22	1:r1:646:LEU:H	1.84	0.41
5:D3:112:PHE:CE1	5:D3:167:ASN:HB2	2.56	0.41
6:E3:109:LEU:HD13	6:E3:119:VAL:HG11	2.02	0.41
10:J3:91:LEU:HD21	10:J3:120:ILE:HD13	2.02	0.41
15:O3:110:ILE:HD13	15:O3:122:VAL:HG23	2.03	0.41
18:R3:24:VAL:HG11	18:R3:43:VAL:HG12	2.03	0.41
19:S3:181:LYS:HB3	19:S3:181:LYS:HE2	1.72	0.41
24:X3:238:LEU:HA	24:X3:241:GLN:HB3	2.02	0.41
25:Y3:102:TRP:HE3	25:Y3:142:LEU:HD23	1.85	0.41
33:63:371:ASP:HA	33:63:372:SER:HA	1.80	0.41
53:s3:426:LEU:HD12	53:s3:426:LEU:HA	1.91	0.41
56:B6:141:ILE:HB	56:B6:190:PRO:HA	2.02	0.41
61:G6:225:LEU:HD23	61:G6:225:LEU:HA	1.87	0.41
65:K6:51:ARG:HA	65:K6:54:ILE:HG22	2.02	0.41
69:O6:218:ARG:HE	69:O6:218:ARG:HB3	1.62	0.41
70:P6:64:LYS:NZ	70:P6:68:CYS:O	2.45	0.41
72:R6:202:ARG:HG3	72:R6:234:GLN:HA	2.02	0.41
78:X6:124:TYR:O	78:X6:308:SER:N	2.43	0.41
78:X6:125:LEU:HD11	78:X6:337:LEU:HD22	2.01	0.41
82:b6:134:PRO:HG3	85:e6:59:ILE:HA	2.01	0.41
86:A6:945:G:H4'	86:A6:946:A:H5''	2.01	0.41
86:A6:1276:A:N1	86:A6:1307:G:O2'	2.50	0.41
86:A6:1412:A:H2'	86:A6:1413:A:C8	2.56	0.41
1:r1:720:TYR:HD2	1:r1:722:PRO:HG3	1.85	0.41
3:A3:2058:C:H1'	26:Z3:88:MET:HE1	2.03	0.41
3:A3:2830:A:N6	3:A3:2837:A:OP2	2.41	0.41
3:A3:2987:U:O2'	3:A3:2991:U:OP1	2.36	0.41
5:D3:175:ALA:HB2	59:E6:84:ARG:CZ	2.51	0.41
13:M3:57:ARG:NH2	13:M3:62:ARG:HH22	2.19	0.41
13:M3:246:ASP:OD1	13:M3:246:ASP:N	2.52	0.41
23:W3:71:ARG:HE	23:W3:71:ARG:HB3	1.66	0.41
33:63:238:THR:OG1	33:63:249:GLN:OE1	2.39	0.41
40:e3:55:ARG:HH11	40:e3:157:LEU:HD23	1.85	0.41
57:C6:60:HIS:NE2	86:A6:1323:A:H4'	2.36	0.41
58:D6:317:HIS:CE1	58:D6:340:ILE:HD11	2.56	0.41
60:F6:160:PRO:HA	87:FE:30:G:H3'	2.01	0.41
63:I6:144:VAL:HB	63:I6:147:ILE:HD11	2.03	0.41
68:N6:110:LEU:HD11	75:U6:125:ARG:HE	1.85	0.41
72:R6:135:ARG:NH2	72:R6:187:GLU:OE2	2.51	0.41
75:U6:39:ILE:HG13	75:U6:40:GLU:OE2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:e6:96:MET:HA	85:e6:97:PRO:HD2	1.96	0.41
1:r1:108:TYR:HB2	1:r1:403:ALA:O	2.20	0.41
3:A3:2841:U:H3'	23:W3:41:ASN:HD21	1.86	0.41
9:I3:46:LYS:HD3	49:o3:31:ALA:HB1	2.03	0.41
11:K3:155:LEU:HD13	52:r3:86:VAL:HG13	2.03	0.41
16:P3:62:ARG:NH2	23:W3:93:GLU:OE2	2.50	0.41
19:S3:110:SER:OG	19:S3:111:GLU:N	2.52	0.41
19:S3:129:ARG:NH2	19:S3:151:LYS:O	2.53	0.41
19:S3:153:LEU:HD11	19:S3:204:LEU:HD12	2.03	0.41
20:T3:135:GLU:HG2	39:d3:278:LYS:HB2	2.03	0.41
33:63:172:PRO:HB2	33:63:174:HIS:CE1	2.55	0.41
33:63:310:THR:O	33:63:311:MET:HE2	2.21	0.41
37:b3:26:LEU:HD12	37:b3:26:LEU:HA	1.94	0.41
38:c3:312:ARG:HA	38:c3:313:PRO:HD3	1.95	0.41
1:r1:654:VAL:HA	1:r1:713:TYR:HA	2.02	0.41
3:A3:2174:G:N2	10:J3:102:ARG:O	2.54	0.41
3:A3:2846:G:N2	3:A3:2895:U:O2	2.50	0.41
11:K3:120:THR:HG22	36:a3:119:THR:HG22	2.03	0.41
24:X3:67:ILE:HA	24:X3:68:PRO:HD3	1.87	0.41
26:Z3:112:VAL:HG13	26:Z3:113:VAL:HG13	2.02	0.41
37:b3:110:LEU:HD23	37:b3:110:LEU:HA	1.91	0.41
38:c3:244:GLU:OE1	38:c3:247:LYS:NZ	2.51	0.41
70:P6:112:LYS:HB3	70:P6:112:LYS:HE3	1.77	0.41
84:d6:161:ARG:O	84:d6:165:LYS:N	2.50	0.41
86:A6:1179:G:H2'	86:A6:1180:G:C8	2.54	0.41
89:n:215:ASN:HA	89:n:216:LYS:HA	1.63	0.41
89:n:295:LEU:HD21	89:n:305:LEU:HD11	2.01	0.41
1:r1:43:ASN:HD22	1:r1:45:LYS:HE3	1.86	0.41
3:A3:2194:U:O2'	3:A3:2195:A:O4'	2.38	0.41
6:E3:128:HIS:CG	6:E3:170:LEU:HD21	2.56	0.41
9:I3:86:ILE:HA	9:I3:89:VAL:HG12	2.02	0.41
13:M3:260:LYS:HG3	13:M3:264:GLN:HE21	1.85	0.41
16:P3:63:LYS:HD2	16:P3:75:GLU:HG3	2.02	0.41
16:P3:71:PHE:HB2	23:W3:107:HIS:HA	2.02	0.41
16:P3:176:ARG:HD3	16:P3:178:TYR:HE1	1.86	0.41
20:T3:62:GLN:NE2	20:T3:67:PRO:O	2.54	0.41
24:X3:21:CYS:HB3	24:X3:212:ILE:HD11	2.02	0.41
24:X3:128:THR:OG1	24:X3:129:MET:N	2.54	0.41
43:h3:69:ARG:O	43:h3:72:SER:OG	2.37	0.41
44:i3:48:ASN:HB2	44:i3:51:ARG:HB2	2.03	0.41
46:k3:42:VAL:O	46:k3:46:ASN:N	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:p3:151:LEU:HB3	50:p3:155:ARG:HH21	1.85	0.41
53:s3:119:PRO:HG3	53:s3:394:TRP:CD2	2.55	0.41
60:F6:162:LEU:HD13	87:FE:32:A:N7	2.35	0.41
62:H6:123:SER:OG	62:H6:126:ILE:O	2.34	0.41
67:M6:21:LEU:HD13	67:M6:34:ILE:HG23	2.02	0.41
69:O6:115:VAL:H	69:O6:149:ARG:NH2	2.19	0.41
77:W6:149:LEU:HD23	77:W6:149:LEU:HA	1.88	0.41
80:Z6:85:LEU:HA	80:Z6:88:LEU:HB2	2.03	0.41
81:a6:92:PRO:HB2	81:a6:94:TYR:CE1	2.54	0.41
85:e6:506:LEU:HD12	85:e6:507:GLU:HG2	2.03	0.41
86:A6:679:A:H2'	86:A6:680:G:C8	2.55	0.41
8:D:206:LEU:HA	8:D:223:VAL:HG12	2.03	0.41
1:r1:212:LYS:HB2	1:r1:212:LYS:HE2	1.90	0.41
1:r1:395:LEU:HD11	1:r1:420:LEU:HD11	2.02	0.41
1:r1:420:LEU:HD12	1:r1:420:LEU:HA	1.80	0.41
3:A3:2116:C:O2'	3:A3:2837:A:N3	2.47	0.41
6:E3:103:LYS:HE3	6:E3:289:VAL:HB	2.02	0.41
11:K3:116:LEU:HD23	11:K3:116:LEU:HA	1.87	0.41
13:M3:31:PRO:HG2	49:o3:86:ARG:HH21	1.85	0.41
17:Q3:165:GLU:HB2	17:Q3:168:ASN:HB2	2.03	0.41
17:Q3:243:ILE:HB	17:Q3:245:PHE:CE2	2.56	0.41
25:Y3:116:GLU:HB3	25:Y3:126:MET:HE3	2.03	0.41
27:O3:100:LEU:HD23	27:O3:100:LEU:HA	1.86	0.41
32:53:256:PHE:HD2	32:53:259:ILE:HB	1.86	0.41
35:93:43:PHE:HE1	35:93:53:ILE:HD11	1.85	0.41
38:c3:125:LEU:HD23	38:c3:125:LEU:HA	1.94	0.41
44:i3:35:ARG:NE	44:i3:37:THR:O	2.48	0.41
45:j3:58:PRO:HA	45:j3:59:PRO:HD3	1.93	0.41
48:m3:35:SER:O	48:m3:35:SER:OG	2.36	0.41
50:p3:175:LEU:HD12	50:p3:178:ILE:HD12	2.03	0.41
51:q3:141:GLU:O	51:q3:145:LYS:N	2.49	0.41
56:B6:143:LEU:HB2	56:B6:193:ILE:HG12	2.03	0.41
58:D6:89:PHE:HD1	80:Z6:62:MET:HE2	1.86	0.41
58:D6:304:LYS:HB3	58:D6:335:LYS:HB3	2.02	0.41
59:E6:90:ARG:HH12	86:A6:978:U:H4'	1.86	0.41
61:G6:92:MET:HE2	61:G6:92:MET:HB3	1.82	0.41
61:G6:300:TYR:CZ	78:X6:385:ASN:HB2	2.56	0.41
62:H6:76:LEU:O	62:H6:145:LEU:N	2.45	0.41
62:H6:133:GLN:NE2	86:A6:1456:U:OP1	2.54	0.41
62:H6:178:GLU:HB3	82:b6:147:PHE:CD1	2.56	0.41
63:I6:93:ASN:OD1	63:I6:93:ASN:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:L6:159:SER:HA	66:L6:162:GLN:HG2	2.02	0.41
69:O6:107:ILE:HD11	69:O6:126:PHE:CZ	2.56	0.41
70:P6:127:PRO:HG3	71:Q6:8:ILE:HD13	2.02	0.41
72:R6:237:PRO:HA	72:R6:242:TYR:CD1	2.55	0.41
76:V6:179:GLN:OE1	76:V6:214:LYS:NZ	2.39	0.41
78:X6:83:LEU:HD12	78:X6:87:PHE:HD2	1.86	0.41
78:X6:111:TYR:HD2	78:X6:124:TYR:HE2	1.69	0.41
78:X6:120:PRO:HA	78:X6:302:HIS:HA	2.01	0.41
82:b6:188:LYS:HA	82:b6:191:ILE:HD12	2.03	0.41
83:c6:9:ARG:HB3	83:c6:20:VAL:HB	2.03	0.41
85:e6:221:GLU:O	85:e6:225:THR:N	2.53	0.41
86:A6:995:G:N2	86:A6:1000:A:OP2	2.53	0.41
8:D:211:GLU:HA	8:D:212:PRO:HD3	1.93	0.41
1:r1:90:ASP:OD1	1:r1:96:ARG:HB3	2.21	0.41
3:A3:2872:C:O2'	23:W3:88:CYS:SG	2.79	0.41
5:D3:134:CYS:SG	5:D3:135:ARG:NH1	2.94	0.41
9:I3:104:LEU:HD23	9:I3:104:LEU:HA	1.92	0.41
17:Q3:96:ARG:NE	17:Q3:282:ILE:HG12	2.36	0.41
18:R3:136:LYS:HA	18:R3:137:GLU:HA	1.86	0.41
22:V3:191:LEU:HD11	25:Y3:156:LEU:HD12	2.03	0.41
24:X3:208:LEU:O	24:X3:212:ILE:HG12	2.20	0.41
34:73:77:THR:HG22	39:d3:284:GLY:H	1.86	0.41
40:e3:59:VAL:HB	40:e3:153:LEU:HB3	2.03	0.41
53:s3:245:LYS:HE3	53:s3:245:LYS:HB2	1.98	0.41
53:s3:293:CYS:SG	53:s3:294:TYR:N	2.94	0.41
56:B6:149:ARG:NH1	71:Q6:82:ASP:OD1	2.54	0.41
59:E6:59:ASN:OD1	59:E6:59:ASN:N	2.47	0.41
60:F6:156:ILE:HG21	60:F6:230:ALA:HB2	2.02	0.41
61:G6:198:ARG:O	61:G6:246:ARG:N	2.44	0.41
61:G6:379:ARG:HH12	86:A6:1315:C:H41	1.67	0.41
62:H6:99:ALA:HB2	62:H6:156:TYR:CZ	2.56	0.41
65:K6:35:TRP:HA	65:K6:38:VAL:HB	2.03	0.41
72:R6:212:GLU:O	72:R6:216:ARG:NH1	2.54	0.41
78:X6:75:LEU:HG	78:X6:79:PHE:HE2	1.85	0.41
86:A6:1059:U:H2'	86:A6:1060:A:H8	1.86	0.41
86:A6:1189:C:H2'	86:A6:1190:A:C8	2.56	0.41
87:24:66:U:H2'	87:24:67:A:C8	2.55	0.41
89:n:191:GLU:HG2	89:n:193:VAL:HG22	2.03	0.41
3:A3:1672:C:OP1	20:T3:51:TRP:N	2.54	0.40
3:A3:1800:G:N1	3:A3:1803:A:OP2	2.54	0.40
3:A3:2063:G:N2	23:W3:56:MET:SD	2.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A3:2322:C:H4'	3:A3:2323:A:H5''	2.02	0.40
9:I3:109:LYS:HB2	9:I3:109:LYS:HE3	1.89	0.40
16:P3:44:ALA:HA	16:P3:45:PRO:HD3	1.94	0.40
24:X3:221:LYS:HD3	24:X3:221:LYS:HA	1.87	0.40
32:53:135:LYS:HB3	32:53:135:LYS:HE3	1.83	0.40
40:e3:70:MET:HE2	40:e3:70:MET:HB2	1.86	0.40
62:H6:87:VAL:HG21	62:H6:168:VAL:HG21	2.03	0.40
62:H6:94:PHE:CG	82:b6:114:LEU:HD23	2.55	0.40
65:K6:38:VAL:HG13	80:Z6:52:TYR:CZ	2.56	0.40
70:P6:49:ASP:O	73:S6:65:TYR:OH	2.37	0.40
71:Q6:30:LEU:HB2	71:Q6:36:ILE:HG23	2.02	0.40
72:R6:145:ASP:HB3	72:R6:179:GLY:HA3	2.02	0.40
76:V6:169:MET:H	76:V6:169:MET:HG2	1.74	0.40
86:A6:706:C:O2'	86:A6:846:C:O2	2.26	0.40
7:F3:103:GLN:HE21	7:F3:103:GLN:HB3	1.63	0.40
8:H3:95:GLU:HG3	8:H3:132:ALA:HB3	2.02	0.40
11:K3:171:THR:HG23	52:r3:59:GLU:HG3	2.04	0.40
28:13:24:ALA:HB2	51:q3:124:CYS:HB2	2.03	0.40
44:i3:71:LYS:HA	44:i3:74:ILE:HD12	2.02	0.40
53:s3:302:LEU:HD12	53:s3:363:ASP:HB2	2.03	0.40
57:C6:124:LEU:HD23	57:C6:158:VAL:HG13	2.02	0.40
69:O6:106:PRO:HD2	69:O6:142:VAL:HA	2.03	0.40
73:S6:42:ARG:HH11	73:S6:44:PRO:HA	1.87	0.40
75:U6:30:ARG:HH11	86:A6:715:U:H5'	1.86	0.40
78:X6:335:ASP:OD2	82:b6:300:LYS:NZ	2.53	0.40
81:a6:43:ARG:NH2	86:A6:710:C:OP1	2.54	0.40
86:A6:686:A:H2'	86:A6:687:G:C8	2.57	0.40
86:A6:811:A:H8	86:A6:812:C:H5	1.68	0.40
86:A6:1313:A:N6	86:A6:1319:G:O6	2.55	0.40
86:A6:1385:A:H2'	86:A6:1386:A:C8	2.54	0.40
1:r1:647:GLU:N	1:r1:724:LEU:HD12	2.36	0.40
3:A3:1879:G:H5'	7:F3:95:ILE:HD11	2.02	0.40
3:A3:2919:A:O2'	54:u3:2:A:OP1	2.40	0.40
5:D3:193:ILE:HD11	5:D3:226:ILE:HD13	2.03	0.40
5:D3:217:LEU:HD11	5:D3:227:GLN:HB2	2.02	0.40
5:D3:233:GLN:HB3	5:D3:292:MET:SD	2.61	0.40
14:N3:197:LYS:HA	14:N3:197:LYS:HD3	1.86	0.40
18:R3:96:GLU:O	19:S3:105:GLN:NE2	2.39	0.40
21:U3:47:GLU:OE1	21:U3:47:GLU:N	2.55	0.40
33:63:347:PRO:HA	33:63:348:PRO:HD3	1.88	0.40
37:b3:62:VAL:HG21	38:c3:71:GLU:HG2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:e3:85:SER:H	88:A:101:ARG:HH22	1.69	0.40
43:h3:63:PRO:HA	43:h3:64:GLU:HB2	2.02	0.40
53:s3:89:MET:HE2	53:s3:275:LYS:HB3	2.04	0.40
57:C6:133:TYR:HD2	85:e6:106:PHE:HB3	1.86	0.40
64:J6:59:LYS:HE3	86:A6:830:A:H5'	2.02	0.40
65:K6:91:CYS:SG	65:K6:94:THR:N	2.95	0.40
81:a6:29:ARG:N	81:a6:32:GLN:OE1	2.47	0.40
1:r1:129:ILE:O	1:r1:133:ARG:N	2.34	0.40
1:r1:369:THR:HB	1:r1:420:LEU:HB3	2.03	0.40
1:r1:626:PHE:HA	1:r1:629:ALA:HB3	2.02	0.40
3:A3:2389:C:N4	32:53:308:GLN:HE22	2.20	0.40
8:H3:138:LYS:HE2	8:H3:138:LYS:HB2	1.94	0.40
11:K3:105:LYS:HG3	11:K3:122:MET:HE1	2.04	0.40
13:M3:35:LYS:HE2	13:M3:35:LYS:HB3	1.79	0.40
15:O3:120:MET:HE3	15:O3:120:MET:HB3	1.97	0.40
16:P3:147:PRO:HB2	16:P3:151:GLU:HG2	2.03	0.40
18:R3:123:ARG:HH22	18:R3:143:SER:HB2	1.85	0.40
21:U3:66:ALA:HB2	21:U3:100:ALA:HB2	2.03	0.40
22:V3:53:ASP:HB3	22:V3:143:ARG:HH22	1.86	0.40
22:V3:82:GLN:OE1	22:V3:82:GLN:N	2.49	0.40
40:e3:50:ALA:HA	40:e3:175:GLN:HA	2.04	0.40
52:r3:99:MET:SD	52:r3:116:GLU:HB3	2.61	0.40
56:B6:88:ARG:HB3	56:B6:91:LEU:HD23	2.03	0.40
63:I6:88:ILE:HD12	63:I6:151:VAL:HG22	2.02	0.40
64:J6:94:PHE:HB3	64:J6:124:THR:HG22	2.02	0.40
74:T6:138:GLU:N	74:T6:142:GLU:OE2	2.54	0.40
75:U6:56:LEU:HA	75:U6:59:ARG:HB2	2.02	0.40
78:X6:348:TYR:H	78:X6:386:ALA:HB1	1.85	0.40
81:a6:123:LYS:HE3	81:a6:123:LYS:HB3	1.87	0.40
86:A6:679:A:H2'	86:A6:680:G:H8	1.85	0.40
87:24:45:A:OP1	88:A:51:ARG:NH2	2.54	0.40
3:A3:1934:U:H3	3:A3:1940:A:H61	1.70	0.40
3:A3:2027:A:O2'	3:A3:2048:U:OP1	2.32	0.40
11:K3:178:LEU:HD13	52:r3:95:PRO:HD3	2.03	0.40
13:M3:51:ARG:HB3	13:M3:58:GLN:HA	2.03	0.40
13:M3:154:ILE:HG22	13:M3:156:VAL:HG13	2.04	0.40
13:M3:154:ILE:HD12	13:M3:167:ILE:HD13	2.03	0.40
13:M3:180:ASP:OD1	13:M3:183:SER:OG	2.36	0.40
16:P3:55:LEU:HB3	16:P3:61:ALA:HB2	2.04	0.40
18:R3:31:PHE:O	36:a3:129:TYR:OH	2.39	0.40
26:Z3:139:LEU:HA	26:Z3:145:LEU:HD12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:13:33:LYS:HE2	28:13:33:LYS:HB2	2.00	0.40
32:53:118:LYS:HB3	32:53:118:LYS:HE2	1.84	0.40
39:d3:161:HIS:O	39:d3:260:ARG:NH1	2.55	0.40
40:e3:73:LEU:HD11	88:A:114:ARG:HE	1.86	0.40
45:j3:91:TRP:CE2	49:o3:58:GLN:HG2	2.57	0.40
46:k3:76:MET:HA	52:r3:49:ILE:HB	2.03	0.40
57:C6:70:SER:HB2	57:C6:93:ARG:HH21	1.87	0.40
61:G6:286:TYR:HB3	61:G6:288:HIS:CD2	2.57	0.40
62:H6:99:ALA:HB1	62:H6:104:ILE:HB	2.04	0.40
66:L6:150:LYS:HD3	66:L6:150:LYS:HA	1.89	0.40
76:V6:177:SER:O	76:V6:181:LEU:N	2.51	0.40
79:Y6:365:SER:OG	79:Y6:366:VAL:N	2.54	0.40
85:e6:548:PHE:HD2	85:e6:582:LEU:HD11	1.85	0.40
86:A6:1535:C:OP1	86:A6:1536:C:N4	2.54	0.40
87:FE:18:U:O4	89:n:215:ASN:ND2	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	r1	694/751 (92%)	523 (75%)	159 (23%)	12 (2%)	7	34
5	D3	234/305 (77%)	216 (92%)	17 (7%)	1 (0%)	30	60
6	E3	296/348 (85%)	258 (87%)	38 (13%)	0	100	100
7	F3	248/311 (80%)	224 (90%)	24 (10%)	0	100	100
8	D	78/267 (29%)	60 (77%)	18 (23%)	0	100	100
8	H3	93/267 (35%)	84 (90%)	9 (10%)	0	100	100
9	I3	154/261 (59%)	145 (94%)	9 (6%)	0	100	100
10	J3	138/192 (72%)	124 (90%)	14 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K3	175/178 (98%)	153 (87%)	19 (11%)	3 (2%)	7	34
12	L3	113/145 (78%)	104 (92%)	9 (8%)	0	100	100
13	M3	285/296 (96%)	254 (89%)	30 (10%)	1 (0%)	30	60
14	N3	203/251 (81%)	189 (93%)	12 (6%)	2 (1%)	12	43
15	O3	150/175 (86%)	130 (87%)	19 (13%)	1 (1%)	18	50
16	P3	129/179 (72%)	118 (92%)	11 (8%)	0	100	100
17	Q3	217/292 (74%)	192 (88%)	25 (12%)	0	100	100
18	R3	138/149 (93%)	128 (93%)	10 (7%)	0	100	100
19	S3	154/205 (75%)	139 (90%)	15 (10%)	0	100	100
20	T3	164/212 (77%)	152 (93%)	12 (7%)	0	100	100
21	U3	109/153 (71%)	96 (88%)	13 (12%)	0	100	100
22	V3	183/216 (85%)	155 (85%)	26 (14%)	2 (1%)	11	42
23	W3	109/148 (74%)	103 (94%)	6 (6%)	0	100	100
24	X3	241/256 (94%)	220 (91%)	20 (8%)	1 (0%)	30	60
25	Y3	174/250 (70%)	161 (92%)	12 (7%)	1 (1%)	21	52
26	Z3	118/161 (73%)	108 (92%)	10 (8%)	0	100	100
27	03	106/188 (56%)	94 (89%)	11 (10%)	1 (1%)	14	45
28	13	50/65 (77%)	46 (92%)	3 (6%)	1 (2%)	6	32
29	23	44/92 (48%)	42 (96%)	2 (4%)	0	100	100
30	33	93/188 (50%)	89 (96%)	4 (4%)	0	100	100
31	43	34/103 (33%)	34 (100%)	0	0	100	100
32	53	368/423 (87%)	326 (89%)	40 (11%)	2 (0%)	24	56
33	63	313/380 (82%)	283 (90%)	30 (10%)	0	100	100
34	73	258/338 (76%)	233 (90%)	25 (10%)	0	100	100
35	93	105/137 (77%)	88 (84%)	17 (16%)	0	100	100
36	a3	78/142 (55%)	74 (95%)	4 (5%)	0	100	100
37	b3	146/155 (94%)	132 (90%)	13 (9%)	1 (1%)	18	50
38	c3	271/332 (82%)	251 (93%)	20 (7%)	0	100	100
39	d3	156/306 (51%)	139 (89%)	15 (10%)	2 (1%)	9	38
40	e3	211/279 (76%)	193 (92%)	18 (8%)	0	100	100
41	f3	125/194 (64%)	103 (82%)	19 (15%)	3 (2%)	4	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	g3	127/166 (76%)	119 (94%)	8 (6%)	0	100	100
43	h3	96/158 (61%)	84 (88%)	11 (12%)	1 (1%)	12	43
44	i3	95/128 (74%)	87 (92%)	8 (8%)	0	100	100
45	j3	83/123 (68%)	78 (94%)	4 (5%)	1 (1%)	10	40
46	k3	82/112 (73%)	66 (80%)	16 (20%)	0	100	100
47	l3	21/138 (15%)	21 (100%)	0	0	100	100
48	m3	43/128 (34%)	36 (84%)	7 (16%)	0	100	100
49	o3	92/102 (90%)	86 (94%)	6 (6%)	0	100	100
50	p3	119/206 (58%)	113 (95%)	6 (5%)	0	100	100
51	q3	126/222 (57%)	119 (94%)	5 (4%)	2 (2%)	7	35
52	r3	140/196 (71%)	125 (89%)	15 (11%)	0	100	100
53	s3	366/439 (83%)	340 (93%)	26 (7%)	0	100	100
55	A5	26/435 (6%)	17 (65%)	9 (35%)	0	100	100
56	B6	215/296 (73%)	200 (93%)	15 (7%)	0	100	100
57	C6	130/167 (78%)	122 (94%)	8 (6%)	0	100	100
58	D6	316/430 (74%)	272 (86%)	44 (14%)	0	100	100
59	E6	120/125 (96%)	113 (94%)	6 (5%)	1 (1%)	16	48
60	F6	197/242 (81%)	182 (92%)	14 (7%)	1 (0%)	24	56
61	G6	301/396 (76%)	276 (92%)	25 (8%)	0	100	100
62	H6	120/201 (60%)	103 (86%)	17 (14%)	0	100	100
63	I6	134/194 (69%)	122 (91%)	12 (9%)	0	100	100
64	J6	106/138 (77%)	93 (88%)	13 (12%)	0	100	100
65	K6	99/128 (77%)	88 (89%)	11 (11%)	0	100	100
66	L6	162/257 (63%)	151 (93%)	11 (7%)	0	100	100
67	M6	114/137 (83%)	100 (88%)	14 (12%)	0	100	100
68	N6	105/130 (81%)	93 (89%)	12 (11%)	0	100	100
69	O6	183/258 (71%)	159 (87%)	24 (13%)	0	100	100
70	P6	94/142 (66%)	82 (87%)	12 (13%)	0	100	100
71	Q6	84/87 (97%)	75 (89%)	9 (11%)	0	100	100
72	R6	240/360 (67%)	210 (88%)	30 (12%)	0	100	100
73	S6	124/190 (65%)	110 (89%)	14 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
74	T6	160/173 (92%)	140 (88%)	19 (12%)	1 (1%)	21	52
75	U6	171/205 (83%)	159 (93%)	12 (7%)	0	100	100
76	V6	320/414 (77%)	287 (90%)	33 (10%)	0	100	100
77	W6	95/187 (51%)	81 (85%)	14 (15%)	0	100	100
78	X6	310/398 (78%)	264 (85%)	45 (14%)	1 (0%)	36	65
79	Y6	106/395 (27%)	96 (91%)	10 (9%)	0	100	100
80	Z6	85/106 (80%)	79 (93%)	6 (7%)	0	100	100
81	a6	197/218 (90%)	174 (88%)	23 (12%)	0	100	100
82	b6	252/323 (78%)	223 (88%)	29 (12%)	0	100	100
83	c6	114/118 (97%)	98 (86%)	15 (13%)	1 (1%)	14	45
84	d6	67/199 (34%)	62 (92%)	5 (8%)	0	100	100
85	e6	362/689 (52%)	328 (91%)	29 (8%)	5 (1%)	9	37
88	A	158/206 (77%)	139 (88%)	19 (12%)	0	100	100
89	n	216/286 (76%)	166 (77%)	50 (23%)	0	100	100
All	All	13828/19638 (70%)	12301 (89%)	1479 (11%)	48 (0%)	37	65

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	r1	365	PHE
1	r1	598	PRO
1	r1	623	GLU
1	r1	724	LEU
1	r1	725	PRO
22	V3	101	THR
39	d3	231	LEU
41	f3	51	LYS
85	e6	68	VAL
85	e6	147	PRO
1	r1	599	LEU
1	r1	682	GLU
11	K3	160	GLN
13	M3	265	ILE
22	V3	194	LEU
24	X3	52	ILE
32	53	270	ILE
51	q3	43	GLU

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Mol	Chain	Res	Type
60	F6	161	ILE
1	r1	404	ASP
14	N3	238	LYS
27	03	178	ASP
28	13	63	ARG
41	f3	50	THR
41	f3	85	ASP
51	q3	42	PRO
78	X6	342	PRO
1	r1	679	ASP
5	D3	207	ILE
83	c6	60	GLU
1	r1	403	ALA
11	K3	4	PHE
45	j3	35	ALA
85	e6	146	GLU
85	e6	274	GLN
11	K3	159	THR
14	N3	237	HIS
43	h3	66	LEU
1	r1	79	VAL
32	53	349	GLY
85	e6	149	ILE
39	d3	164	VAL
74	T6	148	PRO
1	r1	341	ILE
25	Y3	203	PRO
59	E6	15	ARG
15	O3	111	PRO
37	b3	117	LYS

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	
1	r1	592/630 (94%)	592 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	D3	190/245 (78%)	190 (100%)	0	100	100
6	E3	255/290 (88%)	255 (100%)	0	100	100
7	F3	217/262 (83%)	217 (100%)	0	100	100
8	D	73/228 (32%)	73 (100%)	0	100	100
8	H3	86/228 (38%)	86 (100%)	0	100	100
9	I3	145/232 (62%)	145 (100%)	0	100	100
10	J3	113/150 (75%)	113 (100%)	0	100	100
11	K3	155/156 (99%)	154 (99%)	1 (1%)	78	79
12	L3	98/124 (79%)	98 (100%)	0	100	100
13	M3	245/249 (98%)	245 (100%)	0	100	100
14	N3	172/211 (82%)	172 (100%)	0	100	100
15	O3	133/150 (89%)	133 (100%)	0	100	100
16	P3	115/154 (75%)	114 (99%)	1 (1%)	70	75
17	Q3	201/256 (78%)	201 (100%)	0	100	100
18	R3	118/126 (94%)	118 (100%)	0	100	100
19	S3	141/180 (78%)	140 (99%)	1 (1%)	76	77
20	T3	146/182 (80%)	146 (100%)	0	100	100
21	U3	99/135 (73%)	99 (100%)	0	100	100
22	V3	169/191 (88%)	169 (100%)	0	100	100
23	W3	91/119 (76%)	91 (100%)	0	100	100
24	X3	217/227 (96%)	217 (100%)	0	100	100
25	Y3	159/223 (71%)	159 (100%)	0	100	100
26	Z3	111/147 (76%)	111 (100%)	0	100	100
27	03	97/164 (59%)	97 (100%)	0	100	100
28	13	49/60 (82%)	49 (100%)	0	100	100
29	23	40/72 (56%)	40 (100%)	0	100	100
30	33	88/166 (53%)	88 (100%)	0	100	100
31	43	35/89 (39%)	35 (100%)	0	100	100
32	53	337/368 (92%)	336 (100%)	1 (0%)	86	83
33	63	266/332 (80%)	266 (100%)	0	100	100
34	73	242/303 (80%)	242 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	93	91/112 (81%)	91 (100%)	0	100	100
36	a3	78/133 (59%)	78 (100%)	0	100	100
37	b3	130/135 (96%)	129 (99%)	1 (1%)	73	76
38	c3	241/288 (84%)	241 (100%)	0	100	100
39	d3	151/274 (55%)	151 (100%)	0	100	100
40	e3	188/236 (80%)	188 (100%)	0	100	100
41	f3	117/173 (68%)	117 (100%)	0	100	100
42	g3	119/148 (80%)	119 (100%)	0	100	100
43	h3	95/148 (64%)	95 (100%)	0	100	100
44	i3	86/110 (78%)	86 (100%)	0	100	100
45	j3	68/97 (70%)	68 (100%)	0	100	100
46	k3	74/90 (82%)	74 (100%)	0	100	100
47	l3	23/116 (20%)	23 (100%)	0	100	100
48	m3	40/113 (35%)	40 (100%)	0	100	100
49	o3	80/87 (92%)	80 (100%)	0	100	100
50	p3	117/181 (65%)	117 (100%)	0	100	100
51	q3	110/178 (62%)	110 (100%)	0	100	100
52	r3	133/169 (79%)	133 (100%)	0	100	100
53	s3	326/381 (86%)	326 (100%)	0	100	100
56	B6	191/249 (77%)	190 (100%)	1 (0%)	81	80
57	C6	115/143 (80%)	115 (100%)	0	100	100
58	D6	269/357 (75%)	269 (100%)	0	100	100
59	E6	104/107 (97%)	104 (100%)	0	100	100
60	F6	178/209 (85%)	178 (100%)	0	100	100
61	G6	265/342 (78%)	265 (100%)	0	100	100
62	H6	112/180 (62%)	112 (100%)	0	100	100
63	I6	104/147 (71%)	104 (100%)	0	100	100
64	J6	93/118 (79%)	93 (100%)	0	100	100
65	K6	91/113 (80%)	91 (100%)	0	100	100
66	L6	152/226 (67%)	152 (100%)	0	100	100
67	M6	95/113 (84%)	95 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
68	N6	93/115 (81%)	93 (100%)	0	100	100
69	O6	166/230 (72%)	166 (100%)	0	100	100
70	P6	87/123 (71%)	87 (100%)	0	100	100
71	Q6	78/79 (99%)	78 (100%)	0	100	100
72	R6	224/318 (70%)	224 (100%)	0	100	100
73	S6	109/164 (66%)	109 (100%)	0	100	100
74	T6	150/157 (96%)	150 (100%)	0	100	100
75	U6	149/174 (86%)	149 (100%)	0	100	100
76	V6	295/364 (81%)	295 (100%)	0	100	100
77	W6	84/158 (53%)	84 (100%)	0	100	100
78	X6	275/351 (78%)	275 (100%)	0	100	100
79	Y6	99/357 (28%)	99 (100%)	0	100	100
80	Z6	80/95 (84%)	80 (100%)	0	100	100
81	a6	176/190 (93%)	176 (100%)	0	100	100
82	b6	237/291 (81%)	237 (100%)	0	100	100
83	c6	99/101 (98%)	99 (100%)	0	100	100
84	d6	63/166 (38%)	63 (100%)	0	100	100
85	e6	226/609 (37%)	226 (100%)	0	100	100
88	A	151/190 (80%)	151 (100%)	0	100	100
89	n	194/254 (76%)	194 (100%)	0	100	100
All	All	12266/16608 (74%)	12260 (100%)	6 (0%)	100	100

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	K3	70	ASN
16	P3	54	ASN
19	S3	118	ASN
32	53	275	ASN
37	b3	123	ASN
56	B6	113	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (122) such sidechains are listed below:

Mol	Chain	Res	Type
1	r1	43	ASN
1	r1	77	HIS
1	r1	196	HIS
1	r1	367	GLN
1	r1	542	GLN
1	r1	672	HIS
1	r1	678	GLN
1	r1	728	GLN
5	D3	165	ASN
5	D3	195	ASN
5	D3	227	GLN
6	E3	72	GLN
6	E3	277	ASN
6	E3	336	ASN
7	F3	63	GLN
9	I3	43	GLN
10	J3	48	GLN
10	J3	103	GLN
12	L3	33	GLN
12	L3	80	GLN
14	N3	138	HIS
14	N3	210	GLN
16	P3	54	ASN
17	Q3	218	ASN
19	S3	179	ASN
20	T3	105	GLN
21	U3	27	GLN
22	V3	73	GLN
24	X3	93	ASN
25	Y3	117	GLN
25	Y3	179	HIS
25	Y3	207	HIS
28	13	31	ASN
29	23	77	GLN
30	33	154	GLN
32	53	250	ASN
32	53	275	ASN
33	63	224	HIS
33	63	295	GLN
33	63	308	GLN
34	73	49	ASN
34	73	247	ASN
34	73	298	GLN

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Mol	Chain	Res	Type
36	a3	71	HIS
37	b3	102	GLN
38	c3	94	ASN
38	c3	122	ASN
38	c3	134	GLN
38	c3	192	GLN
38	c3	222	GLN
39	d3	119	GLN
41	f3	108	GLN
41	f3	115	ASN
42	g3	93	ASN
45	j3	99	GLN
46	k3	26	ASN
46	k3	35	GLN
48	m3	59	GLN
50	p3	163	GLN
51	q3	134	ASN
52	r3	130	ASN
53	s3	179	GLN
53	s3	281	HIS
53	s3	387	ASN
56	B6	120	GLN
56	B6	150	GLN
57	C6	81	HIS
58	D6	288	HIS
58	D6	317	HIS
58	D6	369	HIS
59	E6	54	HIS
60	F6	146	HIS
61	G6	77	GLN
61	G6	220	GLN
61	G6	255	GLN
61	G6	261	GLN
62	H6	130	HIS
63	I6	96	GLN
63	I6	98	GLN
65	K6	117	HIS
66	L6	110	GLN
66	L6	142	HIS
66	L6	172	ASN
67	M6	28	ASN
67	M6	39	ASN

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Mol	Chain	Res	Type
67	M6	100	HIS
69	O6	130	HIS
70	P6	56	ASN
70	P6	71	HIS
70	P6	115	GLN
73	S6	61	GLN
74	T6	18	GLN
74	T6	56	GLN
74	T6	59	ASN
74	T6	122	GLN
74	T6	128	ASN
75	U6	113	ASN
75	U6	159	GLN
75	U6	161	GLN
76	V6	87	HIS
76	V6	134	GLN
76	V6	238	GLN
76	V6	246	ASN
76	V6	329	GLN
76	V6	380	GLN
76	V6	381	GLN
78	X6	190	ASN
78	X6	312	GLN
79	Y6	295	GLN
79	Y6	303	GLN
81	a6	108	ASN
82	b6	268	GLN
82	b6	301	ASN
85	e6	79	ASN
85	e6	115	ASN
85	e6	436	HIS
85	e6	455	ASN
88	A	127	GLN
88	A	158	HIS
89	n	136	ASN
89	n	276	ASN
89	n	281	HIS

5.3.3 RNA ⓘ

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	8	7/1559 (0%)	4 (57%)	0
3	A3	1490/1559 (95%)	415 (27%)	38 (2%)
4	B3	52/73 (71%)	16 (30%)	1 (1%)
54	u3	1/2 (50%)	0	0
86	A6	921/954 (96%)	267 (28%)	14 (1%)
87	24	73/73 (100%)	38 (52%)	1 (1%)
87	FE	73/73 (100%)	38 (52%)	1 (1%)
All	All	2617/4293 (60%)	778 (29%)	55 (2%)

All (778) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	A3	1674	A
3	A3	1676	A
3	A3	1678	C
3	A3	1679	U
3	A3	1680	A
3	A3	1681	G
3	A3	1685	C
3	A3	1689	C
3	A3	1692	A
3	A3	1693	C
3	A3	1694	U
3	A3	1699	C
3	A3	1700	U
3	A3	1701	U
3	A3	1704	U
3	A3	1707	C
3	A3	1708	A
3	A3	1709	G
3	A3	1713	A
3	A3	1714	C
3	A3	1715	C
3	A3	1716	U
3	A3	1717	U
3	A3	1724	A
3	A3	1727	A
3	A3	1728	U
3	A3	1741	A
3	A3	1748	G
3	A3	1750	G

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Mol	Chain	Res	Type
3	A3	1751	A
3	A3	1767	G
3	A3	1770	G
3	A3	1774	U
3	A3	1777	A
3	A3	1780	U
3	A3	1781	A
3	A3	1782	G
3	A3	1791	G
3	A3	1794	A
3	A3	1804	A
3	A3	1805	A
3	A3	1806	U
3	A3	1807	U
3	A3	1808	A
3	A3	1809	U
3	A3	1810	A
3	A3	1811	A
3	A3	1812	C
3	A3	1813	C
3	A3	1817	C
3	A3	1821	A
3	A3	1824	U
3	A3	1827	C
3	A3	1828	A
3	A3	1829	A
3	A3	1832	A
3	A3	1836	A
3	A3	1844	A
3	A3	1849	C
3	A3	1854	U
3	A3	1856	A
3	A3	1867	A
3	A3	1869	A
3	A3	1870	A
3	A3	1872	U
3	A3	1873	A
3	A3	1874	A
3	A3	1878	U
3	A3	1882	A
3	A3	1883	G
3	A3	1887	A

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Mol	Chain	Res	Type
3	A3	1888	G
3	A3	1890	C
3	A3	1893	A
3	A3	1902	C
3	A3	1903	C
3	A3	1909	A
3	A3	1918	G
3	A3	1922	C
3	A3	1935	A
3	A3	1939	G
3	A3	1940	A
3	A3	1944	C
3	A3	1966	G
3	A3	1968	G
3	A3	1974	A
3	A3	1975	U
3	A3	1985	G
3	A3	1987	G
3	A3	1992	C
3	A3	1993	A
3	A3	1994	A
3	A3	1995	A
3	A3	2000	C
3	A3	2001	C
3	A3	2002	G
3	A3	2015	G
3	A3	2020	U
3	A3	2021	U
3	A3	2022	G
3	A3	2029	A
3	A3	2031	A
3	A3	2032	G
3	A3	2036	C
3	A3	2037	U
3	A3	2053	U
3	A3	2055	U
3	A3	2057	C
3	A3	2059	C
3	A3	2060	A
3	A3	2065	A
3	A3	2074	A
3	A3	2079	C

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Mol	Chain	Res	Type
3	A3	2083	U
3	A3	2085	A
3	A3	2093	U
3	A3	2097	A
3	A3	2098	G
3	A3	2099	U
3	A3	2110	A
3	A3	2113	G
3	A3	2124	A
3	A3	2125	C
3	A3	2132	A
3	A3	2135	A
3	A3	2141	U
3	A3	2142	A
3	A3	2147	G
3	A3	2154	A
3	A3	2157	U
3	A3	2159	U
3	A3	2163	A
3	A3	2165	C
3	A3	2166	C
3	A3	2168	U
3	A3	2171	U
3	A3	2172	A
3	A3	2173	G
3	A3	2177	U
3	A3	2180	A
3	A3	2182	G
3	A3	2183	C
3	A3	2184	A
3	A3	2187	C
3	A3	2190	C
3	A3	2193	U
3	A3	2194	U
3	A3	2195	A
3	A3	2197	G
3	A3	2198	A
3	A3	2200	A
3	A3	2202	C
3	A3	2210	C
3	A3	2216	A
3	A3	2229	A

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Mol	Chain	Res	Type
3	A3	2230	A
3	A3	2231	A
3	A3	2233	U
3	A3	2237	A
3	A3	2239	A
3	A3	2241	A
3	A3	2243	A
3	A3	2244	U
3	A3	2245	A
3	A3	2246	A
3	A3	2262	C
3	A3	2263	C
3	A3	2283	C
3	A3	2284	C
3	A3	2285	U
3	A3	2290	A
3	A3	2294	A
3	A3	2297	A
3	A3	2299	U
3	A3	2300	G
3	A3	2309	A
3	A3	2322	C
3	A3	2323	A
3	A3	2324	U
3	A3	2329	C
3	A3	2331	C
3	A3	2332	C
3	A3	2345	G
3	A3	2364	C
3	A3	2369	A
3	A3	2370	A
3	A3	2371	U
3	A3	2372	U
3	A3	2374	A
3	A3	2375	C
3	A3	2379	C
3	A3	2380	C
3	A3	2381	A
3	A3	2387	U
3	A3	2389	C
3	A3	2390	A
3	A3	2393	C

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Mol	Chain	Res	Type
3	A3	2394	A
3	A3	2400	C
3	A3	2401	A
3	A3	2404	U
3	A3	2405	C
3	A3	2407	U
3	A3	2414	C
3	A3	2415	C
3	A3	2416	U
3	A3	2426	C
3	A3	2427	C
3	A3	2429	A
3	A3	2435	G
3	A3	2443	C
3	A3	2444	A
3	A3	2445	U
3	A3	2446	A
3	A3	2447	A
3	A3	2452	A
3	A3	2478	G
3	A3	2493	C
3	A3	2500	A
3	A3	2506	A
3	A3	2508	C
3	A3	2511	C
3	A3	2520	C
3	A3	2521	A
3	A3	2522	U
3	A3	2523	C
3	A3	2524	A
3	A3	2527	A
3	A3	2530	A
3	A3	2531	U
3	A3	2532	U
3	A3	2536	G
3	A3	2539	A
3	A3	2540	C
3	A3	2557	C
3	A3	2558	A
3	A3	2559	U
3	A3	2560	G
3	A3	2563	U

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Mol	Chain	Res	Type
3	A3	2567	G
3	A3	2570	C
3	A3	2581	A
3	A3	2582	A
3	A3	2592	G
3	A3	2593	G
3	A3	2594	U
3	A3	2596	G
3	A3	2601	A
3	A3	2603	C
3	A3	2618	U
3	A3	2626	U
3	A3	2627	G
3	A3	2629	A
3	A3	2630	U
3	A3	2632	A
3	A3	2633	A
3	A3	2634	U
3	A3	2635	G
3	A3	2643	G
3	A3	2645	G
3	A3	2654	U
3	A3	2655	G
3	A3	2656	U
3	A3	2660	U
3	A3	2683	C
3	A3	2686	G
3	A3	2694	A
3	A3	2696	A
3	A3	2706	A
3	A3	2708	C
3	A3	2709	A
3	A3	2718	C
3	A3	2719	G
3	A3	2723	A
3	A3	2724	G
3	A3	2725	A
3	A3	2732	G
3	A3	2733	G
3	A3	2740	A
3	A3	2745	A
3	A3	2749	A

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Mol	Chain	Res	Type
3	A3	2750	U
3	A3	2757	A
3	A3	2758	G
3	A3	2761	C
3	A3	2762	C
3	A3	2763	U
3	A3	2764	A
3	A3	2765	A
3	A3	2766	C
3	A3	2767	A
3	A3	2768	A
3	A3	2769	A
3	A3	2771	C
3	A3	2773	A
3	A3	2774	C
3	A3	2775	A
3	A3	2776	G
3	A3	2777	G
3	A3	2778	U
3	A3	2779	C
3	A3	2780	C
3	A3	2781	U
3	A3	2782	A
3	A3	2783	A
3	A3	2784	A
3	A3	2785	C
3	A3	2786	U
3	A3	2787	A
3	A3	2788	C
3	A3	2789	C
3	A3	2790	A
3	A3	2791	A
3	A3	2792	A
3	A3	2804	A
3	A3	2810	G
3	A3	2814	G
3	A3	2823	U
3	A3	2831	G
3	A3	2832	A
3	A3	2833	A
3	A3	2842	C
3	A3	2844	G

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Mol	Chain	Res	Type
3	A3	2847	C
3	A3	2851	A
3	A3	2854	U
3	A3	2861	A
3	A3	2864	U
3	A3	2865	C
3	A3	2870	G
3	A3	2871	U
3	A3	2879	A
3	A3	2893	A
3	A3	2896	G
3	A3	2901	A
3	A3	2906	C
3	A3	2910	A
3	A3	2913	A
3	A3	2916	G
3	A3	2917	G
3	A3	2918	A
3	A3	2919	A
3	A3	2922	A
3	A3	2926	A
3	A3	2928	C
3	A3	2932	G
3	A3	2934	G
3	A3	2935	A
3	A3	2936	U
3	A3	2955	U
3	A3	2956	A
3	A3	2963	A
3	A3	2968	A
3	A3	2971	A
3	A3	2981	A
3	A3	2989	G
3	A3	2990	A
3	A3	2991	U
3	A3	2992	G
3	A3	2994	U
3	A3	3000	A
3	A3	3005	A
3	A3	3012	U
3	A3	3016	G
3	A3	3022	G

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Mol	Chain	Res	Type
3	A3	3029	A
3	A3	3041	U
3	A3	3042	U
3	A3	3053	A
3	A3	3054	G
3	A3	3056	C
3	A3	3060	C
3	A3	3063	G
3	A3	3065	U
3	A3	3070	G
3	A3	3072	U
3	A3	3077	C
3	A3	3086	U
3	A3	3089	A
3	A3	3093	C
3	A3	3096	U
3	A3	3100	U
3	A3	3102	U
3	A3	3108	U
3	A3	3109	U
3	A3	3114	U
3	A3	3123	G
3	A3	3124	U
3	A3	3128	A
3	A3	3129	A
3	A3	3131	G
3	A3	3135	A
3	A3	3141	A
3	A3	3150	U
3	A3	3155	C
3	A3	3157	C
3	A3	3158	A
3	A3	3160	A
3	A3	3161	G
3	A3	3162	C
3	A3	3168	C
3	A3	3169	C
3	A3	3172	C
3	A3	3176	A
3	A3	3180	A
3	A3	3184	C
3	A3	3189	C

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Mol	Chain	Res	Type
3	A3	3190	A
3	A3	3202	U
3	A3	3204	C
3	A3	3207	A
3	A3	3217	A
3	A3	3218	A
3	A3	3220	A
3	A3	3228	U
4	B3	1607	U
4	B3	1608	G
4	B3	1609	U
4	B3	1611	G
4	B3	1614	U
4	B3	1615	A
4	B3	1625	A
4	B3	1631	C
4	B3	1632	U
4	B3	1634	A
4	B3	1641	G
4	B3	1644	G
4	B3	1645	A
4	B3	1663	C
4	B3	1665	C
4	B3	1667	C
86	A6	654	U
86	A6	655	A
86	A6	675	U
86	A6	678	U
86	A6	682	U
86	A6	684	U
86	A6	686	A
86	A6	692	A
86	A6	694	U
86	A6	695	A
86	A6	698	C
86	A6	701	G
86	A6	707	A
86	A6	708	U
86	A6	709	C
86	A6	715	U
86	A6	716	C
86	A6	717	C

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Mol	Chain	Res	Type
86	A6	722	A
86	A6	724	U
86	A6	725	U
86	A6	726	C
86	A6	727	A
86	A6	749	A
86	A6	757	A
86	A6	761	A
86	A6	765	A
86	A6	768	A
86	A6	770	G
86	A6	774	C
86	A6	775	A
86	A6	777	U
86	A6	786	A
86	A6	787	A
86	A6	792	U
86	A6	795	G
86	A6	797	C
86	A6	798	U
86	A6	799	A
86	A6	800	G
86	A6	811	A
86	A6	812	C
86	A6	813	G
86	A6	816	A
86	A6	818	A
86	A6	819	C
86	A6	820	A
86	A6	821	G
86	A6	831	A
86	A6	834	U
86	A6	836	U
86	A6	839	C
86	A6	840	A
86	A6	850	A
86	A6	851	G
86	A6	853	U
86	A6	857	C
86	A6	859	A
86	A6	865	U
86	A6	869	A

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Mol	Chain	Res	Type
86	A6	872	C
86	A6	873	C
86	A6	874	C
86	A6	884	C
86	A6	886	A
86	A6	887	U
86	A6	889	U
86	A6	894	C
86	A6	903	G
86	A6	907	U
86	A6	908	C
86	A6	909	A
86	A6	923	A
86	A6	924	G
86	A6	931	G
86	A6	937	G
86	A6	938	G
86	A6	942	A
86	A6	943	A
86	A6	946	A
86	A6	947	G
86	A6	951	U
86	A6	952	U
86	A6	954	A
86	A6	957	U
86	A6	958	C
86	A6	959	A
86	A6	970	A
86	A6	971	A
86	A6	981	A
86	A6	982	A
86	A6	989	U
86	A6	992	G
86	A6	996	U
86	A6	997	A
86	A6	1005	C
86	A6	1006	C
86	A6	1011	G
86	A6	1012	A
86	A6	1015	C
86	A6	1018	A
86	A6	1019	A

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Mol	Chain	Res	Type
86	A6	1023	A
86	A6	1026	A
86	A6	1032	G
86	A6	1035	G
86	A6	1036	C
86	A6	1038	U
86	A6	1043	A
86	A6	1046	U
86	A6	1050	A
86	A6	1053	A
86	A6	1056	C
86	A6	1069	C
86	A6	1085	U
86	A6	1086	A
86	A6	1102	C
86	A6	1107	A
86	A6	1109	C
86	A6	1110	C
86	A6	1113	A
86	A6	1125	A
86	A6	1129	A
86	A6	1130	A
86	A6	1133	U
86	A6	1141	A
86	A6	1142	G
86	A6	1146	A
86	A6	1148	U
86	A6	1155	C
86	A6	1157	C
86	A6	1158	A
86	A6	1170	A
86	A6	1171	A
86	A6	1183	G
86	A6	1184	U
86	A6	1189	C
86	A6	1191	U
86	A6	1192	A
86	A6	1193	U
86	A6	1194	C
86	A6	1195	C
86	A6	1196	C
86	A6	1198	C

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Mol	Chain	Res	Type
86	A6	1207	C
86	A6	1210	G
86	A6	1218	A
86	A6	1219	U
86	A6	1220	C
86	A6	1224	A
86	A6	1226	A
86	A6	1227	C
86	A6	1229	C
86	A6	1230	C
86	A6	1233	U
86	A6	1235	A
86	A6	1236	A
86	A6	1241	A
86	A6	1247	U
86	A6	1249	U
86	A6	1250	U
86	A6	1251	G
86	A6	1252	C
86	A6	1254	C
86	A6	1255	A
86	A6	1256	G
86	A6	1258	C
86	A6	1261	U
86	A6	1265	C
86	A6	1274	U
86	A6	1275	C
86	A6	1276	A
86	A6	1287	A
86	A6	1288	U
86	A6	1289	G
86	A6	1291	A
86	A6	1294	C
86	A6	1296	A
86	A6	1297	C
86	A6	1298	A
86	A6	1299	A
86	A6	1300	A
86	A6	1301	G
86	A6	1304	A
86	A6	1330	A
86	A6	1331	G

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Mol	Chain	Res	Type
86	A6	1333	U
86	A6	1334	C
86	A6	1336	A
86	A6	1346	C
86	A6	1347	A
86	A6	1348	U
86	A6	1355	G
86	A6	1357	A
86	A6	1358	A
86	A6	1359	G
86	A6	1360	A
86	A6	1363	U
86	A6	1371	A
86	A6	1372	U
86	A6	1373	U
86	A6	1375	U
86	A6	1380	C
86	A6	1381	C
86	A6	1382	C
86	A6	1383	A
86	A6	1385	A
86	A6	1394	A
86	A6	1395	U
86	A6	1397	G
86	A6	1400	C
86	A6	1401	U
86	A6	1406	A
86	A6	1407	A
86	A6	1420	A
86	A6	1421	A
86	A6	1423	G
86	A6	1424	U
86	A6	1428	U
86	A6	1434	A
86	A6	1436	U
86	A6	1441	U
86	A6	1444	G
86	A6	1448	A
86	A6	1451	G
86	A6	1452	U
86	A6	1456	U
86	A6	1458	G

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Mol	Chain	Res	Type
86	A6	1460	U
86	A6	1466	G
86	A6	1469	C
86	A6	1470	C
86	A6	1485	C
86	A6	1486	A
86	A6	1498	C
86	A6	1506	A
86	A6	1516	A
86	A6	1521	A
86	A6	1522	C
86	A6	1529	C
86	A6	1531	A
86	A6	1536	C
86	A6	1537	C
86	A6	1538	C
86	A6	1539	U
86	A6	1540	A
86	A6	1541	C
86	A6	1542	G
86	A6	1543	C
86	A6	1544	A
86	A6	1545	U
86	A6	1547	U
86	A6	1551	U
86	A6	1562	A
86	A6	1563	G
86	A6	1566	G
86	A6	1568	A
86	A6	1572	U
86	A6	1575	U
86	A6	1576	A
86	A6	1586	G
86	A6	1588	A
86	A6	1595	C
86	A6	1598	G
86	A6	1599	G
86	A6	1603	A
86	A6	1604	A
87	24	2	U
87	24	3	U
87	24	7	G

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Mol	Chain	Res	Type
87	24	8	U
87	24	9	A
87	24	12	U
87	24	13	U
87	24	14	A
87	24	16	A
87	24	17	U
87	24	18	U
87	24	19	A
87	24	20	U
87	24	21	C
87	24	22	A
87	24	27	A
87	24	28	A
87	24	30	G
87	24	31	C
87	24	32	A
87	24	35	G
87	24	41	G
87	24	45	A
87	24	46	G
87	24	51	G
87	24	52	C
87	24	54	U
87	24	55	C
87	24	56	A
87	24	57	C
87	24	58	A
87	24	59	G
87	24	62	C
87	24	65	U
87	24	67	A
87	24	71	C
87	24	72	C
87	24	73	A
3	8	18	A
3	8	19	A
3	8	21	U
3	8	23	A
87	FE	2	U
87	FE	3	U
87	FE	7	G

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Mol	Chain	Res	Type
87	FE	8	U
87	FE	9	A
87	FE	12	U
87	FE	13	U
87	FE	14	A
87	FE	16	A
87	FE	17	U
87	FE	18	U
87	FE	19	A
87	FE	20	U
87	FE	21	C
87	FE	22	A
87	FE	27	A
87	FE	28	A
87	FE	30	G
87	FE	31	C
87	FE	32	A
87	FE	35	G
87	FE	41	G
87	FE	45	A
87	FE	46	G
87	FE	51	G
87	FE	52	C
87	FE	54	U
87	FE	55	C
87	FE	56	A
87	FE	57	C
87	FE	58	A
87	FE	59	G
87	FE	62	C
87	FE	65	U
87	FE	67	A
87	FE	71	C
87	FE	72	C
87	FE	73	A

All (55) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	A3	1703	C
3	A3	1805	A
3	A3	1806	U

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Mol	Chain	Res	Type
3	A3	1807	U
3	A3	1809	U
3	A3	1823	A
3	A3	1871	A
3	A3	1901	C
3	A3	1994	A
3	A3	2165	C
3	A3	2172	A
3	A3	2182	G
3	A3	2186	C
3	A3	2243	A
3	A3	2245	A
3	A3	2315	A
3	A3	2374	A
3	A3	2507	A
3	A3	2523	C
3	A3	2530	A
3	A3	2558	A
3	A3	2559	U
3	A3	2628	U
3	A3	2653	C
3	A3	2744	U
3	A3	2757	A
3	A3	2779	C
3	A3	2784	A
3	A3	2788	C
3	A3	2789	C
3	A3	2905	A
3	A3	2989	G
3	A3	3041	U
3	A3	3092	U
3	A3	3123	G
3	A3	3157	C
3	A3	3201	A
3	A3	3206	C
4	B3	1607	U
86	A6	721	G
86	A6	797	C
86	A6	886	A
86	A6	1025	U
86	A6	1034	G
86	A6	1045	A

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Mol	Chain	Res	Type
86	A6	1170	A
86	A6	1193	U
86	A6	1250	U
86	A6	1335	A
86	A6	1419	G
86	A6	1433	C
86	A6	1538	C
86	A6	1541	C
87	24	1	G
87	FE	1	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 138 ligands modelled in this entry, 135 are monoatomic - leaving 3 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	$\# Z > 2$
95	GDP	X6	500	-	29,30,30	1.18	3 (10%)	45,47,47	1.84	8 (17%)
93	SPD	A3	3396	-	9,9,9	0.35	0	8,8,8	0.48	0
91	GCP	r1	801	92	32,34,34	3.34	16 (50%)	49,54,54	4.53	18 (36%)

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
95	GDP	X6	500	-	-	6/16/32/32	0/3/3/3
93	SPD	A3	3396	-	-	6/7/7/7	-
91	GCP	r1	801	92	-	7/19/38/38	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
91	r1	801	GCP	O6-C6	8.71	1.40	1.23
91	r1	801	GCP	C2'-C3'	-8.24	1.31	1.53
91	r1	801	GCP	PB-O3A	6.26	1.65	1.58
91	r1	801	GCP	O4'-C1'	-5.48	1.29	1.42
91	r1	801	GCP	C2-N2	5.21	1.46	1.34
91	r1	801	GCP	PA-O3A	4.53	1.64	1.59
91	r1	801	GCP	O4'-C4'	4.16	1.54	1.45
91	r1	801	GCP	C6-N1	-3.26	1.32	1.38
91	r1	801	GCP	C5'-C4'	-3.12	1.42	1.51
95	X6	500	GDP	C5-C4	3.12	1.47	1.38
91	r1	801	GCP	O3'-C3'	2.98	1.50	1.43
91	r1	801	GCP	C2'-C1'	2.73	1.62	1.53
95	X6	500	GDP	C6-N1	-2.55	1.34	1.38
91	r1	801	GCP	C5-N7	-2.47	1.34	1.39
91	r1	801	GCP	C8-N9	-2.36	1.32	1.37
91	r1	801	GCP	PG-O3G	-2.27	1.49	1.55
91	r1	801	GCP	PB-O2B	-2.20	1.51	1.56
95	X6	500	GDP	C5-N7	-2.19	1.34	1.39
91	r1	801	GCP	PG-O2G	-2.06	1.50	1.55

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
91	r1	801	GCP	O3G-PG-C3B	-16.88	65.45	106.40
91	r1	801	GCP	O3G-PG-O1G	-14.68	74.41	112.39
91	r1	801	GCP	O1G-PG-C3B	12.89	139.50	111.37
91	r1	801	GCP	O3G-PG-O2G	12.39	143.27	107.96
95	X6	500	GDP	C5-C4-N3	-6.35	118.29	128.39
95	X6	500	GDP	C2-N3-C4	5.16	121.19	112.30
91	r1	801	GCP	C5-C4-N3	-4.95	120.51	128.39
95	X6	500	GDP	N9-C4-N3	4.69	135.33	125.95
91	r1	801	GCP	C2-N3-C4	4.32	119.74	112.30
91	r1	801	GCP	C4'-O4'-C1'	-4.26	100.05	109.47
91	r1	801	GCP	PB-O3A-PA	-3.93	119.55	132.37
91	r1	801	GCP	C6-C5-N7	3.35	136.38	130.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
91	r1	801	GCP	N9-C4-N3	3.16	132.28	125.95
95	X6	500	GDP	C6-C5-N7	3.10	135.94	130.29
91	r1	801	GCP	C2-N1-C6	-2.89	119.88	125.11
91	r1	801	GCP	N9-C8-N7	-2.80	108.20	113.40
91	r1	801	GCP	C8-N7-C5	2.77	109.20	104.26
91	r1	801	GCP	C4-C5-N7	-2.73	106.34	110.67
91	r1	801	GCP	C3'-C2'-C1'	2.70	106.58	101.46
91	r1	801	GCP	C5-C6-N1	2.69	120.11	113.25
95	X6	500	GDP	C3'-C2'-C1'	2.67	106.51	101.46
91	r1	801	GCP	O6-C6-C5	-2.60	119.68	126.53
95	X6	500	GDP	C4-C5-N7	-2.49	106.73	110.67
95	X6	500	GDP	O4'-C1'-N9	2.40	113.79	108.36
91	r1	801	GCP	O2G-PG-O1G	-2.33	106.37	112.39
95	X6	500	GDP	O6-C6-C5	-2.07	121.07	126.53

There are no chirality outliers.

All (19) torsion outliers are listed below:

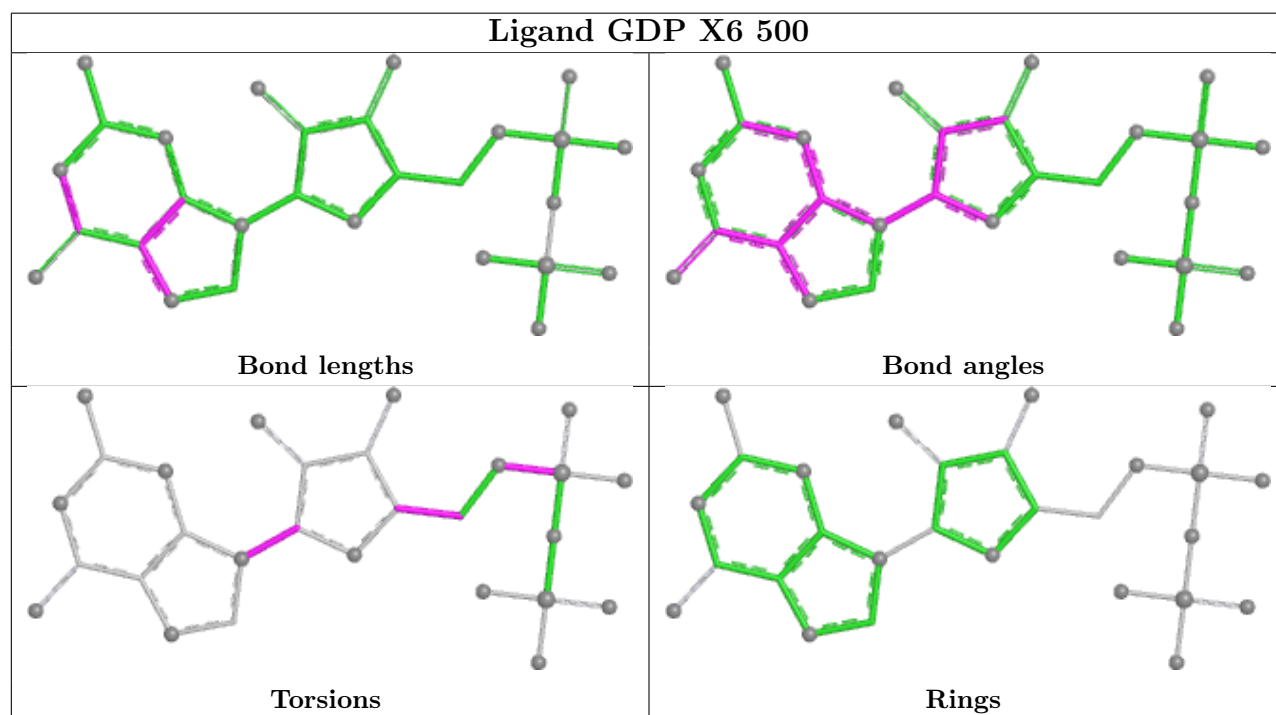
Mol	Chain	Res	Type	Atoms
91	r1	801	GCP	PG-C3B-PB-O1B
91	r1	801	GCP	PG-C3B-PB-O2B
91	r1	801	GCP	PG-C3B-PB-O3A
91	r1	801	GCP	C5'-O5'-PA-O1A
95	X6	500	GDP	C5'-O5'-PA-O3A
95	X6	500	GDP	C5'-O5'-PA-O1A
95	X6	500	GDP	C3'-C4'-C5'-O5'
95	X6	500	GDP	O4'-C1'-N9-C8
93	A3	3396	SPD	N6-C7-C8-C9
93	A3	3396	SPD	C3-C4-C5-N6
95	X6	500	GDP	O4'-C4'-C5'-O5'
95	X6	500	GDP	O4'-C1'-N9-C4
93	A3	3396	SPD	C8-C7-N6-C5
91	r1	801	GCP	O4'-C4'-C5'-O5'
91	r1	801	GCP	C3'-C4'-C5'-O5'
93	A3	3396	SPD	N1-C2-C3-C4
93	A3	3396	SPD	C7-C8-C9-N10
91	r1	801	GCP	C4'-C5'-O5'-PA
93	A3	3396	SPD	C2-C3-C4-C5

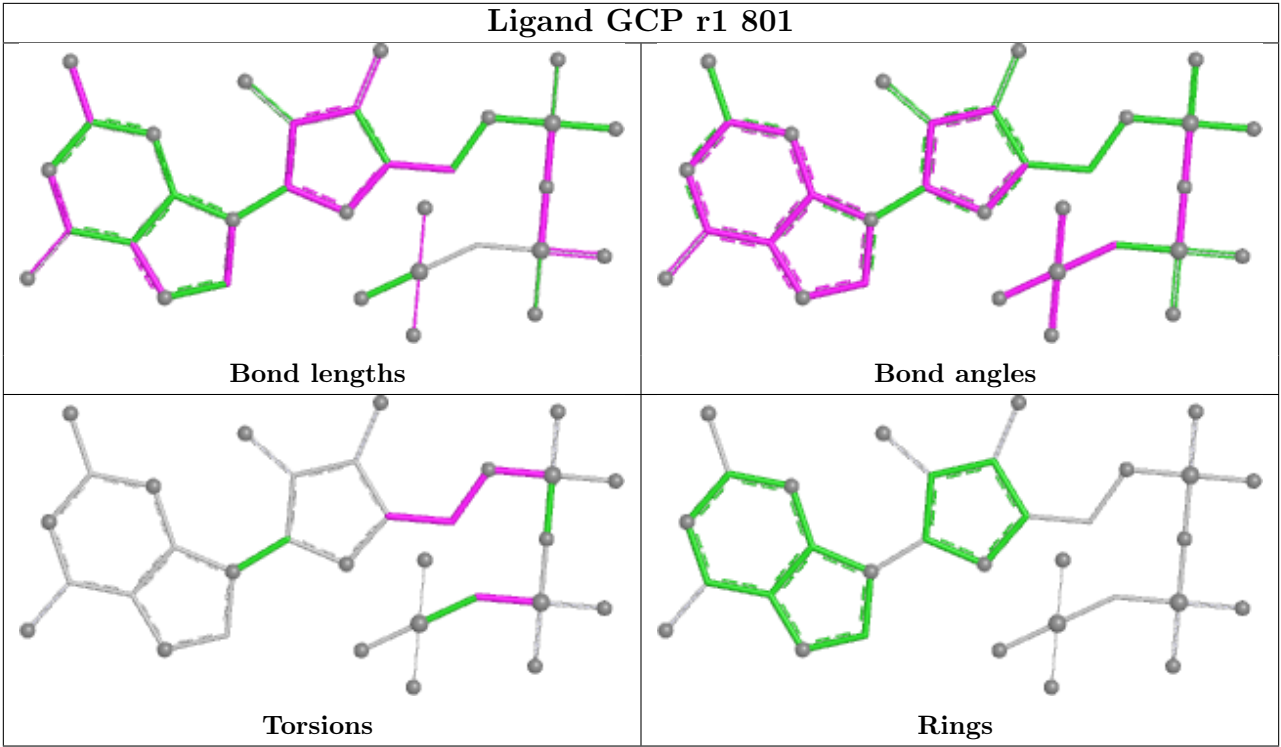
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
95	X6	500	GDP	1	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
13	M3	1
25	Y3	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M3	61:THR	C	62:ARG	N	1.19
1	Y3	123:ARG	C	124:LEU	N	1.19

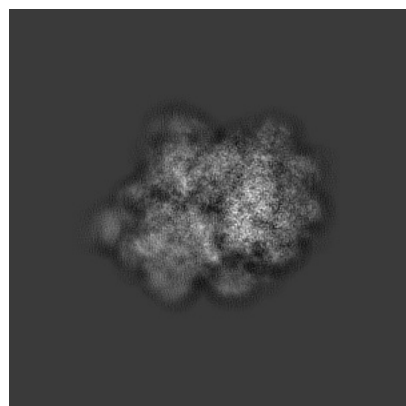
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11646. These allow visual inspection of the internal detail of the map and identification of artifacts.

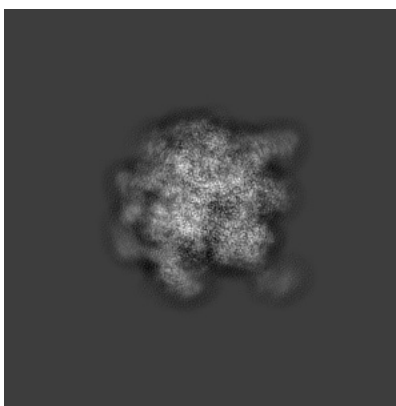
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

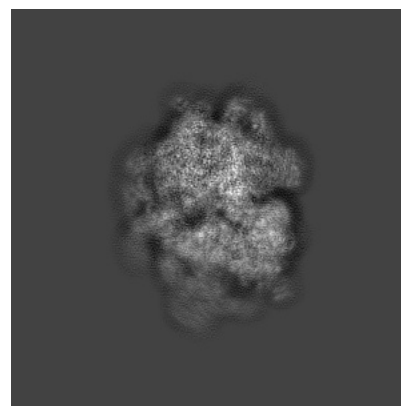
6.1.1 Primary map



X

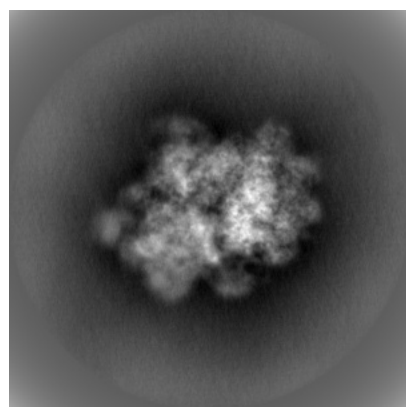


Y

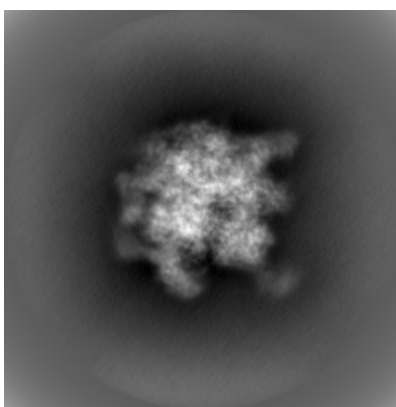


Z

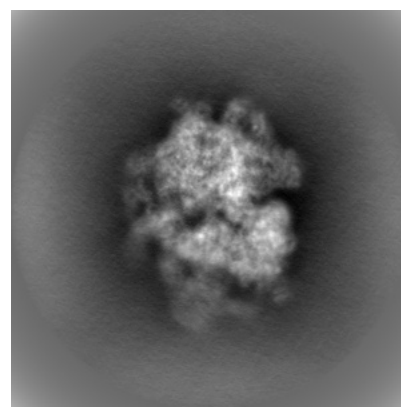
6.1.2 Raw map



X



Y

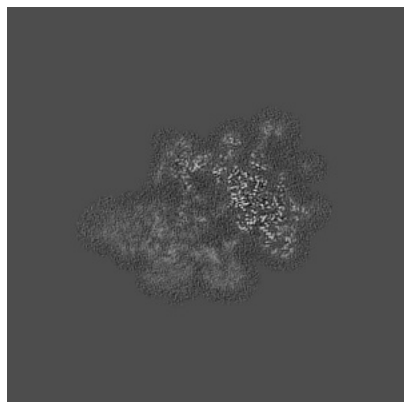


Z

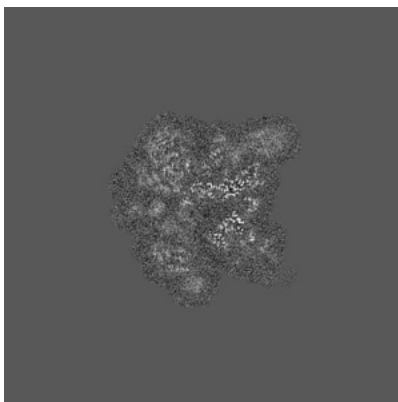
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

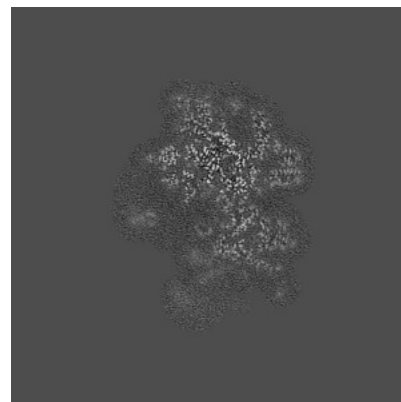
6.2.1 Primary map



X Index: 256

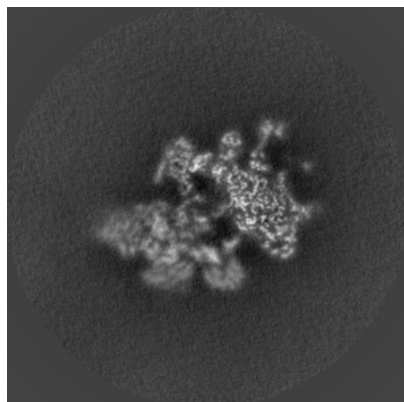


Y Index: 256

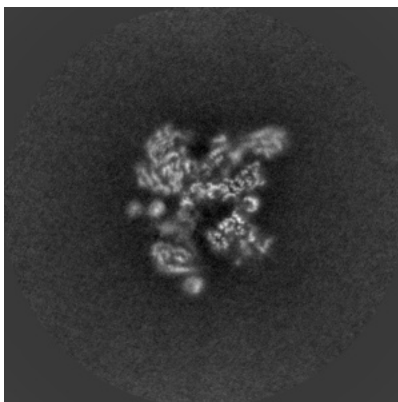


Z Index: 256

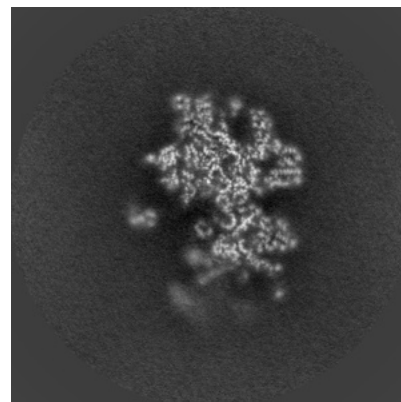
6.2.2 Raw map



X Index: 256



Y Index: 256

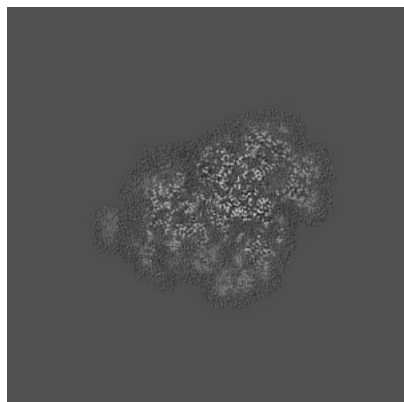


Z Index: 256

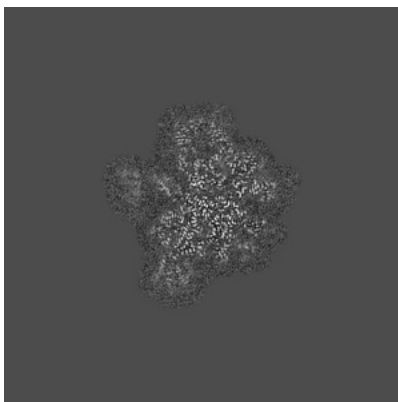
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

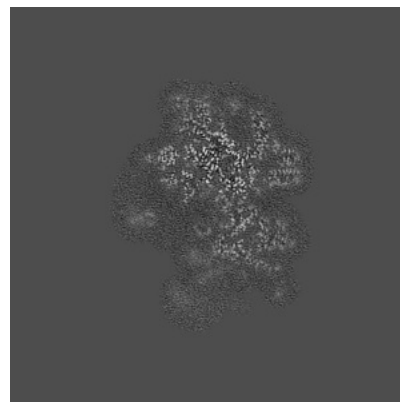
6.3.1 Primary map



X Index: 286

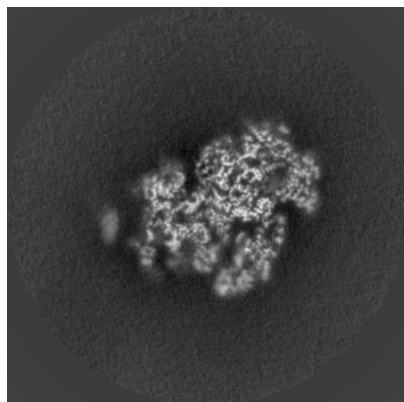


Y Index: 305

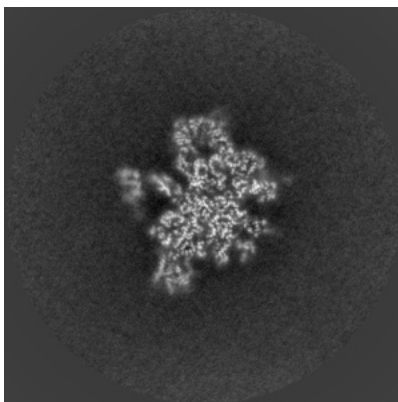


Z Index: 256

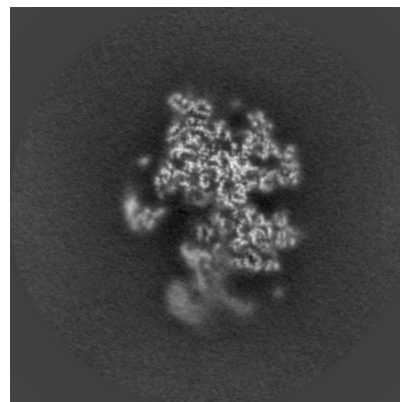
6.3.2 Raw map



X Index: 286



Y Index: 305

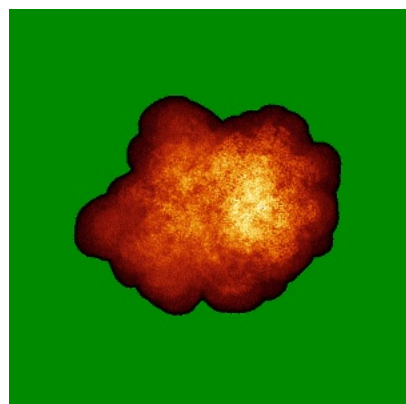


Z Index: 247

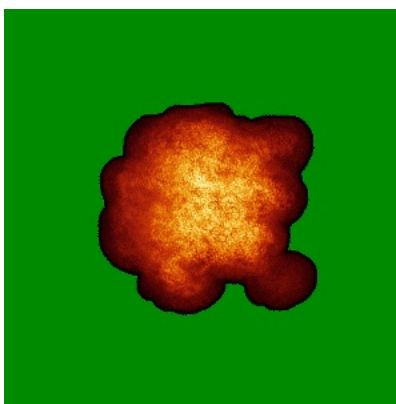
The images above show the largest variance slices of the map in three orthogonal directions.

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

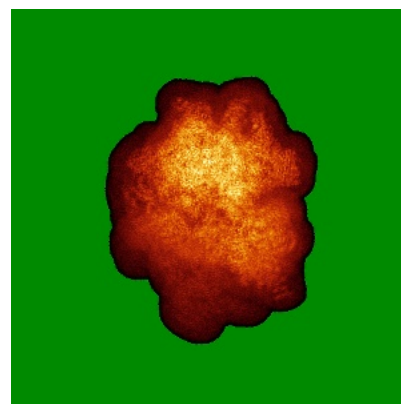
6.4.1 Primary map



X

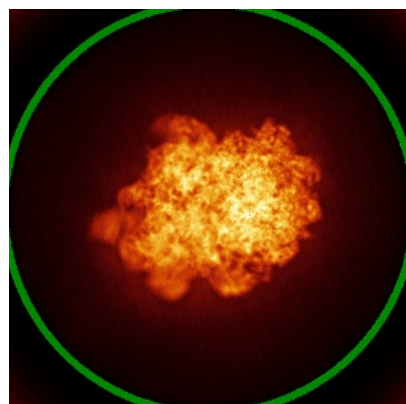


Y

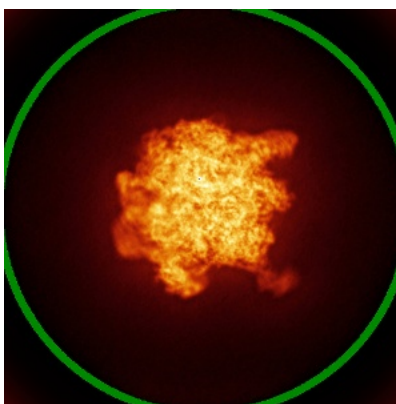


Z

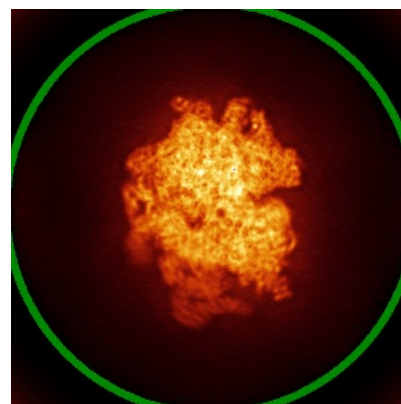
6.4.2 Raw map



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](#)

This section was not generated.

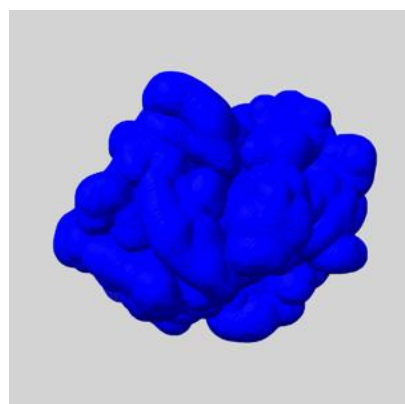
6.6 Mask visualisation [i](#)

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

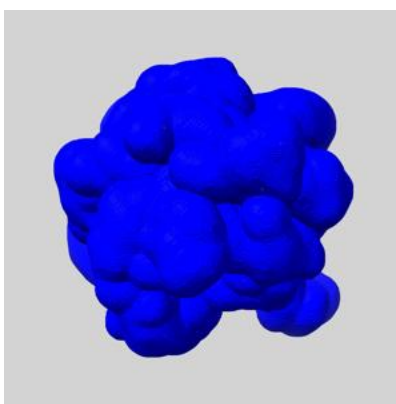
A mask typically either:

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

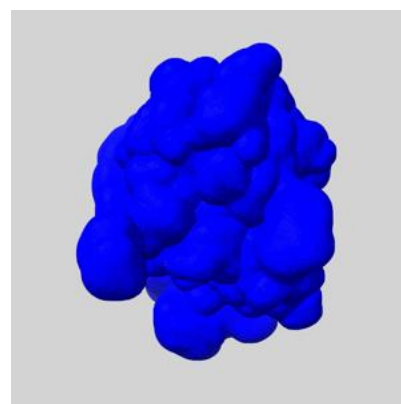
6.6.1 emd_11646_msk_1.map [i](#)



X



Y

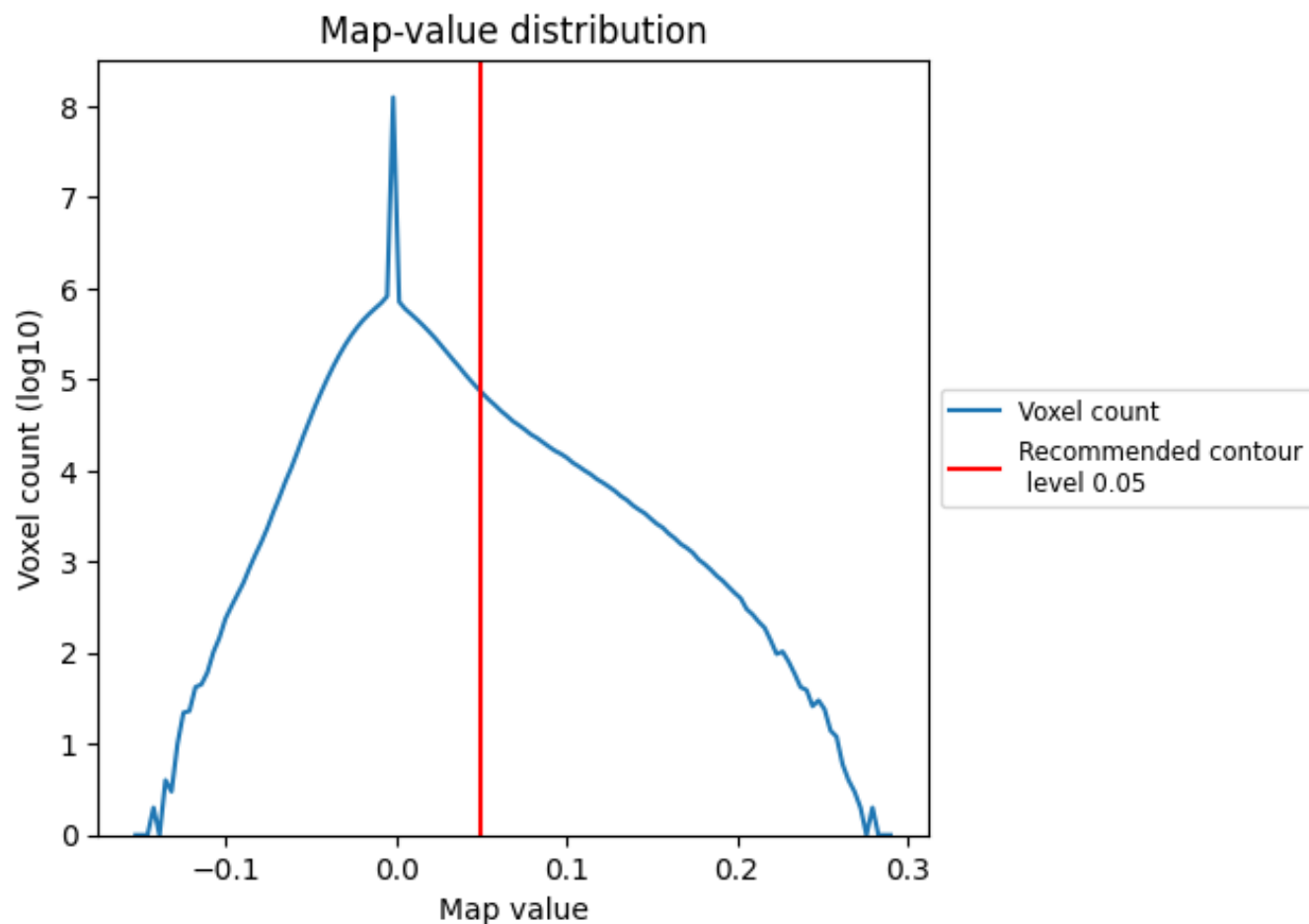


Z

7 Map analysis [i](#)

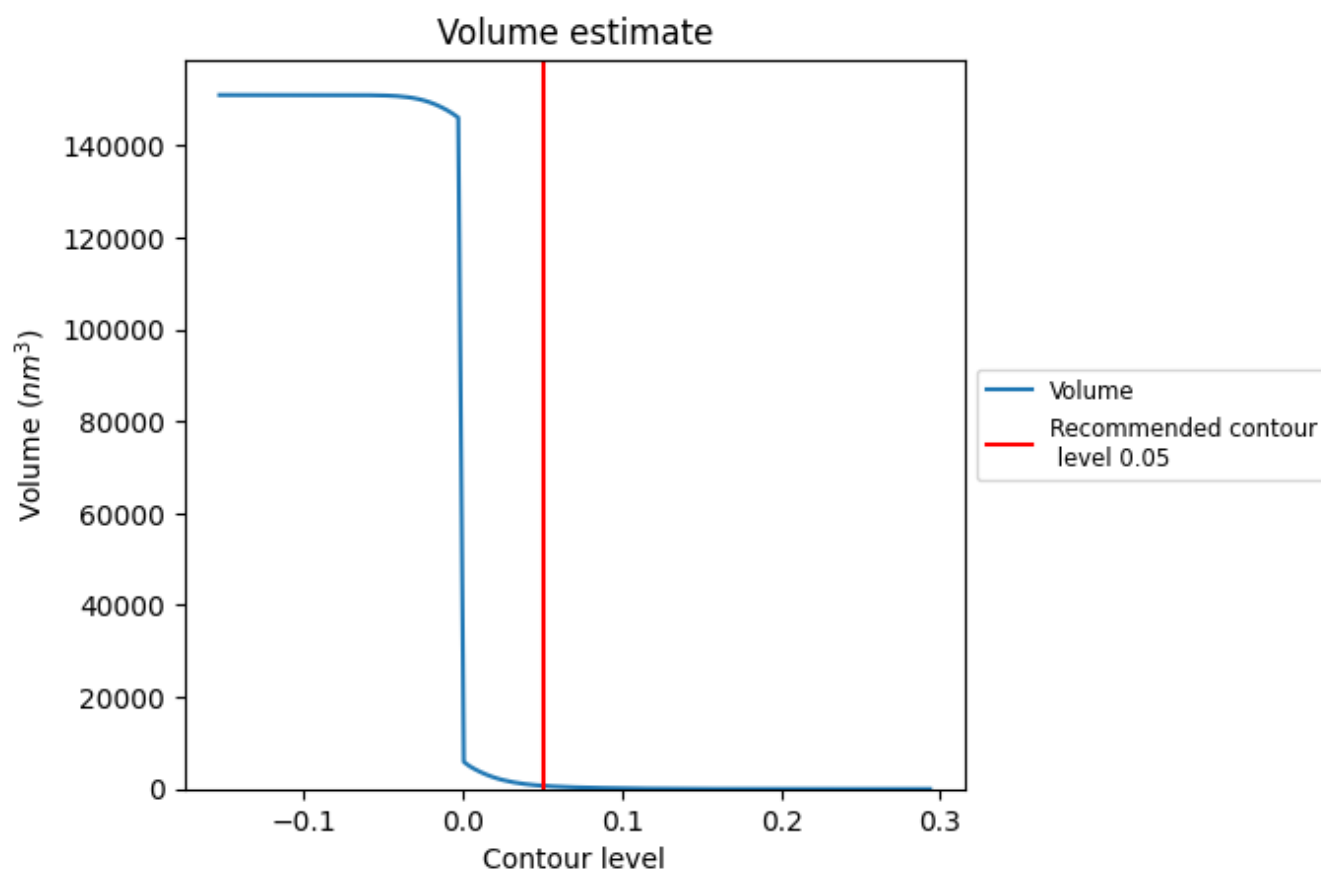
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

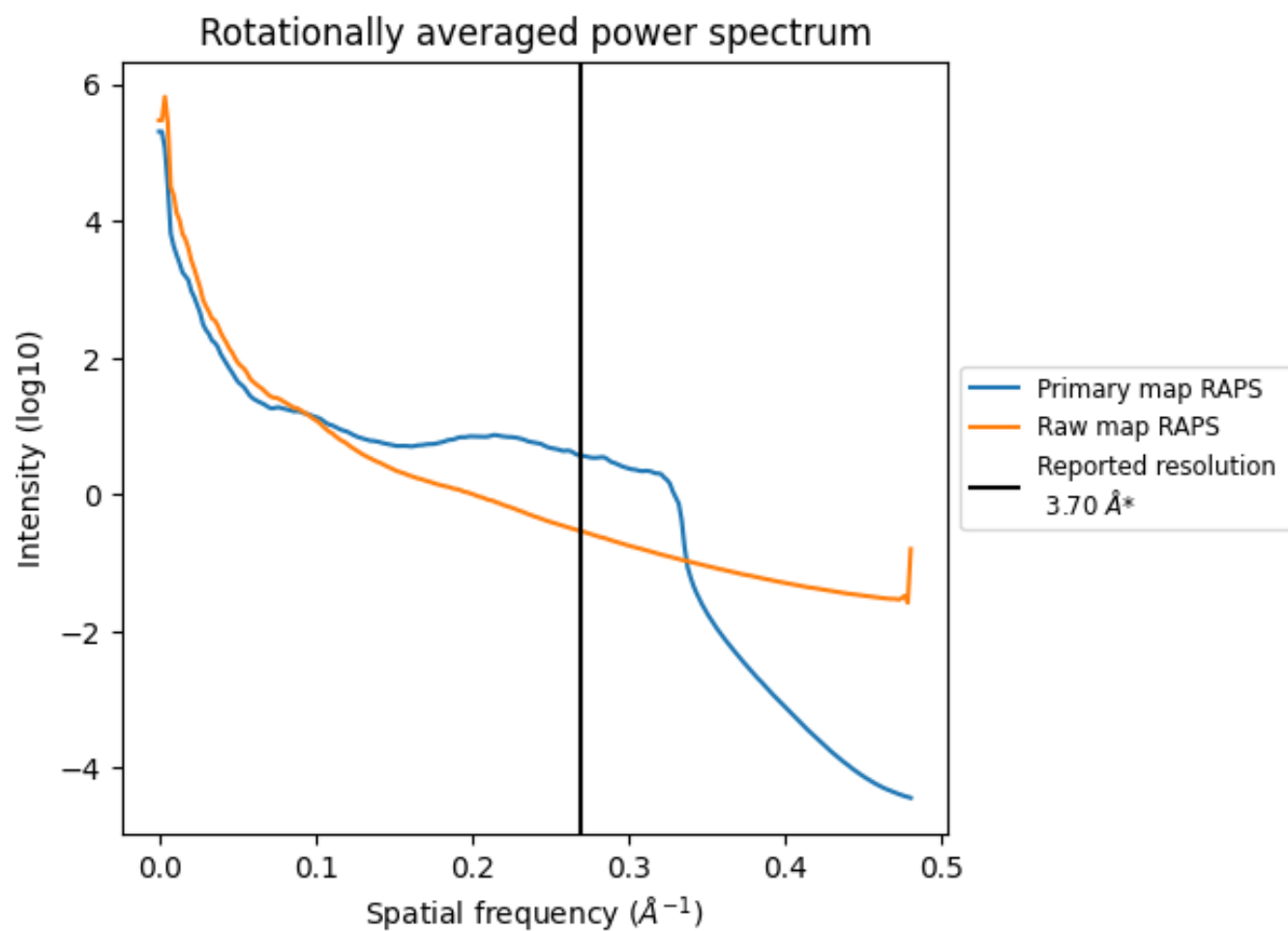
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 706 nm^3 ; this corresponds to an approximate mass of 638 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 ⓘ

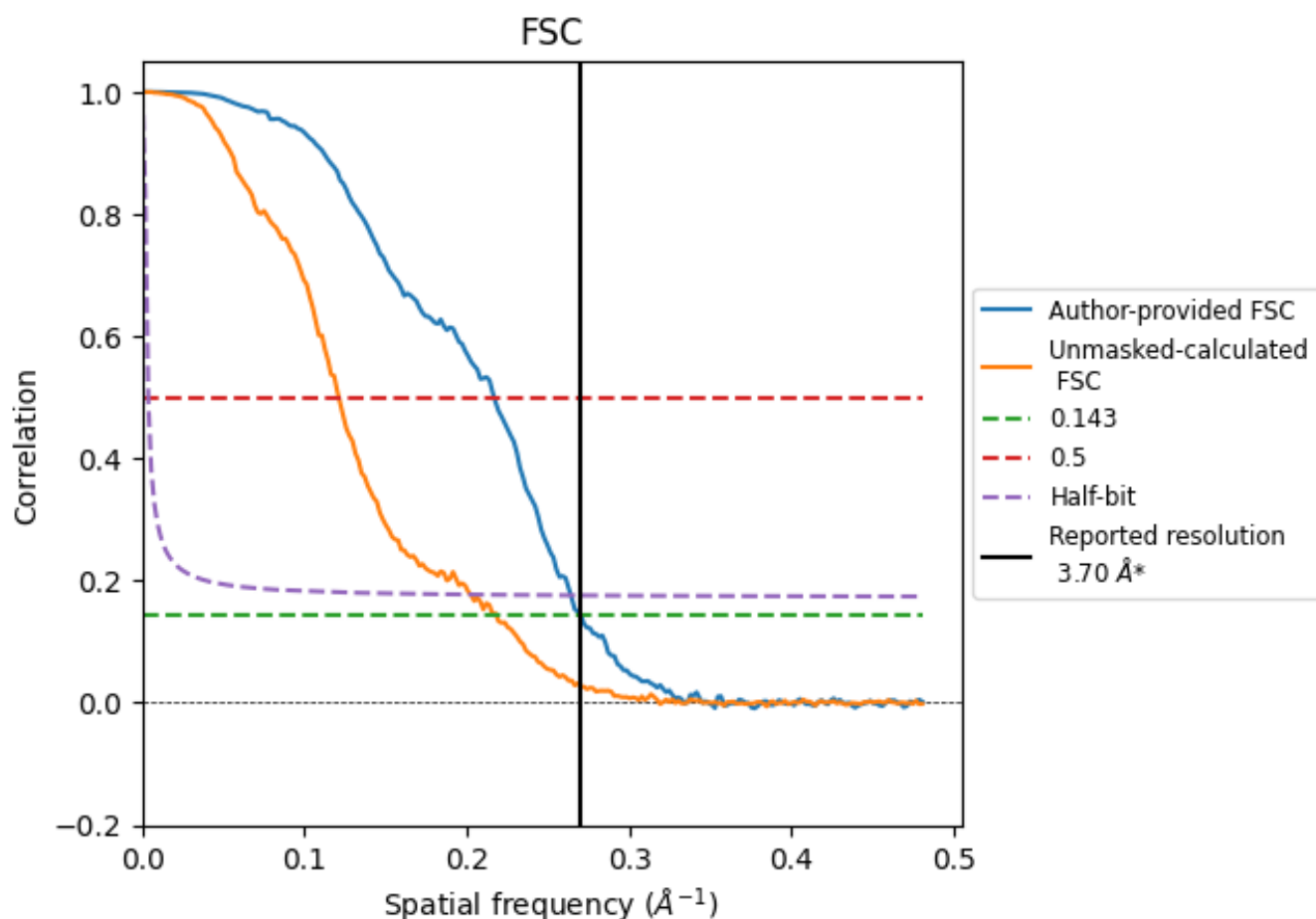


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.270 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

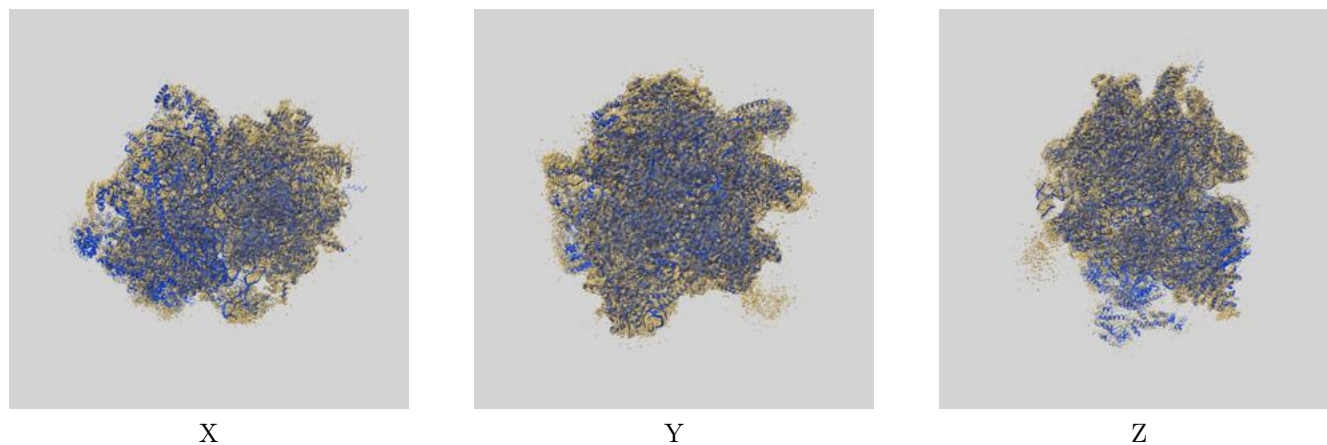
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.70	4.61	3.78
Unmasked-calculated*	4.58	8.26	4.94

*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 4.58 differs from the reported value 3.7 by more than 10 %

9 Map-model fit [i](#)

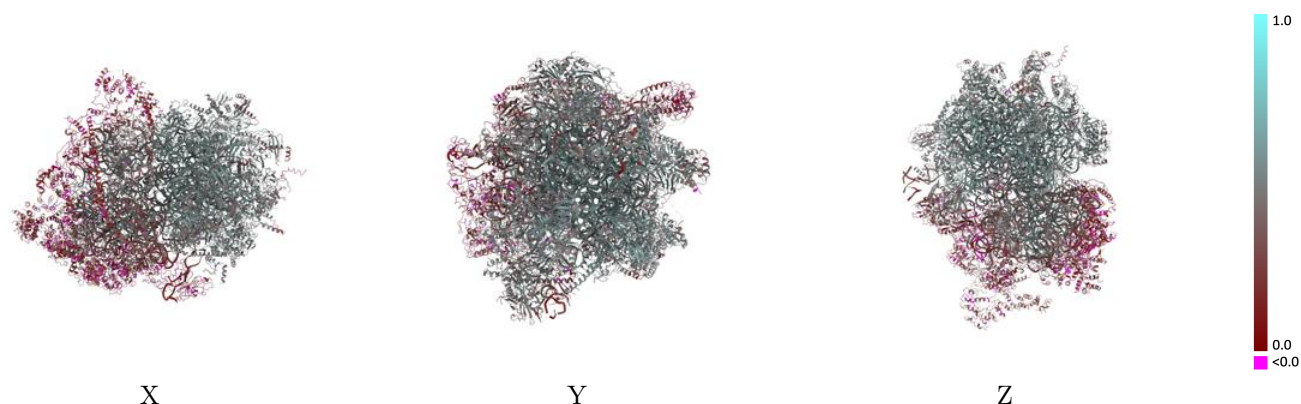
This section contains information regarding the fit between EMDB map EMD-11646 and PDB model 7A5K. Per-residue inclusion information can be found in [section 3](#) on [page 23](#).

9.1 Map-model overlay [i](#)



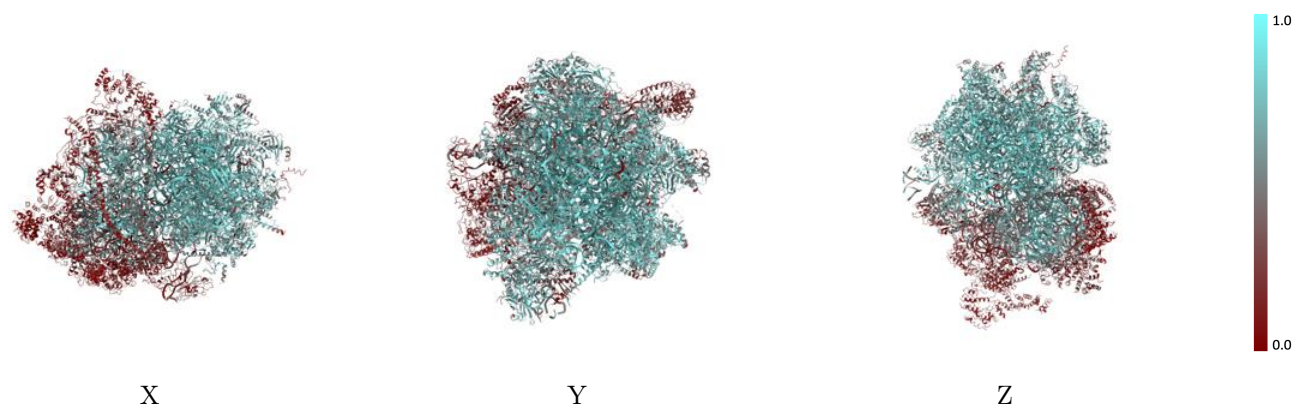
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



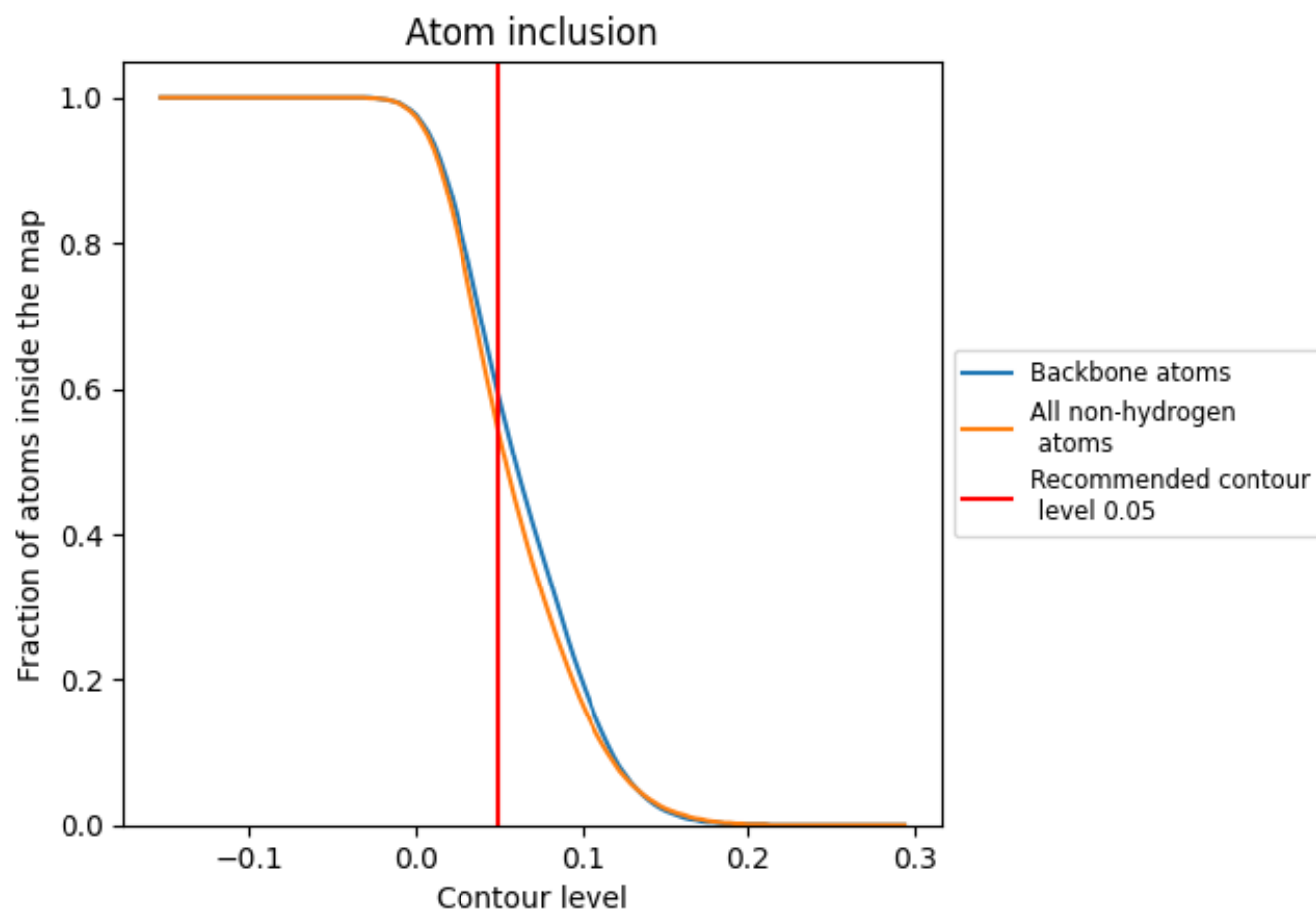
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 59% of all backbone atoms, 54% 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	 0.5400	 0.4080
03	 0.6660	 0.5020
13	 0.6710	 0.5060
23	 0.7890	 0.5720
24	 0.1140	 0.2090
33	 0.7810	 0.5610
43	 0.7850	 0.5670
53	 0.6440	 0.4830
63	 0.6390	 0.4690
73	 0.6060	 0.4670
8	 0.1490	 0.2980
93	 0.6360	 0.4920
A	 0.2200	 0.2810
A3	 0.8370	 0.5250
A5	 0.0000	 0.1500
A6	 0.5830	 0.3810
B	 0.3000	 0.2660
B3	 0.6330	 0.3450
B6	 0.3390	 0.2780
C6	 0.0750	 0.2080
D	 0.2000	 0.1820
D3	 0.6720	 0.5180
D6	 0.3430	 0.3350
E3	 0.7270	 0.5350
E6	 0.2540	 0.3260
F3	 0.7220	 0.5300
F6	 0.0370	 0.1600
FE	 0.2860	 0.1670
G6	 0.1460	 0.2350
H3	 0.5830	 0.4720
H6	 0.0960	 0.2350
I3	 0.4940	 0.4020
I6	 0.2780	 0.2790
J3	 0.3240	 0.2230
J6	 0.5640	 0.4780



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Chain	Atom inclusion	Q-score
K3	 0.7540	 0.5410
K6	 0.1150	 0.2420
L3	 0.6370	 0.5200
L6	 0.3700	 0.3710
M3	 0.7180	 0.5220
M6	 0.3200	 0.2340
N3	 0.7010	 0.5390
N6	 0.4550	 0.3900
O3	 0.7110	 0.5300
O6	 0.2780	 0.2210
P3	 0.6710	 0.5040
P6	 0.2850	 0.3080
Q3	 0.6370	 0.5090
Q6	 0.4080	 0.3860
R3	 0.7290	 0.5440
R6	 0.1850	 0.1630
S3	 0.7250	 0.5330
S6	 0.2380	 0.2250
T3	 0.7150	 0.5450
T6	 0.3370	 0.2540
U3	 0.7560	 0.5250
U6	 0.2360	 0.2430
V3	 0.5650	 0.4560
V6	 0.1580	 0.1990
W3	 0.7370	 0.5490
W6	 0.1950	 0.2390
X3	 0.6320	 0.4940
X6	 0.0480	 0.1740
Y2	 0.1660	 0.3110
Y3	 0.6990	 0.5070
Y6	 0.0630	 0.1760
Z3	 0.7310	 0.5420
Z6	 0.0770	 0.1940
a3	 0.7130	 0.5240
a6	 0.2410	 0.2380
b3	 0.7140	 0.5250
b6	 0.0750	 0.1920
c3	 0.6530	 0.4930
c6	 0.2300	 0.2880
d3	 0.5690	 0.4410
d6	 0.5450	 0.4610
e3	 0.2200	 0.2680

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Chain	Atom inclusion	Q-score
e6	 0.0490	 0.2010
f3	 0.3720	 0.3680
g3	 0.6990	 0.5070
h3	 0.5670	 0.4430
i3	 0.7470	 0.5450
j3	 0.6660	 0.4960
k3	 0.4540	 0.3670
l3	 0.7140	 0.5040
m3	 0.3600	 0.3560
n	 0.0910	 0.1670
o3	 0.7550	 0.5390
p3	 0.5770	 0.4600
q3	 0.5620	 0.4570
r1	 0.4440	 0.3990
r3	 0.7460	 0.5270
s3	 0.6870	 0.5100
u3	 0.8570	 0.5160