Full wwPDB EM Validation Report ⓘ

Oct 24, 2026 – 11:28 am BST

PDB ID	:	9TS7 / pdb_00009ts7
EMDB ID	:	EMD-56210
Title	:	Structure of the Plant mitochondrial initiation complex, (SSU, LSU, initiator tRNA, mRNA)
Authors	:	Skaltsogiannis, V.; Giege, P.; Soufari, H.
Deposited on	:	2025-12-29
Resolution	:	2.92 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:

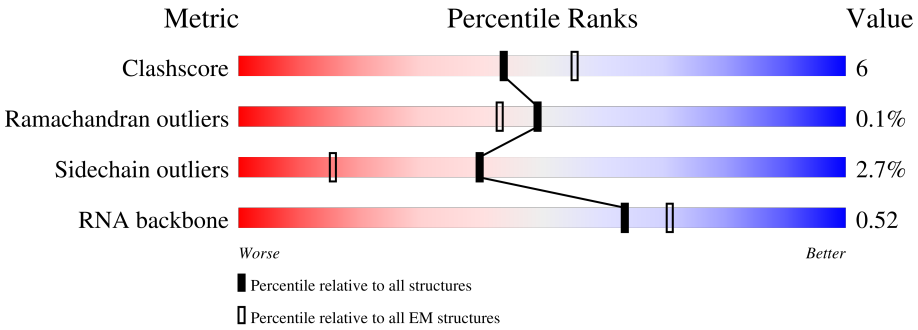
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)	:	2.51

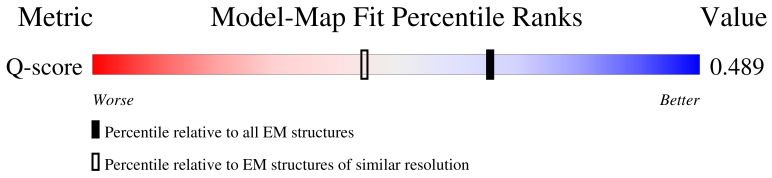
1 Overall quality at a glance

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

The reported resolution of this entry is 2.92 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	13007 (2.42 - 3.42)

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 <=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	1	2923	17% 64% 32% 5%
2	1B	217	6% 73% 7% • 18%
3	1C	286	40% 64% 10% 25%

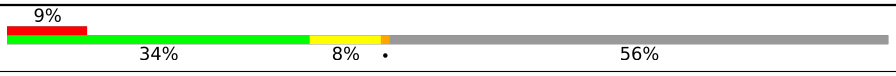
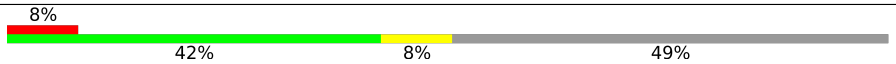
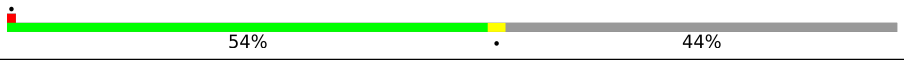
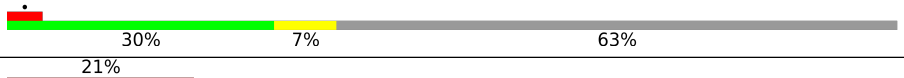
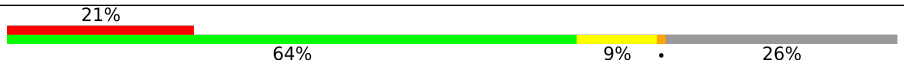
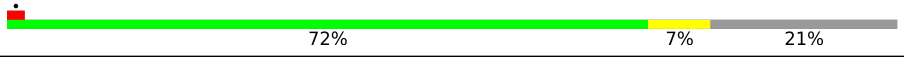
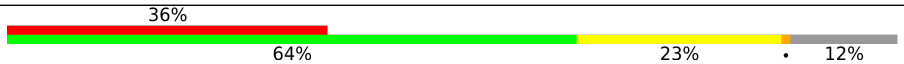
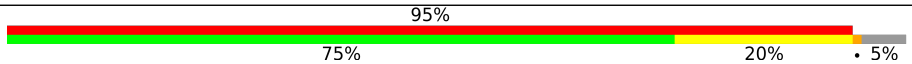
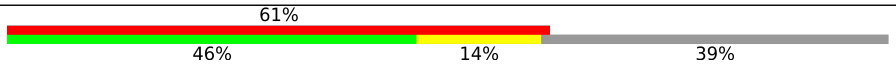
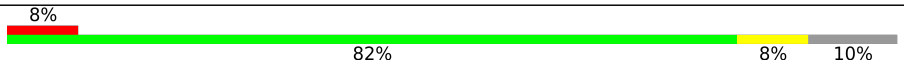
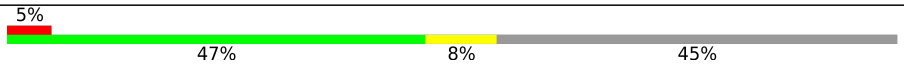
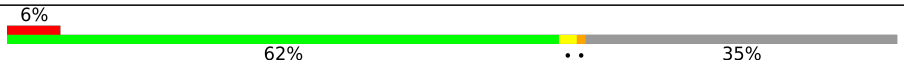
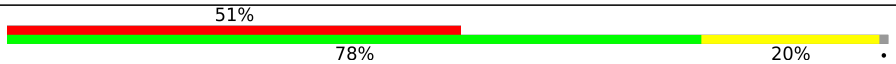
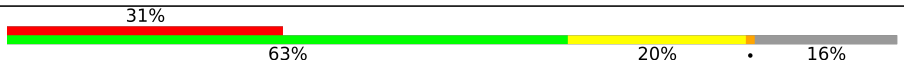
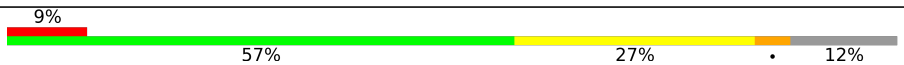
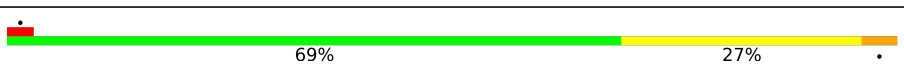
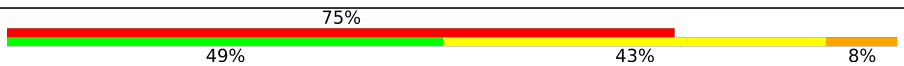
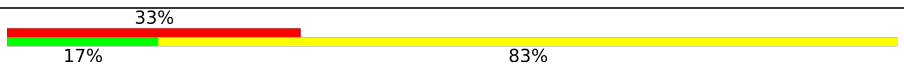
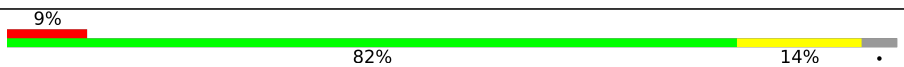
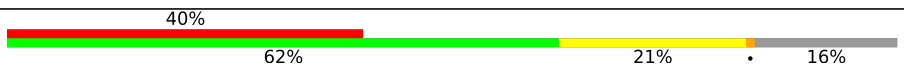
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Mol	Chain	Length	Quality of chain
4	1D	319	73% 10% 17%
5	1E	296	69% 6% 25%
6	1F	185	14% 66% 18% 15%
7	1G	102	88% 87% 9%
8	1H	220	6% 24% 6% 70%
9	1I	170	76% 53% 22% 24%
10	1J	156	94% 69% 26% 6%
11	1K	204	10% 83% 10% 7%
12	1L	176	62% 10% 28%
13	1M	281	66% 8% 25%
14	1N	179	21% 69% 13% 17%
15	1O	160	84% 10% 6%
16	1P	114	82% 17%
17	1Q	233	46% 6% 48%
18	1R	126	78% 10% 13%
19	1S	270	49% 5% 46%
20	1T	264	53% 5% 41%
21	1U	180	7% 64% 8% 28%
22	1V	159	89% 11%
23	1W	238	85% 63% 23% 14%
24	1X	271	18% 68% 11% 20%
25	1Y	156	8% 54% 8% 37%
26	1Z	215	32% 70% 12% 18%
27	1a	144	65% 11% 24%
28	1b	109	85% 6% 8%

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Mol	Chain	Length	Quality of chain
29	1c	135	
30	1d	139	
31	1e	106	
32	1f	146	
33	1g	162	
34	1h	103	
35	1i	247	
36	1j	90	
37	1k	119	
38	1l	239	
39	1m	128	
40	1o	125	
41	1p	130	
42	1q	78	
43	1r	167	
44	1s	181	
45	1t	491	
46	1u	751	
47	1v	514	
48	2	1766	
49	3	118	
50	5	77	
51	6	6	
52	A	212	
53	B	554	

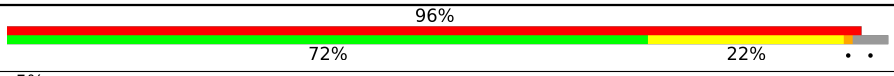
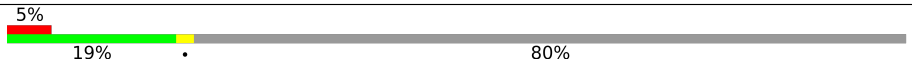
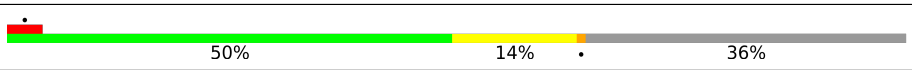
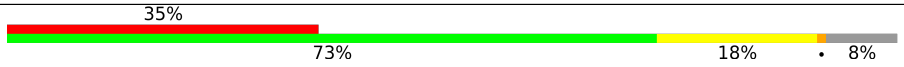
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Mol	Chain	Length	Quality of chain
54	C	362	11% 69% 22% 8%
55	D	501	26% 68% 14% 17%
56	E	138	63% 10% 27%
57	F	157	96% 78% 22%
58	G	129	88% 11%
59	H	383	16% 43% 12% 44%
60	I	228	36% 13% 50%
61	J	304	7% 34% 8% 58%
62	K	125	7% 78% 21%
63	L	154	10% 64% 13% 23%
64	M	155	55% 9% 35%
65	N	414	24% 72%
66	O	136	65% 15% 19%
67	P	110	10% 76% 6% 17%
68	Q	237	33% 5% 62%
69	R	212	50% 65% 13% 22%
70	S	100	20% 57% 18% 25%
71	T	94	46% 7% 47%
72	U	192	43% 51% 15% 34%
73	V	193	13% 68% 16% 15%
74	W	483	24% 63% 16% 21%
75	X	496	18% 30% 10% 59%
76	Y	102	21% 74% 20%
77	Z	153	20% 39% 13% 48%
78	a	424	40% 57% 16% 26%

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Mol	Chain	Length	Quality of chain
79	b	80	
80	c	128	
81	d	110	
82	e	383	
83	f	410	
84	h	384	
85	i	725	
86	k	153	

2 Entry composition (i)

There are 91 unique types of molecules in this entry. The entry contains 207751 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 RNA chain called 26S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	2922	62518	27942	11365	20289	2922	5	0

- Molecule 2 is a protein called Large ribosomal subunit protein uL2 C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1B	177	1325	819	259	233	14	0	0

- Molecule 3 is a protein called uL2m N-ter mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	1C	215	1696	1078	316	296	6	0	0

- Molecule 4 is a protein called 50S ribosomal protein L3-2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	1D	264	2045	1309	367	358	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	1E	221	1753	1104	334	308	7	0	0

- Molecule 6 is a protein called Large ribosomal subunit protein uL5m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	1F	158	1286	829	212	236	9	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1F	12	LEU	SER	conflict	UNP A0A068BF07
1F	16	LEU	PRO	conflict	UNP A0A068BF07
1F	20	LEU	PRO	conflict	UNP A0A068BF07
1F	22	TYR	HIS	conflict	UNP A0A068BF07
1F	31	LEU	SER	conflict	UNP A0A068BF07
1F	57	CYS	ARG	conflict	UNP A0A068BF07
1F	106	LEU	SER	conflict	UNP A0A068BF07
1F	110	LEU	SER	conflict	UNP A0A068BF07
1F	160	ILE	VAL	conflict	UNP A0A068BF07
1F	171	LEU	PRO	conflict	UNP A0A068BF07

- Molecule 7 is a protein called Large ribosomal subunit protein uL6 alpha-beta domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	1G	98	Total	C	N	O	S	0	0
			779	508	136	130	5		

- Molecule 8 is a protein called Large ribosomal subunit protein bL9c.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	1H	66	Total	C	N	O	S	0	0
			539	345	98	94	2		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1H	19	THR	LYS	conflict	UNP A0A0D3EAI8
1H	24	THR	SER	conflict	UNP A0A0D3EAI8
1H	69	PHE	LEU	conflict	UNP A0A0D3EAI8
1H	99	TYR	PHE	conflict	UNP A0A0D3EAI8
1H	104	GLU	VAL	conflict	UNP A0A0D3EAI8
1H	105	GLU	VAL	conflict	UNP A0A0D3EAI8
1H	106	VAL	HIS	conflict	UNP A0A0D3EAI8
1H	108	SER	THR	conflict	UNP A0A0D3EAI8
1H	160	ILE	LEU	conflict	UNP A0A0D3EAI8
1H	173	ASP	ASN	conflict	UNP A0A0D3EAI8
1H	184	ALA	THR	conflict	UNP A0A0D3EAI8
1H	212	VAL	LEU	conflict	UNP A0A0D3EAI8

- Molecule 9 is a protein called Large ribosomal subunit protein uL10c.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	1I	130	Total	C	N	O	S	0	0
			1036	669	178	184	5		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1I	118	LYS	GLU	conflict	UNP A0A0D3AE97
1I	124	GLN	LYS	conflict	UNP A0A0D3AE97

- Molecule 10 is a protein called Large ribosomal subunit protein uL11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	1J	147	Total	C	N	O	S	0	0
			1129	722	193	205	9		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1J	78	SER	THR	conflict	UNP A0A3P6F9L4
1J	79	VAL	PHE	conflict	UNP A0A3P6F9L4
1J	83	THR	SER	conflict	UNP A0A3P6F9L4

- Molecule 11 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	1K	189	Total	C	N	O	S	0	0
			1526	955	299	265	7		

- Molecule 12 is a protein called uL14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1L	127	Total	C	N	O	S	0	0
			966	609	184	168	5		

- Molecule 13 is a protein called Large ribosomal subunit protein uL15/eL18 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	1M	210	Total	C	N	O	S	0	0
			1649	1052	321	273	3		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1M	46	SER	PRO	conflict	UNP A0A0D3BF13
1M	58	ILE	MET	conflict	UNP A0A0D3BF13
1M	127	LYS	ASN	conflict	UNP A0A0D3BF13
1M	249	LEU	GLN	conflict	UNP A0A0D3BF13
1M	280	GLU	GLY	conflict	UNP A0A0D3BF13

- Molecule 14 is a protein called Large ribosomal subunit protein uL16m|.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	1N	148	Total	C	N	O	S	0	0
			1160	731	230	192	7		

- Molecule 15 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	1O	151	Total	C	N	O	S	0	0
			1231	767	244	214	6		

- Molecule 16 is a protein called Ribosomal protein L18e/L15P domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	1P	113	Total	C	N	O	S	0	0
			878	564	160	149	5		

- Molecule 17 is a protein called bL19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	1Q	122	Total	C	N	O	S	0	0
			1008	641	198	166	3		

- Molecule 18 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	1R	110	Total	C	N	O	S	0	0
			915	572	184	154	5		

- Molecule 19 is a protein called bL21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	1S	145	Total	C	N	O	S	0	0
			1170	750	207	211	2		

- Molecule 20 is a protein called Large ribosomal subunit protein uL22c.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	1T	155	Total	C	N	O	S	0	0
			1241	782	249	205	5		

- Molecule 21 is a protein called Large ribosomal subunit protein uL23m.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	1U	130	Total	C	N	O	S	0	0
			1048	675	190	181	2		

- Molecule 22 is a protein called KOW domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	1V	158	Total	C	N	O	S	0	0
			1223	770	229	220	4		

- Molecule 23 is a protein called bL25-2m.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	1W	205	Total	C	N	O	S	0	0
			1588	1006	284	294	4		

- Molecule 24 is a protein called bL25m.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	1X	216	Total	C	N	O	S	0	0
			1670	1069	298	302	1		

- Molecule 25 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	1Y	98	Total	C	N	O	S	0	0
			768	484	152	131	1		

- Molecule 26 is a protein called Large ribosomal subunit protein bL28m.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	1Z	177	Total	C	N	O	S	0	0
			1441	911	266	255	9		

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1Z	20	ASN	THR	conflict	UNP A0A3P6BNQ4
1Z	21	ILE	LEU	conflict	UNP A0A3P6BNQ4
1Z	27	GLU	GLY	conflict	UNP A0A3P6BNQ4
1Z	36	THR	SER	conflict	UNP A0A3P6BNQ4
1Z	87	SER	ARG	conflict	UNP A0A3P6BNQ4
1Z	126	TYR	PHE	conflict	UNP A0A3P6BNQ4
1Z	133	ALA	GLN	conflict	UNP A0A3P6BNQ4
1Z	148	PRO	ALA	conflict	UNP A0A3P6BNQ4
1Z	154	LEU	PHE	conflict	UNP A0A3P6BNQ4
1Z	174	ARG	LYS	conflict	UNP A0A3P6BNQ4
1Z	175	THR	GLU	conflict	UNP A0A3P6BNQ4
1Z	176	PHE	ALA	conflict	UNP A0A3P6BNQ4
1Z	178	LYS	ARG	conflict	UNP A0A3P6BNQ4

- Molecule 27 is a protein called Cation-transporting P-type ATPase N-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	1a	110	Total	C	N	O	S	0	0
			928	588	172	158	10		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1a	24	THR	ALA	conflict	UNP A0A3P6EWC5
1a	143	GLY	ALA	conflict	UNP A0A3P6EWC5

- Molecule 28 is a protein called Large ribosomal subunit protein uL30m.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	1b	100	Total	C	N	O	S	0	0
			803	504	160	134	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1b	17	GLN	GLU	conflict	UNP A0A0D3EB87

- Molecule 29 is a protein called bL31m.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	1c	59	Total	C	N	O	S	0	0
			489	313	98	73	5		

- Molecule 30 is a protein called Large ribosomal subunit protein bL32m.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	1d	49	Total	C	N	O	S	0	0
			379	240	80	55	4		

- Molecule 31 is a protein called bL33m.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	1e	54	Total	C	N	O	S	0	0
			459	300	85	72	2		

- Molecule 32 is a protein called Large ribosomal subunit protein bL34m.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	1f	44	Total	C	N	O	0	0
			364	224	88	52		

- Molecule 33 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	1g	91	Total	C	N	O	S	0	0
			770	496	152	119	3		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1g	30	ILE	LEU	conflict	UNP A0A0D3AUD0
1g	54	ARG	THR	conflict	UNP A0A0D3AUD0
1g	127	ASP	TYR	conflict	UNP A0A0D3AUD0

- Molecule 34 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	1h	38	Total	C	N	O	S	0	0
			309	190	65	49	5		

- Molecule 35 is a protein called mL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	1i	183	Total	C	N	O	S	0	0
			1424	885	255	274	10		

- Molecule 36 is a protein called 39S ribosomal protein L41-A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	1j	71	Total	C	N	O	S	0	0
			570	369	102	97	2		

- Molecule 37 is a protein called Large ribosomal subunit protein mL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	1k	118	Total	C	N	O	S	0	0
			952	599	184	165	4		

- Molecule 38 is a protein called Large ribosomal subunit protein mL46.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	1l	211	Total	C	N	O	S	0	0
			1741	1131	286	316	8		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1l	25	ASP	GLU	conflict	UNP A0A0D3B6Y5
1l	126	LYS	GLU	conflict	UNP A0A0D3B6Y5
1l	154	VAL	LEU	conflict	UNP A0A0D3B6Y5
1l	179	MET	THR	conflict	UNP A0A0D3B6Y5
1l	201	ASP	ASN	conflict	UNP A0A0D3B6Y5
1l	220	PHE	LEU	conflict	UNP A0A0D3B6Y5

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	1m	122	Total	C	N	O	S	0	0
			970	610	170	184	6		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
40	1o	76	Total	C	N	O	0	0
			626	397	114	115		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1o	4	CYS	TYR	conflict	UNP A0A3P6AZ01
1o	63	ARG	GLY	conflict	UNP A0A3P6AZ01

- Molecule 41 is a protein called MRPL25 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	1p	117	Total	C	N	O	S	0	0
			992	626	189	169	8		

- Molecule 42 is a protein called mL60.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	1q	50	Total	C	N	O	S	0	0
			390	243	79	67	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1q	63	ALA	SER	conflict	UNP A0A0D3BIE3

- Molecule 43 is a protein called mL80.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	1r	92	Total	C	N	O	S	0	0
			735	469	139	122	5		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1r	5	GLY	-	insertion	UNP A0A0D3D0H7
1r	6	VAL	-	insertion	UNP A0A0D3D0H7
1r	20	LEU	PHE	conflict	UNP A0A0D3D0H7
1r	22	LYS	ASN	conflict	UNP A0A0D3D0H7
1r	63	ASP	GLU	conflict	UNP A0A0D3D0H7
1r	130	PRO	ILE	conflict	UNP A0A0D3D0H7
1r	136	PRO	-	insertion	UNP A0A0D3D0H7
1r	137	VAL	-	insertion	UNP A0A0D3D0H7
1r	138	ALA	-	insertion	UNP A0A0D3D0H7
1r	139	ALA	-	insertion	UNP A0A0D3D0H7
1r	140	ALA	-	insertion	UNP A0A0D3D0H7
1r	141	ALA	LEU	conflict	UNP A0A0D3D0H7

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Chain	Residue	Modelled	Actual	Comment	Reference
1r	144	ALA	THR	conflict	UNP A0A0D3D0H7
1r	145	ALA	PRO	conflict	UNP A0A0D3D0H7
1r	149	THR	-	insertion	UNP A0A0D3D0H7
1r	150	THR	-	insertion	UNP A0A0D3D0H7
1r	151	ASP	-	insertion	UNP A0A0D3D0H7
1r	152	LYS	GLU	conflict	UNP A0A0D3D0H7
1r	156	ALA	GLN	conflict	UNP A0A0D3D0H7
1r	157	PHE	THR	conflict	UNP A0A0D3D0H7

- Molecule 44 is a protein called mL87.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	1s	118	Total	C	N	O	S	0	0
			985	617	203	163	2		

- Molecule 45 is a protein called Pentacotripeptide-repeat region of PRORP domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	1t	484	Total	C	N	O	S	0	0
			3856	2433	665	733	25		

- Molecule 46 is a protein called mL102.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	1u	666	Total	C	N	O	S	0	0
			5264	3316	915	991	42		

- Molecule 47 is a protein called mL104.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	1v	433	Total	C	N	O	S	0	0
			3440	2173	599	640	28		

- Molecule 48 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	2	1560	Total	C	N	O	P	0	0
			33425	14925	6097	10843	1560		

- Molecule 49 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	3	118	Total	C	N	O	P	0	0
			2513	1124	453	819	117		

- Molecule 50 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	5	77	Total	C	N	O	P	0	0
			1641	733	294	537	77		

- Molecule 51 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	6	6	Total	C	N	O	P	0	0
			129	58	24	41	6		

- Molecule 52 is a protein called Ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	A	204	Total	C	N	O	S	0	0
			1611	1032	284	285	10		

- Molecule 53 is a protein called Small ribosomal subunit protein uS3m.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	B	467	Total	C	N	O	S	0	0
			3877	2520	701	643	13		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	22	TRP	ARG	conflict	UNP A0A068BCX1
B	172	LEU	SER	conflict	UNP A0A068BCX1
B	202	LYS	ARG	conflict	UNP A0A068BCX1
B	296	LEU	SER	conflict	UNP A0A068BCX1
B	512	CYS	ARG	conflict	UNP A0A068BCX1
B	524	VAL	ALA	conflict	UNP A0A068BCX1
B	533	LEU	SER	conflict	UNP A0A068BCX1

- Molecule 54 is a protein called uS4m.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	C	333	Total	C	N	O	S	0	0
			2811	1798	540	462	11		

- Molecule 55 is a protein called S5 DRBM domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	D	417	Total	C	N	O	S	0	0
			3425	2146	603	664	12		

- Molecule 56 is a protein called bS6m.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	E	101	Total	C	N	O	S	0	0
			823	535	145	138	5		

- Molecule 57 is a protein called uS7m.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	F	157	Total	C	N	O	S	0	0
			1254	793	244	213	4		

- Molecule 58 is a protein called uS8m.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	G	128	Total	C	N	O	S	0	0
			1037	652	193	189	3		

- Molecule 59 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	H	213	Total	C	N	O	S	0	0
			1682	1054	312	311	5		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	50	SER	PRO	conflict	UNP A0A3P6FWE0
H	94	SER	ASN	conflict	UNP A0A3P6FWE0

- Molecule 60 is a protein called Small ribosomal subunit protein uS10 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	I	113	Total	C	N	O	S	0	0
			941	602	174	159	6		

- Molecule 61 is a protein called Ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	J	127	Total	C	N	O	S	0	0
			988	608	195	181	4		

- Molecule 62 is a protein called uS12m.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	K	124	Total	C	N	O	S	0	0
			992	613	208	167	4		

- Molecule 63 is a protein called uS13m.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	L	119	Total	C	N	O	S	0	0
			940	572	200	163	5		

- Molecule 64 is a protein called Small ribosomal subunit protein uS14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	M	101	Total	C	N	O	S	0	0
			843	524	174	140	5		

- Molecule 65 is a protein called Small ribosomal subunit protein uS15c.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	N	116	Total	C	N	O	S	0	0
			941	593	170	171	7		

- Molecule 66 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	O	110	Total	C	N	O	S	0	0
			869	550	169	144	6		

- Molecule 67 is a protein called Small ribosomal subunit protein uS17c.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	P	91	Total	C	N	O	S	0	0
			717	455	135	124	3		

- Molecule 68 is a protein called bS18m.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Q	90	Total	C	N	O	S	0	0
			724	460	127	134	3		

- Molecule 69 is a protein called uS19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	R	166	Total	C	N	O	S	0	0
			1299	819	236	237	7		

- Molecule 70 is a protein called Ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	S	75	Total	C	N	O	S	0	0
			611	386	120	103	2		

- Molecule 71 is a protein called 30S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	T	50	Total	C	N	O	S	0	0
			408	260	79	68	1		

- Molecule 72 is a protein called Small ribosomal subunit protein mS23.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	U	127	Total	C	N	O	S	0	0
			1014	647	184	178	5		

- Molecule 73 is a protein called mS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	V	164	Total	C	N	O	S	0	0
			1399	874	266	255	4		

- Molecule 74 is a protein called Small ribosomal subunit protein mS29.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	W	380	Total	C	N	O	S	0	0
			3062	1955	535	559	13		

- Molecule 75 is a protein called mS31/mS46.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	X	204	Total	C	N	O	S	0	0
			1613	1011	262	329	11		

- Molecule 76 is a protein called MOSC domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Y	98	Total	C	N	O	S	0	0
			793	495	159	137	2		

- Molecule 77 is a protein called mS34.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Z	80	Total	C	N	O	S	0	0
			649	422	121	104	2		

- Molecule 78 is a protein called Small ribosomal subunit protein mS35 mitochondrial conserved domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	a	315	Total	C	N	O	S	0	0
			2487	1547	448	482	10		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	186	GLU	ASP	conflict	UNP A0A3P6FE97
a	239	ALA	PRO	conflict	UNP A0A3P6FE97

- Molecule 79 is a protein called mS37.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	b	77	Total	C	N	O	S	0	0
			610	378	116	108	8		

- Molecule 80 is a protein called Small ribosomal subunit protein mS38.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	c	26	Total	C	N	O	S	0	0
			232	145	54	32	1		

- Molecule 81 is a protein called Small ribosomal subunit protein mS41 SAM domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	d	78	Total	C	N	O	S	0	0
			616	403	110	102	1		

- Molecule 82 is a protein called mS45.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	e	246	Total	C	N	O	S	0	0
			2074	1310	374	380	10		

- Molecule 83 is a protein called mS47.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	f	377	Total	C	N	O	S	0	0
			2922	1843	486	573	20		

- Molecule 84 is a protein called Adenylyl cyclase.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	h	310	Total	C	N	O	S	0	0
			2460	1551	436	458	15		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
h	?	-	THR	deletion	UNP A0A3P6FIH7
h	?	-	ILE	deletion	UNP A0A3P6FIH7
h	?	-	SER	deletion	UNP A0A3P6FIH7
h	?	-	SER	deletion	UNP A0A3P6FIH7
h	?	-	PHE	deletion	UNP A0A3P6FIH7
h	?	-	HIS	deletion	UNP A0A3P6FIH7
h	?	-	ALA	deletion	UNP A0A3P6FIH7
h	?	-	PHE	deletion	UNP A0A3P6FIH7
h	?	-	LEU	deletion	UNP A0A3P6FIH7
h	?	-	GLN	deletion	UNP A0A3P6FIH7
h	?	-	TRP	deletion	UNP A0A3P6FIH7
h	?	-	VAL	deletion	UNP A0A3P6FIH7
h	?	-	PHE	deletion	UNP A0A3P6FIH7
h	?	-	LEU	deletion	UNP A0A3P6FIH7
h	?	-	TYR	deletion	UNP A0A3P6FIH7
h	?	-	ALA	deletion	UNP A0A3P6FIH7
h	152	GLN	ARG	conflict	UNP A0A3P6FIH7
h	189	MET	LEU	conflict	UNP A0A3P6FIH7
h	190	MET	LEU	conflict	UNP A0A3P6FIH7

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Chain	Residue	Modelled	Actual	Comment	Reference
h	203	GLU	ASP	conflict	UNP A0A3P6FIH7
h	330	LYS	PHE	conflict	UNP A0A3P6FIH7
h	331	GLU	LYS	conflict	UNP A0A3P6FIH7

- Molecule 85 is a protein called PROP1-like PPR domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	i	306	Total	C	N	O	S	0	0
			2487	1567	419	487	14		

- Molecule 86 is a protein called RRM domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	k	47	Total	C	N	O	S	0	0
			314	194	61	55	4		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	23	SER	ALA	conflict	UNP A0A3P6FEP3
k	38	ILE	LEU	conflict	UNP A0A3P6FEP3
k	46	SER	THR	conflict	UNP A0A3P6FEP3
k	50	GLU	ASP	conflict	UNP A0A3P6FEP3
k	51	LEU	ILE	conflict	UNP A0A3P6FEP3

- Molecule 87 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
87	1	251	Total	Mg	0
			251	251	
87	1D	1	Total	Mg	0
			1	1	
87	1j	1	Total	Mg	0
			1	1	
87	1q	1	Total	Mg	0
			1	1	
87	2	97	Total	Mg	0
			97	97	
87	3	3	Total	Mg	0
			3	3	
87	D	1	Total	Mg	0
			1	1	

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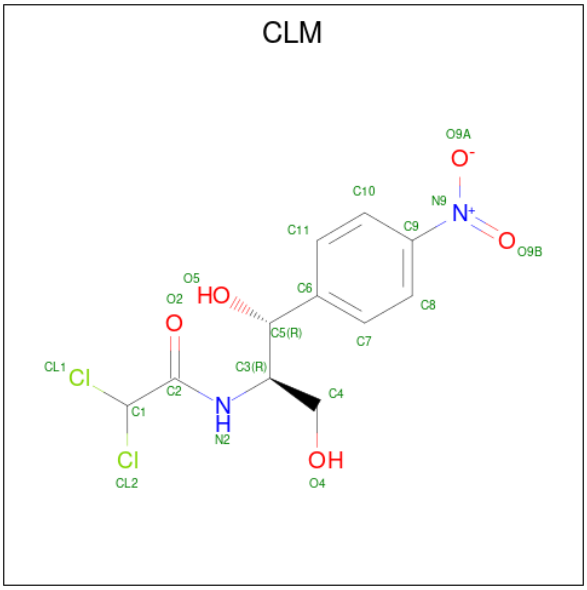
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Mol	Chain	Residues	Atoms	AltConf
87	T	1	Total Mg 1 1	0
87	W	1	Total Mg 1 1	0

- Molecule 88 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
88	1	57	Total K 57 57	0
88	1B	2	Total K 2 2	0
88	1E	1	Total K 1 1	0
88	2	14	Total K 14 14	0

- Molecule 89 is CHLORAMPHENICOL (CCD ID: CLM) (formula: $C_{11}H_{12}Cl_2N_2O_5$).

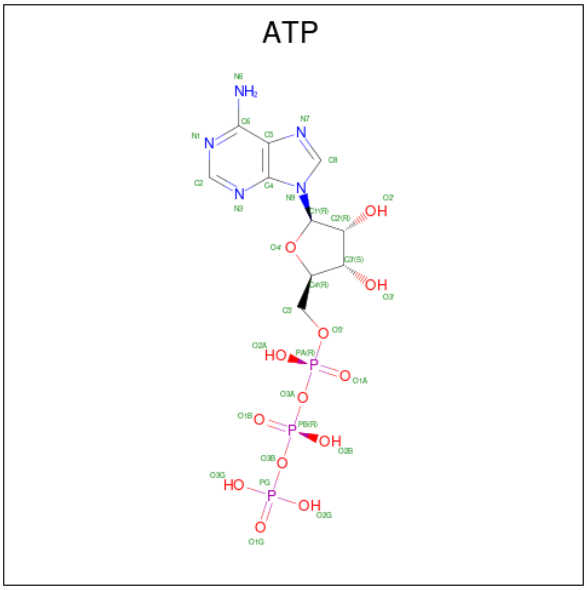


Mol	Chain	Residues	Atoms	AltConf
89	1	1	Total C Cl N O 20 11 2 2 5	0

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

Mol	Chain	Residues	Atoms	AltConf
90	1d	1	Total Zn 1 1	0
90	1h	1	Total Zn 1 1	0

- Molecule 91 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
91	W	1	Total C N O P 31 10 5 13 3	0

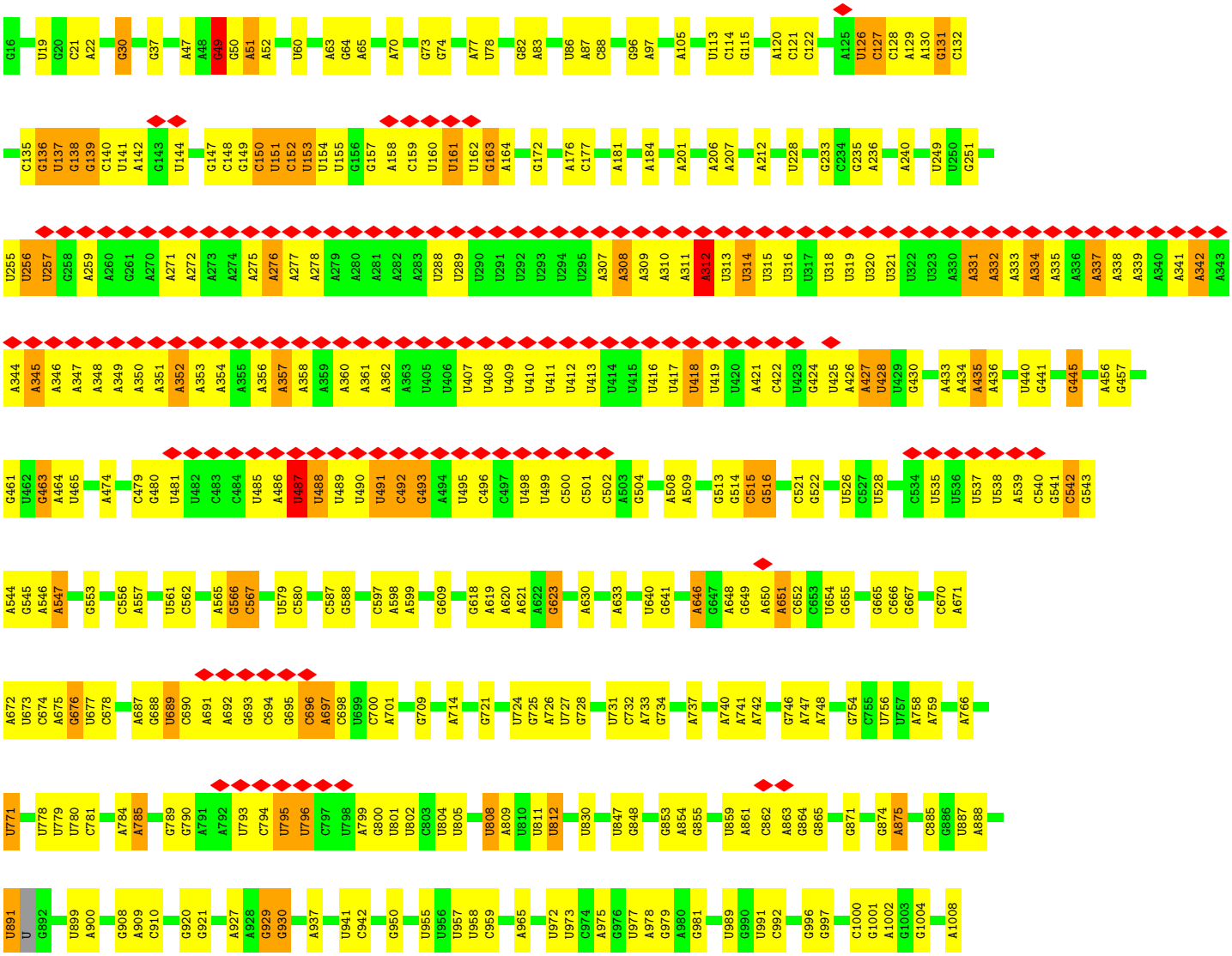
3 Residue-property plots (i)

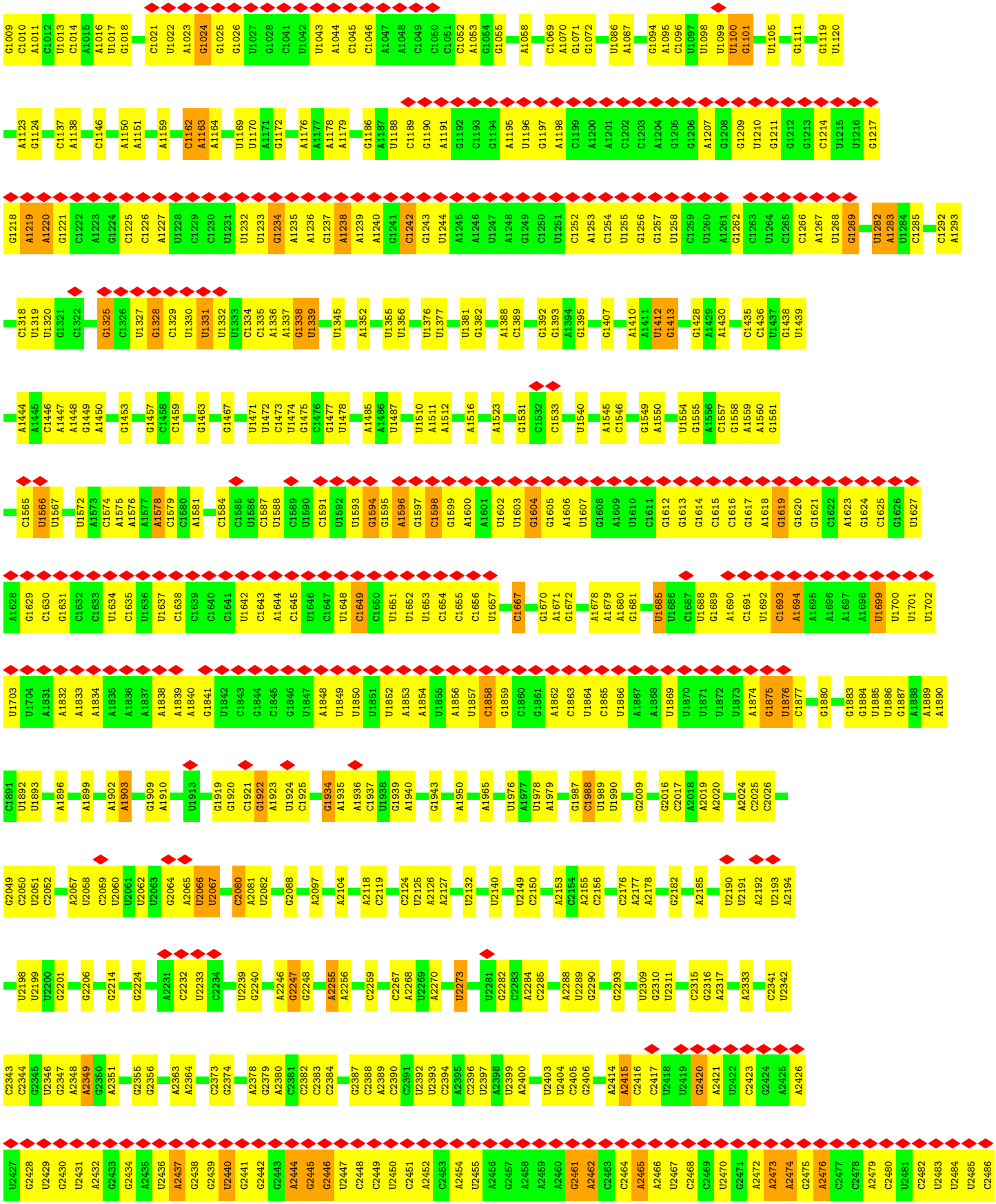
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

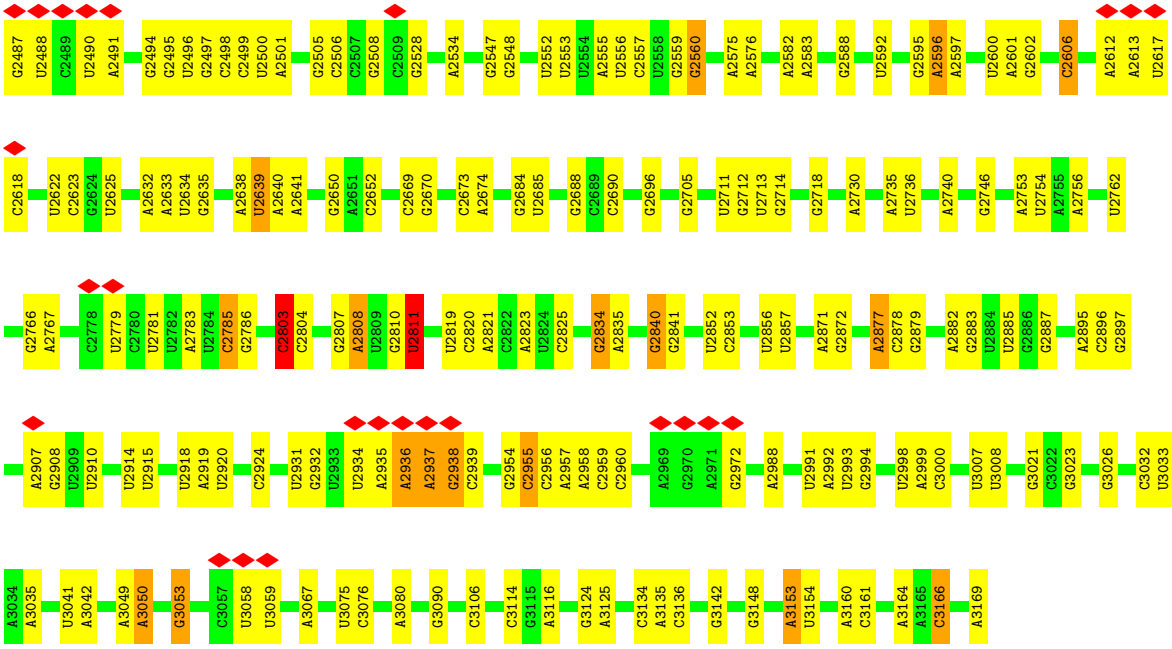
- Molecule 1: 26S rRNA

Chain 1:





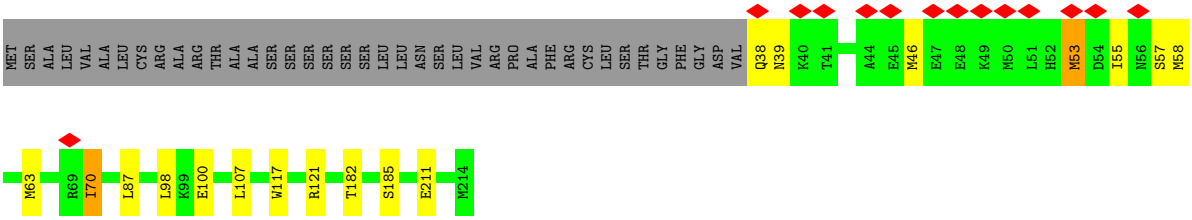

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A1123 G1124 C1137 A1138 C1146 A1150 A1151 A1159 C1162 A1163 A1164 U1169 U1170 A1171 G1172 A1176 A1177 A1178 A1179 G1186 A1187 U1188 C1189 G1190 A1191 G1192 C1193 G1194 A1195 U1196 G1197 A1198 C1199 A1200 A1201 C1202 C1203 A1204 G1205 G1206 A1207 G1208 G1209 U1210 G1211 G1212 G1213 C1214 U1215 U1216 G1217
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U2198 U2199 U2200 G2201 G2206 G2214 G2224 A2231 C2232 U2233 C2234 U2239 G2240 A2246 G2247 G2248 A2255 A2256 C2259 C2267 A2268 U2269 A2270 U2273 U2281 G2282 C2283 A2284 C2285 A2288 U2289 G2290 G2293 U2309 G2310 U2311 C2315 G2316 A2317 A2333 C2341 U2342
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• Molecule 2: Large ribosomal subunit protein uL2 C-terminal domain-containing protein

Chain 1B:

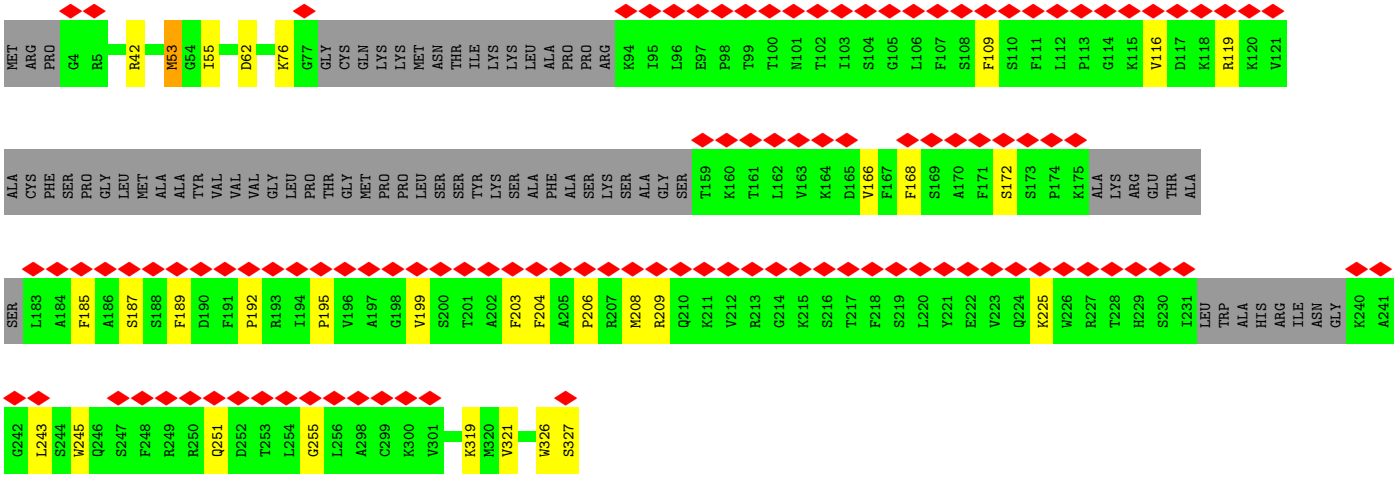




• Molecule 3: uL2m N-ter mitochondrial

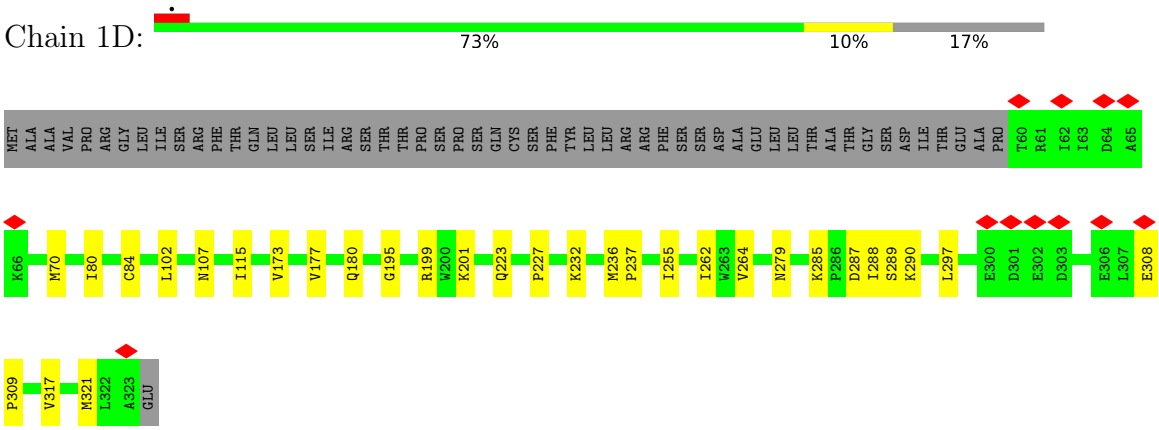
Chain 1C:





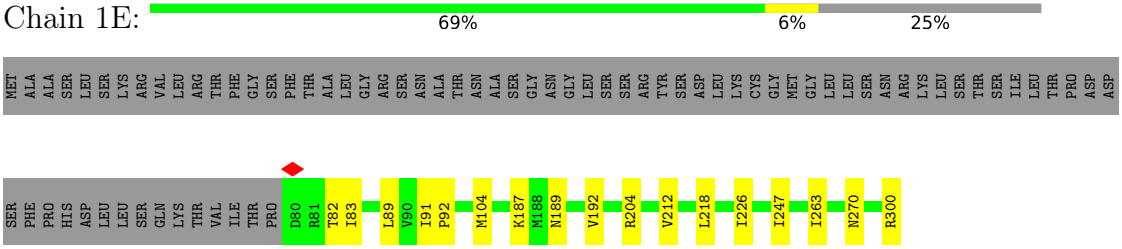
• Molecule 4: 50S ribosomal protein L3-2, chloroplastic

Chain 1D:



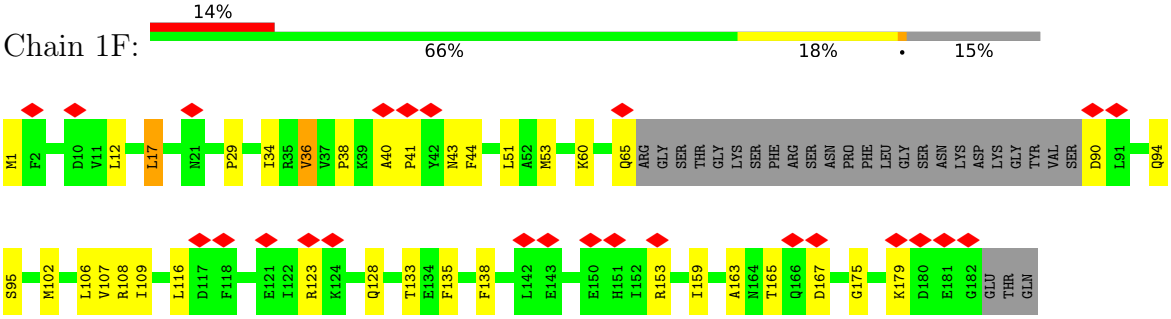
• Molecule 5: Large ribosomal subunit protein uL4m

Chain 1E:



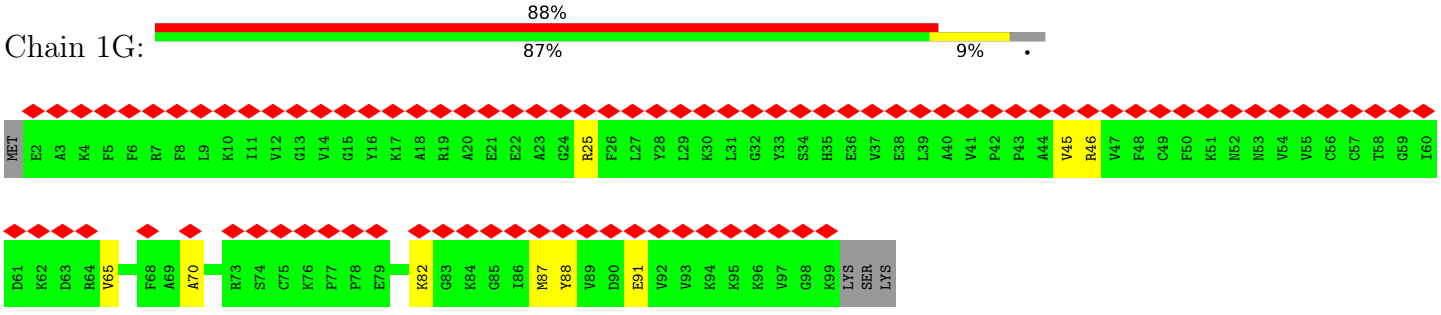
• Molecule 6: Large ribosomal subunit protein uL5m

Chain 1F:



• Molecule 7: Large ribosomal subunit protein uL6 alpha-beta domain-containing protein

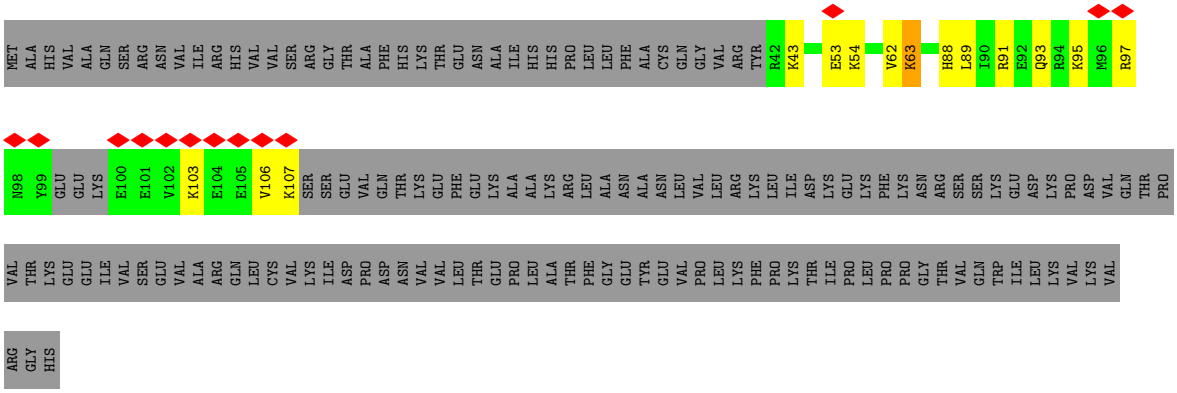
Chain 1G:



• Molecule 8: Large ribosomal subunit protein bL9c

Chain 1H:

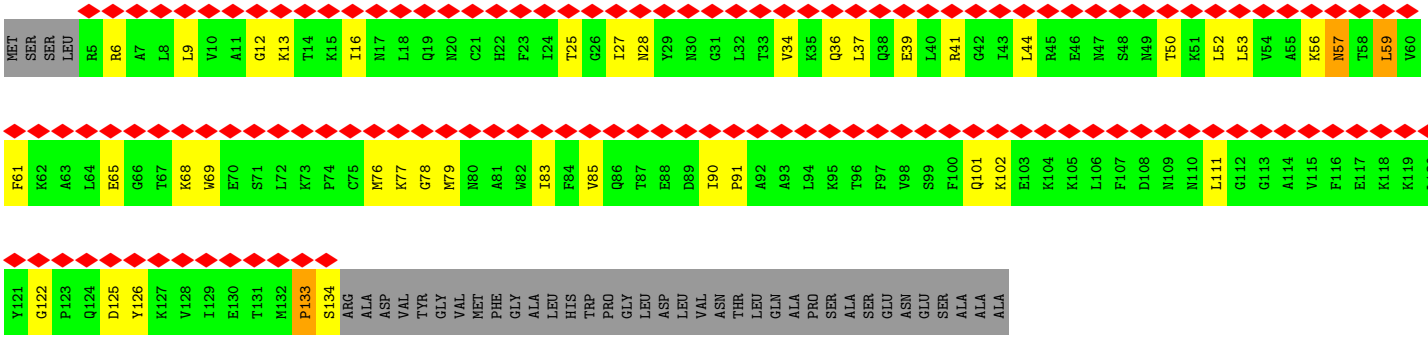




• Molecule 9: Large ribosomal subunit protein uL10c

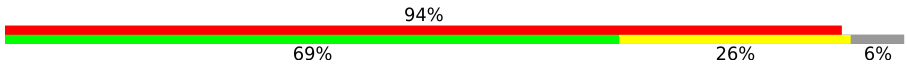
Chain 1I:

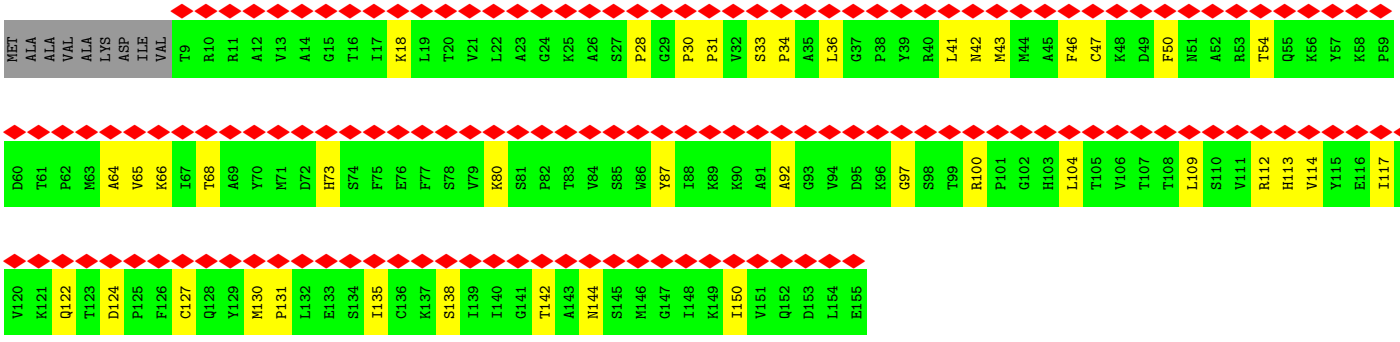




• Molecule 10: Large ribosomal subunit protein uL11m

Chain 1J:

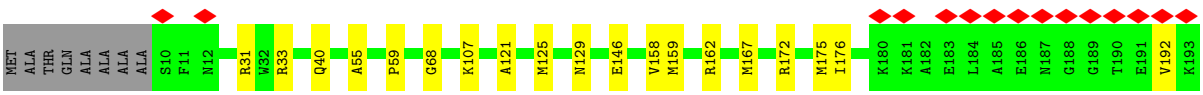


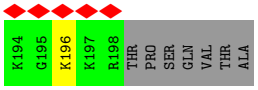


• Molecule 11: 50S ribosomal protein L13

Chain 1K:





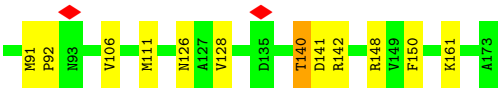


• Molecule 12: uL14m

Chain 1L:



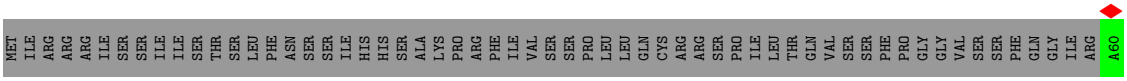


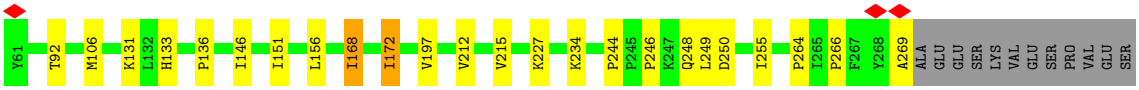


• Molecule 13: Large ribosomal subunit protein uL15/eL18 domain-containing protein

Chain 1M:



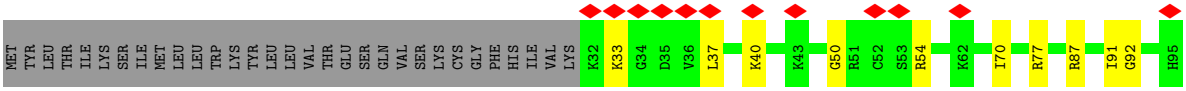


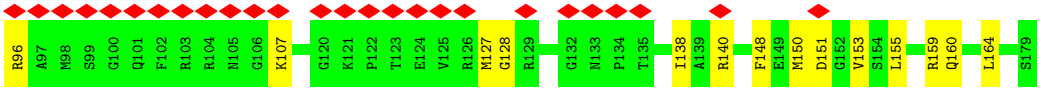


• Molecule 14: Large ribosomal subunit protein uL16m|

Chain 1N:



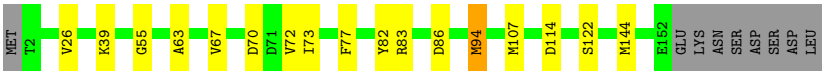




• Molecule 15: 50S ribosomal protein L17

Chain 1O:

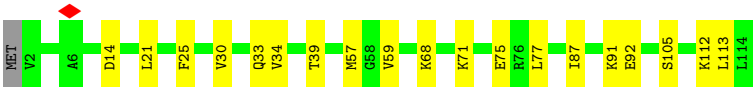




• Molecule 16: Ribosomal protein L18e/L15P domain-containing protein

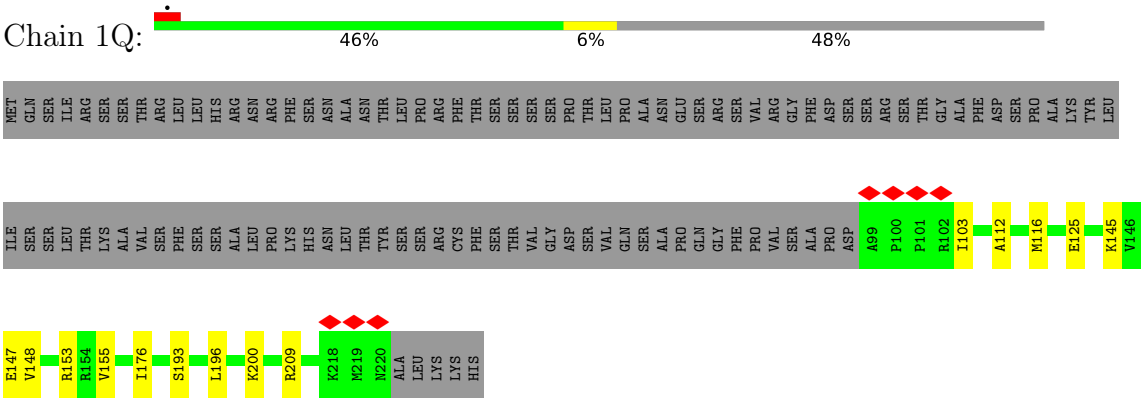
Chain 1P:





• Molecule 17: bL19m

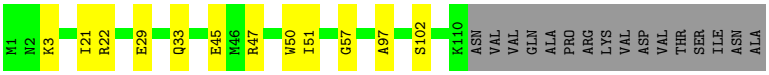
Chain 1Q:



• Molecule 18: 50S ribosomal protein L20

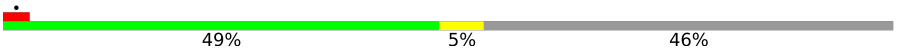
Chain 1R:

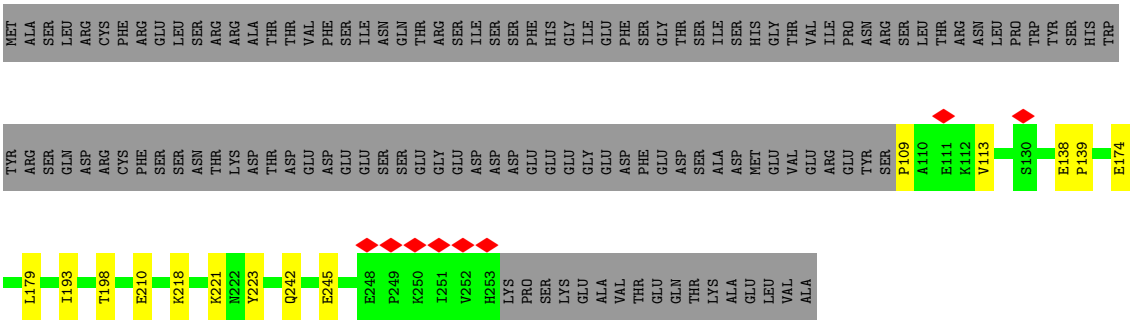




• Molecule 19: bL21m

Chain 1S:

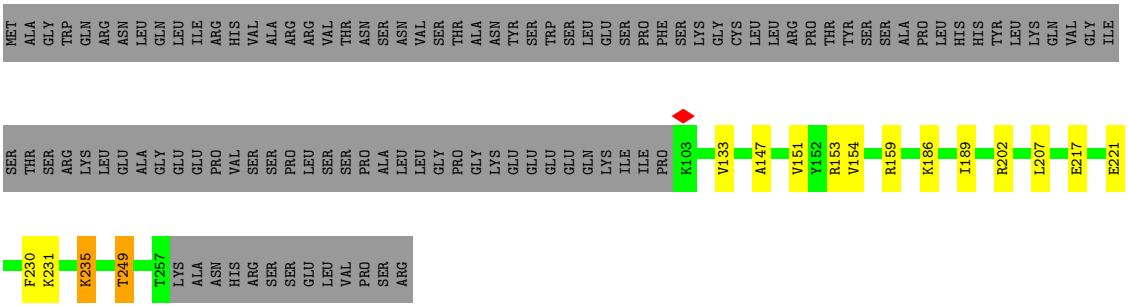




• Molecule 20: Large ribosomal subunit protein uL22c

Chain 1T:

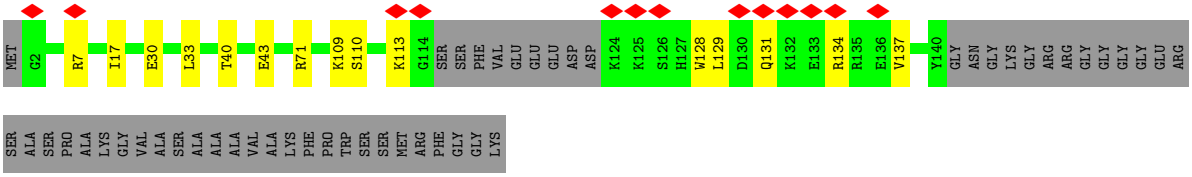




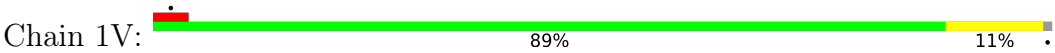
• Molecule 21: Large ribosomal subunit protein uL23m

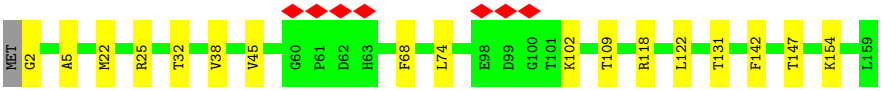
Chain 1U:



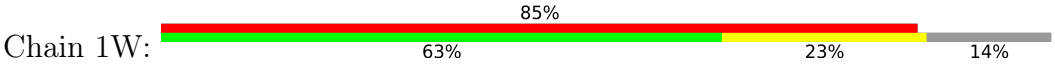


• Molecule 22: KOW domain-containing protein

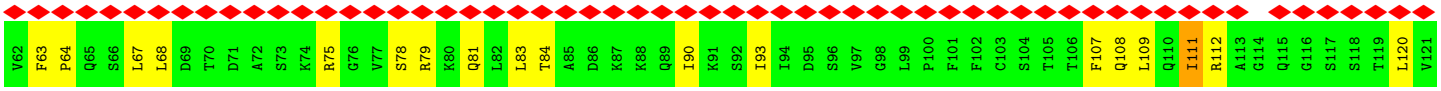


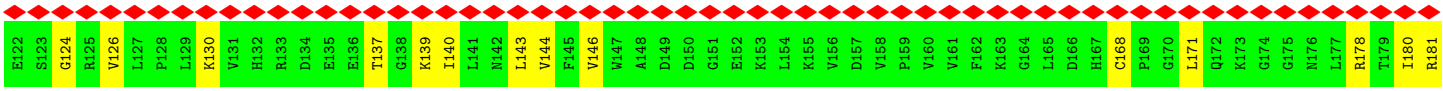


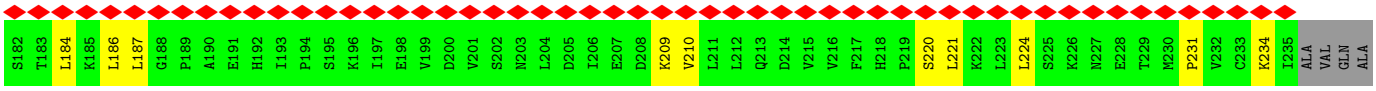
• Molecule 23: bL25-2m





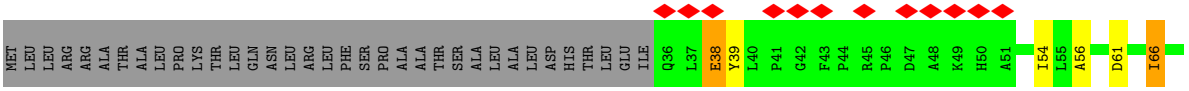


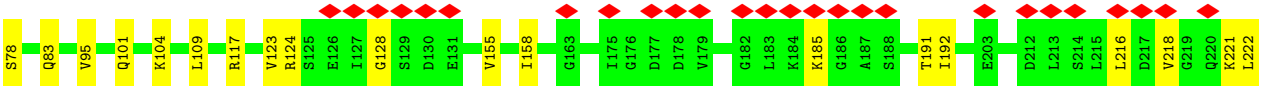


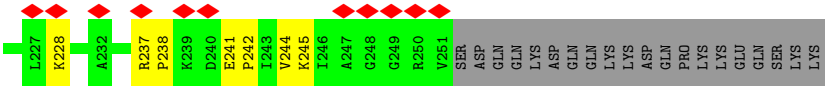


• Molecule 24: bL25m



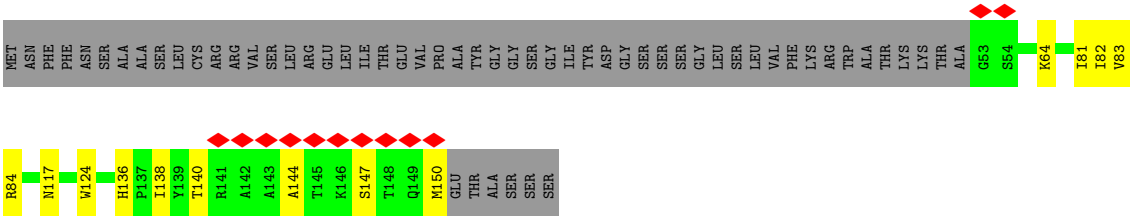






• Molecule 25: 50S ribosomal protein L27

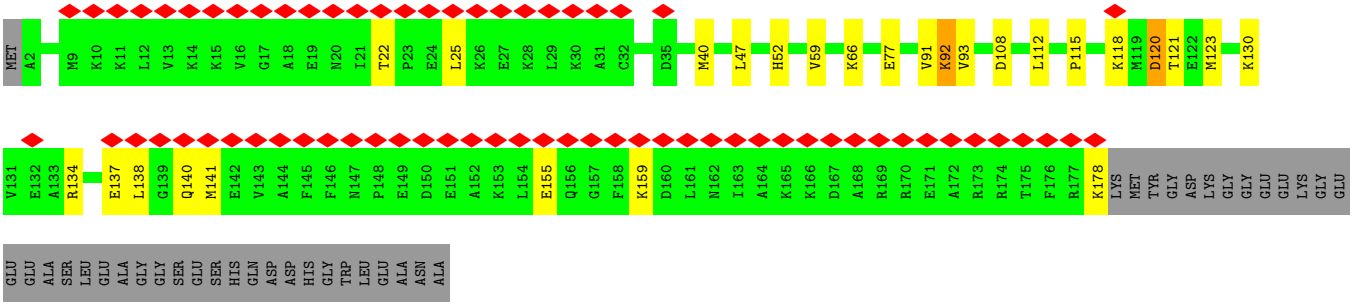




• Molecule 26: Large ribosomal subunit protein bL28m

Chain 1Z:

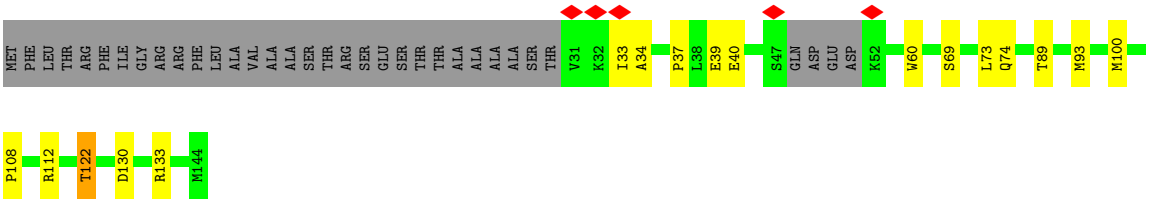




• Molecule 27: Cation-transporting P-type ATPase N-terminal domain-containing protein

Chain 1a:

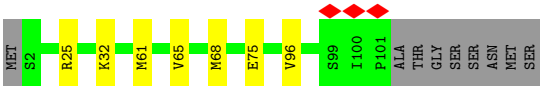




• Molecule 28: Large ribosomal subunit protein uL30m

Chain 1b:

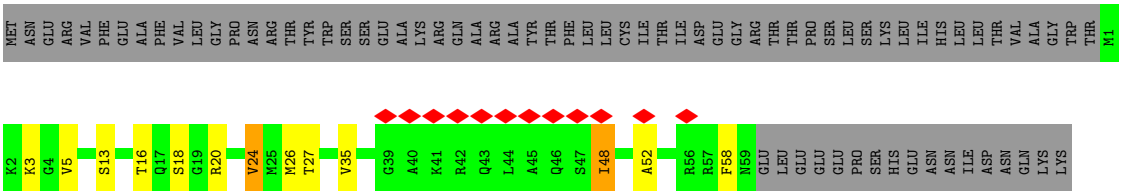




• Molecule 29: bL31m

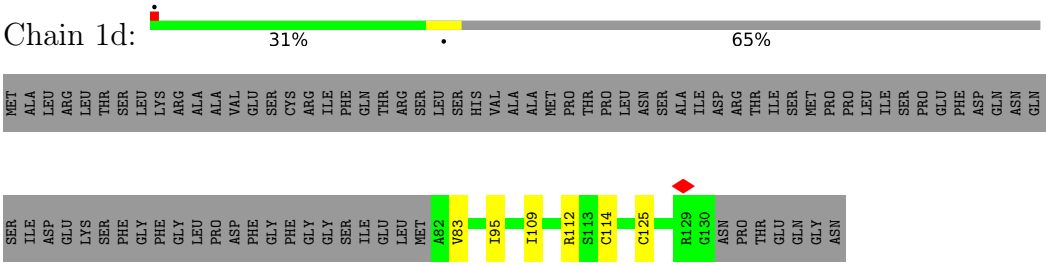
Chain 1c:





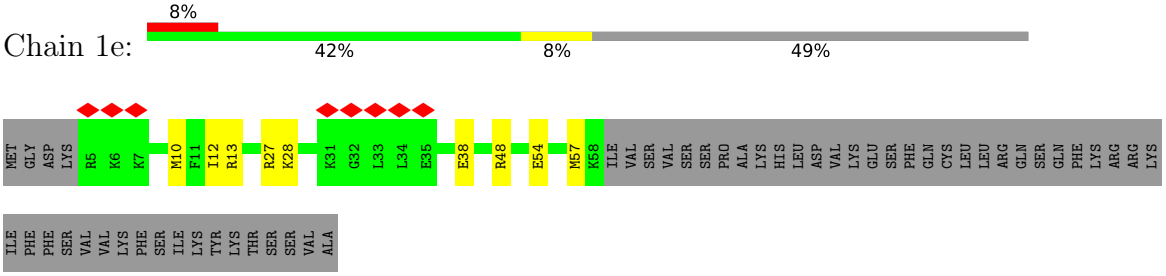
• Molecule 30: Large ribosomal subunit protein bL32m

Chain 1d:



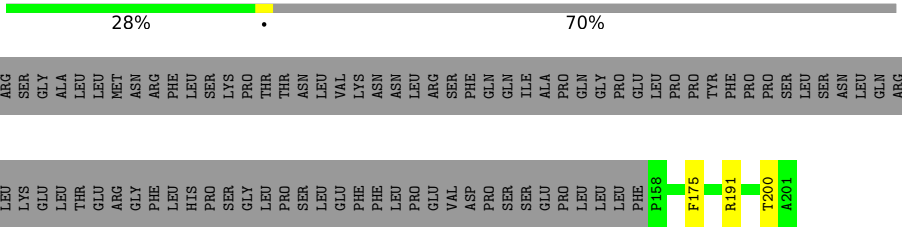
• Molecule 31: bL33m

Chain 1e:



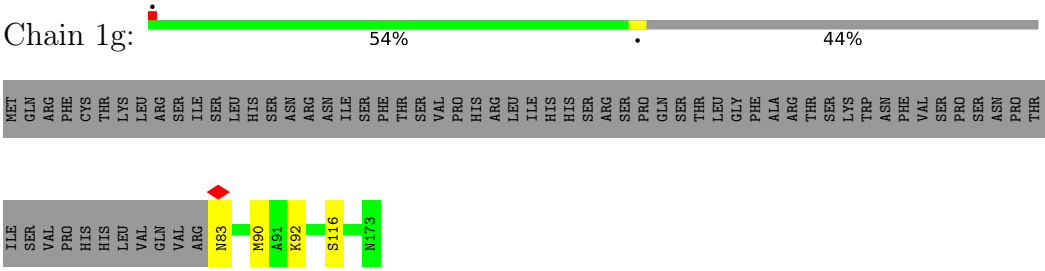
• Molecule 32: Large ribosomal subunit protein bL34m

Chain 1f:



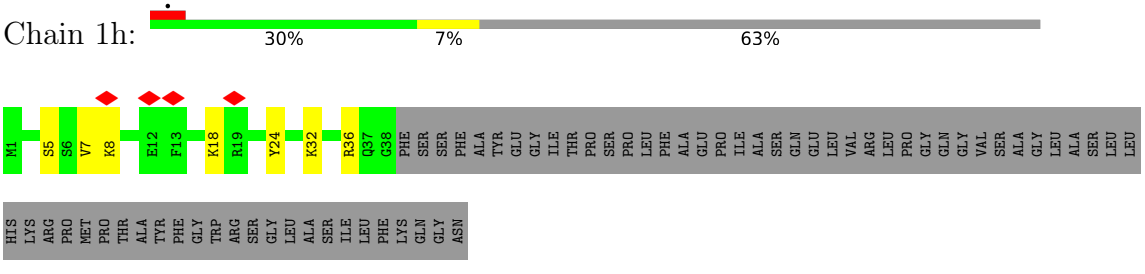
• Molecule 33: 50S ribosomal protein L35

Chain 1g:



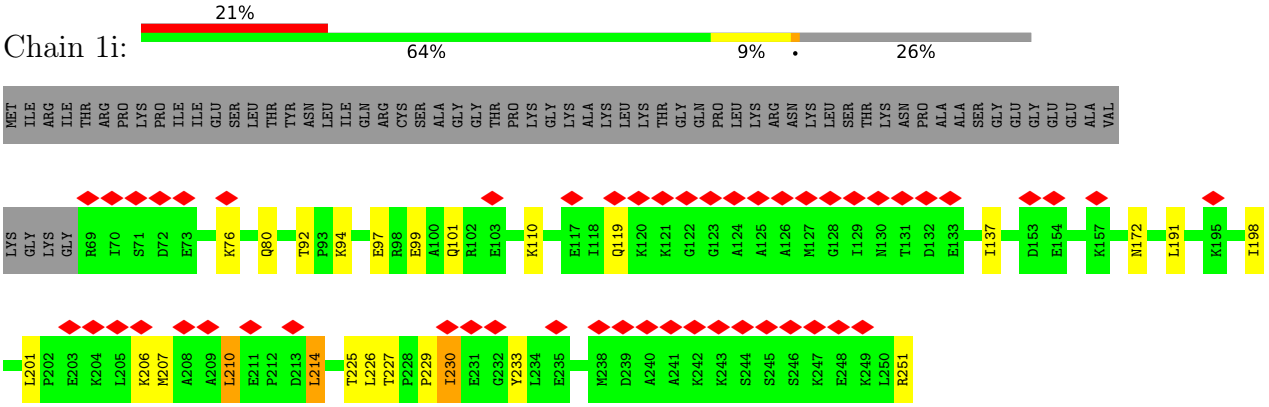
• Molecule 34: Ribosomal protein

Chain 1h:



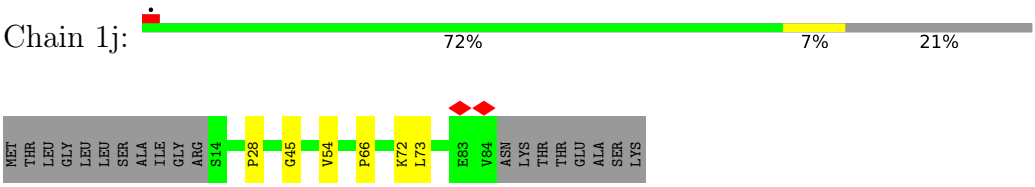
• Molecule 35: mL40

Chain 1i:



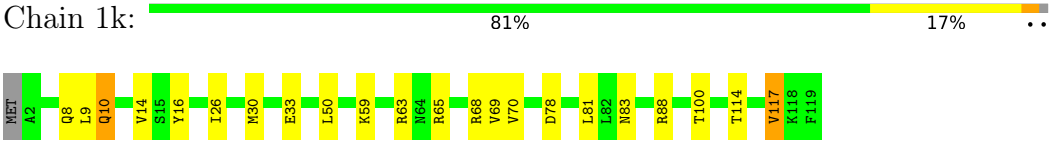
• Molecule 36: 39S ribosomal protein L41-A, mitochondrial

Chain 1j:



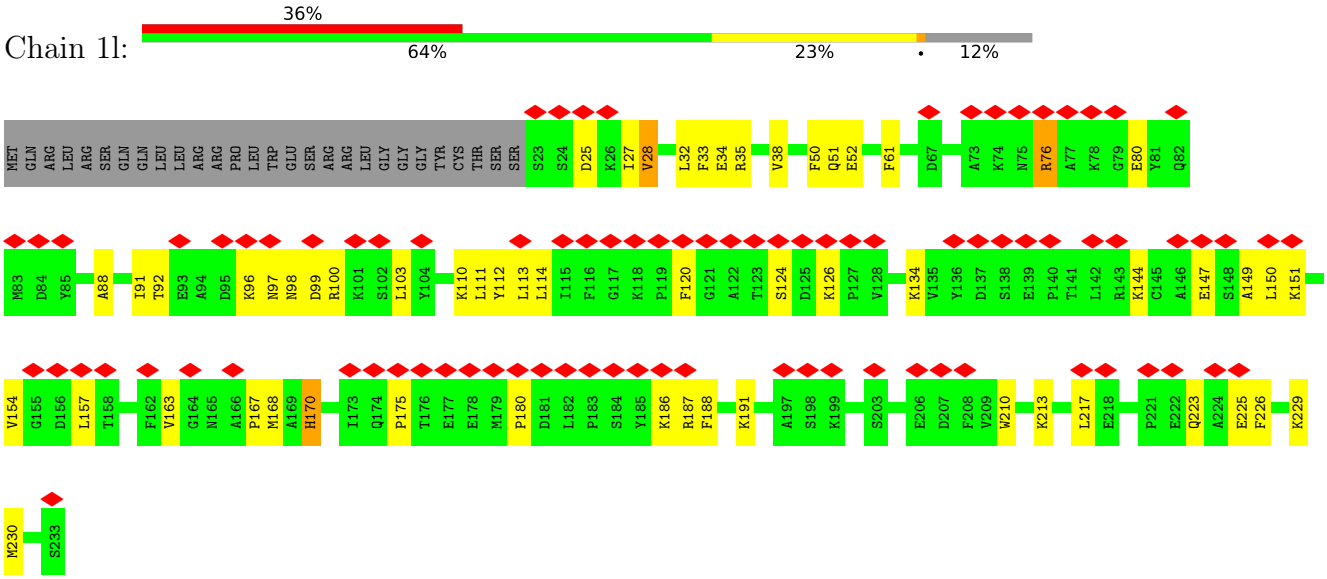
• Molecule 37: Large ribosomal subunit protein mL43

Chain 1k:



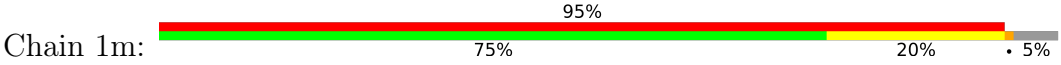
• Molecule 38: Large ribosomal subunit protein mL46

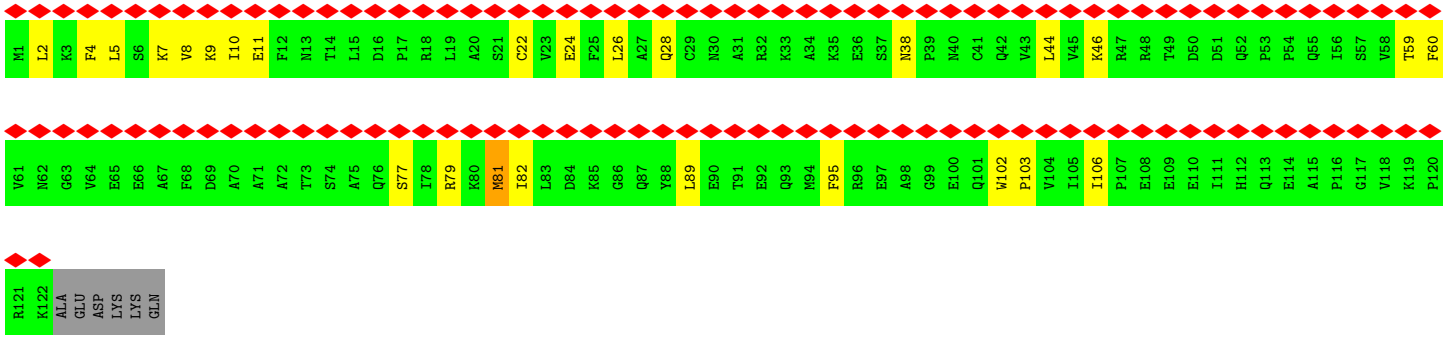
Chain 1l:



• Molecule 39: Large ribosomal subunit protein mL53

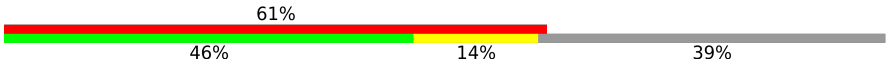
Chain 1m:

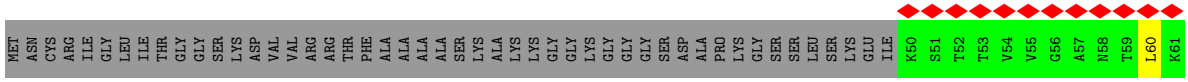


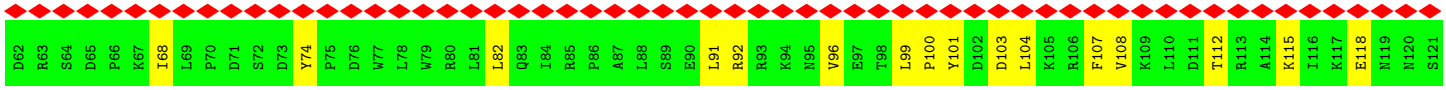


• Molecule 40: Large ribosomal subunit protein mL54

Chain 1o:







• Molecule 41: MRPL25 domain-containing protein

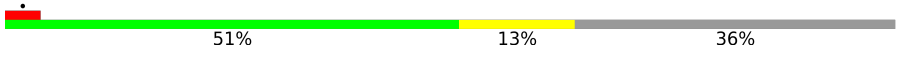
Chain 1p:

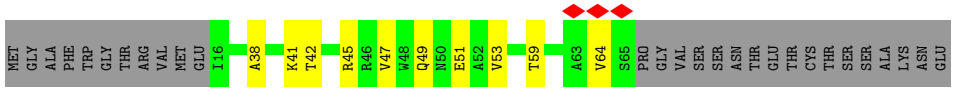




• Molecule 42: mL60

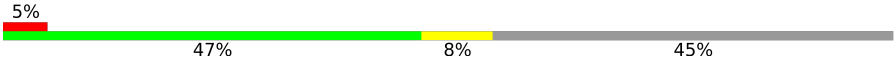
Chain 1q:

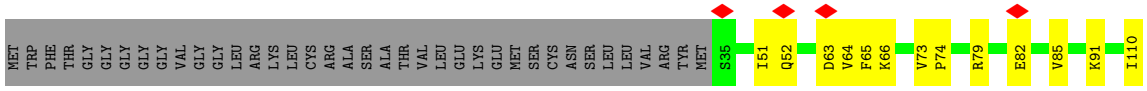


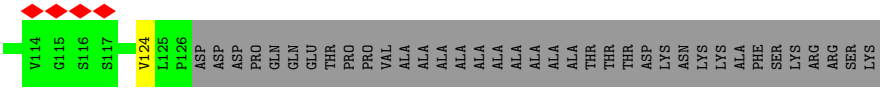


• Molecule 43: mL80

Chain 1r:



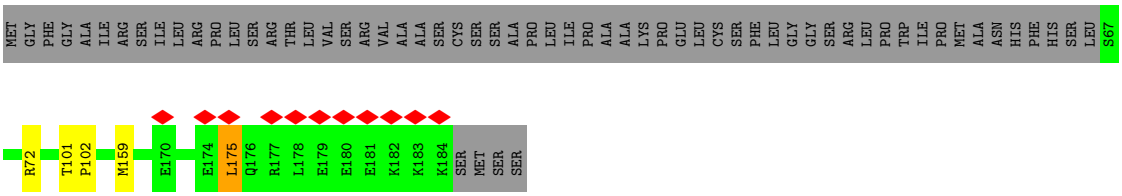




• Molecule 44: mL87

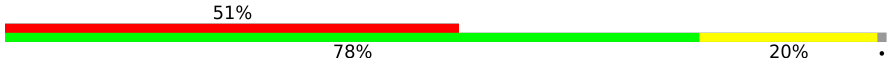
Chain 1s:



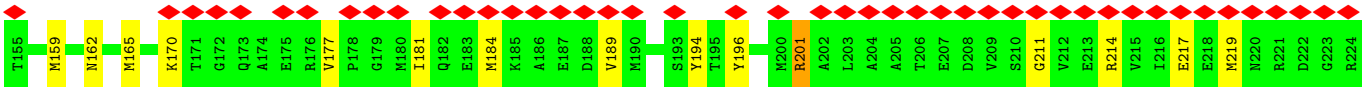


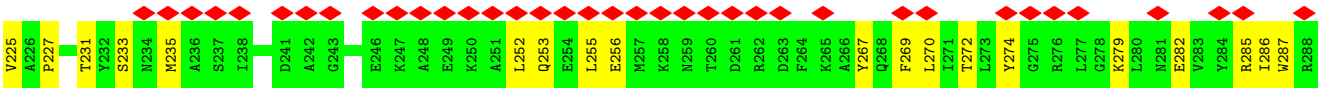
• Molecule 45: Pentacotripeptide-repeat region of PRORP domain-containing protein

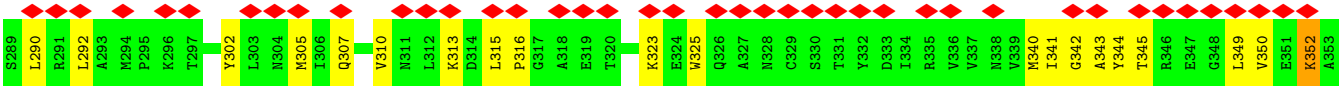
Chain 1t:

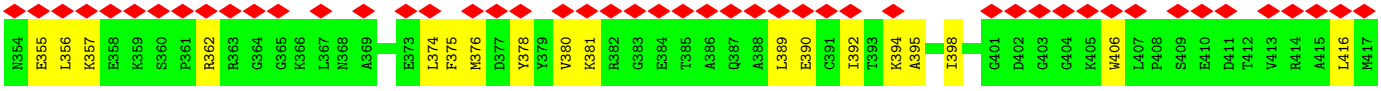


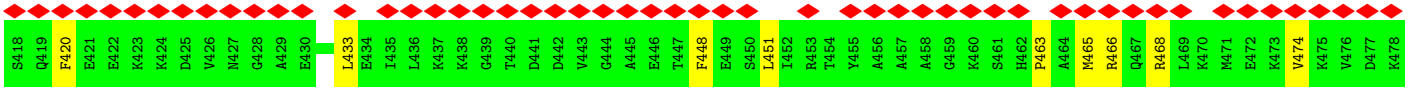


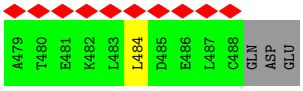










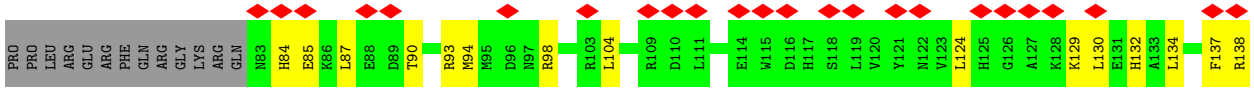


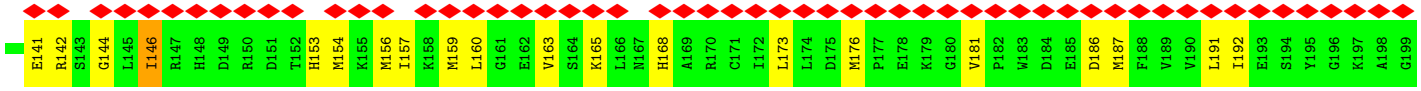
• Molecule 46: mL102

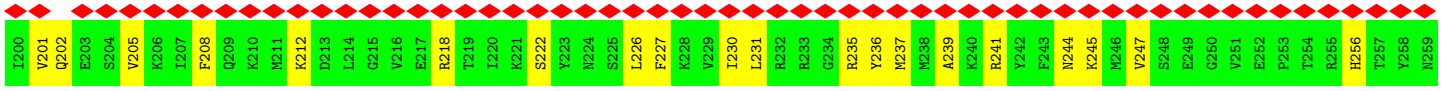
Chain 1u:

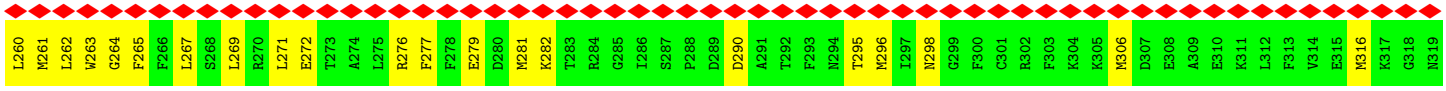


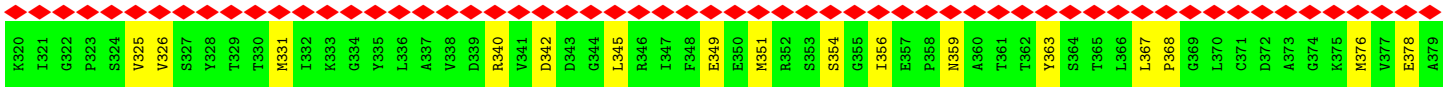


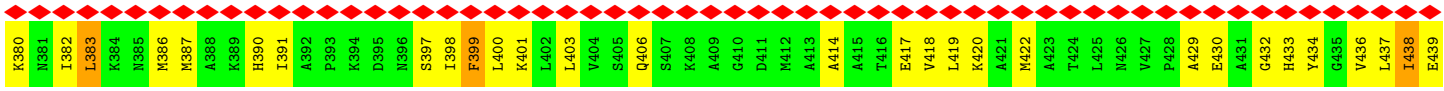


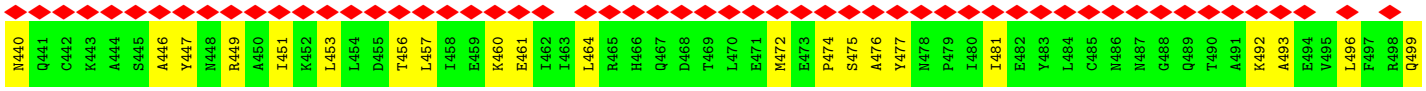


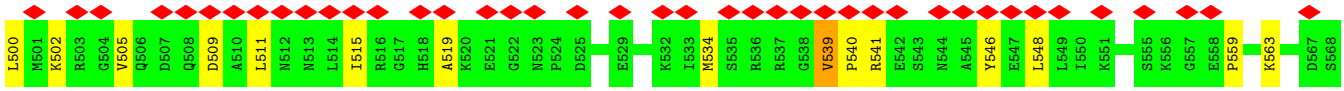


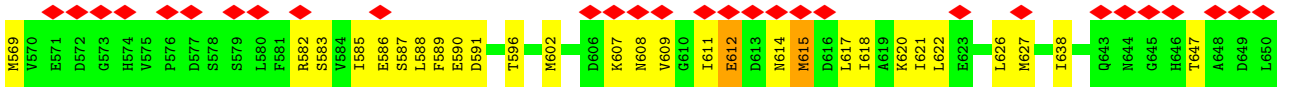


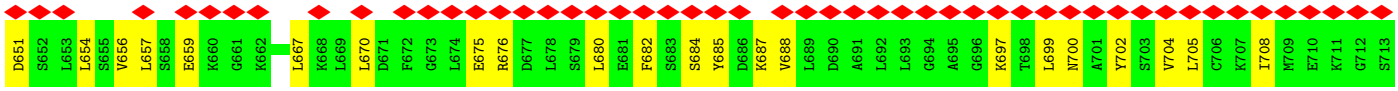


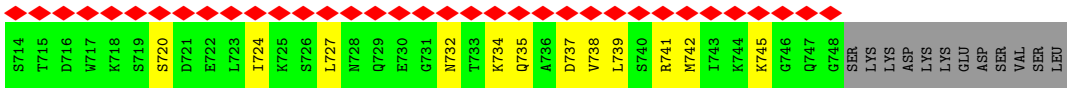








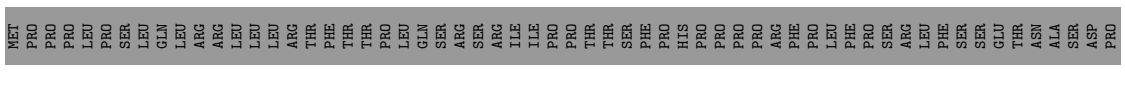


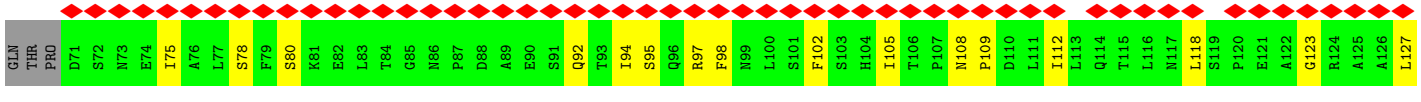


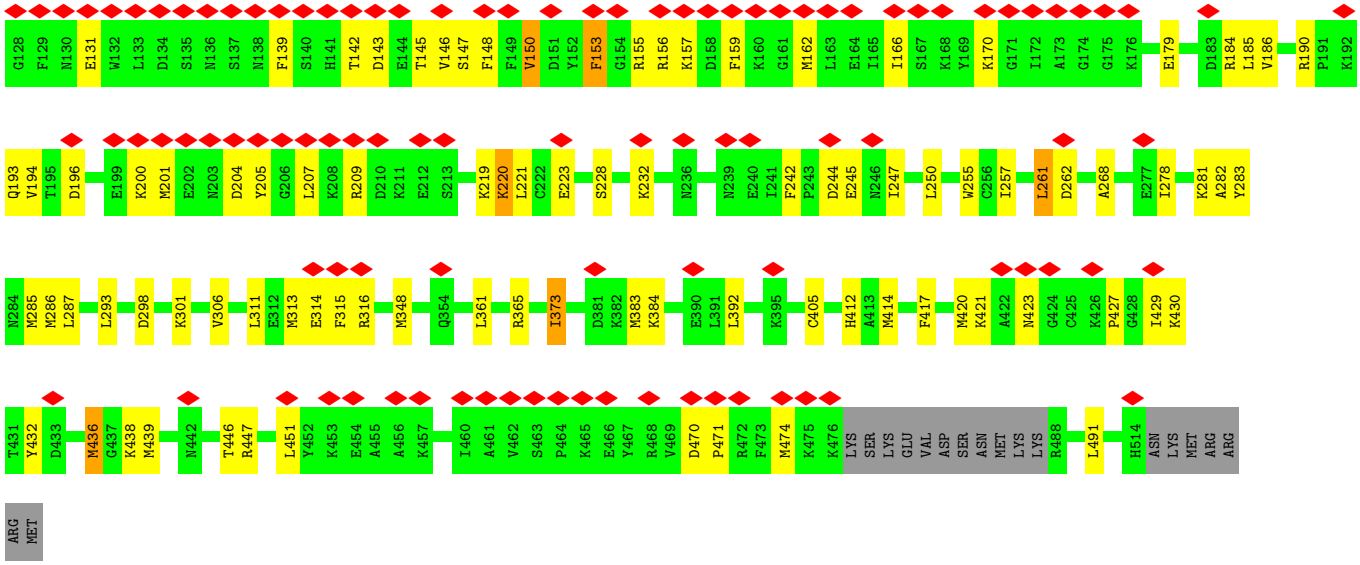
• Molecule 47: mL104

Chain 1v:





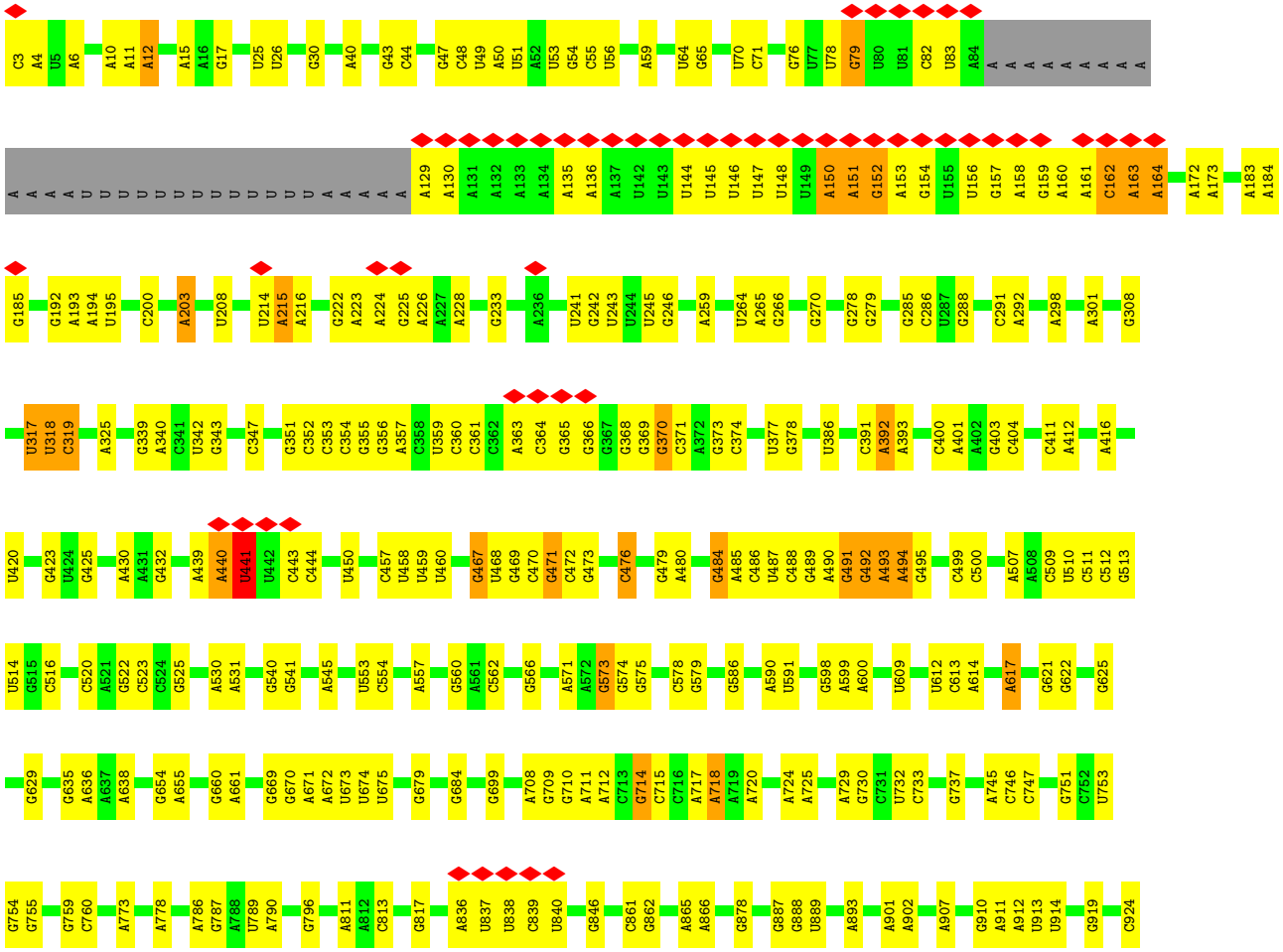


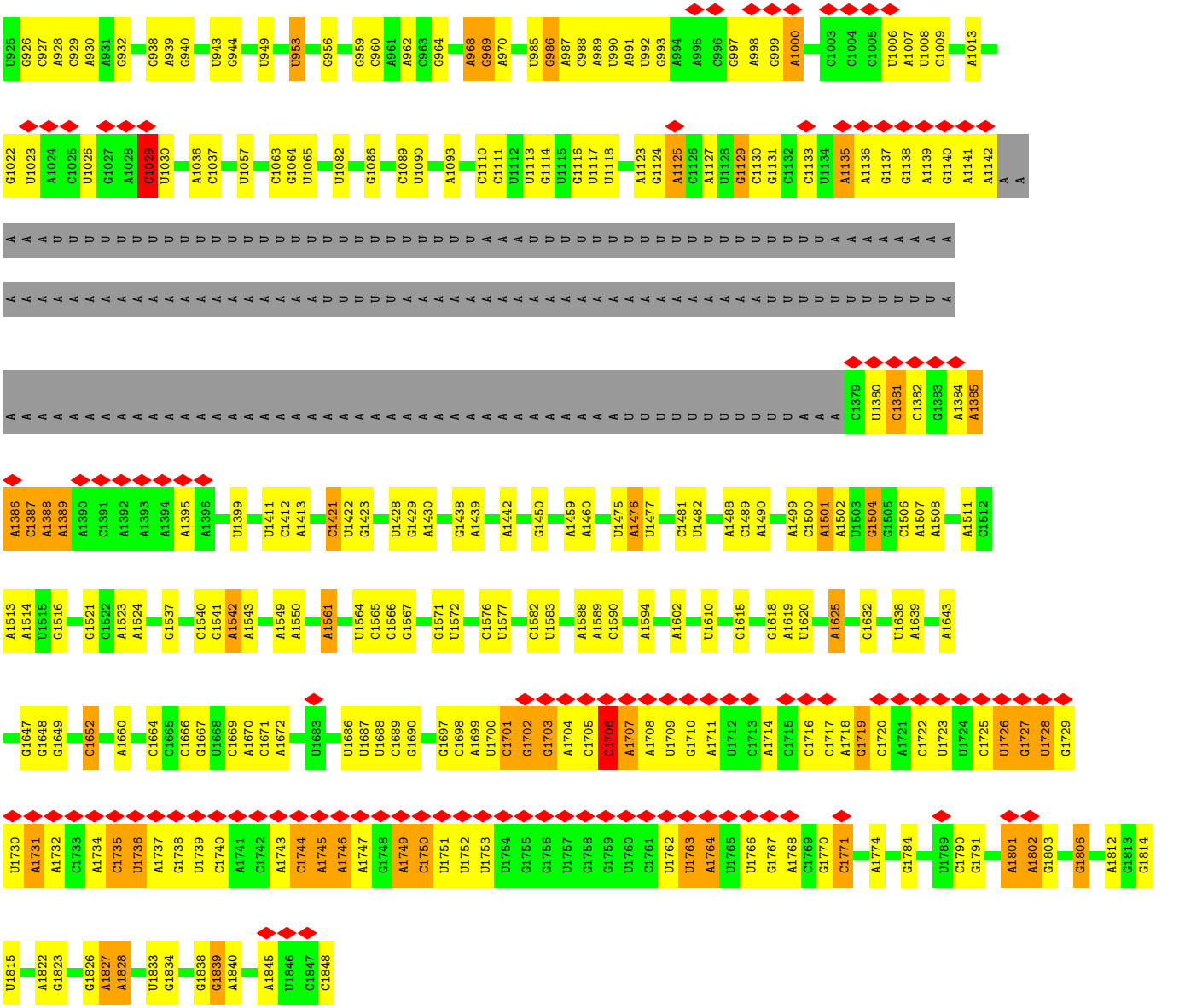


- Molecule 48: 18S rRNA

Chain 2:



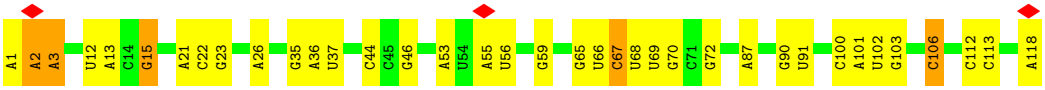




• Molecule 49: 5S rRNA

Chain 3:

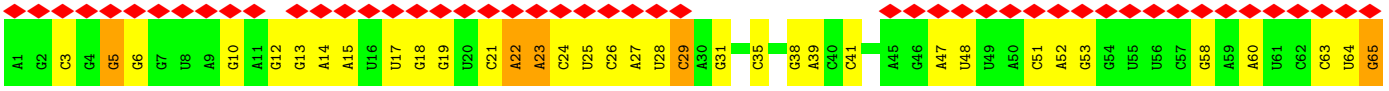


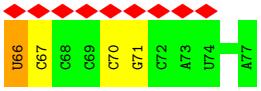


• Molecule 50: tRNA

Chain 5:



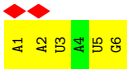




• Molecule 51: mRNA

Chain 6:

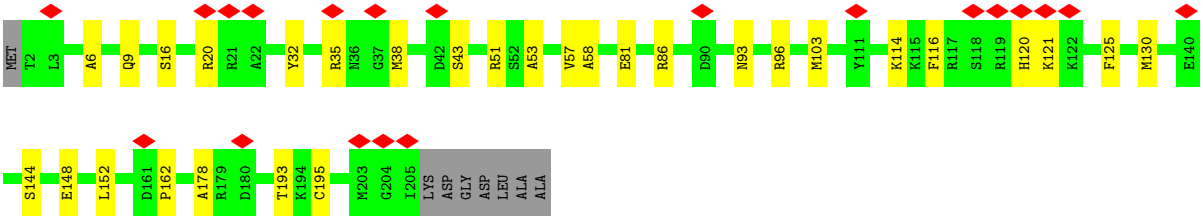




• Molecule 52: Ribosomal protein S2

Chain A:

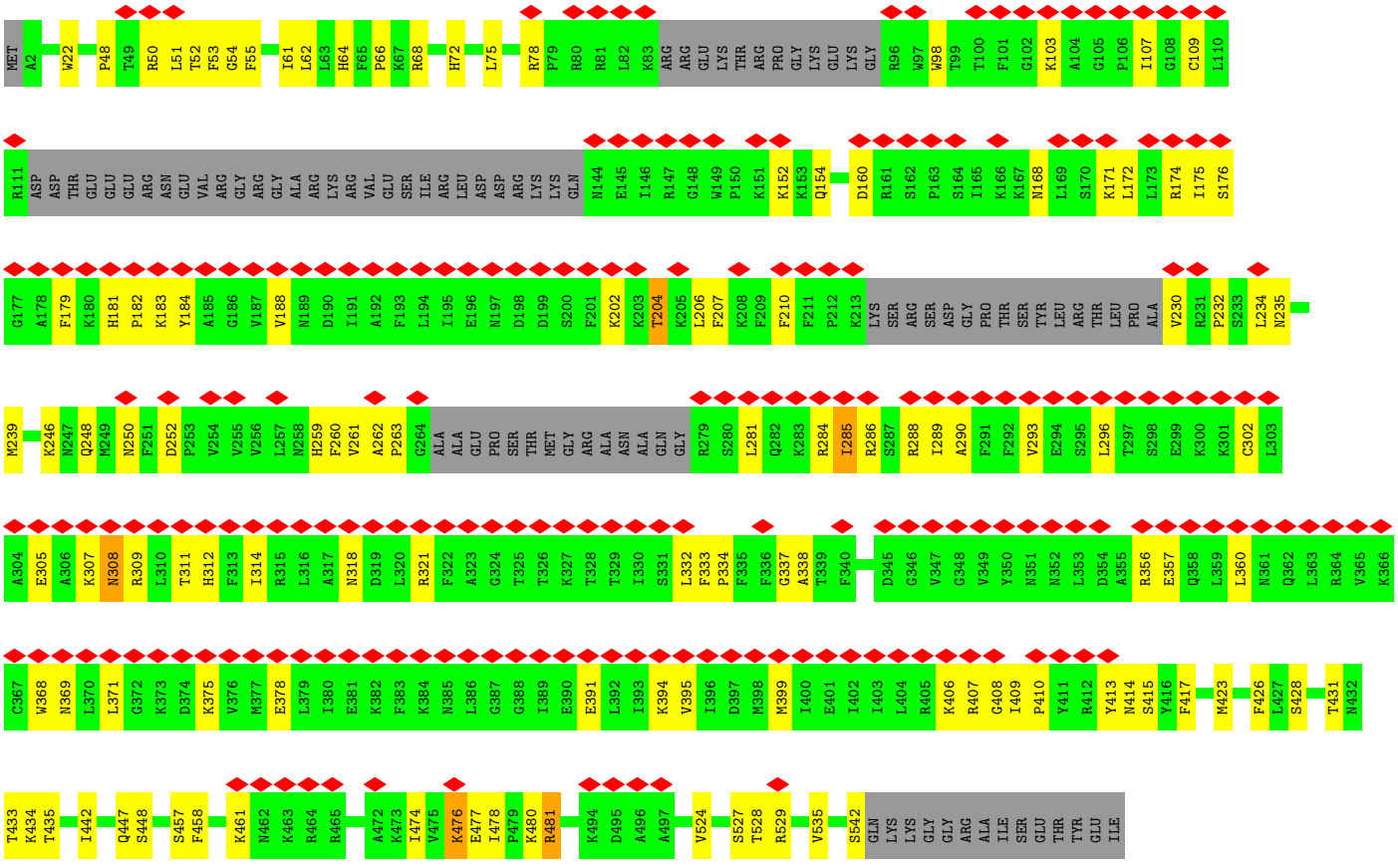




• Molecule 53: Small ribosomal subunit protein uS3m

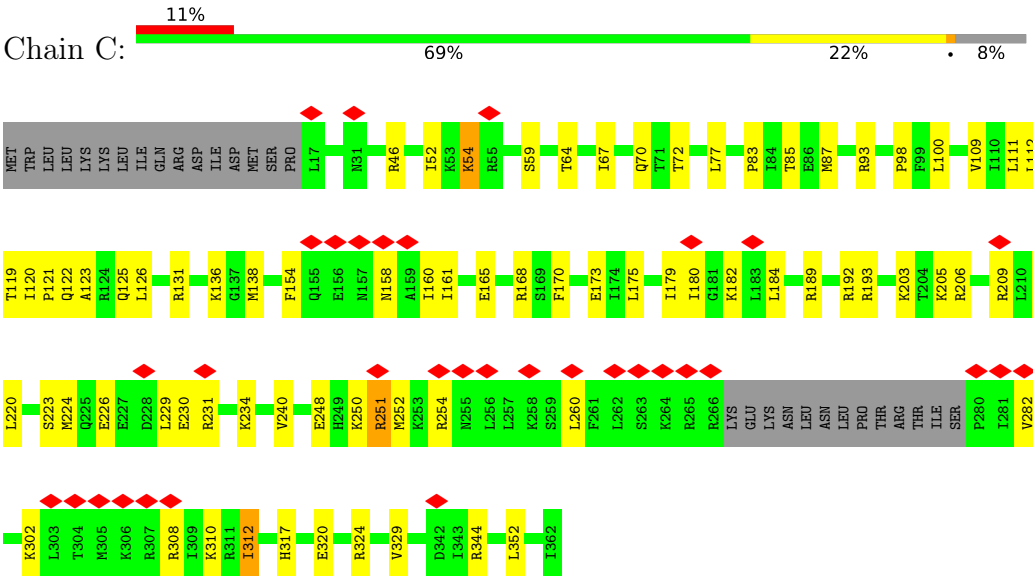
Chain B:





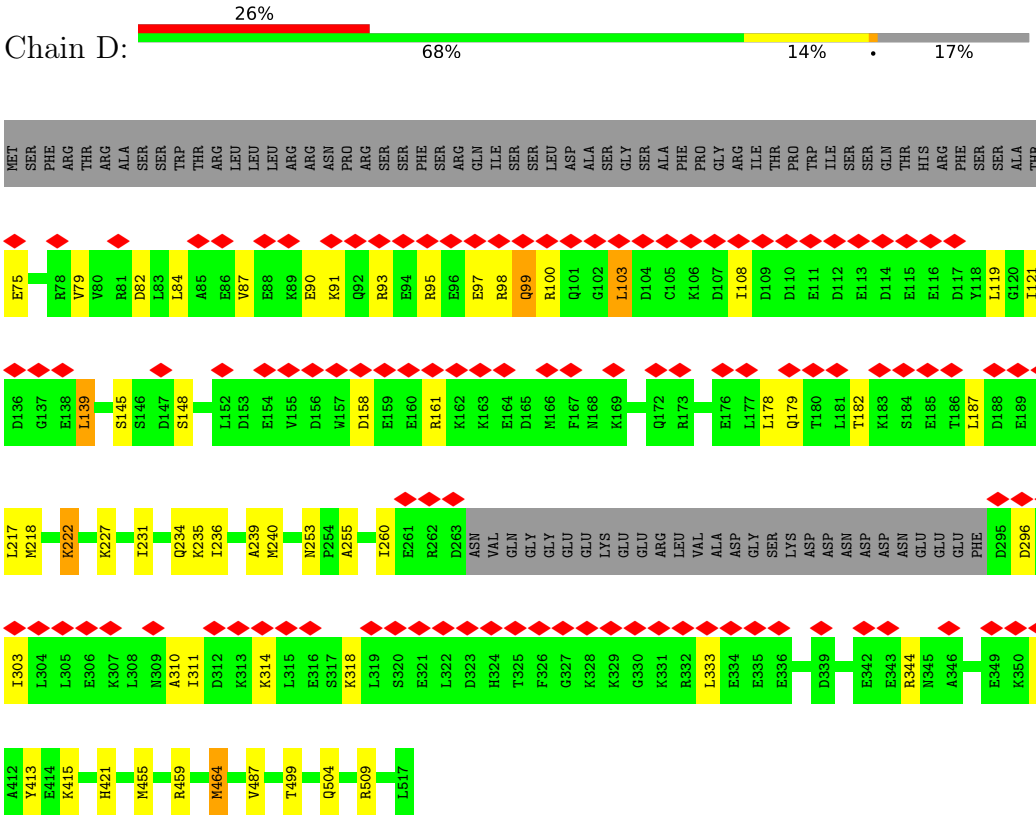
• Molecule 54: uS4m

Chain C:



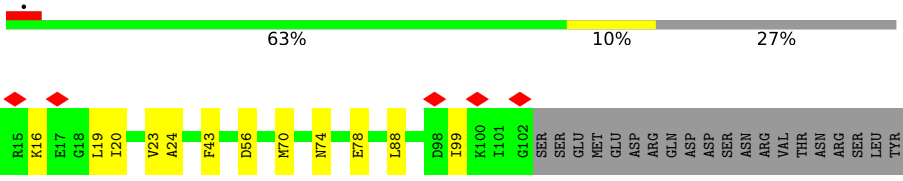
• Molecule 55: S5 DRBM domain-containing protein

Chain D:



• Molecule 56: bS6m

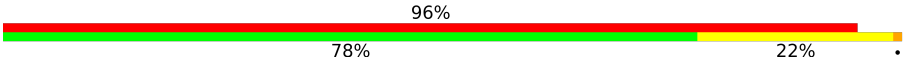
Chain E:

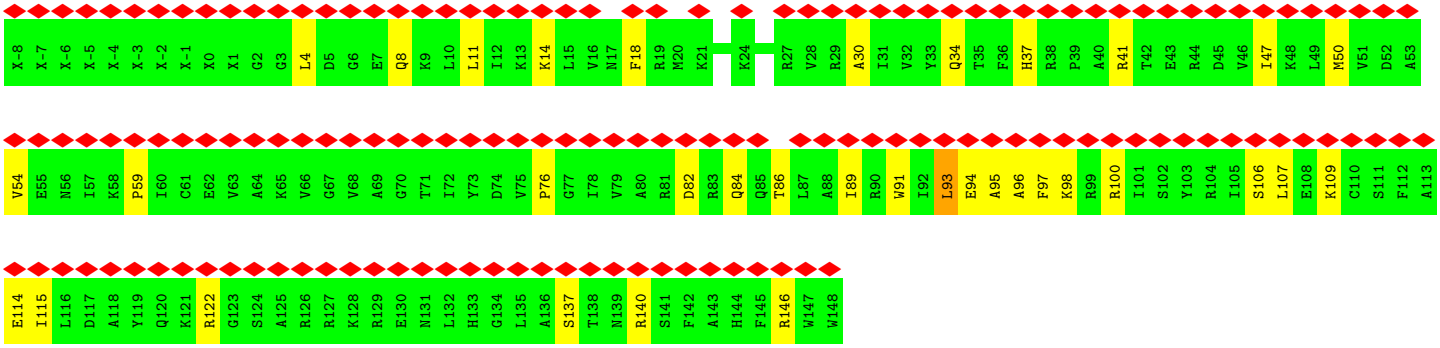




• Molecule 57: uS7m

Chain F:





• Molecule 58: uS8m

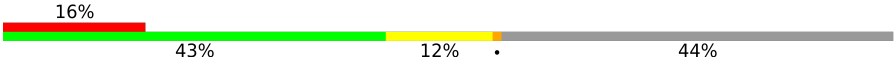
Chain G:

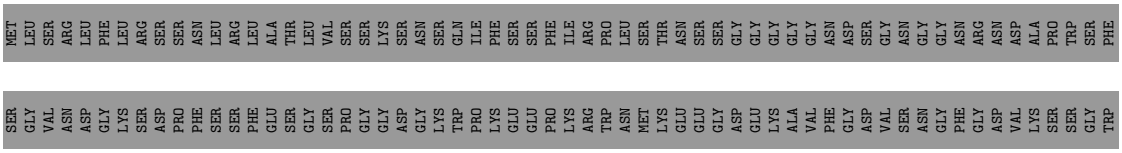


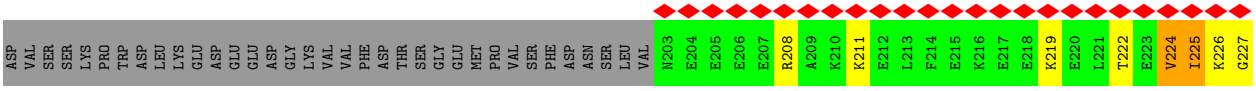


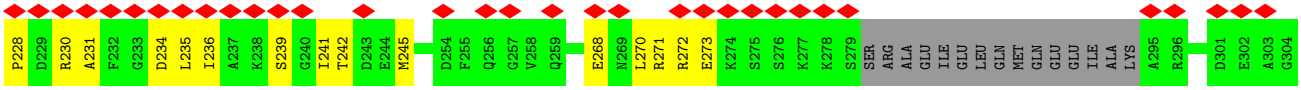
• Molecule 59: 30S ribosomal protein S9

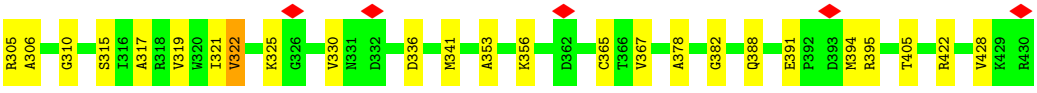
Chain H:









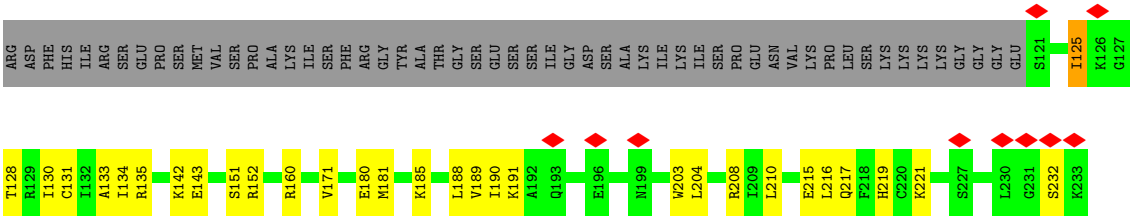


• Molecule 60: Small ribosomal subunit protein uS10 domain-containing protein

Chain I:

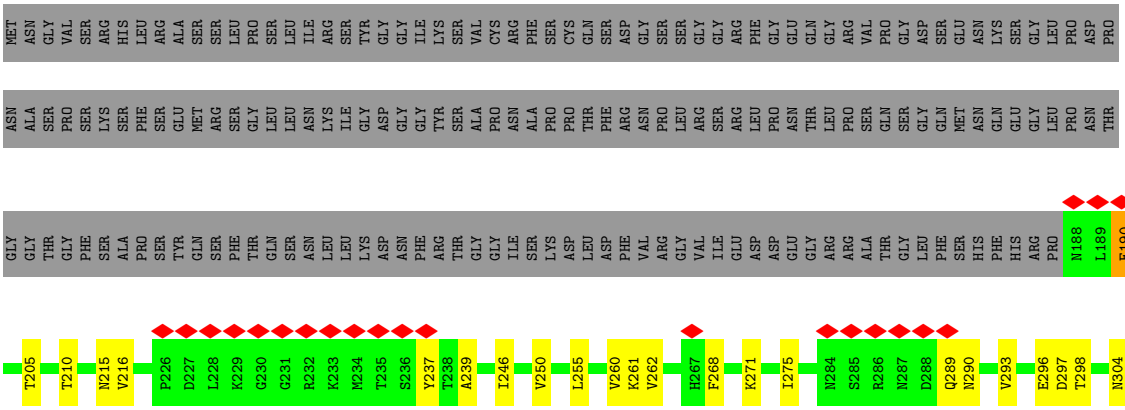




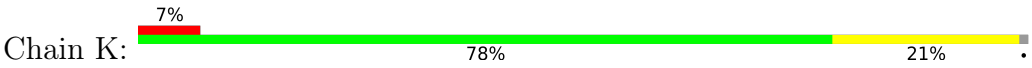


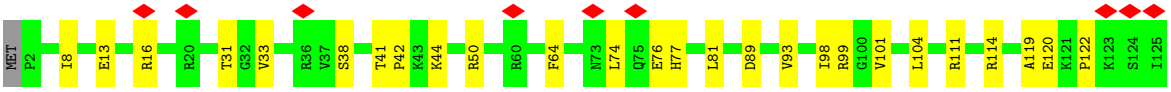
• Molecule 61: Ribosomal protein S11





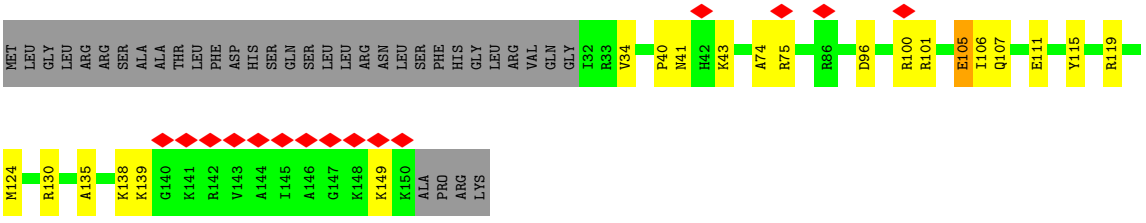
• Molecule 62: uS12m





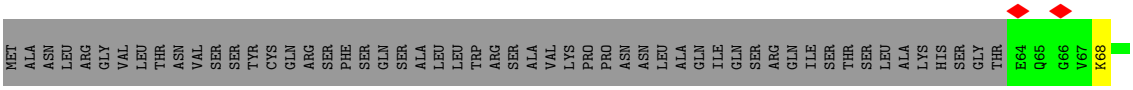
• Molecule 63: uS13m

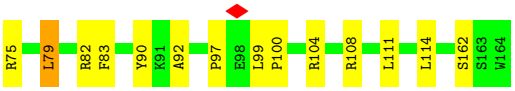




• Molecule 64: Small ribosomal subunit protein uS14m



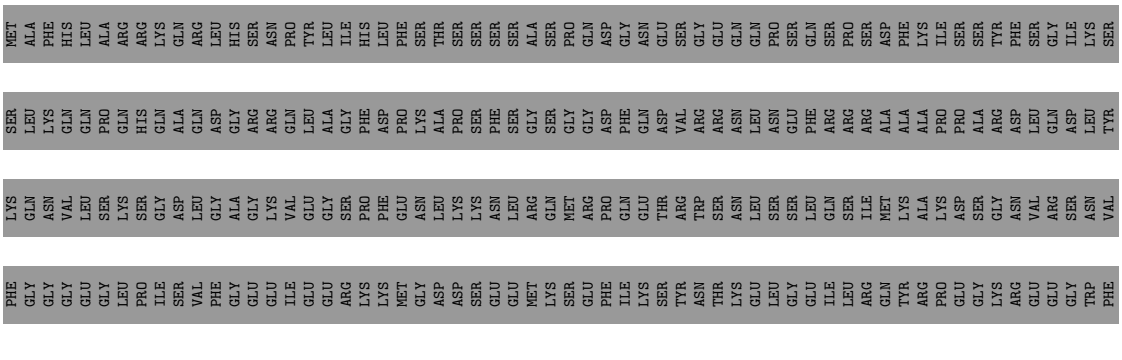




• Molecule 65: Small ribosomal subunit protein uS15c

Chain N:

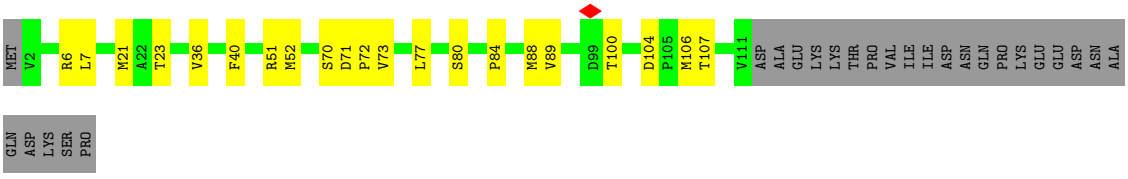




• Molecule 66: 30S ribosomal protein S16

Chain O:

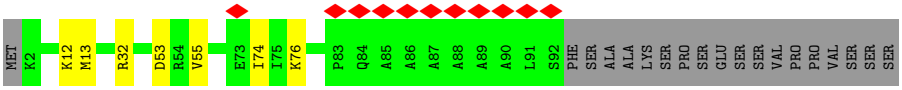




• Molecule 67: Small ribosomal subunit protein uS17c

Chain P:

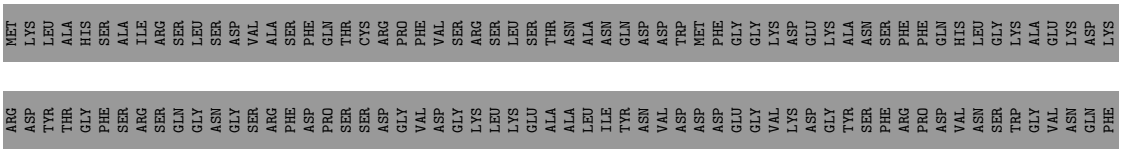




• Molecule 68: bS18m

Chain Q:

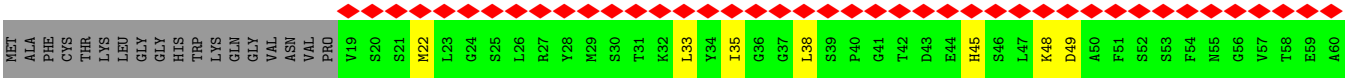


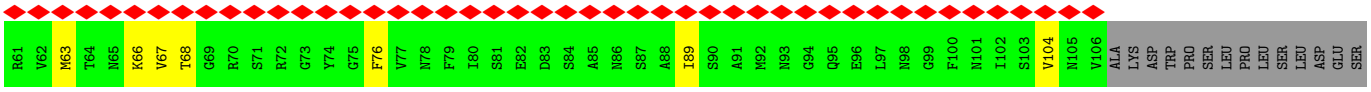


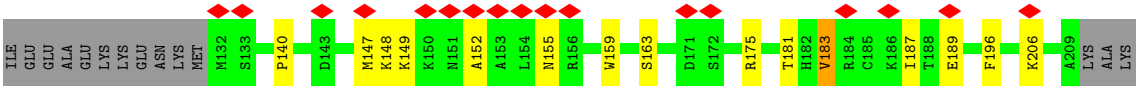


• Molecule 69: uS19m



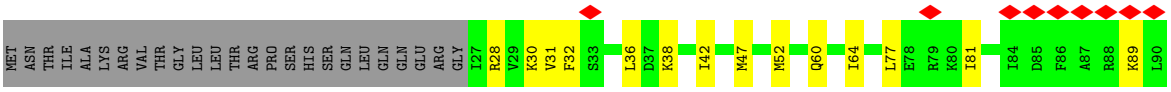


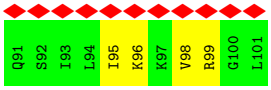




• Molecule 70: Ribosomal protein S21

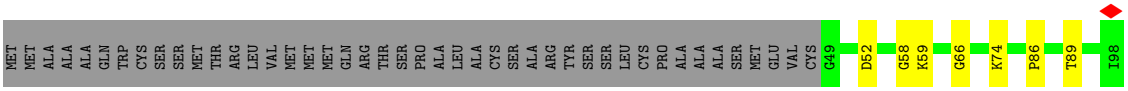




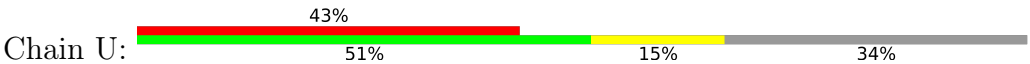


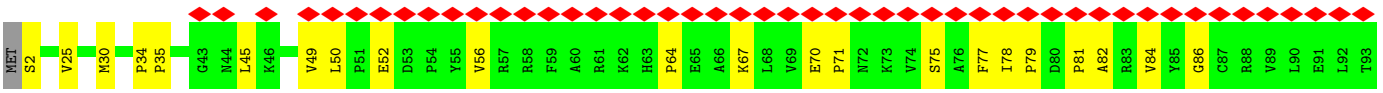
• Molecule 71: 30S ribosomal protein S31, mitochondrial

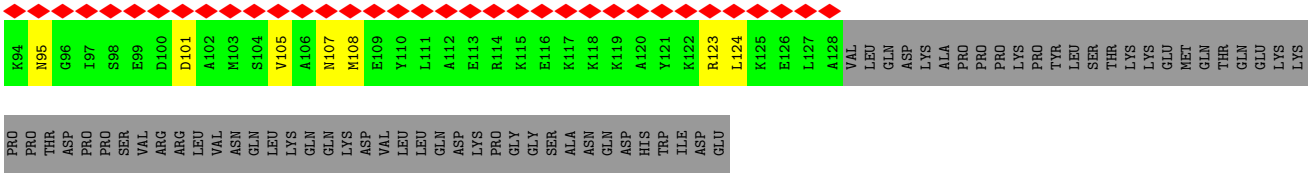




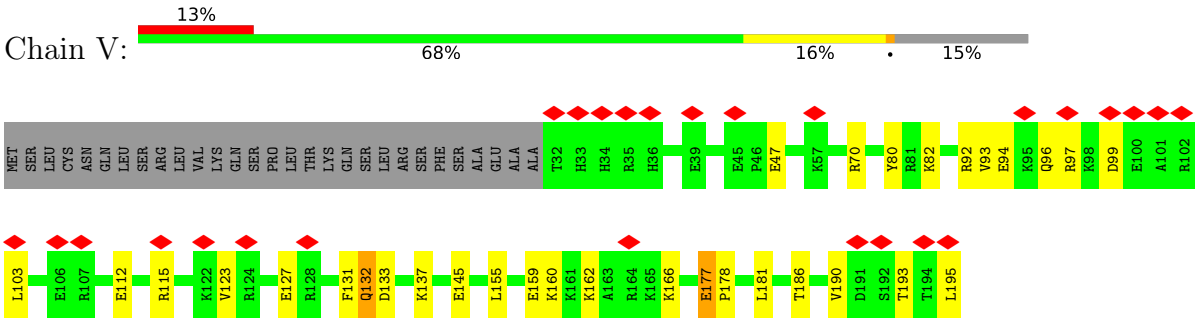
• Molecule 72: Small ribosomal subunit protein mS23



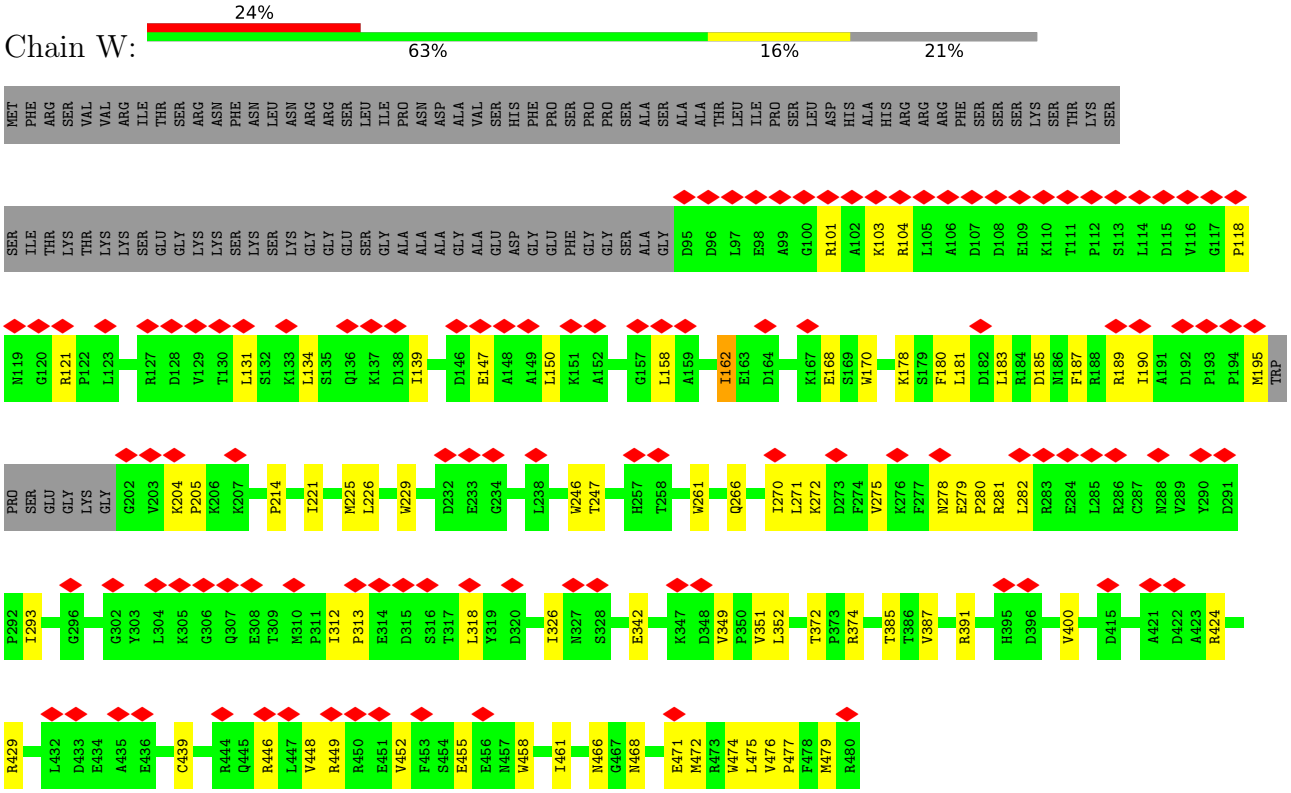




• Molecule 73: mS26

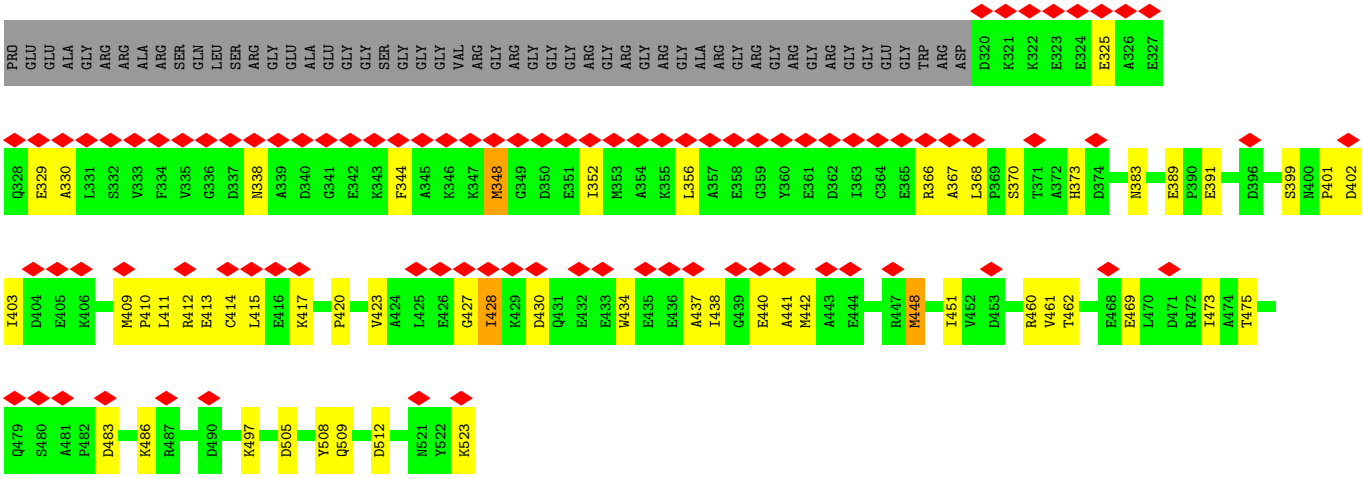


• Molecule 74: Small ribosomal subunit protein mS29



• Molecule 75: mS31/mS46

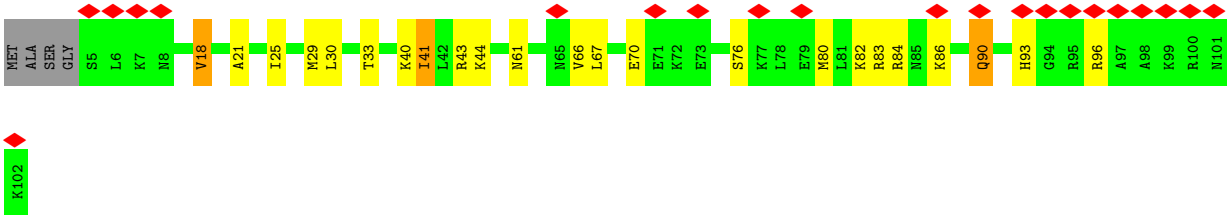




• Molecule 76: MOSC domain-containing protein

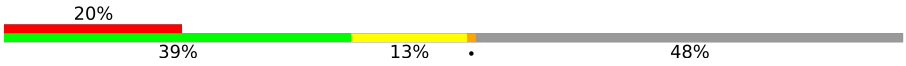
Chain Y:

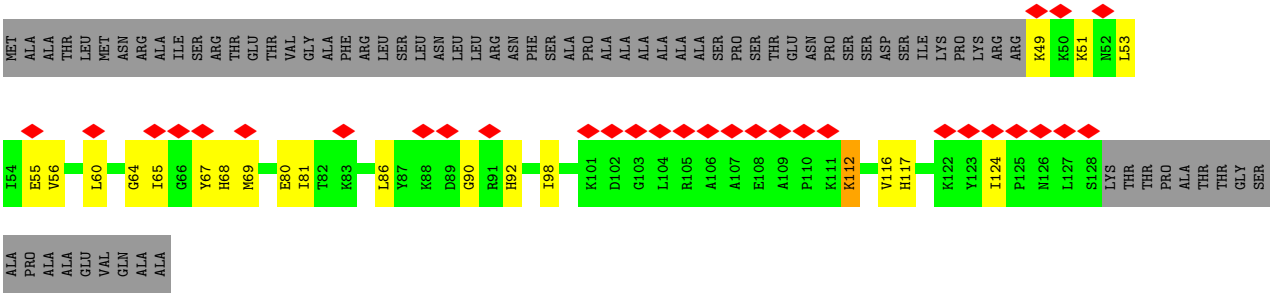




• Molecule 77: mS34

Chain Z:

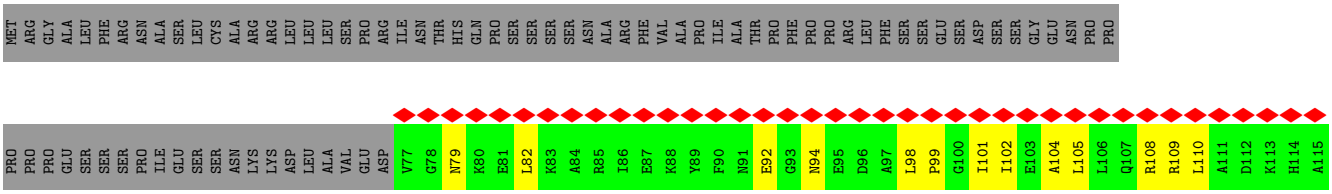


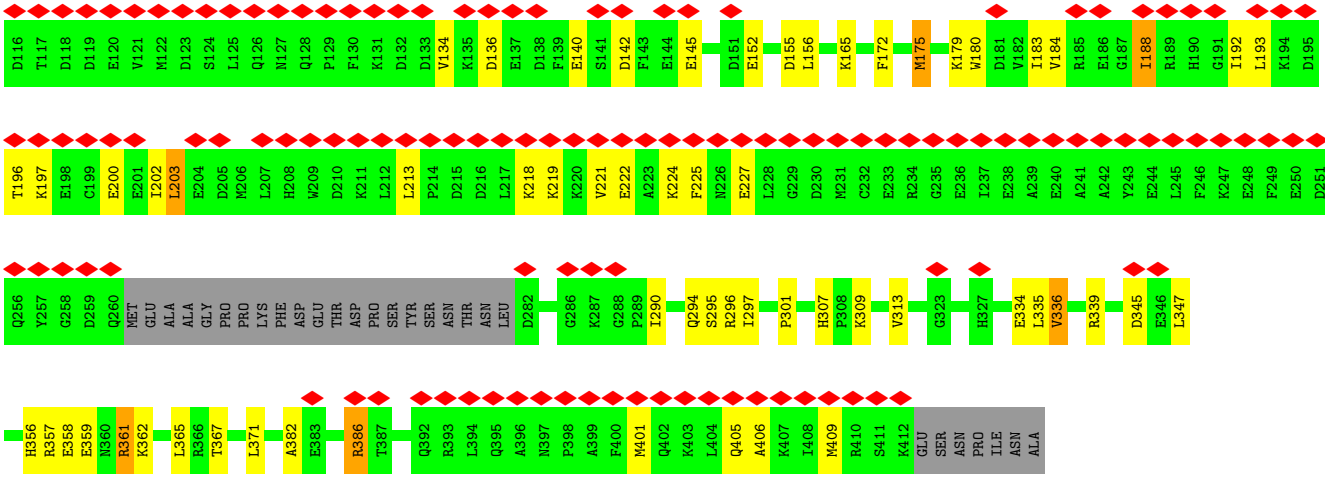


• Molecule 78: Small ribosomal subunit protein mS35 mitochondrial conserved domain-containing protein

Chain a:

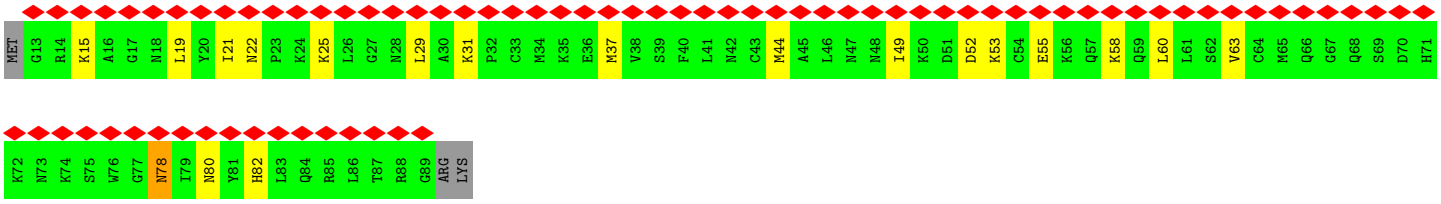






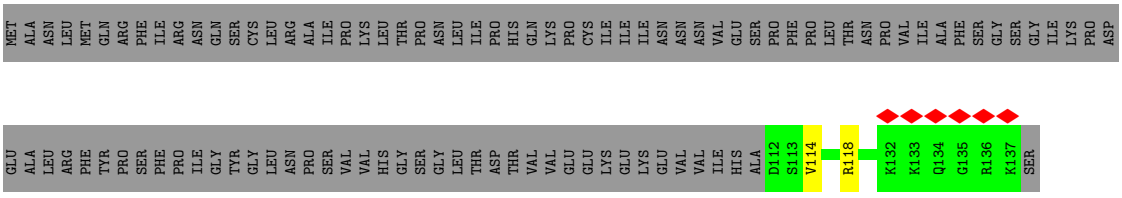
• Molecule 79: mS37





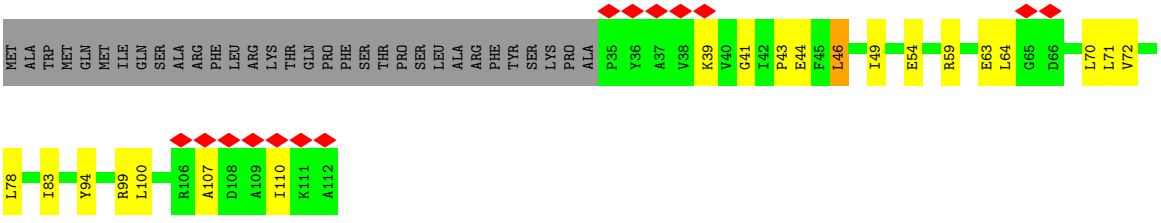
• Molecule 80: Small ribosomal subunit protein mS38





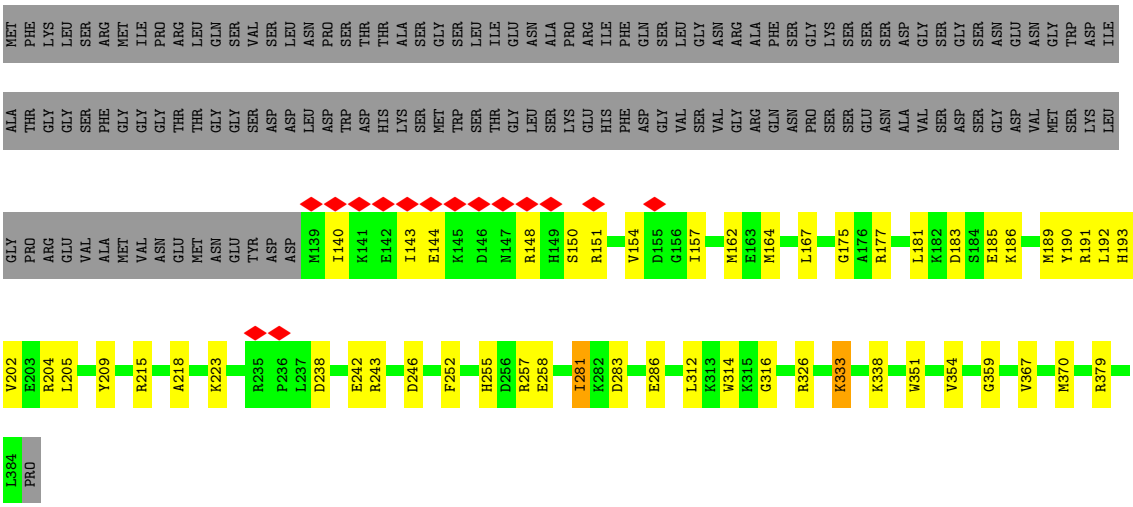
• Molecule 81: Small ribosomal subunit protein mS41 SAM domain-containing protein





• Molecule 82: mS45

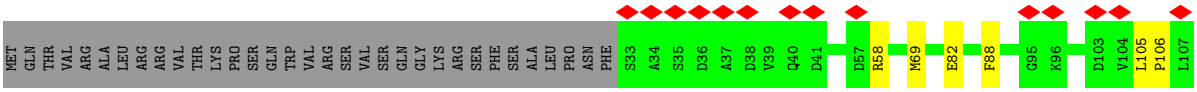


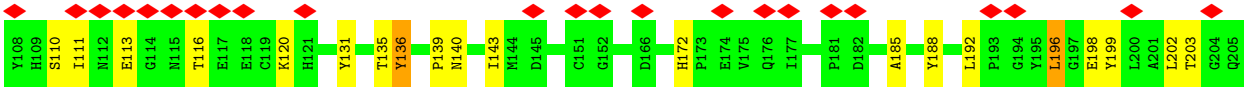


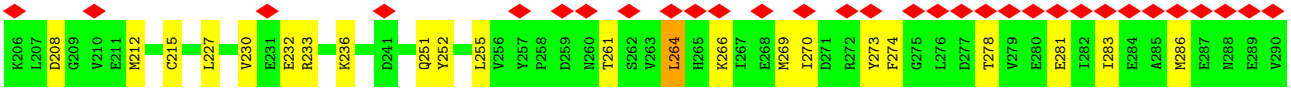
• Molecule 83: mS47

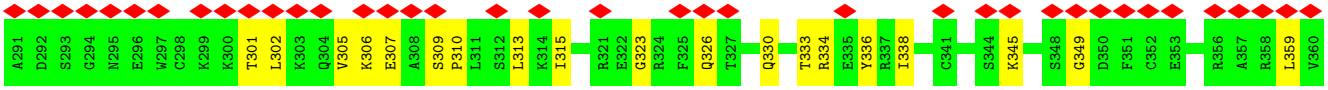
Chain f:

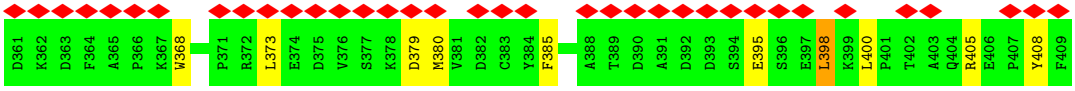








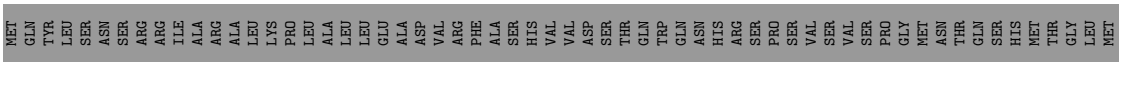


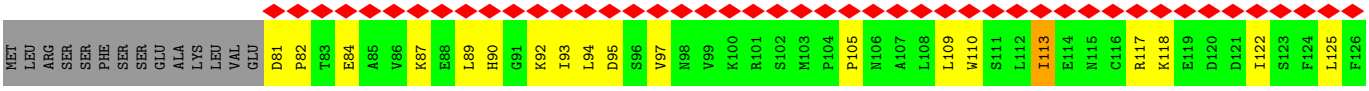


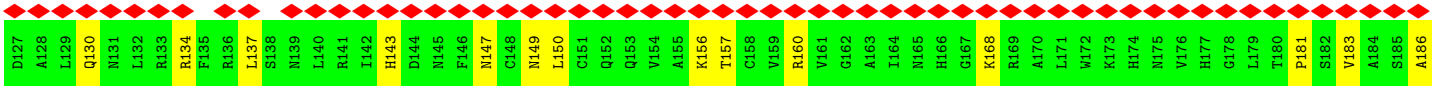
• Molecule 84: Adenylyl cyclase

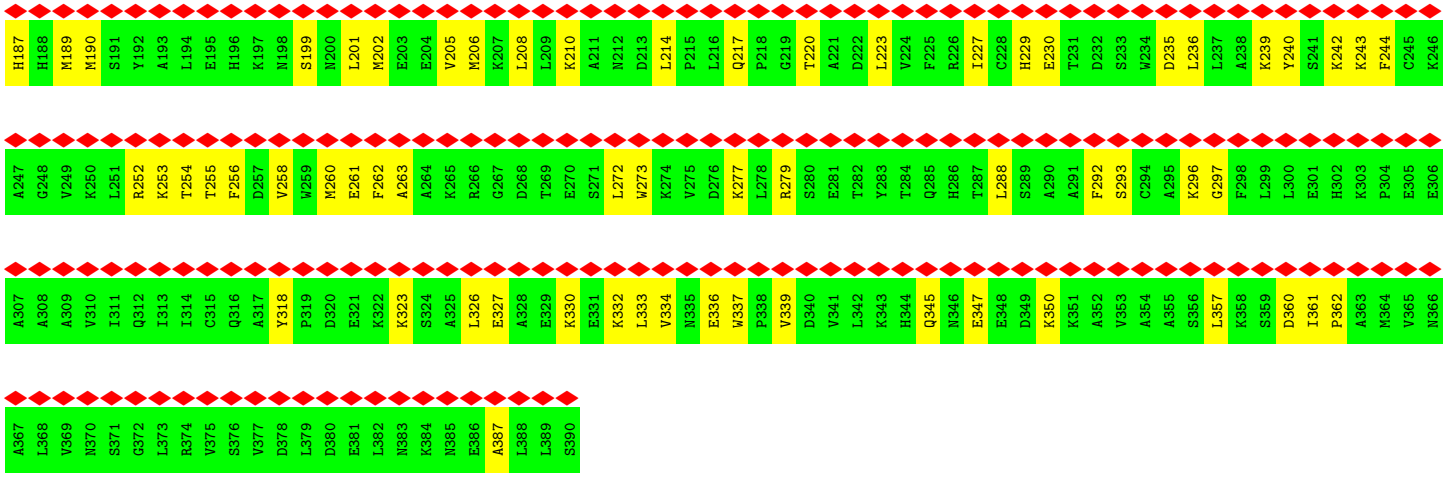
Chain h:





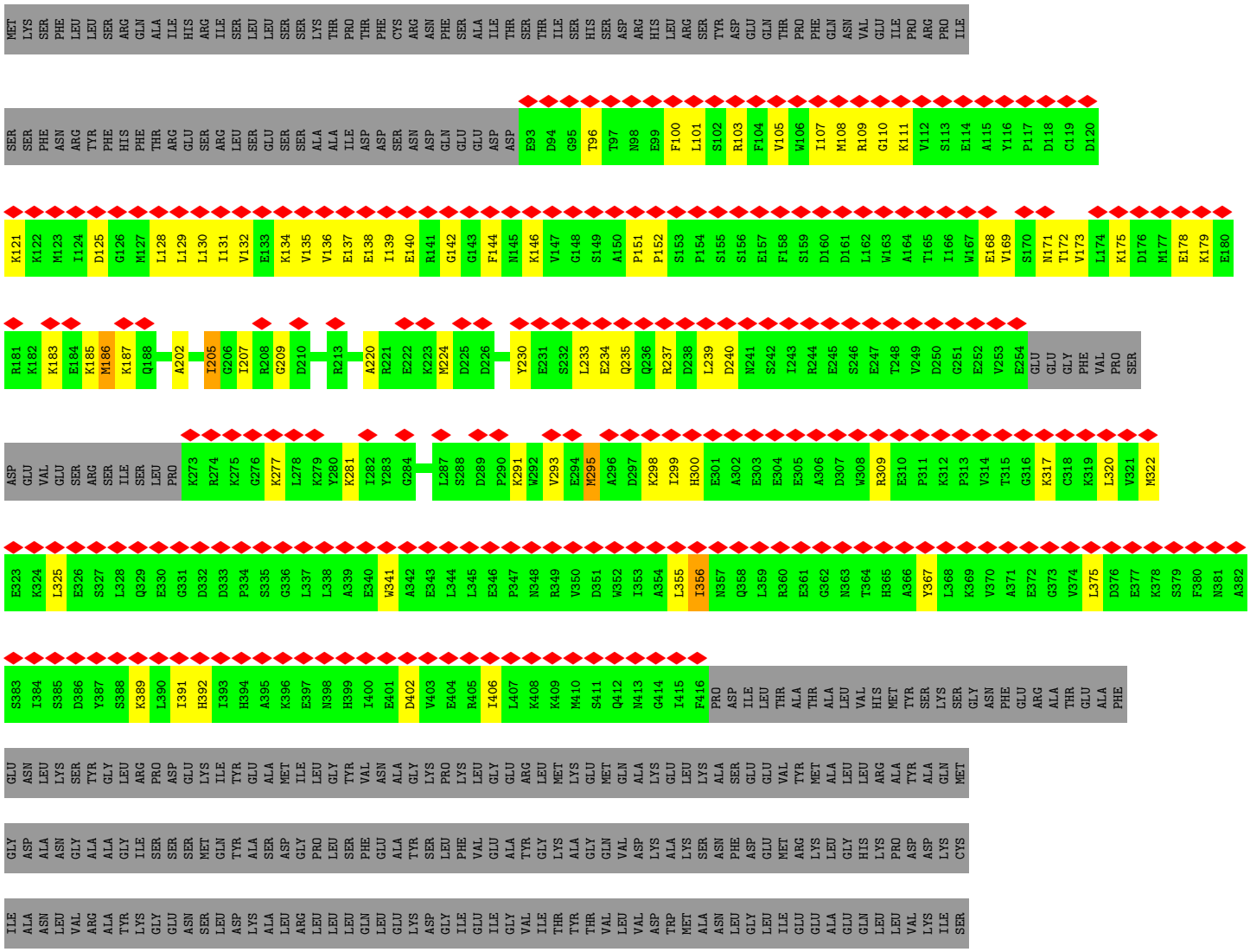


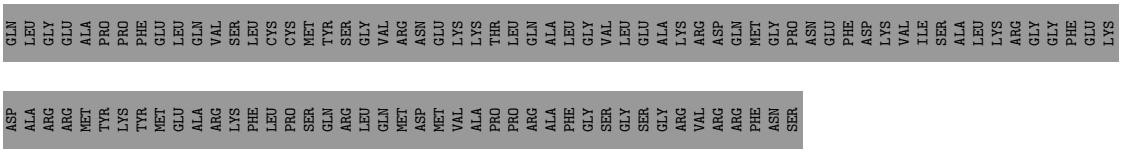




- Molecule 85: PROP1-like PPR domain-containing protein



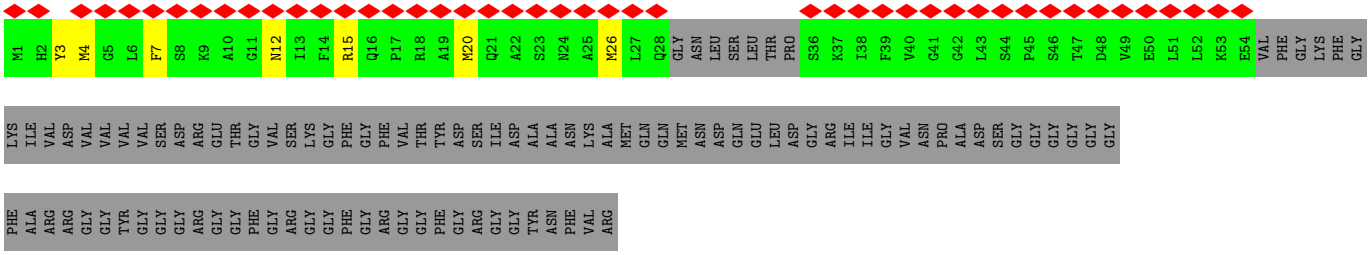




• Molecule 86: RRM domain-containing protein

Chain k:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	18503	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	3.011	Depositor
Minimum map value	-0.579	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	730.296, 730.296, 730.296	wwPDB
Map dimensions	756, 756, 756	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.94, 0.94, 0.94	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, MG, OMG, ZN, 5MU, 4OC, PSU, CLM, H2U, OMC, 2MA, OMU, MA6, UR3, K, 2MG, G7M

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	1	0.35	0/69733	0.77	33/108691 (0.0%)
2	1B	0.16	0/1347	0.37	0/1797
3	1C	0.16	0/1727	0.36	0/2311
4	1D	0.17	0/2099	0.34	0/2836
5	1E	0.15	0/1786	0.30	0/2412
6	1F	0.15	0/1313	0.37	0/1772
7	1G	0.15	0/796	0.39	0/1067
8	1H	0.14	0/547	0.37	0/731
9	1I	0.14	0/1054	0.39	0/1417
10	1J	0.17	0/1155	0.47	0/1563
11	1K	0.17	0/1553	0.32	0/2080
12	1L	0.15	0/976	0.35	0/1304
13	1M	0.17	0/1682	0.37	0/2248
14	1N	0.16	0/1184	0.35	0/1580
15	1O	0.16	0/1255	0.33	0/1687
16	1P	0.15	0/895	0.38	0/1206
17	1Q	0.15	0/1022	0.31	0/1368
18	1R	0.17	0/930	0.30	0/1234
19	1S	0.17	0/1192	0.33	0/1602
20	1T	0.18	0/1259	0.36	0/1687
21	1U	0.16	0/1065	0.37	0/1421
22	1V	0.16	0/1247	0.34	0/1681
23	1W	0.15	0/1613	0.41	0/2180
24	1X	0.14	0/1703	0.36	0/2307
25	1Y	0.16	0/785	0.31	0/1051
26	1Z	0.15	0/1466	0.39	1/1954 (0.1%)
27	1a	0.16	0/946	0.36	0/1262
28	1b	0.17	0/818	0.40	0/1099
29	1c	0.13	0/501	0.33	0/666
30	1d	0.17	0/387	0.30	0/514
31	1e	0.16	0/468	0.30	0/618

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	1f	0.17	0/370	0.29	0/486
33	1g	0.17	0/789	0.34	0/1048
34	1h	0.12	0/312	0.28	0/409
35	1i	0.13	0/1440	0.32	0/1927
36	1j	0.17	0/586	0.33	0/789
37	1k	0.16	0/970	0.35	0/1309
38	1l	0.16	0/1792	0.44	1/2423 (0.0%)
39	1m	0.12	0/987	0.35	0/1331
40	1o	0.15	0/637	0.44	0/860
41	1p	0.15	0/1014	0.35	0/1349
42	1q	0.16	0/394	0.31	0/527
43	1r	0.17	0/750	0.40	0/1005
44	1s	0.17	0/1001	0.35	0/1327
45	1t	0.15	0/3919	0.41	0/5272
46	1u	0.17	0/5345	0.48	1/7180 (0.0%)
47	1v	0.15	0/3497	0.38	0/4681
48	2	0.31	0/37259	0.74	13/58092 (0.0%)
49	3	0.31	0/2810	0.79	1/4378 (0.0%)
50	5	0.31	0/1834	0.80	1/2854 (0.0%)
51	6	0.80	0/144	1.06	0/222
52	A	0.16	0/1647	0.36	0/2227
53	B	0.16	0/3969	0.41	0/5320
54	C	0.15	0/2865	0.38	0/3836
55	D	0.19	0/3474	0.45	3/4647 (0.1%)
56	E	0.16	0/838	0.37	0/1121
57	F	0.16	0/1225	0.45	0/1641
58	G	0.15	0/1054	0.33	0/1418
59	H	0.18	0/1707	0.44	0/2287
60	I	0.16	0/964	0.40	0/1293
61	J	0.15	0/1000	0.36	0/1340
62	K	0.17	0/1009	0.38	0/1345
63	L	0.15	0/950	0.44	0/1263
64	M	0.17	0/856	0.39	0/1134
65	N	0.15	0/958	0.34	0/1280
66	O	0.18	0/890	0.41	0/1196
67	P	0.14	0/730	0.33	0/984
68	Q	0.15	0/733	0.38	0/978
69	R	0.14	0/1323	0.43	0/1772
70	S	0.15	0/614	0.34	0/809
71	T	0.15	0/416	0.29	0/547
72	U	0.17	0/1036	0.44	0/1395
73	V	0.14	0/1423	0.37	0/1895
74	W	0.15	0/3139	0.37	0/4250

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
75	X	0.17	0/1644	0.44	0/2216
76	Y	0.15	0/807	0.37	0/1077
77	Z	0.14	0/669	0.42	0/900
78	a	0.17	0/2524	0.42	0/3387
79	b	0.15	0/618	0.41	0/822
80	c	0.13	0/233	0.24	0/296
81	d	0.14	0/628	0.43	0/840
82	e	0.16	0/2118	0.40	0/2828
83	f	0.16	0/2981	0.42	0/4033
84	h	0.15	0/2507	0.42	0/3384
85	i	0.14	0/2532	0.39	0/3400
86	k	0.15	0/317	0.43	0/424
All	All	0.26	0/220752	0.62	54/320400 (0.0%)

There are no bond length outliers.

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	3166[A]	C	N1-C2-O2	8.46	123.98	118.90
1	1	2811	U	C2-N1-C1'	8.19	127.52	117.70
1	1	3166[A]	C	C2-N1-C1'	8.14	127.75	118.80
48	2	1706	C	C2-N1-C1'	7.32	126.86	118.80
48	2	1387	C	C2-N1-C1'	7.32	126.85	118.80
1	1	1471	U	C2-N1-C1'	7.28	126.43	117.70
1	1	3166[A]	C	N3-C2-O2	-7.17	116.88	121.90
1	1	1667	C	C2-N1-C1'	7.07	126.58	118.80
1	1	1667	C	N1-C2-O2	6.80	122.98	118.90
1	1	2080	C	N3-C2-O2	-6.71	117.20	121.90
1	1	137	U	C2-N1-C1'	6.71	125.75	117.70
48	2	1387	C	N1-C2-O2	6.62	122.87	118.90
1	1	2811	U	N1-C2-O2	6.61	127.42	122.80
26	1Z	120	ASP	N-CA-CB	-6.48	106.79	114.17
1	1	137	U	N1-C2-O2	6.34	127.23	122.80
1	1	137	U	N3-C2-O2	-6.28	117.80	122.20
1	1	3106	C	C2-N1-C1'	6.16	125.57	118.80
50	5	29	C	C2-N1-C1'	5.93	125.32	118.80
38	1l	76	ARG	CA-CB-CG	5.80	125.70	114.10
1	1	1685	U	C2-N1-C1'	5.76	124.61	117.70
1	1	1667	C	N3-C2-O2	-5.75	117.87	121.90
1	1	2811	U	C6-N1-C1'	-5.69	113.23	121.20
49	3	67	C	C2-N1-C1'	5.65	125.01	118.80
1	1	1921	C	C2-N1-C1'	5.64	125.00	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	3166[A]	C	C6-N1-C1'	-5.59	114.09	120.80
48	2	441	U	C2-N1-C1'	5.59	124.41	117.70
48	2	1750	C	N1-C2-O2	5.58	122.25	118.90
48	2	1750	C	C2-N1-C1'	5.54	124.89	118.80
48	2	1706	C	C6-N1-C1'	-5.53	114.17	120.80
1	1	1242	C	C2-N1-C1'	5.46	124.81	118.80
1	1	3166[A]	C	C6-N1-C2	-5.46	118.12	120.30
1	1	49	G	C4-N9-C1'	5.45	133.59	126.50
48	2	1421	C	C2-N1-C1'	5.42	124.77	118.80
1	1	646	A	O5'-C5'-C4'	5.39	113.71	109.40
55	D	103	LEU	CA-CB-CG	5.34	134.99	116.30
1	1	2606	C	C2-N1-C1'	5.34	124.67	118.80
1	1	1217	G	N9-C1'-C2'	5.33	117.87	112.00
1	1	2811	U	N3-C2-O2	-5.33	118.47	122.20
48	2	1387	C	N3-C2-O2	-5.30	118.19	121.90
1	1	2255	A	O5'-C5'-C4'	5.29	113.64	109.40
1	1	496	C	N1-C2-O2	5.25	122.05	118.90
48	2	400	C	C2-N1-C1'	5.25	124.57	118.80
1	1	1471	U	N1-C2-O2	5.24	126.47	122.80
1	1	1598	C	P-O3'-C3'	5.17	125.90	119.70
48	2	1029	C	C2-N1-C1'	5.13	124.45	118.80
1	1	312	A	P-O3'-C3'	5.12	125.84	119.70
55	D	99	GLN	CA-C-N	-5.11	112.92	120.28
55	D	99	GLN	C-N-CA	-5.11	112.92	120.28
1	1	2811	U	C5-C6-N1	5.06	125.23	122.70
1	1	1472	U	C2-N1-C1'	5.06	123.77	117.70
46	1u	191	LEU	CA-CB-CG	5.05	133.99	116.30
48	2	1387	C	C6-N1-C1'	-5.04	114.76	120.80
1	1	487	U	P-O3'-C3'	5.02	125.73	119.70
48	2	476	C	N1-C2-O2	5.01	121.90	118.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	62518	0	31502	513	0
2	1B	1325	0	1398	11	0
3	1C	1696	0	1745	22	0
4	1D	2045	0	2080	15	0
5	1E	1753	0	1815	10	0
6	1F	1286	0	1280	24	0
7	1G	779	0	810	8	0
8	1H	539	0	574	9	0
9	1I	1036	0	1084	26	0
10	1J	1129	0	1166	30	0
11	1K	1526	0	1586	12	0
12	1L	966	0	1048	13	0
13	1M	1649	0	1765	11	0
14	1N	1160	0	1206	16	0
15	1O	1231	0	1262	9	0
16	1P	878	0	939	10	0
17	1Q	1008	0	1101	7	0
18	1R	915	0	946	7	0
19	1S	1170	0	1226	8	0
20	1T	1241	0	1346	12	0
21	1U	1048	0	1123	10	0
22	1V	1223	0	1277	16	0
23	1W	1588	0	1663	35	0
24	1X	1670	0	1751	17	0
25	1Y	768	0	792	7	0
26	1Z	1441	0	1485	20	0
27	1a	928	0	959	11	0
28	1b	803	0	845	5	0
29	1c	489	0	511	11	0
30	1d	379	0	416	3	0
31	1e	459	0	491	3	0
32	1f	364	0	398	2	0
33	1g	770	0	841	3	0
34	1h	309	0	337	3	0
35	1i	1424	0	1482	19	0
36	1j	570	0	593	7	0
37	1k	952	0	987	11	0
38	1l	1741	0	1707	34	0
39	1m	970	0	979	16	0
40	1o	626	0	657	17	0
41	1p	992	0	1027	8	0
42	1q	390	0	421	4	0
43	1r	735	0	781	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	1s	985	0	1072	4	0
45	1t	3856	0	3912	79	0
46	1u	5264	0	5353	154	0
47	1v	3440	0	3497	71	0
48	2	33425	0	16848	294	0
49	3	2513	0	1275	11	0
50	5	1641	0	831	22	0
51	6	129	0	65	3	0
52	A	1611	0	1633	19	0
53	B	3877	0	4008	91	0
54	C	2811	0	2986	63	0
55	D	3425	0	3453	62	0
56	E	823	0	879	9	0
57	F	1254	0	1268	25	0
58	G	1037	0	1058	8	0
59	H	1682	0	1726	43	0
60	I	941	0	970	21	0
61	J	988	0	1022	17	0
62	K	992	0	1051	15	0
63	L	940	0	989	17	0
64	M	843	0	884	10	0
65	N	941	0	978	8	0
66	O	869	0	898	14	0
67	P	717	0	755	4	0
68	Q	724	0	744	10	0
69	R	1299	0	1307	20	0
70	S	611	0	687	14	0
71	T	408	0	444	4	0
72	U	1014	0	1061	23	0
73	V	1399	0	1427	26	0
74	W	3062	0	3030	48	0
75	X	1613	0	1559	42	0
76	Y	793	0	834	16	0
77	Z	649	0	662	14	0
78	a	2487	0	2382	62	0
79	b	610	0	626	17	0
80	c	232	0	278	1	0
81	d	616	0	674	12	0
82	e	2074	0	2074	46	0
83	f	2922	0	2870	52	0
84	h	2460	0	2478	73	0
85	i	2487	0	2450	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	k	314	0	261	8	0
87	1	251	0	0	0	0
87	1D	1	0	0	0	0
87	1j	1	0	0	0	0
87	1q	1	0	0	0	0
87	2	97	0	0	0	0
87	3	3	0	0	0	0
87	D	1	0	0	0	0
87	T	1	0	0	0	0
87	W	1	0	0	0	0
88	1	57	0	0	0	0
88	1B	2	0	0	0	0
88	1E	1	0	0	0	0
88	2	14	0	0	0	0
89	1	20	0	11	1	0
90	1d	1	0	0	0	0
90	1h	1	0	0	0	0
91	W	31	0	12	0	0
All	All	207751	0	160684	2384	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 6.

All (2384) 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)
48:2:1726:U:H3	48:2:1744:C:N4	1.66	0.94
48:2:1726:U:H3	48:2:1744:C:H42	0.90	0.88
37:1k:10:GLN:HE22	37:1k:63:ARG:HG2	1.38	0.88
53:B:234:LEU:HD21	75:X:441:ALA:HB2	1.57	0.85
1:1:1257:G:H5"	9:1I:57:ASN:HD21	1.42	0.85
48:2:1737:A:H3'	48:2:1738:G:H21	1.42	0.84
54:C:310:LYS:H	54:C:310:LYS:HD3	1.45	0.81
48:2:161:A:H2'	48:2:162:C:H4'	1.60	0.81
47:1v:190:ARG:HG2	47:1v:193:GLN:HG3	1.62	0.80
53:B:391:GLU:HG2	78:a:109:ARG:HE	1.48	0.79
1:1:1594:G:H1	1:1:1657:U:H3	0.80	0.79
48:2:1745:A:H5'	84:h:110:TRP:HE1	1.47	0.79
1:1:2270:A:H61	12:1L:50:MET:HE3	1.48	0.78
79:b:55:GLU:HA	79:b:58:LYS:HG2	1.66	0.78
74:W:131:LEU:HD22	74:W:134:LEU:HD11	1.64	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:1t:380:VAL:HG12	45:1t:416:LEU:HD13	1.65	0.76
78:a:192:ILE:HG23	78:a:193:LEU:HD22	1.65	0.76
54:C:231:ARG:HH12	54:C:308:ARG:HG3	1.50	0.76
54:C:117:LEU:HD23	54:C:122:GLN:HG2	1.67	0.76
46:1u:534:MET:HE3	46:1u:539:VAL:HB	1.68	0.75
56:E:16:LYS:O	56:E:20:ILE:HD12	1.87	0.75
82:e:312:LEU:HD21	82:e:370:MET:HE1	1.69	0.75
77:Z:69:MET:HG3	77:Z:81:ILE:HD11	1.68	0.75
1:1:2415:A:H61	1:1:2495:G:H1	1.32	0.75
1:1:228:U:H3	1:1:240:A:H2	1.34	0.75
1:1:3000:C:H5'	1:1:3153:A:H5'	1.67	0.75
77:Z:51:LYS:HB3	77:Z:55:GLU:HB2	1.69	0.75
75:X:423:VAL:HG22	75:X:428:ILE:HD11	1.68	0.74
1:1:1026:G:H1	1:1:1043:U:H3	1.35	0.74
48:2:669:G:H2'	48:2:670:G:C8	2.22	0.74
82:e:283:ASP:HB3	82:e:286:GLU:HG2	1.70	0.74
1:1:1575:A:H5'	45:1t:91:SER:HB3	1.69	0.74
82:e:162:MET:HA	82:e:162:MET:HE3	1.69	0.74
84:h:292:PHE:HZ	84:h:333:LEU:HB2	1.52	0.74
24:1X:124:ARG:HH21	24:1X:128:GLY:H	1.36	0.74
83:f:230:VAL:HG22	83:f:252:TYR:HB3	1.69	0.73
72:U:67:LYS:HB3	72:U:81:PRO:HG3	1.69	0.73
54:C:289:LEU:HG	82:e:154:VAL:HG21	1.70	0.73
55:D:239:ALA:HB2	85:i:205:ILE:HD11	1.70	0.73
48:2:26:U:H3	48:2:910:G:H1	1.35	0.73
59:H:219:LYS:HZ3	72:U:124:LEU:HA	1.52	0.73
46:1u:612:GLU:HA	46:1u:615:MET:HG2	1.70	0.73
57:F:14:LYS:HD2	57:F:89:ILE:HD12	1.70	0.73
59:H:391:GLU:HG2	59:H:394:MET:HE2	1.71	0.73
2:1B:55:ILE:HA	2:1B:58:MET:HE3	1.71	0.72
46:1u:735:GLN:CD	46:1u:735:GLN:H	1.96	0.72
61:J:205:THR:HG21	61:J:239:ALA:HA	1.70	0.72
46:1u:173:LEU:HD11	46:1u:187:MET:HG2	1.70	0.72
3:1C:168:PHE:O	3:1C:172:SER:HB3	1.89	0.72
59:H:272:ARG:HH11	59:H:273:GLU:HA	1.53	0.72
73:V:93:VAL:HA	73:V:96:GLN:HE21	1.54	0.72
45:1t:468:ARG:H	45:1t:468:ARG:HD2	1.54	0.72
48:2:151:A:H5"	48:2:152:G:H5'	1.71	0.72
52:A:9:GLN:HE22	59:H:236:ILE:HG12	1.54	0.72
24:1X:54:ILE:HA	24:1X:101:GLN:HE22	1.55	0.71
62:K:114:ARG:HB2	62:K:119:ALA:HB3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1026:G:N2	1:1:1043:U:O2	2.23	0.71
60:I:131:CYS:HB2	60:I:217:GLN:HB2	1.73	0.71
48:2:660:G:H22	48:2:737:G:H1	1.39	0.71
83:f:136:TYR:HD2	83:f:140:ASN:HD22	1.35	0.71
48:2:163:A:H4'	48:2:164:A:H5'	1.73	0.71
1:1:1325:G:H1	1:1:1331:U:H3	1.38	0.70
38:1l:27:ILE:HG22	38:1l:186:LYS:H	1.56	0.70
46:1u:239:ALA:HB1	46:1u:261:MET:HE1	1.71	0.70
26:1Z:77:GLU:HG3	26:1Z:92:LYS:HG3	1.73	0.70
79:b:22:ASN:HB2	79:b:25:LYS:HB2	1.72	0.70
84:h:168:LYS:HA	84:h:189:MET:HE1	1.73	0.70
45:1t:465:MET:HE3	45:1t:484:LEU:HD22	1.73	0.70
21:1U:131:GLN:HE21	21:1U:134:ARG:HD2	1.54	0.70
74:W:183:LEU:HD21	74:W:226:LEU:HD22	1.74	0.70
85:i:291:LYS:O	85:i:295:MET:HB2	1.92	0.70
35:1i:230:ILE:HB	35:1i:233:TYR:HB2	1.74	0.70
79:b:44:MET:HG3	79:b:49:ILE:HA	1.73	0.70
83:f:310:PRO:HB3	83:f:373:LEU:HB3	1.74	0.70
48:2:613:C:H2'	48:2:614:A:H8	1.57	0.70
53:B:318:ASN:HA	53:B:321:ARG:HE	1.57	0.70
48:2:670:G:H2'	48:2:671:A:H8	1.56	0.69
23:1W:67:LEU:HA	23:1W:75:ARG:HG3	1.73	0.69
46:1u:367:LEU:HD11	46:1u:386:MET:HE1	1.74	0.69
48:2:710:G:H2'	48:2:711:A:C8	2.27	0.69
52:A:58:ALA:HB2	52:A:195:CYS:HB3	1.74	0.69
45:1t:219:MET:HE1	45:1t:227:PRO:HG3	1.73	0.69
45:1t:255:LEU:HD22	45:1t:270:LEU:HD21	1.73	0.69
47:1v:439:MET:HE1	47:1v:451:LEU:HD12	1.74	0.68
48:2:1524:A:H2	48:2:1537:G:H21	1.39	0.68
7:1G:25:ARG:HG2	7:1G:46:ARG:HH12	1.56	0.68
64:M:108:ARG:HG3	69:R:147:MET:HE1	1.74	0.68
1:1:1255:U:H2'	1:1:1256:G:H8	1.57	0.68
14:1N:70:ILE:HG22	14:1N:148:PHE:HB2	1.75	0.68
74:W:131:LEU:HD12	74:W:229:TRP:HB2	1.75	0.68
83:f:315:ILE:HG23	83:f:385:PHE:HE1	1.57	0.68
59:H:388:GLN:HG3	59:H:395:ARG:HG3	1.75	0.68
82:e:333:LYS:HZ3	82:e:354:VAL:HG13	1.59	0.68
53:B:286:ARG:HG2	53:B:321:ARG:HH22	1.57	0.68
1:1:1581:A:N3	45:1t:272:THR:HG21	2.09	0.68
45:1t:448:PHE:HA	45:1t:451:LEU:HB2	1.74	0.68
48:2:709:G:H2'	48:2:710:G:C8	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:W:372:THR:HG22	74:W:374:ARG:H	1.57	0.68
1:1:1001:G:H2'	1:1:1002:A:C8	2.29	0.68
60:I:180:GLU:HG2	64:M:162:SER:HB2	1.76	0.68
47:1v:109:PRO:HD3	47:1v:139:PHE:HE1	1.57	0.67
60:I:125:ILE:HG21	60:I:189:VAL:HG11	1.74	0.67
1:1:2420:G:H1	1:1:2490:U:H3	1.42	0.67
12:1L:91:MET:HE3	12:1L:92:PRO:HD2	1.75	0.67
55:D:464:MET:HE1	55:D:487:VAL:HG22	1.76	0.67
57:F:8:GLN:HB3	57:F:47:ILE:HD11	1.76	0.67
78:a:175:MET:HA	78:a:179:LYS:HD2	1.75	0.67
48:2:1618:G:H2'	48:2:1619:A:C8	2.30	0.67
48:2:172:A:H5'	48:2:173:A:H5"	1.76	0.67
1:1:565:A:H5"	1:1:566:G:H5"	1.77	0.67
53:B:308:ASN:O	53:B:312:HIS:HB2	1.94	0.67
46:1u:331:MET:HE2	46:1u:331:MET:HA	1.77	0.67
52:A:16:SER:HB2	52:A:178:ALA:HB1	1.77	0.67
47:1v:94:ILE:H	47:1v:94:ILE:HD12	1.58	0.66
1:1:1866:U:H3	45:1t:362:ARG:HH21	1.43	0.66
14:1N:127:MET:HE2	14:1N:127:MET:HA	1.78	0.66
59:H:219:LYS:HZ2	72:U:124:LEU:HD23	1.59	0.66
23:1W:38:ALA:HB1	23:1W:83:LEU:HD21	1.75	0.66
53:B:248:GLN:HG3	75:X:460:ARG:HB3	1.77	0.66
45:1t:345:THR:HB	45:1t:378:TYR:HB2	1.77	0.66
73:V:94:GLU:HG2	73:V:97:ARG:HH21	1.60	0.66
70:S:89:LYS:HD3	79:b:19:LEU:HD21	1.77	0.66
29:1c:16:THR:HG23	29:1c:18:SER:H	1.60	0.66
1:1:346:A:H2'	1:1:347:A:H8	1.61	0.65
25:1Y:82:ILE:HG22	25:1Y:83:VAL:HG23	1.77	0.65
46:1u:231:LEU:HD13	46:1u:264:GLY:HA3	1.77	0.65
83:f:270:ILE:O	83:f:274:PHE:HB2	1.96	0.65
49:3:1:A:HO2'	49:3:2:A:H8	1.43	0.65
69:R:35:ILE:HG22	69:R:38:LEU:HD21	1.79	0.65
78:a:406:ALA:HA	78:a:409:MET:HE3	1.78	0.65
48:2:458:U:H4'	54:C:131:ARG:NH2	2.12	0.65
1:1:2494:G:H2'	1:1:2495:G:C8	2.30	0.65
47:1v:287:LEU:HD11	47:1v:306:VAL:HG23	1.79	0.65
53:B:202:LYS:HA	53:B:207:PHE:HD2	1.61	0.65
53:B:480:LYS:HG2	53:B:481:ARG:H	1.62	0.65
46:1u:383:LEU:HA	46:1u:386:MET:HG3	1.78	0.65
66:O:40:PHE:HD1	66:O:52:MET:HB2	1.61	0.65
74:W:204:LYS:HD3	74:W:205:PRO:HD2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:1W:58:ILE:HG21	23:1W:140:ILE:HG13	1.77	0.65
46:1u:705:LEU:HD22	46:1u:708:ILE:HD11	1.79	0.64
48:2:1141:A:H61	48:2:1381:C:H4'	1.62	0.64
1:1:2639:U:H5	16:1P:91:LYS:HE3	1.62	0.64
53:B:239:MET:HA	75:X:448:MET:HE1	1.79	0.64
84:h:210:LYS:HE3	84:h:243:LYS:HE3	1.79	0.64
1:1:1186:G:H1	1:1:1269:G:H22	1.43	0.64
1:1:30:G:H22	1:1:655:G:H1'	1.62	0.64
9:1I:6:ARG:HA	9:1I:9:LEU:HD12	1.80	0.64
38:1l:76:ARG:O	38:1l:76:ARG:HD2	1.97	0.64
63:L:135:ALA:HB3	63:L:139:LYS:HE2	1.78	0.64
37:1k:10:GLN:NE2	37:1k:63:ARG:HG2	2.09	0.64
76:Y:18:VAL:HG22	78:a:335:LEU:HD13	1.78	0.64
10:1J:64:ALA:HB3	10:1J:80:LYS:HB3	1.79	0.64
48:2:1833:U:H2'	48:2:1834:G:C8	2.32	0.64
63:L:41:ASN:HB3	63:L:75:ARG:HB3	1.79	0.64
83:f:192:LEU:HD22	83:f:196:LEU:HB3	1.80	0.64
1:1:513:G:N2	1:1:515:C:H5'	2.13	0.63
35:1i:225:THR:HG22	35:1i:226:LEU:H	1.62	0.63
52:A:86:ARG:HG2	52:A:193:THR:HG23	1.78	0.63
24:1X:221:LYS:HB3	24:1X:245:LYS:HG3	1.79	0.63
47:1v:92:GLN:HB2	47:1v:97:ARG:HH22	1.64	0.63
39:1m:10:ILE:HD11	39:1m:22:CYS:HB2	1.78	0.63
77:Z:86:LEU:HD11	77:Z:90:GLY:HA2	1.79	0.63
83:f:398:LEU:HD21	83:f:400:LEU:HD21	1.80	0.63
5:1E:189:ASN:HB2	5:1E:192:VAL:HG23	1.81	0.63
46:1u:608:ASN:HA	46:1u:611:ILE:HD11	1.81	0.63
48:2:11:A:H5"	48:2:12:A:H5'	1.81	0.63
38:1l:175:PRO:HB3	38:1l:180:PRO:HA	1.80	0.63
48:2:129:A:H2'	48:2:130:A:H8	1.63	0.63
65:N:315:HIS:CD2	65:N:316:PRO:HD2	2.34	0.63
84:h:206:MET:HE2	84:h:240:TYR:HD2	1.62	0.63
46:1u:611:ILE:HD12	46:1u:611:ILE:H	1.64	0.63
10:1J:127:CYS:HA	10:1J:130:MET:HE3	1.81	0.63
74:W:472:MET:O	74:W:476:VAL:HG13	1.98	0.63
12:1L:66:MET:HE3	12:1L:88:LYS:HE3	1.79	0.63
6:1F:167:ASP:HB2	35:1i:214:LEU:HD11	1.79	0.62
1:1:461:G:H5'	22:1V:5:ALA:HB1	1.80	0.62
1:1:1615:C:H41	1:1:1637:U:H3	1.45	0.62
46:1u:446:ALA:HA	46:1u:449:ARG:HH21	1.65	0.62
53:B:103:LYS:HG2	53:B:408:GLY:HA3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:K:99:ARG:HD2	62:K:104:LEU:HD21	1.81	0.62
48:2:1412:C:H2'	48:2:1413:A:H8	1.65	0.62
75:X:412:ARG:HH21	75:X:442:MET:HG3	1.63	0.62
38:1l:32:LEU:HD21	38:1l:112:TYR:HD2	1.65	0.62
47:1v:405:CYS:HB3	47:1v:438:LYS:HZ2	1.63	0.62
1:1:30:G:N2	1:1:655:G:H1'	2.15	0.62
46:1u:437:LEU:HD11	46:1u:453:LEU:HD13	1.79	0.62
48:2:778:A:H62	48:2:796:G:H21	1.48	0.62
48:2:997:G:H22	48:2:1029:C:H5	1.47	0.62
70:S:95:ILE:HA	70:S:98:VAL:HG12	1.80	0.62
53:B:262:ALA:HB2	53:B:332:LEU:HD11	1.81	0.62
82:e:189:MET:HG2	82:e:205:LEU:HD22	1.82	0.62
1:1:345:A:H2'	1:1:346:A:C8	2.35	0.62
1:1:732:C:H2'	1:1:733:A:H8	1.64	0.62
20:1T:249:THR:HG23	30:1d:112:ARG:HD2	1.81	0.62
1:1:277:A:H2'	1:1:278:A:H8	1.64	0.62
29:1c:16:THR:HG22	29:1c:20:ARG:H	1.65	0.62
39:1m:2:LEU:HG	39:1m:38:ASN:HB2	1.80	0.62
53:B:22:TRP:HB3	53:B:64:HIS:HB2	1.82	0.62
1:1:427:A:H2'	1:1:430:G:C8	2.34	0.61
1:1:1594:G:N2	1:1:1657:U:O2	2.26	0.61
53:B:260:PHE:HD1	53:B:333:PHE:HB2	1.65	0.61
53:B:423:MET:HA	53:B:426:PHE:CE2	2.35	0.61
6:1F:36:VAL:HG13	6:1F:95:SER:HB2	1.81	0.61
10:1J:36:LEU:HD22	10:1J:41:LEU:HD12	1.82	0.61
38:1l:35:ARG:HD3	38:1l:103:LEU:HD22	1.82	0.61
46:1u:138:ARG:HB3	46:1u:142:ARG:HH12	1.63	0.61
48:2:1734:A:H2'	48:2:1735:C:H4'	1.83	0.61
59:H:305:ARG:HG2	59:H:322:VAL:HG22	1.82	0.61
85:i:105:VAL:O	85:i:109:ARG:HG2	1.99	0.61
1:1:2957:A:H2'	1:1:2958:A:H8	1.64	0.61
37:1k:59:LYS:HG3	37:1k:69:VAL:HG22	1.82	0.61
48:2:959:G:N2	50:5:35:C:H5'	2.16	0.61
53:B:181:HIS:CD2	53:B:182:PRO:HD2	2.34	0.61
57:F:106:SER:HB2	57:F:109:LYS:HG3	1.81	0.61
48:2:613:C:H2'	48:2:614:A:C8	2.34	0.61
48:2:968:A:H4'	48:2:969:G:H5"	1.82	0.61
53:B:174:ARG:HG3	53:B:175:ILE:HG23	1.80	0.61
60:I:152:ARG:HB2	60:I:189:VAL:HB	1.81	0.61
1:1:151:U:HO2'	1:1:152:C:H6	1.47	0.61
1:1:1594:G:O6	1:1:1657:U:O4	2.18	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1U:110:SER:HA	21:1U:113:LYS:HE2	1.82	0.61
48:2:25:U:H2'	48:2:26:U:C6	2.35	0.61
54:C:136:LYS:HB3	66:O:106:MET:HG2	1.81	0.61
77:Z:65:ILE:HG22	77:Z:81:ILE:HG22	1.82	0.61
78:a:142:ASP:HA	78:a:145:GLU:HG2	1.82	0.61
19:1S:198:THR:HB	19:1S:242:GLN:HB2	1.82	0.61
46:1u:451:ILE:HD12	46:1u:492:LYS:HZ1	1.65	0.61
48:2:1839:G:H2'	48:2:1840:A:C8	2.35	0.61
1:1:1189:C:H42	1:1:1266:C:H42	1.49	0.61
1:1:1576:A:C4	45:1t:159:MET:HE1	2.36	0.61
6:1F:123:ARG:HH21	6:1F:128:GLN:HB2	1.65	0.61
10:1J:100:ARG:HB3	10:1J:104:LEU:HD13	1.83	0.61
52:A:53:ALA:O	52:A:57:VAL:HG23	2.00	0.61
72:U:95:ASN:HA	85:i:389:LYS:HD3	1.83	0.61
85:i:185:LYS:HG2	85:i:224:MET:SD	2.41	0.61
1:1:346:A:H2'	1:1:347:A:C8	2.35	0.61
24:1X:61:ASP:HB3	24:1X:66:ILE:HG12	1.83	0.61
45:1t:341:ILE:HD11	45:1t:356:LEU:HB3	1.83	0.61
47:1v:417:PHE:O	47:1v:421:LYS:HG2	2.00	0.61
66:O:71:ASP:OD1	66:O:72:PRO:HD3	2.01	0.61
74:W:162:ILE:HG13	74:W:221:ILE:HG12	1.82	0.61
4:1D:70:MET:HG2	4:1D:288:ILE:HG23	1.82	0.60
24:1X:83:GLN:HG3	24:1X:158:ILE:HD11	1.81	0.60
47:1v:439:MET:SD	47:1v:447:ARG:HG2	2.41	0.60
52:A:20:ARG:H	52:A:162:PRO:HG2	1.66	0.60
84:h:186:ALA:O	84:h:190:MET:HG2	2.01	0.60
84:h:260:MET:HG3	84:h:293:SER:HB2	1.83	0.60
1:1:2415:A:N6	1:1:2495:G:H1	1.99	0.60
52:A:35:ARG:HH12	72:U:50:LEU:HG	1.67	0.60
73:V:99:ASP:O	73:V:103:LEU:HG	2.02	0.60
23:1W:39:ILE:HD13	23:1W:57:ARG:HH22	1.66	0.60
38:1l:151:LYS:HD3	38:1l:157:LEU:HG	1.82	0.60
48:2:1113:U:H2'	48:2:1114:G:H8	1.65	0.60
53:B:107:ILE:HG22	53:B:109:CYS:H	1.65	0.60
55:D:91:LYS:O	55:D:95:ARG:HG3	2.00	0.60
70:S:77:LEU:O	70:S:81:ILE:HG23	2.01	0.60
54:C:260:LEU:HD11	55:D:182:THR:HA	1.84	0.60
62:K:42:PRO:HB3	62:K:89:ASP:HB3	1.83	0.60
77:Z:60:LEU:HD23	77:Z:64:GLY:HA2	1.84	0.60
83:f:315:ILE:HG23	83:f:385:PHE:CE1	2.36	0.60
84:h:201:LEU:O	84:h:205:VAL:HG12	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:1u:256:HIS:O	46:1u:260:LEU:HD12	2.02	0.60
83:f:192:LEU:HD11	83:f:215:CYS:HB3	1.82	0.60
85:i:317:LYS:HE3	85:i:320:LEU:HD11	1.83	0.60
39:1m:102:TRP:CE3	39:1m:103:PRO:HA	2.36	0.60
16:1P:87:ILE:HD11	16:1P:113:LEU:HD22	1.84	0.60
48:2:939:A:H2'	48:2:940:G:C8	2.37	0.60
23:1W:58:ILE:HG12	23:1W:140:ILE:HG23	1.84	0.59
84:h:296:LYS:HZ3	84:h:337:TRP:CD1	2.20	0.59
48:2:939:A:H2'	48:2:940:G:H8	1.66	0.59
74:W:101:ARG:HA	74:W:104:ARG:HE	1.67	0.59
74:W:266:GLN:O	74:W:270:ILE:HD12	2.01	0.59
1:1:275:A:H2'	1:1:276:A:H8	1.67	0.59
46:1u:230:ILE:HD11	46:1u:235:ARG:HD3	1.84	0.59
46:1u:738:VAL:HA	46:1u:741:ARG:HD2	1.82	0.59
54:C:46:ARG:CZ	55:D:148:SER:HB3	2.33	0.59
63:L:107:GLN:OE1	63:L:111:GLU:HG2	2.02	0.59
76:Y:40:LYS:HA	76:Y:43:ARG:HD3	1.84	0.59
78:a:367:THR:O	78:a:371:LEU:HD13	2.02	0.59
38:1l:134:LYS:HB3	38:1l:149:ALA:HB2	1.83	0.59
23:1W:187:LEU:HD11	23:1W:224:LEU:HD13	1.84	0.59
47:1v:155:ARG:HB2	47:1v:184:ARG:HH21	1.68	0.59
46:1u:271:LEU:HD23	46:1u:271:LEU:H	1.67	0.59
48:2:1113:U:H2'	48:2:1114:G:C8	2.38	0.59
1:1:1596:A:C6	45:1t:292:LEU:HD12	2.37	0.59
46:1u:626:LEU:HD13	46:1u:657:LEU:HD11	1.84	0.59
48:2:654:G:H2'	48:2:655:A:H8	1.68	0.59
84:h:292:PHE:CE2	84:h:296:LYS:HE3	2.37	0.59
1:1:2957:A:H2'	1:1:2958:A:C8	2.37	0.59
82:e:144:GLU:O	82:e:148:ARG:HG2	2.02	0.59
4:1D:308:GLU:HG2	4:1D:309:PRO:HD2	1.83	0.59
3:1C:199:VAL:HG13	8:1H:97:ARG:HD2	1.85	0.59
74:W:474:TRP:HE3	74:W:475:LEU:HD22	1.68	0.59
84:h:181:PRO:HB2	84:h:214:LEU:HD11	1.84	0.59
1:1:732:C:H2'	1:1:733:A:C8	2.38	0.58
10:1J:42:ASN:HB2	10:1J:73:HIS:CE1	2.38	0.58
58:G:39:ILE:HD11	58:G:109:ILE:HG22	1.85	0.58
1:1:542:C:H2'	1:1:543:G:H8	1.68	0.58
1:1:1226:C:H2'	1:1:1227:A:H8	1.67	0.58
45:1t:231:THR:O	45:1t:235:MET:HG3	2.03	0.58
60:I:128:THR:HA	60:I:219:HIS:O	2.03	0.58
45:1t:376:MET:O	45:1t:380:VAL:HG22	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:321:MET:HE2	17:1Q:153:ARG:HG3	1.84	0.58
53:B:286:ARG:HB3	53:B:321:ARG:HH12	1.67	0.58
85:i:101:LEU:O	85:i:105:VAL:HG12	2.04	0.58
85:i:103:ARG:HD3	85:i:173:VAL:HG13	1.84	0.58
1:1:689:U:P	37:1k:65:ARG:HH21	2.26	0.58
31:1e:12:ILE:HD13	31:1e:54:GLU:HG3	1.84	0.58
47:1v:186:VAL:HG22	47:1v:221:LEU:HD23	1.86	0.58
53:B:262:ALA:H	78:a:196:THR:HG21	1.68	0.58
57:F:82:ASP:O	57:F:86:THR:HG23	2.04	0.58
83:f:199:TYR:O	83:f:203:THR:HG22	2.03	0.58
1:1:2024:A:H2'	1:1:2025:C:C6	2.39	0.58
23:1W:63:PHE:HE1	23:1W:68:LEU:HD12	1.67	0.58
35:1i:230:ILE:HD13	38:1l:88:ALA:HB2	1.84	0.58
59:H:272:ARG:NH1	59:H:273:GLU:HA	2.18	0.58
62:K:74:LEU:HD11	62:K:104:LEU:HB2	1.86	0.58
3:1C:119:ARG:HH11	26:1Z:140:GLN:HG3	1.67	0.58
45:1t:145:LEU:O	45:1t:149:MET:HG2	2.03	0.58
83:f:278:THR:HG23	83:f:281:GLU:H	1.68	0.58
59:H:235:LEU:O	59:H:239:SER:HB3	2.03	0.58
48:2:1766:U:H2'	48:2:1767:G:H8	1.69	0.58
1:1:855:G:H1	1:1:865:G:H1	1.50	0.58
1:1:2414:A:H2'	1:1:2415:A:C8	2.38	0.58
1:1:2445:G:H2'	1:1:2446:G:H8	1.69	0.58
45:1t:342:GLY:HA3	45:1t:374:LEU:HD13	1.85	0.58
48:2:241:U:H2'	48:2:242:G:H8	1.69	0.58
61:J:296:GLU:OE1	70:S:28:ARG:HB3	2.04	0.58
1:1:2177:A:H2'	1:1:2178:A:C8	2.39	0.57
69:R:189:GLU:H	69:R:189:GLU:CD	2.12	0.57
76:Y:84:ARG:HG2	76:Y:86:LYS:HG2	1.86	0.57
84:h:229:HIS:HD1	84:h:230:GLU:HG3	1.69	0.57
1:1:2600:U:H2'	1:1:2601:A:C8	2.39	0.57
8:1H:53:GLU:HG2	8:1H:54:LYS:HD3	1.86	0.57
8:1H:89:LEU:O	8:1H:93:GLN:HG3	2.04	0.57
26:1Z:115:PRO:HG2	26:1Z:118:LYS:HD3	1.86	0.57
47:1v:405:CYS:HB3	47:1v:438:LYS:NZ	2.19	0.57
48:2:654:G:H2'	48:2:655:A:C8	2.39	0.57
82:e:333:LYS:NZ	82:e:354:VAL:HG13	2.19	0.57
16:1P:71:LYS:O	16:1P:75:GLU:HG2	2.04	0.57
38:1l:144:LYS:HA	38:1l:147:GLU:OE1	2.04	0.57
75:X:325:GLU:O	75:X:329:GLU:HG3	2.03	0.57
1:1:126:U:O2'	1:1:127:C:H5'	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:2:1717:C:H4'	84:h:105:PRO:HG3	1.87	0.57
75:X:410:PRO:HG2	75:X:413:GLU:HG3	1.86	0.57
38:1l:168:MET:HE2	38:1l:230:MET:HE3	1.86	0.57
38:1l:92:THR:O	38:1l:96:LYS:HD2	2.05	0.57
47:1v:109:PRO:HA	47:1v:112:ILE:HG12	1.87	0.57
4:1D:287:ASP:HB3	4:1D:290:LYS:HG3	1.86	0.57
45:1t:349:LEU:HB3	45:1t:352:LYS:HD2	1.86	0.57
48:2:64:U:H2'	48:2:65:G:H8	1.70	0.57
1:1:1255:U:H2'	1:1:1256:G:C8	2.40	0.57
1:1:2718:G:H4'	33:1g:90:MET:HE1	1.87	0.57
48:2:1000:A:H62	48:2:1026:U:H3	1.53	0.57
85:i:322:MET:HA	85:i:325:LEU:HD12	1.86	0.57
48:2:129:A:H2'	48:2:130:A:C8	2.40	0.57
48:2:1671:C:H2'	48:2:1672:A:H8	1.70	0.57
55:D:314:LYS:O	55:D:318:LYS:HG2	2.04	0.57
73:V:92:ARG:HB2	73:V:92:ARG:HH11	1.69	0.57
74:W:318:LEU:HD21	74:W:342:GLU:HG2	1.87	0.57
1:1:2440:U:H2'	1:1:2441:G:H8	1.70	0.57
54:C:324:ARG:HG2	82:e:238:ASP:O	2.05	0.57
84:h:206:MET:HG2	84:h:240:TYR:HE2	1.69	0.57
1:1:544:A:H2'	1:1:545:G:C8	2.39	0.56
1:1:2634:U:H2'	1:1:2635:G:C8	2.40	0.56
10:1J:112:ARG:HG2	40:1o:74:TYR:HE2	1.70	0.56
16:1P:21:LEU:HD23	16:1P:87:ILE:HD12	1.87	0.56
48:2:377:U:H2'	48:2:378:G:H8	1.69	0.56
48:2:1135:A:H5"	69:R:66:LYS:HG3	1.87	0.56
81:d:78:LEU:HB3	81:d:83:ILE:HD11	1.87	0.56
82:e:193:HIS:HB2	82:e:205:LEU:HD11	1.86	0.56
84:h:217:GLN:HB2	84:h:220:THR:HG23	1.87	0.56
1:1:407:U:H2'	1:1:408:U:C6	2.40	0.56
7:1G:88:TYR:HB2	7:1G:91:GLU:HB3	1.87	0.56
59:H:224:VAL:O	59:H:225:ILE:HG12	2.05	0.56
85:i:317:LYS:HD2	85:i:320:LEU:HD21	1.86	0.56
27:1a:34:ALA:HB1	27:1a:39:GLU:HB2	1.86	0.56
40:1o:96:VAL:HA	40:1o:99:LEU:HD12	1.86	0.56
46:1u:434:TYR:HD2	46:1u:457:LEU:HB2	1.71	0.56
48:2:318:U:H5'	48:2:319:C:C6	2.41	0.56
48:2:670:G:H2'	48:2:671:A:C8	2.38	0.56
48:2:711:A:H2'	48:2:712:A:C8	2.39	0.56
68:Q:227:MET:HE2	70:S:52:MET:HG2	1.86	0.56
76:Y:21:ALA:O	76:Y:25:ILE:HG23	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:Y:41:ILE:HA	76:Y:44:LYS:HE3	1.87	0.56
77:Z:92:HIS:HD2	77:Z:117:HIS:HD2	1.51	0.56
48:2:1549:A:H2'	48:2:1550:A:C8	2.40	0.56
84:h:323:LYS:HA	84:h:326:LEU:HD12	1.87	0.56
1:1:434:A:H5"	22:1V:109:THR:HG23	1.86	0.56
1:1:1680:A:H61	1:1:1886:U:H3	1.52	0.56
38:1l:33:PHE:HB3	38:1l:113:LEU:HB3	1.88	0.56
46:1u:90:THR:O	46:1u:94:MET:HG2	2.05	0.56
46:1u:464:LEU:HD21	46:1u:499:GLN:HB3	1.88	0.56
48:2:997:G:H1	48:2:1029:C:H41	1.52	0.56
54:C:175:LEU:HA	54:C:179:ILE:HD12	1.88	0.56
81:d:71:LEU:HD11	81:d:99:ARG:HB3	1.87	0.56
84:h:254:THR:O	84:h:258:VAL:HG23	2.05	0.56
1:1:855:G:H22	1:1:865:G:H22	1.51	0.56
1:1:958:U:H2'	1:1:959:C:C6	2.41	0.56
20:1T:186:LYS:HE2	20:1T:202:ARG:HB2	1.86	0.56
54:C:117:LEU:HD21	54:C:126:LEU:HD22	1.86	0.56
85:i:103:ARG:O	85:i:107:ILE:HG12	2.05	0.56
1:1:1009:G:H2'	1:1:1010:C:C6	2.41	0.56
78:a:79:ASN:HA	78:a:82:LEU:HB2	1.87	0.56
1:1:1252:C:H2'	1:1:1253:A:H8	1.70	0.56
2:1B:98:LEU:HB2	2:1B:107:LEU:HD23	1.86	0.56
46:1u:704:VAL:O	46:1u:708:ILE:HG12	2.06	0.56
53:B:480:LYS:HG2	53:B:481:ARG:N	2.20	0.56
78:a:98:LEU:HA	78:a:101:ILE:HG22	1.87	0.56
84:h:157:THR:HA	84:h:160:ARG:HD3	1.88	0.56
1:1:1254:C:H5'	40:1o:115:LYS:HZ3	1.71	0.56
1:1:2126:A:H2'	1:1:2127:A:C8	2.40	0.56
11:1K:55:ALA:HB2	11:1K:68:GLY:HA2	1.88	0.56
24:1X:56:ALA:HB3	24:1X:123:VAL:HG22	1.87	0.56
46:1u:474:PRO:HA	46:1u:477:TYR:CZ	2.41	0.56
48:2:1801:A:H5'	62:K:44:LYS:HE3	1.88	0.56
57:F:14:LYS:HG2	57:F:18:PHE:CE1	2.41	0.56
78:a:200:GLU:HA	78:a:203:LEU:HD23	1.88	0.56
84:h:357:LEU:O	84:h:361:ILE:HG13	2.05	0.56
1:1:855:G:H1	1:1:865:G:H22	1.54	0.56
10:1J:114:VAL:HA	10:1J:117:ILE:HD12	1.87	0.56
46:1u:241:ARG:O	46:1u:245:LYS:HG2	2.06	0.56
47:1v:153:PHE:HB3	47:1v:162:MET:HB3	1.86	0.56
55:D:158:ASP:HA	55:D:161:ARG:HG2	1.88	0.56
68:Q:230:LYS:HD2	68:Q:238:MET:HA	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
84:h:330:LYS:O	84:h:334:VAL:HG23	2.06	0.56
46:1u:159:MET:O	46:1u:163:VAL:HG22	2.05	0.55
47:1v:150:VAL:HG22	47:1v:162:MET:HE2	1.88	0.55
75:X:505:ASP:HA	75:X:508:TYR:CE2	2.41	0.55
1:1:153:U:H2'	1:1:154:U:C6	2.41	0.55
1:1:556:C:H2'	1:1:557:A:C8	2.41	0.55
38:1l:28:VAL:HG13	38:1l:187:ARG:HG3	1.88	0.55
46:1u:519:ALA:HB3	46:1u:548:LEU:HD23	1.87	0.55
47:1v:436:MET:HA	47:1v:439:MET:HE3	1.87	0.55
54:C:168:ARG:HA	55:D:119:LEU:HD13	1.88	0.55
1:1:1978:U:H2'	1:1:1979:A:H8	1.70	0.55
14:1N:87:ARG:O	14:1N:91:ILE:HG23	2.07	0.55
35:1i:97:GLU:CD	35:1i:97:GLU:H	2.14	0.55
47:1v:228:SER:O	47:1v:232:LYS:HG2	2.06	0.55
48:2:158:A:H2'	48:2:159:G:C8	2.41	0.55
59:H:317:ALA:HB2	59:H:367:VAL:HG23	1.88	0.55
68:Q:198:GLN:NE2	68:Q:199:THR:HG23	2.21	0.55
4:1D:84:CYS:HA	17:1Q:112:ALA:HB1	1.88	0.55
45:1t:287:TRP:HZ2	45:1t:302:TYR:HE1	1.54	0.55
45:1t:465:MET:H	45:1t:468:ARG:NH1	2.05	0.55
48:2:612:U:H2'	48:2:613:C:C6	2.41	0.55
48:2:1618:G:H2'	48:2:1619:A:H8	1.69	0.55
54:C:329:VAL:HG11	82:e:218:ALA:HB1	1.89	0.55
79:b:29:LEU:HD23	79:b:29:LEU:H	1.71	0.55
1:1:1511:A:H2'	1:1:1512:A:C8	2.41	0.55
3:1C:326:TRP:HE3	3:1C:327:SER:H	1.55	0.55
47:1v:261:LEU:HD23	47:1v:293:LEU:HD12	1.88	0.55
60:I:135:ARG:HG2	60:I:185:LYS:HG3	1.89	0.55
48:2:79:G:H22	48:2:161:A:H2	1.55	0.55
48:2:1749:A:H2'	48:2:1750:C:H6	1.71	0.55
48:2:1770:G:H3'	48:2:1771:C:H4'	1.88	0.55
64:M:97:PRO:HA	64:M:104:ARG:HH12	1.71	0.55
53:B:232:PRO:HB2	53:B:333:PHE:CZ	2.41	0.55
55:D:318:LYS:HB3	55:D:333:LEU:HD11	1.89	0.55
1:1:1234:G:H2'	1:1:1235:A:C8	2.41	0.55
1:1:2382:C:H2'	1:1:2383:C:H6	1.71	0.55
6:1F:123:ARG:NH2	6:1F:128:GLN:HB2	2.22	0.55
48:2:887:G:H2'	48:2:888:G:H8	1.72	0.55
53:B:285:ILE:O	53:B:289:ILE:HG13	2.06	0.55
83:f:334:ARG:HH12	83:f:338:ILE:HD11	1.71	0.55
23:1W:58:ILE:HD13	23:1W:90:ILE:HD12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1Z:121:THR:HG22	26:1Z:123:MET:H	1.72	0.55
46:1u:244:ASN:HA	46:1u:247:VAL:HG22	1.89	0.55
46:1u:627:MET:HA	46:1u:627:MET:HE2	1.87	0.55
48:2:352:C:H2'	48:2:353:C:H6	1.72	0.55
48:2:1746:A:H2'	48:2:1747:A:C8	2.42	0.55
76:Y:76:SER:O	76:Y:80:MET:HG3	2.07	0.55
1:1:864:G:H2'	1:1:865:G:H8	1.72	0.55
13:1M:168:ILE:HG21	13:1M:172:ILE:HG22	1.89	0.55
24:1X:237:ARG:HD3	24:1X:238:PRO:HD2	1.87	0.55
38:1l:34:GLU:OE1	38:1l:110:LYS:HB3	2.07	0.55
45:1t:130:LEU:HD23	45:1t:145:LEU:HD23	1.89	0.55
53:B:176:SER:HG	53:B:230:VAL:N	2.03	0.55
74:W:468:ASN:O	74:W:472:MET:HG3	2.08	0.55
82:e:148:ARG:HA	82:e:151:ARG:HD2	1.88	0.55
3:1C:189:PHE:HB2	26:1Z:134:ARG:HH22	1.71	0.54
46:1u:737:ASP:O	46:1u:741:ARG:HG3	2.07	0.54
77:Z:80:GLU:HB3	77:Z:98:ILE:HG22	1.87	0.54
1:1:801:U:H2'	1:1:802:U:C6	2.42	0.54
42:1q:38:ALA:O	42:1q:42:THR:HG23	2.08	0.54
1:1:1446:C:H2'	1:1:1447:A:H8	1.73	0.54
1:1:2639:U:C5	16:1P:91:LYS:HE3	2.41	0.54
46:1u:376:MET:H	46:1u:376:MET:HE3	1.72	0.54
48:2:1704:A:H2	48:2:1706:C:H41	1.55	0.54
54:C:192:ARG:HH22	55:D:132:ASN:HA	1.72	0.54
72:U:101:ASP:O	72:U:105:VAL:HG13	2.06	0.54
78:a:336:VAL:HG22	78:a:339:ARG:HB2	1.89	0.54
83:f:266:LYS:O	83:f:270:ILE:HG12	2.08	0.54
1:1:1186:G:H1	1:1:1269:G:N2	2.05	0.54
1:1:2389:A:H2'	1:1:2390:C:C6	2.42	0.54
45:1t:110:GLU:O	45:1t:114:VAL:HG23	2.08	0.54
45:1t:389:LEU:HA	45:1t:392:ILE:HG22	1.89	0.54
84:h:229:HIS:HD2	84:h:262:PHE:HB2	1.73	0.54
5:1E:218:LEU:HD11	5:1E:226:ILE:HD11	1.90	0.54
14:1N:155:LEU:O	14:1N:159:ARG:HG3	2.07	0.54
56:E:99:ILE:HD13	68:Q:176:ASP:HB2	1.88	0.54
59:H:230:ARG:HD3	72:U:79:PRO:HG2	1.88	0.54
1:1:977:U:H2'	1:1:978:A:H8	1.73	0.54
53:B:68:ARG:HE	53:B:434:LYS:NZ	2.06	0.54
57:F:137:SER:O	57:F:140:ARG:HG2	2.08	0.54
59:H:245:MET:HE1	85:i:295:MET:HE1	1.89	0.54
74:W:387:VAL:O	74:W:391:ARG:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1119:G:OP1	28:1b:32:LYS:HG2	2.08	0.54
1:1:1178:A:H2'	1:1:1179:A:C8	2.42	0.54
1:1:2343:C:H2'	1:1:2344:C:C6	2.42	0.54
23:1W:180:ILE:HG22	23:1W:181:ARG:HE	1.72	0.54
45:1t:352:LYS:O	45:1t:355:GLU:HG2	2.07	0.54
47:1v:166:ILE:HG13	47:1v:205:TYR:HE2	1.73	0.54
48:2:15:A:H5'	48:2:317:U:H5"	1.90	0.54
74:W:468:ASN:HB3	74:W:471:GLU:HB2	1.89	0.54
1:1:630:A:O2'	20:1T:153:ARG:HD3	2.08	0.54
1:1:2632:A:H2'	1:1:2633:A:C8	2.43	0.54
46:1u:130:LEU:HD13	46:1u:163:VAL:HG21	1.88	0.54
48:2:48:C:H2'	48:2:49:U:C6	2.42	0.54
48:2:609:U:H3	48:2:625:G:H22	1.56	0.54
73:V:123:VAL:O	73:V:127:GLU:HG3	2.07	0.54
84:h:239:LYS:HA	84:h:242:LYS:HE3	1.90	0.54
1:1:1024:G:H2'	1:1:1025:G:C8	2.43	0.54
1:1:1447:A:H2'	1:1:1448:A:C8	2.43	0.54
16:1P:34:VAL:HG21	16:1P:77:LEU:HD11	1.90	0.54
43:1r:51:ILE:HD12	43:1r:52:GLN:N	2.23	0.54
47:1v:108:ASN:O	47:1v:112:ILE:HG23	2.08	0.54
47:1v:196:ASP:O	47:1v:200:LYS:HG2	2.07	0.54
48:2:1730:U:H2'	48:2:1731:A:C8	2.42	0.54
53:B:202:LYS:HA	53:B:207:PHE:CD2	2.40	0.54
53:B:371:LEU:HB3	75:X:344:PHE:HE2	1.71	0.54
75:X:420:PRO:HB2	78:a:202:ILE:HD11	1.89	0.54
1:1:855:G:H22	1:1:865:G:N2	2.06	0.54
1:1:1838:A:H5"	1:1:1839:A:C8	2.42	0.54
1:1:2783:A:H5'	34:1h:32:LYS:HE3	1.88	0.54
26:1Z:22:THR:HG22	26:1Z:25:LEU:HB2	1.88	0.54
59:H:227:GLY:O	59:H:230:ARG:HG3	2.08	0.54
78:a:104:ALA:O	78:a:108:ARG:HG2	2.08	0.54
1:1:275:A:H1'	46:1u:387:MET:SD	2.47	0.53
1:1:1150:A:H2'	1:1:1151:A:C8	2.43	0.53
48:2:150:A:H2'	48:2:151:A:C4	2.43	0.53
48:2:520:C:H41	62:K:50:ARG:HH22	1.56	0.53
50:5:24:C:H2'	50:5:25:U:C6	2.43	0.53
84:h:113:ILE:HG23	84:h:125:LEU:HD21	1.89	0.53
47:1v:179:GLU:HG2	47:1v:220:LYS:HE2	1.89	0.53
53:B:333:PHE:CG	53:B:333:PHE:O	2.62	0.53
60:I:133:ALA:HB3	60:I:215:GLU:HB3	1.90	0.53
68:Q:198:GLN:HE22	68:Q:199:THR:HG23	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1X:192:ILE:HD12	24:1X:242:PRO:HB2	1.90	0.53
45:1t:177:VAL:HG12	45:1t:181:ILE:HD11	1.89	0.53
45:1t:416:LEU:HG	45:1t:420:PHE:CZ	2.44	0.53
47:1v:204:ASP:HB3	47:1v:205:TYR:CD1	2.44	0.53
69:R:149:LYS:HG3	69:R:152:ALA:HB3	1.91	0.53
77:Z:67:TYR:HD1	77:Z:68:HIS:H	1.56	0.53
85:i:108:MET:HG2	85:i:111:LYS:HE2	1.90	0.53
1:1:2485:U:H2'	1:1:2486:C:C6	2.43	0.53
46:1u:739:LEU:HA	46:1u:742:MET:SD	2.48	0.53
48:2:203:A:H62	48:2:243:U:H3	1.55	0.53
48:2:458:U:H4'	54:C:131:ARG:HH22	1.73	0.53
48:2:1489:C:H3'	63:L:124:MET:HE1	1.91	0.53
48:2:1745:A:OP1	84:h:149:ASN:HB3	2.08	0.53
84:h:137:LEU:HD12	84:h:143:HIS:HA	1.91	0.53
1:1:556:C:H2'	1:1:557:A:H8	1.73	0.53
1:1:1978:U:H2'	1:1:1979:A:C8	2.42	0.53
10:1J:92:ALA:HB2	10:1J:109:LEU:HD11	1.91	0.53
60:I:216:LEU:HB2	78:a:297:ILE:HB	1.91	0.53
83:f:408:TYR:CD1	85:i:187:LYS:HG2	2.44	0.53
1:1:1624:G:H21	1:1:1625:C:H41	1.57	0.53
10:1J:87:TYR:CD1	10:1J:117:ILE:HG12	2.44	0.53
39:1m:5:LEU:HD12	39:1m:60:PHE:HE1	1.74	0.53
46:1u:727:LEU:O	46:1u:732:ASN:HB2	2.09	0.53
53:B:410:PRO:HB2	53:B:413:TYR:HB2	1.90	0.53
1:1:1219:A:H4'	1:1:1220:A:C8	2.44	0.53
46:1u:351:MET:O	46:1u:351:MET:HE3	2.09	0.53
47:1v:268:ALA:HB2	47:1v:286:MET:HE1	1.90	0.53
48:2:65:G:H1	48:2:374:C:H5	1.56	0.53
50:5:38:G:H3'	50:5:39:A:H8	1.74	0.53
54:C:206:ARG:HA	54:C:209:ARG:HH12	1.73	0.53
85:i:125:ASP:O	85:i:129:LEU:HG	2.08	0.53
1:1:341:A:H62	46:1u:235:ARG:NH1	2.07	0.53
1:1:347:A:H2'	1:1:348:A:C8	2.44	0.53
11:1K:175:MET:HE3	11:1K:176:ILE:HD13	1.91	0.53
26:1Z:47:LEU:HB2	26:1Z:93:VAL:HG12	1.90	0.53
55:D:504:GLN:HG3	55:D:509:ARG:O	2.08	0.53
75:X:469:GLU:O	75:X:473:ILE:HG22	2.09	0.53
39:1m:77:SER:O	39:1m:81:MET:HG2	2.09	0.53
40:1o:92:ARG:HA	40:1o:107:PHE:HZ	1.74	0.53
47:1v:383:MET:HE3	47:1v:392:LEU:HD11	1.90	0.53
48:2:147:U:H2'	48:2:148:U:C6	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:B:457:SER:O	53:B:461:LYS:HG2	2.08	0.53
55:D:367:VAL:HG21	55:D:409:MET:HE2	1.91	0.53
61:J:297:ASP:OD2	70:S:47:MET:HE1	2.09	0.53
81:d:49:ILE:HG12	81:d:94:TYR:HD2	1.73	0.53
84:h:296:LYS:HZ3	84:h:337:TRP:CG	2.26	0.53
1:1:356:A:H2'	1:1:357:A:C8	2.44	0.53
40:1o:100:PRO:HD2	40:1o:103:ASP:HB2	1.91	0.53
45:1t:463:PRO:HG2	45:1t:468:ARG:HH12	1.74	0.53
48:2:64:U:H2'	48:2:65:G:C8	2.45	0.53
48:2:1710:G:H2'	48:2:1711:A:C8	2.44	0.53
50:5:51:C:H2'	50:5:52:A:H8	1.74	0.53
55:D:99:GLN:CD	55:D:99:GLN:C	2.77	0.53
69:R:67:VAL:HG13	69:R:68:THR:HG23	1.90	0.53
13:1M:146:ILE:HD12	13:1M:151:ILE:HB	1.91	0.52
45:1t:117:PRO:HD2	45:1t:120:SER:HB2	1.91	0.52
48:2:708:A:H2'	48:2:709:G:C8	2.44	0.52
57:F:41:ARG:HH21	74:W:168:GLU:HG2	1.74	0.52
57:F:93:LEU:HD12	57:F:97:PHE:CZ	2.44	0.52
85:i:136:VAL:HA	85:i:139:ILE:HG12	1.92	0.52
1:1:696:C:H1'	1:1:697:A:C8	2.44	0.52
1:1:1579:C:H1'	45:1t:201:ARG:HH22	1.74	0.52
1:1:1832:A:H2'	1:1:1833:A:C8	2.43	0.52
6:1F:109:ILE:HG13	6:1F:135:PHE:CZ	2.44	0.52
25:1Y:147:SER:HA	25:1Y:150:MET:HG2	1.91	0.52
43:1r:79:ARG:HA	43:1r:82:GLU:OE1	2.09	0.52
48:2:1686:U:H2'	48:2:1687:U:C6	2.44	0.52
65:N:348:VAL:O	65:N:352:GLN:HG3	2.10	0.52
1:1:733:A:H2'	1:1:734:G:H8	1.75	0.52
1:1:2486:C:H2'	1:1:2487:G:O4'	2.09	0.52
48:2:887:G:H2'	48:2:888:G:C8	2.45	0.52
48:2:1737:A:H3'	48:2:1738:G:N2	2.20	0.52
55:D:217:LEU:HD11	85:i:207:ILE:HD11	1.92	0.52
59:H:319:VAL:HG12	59:H:365:CYS:HB3	1.91	0.52
78:a:136:ASP:O	78:a:140:GLU:HG2	2.08	0.52
85:i:356:ILE:HG23	85:i:367:TYR:HE1	1.74	0.52
1:1:49:G:N2	47:1v:491:LEU:HD22	2.24	0.52
1:1:2955:C:H5	1:1:3041:U:H2'	1.74	0.52
45:1t:463:PRO:HG2	45:1t:468:ARG:NH1	2.23	0.52
47:1v:361:LEU:O	47:1v:365:ARG:HG3	2.09	0.52
59:H:224:VAL:HG12	59:H:225:ILE:H	1.73	0.52
70:S:99:ARG:HH12	86:k:26:MET:HG3	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:c:114:VAL:O	80:c:118:ARG:HG3	2.09	0.52
1:1:740:A:H2'	1:1:741:A:H8	1.75	0.52
1:1:2441:G:H2'	1:1:2442:G:C8	2.44	0.52
3:1C:251:GLN:HA	3:1C:255:GLY:HA2	1.91	0.52
4:1D:195:GLY:O	4:1D:199:ARG:HB2	2.09	0.52
48:2:598:G:H2'	48:2:599:A:H8	1.75	0.52
78:a:347:LEU:HD21	78:a:371:LEU:HD23	1.91	0.52
1:1:349:A:H2'	1:1:350:A:C8	2.45	0.52
46:1u:376:MET:HG2	46:1u:380:LYS:HD2	1.92	0.52
48:2:1700:U:H2'	48:2:1701:C:C6	2.45	0.52
48:2:1710:G:H2'	48:2:1711:A:H8	1.75	0.52
53:B:48:PRO:HG3	53:B:54:GLY:HA3	1.91	0.52
84:h:242:LYS:HD2	84:h:243:LYS:N	2.24	0.52
1:1:347:A:H2'	1:1:348:A:H8	1.74	0.52
1:1:1186:G:H22	1:1:1269:G:N2	2.08	0.52
1:1:1700:U:H2'	1:1:1701:U:C6	2.44	0.52
1:1:2382:C:H2'	1:1:2383:C:C6	2.44	0.52
1:1:2896:C:H2'	1:1:2897:G:H8	1.75	0.52
5:1E:104:MET:HE3	5:1E:212:VAL:HG11	1.92	0.52
9:1I:101:GLN:HB3	9:1I:102:LYS:HZ2	1.75	0.52
13:1M:246:PRO:HA	13:1M:249:LEU:HD12	1.91	0.52
35:1i:207:MET:N	35:1i:207:MET:HE3	2.25	0.52
48:2:146:U:H2'	48:2:147:U:C6	2.44	0.52
63:L:96:ASP:O	63:L:100:ARG:HG3	2.09	0.52
72:U:70:GLU:HG2	86:k:15:ARG:HD3	1.90	0.52
75:X:409:MET:HE1	75:X:414:CYS:HA	1.92	0.52
84:h:252:ARG:HB3	84:h:255:THR:HG22	1.92	0.52
21:1U:40:THR:HB	21:1U:43:GLU:HG3	1.90	0.52
40:1o:91:LEU:HB3	40:1o:107:PHE:CE1	2.44	0.52
46:1u:157:ILE:HG13	46:1u:173:LEU:HD13	1.92	0.52
48:2:356:G:H2'	48:2:357:A:C8	2.45	0.52
48:2:1718:A:H2'	48:2:1719:G:H8	1.75	0.52
82:e:183:ASP:HB3	82:e:246:ASP:OD2	2.10	0.52
1:1:2552:U:H2'	1:1:2553:U:C6	2.45	0.52
22:1V:142:PHE:CG	36:1j:72:LYS:HD2	2.45	0.52
23:1W:178:ARG:HB2	23:1W:234:LYS:HD2	1.92	0.52
45:1t:392:ILE:HD12	45:1t:406:TRP:CZ3	2.45	0.52
48:2:1718:A:H2'	48:2:1719:G:C8	2.44	0.52
75:X:437:ALA:O	75:X:440:GLU:HG3	2.09	0.52
1:1:277:A:H2'	1:1:278:A:C8	2.44	0.52
1:1:811:U:H2'	1:1:812:U:O4'	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:53:MET:HG3	2:1B:57:SER:OG	2.09	0.52
29:1c:13:SER:HB2	29:1c:35:VAL:HG13	1.91	0.52
37:1k:70:VAL:HG11	37:1k:83:ASN:HD22	1.74	0.52
48:2:411:C:H2'	48:2:412:A:C8	2.45	0.52
48:2:490:A:H2'	48:2:491:G:C8	2.44	0.52
48:2:553:U:H2'	48:2:554:C:C6	2.45	0.52
48:2:1388:A:O2'	48:2:1389:A:H8	1.92	0.52
50:5:13:G:H21	50:5:23:A:H62	1.56	0.52
74:W:139:ILE:HD12	74:W:178:LYS:HG3	1.91	0.52
78:a:356:HIS:HB2	78:a:359:GLU:HG2	1.91	0.52
85:i:234:GLU:HG3	85:i:237:ARG:HH21	1.75	0.52
46:1u:500:LEU:HG	46:1u:505:VAL:HG21	1.92	0.51
47:1v:142:THR:H	47:1v:145:THR:HG22	1.75	0.51
47:1v:244:ASP:H	47:1v:247:ILE:HD12	1.75	0.51
48:2:411:C:H2'	48:2:412:A:H8	1.74	0.51
55:D:405:GLY:O	55:D:409:MET:HG3	2.10	0.51
74:W:455:GLU:HA	74:W:458:TRP:CD1	2.45	0.51
84:h:117:ARG:HG2	84:h:118:LYS:HG3	1.92	0.51
1:1:1388:A:H2'	1:1:1389:C:H6	1.76	0.51
1:1:1856:A:H2'	1:1:1857:U:O4'	2.10	0.51
1:1:2441:G:H2'	1:1:2442:G:H8	1.75	0.51
59:H:208:ARG:HA	59:H:211:LYS:HD2	1.92	0.51
84:h:84:GLU:HA	84:h:87:LYS:HG2	1.93	0.51
1:1:3090:G:H1'	20:1T:230:PHE:HE2	1.75	0.51
3:1C:116:VAL:HG12	46:1u:142:ARG:HG2	1.91	0.51
46:1u:720:SER:O	46:1u:724:ILE:HG23	2.10	0.51
47:1v:155:ARG:HA	47:1v:184:ARG:HE	1.74	0.51
48:2:553:U:H2'	48:2:554:C:H6	1.76	0.51
48:2:1729:G:H2'	48:2:1730:U:H6	1.75	0.51
63:L:111:GLU:OE2	63:L:111:GLU:HA	2.11	0.51
72:U:81:PRO:HA	72:U:84:VAL:HG12	1.93	0.51
73:V:92:ARG:HB2	73:V:92:ARG:NH1	2.26	0.51
84:h:339:VAL:HG13	84:h:387:ALA:HB2	1.92	0.51
85:i:130:LEU:HD12	85:i:131:ILE:HG13	1.92	0.51
1:1:1101:G:C5	14:1N:54:ARG:HD3	2.45	0.51
21:1U:128:TRP:CD1	21:1U:129:LEU:HD13	2.46	0.51
23:1W:209:LYS:HD2	23:1W:231:PRO:HG3	1.91	0.51
29:1c:48:ILE:HG23	29:1c:52:ALA:HB3	1.92	0.51
48:2:1488:A:N3	69:R:206:LYS:HE2	2.24	0.51
55:D:103:LEU:HD12	55:D:103:LEU:O	2.11	0.51
77:Z:56:VAL:HG23	77:Z:69:MET:HE1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1024:G:H2'	1:1:1025:G:H8	1.75	0.51
53:B:302:CYS:SG	53:B:305:GLU:HB2	2.50	0.51
63:L:101:ARG:O	63:L:105:GLU:HG2	2.11	0.51
84:h:252:ARG:HG2	84:h:253:LYS:H	1.76	0.51
38:1l:35:ARG:NH1	38:1l:38:VAL:HG23	2.25	0.51
48:2:1476:A:H4'	76:Y:96:ARG:HH21	1.76	0.51
48:2:1502:A:H62	48:2:1561:A:H61	1.58	0.51
48:2:1766:U:H2'	48:2:1767:G:C8	2.45	0.51
83:f:82:GLU:OE1	85:i:209:GLY:HA2	2.11	0.51
1:1:314:U:H2'	1:1:315:U:H6	1.75	0.51
1:1:741:A:H2'	1:1:742:A:C8	2.46	0.51
12:1L:140:THR:O	12:1L:142:ARG:HD2	2.11	0.51
23:1W:34:GLN:HB2	23:1W:107:PHE:CD1	2.46	0.51
59:H:219:LYS:O	59:H:222:THR:HG22	2.10	0.51
63:L:41:ASN:HA	63:L:74:ALA:HB3	1.93	0.51
74:W:352:LEU:HD11	74:W:400:VAL:HG23	1.92	0.51
77:Z:92:HIS:HD2	77:Z:117:HIS:CD2	2.29	0.51
84:h:199:SER:HA	84:h:202:MET:HE3	1.93	0.51
1:1:312:A:H61	46:1u:269:LEU:HD13	1.76	0.51
1:1:320:U:H2'	1:1:321:U:C6	2.46	0.51
1:1:1511:A:H2'	1:1:1512:A:H8	1.74	0.51
48:2:1567:G:H21	48:2:1594:A:H2	1.59	0.51
55:D:239:ALA:CB	85:i:205:ILE:HD11	2.40	0.51
83:f:336:TYR:CD2	83:f:398:LEU:HB2	2.45	0.51
1:1:412:U:H2'	1:1:413:U:C6	2.46	0.51
1:1:2756:A:C2	89:1:3238:CLM:H10	2.45	0.51
9:1I:41:ARG:HG3	9:1I:52:LEU:HB2	1.93	0.51
45:1t:233:SER:HB2	45:1t:269:PHE:HD2	1.75	0.51
46:1u:124:LEU:HD21	46:1u:156:MET:HG2	1.93	0.51
48:2:573:G:O2'	48:2:817:G:H5'	2.11	0.51
49:3:2:A:O2'	49:3:3:A:H8	1.93	0.51
49:3:102:U:H2'	49:3:103:G:H8	1.76	0.51
50:5:10:G:N2	50:5:27:A:H1'	2.26	0.51
53:B:415:SER:HB2	78:a:134:VAL:HG21	1.93	0.51
57:F:97:PHE:CD1	57:F:107:LEU:HD11	2.46	0.51
68:Q:169:GLU:O	68:Q:173:LYS:HG3	2.10	0.51
74:W:246:TRP:CZ2	74:W:270:ILE:HG12	2.46	0.51
1:1:275:A:H2'	1:1:276:A:C8	2.46	0.51
1:1:427:A:H4'	1:1:428:U:OP2	2.09	0.51
23:1W:168:CYS:HB3	23:1W:171:LEU:HB3	1.92	0.51
45:1t:252:LEU:HD23	45:1t:274:TYR:CE1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:1u:359:ASN:C	46:1u:391:ILE:HD11	2.35	0.51
46:1u:656:VAL:HA	46:1u:659:GLU:HG2	1.92	0.51
47:1v:159:PHE:HE2	47:1v:185:LEU:HG	1.76	0.51
47:1v:429:ILE:HG23	47:1v:430:LYS:HE2	1.91	0.51
48:2:510:U:H2'	48:2:511:C:C6	2.45	0.51
55:D:121:ILE:HA	55:D:124:PHE:HD2	1.75	0.51
55:D:122:GLU:O	55:D:126:GLU:HG2	2.10	0.51
74:W:118:PRO:O	74:W:121:ARG:HD3	2.11	0.51
1:1:1338:G:H5'	1:1:1339:U:OP1	2.11	0.50
1:1:1615:C:N4	1:1:1637:U:H3	2.08	0.50
31:1e:13:ARG:HG3	31:1e:57:MET:SD	2.51	0.50
45:1t:310:VAL:HG21	45:1t:343:ALA:HB2	1.92	0.50
46:1u:227:PHE:HA	46:1u:230:ILE:HG22	1.91	0.50
57:F:100:ARG:HG3	57:F:107:LEU:HD13	1.92	0.50
23:1W:51:ARG:O	23:1W:55:ILE:HG13	2.11	0.50
48:2:1506:C:H2'	48:2:1507:A:H8	1.76	0.50
48:2:1513:A:H2'	48:2:1514:A:C8	2.45	0.50
53:B:239:MET:CA	75:X:448:MET:HE1	2.41	0.50
69:R:45:HIS:HA	69:R:48:LYS:HD3	1.91	0.50
83:f:283:ILE:HA	83:f:286:MET:SD	2.51	0.50
84:h:89:LEU:HD23	84:h:92:LYS:HD3	1.92	0.50
1:1:864:G:H2'	1:1:865:G:C8	2.46	0.50
13:1M:197:VAL:HG21	13:1M:212:VAL:HG11	1.92	0.50
32:1f:175:PHE:HA	32:1f:200:THR:HG21	1.94	0.50
45:1t:323:LYS:HD2	45:1t:323:LYS:O	2.12	0.50
46:1u:682:PHE:HA	46:1u:685:TYR:HD2	1.76	0.50
48:2:1806:G:H1'	48:2:1827:MA6:H2	1.92	0.50
52:A:93:ASN:HB2	52:A:96:ARG:HB3	1.93	0.50
54:C:203:LYS:HE3	55:D:122:GLU:HG3	1.93	0.50
1:1:561:U:H2'	1:1:562:C:C6	2.47	0.50
10:1J:18:LYS:HG2	10:1J:66:LYS:HB3	1.93	0.50
23:1W:40:PRO:HD3	23:1W:112:ARG:O	2.11	0.50
45:1t:344:TYR:CD2	45:1t:352:LYS:HG3	2.47	0.50
53:B:250:ASN:HB3	75:X:402:ASP:OD2	2.11	0.50
53:B:288:ARG:HB3	78:a:213:LEU:HD11	1.92	0.50
54:C:112:LEU:HD22	54:C:120:ILE:HG12	1.94	0.50
60:I:143:GLU:HG2	60:I:210:LEU:HD12	1.93	0.50
60:I:221:LYS:HB3	78:a:290:ILE:HD11	1.92	0.50
61:J:262:VAL:O	61:J:297:ASP:HA	2.11	0.50
66:O:21:MET:HE1	66:O:36:VAL:HG22	1.93	0.50
1:1:138:G:H1'	1:1:139:G:H5'	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:341:A:H5'	1:1:342:A:H5'	1.93	0.50
1:1:1410:A:H5'	18:1R:22:ARG:HH12	1.77	0.50
46:1u:481:ILE:HD13	46:1u:493:ALA:HB1	1.93	0.50
53:B:174:ARG:CZ	75:X:366:ARG:HB3	2.41	0.50
54:C:217:LEU:HD23	54:C:220:LEU:HD12	1.93	0.50
59:H:353:ALA:O	59:H:356:LYS:HE2	2.11	0.50
1:1:1257:G:H5"	9:1I:57:ASN:ND2	2.21	0.50
4:1D:102:LEU:HB2	4:1D:262:ILE:HG23	1.93	0.50
47:1v:201:MET:HE2	47:1v:209:ARG:HG3	1.94	0.50
53:B:408:GLY:O	53:B:409:ILE:HG22	2.11	0.50
59:H:231:ALA:HB1	59:H:234:ASP:HB2	1.92	0.50
27:1a:89:THR:HG22	27:1a:93:MET:HE3	1.94	0.50
46:1u:192:ILE:HG21	46:1u:226:LEU:HD22	1.94	0.50
48:2:1013:A:H2	48:2:1482:U:H1'	1.76	0.50
55:D:145:SER:HB2	55:D:148:SER:HB2	1.92	0.50
58:G:35:SER:O	58:G:39:ILE:HG13	2.11	0.50
83:f:202:LEU:HD22	83:f:313:LEU:HD13	1.93	0.50
1:1:899:U:H2'	1:1:900:A:H8	1.77	0.50
1:1:1653:U:H2'	1:1:1654:C:C6	2.47	0.50
1:1:2051:U:H2'	1:1:2052:C:H6	1.76	0.50
1:1:2633:A:H2'	1:1:2634:U:C6	2.46	0.50
37:1k:16:TYR:CE1	37:1k:30:MET:HE1	2.47	0.50
46:1u:622:LEU:HD13	46:1u:638:ILE:HD11	1.93	0.50
47:1v:159:PHE:O	47:1v:162:MET:HG3	2.12	0.50
47:1v:420:MET:HE3	47:1v:427:PRO:HG3	1.92	0.50
55:D:260:ILE:HB	55:D:356:TYR:HD1	1.77	0.50
75:X:389:GLU:HG2	75:X:391:GLU:H	1.77	0.50
83:f:131:TYR:O	83:f:135:THR:HG22	2.12	0.50
9:1I:77:LYS:HD2	9:1I:78:GLY:H	1.76	0.50
37:1k:33:GLU:HG2	37:1k:81:LEU:HD22	1.94	0.50
46:1u:130:LEU:HD23	46:1u:130:LEU:H	1.75	0.50
46:1u:262:LEU:HD13	46:1u:296:MET:HE1	1.94	0.50
55:D:187:LEU:HD21	85:i:240:ASP:HB3	1.93	0.50
55:D:227:LYS:O	55:D:231:ILE:HG12	2.11	0.50
55:D:310:ALA:O	55:D:314:LYS:HG3	2.12	0.50
59:H:225:ILE:HG13	59:H:226:LYS:N	2.27	0.50
63:L:100:ARG:NH1	63:L:100:ARG:HB3	2.27	0.50
64:M:75:ARG:O	64:M:79:LEU:HD12	2.12	0.50
76:Y:66:VAL:O	76:Y:70:GLU:HG3	2.11	0.50
84:h:157:THR:O	84:h:160:ARG:HG2	2.12	0.50
1:1:1559:A:H2'	1:1:1560:A:C8	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1693:C:H2'	1:1:1694:A:C8	2.47	0.49
1:1:2600:U:H2'	1:1:2601:A:H8	1.76	0.49
1:1:3134:C:H2'	1:1:3135:A:H8	1.77	0.49
6:1F:108:ARG:HG3	29:1c:24:VAL:HG11	1.94	0.49
45:1t:357:LYS:HD3	45:1t:375:PHE:CE2	2.48	0.49
48:2:1385:A:H2'	48:2:1386:A:C5	2.47	0.49
58:G:10:LEU:HB3	58:G:71:CYS:HB2	1.94	0.49
78:a:405:GLN:O	78:a:409:MET:HG3	2.11	0.49
84:h:147:ASN:OD1	84:h:150:LEU:HD23	2.12	0.49
1:1:1700:U:H2'	1:1:1701:U:H6	1.78	0.49
1:1:2388:C:H2'	1:1:2389:A:H8	1.77	0.49
2:1B:121:ARG:HG2	3:1C:326:TRP:HE1	1.77	0.49
7:1G:46:ARG:HD3	39:1m:106:ILE:HG12	1.94	0.49
9:1I:9:LEU:HD11	40:1o:108:VAL:HG11	1.94	0.49
21:1U:71:ARG:HG2	21:1U:71:ARG:O	2.12	0.49
46:1u:306:MET:HB2	46:1u:340:ARG:HH12	1.77	0.49
74:W:278:ASN:HB3	74:W:282:LEU:HD23	1.94	0.49
78:a:313:VAL:HG11	78:a:361:ARG:HG3	1.92	0.49
1:1:1691:C:H2'	1:1:1692:U:C6	2.47	0.49
14:1N:37:LEU:HD23	14:1N:37:LEU:H	1.78	0.49
23:1W:83:LEU:HD13	23:1W:84:THR:N	2.26	0.49
24:1X:124:ARG:NH2	24:1X:128:GLY:H	2.08	0.49
26:1Z:22:THR:HG23	26:1Z:25:LEU:H	1.77	0.49
45:1t:282:GLU:HA	45:1t:285:ARG:HB3	1.94	0.49
46:1u:380:LYS:HA	46:1u:383:LEU:HD23	1.94	0.49
46:1u:511:LEU:O	46:1u:515:ILE:HG12	2.12	0.49
57:F:146:ARG:HH21	79:b:31:LYS:HG2	1.77	0.49
78:a:180:TRP:O	78:a:184:VAL:HG22	2.12	0.49
84:h:206:MET:HE2	84:h:240:TYR:CD2	2.45	0.49
1:1:847:U:H2'	1:1:848:G:O4'	2.12	0.49
1:1:977:U:H2'	1:1:978:A:C8	2.46	0.49
1:1:1838:A:H3'	1:1:1839:A:H8	1.77	0.49
1:1:2201:G:H5"	33:1g:83:ASN:HD21	1.77	0.49
1:1:2404:U:H2'	1:1:2405:C:C6	2.46	0.49
22:1V:147:THR:HG22	27:1a:69:SER:HB2	1.94	0.49
48:2:724:A:H2'	48:2:725:A:C8	2.47	0.49
53:B:179:PHE:HA	53:B:184:TYR:HD2	1.75	0.49
83:f:333:THR:HA	83:f:398:LEU:HD22	1.93	0.49
1:1:2834:G:H5"	1:1:2835:A:H5"	1.94	0.49
15:1O:144:MET:HG2	17:1Q:103:ILE:HD13	1.94	0.49
38:1l:150:LEU:O	38:1l:154:VAL:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:1t:352:LYS:HA	45:1t:355:GLU:CD	2.37	0.49
48:2:1719:G:H1	48:2:1752:U:H3	1.59	0.49
49:3:35:G:H2'	49:3:36:A:C8	2.47	0.49
53:B:357:GLU:HA	53:B:360:LEU:HD12	1.94	0.49
54:C:320:GLU:HB3	54:C:329:VAL:HG12	1.95	0.49
85:i:186:MET:HE2	85:i:220:ALA:HB1	1.95	0.49
1:1:1226:C:H2'	1:1:1227:A:C8	2.47	0.49
9:1I:50:THR:HG22	9:1I:85:VAL:HG13	1.93	0.49
10:1J:150:ILE:HG13	40:1o:82:LEU:HD11	1.94	0.49
21:1U:17:ILE:HG23	21:1U:33:LEU:HD13	1.93	0.49
27:1a:74:GLN:HE21	36:1j:66:PRO:HD3	1.76	0.49
46:1u:137:PHE:CD1	46:1u:156:MET:HG3	2.48	0.49
46:1u:432:GLY:O	46:1u:436:VAL:HG22	2.13	0.49
46:1u:496:LEU:HA	46:1u:499:GLN:OE1	2.12	0.49
48:2:1697:G:H2'	48:2:1698:C:C6	2.48	0.49
70:S:60:GLN:HG3	70:S:64:ILE:HD11	1.93	0.49
1:1:758:A:H2'	1:1:759:A:C8	2.47	0.49
1:1:1234:G:H1'	1:1:1255:U:O2'	2.13	0.49
1:1:1858:C:H2'	1:1:1859:G:C8	2.48	0.49
45:1t:184:MET:HE2	45:1t:189:VAL:HG12	1.94	0.49
48:2:1729:G:OP1	84:h:156:LYS:HE3	2.11	0.49
59:H:241:ILE:HA	85:i:295:MET:HE2	1.94	0.49
83:f:232:GLU:O	83:f:236:LYS:HG2	2.12	0.49
1:1:740:A:H2'	1:1:741:A:C8	2.47	0.49
10:1J:33:SER:HA	10:1J:43:MET:HE3	1.94	0.49
45:1t:315:LEU:HB3	45:1t:316:PRO:HD3	1.95	0.49
48:2:10:A:N6	82:e:379:ARG:HG2	2.28	0.49
48:2:222:G:H2'	48:2:223:A:H8	1.78	0.49
48:2:1638:U:H2'	48:2:1639:A:C8	2.48	0.49
53:B:337:GLY:HA3	78:a:180:TRP:HH2	1.78	0.49
75:X:415:LEU:HD13	75:X:438:ILE:HD12	1.94	0.49
75:X:427:GLY:C	75:X:428:ILE:HG13	2.38	0.49
77:Z:124:ILE:HD12	77:Z:124:ILE:O	2.13	0.49
82:e:201:THR:HG23	82:e:204:ARG:H	1.78	0.49
1:1:2403:U:H2'	1:1:2404:U:C6	2.48	0.49
13:1M:156:LEU:HD13	13:1M:264:PRO:HB3	1.94	0.49
24:1X:191:THR:HA	24:1X:244:VAL:HG12	1.94	0.49
47:1v:432:TYR:HB3	47:1v:436:MET:HE3	1.93	0.49
48:2:929:C:H2'	48:2:930:A:H8	1.77	0.49
48:2:1481:C:H2'	48:2:1482:U:C6	2.48	0.49
48:2:1687:U:H2'	48:2:1688:U:C6	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:2:1689:C:H2'	48:2:1690:G:H8	1.78	0.49
50:5:63:C:H2'	50:5:64:U:C6	2.48	0.49
53:B:369:ASN:HD22	75:X:338:ASN:HA	1.78	0.49
73:V:93:VAL:HA	73:V:96:GLN:NE2	2.24	0.49
1:1:445:G:H21	1:1:465:U:H3'	1.78	0.49
1:1:677:U:H2'	1:1:678:C:C6	2.48	0.49
1:1:958:U:H2'	1:1:959:C:H6	1.78	0.49
2:1B:46:MET:HG2	3:1C:53:MET:HE1	1.95	0.49
12:1L:54:LEU:HD23	12:1L:126:ASN:HB3	1.95	0.49
12:1L:140:THR:HG22	12:1L:141:ASP:H	1.77	0.49
27:1a:108:PRO:O	27:1a:112:ARG:HG3	2.13	0.49
46:1u:212:LYS:HB2	46:1u:218:ARG:HH21	1.78	0.49
48:2:146:U:H2'	48:2:147:U:H6	1.77	0.49
48:2:599:A:H2'	48:2:600:A:H8	1.78	0.49
48:2:718:A:H2	48:2:729:A:H61	1.61	0.49
53:B:406:LYS:HD2	53:B:407:ARG:HH11	1.77	0.49
79:b:52:ASP:O	79:b:53:LYS:HG2	2.13	0.49
84:h:206:MET:O	84:h:210:LYS:HG3	2.13	0.49
85:i:171:ASN:O	85:i:175:LYS:HG2	2.13	0.49
1:1:2445:G:H4'	1:1:2446:G:OP1	2.12	0.48
1:1:2465:A:H5"	1:1:2476:A:C8	2.47	0.48
1:1:2508:G:N2	1:1:2528:G:C5	2.81	0.48
6:1F:38:PRO:HD3	6:1F:53:MET:HE3	1.95	0.48
9:1I:68:LYS:HE3	9:1I:69:TRP:CE2	2.47	0.48
22:1V:118:ARG:HE	22:1V:122:LEU:HD12	1.78	0.48
45:1t:349:LEU:HD23	45:1t:352:LYS:HD2	1.95	0.48
46:1u:437:LEU:HA	46:1u:440:ASN:OD1	2.12	0.48
49:3:1:A:O2'	49:3:2:A:H8	1.95	0.48
54:C:64:THR:HG21	55:D:459:ARG:HG3	1.94	0.48
62:K:81:LEU:HD22	62:K:101:VAL:HG11	1.94	0.48
84:h:347:GLU:HA	84:h:350:LYS:HD2	1.96	0.48
85:i:235:GLN:O	85:i:239:LEU:HG	2.13	0.48
1:1:855:G:N2	1:1:865:G:H22	2.11	0.48
1:1:1100:U:H4'	1:1:1101:G:O5'	2.13	0.48
6:1F:65:GLN:HA	6:1F:90:ASP:N	2.29	0.48
10:1J:33:SER:HB3	10:1J:34:PRO:HD3	1.94	0.48
45:1t:36:GLU:HG3	45:1t:40:ARG:HD2	1.94	0.48
47:1v:373:ILE:HB	47:1v:412:HIS:CE1	2.48	0.48
48:2:638:A:C8	58:G:106:PRO:HA	2.48	0.48
48:2:1388:A:C8	48:2:1389:A:C8	3.00	0.48
57:F:50:MET:SD	57:F:115:ILE:HD13	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:O:6:ARG:HA	66:O:73:VAL:HG21	1.95	0.48
83:f:269:MET:O	83:f:273:TYR:HD1	1.96	0.48
1:1:77:A:H2'	1:1:78:U:C6	2.48	0.48
1:1:733:A:H2'	1:1:734:G:C8	2.48	0.48
1:1:965:A:H4'	1:1:981:G:H22	1.78	0.48
1:1:1188:U:H3	1:1:1267:A:H61	1.60	0.48
1:1:1233:U:O3'	1:1:1234:G:H8	1.96	0.48
1:1:2392:U:H2'	1:1:2393:U:C6	2.48	0.48
13:1M:244:PRO:HD3	13:1M:255:ILE:HG12	1.95	0.48
23:1W:186:LEU:HD23	23:1W:221:LEU:HD21	1.95	0.48
25:1Y:117:ASN:HB2	25:1Y:124:TRP:HZ3	1.79	0.48
42:1q:47:VAL:O	42:1q:51:GLU:HG2	2.13	0.48
47:1v:80:SER:HB2	47:1v:118:LEU:HD21	1.94	0.48
48:2:48:C:H2'	48:2:49:U:H6	1.79	0.48
48:2:278:G:H2'	48:2:279:G:H8	1.77	0.48
48:2:732:U:H2'	48:2:733:C:C6	2.48	0.48
48:2:1501:A:H2	48:2:1504:G:N3	2.11	0.48
53:B:261:VAL:HG12	53:B:263:PRO:HD3	1.94	0.48
53:B:286:ARG:HB3	53:B:321:ARG:NH1	2.28	0.48
54:C:240:VAL:HG11	55:D:218:MET:HE3	1.94	0.48
76:Y:25:ILE:HD12	78:a:371:LEU:HD12	1.94	0.48
1:1:411:U:H2'	1:1:412:U:C6	2.48	0.48
1:1:1688:U:H2'	1:1:1689:G:H8	1.78	0.48
1:1:2931:U:H2'	1:1:2932:G:C8	2.49	0.48
14:1N:160:GLN:O	14:1N:164:LEU:HG	2.13	0.48
26:1Z:155:GLU:HG3	26:1Z:159:LYS:HE3	1.94	0.48
35:1i:137:ILE:HG13	38:1l:52:GLU:HG3	1.95	0.48
38:1l:91:ILE:HG22	38:1l:96:LYS:HE3	1.95	0.48
39:1m:9:LYS:HE2	39:1m:44:LEU:HD13	1.96	0.48
48:2:990:U:H2'	48:2:991:A:C8	2.48	0.48
83:f:301:THR:O	83:f:305:VAL:HG22	2.13	0.48
9:1I:56:LYS:HB3	9:1I:59:LEU:HB3	1.96	0.48
30:1d:114:CYS:HB3	30:1d:125:CYS:SG	2.52	0.48
39:1m:24:GLU:O	39:1m:28:GLN:HG2	2.12	0.48
60:I:125:ILE:HD11	60:I:191:LYS:HD3	1.94	0.48
82:e:181:LEU:HD11	82:e:209:TYR:HD2	1.78	0.48
83:f:345:LYS:HE2	83:f:349:GLY:HA2	1.94	0.48
84:h:345:GLN:C	84:h:350:LYS:HE3	2.37	0.48
1:1:513:G:H21	1:1:515:C:H5'	1.78	0.48
1:1:1256:G:C2	1:1:1257:G:C5	3.02	0.48
1:1:1412:U:H5"	1:1:1413:G:H5"	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2383:C:H2'	1:1:2384:C:H6	1.79	0.48
7:1G:45:VAL:HG13	7:1G:65:VAL:HG22	1.95	0.48
25:1Y:81:ILE:HD13	25:1Y:84:ARG:HH21	1.78	0.48
47:1v:185:LEU:HB3	47:1v:194:VAL:HG22	1.94	0.48
53:B:337:GLY:HA3	78:a:180:TRP:CH2	2.49	0.48
54:C:287:LEU:HD22	55:D:178:LEU:HD13	1.95	0.48
57:F:140:ARG:HD2	61:J:237:TYR:OH	2.14	0.48
62:K:120:GLU:HA	62:K:120:GLU:OE2	2.13	0.48
83:f:120:LYS:HG2	83:f:336:TYR:OH	2.13	0.48
1:1:361:A:H2'	1:1:362:A:H8	1.78	0.48
1:1:1902:A:H4'	1:1:1903:A:H5"	1.96	0.48
1:1:2349:A:C6	1:1:2803:OMC:H1'	2.48	0.48
3:1C:76:LYS:HB3	3:1C:76:LYS:HE2	1.51	0.48
46:1u:589:PHE:CZ	46:1u:620:LYS:HD3	2.49	0.48
52:A:6:ALA:O	52:A:9:GLN:HG3	2.14	0.48
53:B:181:HIS:ND1	53:B:183:LYS:HG2	2.29	0.48
69:R:89:ILE:HG12	69:R:104:VAL:HG12	1.95	0.48
73:V:92:ARG:O	73:V:96:GLN:HG3	2.14	0.48
1:1:542:C:H2'	1:1:543:G:C8	2.48	0.48
1:1:2342:U:H2'	1:1:2343:C:C6	2.49	0.48
8:1H:106:VAL:HG12	8:1H:107:LYS:HG3	1.96	0.48
9:1I:12:GLY:O	9:1I:16:ILE:HG22	2.12	0.48
10:1J:42:ASN:H	10:1J:73:HIS:HE1	1.61	0.48
14:1N:50:GLY:HA3	14:1N:140:ARG:HH22	1.79	0.48
15:1O:107:MET:HA	15:1O:107:MET:HE2	1.95	0.48
19:1S:109:PRO:O	19:1S:113:VAL:HG23	2.13	0.48
23:1W:90:ILE:HG21	23:1W:140:ILE:HG21	1.95	0.48
41:1p:88:ARG:O	41:1p:92:GLU:HG2	2.14	0.48
45:1t:165:MET:HE3	45:1t:181:ILE:HG13	1.95	0.48
48:2:956:G:N2	60:I:171:VAL:HG11	2.29	0.48
53:B:286:ARG:CG	53:B:321:ARG:HH22	2.24	0.48
54:C:282:VAL:HG21	82:e:143:ILE:HD12	1.94	0.48
59:H:306:ALA:HB3	59:H:321:ILE:HG12	1.95	0.48
64:M:82:ARG:HB3	64:M:83:PHE:HD1	1.79	0.48
64:M:83:PHE:HD2	64:M:114:LEU:HD22	1.79	0.48
75:X:427:GLY:O	75:X:428:ILE:HG13	2.14	0.48
85:i:134:LYS:O	85:i:137:GLU:HG2	2.13	0.48
1:1:334:A:H2'	1:1:335:A:C8	2.49	0.48
1:1:1052:C:H2'	1:1:1053:A:H8	1.79	0.48
1:1:1688:U:H2'	1:1:1689:G:C8	2.49	0.48
14:1N:107:LYS:HB2	14:1N:107:LYS:HE3	1.69	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:1R:29:GLU:O	18:1R:33:GLN:HG3	2.13	0.48
21:1U:30:GLU:OE2	21:1U:137:VAL:HA	2.14	0.48
35:1i:76:LYS:O	35:1i:80:GLN:HG2	2.14	0.48
39:1m:95:PHE:HB2	39:1m:102:TRP:HE1	1.79	0.48
48:2:50:A:H2'	48:2:51:U:C6	2.49	0.48
48:2:1063:C:H2'	48:2:1064:G:H8	1.79	0.48
48:2:1709:U:H2'	48:2:1710:G:H8	1.78	0.48
52:A:43:SER:HB2	86:k:4:MET:SD	2.54	0.48
1:1:795:U:O2'	46:1u:667:LEU:HD11	2.14	0.48
1:1:1693:C:H2'	1:1:1694:A:H8	1.78	0.48
1:1:2494:G:H2'	1:1:2495:G:H8	1.75	0.48
45:1t:162:ASN:HB3	45:1t:194:TYR:HD2	1.79	0.48
48:2:356:G:H2'	48:2:357:A:H8	1.78	0.48
48:2:1438:G:H2'	48:2:1439:A:H8	1.78	0.48
48:2:1638:U:H2'	48:2:1639:A:H8	1.78	0.48
61:J:298:THR:HG22	68:Q:228:GLY:HA2	1.96	0.48
84:h:272:LEU:HD23	84:h:297:GLY:HA3	1.96	0.48
1:1:121:C:H2'	1:1:122:C:C6	2.50	0.47
1:1:235:G:H2'	1:1:236:A:C8	2.48	0.47
1:1:941:U:H2'	1:1:942:C:C6	2.49	0.47
55:D:299:GLU:O	55:D:303:ILE:HG12	2.14	0.47
59:H:239:SER:OG	59:H:241:ILE:HG22	2.14	0.47
76:Y:61:ASN:HA	76:Y:67:LEU:HD11	1.95	0.47
81:d:41:GLY:H	81:d:44:GLU:HG2	1.79	0.47
1:1:408:U:H2'	1:1:409:U:C6	2.48	0.47
1:1:1463:G:H22	1:1:1965:A:H2	1.61	0.47
6:1F:17:LEU:HD21	35:1i:191:LEU:HB2	1.96	0.47
12:1L:106:VAL:HA	12:1L:128:VAL:HG12	1.95	0.47
48:2:1648:G:H2'	48:2:1649:G:H8	1.79	0.47
54:C:250:LYS:O	54:C:254:ARG:HG3	2.14	0.47
55:D:127:LYS:N	55:D:127:LYS:HD3	2.29	0.47
60:I:130:ILE:HB	60:I:190:ILE:HB	1.95	0.47
74:W:439:CYS:SG	74:W:458:TRP:HB2	2.54	0.47
85:i:356:ILE:HG23	85:i:367:TYR:CE1	2.48	0.47
1:1:361:A:H5'	47:1v:446:THR:HB	1.95	0.47
1:1:1840:A:H2'	1:1:1841:G:H8	1.79	0.47
1:1:2444:A:H4'	1:1:2445:G:O4'	2.15	0.47
1:1:2956:C:H2'	1:1:2957:A:H8	1.79	0.47
23:1W:49:SER:O	23:1W:53:ARG:HG2	2.15	0.47
23:1W:112:ARG:HG2	23:1W:120:LEU:HG	1.96	0.47
45:1t:129:LEU:HA	45:1t:132:CYS:SG	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:1v:316:ARG:HD2	47:1v:316:ARG:N	2.29	0.47
48:2:1726:U:H2'	48:2:1727:G:C8	2.49	0.47
53:B:395:VAL:HG13	78:a:105:LEU:HD11	1.94	0.47
64:M:108:ARG:O	64:M:108:ARG:HD3	2.14	0.47
74:W:272:LYS:HG3	74:W:326:ILE:HD13	1.96	0.47
9:1I:28:ASN:HA	9:1I:79:MET:O	2.14	0.47
45:1t:395:ALA:HB3	45:1t:406:TRP:CZ3	2.50	0.47
47:1v:127:LEU:O	47:1v:131:GLU:HG2	2.15	0.47
48:2:160:A:H2'	48:2:161:A:C8	2.49	0.47
49:3:102:U:H2'	49:3:103:G:C8	2.50	0.47
64:M:99:LEU:HG	64:M:100:PRO:HD2	1.95	0.47
72:U:56:VAL:HG13	72:U:82:ALA:HB1	1.97	0.47
74:W:449:ARG:HB2	74:W:452:VAL:HG22	1.95	0.47
82:e:338:LYS:HD3	82:e:351:TRP:HE3	1.78	0.47
1:1:1052:C:C2	1:1:1053:A:C8	3.03	0.47
1:1:1934:G:C4	44:1s:72:ARG:HG2	2.49	0.47
6:1F:106:LEU:HA	6:1F:109:ILE:HG22	1.97	0.47
15:1O:63:ALA:O	15:1O:67:VAL:HG22	2.14	0.47
35:1i:110:LYS:HD2	35:1i:110:LYS:HA	1.67	0.47
46:1u:295:THR:HA	46:1u:298:ASN:HD21	1.79	0.47
53:B:98:TRP:HB2	75:X:330:ALA:HB1	1.96	0.47
53:B:281:LEU:O	53:B:284:ARG:HB2	2.13	0.47
58:G:81:LYS:HB2	58:G:84:GLU:HG3	1.95	0.47
1:1:1267:A:H2'	1:1:1268:U:C6	2.50	0.47
26:1Z:40:MET:HG2	26:1Z:52:HIS:NE2	2.30	0.47
31:1e:12:ILE:HG21	31:1e:28:LYS:HD2	1.96	0.47
45:1t:196:TYR:HE2	45:1t:225:VAL:HG21	1.80	0.47
48:2:1736:U:H4'	48:2:1737:A:C8	2.48	0.47
50:5:52:A:H2'	50:5:53:G:O4'	2.15	0.47
53:B:312:HIS:HE1	53:B:314:ILE:HD11	1.80	0.47
57:F:96:ALA:HA	57:F:114:GLU:OE1	2.14	0.47
69:R:63:MET:HE3	69:R:76:PHE:HD2	1.80	0.47
74:W:278:ASN:O	74:W:282:LEU:HD23	2.13	0.47
1:1:1095:A:H2'	1:1:1096:C:C6	2.49	0.47
1:1:2388:C:H2'	1:1:2389:A:C8	2.50	0.47
1:1:2811:U:H2'	1:1:2811:U:O2	2.15	0.47
1:1:2924:C:O2	4:1D:236:MET:HE1	2.14	0.47
10:1J:109:LEU:HD22	10:1J:113:HIS:ND1	2.29	0.47
10:1J:124:ASP:OD1	10:1J:127:CYS:HB2	2.14	0.47
10:1J:131:PRO:O	10:1J:135:ILE:HG13	2.15	0.47
18:1R:97:ALA:HB1	28:1b:96:VAL:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:1o:68:ILE:HD12	40:1o:68:ILE:O	2.15	0.47
48:2:78:U:O2'	48:2:79:G:H5'	2.15	0.47
48:2:1707:A:H2'	48:2:1708:A:H8	1.78	0.47
54:C:248:GLU:HA	54:C:251:ARG:HG2	1.97	0.47
55:D:253:ASN:HD21	55:D:255:ALA:HB3	1.79	0.47
78:a:218:LYS:HA	78:a:221:VAL:HG12	1.97	0.47
79:b:58:LYS:HD3	79:b:58:LYS:N	2.30	0.47
82:e:200:TYR:HD1	82:e:204:ARG:HD2	1.80	0.47
84:h:89:LEU:HA	84:h:92:LYS:HG2	1.96	0.47
84:h:223:LEU:O	84:h:227:ILE:HG12	2.15	0.47
1:1:721:G:H2'	1:1:2348:A:N7	2.29	0.47
1:1:2363:A:H2'	1:1:2364:A:H8	1.80	0.47
24:1X:185:LYS:HD2	24:1X:218:VAL:HG21	1.96	0.47
47:1v:315:PHE:CD1	47:1v:315:PHE:C	2.93	0.47
48:2:10:A:C6	82:e:379:ARG:HG2	2.49	0.47
48:2:598:G:H2'	48:2:599:A:C8	2.49	0.47
48:2:938:G:C2	48:2:939:A:C8	3.03	0.47
58:G:29:ILE:HG21	58:G:60:ILE:HG13	1.95	0.47
83:f:120:LYS:NZ	83:f:395:GLU:HB3	2.29	0.47
85:i:135:VAL:HA	85:i:138:GLU:OE2	2.15	0.47
1:1:176:A:H2'	1:1:177:C:C6	2.50	0.47
1:1:417:U:O3'	1:1:418:U:H4'	2.15	0.47
1:1:463:G:H2'	22:1V:25:ARG:HH12	1.80	0.47
1:1:648:A:H8	1:1:651:A:H2	1.61	0.47
1:1:1591:C:H3'	1:1:1591:C:OP1	2.15	0.47
1:1:2555:A:H2'	1:1:2556:U:C6	2.49	0.47
9:1I:57:ASN:HB2	9:1I:76:MET:SD	2.55	0.47
9:1I:90:ILE:N	9:1I:91:PRO:HD2	2.29	0.47
21:1U:129:LEU:HD21	45:1t:110:GLU:OE2	2.14	0.47
46:1u:146:ILE:HA	46:1u:146:ILE:HD13	1.76	0.47
47:1v:143:ASP:HA	47:1v:146:VAL:HG22	1.96	0.47
48:2:278:G:H2'	48:2:279:G:C8	2.49	0.47
48:2:679:G:N2	61:J:215:ASN:HA	2.30	0.47
52:A:114:LYS:HB2	52:A:125:PHE:CE1	2.50	0.47
57:F:59:PRO:O	57:F:84:GLN:HG2	2.15	0.47
1:1:360:A:H2'	1:1:361:A:C8	2.50	0.47
1:1:1558:G:H2'	1:1:1559:A:H8	1.80	0.47
1:1:1579:C:C1'	45:1t:201:ARG:HH22	2.28	0.47
1:1:2820:C:H2'	1:1:2821:A:H8	1.80	0.47
17:1Q:200:LYS:HB2	17:1Q:200:LYS:HE3	1.67	0.47
22:1V:142:PHE:CD1	36:1j:72:LYS:HD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:1W:38:ALA:HB3	23:1W:111:ILE:HA	1.96	0.47
46:1u:368:PRO:HG3	46:1u:398:ILE:HD12	1.97	0.47
48:2:1671:C:H2'	48:2:1672:A:C8	2.50	0.47
53:B:172:LEU:O	53:B:176:SER:HB3	2.15	0.47
55:D:411:LYS:O	55:D:415:LYS:HG2	2.14	0.47
75:X:523:LYS:HE2	75:X:523:LYS:HB2	1.81	0.47
1:1:135:C:O2'	1:1:136:G:H5'	2.15	0.46
1:1:271:A:H2'	1:1:272:A:H8	1.79	0.46
1:1:2625:U:H3	1:1:2638:A:N6	2.13	0.46
45:1t:395:ALA:HA	45:1t:398:ILE:HG22	1.96	0.46
46:1u:702:TYR:HD1	46:1u:702:TYR:O	1.98	0.46
48:2:1507:A:H2'	48:2:1508:A:H8	1.80	0.46
48:2:1746:A:H2'	48:2:1747:A:H8	1.80	0.46
52:A:120:HIS:CG	52:A:121:LYS:H	2.33	0.46
53:B:338:ALA:HB3	75:X:383:ASN:HD21	1.80	0.46
59:H:235:LEU:O	59:H:239:SER:CB	2.63	0.46
62:K:8:ILE:HD11	67:P:32:ARG:HB2	1.97	0.46
65:N:338:MET:SD	65:N:347:ARG:HD3	2.55	0.46
1:1:1449:G:H2'	1:1:1450:A:C8	2.49	0.46
1:1:1987:G:H5"	1:1:1988:C:H5'	1.95	0.46
1:1:2118:A:H2'	1:1:2119:C:C6	2.50	0.46
10:1J:138:SER:O	10:1J:142:THR:HG23	2.15	0.46
23:1W:64:PRO:HD2	23:1W:78:SER:OG	2.15	0.46
26:1Z:59:VAL:HG22	26:1Z:66:LYS:HG2	1.96	0.46
35:1i:172:ASN:HD22	38:1l:50:PHE:HB3	1.78	0.46
48:2:732:U:H2'	48:2:733:C:H6	1.80	0.46
66:O:7:LEU:HD13	66:O:73:VAL:HG22	1.97	0.46
1:1:21:C:H2'	1:1:22:A:C8	2.50	0.46
1:1:1009:G:H2'	1:1:1010:C:H6	1.80	0.46
1:1:1376:U:H2'	1:1:1377:U:C6	2.51	0.46
1:1:1934:G:C5	44:1s:72:ARG:HG2	2.50	0.46
13:1M:266:PRO:HB2	13:1M:269:ALA:HB3	1.97	0.46
17:1Q:193:SER:HB3	17:1Q:196:LEU:HD23	1.98	0.46
46:1u:734:LYS:O	46:1u:738:VAL:HG13	2.15	0.46
48:2:457:C:H2'	48:2:458:U:O2	2.15	0.46
48:2:467:G:H2'	48:2:468:U:C6	2.51	0.46
53:B:53:PHE:HB2	53:B:78:ARG:HG3	1.97	0.46
54:C:170:PHE:O	54:C:173:GLU:HG3	2.16	0.46
75:X:413:GLU:O	75:X:417:LYS:HD2	2.15	0.46
75:X:434:TRP:O	75:X:438:ILE:HG12	2.16	0.46
76:Y:82:LYS:HB3	76:Y:82:LYS:HE2	1.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:a:219:LYS:O	78:a:222:GLU:HG3	2.16	0.46
1:1:479:C:H2'	1:1:480:G:C8	2.51	0.46
1:1:1388:A:H2'	1:1:1389:C:C6	2.50	0.46
1:1:1474:U:H2'	1:1:1475:G:H8	1.80	0.46
1:1:1840:A:H2'	1:1:1841:G:C8	2.50	0.46
1:1:2556:U:H2'	1:1:2557:C:H6	1.80	0.46
1:1:2766:G:H2'	1:1:2767:A:C8	2.51	0.46
1:1:2852:U:H2'	1:1:2853:C:C6	2.51	0.46
10:1J:18:LYS:HG2	10:1J:66:LYS:CB	2.45	0.46
10:1J:30:PRO:HB2	10:1J:31:PRO:HD3	1.96	0.46
39:1m:11:GLU:HB3	39:1m:46:LYS:HB3	1.98	0.46
46:1u:165:LYS:HG3	46:1u:168:HIS:ND1	2.30	0.46
46:1u:399:PHE:HB3	46:1u:422:MET:HE1	1.97	0.46
46:1u:403:LEU:HG	46:1u:418:VAL:HG11	1.97	0.46
46:1u:430:GLU:HB2	46:1u:433:HIS:CG	2.51	0.46
48:2:265:A:C2	48:2:301:A:C5	3.04	0.46
48:2:476:C:H41	66:O:88:MET:HE3	1.79	0.46
53:B:168:ASN:HB3	75:X:451:ILE:HD11	1.97	0.46
59:H:225:ILE:HA	59:H:228:PRO:HG3	1.95	0.46
1:1:21:C:H2'	1:1:22:A:H8	1.81	0.46
1:1:130:A:O2'	1:1:131:G:H5'	2.15	0.46
1:1:361:A:H2'	1:1:362:A:C8	2.49	0.46
1:1:1612:G:H2'	1:1:1613:G:C8	2.50	0.46
1:1:2595:G:H4'	1:1:2596:A:O4'	2.15	0.46
23:1W:60:ALA:HB2	23:1W:143:LEU:HB2	1.97	0.46
48:2:1008:U:H2'	48:2:1009:C:H6	1.80	0.46
48:2:1129:G:H4'	78:a:345:ASP:OD2	2.15	0.46
53:B:66:PRO:HA	78:a:301:PRO:HA	1.98	0.46
73:V:166:LYS:HB3	73:V:166:LYS:NZ	2.31	0.46
79:b:21:ILE:H	79:b:80:ASN:HD21	1.63	0.46
84:h:81:ASP:HB2	84:h:82:PRO:HD3	1.98	0.46
1:1:149:G:O2'	1:1:150:C:H5'	2.16	0.46
1:1:1862:A:H2'	1:1:1863:C:H6	1.81	0.46
14:1N:77:ARG:HB3	14:1N:138:ILE:HD11	1.97	0.46
24:1X:104:LYS:HB3	24:1X:104:LYS:HE2	1.70	0.46
41:1p:67:ASP:HB3	46:1u:502:LYS:HD3	1.97	0.46
48:2:786:A:H2'	48:2:787:G:C8	2.51	0.46
50:5:38:G:H3'	50:5:39:A:C8	2.51	0.46
53:B:458:PHE:HA	53:B:461:LYS:HG2	1.98	0.46
59:H:219:LYS:NZ	72:U:124:LEU:HD23	2.29	0.46
59:H:271:ARG:HH11	59:H:271:ARG:HG3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:i:325:LEU:HD13	85:i:355:LEU:HD11	1.98	0.46
1:1:1318:C:H2'	1:1:1319:U:C6	2.51	0.46
1:1:1336:A:H2'	1:1:1337:A:C8	2.51	0.46
38:1l:225:GLU:HG2	38:1l:226:PHE:N	2.31	0.46
46:1u:429:ALA:HB1	46:1u:434:TYR:CE1	2.51	0.46
48:2:488:C:H2'	48:2:489:G:H8	1.81	0.46
48:2:943:U:H2'	48:2:944:G:C8	2.50	0.46
53:B:391:GLU:HG2	78:a:109:ARG:NE	2.25	0.46
57:F:91:TRP:HA	57:F:94:GLU:HG2	1.96	0.46
59:H:231:ALA:HB2	72:U:78:ILE:HD12	1.98	0.46
63:L:115:TYR:O	63:L:119:ARG:HG2	2.16	0.46
1:1:1654:C:H2'	1:1:1655:C:H6	1.79	0.46
1:1:1920:G:O6	47:1v:190:ARG:HD3	2.15	0.46
1:1:2346:U:H2'	1:1:2347:G:C8	2.51	0.46
1:1:2555:A:H2'	1:1:2556:U:H6	1.80	0.46
23:1W:67:LEU:HB2	23:1W:78:SER:OG	2.15	0.46
53:B:305:GLU:O	53:B:309:ARG:HD3	2.16	0.46
59:H:319:VAL:HG21	59:H:382:GLY:C	2.41	0.46
60:I:189:VAL:C	60:I:190:ILE:HD13	2.41	0.46
75:X:411:LEU:HD22	75:X:442:MET:HE1	1.97	0.46
75:X:497:LYS:HE3	75:X:497:LYS:HB2	1.75	0.46
1:1:1328:G:H8	1:1:1330:U:O2	1.99	0.46
1:1:1618:A:H2'	1:1:1619:G:C8	2.50	0.46
1:1:2446:G:H2'	1:1:2447:U:C6	2.51	0.46
6:1F:116:LEU:HD11	6:1F:138:PHE:CD2	2.51	0.46
20:1T:133:VAL:HG11	20:1T:159:ARG:HD3	1.98	0.46
27:1a:60:TRP:HH2	36:1j:73:LEU:HD22	1.80	0.46
29:1c:26:MET:HE2	29:1c:26:MET:HB3	1.70	0.46
46:1u:137:PHE:CG	46:1u:156:MET:HE2	2.51	0.46
47:1v:383:MET:HE2	47:1v:383:MET:HB3	1.85	0.46
48:2:1845:A:N1	79:b:21:ILE:HG23	2.30	0.46
49:3:15:G:H5"	49:3:106:C:OP2	2.16	0.46
50:5:5:G:H2'	50:5:6:G:H8	1.80	0.46
53:B:474:ILE:O	53:B:478:ILE:HB	2.16	0.46
54:C:312:ILE:HG22	82:e:252:PHE:HD1	1.81	0.46
56:E:8:LEU:HD23	56:E:88:LEU:HD11	1.98	0.46
59:H:325:LYS:O	59:H:325:LYS:HG2	2.15	0.46
83:f:110:SER:O	83:f:113:GLU:HG2	2.15	0.46
85:i:142:GLY:HA3	85:i:146:LYS:HD3	1.97	0.46
1:1:1477:G:H2'	1:1:1478:U:C6	2.51	0.46
1:1:1885:U:H2'	1:1:1886:U:C6	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:1b:61:MET:O	28:1b:65:VAL:HG22	2.16	0.46
40:1o:112:THR:HG23	40:1o:115:LYS:HE3	1.97	0.46
40:1o:112:THR:O	40:1o:115:LYS:HG3	2.16	0.46
43:1r:63:ASP:HA	43:1r:66:LYS:HG2	1.98	0.46
45:1t:71:TYR:CD2	45:1t:102:LYS:HB3	2.51	0.46
48:2:403:G:H2'	48:2:404:C:C6	2.51	0.46
48:2:522:G:H2'	48:2:523:C:C6	2.51	0.46
48:2:1583:U:H4'	63:L:115:TYR:CE2	2.51	0.46
50:5:26:C:H2'	50:5:27:A:O4'	2.16	0.46
52:A:51:ARG:C	83:f:251:GLN:HE22	2.24	0.46
53:B:204:THR:HG22	53:B:206:LEU:H	1.81	0.46
55:D:98:ARG:HB3	55:D:103:LEU:HD11	1.96	0.46
73:V:132:GLN:NE2	73:V:132:GLN:HA	2.31	0.46
78:a:295:SER:HB2	78:a:357:ARG:HD3	1.97	0.46
84:h:206:MET:HE1	84:h:244:PHE:HE1	1.80	0.46
1:1:965:A:H4'	1:1:981:G:N2	2.31	0.45
1:1:1234:G:OP1	9:1I:53:LEU:HD12	2.16	0.45
5:1E:204:ARG:HD3	5:1E:204:ARG:HA	1.73	0.45
24:1X:216:LEU:HD11	24:1X:222:LEU:HD13	1.98	0.45
48:2:1129:G:H2'	48:2:1130:C:C6	2.50	0.45
48:2:1540:C:O2'	48:2:1542:A:H8	1.99	0.45
52:A:51:ARG:HB3	83:f:251:GLN:NE2	2.31	0.45
53:B:61:ILE:HB	53:B:72:HIS:HB2	1.98	0.45
54:C:119:THR:HB	54:C:121:PRO:HD2	1.98	0.45
54:C:252:MET:HE2	82:e:150:SER:HB3	1.97	0.45
65:N:298:PRO:HG2	65:N:301:LEU:HD12	1.98	0.45
66:O:70:SER:OG	66:O:72:PRO:HD2	2.16	0.45
68:Q:169:GLU:CD	68:Q:169:GLU:H	2.24	0.45
71:T:59:LYS:HE3	71:T:66:GLY:HA3	1.99	0.45
81:d:41:GLY:H	81:d:44:GLU:CG	2.28	0.45
84:h:263:ALA:HB3	84:h:272:LEU:HD13	1.97	0.45
1:1:654:U:H4'	1:1:1392:G:H4'	1.98	0.45
1:1:1886:U:H2'	1:1:1887:G:O4'	2.16	0.45
1:1:2497:G:H2'	1:1:2498:C:C6	2.52	0.45
2:1B:70:ILE:HG12	2:1B:100:GLU:HG2	1.97	0.45
38:1l:163:VAL:HG22	38:1l:191:LYS:HG2	1.99	0.45
39:1m:10:ILE:HG21	39:1m:26:LEU:HD21	1.97	0.45
40:1o:92:ARG:HA	40:1o:107:PHE:CZ	2.51	0.45
43:1r:110:ILE:C	43:1r:110:ILE:HD12	2.42	0.45
46:1u:295:THR:HA	46:1u:298:ASN:ND2	2.31	0.45
46:1u:376:MET:HE3	46:1u:376:MET:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:2:53:U:H2'	48:2:54:G:H8	1.80	0.45
48:2:215:A:H2'	48:2:216:A:C8	2.50	0.45
48:2:392:A:H2'	48:2:393:A:H8	1.81	0.45
48:2:512:C:H2'	48:2:513:G:H8	1.80	0.45
49:3:21:A:H2'	49:3:22:C:C6	2.51	0.45
59:H:341:MET:HE2	59:H:341:MET:HB2	1.77	0.45
62:K:111:ARG:HD2	62:K:122:PRO:HG3	1.98	0.45
75:X:366:ARG:HG3	75:X:367:ALA:N	2.29	0.45
84:h:332:LYS:HA	84:h:336:GLU:OE1	2.16	0.45
1:1:665:G:H2'	1:1:666:C:C6	2.51	0.45
1:1:859:U:H2'	1:1:861:A:C8	2.52	0.45
1:1:978:A:H2'	1:1:979:G:H8	1.81	0.45
1:1:1123:A:H5"	19:1S:221:LYS:HD2	1.98	0.45
8:1H:88:HIS:HA	8:1H:91:ARG:HH12	1.81	0.45
10:1J:122:GLN:HA	10:1J:127:CYS:SG	2.57	0.45
20:1T:202:ARG:HE	20:1T:202:ARG:HB3	1.59	0.45
37:1k:8:GLN:HA	37:1k:63:ARG:HG3	1.99	0.45
48:2:1006:U:C2	75:X:509:GLN:HG2	2.51	0.45
1:1:314:U:H2'	1:1:315:U:C6	2.51	0.45
1:1:731:U:H2'	1:1:732:C:C6	2.50	0.45
1:1:756:U:C5	5:1E:300:ARG:HD3	2.52	0.45
6:1F:43:ASN:O	6:1F:44:PHE:HB2	2.15	0.45
46:1u:583:SER:O	46:1u:586:GLU:HG3	2.16	0.45
46:1u:684:SER:O	46:1u:688:VAL:HG12	2.17	0.45
48:2:1610:U:H4'	59:H:422:ARG:HG3	1.98	0.45
48:2:1839:G:H2'	48:2:1840:A:H8	1.79	0.45
53:B:55:PHE:CD1	53:B:75:LEU:HD21	2.51	0.45
60:I:217:GLN:OE1	78:a:296:ARG:HG2	2.16	0.45
63:L:138:LYS:HA	63:L:138:LYS:HD2	1.77	0.45
73:V:155:LEU:O	73:V:159:GLU:HG2	2.16	0.45
74:W:189:ARG:HB3	74:W:189:ARG:NH1	2.31	0.45
78:a:224:LYS:O	78:a:227:GLU:HG3	2.16	0.45
78:a:382:ALA:HB1	78:a:386:ARG:HH21	1.80	0.45
83:f:198:GLU:O	83:f:202:LEU:HG	2.16	0.45
1:1:334:A:H5'	46:1u:272:GLU:HG3	1.98	0.45
1:1:2877:A:H5"	1:1:2879:G:H4'	1.99	0.45
3:1C:53:MET:HB3	3:1C:76:LYS:HB2	1.97	0.45
41:1p:41:MET:HE3	41:1p:41:MET:HB3	1.87	0.45
49:3:2:A:HO2'	49:3:3:A:H8	1.62	0.45
54:C:100:LEU:HD12	54:C:352:LEU:HD21	1.98	0.45
55:D:311:ILE:HD11	55:D:344:ARG:HD3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:L:40:PRO:HB2	63:L:43:LYS:HG3	1.98	0.45
66:O:104:ASP:OD2	66:O:107:THR:HG22	2.16	0.45
70:S:38:LYS:O	70:S:42:ILE:HG13	2.16	0.45
73:V:186:THR:O	73:V:190:VAL:HG13	2.17	0.45
82:e:326:ARG:HG2	82:e:326:ARG:HH11	1.80	0.45
1:1:308:A:C8	46:1u:326:VAL:HG11	2.51	0.45
1:1:337:A:H2'	1:1:338:A:C8	2.51	0.45
1:1:2118:A:H2'	1:1:2119:C:H6	1.82	0.45
20:1T:235:LYS:HE2	20:1T:235:LYS:HB3	1.77	0.45
23:1W:36:ILE:HD11	23:1W:93:ILE:HG13	1.98	0.45
23:1W:109:LEU:HB2	23:1W:126:VAL:HG21	1.99	0.45
41:1p:109:LEU:HD23	41:1p:109:LEU:HA	1.77	0.45
46:1u:236:TYR:HB2	46:1u:265:PHE:CE1	2.51	0.45
46:1u:276:ARG:O	46:1u:279:GLU:HG3	2.16	0.45
48:2:78:U:O2'	48:2:79:G:H8	1.99	0.45
48:2:1707:A:H2'	48:2:1708:A:C8	2.51	0.45
48:2:1709:U:H2'	48:2:1710:G:C8	2.51	0.45
54:C:324:ARG:HG3	82:e:242:GLU:OE2	2.14	0.45
57:F:94:GLU:HG3	57:F:95:ALA:N	2.32	0.45
66:O:52:MET:HE1	66:O:80:SER:HB3	1.97	0.45
1:1:874:G:H5'	1:1:875:A:H5"	1.98	0.45
1:1:1699:U:H2'	1:1:1700:U:C6	2.52	0.45
8:1H:95:LYS:HE2	8:1H:95:LYS:HB2	1.80	0.45
12:1L:141:ASP:HB2	12:1L:161:LYS:O	2.17	0.45
35:1i:101:GLN:HG2	41:1p:116:TRP:CH2	2.51	0.45
38:1l:170:HIS:C	38:1l:170:HIS:ND1	2.75	0.45
46:1u:453:LEU:HA	46:1u:456:THR:HG22	1.98	0.45
48:2:1499:A:H4'	48:2:1566:G:H4'	1.98	0.45
48:2:1571:G:H5'	63:L:106:ILE:HD11	1.97	0.45
48:2:1625:A:N3	48:2:1625:A:H2'	2.31	0.45
82:e:164:MET:HE2	82:e:164:MET:HB2	1.77	0.45
84:h:92:LYS:HB2	84:h:92:LYS:HE3	1.80	0.45
1:1:126:U:HO2'	1:1:127:C:H6	1.65	0.45
1:1:256:U:H4'	1:1:257:U:H5	1.82	0.45
1:1:318:U:H2'	1:1:319:U:C6	2.52	0.45
1:1:2582:A:H2'	1:1:2583:A:C8	2.52	0.45
3:1C:245:TRP:CH2	26:1Z:47:LEU:HD21	2.52	0.45
4:1D:70:MET:HG2	4:1D:288:ILE:HD12	1.99	0.45
6:1F:29:PRO:HB3	6:1F:163:ALA:HA	1.99	0.45
46:1u:587:SER:HA	46:1u:590:GLU:HG3	1.99	0.45
48:2:359:U:H3	48:2:368:G:H1	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:2:491:G:H2'	48:2:492:G:C5	2.52	0.45
48:2:1652:C:H5'	79:b:15:LYS:HB2	1.99	0.45
48:2:1739:U:H2'	48:2:1740:C:H6	1.80	0.45
54:C:117:LEU:HD22	54:C:123:ALA:HA	1.99	0.45
69:R:33:LEU:HD11	69:R:104:VAL:HG13	1.98	0.45
74:W:187:PHE:O	74:W:190:ILE:HG22	2.17	0.45
84:h:208:LEU:HD12	84:h:208:LEU:HA	1.88	0.45
84:h:236:LEU:O	84:h:240:TYR:HD1	1.99	0.45
85:i:109:ARG:HG3	85:i:110:GLY:N	2.31	0.45
1:1:1163:A:H2'	1:1:1164:A:H8	1.82	0.45
1:1:1604:G:H8	1:1:1649:C:H42	1.61	0.45
1:1:2363:A:H2'	1:1:2364:A:C8	2.51	0.45
1:1:2840:G:C2	1:1:2841:G:C8	3.05	0.45
12:1L:148:ARG:HH21	12:1L:150:PHE:HE1	1.64	0.45
26:1Z:130:LYS:HB3	26:1Z:130:LYS:HE3	1.53	0.45
46:1u:406:GLN:NE2	46:1u:414:ALA:HB3	2.32	0.45
46:1u:697:LYS:HB3	46:1u:700:ASN:HB2	1.99	0.45
47:1v:95:SER:HA	47:1v:98:PHE:CE2	2.52	0.45
47:1v:421:LYS:HZ2	47:1v:427:PRO:HG2	1.82	0.45
48:2:3:C:O2'	48:2:4:A:H2'	2.16	0.45
48:2:990:U:H2'	48:2:991:A:H8	1.82	0.45
48:2:1728:U:O2'	48:2:1729:G:H8	2.00	0.45
67:P:13:MET:HB2	67:P:13:MET:HE3	1.73	0.45
83:f:310:PRO:HD3	83:f:368:TRP:CD1	2.52	0.45
84:h:258:VAL:O	84:h:261:GLU:HG2	2.17	0.45
85:i:402:ASP:O	85:i:406:ILE:HG22	2.17	0.45
1:1:609:G:OP2	32:1f:191:ARG:HD3	2.17	0.45
1:1:1558:G:H2'	1:1:1559:A:C8	2.52	0.45
1:1:1701:U:H2'	1:1:1702:U:C6	2.52	0.45
1:1:2896:C:H2'	1:1:2897:G:C8	2.52	0.45
3:1C:208:MET:SD	26:1Z:141:MET:HE2	2.57	0.45
22:1V:38:VAL:HG22	22:1V:45:VAL:HG12	2.00	0.45
46:1u:98:ARG:HB2	46:1u:104:LEU:HD22	1.99	0.45
46:1u:138:ARG:HB3	46:1u:142:ARG:NH1	2.31	0.45
46:1u:176:MET:HB3	46:1u:181:VAL:HG23	1.98	0.45
48:2:354:C:H2'	48:2:355:G:H8	1.81	0.45
48:2:1589:A:H2'	48:2:1590:C:C6	2.51	0.45
60:I:160:ARG:HA	60:I:181:MET:O	2.17	0.45
60:I:203:TRP:HA	60:I:203:TRP:CE3	2.52	0.45
73:V:131:PHE:C	73:V:131:PHE:CD1	2.94	0.45
1:1:51:A:H2'	1:1:52:A:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:487:U:H1'	1:1:488:U:OP2	2.17	0.44
1:1:566:G:H1'	1:1:567:C:H5'	1.99	0.44
1:1:1549:G:O2'	1:1:1550:A:H5'	2.17	0.44
1:1:1554:U:H2'	1:1:1555:G:C8	2.53	0.44
1:1:1656:C:H2'	1:1:1657:U:C6	2.52	0.44
1:1:2051:U:H2'	1:1:2052:C:C6	2.51	0.44
2:1B:38:GLN:HG2	2:1B:39:ASN:N	2.32	0.44
9:1I:122:GLY:N	9:1I:125:ASP:HB2	2.32	0.44
46:1u:137:PHE:CD2	46:1u:156:MET:HE2	2.52	0.44
50:5:35:C:H42	51:6:6:G:H1	1.64	0.44
54:C:320:GLU:OE2	82:e:215:ARG:HG3	2.16	0.44
57:F:11:LEU:HD11	57:F:54:VAL:HG21	1.97	0.44
72:U:123:ARG:HA	72:U:123:ARG:HD3	1.82	0.44
84:h:94:LEU:HA	84:h:97:VAL:HG22	1.99	0.44
1:1:794:C:H3'	46:1u:699:LEU:HD11	1.99	0.44
1:1:2316:G:H2'	1:1:2317:A:H8	1.82	0.44
11:1K:192:VAL:O	11:1K:196:LYS:HB2	2.18	0.44
18:1R:3:LYS:HG3	18:1R:21:ILE:HD13	1.99	0.44
47:1v:278:ILE:HG12	47:1v:283:TYR:CE1	2.52	0.44
48:2:476:C:N4	66:O:88:MET:HE3	2.32	0.44
48:2:911:A:H2'	48:2:912:A:C8	2.51	0.44
48:2:969:G:H22	48:2:1625:A:H5'	1.81	0.44
50:5:12:G:H2'	50:5:13:G:O4'	2.17	0.44
54:C:131:ARG:HH11	54:C:158:ASN:ND2	2.15	0.44
56:E:74:ASN:O	56:E:78:GLU:HG2	2.17	0.44
74:W:104:ARG:HD2	74:W:446:ARG:HD3	1.99	0.44
1:1:408:U:H2'	1:1:409:U:H6	1.82	0.44
1:1:2355:G:H2'	1:1:2356:G:C8	2.53	0.44
5:1E:187:LYS:NZ	5:1E:187:LYS:HB3	2.33	0.44
10:1J:144:ASN:ND2	10:1J:144:ASN:O	2.44	0.44
26:1Z:108:ASP:O	26:1Z:112:LEU:HD23	2.16	0.44
38:1l:114:LEU:HD23	38:1l:114:LEU:HA	1.79	0.44
46:1u:263:TRP:CZ3	46:1u:267:LEU:HD22	2.53	0.44
46:1u:401:LYS:HD2	46:1u:401:LYS:HA	1.79	0.44
46:1u:438:ILE:HD11	46:1u:453:LEU:HB3	1.99	0.44
47:1v:432:TYR:O	47:1v:436:MET:HE3	2.18	0.44
48:2:43:G:H2'	48:2:44:C:C6	2.53	0.44
48:2:578:C:H2'	48:2:579:G:O4'	2.18	0.44
48:2:1428:U:H2'	48:2:1429:G:O4'	2.18	0.44
48:2:1588:A:H2'	48:2:1589:A:H8	1.82	0.44
48:2:1719:G:H2'	48:2:1720:C:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:B:442:ILE:HD13	78:a:156:LEU:HD21	2.00	0.44
54:C:126:LEU:HD21	54:C:154:PHE:HE1	1.82	0.44
55:D:75:GLU:O	55:D:79:VAL:HG12	2.18	0.44
72:U:45:LEU:HD12	72:U:45:LEU:HA	1.82	0.44
82:e:190:TYR:CD2	82:e:223:LYS:HB3	2.53	0.44
85:i:109:ARG:HB3	85:i:128:LEU:HD21	1.99	0.44
1:1:352:A:H2	1:1:487:U:H5"	1.82	0.44
1:1:899:U:H2'	1:1:900:A:C8	2.53	0.44
1:1:1690:A:H2'	1:1:1691:C:C6	2.53	0.44
4:1D:201:LYS:HB2	4:1D:201:LYS:HE2	1.73	0.44
6:1F:34:ILE:HG12	6:1F:159:ILE:HG12	2.00	0.44
10:1J:46:PHE:CE1	10:1J:65:VAL:HG11	2.53	0.44
29:1c:58:PHE:CD1	69:R:140:PRO:HD3	2.53	0.44
45:1t:466:ARG:HE	47:1v:242:PHE:HE2	1.65	0.44
46:1u:670:LEU:HD22	46:1u:688:VAL:HG11	2.00	0.44
47:1v:95:SER:HA	47:1v:98:PHE:HE2	1.82	0.44
47:1v:102:PHE:HD1	47:1v:105:ILE:HD12	1.81	0.44
48:2:53:U:H2'	48:2:54:G:C8	2.53	0.44
48:2:499:C:H2'	48:2:500:C:C6	2.53	0.44
53:B:356:ARG:HA	75:X:368:LEU:HD21	2.00	0.44
54:C:112:LEU:HD23	54:C:113:ARG:NH1	2.32	0.44
55:D:122:GLU:HB2	55:D:123:PRO:HD3	1.99	0.44
55:D:131:GLN:HA	55:D:134:LYS:HG2	1.98	0.44
55:D:362:VAL:HG21	55:D:413:TYR:HE1	1.83	0.44
55:D:455:MET:HE3	55:D:455:MET:HB2	1.81	0.44
76:Y:90:GLN:HB3	76:Y:93:HIS:HB2	1.99	0.44
85:i:103:ARG:HE	85:i:173:VAL:HG22	1.82	0.44
85:i:132:VAL:HA	85:i:135:VAL:HG12	1.99	0.44
1:1:51:A:H2'	1:1:52:A:H8	1.83	0.44
1:1:747:A:H2'	1:1:748:A:C8	2.53	0.44
1:1:1219:A:H4'	1:1:1220:A:H8	1.82	0.44
1:1:1319:U:H2'	1:1:1320:U:C6	2.52	0.44
1:1:1355:U:H2'	1:1:1356:U:H6	1.83	0.44
1:1:1864:U:H2'	1:1:1865:C:C6	2.52	0.44
35:1i:80:GLN:HG2	35:1i:80:GLN:H	1.62	0.44
45:1t:211:GLY:HA2	45:1t:214:ARG:HH21	1.83	0.44
46:1u:439:GLU:OE2	46:1u:475:SER:HB2	2.17	0.44
47:1v:75:ILE:HD12	47:1v:105:ILE:HG21	1.98	0.44
48:2:617:A:OP2	48:2:617:A:H8	2.00	0.44
48:2:1730:U:H2'	48:2:1731:A:H8	1.83	0.44
50:5:51:C:H2'	50:5:52:A:C8	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:B:524:VAL:HG12	53:B:535:VAL:HB	2.00	0.44
71:T:52:ASP:O	71:T:58:GLY:HA3	2.18	0.44
74:W:185:ASP:O	74:W:189:ARG:HG3	2.17	0.44
78:a:165:LYS:HD2	78:a:165:LYS:HA	1.86	0.44
81:d:39:LYS:HB3	81:d:39:LYS:HE2	1.58	0.44
82:e:148:ARG:HA	82:e:151:ARG:CD	2.47	0.44
1:1:1227:A:C2	1:1:1238:A:H2'	2.53	0.44
1:1:1667:C:O2	1:1:1667:C:H2'	2.18	0.44
1:1:3049:A:H2'	1:1:3050:A:C8	2.52	0.44
3:1C:225:LYS:HE2	3:1C:225:LYS:HB3	1.84	0.44
11:1K:146:GLU:OE1	11:1K:146:GLU:N	2.51	0.44
45:1t:211:GLY:O	45:1t:214:ARG:HG2	2.17	0.44
46:1u:559:PRO:HB2	46:1u:588:LEU:HD23	2.00	0.44
46:1u:735:GLN:CD	46:1u:735:GLN:N	2.72	0.44
47:1v:142:THR:O	47:1v:146:VAL:HG13	2.16	0.44
48:2:959:G:H2'	48:2:960:C:C6	2.52	0.44
48:2:1481:C:H2'	48:2:1482:U:H6	1.83	0.44
53:B:308:ASN:HA	53:B:311:THR:HG22	1.98	0.44
55:D:99:GLN:NE2	55:D:100:ARG:N	2.65	0.44
61:J:268:PHE:HD1	61:J:271:LYS:HD2	1.82	0.44
69:R:22:MET:HE3	69:R:22:MET:HB2	1.86	0.44
72:U:52:GLU:HB3	72:U:86:GLY:HA3	2.00	0.44
73:V:82:LYS:HA	73:V:82:LYS:HD3	1.91	0.44
79:b:60:LEU:O	79:b:63:VAL:HG12	2.18	0.44
85:i:277:LYS:HE3	85:i:277:LYS:HB2	1.77	0.44
1:1:308:A:H4'	46:1u:263:TRP:NE1	2.33	0.44
1:1:771:U:C5	5:1E:300:ARG:HA	2.52	0.44
1:1:862:C:H3'	1:1:863:A:H8	1.82	0.44
1:1:2126:A:H2'	1:1:2127:A:H8	1.82	0.44
1:1:2634:U:H2'	1:1:2635:G:H8	1.81	0.44
1:1:2819:U:H2'	1:1:2820:C:C6	2.53	0.44
1:1:2959:C:H2'	1:1:2960:C:H6	1.83	0.44
1:1:2991:U:H2'	1:1:2992:A:H8	1.82	0.44
1:1:3007:U:H2'	1:1:3008:U:C6	2.53	0.44
4:1D:173:VAL:HG13	4:1D:255:ILE:HG23	1.99	0.44
12:1L:141:ASP:OD1	12:1L:141:ASP:C	2.60	0.44
24:1X:228:LYS:HD2	24:1X:228:LYS:C	2.43	0.44
38:1l:97:ASN:OD1	38:1l:99:ASP:HB2	2.17	0.44
41:1p:95:GLU:O	41:1p:99:LYS:HG3	2.18	0.44
46:1u:129:LYS:HB2	46:1u:132:HIS:CD2	2.52	0.44
48:2:342:U:H2'	48:2:343:G:O4'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:A:32:TYR:CD1	52:A:32:TYR:C	2.95	0.44
55:D:421:HIS:NE2	72:U:2:SER:HB2	2.33	0.44
57:F:30:ALA:O	57:F:34:GLN:HG3	2.17	0.44
66:O:106:MET:HE1	82:e:316:GLY:HA2	2.00	0.44
81:d:64:LEU:HD13	81:d:70:LEU:HD23	1.99	0.44
82:e:192:LEU:HD22	82:e:200:TYR:CE2	2.53	0.44
84:h:90:HIS:O	84:h:93:ILE:HG13	2.18	0.44
85:i:132:VAL:O	85:i:135:VAL:HG12	2.18	0.44
85:i:179:LYS:O	85:i:183:LYS:HG2	2.18	0.44
1:1:288:U:H2'	1:1:289:U:C6	2.53	0.44
1:1:1016:A:OP1	14:1N:40:LYS:HD2	2.18	0.44
1:1:1086:U:H2'	1:1:1087:A:H8	1.83	0.44
1:1:2496:U:H2'	1:1:2497:G:H8	1.83	0.44
14:1N:92:GLY:O	14:1N:96:ARG:HG3	2.18	0.44
20:1T:154:VAL:HG21	20:1T:207:LEU:HD23	2.00	0.44
41:1p:77:MET:HE2	41:1p:77:MET:HB3	1.90	0.44
45:1t:356:LEU:HD12	45:1t:356:LEU:HA	1.83	0.44
46:1u:546:TYR:CG	46:1u:569:MET:HG3	2.52	0.44
46:1u:582:ARG:HH21	46:1u:614:ASN:HA	1.83	0.44
47:1v:474:MET:HE2	47:1v:474:MET:HB3	1.88	0.44
48:2:493:A:H4'	48:2:494:A:OP1	2.17	0.44
48:2:746:C:H2'	48:2:747:C:C6	2.52	0.44
48:2:1822:A:H2'	48:2:1823:G:C8	2.53	0.44
54:C:111:LEU:HD23	54:C:111:LEU:HA	1.86	0.44
54:C:179:ILE:HG22	54:C:184:LEU:HD22	1.99	0.44
60:I:142:LYS:HB3	60:I:143:GLU:OE1	2.17	0.44
61:J:210:THR:HG22	61:J:216:VAL:HA	2.00	0.44
62:K:81:LEU:HD23	62:K:98:ILE:HD12	2.00	0.44
64:M:92:ALA:HB2	76:Y:41:ILE:HD11	1.99	0.44
74:W:261:TRP:O	74:W:385:THR:HG23	2.17	0.44
83:f:323:GLY:HA2	83:f:326:GLN:HB2	1.99	0.44
85:i:175:LYS:O	85:i:178:GLU:HG3	2.17	0.44
1:1:150:C:O2'	1:1:151:U:H5'	2.18	0.44
1:1:1186:G:H22	1:1:1269:G:H22	1.66	0.44
1:1:1258:U:H5'	9:1I:77:LYS:NZ	2.32	0.44
1:1:1559:A:H2'	1:1:1560:A:H8	1.81	0.44
3:1C:203:PHE:CE1	3:1C:225:LYS:HD3	2.52	0.44
15:1O:55:GLY:HA2	15:1O:77:PHE:CE2	2.52	0.44
38:1l:35:ARG:HH21	38:1l:111:LEU:HG	1.83	0.44
45:1t:282:GLU:O	45:1t:286:ILE:HG12	2.17	0.44
46:1u:724:ILE:HG22	46:1u:739:LEU:HD23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:1v:282:ALA:O	47:1v:286:MET:HG3	2.18	0.44
48:2:949:U:O2	48:2:953:U:H5	2.01	0.44
48:2:1013:A:H1'	69:R:159:TRP:HB2	1.98	0.44
48:2:1576:C:H2'	48:2:1577:U:C6	2.53	0.44
50:5:5:G:H2'	50:5:6:G:C8	2.52	0.44
65:N:393:ASP:OD1	65:N:396:SER:HB2	2.18	0.44
76:Y:18:VAL:HG11	78:a:334:GLU:OE2	2.17	0.44
77:Z:53:LEU:HD13	77:Z:116:VAL:HG12	2.00	0.44
82:e:183:ASP:HA	82:e:186:LYS:HD2	1.99	0.44
84:h:206:MET:HG2	84:h:240:TYR:CE2	2.51	0.44
1:1:212:A:C2	1:1:2712:G:H1'	2.53	0.43
1:1:433:A:H2'	1:1:434:A:C8	2.53	0.43
1:1:1474:U:H2'	1:1:1475:G:C8	2.53	0.43
1:1:1565:C:H3'	1:1:1566:U:H5'	1.99	0.43
1:1:2246:A:H2'	1:1:2247:G:O4'	2.18	0.43
10:1J:50:PHE:O	10:1J:54:THR:HG22	2.18	0.43
15:1O:83:ARG:HD2	15:1O:114:ASP:O	2.18	0.43
17:1Q:147:GLU:HB2	17:1Q:155:VAL:HG22	1.99	0.43
39:1m:79:ARG:HA	39:1m:82:ILE:HG12	2.00	0.43
43:1r:65:PHE:HB3	43:1r:124:VAL:HG13	2.00	0.43
46:1u:684:SER:HA	46:1u:687:LYS:HB3	1.99	0.43
48:2:440:A:H3'	48:2:441:U:H4'	2.00	0.43
48:2:488:C:H2'	48:2:489:G:C8	2.53	0.43
53:B:318:ASN:O	53:B:321:ARG:HG2	2.17	0.43
67:P:55:VAL:HG12	67:P:74:ILE:HG12	2.00	0.43
71:T:86:PRO:O	71:T:89:THR:HG22	2.17	0.43
74:W:195:MET:HE3	74:W:195:MET:HB3	1.80	0.43
74:W:214:PRO:HB2	74:W:429:ARG:HE	1.83	0.43
74:W:461:ILE:HD12	74:W:479:MET:HE2	1.99	0.43
83:f:326:GLN:OE1	83:f:334:ARG:HD2	2.18	0.43
1:1:727:U:H2'	1:1:728:G:C8	2.52	0.43
1:1:1162:C:C2	11:1K:162:ARG:HD3	2.52	0.43
23:1W:79:ARG:H	23:1W:79:ARG:HG2	1.67	0.43
45:1t:267:TYR:HD2	45:1t:290:LEU:HB2	1.83	0.43
46:1u:263:TRP:HZ3	46:1u:267:LEU:HD22	1.82	0.43
48:2:129:A:C5	48:2:150:A:N1	2.87	0.43
53:B:476:LYS:HG3	53:B:477:GLU:N	2.32	0.43
55:D:97:GLU:HG2	55:D:100:ARG:NH2	2.33	0.43
56:E:70:MET:HE3	65:N:313:TYR:CZ	2.53	0.43
59:H:219:LYS:NZ	72:U:124:LEU:HA	2.27	0.43
78:a:401:MET:HE2	78:a:401:MET:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:e:243:ARG:HA	82:e:243:ARG:NE	2.33	0.43
84:h:357:LEU:HA	84:h:360:ASP:OD1	2.18	0.43
1:1:357:A:H2'	1:1:358:A:C8	2.53	0.43
1:1:435:A:H5"	22:1V:109:THR:OG1	2.19	0.43
1:1:709:G:OP1	11:1K:129:ASN:HB2	2.18	0.43
1:1:1656:C:H2'	1:1:1657:U:H6	1.82	0.43
1:1:2485:U:H2'	1:1:2486:C:H6	1.83	0.43
1:1:3124:G:H2'	1:1:3125:A:H8	1.83	0.43
45:1t:253:GLN:O	45:1t:256:GLU:HG2	2.18	0.43
46:1u:153:HIS:CD2	46:1u:176:MET:HE2	2.53	0.43
48:2:635:G:C2	48:2:636:A:C8	3.06	0.43
48:2:1745:A:H5'	84:h:110:TRP:NE1	2.24	0.43
54:C:93:ARG:HD2	54:C:98:PRO:HG2	2.00	0.43
55:D:222:LYS:H	55:D:222:LYS:HG2	1.54	0.43
1:1:409:U:H2'	1:1:410:U:C6	2.53	0.43
1:1:1013:U:H2'	1:1:1014:C:C6	2.53	0.43
1:1:1235:A:H2'	1:1:1236:A:C8	2.53	0.43
1:1:2431:U:H2'	1:1:2432:A:N7	2.34	0.43
1:1:2993:U:H2'	1:1:2994:G:H8	1.83	0.43
2:1B:38:GLN:HG2	2:1B:39:ASN:H	1.83	0.43
4:1D:177:VAL:O	4:1D:180:GLN:HG2	2.18	0.43
9:1I:133:PRO:HB2	9:1I:134:SER:H	1.61	0.43
23:1W:130:LYS:HB3	23:1W:144:VAL:CG2	2.48	0.43
46:1u:351:MET:HE1	46:1u:354:SER:HB3	1.99	0.43
46:1u:378:GLU:O	46:1u:382:ILE:HG12	2.18	0.43
46:1u:446:ALA:HB1	46:1u:449:ARG:HE	1.83	0.43
47:1v:470:ASP:HA	47:1v:471:PRO:HD3	1.89	0.43
50:5:22:A:N6	50:5:47:A:H1'	2.33	0.43
54:C:223:SER:O	54:C:226:GLU:HG3	2.19	0.43
74:W:221:ILE:O	74:W:225:MET:HG3	2.18	0.43
83:f:227:LEU:HD12	83:f:227:LEU:HA	1.85	0.43
83:f:379:ASP:OD1	83:f:380:MET:N	2.51	0.43
83:f:405:ARG:HA	83:f:405:ARG:HD3	1.82	0.43
85:i:300:HIS:HB3	85:i:309:ARG:HH22	1.83	0.43
1:1:2684:G:H2'	1:1:2685:U:C6	2.53	0.43
12:1L:91:MET:HE3	12:1L:91:MET:HB3	1.87	0.43
27:1a:130:ASP:HB3	27:1a:133:ARG:HB2	2.00	0.43
35:1i:92:THR:HG22	35:1i:94:LYS:H	1.84	0.43
45:1t:279:LYS:HB2	45:1t:282:GLU:HG2	2.00	0.43
48:2:439:A:H2'	48:2:441:U:H1'	1.99	0.43
48:2:888:G:H2'	48:2:889:U:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:B:50:ARG:HD3	53:B:51:LEU:N	2.33	0.43
54:C:209:ARG:NH1	54:C:209:ARG:HB3	2.34	0.43
54:C:317:HIS:HB3	82:e:255:HIS:O	2.19	0.43
57:F:11:LEU:HD12	57:F:89:ILE:HD11	2.00	0.43
57:F:76:PRO:HG2	79:b:37:MET:HE3	2.01	0.43
59:H:235:LEU:HD21	85:i:299:ILE:HG12	2.00	0.43
60:I:203:TRP:HA	60:I:203:TRP:HE3	1.84	0.43
66:O:106:MET:HE2	66:O:106:MET:HB2	1.86	0.43
78:a:188:ILE:HD12	78:a:188:ILE:HA	1.86	0.43
86:k:4:MET:HE2	86:k:4:MET:HB2	1.80	0.43
1:1:996:G:H2'	1:1:997:G:H8	1.84	0.43
1:1:1381:U:H2'	1:1:1382:G:C8	2.54	0.43
6:1F:165:THR:HB	6:1F:167:ASP:OD1	2.18	0.43
10:1J:28:PRO:HG3	10:1J:47:CYS:SG	2.59	0.43
11:1K:167:MET:HE2	11:1K:172:ARG:HA	2.01	0.43
12:1L:47:PHE:HB3	12:1L:76:GLY:HA3	2.00	0.43
40:1o:118:GLU:O	40:1o:122:ILE:HG22	2.19	0.43
46:1u:378:GLU:H	46:1u:378:GLU:CD	2.26	0.43
48:2:192:G:H2'	48:2:193:A:C8	2.53	0.43
48:2:943:U:H2'	48:2:944:G:H8	1.83	0.43
48:2:986:G:H2'	48:2:988:C:H41	1.83	0.43
48:2:1110:C:H1'	48:2:1442:A:C4	2.54	0.43
48:2:1541:G:H3'	78:a:309:LYS:HE3	2.01	0.43
48:2:1687:U:H2'	48:2:1688:U:H6	1.83	0.43
55:D:91:LYS:HE2	55:D:108:ILE:HG22	2.01	0.43
69:R:163:SER:HB2	69:R:196:PHE:HD2	1.84	0.43
74:W:131:LEU:CD1	74:W:229:TRP:HB2	2.46	0.43
75:X:428:ILE:HD12	75:X:428:ILE:O	2.18	0.43
1:1:1225:C:H2'	1:1:1226:C:C6	2.54	0.43
1:1:1325:G:O6	1:1:1331:U:O4	2.36	0.43
1:1:1334:C:H2'	1:1:1335:C:C6	2.54	0.43
19:1S:174:GLU:OE2	19:1S:198:THR:HG23	2.19	0.43
20:1T:217:GLU:O	20:1T:221:GLU:HG3	2.18	0.43
29:1c:26:MET:HG2	29:1c:27:THR:N	2.34	0.43
48:2:1666:C:H2'	48:2:1667:G:C8	2.53	0.43
59:H:239:SER:HA	85:i:298:LYS:HZ2	1.84	0.43
59:H:336:ASP:OD2	74:W:466:ASN:HB3	2.19	0.43
82:e:140:ILE:HD12	82:e:143:ILE:HD11	1.99	0.43
83:f:58:ARG:HE	83:f:69:MET:HE2	1.82	0.43
1:1:804:U:H2'	1:1:805:U:C6	2.54	0.43
1:1:1864:U:H2'	1:1:1865:C:H6	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1943:G:H5'	36:1j:28:PRO:HB2	2.01	0.43
1:1:2178:A:N6	1:1:2206:G:H1'	2.34	0.43
22:1V:102:LYS:HB3	22:1V:102:LYS:HE3	1.85	0.43
42:1q:49:GLN:O	42:1q:53:VAL:HG23	2.19	0.43
46:1u:165:LYS:HG3	46:1u:168:HIS:CG	2.54	0.43
48:2:200:C:H5	48:2:246:G:H1	1.67	0.43
48:2:992:U:H2'	48:2:993:G:H8	1.83	0.43
48:2:1763:U:H5'	48:2:1764:A:H5'	2.01	0.43
53:B:206:LEU:HD13	78:a:183:ILE:HG23	2.01	0.43
53:B:375:LYS:NZ	78:a:102:ILE:HG23	2.34	0.43
54:C:229:LEU:HD22	82:e:162:MET:SD	2.59	0.43
72:U:107:ASN:OD1	72:U:107:ASN:C	2.62	0.43
74:W:150:LEU:HD13	74:W:158:LEU:HD21	1.99	0.43
74:W:271:LEU:O	74:W:275:VAL:HG13	2.19	0.43
83:f:185:ALA:HA	83:f:188:TYR:CE2	2.54	0.43
1:1:154:U:H2'	1:1:155:U:O2	2.19	0.43
1:1:618:G:N7	22:1V:2:GLY:HA3	2.33	0.43
1:1:978:A:H2'	1:1:979:G:C8	2.53	0.43
1:1:1162:C:N4	11:1K:159:MET:HE3	2.34	0.43
1:1:1355:U:H2'	1:1:1356:U:C6	2.54	0.43
1:1:1560:A:H2'	1:1:1561:G:C8	2.54	0.43
1:1:1613:G:H2'	1:1:1614:G:C8	2.54	0.43
1:1:2267:C:H2'	1:1:2268:A:C8	2.54	0.43
1:1:2348:A:C2	1:1:2804:C:H5"	2.54	0.43
1:1:2673:C:H2'	1:1:2674:A:H8	1.84	0.43
2:1B:117:TRP:HD1	2:1B:211:GLU:HG2	1.84	0.43
9:1I:27:ILE:HG12	9:1I:111:LEU:HD23	1.99	0.43
22:1V:22:MET:HG3	22:1V:32:THR:HG22	2.01	0.43
23:1W:63:PHE:O	23:1W:146:VAL:HA	2.19	0.43
24:1X:78:SER:HB3	24:1X:95:VAL:HG23	2.00	0.43
25:1Y:140:THR:O	25:1Y:144:ALA:HB3	2.19	0.43
39:1m:5:LEU:HD12	39:1m:60:PHE:CE1	2.54	0.43
45:1t:357:LYS:HE3	45:1t:357:LYS:HB3	1.85	0.43
46:1u:472:MET:HG3	46:1u:476:ALA:HB3	2.00	0.43
78:a:109:ARG:HH11	78:a:110:LEU:HD22	1.84	0.43
84:h:168:LYS:HB3	84:h:168:LYS:HE3	1.88	0.43
1:1:1086:U:H2'	1:1:1087:A:C8	2.54	0.43
1:1:1123:A:H5'	1:1:1345:U:H1'	2.01	0.43
1:1:1214:C:H5'	10:1J:97:GLY:HA3	2.01	0.43
1:1:1473:C:H2'	1:1:1474:U:C6	2.54	0.43
1:1:1838:A:P	45:1t:362:ARG:HH22	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2342:U:H2'	1:1:2343:C:H6	1.84	0.43
5:1E:91:ILE:HG13	5:1E:92:PRO:HD2	2.00	0.43
9:1I:111:LEU:HB3	9:1I:126:TYR:OH	2.19	0.43
27:1a:73:LEU:HD23	27:1a:73:LEU:HA	1.85	0.43
37:1k:114:THR:HG22	37:1k:117:VAL:HG23	2.00	0.43
39:1m:60:PHE:HD2	39:1m:89:LEU:HD12	1.83	0.43
46:1u:447:TYR:O	46:1u:451:ILE:HG12	2.19	0.43
46:1u:563:LYS:HG3	46:1u:596:THR:HG22	1.99	0.43
46:1u:741:ARG:O	46:1u:745:LYS:HG2	2.18	0.43
48:2:715:C:C2	68:Q:193:LEU:HD12	2.54	0.43
48:2:1421:C:C4	48:2:1423:G:C8	3.07	0.43
48:2:1686:U:H2'	48:2:1687:U:H6	1.83	0.43
53:B:51:LEU:HD12	53:B:52:THR:HG23	2.00	0.43
53:B:307:LYS:HA	53:B:307:LYS:HD3	1.91	0.43
54:C:83:PRO:O	54:C:87:MET:HG3	2.18	0.43
54:C:136:LYS:HG3	82:e:314:TRP:CE3	2.53	0.43
61:J:250:VAL:HG13	61:J:255:LEU:HB2	2.01	0.43
74:W:312:ILE:HD12	74:W:313:PRO:HD2	2.01	0.43
76:Y:25:ILE:CD1	78:a:371:LEU:HD12	2.49	0.43
82:e:191:ARG:HG3	82:e:192:LEU:N	2.33	0.43
83:f:286:MET:HE1	83:f:302:LEU:HD13	2.01	0.43
83:f:307:GLU:HA	83:f:307:GLU:OE2	2.19	0.43
1:1:801:U:H2'	1:1:802:U:H6	1.83	0.42
1:1:2445:G:H2'	1:1:2446:G:C8	2.52	0.42
1:1:2958:A:H2'	1:1:2959:C:C6	2.53	0.42
7:1G:25:ARG:HG2	7:1G:46:ARG:NH1	2.30	0.42
21:1U:109:LYS:HD2	21:1U:109:LYS:C	2.44	0.42
22:1V:68:PHE:N	22:1V:68:PHE:CD1	2.87	0.42
28:1b:75:GLU:OE1	28:1b:75:GLU:N	2.49	0.42
45:1t:214:ARG:O	45:1t:217:GLU:HG2	2.19	0.42
46:1u:230:ILE:HA	46:1u:230:ILE:HD12	1.73	0.42
46:1u:654:LEU:HD12	46:1u:654:LEU:HA	1.81	0.42
48:2:1501:A:N7	48:2:1565:C:H1'	2.34	0.42
56:E:43:PHE:HB3	73:V:195:LEU:HD23	2.00	0.42
57:F:146:ARG:NH2	79:b:31:LYS:HG2	2.34	0.42
73:V:115:ARG:HB3	73:V:115:ARG:CZ	2.48	0.42
74:W:103:LYS:HD2	74:W:103:LYS:C	2.44	0.42
74:W:147:GLU:O	74:W:150:LEU:HG	2.19	0.42
83:f:143:ILE:N	83:f:143:ILE:HD12	2.34	0.42
83:f:309:SER:HA	83:f:368:TRP:CD1	2.54	0.42
1:1:409:U:H2'	1:1:410:U:H6	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:456:A:H5'	1:1:474:A:H1'	2.00	0.42
1:1:579:U:H2'	1:1:580:C:C6	2.54	0.42
1:1:621:A:N3	1:1:623:G:H5"	2.34	0.42
1:1:640:U:H2'	1:1:641:G:O4'	2.19	0.42
1:1:676:G:H2'	1:1:677:U:C6	2.53	0.42
1:1:1334:C:H2'	1:1:1335:C:H6	1.84	0.42
1:1:1651:U:H2'	1:1:1652:U:C6	2.53	0.42
1:1:2473:A:H1'	1:1:2474:A:C8	2.54	0.42
1:1:2496:U:C2	1:1:2497:G:C8	3.07	0.42
1:1:2560:OMG:HM23	1:1:2560:OMG:H1'	1.74	0.42
1:1:2612:A:O3'	6:1F:123:ARG:HD3	2.19	0.42
1:1:3136:C:OP1	43:1r:91:LYS:HG3	2.19	0.42
6:1F:12:LEU:HD21	6:1F:175:GLY:HA3	2.02	0.42
6:1F:41:PRO:HG2	6:1F:153:ARG:NH2	2.33	0.42
14:1N:150:MET:HE3	14:1N:150:MET:HB2	1.92	0.42
14:1N:151:ASP:OD1	14:1N:151:ASP:C	2.61	0.42
24:1X:38:GLU:HG3	24:1X:39:TYR:N	2.34	0.42
38:1l:98:ASN:HB3	38:1l:100:ARG:HH12	1.84	0.42
45:1t:98:ASP:OD1	45:1t:102:LYS:HD2	2.19	0.42
46:1u:417:GLU:HA	46:1u:420:LYS:HG2	2.01	0.42
47:1v:78:SER:OG	47:1v:102:PHE:HZ	2.02	0.42
48:2:486:C:H2'	48:2:487:U:C6	2.54	0.42
48:2:674:U:H2'	48:2:675:U:C6	2.54	0.42
48:2:989:A:H2'	48:2:990:U:C6	2.54	0.42
48:2:1507:A:H2'	48:2:1508:A:C8	2.54	0.42
58:G:51:VAL:HG22	58:G:60:ILE:HG12	2.01	0.42
78:a:197:LYS:O	78:a:200:GLU:HG3	2.18	0.42
82:e:192:LEU:HD22	82:e:200:TYR:CD2	2.54	0.42
83:f:330:GLN:O	83:f:334:ARG:HG2	2.18	0.42
84:h:239:LYS:CA	84:h:242:LYS:HE3	2.49	0.42
84:h:345:GLN:HB2	84:h:350:LYS:HE3	2.01	0.42
1:1:151:U:H1'	1:1:152:C:H5'	2.01	0.42
1:1:1892:U:H2'	1:1:1893:U:C6	2.54	0.42
1:1:1939:G:H5"	1:1:1940:A:H5'	2.01	0.42
1:1:2497:G:H2'	1:1:2498:C:H6	1.84	0.42
6:1F:40:ALA:HB3	6:1F:41:PRO:HD3	2.02	0.42
10:1J:113:HIS:O	10:1J:117:ILE:HG13	2.19	0.42
15:1O:82:TYR:CE1	44:1s:175:LEU:HD23	2.54	0.42
46:1u:539:VAL:HG12	46:1u:540:PRO:HD2	2.01	0.42
48:2:759:G:H2'	48:2:760:C:C6	2.54	0.42
48:2:1130:C:H2'	48:2:1131:G:H8	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:A:130:MET:HA	52:A:130:MET:HE2	2.00	0.42
53:B:334:PRO:HG3	78:a:180:TRP:NE1	2.35	0.42
54:C:193:ARG:HA	55:D:132:ASN:HD21	1.85	0.42
69:R:175:ARG:HA	69:R:183:VAL:O	2.19	0.42
74:W:131:LEU:HD21	74:W:180:PHE:HE2	1.84	0.42
85:i:151:PRO:HA	85:i:152:PRO:HD3	1.89	0.42
85:i:202:ALA:O	85:i:205:ILE:HG22	2.19	0.42
1:1:545:G:H2'	1:1:546:A:C8	2.54	0.42
1:1:1008:A:H2'	1:1:1009:G:C8	2.55	0.42
1:1:2936:A:H5"	1:1:2937:A:N7	2.34	0.42
13:1M:168:ILE:HD13	13:1M:168:ILE:HA	1.81	0.42
47:1v:384:LYS:NZ	47:1v:423:ASN:HD21	2.18	0.42
48:2:369:G:H2'	48:2:370:G:C8	2.54	0.42
48:2:913:U:H2'	48:2:914:U:C6	2.54	0.42
48:2:1698:C:H2'	48:2:1699:A:H8	1.84	0.42
48:2:1700:U:H2'	48:2:1701:C:H6	1.82	0.42
55:D:90:GLU:HA	55:D:93:ARG:HG2	2.00	0.42
55:D:187:LEU:CD1	85:i:237:ARG:HG2	2.50	0.42
84:h:113:ILE:HG23	84:h:125:LEU:CD2	2.50	0.42
84:h:130:GLN:NE2	84:h:134:ARG:HG3	2.34	0.42
1:1:357:A:H2'	1:1:358:A:H8	1.85	0.42
1:1:410:U:H2'	1:1:411:U:C6	2.55	0.42
1:1:440:U:H2'	1:1:441:G:O4'	2.20	0.42
1:1:488:U:H2'	1:1:489:U:C6	2.54	0.42
1:1:1169:U:H2'	1:1:1170:U:C6	2.55	0.42
1:1:2149:U:H2'	1:1:2150:C:C6	2.54	0.42
9:1I:25:THR:OG1	9:1I:83:ILE:HB	2.19	0.42
14:1N:33:LYS:HE3	14:1N:33:LYS:HB3	1.68	0.42
21:1U:7:ARG:HB3	21:1U:7:ARG:CZ	2.49	0.42
23:1W:57:ARG:HH21	23:1W:84:THR:HG23	1.85	0.42
23:1W:60:ALA:HA	23:1W:143:LEU:O	2.20	0.42
23:1W:108:GLN:HG2	23:1W:124:GLY:O	2.19	0.42
25:1Y:64:LYS:HD3	25:1Y:64:LYS:HA	1.87	0.42
26:1Z:121:THR:HG22	26:1Z:123:MET:N	2.34	0.42
45:1t:305:MET:HE2	45:1t:305:MET:HB3	1.89	0.42
45:1t:313:LYS:HE2	45:1t:313:LYS:HB2	1.65	0.42
46:1u:87:LEU:O	46:1u:90:THR:HG22	2.20	0.42
47:1v:257:ILE:HD12	47:1v:257:ILE:HA	1.83	0.42
48:2:943:U:OP2	63:L:130:ARG:HD2	2.18	0.42
48:2:1124:G:H2'	48:2:1125:A:O4'	2.19	0.42
48:2:1430:A:H5'	79:b:82:HIS:NE2	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:2:1669:C:C2	48:2:1670:A:C8	3.07	0.42
48:2:1688:U:H2'	48:2:1689:C:C6	2.54	0.42
53:B:431:THR:OG1	53:B:433:THR:HG22	2.20	0.42
54:C:165:GLU:HA	54:C:168:ARG:HH12	1.84	0.42
54:C:344:ARG:H	54:C:344:ARG:HG3	1.68	0.42
55:D:194:MET:HE3	55:D:195:THR:N	2.35	0.42
66:O:84:PRO:HD3	73:V:80:TYR:CD2	2.54	0.42
73:V:177:GLU:CD	73:V:178:PRO:HD2	2.45	0.42
83:f:105:LEU:HB2	83:f:106:PRO:HD3	2.00	0.42
1:1:256:U:H4'	1:1:257:U:C5	2.54	0.42
1:1:874:G:O2'	1:1:908:G:H4'	2.19	0.42
1:1:2785:C:H2'	1:1:2786:G:O4'	2.19	0.42
7:1G:87:MET:HE1	7:1G:91:GLU:O	2.19	0.42
11:1K:121:ALA:O	11:1K:125:MET:HG3	2.20	0.42
45:1t:170:LYS:HD3	45:1t:170:LYS:HA	1.83	0.42
45:1t:376:MET:HE3	45:1t:376:MET:HB2	1.89	0.42
47:1v:201:MET:HE3	47:1v:207:LEU:CB	2.49	0.42
48:2:360:C:H2'	48:2:361:C:C6	2.54	0.42
48:2:1384:A:H2'	48:2:1385:A:C8	2.55	0.42
48:2:1499:A:H2'	48:2:1500:C:C6	2.54	0.42
48:2:1571:G:H2'	48:2:1572:U:C6	2.55	0.42
53:B:448:SER:OG	78:a:156:LEU:HB2	2.20	0.42
61:J:260:VAL:HG11	61:J:275:ILE:HD12	2.02	0.42
61:J:293:VAL:O	70:S:31:VAL:HG12	2.20	0.42
62:K:76:GLU:HG2	62:K:77:HIS:ND1	2.35	0.42
73:V:133:ASP:O	73:V:137:LYS:HG2	2.20	0.42
75:X:410:PRO:O	75:X:414:CYS:HB2	2.19	0.42
82:e:281:ILE:H	82:e:281:ILE:HD12	1.85	0.42
85:i:356:ILE:HD13	85:i:356:ILE:HA	1.90	0.42
1:1:1119:G:H2'	1:1:1120:U:C6	2.54	0.42
1:1:1209:G:H2'	1:1:1210:U:C5	2.55	0.42
1:1:1449:G:H2'	1:1:1450:A:H8	1.82	0.42
1:1:1702:U:H2'	1:1:1703:U:C6	2.55	0.42
1:1:2383:C:H2'	1:1:2384:C:C6	2.55	0.42
1:1:2437:A:C2	1:1:2472:A:H2'	2.55	0.42
1:1:2446:G:H2'	1:1:2447:U:H6	1.85	0.42
1:1:2669:C:H2'	1:1:2670:G:O4'	2.19	0.42
1:1:2882:A:H2'	1:1:2919:A:N6	2.35	0.42
1:1:2895:A:H2'	1:1:2896:C:H6	1.85	0.42
1:1:2958:A:H2'	1:1:2959:C:H6	1.84	0.42
37:1k:14:VAL:HG13	37:1k:26:ILE:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:1r:63:ASP:OD1	43:1r:64:VAL:N	2.53	0.42
46:1u:160:LEU:HD22	46:1u:165:LYS:HB3	2.02	0.42
46:1u:387:MET:HA	46:1u:390:HIS:H	1.85	0.42
46:1u:675:GLU:C	46:1u:675:GLU:OE1	2.62	0.42
47:1v:298:ASP:OD1	47:1v:301:LYS:HB2	2.20	0.42
48:2:70:U:H2'	48:2:71:C:C6	2.55	0.42
48:2:223:A:H2'	48:2:224:A:C8	2.55	0.42
48:2:354:C:C2	48:2:355:G:C8	3.07	0.42
48:2:403:G:H2'	48:2:404:C:H6	1.84	0.42
48:2:484:G:C4	48:2:485:A:C8	3.08	0.42
48:2:1749:A:H2'	48:2:1750:C:C6	2.52	0.42
53:B:171:LYS:HA	53:B:174:ARG:HG2	2.02	0.42
53:B:290:ALA:HA	53:B:293:VAL:HG22	2.00	0.42
53:B:399:MET:HE2	78:a:102:ILE:HD12	2.01	0.42
55:D:99:GLN:C	55:D:99:GLN:NE2	2.78	0.42
63:L:149:LYS:HA	63:L:149:LYS:HD2	1.81	0.42
74:W:139:ILE:HD11	74:W:181:LEU:HD12	2.01	0.42
75:X:401:PRO:HD2	78:a:365:LEU:HD22	2.01	0.42
81:d:43:PRO:HG2	81:d:44:GLU:OE1	2.19	0.42
84:h:272:LEU:HD12	84:h:272:LEU:HA	1.87	0.42
85:i:341:TRP:CZ3	85:i:355:LEU:HD22	2.54	0.42
1:1:176:A:H2'	1:1:177:C:H6	1.85	0.42
1:1:508:A:H2'	1:1:509:A:H8	1.85	0.42
1:1:758:A:H2'	1:1:759:A:H8	1.84	0.42
1:1:1909:G:H2'	1:1:1910:A:C8	2.55	0.42
22:1V:154:LYS:HB3	22:1V:154:LYS:HE3	1.80	0.42
26:1Z:178:LYS:HE2	26:1Z:178:LYS:HB3	1.90	0.42
48:2:672:A:H2'	48:2:673:U:H6	1.85	0.42
48:2:1385:A:OP2	48:2:1385:A:H8	2.02	0.42
48:2:1430:A:H8	79:b:78:ASN:OD1	2.03	0.42
48:2:1701:C:H2'	48:2:1702:G:C8	2.55	0.42
48:2:1790:C:H2'	48:2:1791:G:C8	2.55	0.42
50:5:28:U:H2'	50:5:29:C:H6	1.84	0.42
69:R:48:LYS:HG2	69:R:49:ASP:N	2.35	0.42
69:R:155:ASN:CG	69:R:155:ASN:O	2.62	0.42
74:W:281:ARG:HD2	74:W:349:VAL:HG11	2.02	0.42
78:a:98:LEU:HD23	78:a:99:PRO:HD3	2.01	0.42
85:i:391:ILE:HG13	85:i:392:HIS:N	2.35	0.42
1:1:162:U:O3'	1:1:163:G:H3'	2.20	0.42
1:1:746:G:H2'	1:1:747:A:H8	1.85	0.42
1:1:887:U:H2'	1:1:888:A:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:955:U:O4	13:1M:92:THR:HG22	2.19	0.42
1:1:1282:U:H3'	1:1:1283:A:H5"	2.01	0.42
1:1:2049:G:H2'	1:1:2050:C:H6	1.85	0.42
1:1:2416:C:H2'	1:1:2417:C:H6	1.84	0.42
10:1J:124:ASP:OD1	10:1J:124:ASP:C	2.63	0.42
18:1R:47:ARG:HA	18:1R:50:TRP:CE3	2.55	0.42
25:1Y:136:HIS:ND1	25:1Y:138:ILE:HG22	2.34	0.42
36:1j:72:LYS:HE2	36:1j:72:LYS:HB3	1.83	0.42
45:1t:302:TYR:HD2	45:1t:325:TRP:CD1	2.38	0.42
45:1t:390:GLU:O	45:1t:394:LYS:HG2	2.19	0.42
48:2:423:G:H4'	48:2:460:U:O2	2.19	0.42
48:2:1411:U:H2'	48:2:1412:C:O4'	2.20	0.42
51:6:1:A:N3	51:6:1:A:H2'	2.34	0.42
54:C:67:ILE:HD13	54:C:67:ILE:HA	1.93	0.42
54:C:297:PHE:CE1	82:e:157:ILE:HD11	2.55	0.42
84:h:183:VAL:HG22	84:h:214:LEU:HD22	2.02	0.42
1:1:427:A:H8	1:1:427:A:H5"	1.84	0.42
1:1:521:C:H2'	1:1:522:G:C8	2.55	0.42
1:1:2177:A:H2'	1:1:2178:A:H8	1.83	0.42
1:1:2461:G:H4'	1:1:2462:A:O5'	2.19	0.42
9:1I:34:VAL:O	9:1I:37:LEU:HG	2.19	0.42
16:1P:57:MET:HE2	16:1P:68:LYS:HD2	2.02	0.42
17:1Q:148:VAL:O	17:1Q:153:ARG:HA	2.18	0.42
23:1W:137:THR:OG1	23:1W:139:LYS:HG3	2.19	0.42
33:1g:92:LYS:HE2	33:1g:92:LYS:HB2	1.83	0.42
34:1h:24:TYR:CE1	34:1h:36:ARG:HG3	2.55	0.42
35:1i:201:LEU:HD12	35:1i:206:LYS:HA	2.02	0.42
39:1m:7:LYS:HB2	39:1m:59:THR:HG22	2.02	0.42
42:1q:41:LYS:O	42:1q:45:ARG:HG3	2.19	0.42
45:1t:252:LEU:HD12	45:1t:252:LEU:HA	1.82	0.42
46:1u:400:LEU:HD13	46:1u:433:HIS:HD2	1.84	0.42
46:1u:620:LYS:HD2	46:1u:621:ILE:HD12	2.02	0.42
47:1v:123:GLY:H	47:1v:156:ARG:NH1	2.16	0.42
47:1v:219:LYS:HA	47:1v:250:LEU:HD12	2.02	0.42
48:2:1716:C:H2'	48:2:1717:C:C6	2.55	0.42
49:3:100:C:C2	49:3:101:A:C8	3.08	0.42
50:5:22:A:H3'	50:5:47:A:H62	1.84	0.42
54:C:109:VAL:O	54:C:113:ARG:HG2	2.20	0.42
75:X:483:ASP:HA	75:X:486:LYS:HG3	2.02	0.42
1:1:105:A:O2'	27:1a:122:THR:HG21	2.19	0.41
1:1:2819:U:H2'	1:1:2820:C:H6	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:3053:G:O2'	7:1G:70:ALA:HB1	2.19	0.41
10:1J:42:ASN:HB2	10:1J:73:HIS:NE2	2.35	0.41
11:1K:31:ARG:HB3	11:1K:33:ARG:HD2	2.01	0.41
47:1v:474:MET:H	47:1v:474:MET:HG2	1.62	0.41
48:2:540:G:H2'	48:2:541:G:H8	1.85	0.41
48:2:901:A:H2'	48:2:902:A:H8	1.85	0.41
50:5:64:U:H2'	50:5:65:G:O4'	2.20	0.41
50:5:66:U:H2'	50:5:67:C:C6	2.56	0.41
60:I:143:GLU:OE1	60:I:143:GLU:N	2.53	0.41
62:K:76:GLU:HG2	62:K:77:HIS:CE1	2.54	0.41
70:S:96:LYS:HA	86:k:26:MET:CE	2.50	0.41
83:f:306:LYS:HD2	83:f:306:LYS:HA	1.81	0.41
1:1:1435:C:H2'	1:1:1436:C:C6	2.55	0.41
1:1:2396:C:H2'	1:1:2397:U:C6	2.55	0.41
1:1:3075:U:H2'	1:1:3076:C:C6	2.55	0.41
2:1B:63:MET:HB3	2:1B:63:MET:HE2	1.76	0.41
3:1C:185:PHE:HE1	26:1Z:137:GLU:HB3	1.85	0.41
4:1D:223:GLN:HB2	4:1D:227:PRO:HD3	2.00	0.41
16:1P:25:PHE:HD1	16:1P:30:VAL:HG12	1.85	0.41
19:1S:218:LYS:HD2	19:1S:223:TYR:CD2	2.56	0.41
24:1X:78:SER:HA	24:1X:155:VAL:O	2.19	0.41
29:1c:18:SER:HB2	35:1i:229:PRO:HB3	2.02	0.41
35:1i:210:LEU:HD12	35:1i:210:LEU:HA	1.84	0.41
37:1k:9:LEU:HD22	37:1k:88:ARG:HA	2.01	0.41
38:1l:120:PHE:CD1	38:1l:120:PHE:C	2.98	0.41
38:1l:229:LYS:HB2	38:1l:229:LYS:HE3	1.82	0.41
39:1m:89:LEU:HD23	39:1m:89:LEU:HA	1.90	0.41
40:1o:101:TYR:O	40:1o:104:LEU:HG	2.20	0.41
45:1t:448:PHE:CZ	45:1t:474:VAL:HG21	2.54	0.41
46:1u:417:GLU:O	46:1u:420:LYS:HG2	2.21	0.41
46:1u:460:LYS:C	46:1u:461:GLU:HG3	2.46	0.41
46:1u:509:ASP:OD1	46:1u:509:ASP:N	2.53	0.41
46:1u:626:LEU:HA	46:1u:626:LEU:HD23	1.78	0.41
48:2:590:A:H2'	48:2:591:U:H6	1.85	0.41
52:A:144:SER:O	52:A:148:GLU:HG3	2.20	0.41
56:E:19:LEU:O	56:E:23:VAL:HG23	2.21	0.41
59:H:219:LYS:HE3	59:H:219:LYS:HB3	1.80	0.41
69:R:148:LYS:HD2	69:R:149:LYS:HB2	2.02	0.41
72:U:75:SER:HB2	72:U:78:ILE:HD13	2.00	0.41
78:a:196:THR:O	78:a:200:GLU:HG2	2.20	0.41
83:f:232:GLU:HG3	83:f:233:ARG:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
84:h:273:TRP:O	84:h:277:LYS:HE3	2.20	0.41
1:1:1699:U:H2'	1:1:1700:U:H6	1.85	0.41
1:1:2019:A:H2'	1:1:2020:A:H8	1.84	0.41
1:1:2155:A:H2'	1:1:2156:C:C6	2.55	0.41
20:1T:147:ALA:O	20:1T:151:VAL:HG23	2.20	0.41
23:1W:36:ILE:HD13	23:1W:36:ILE:HA	1.90	0.41
26:1Z:120:ASP:OD1	26:1Z:120:ASP:O	2.38	0.41
34:1h:7:VAL:O	34:1h:8:LYS:HD2	2.20	0.41
38:1l:167:PRO:HB3	38:1l:188:PHE:HB3	2.01	0.41
45:1t:51:LYS:HD3	45:1t:51:LYS:HA	1.88	0.41
45:1t:233:SER:HB2	45:1t:269:PHE:CD2	2.54	0.41
45:1t:340:MET:HB3	45:1t:340:MET:HE2	1.62	0.41
45:1t:381:LYS:HA	45:1t:381:LYS:HD2	1.80	0.41
45:1t:448:PHE:HZ	45:1t:474:VAL:HG21	1.86	0.41
46:1u:607:LYS:HD3	46:1u:607:LYS:HA	1.73	0.41
47:1v:432:TYR:O	47:1v:436:MET:HG2	2.19	0.41
48:2:969:G:H5'	48:2:1620:U:O2'	2.20	0.41
48:2:1845:A:H2	79:b:22:ASN:H	1.67	0.41
51:6:5:U:H2'	51:6:6:G:C8	2.55	0.41
53:B:230:VAL:HG11	53:B:235:ASN:HB2	2.01	0.41
54:C:206:ARG:H	54:C:206:ARG:HG2	1.60	0.41
54:C:211:LEU:O	54:C:217:LEU:HD12	2.20	0.41
55:D:122:GLU:CD	55:D:122:GLU:H	2.28	0.41
55:D:296:ASP:O	55:D:299:GLU:HG3	2.20	0.41
61:J:190:GLU:HB3	68:Q:247:TYR:CZ	2.54	0.41
73:V:112:GLU:HG2	73:V:115:ARG:NH2	2.35	0.41
78:a:109:ARG:HD3	78:a:110:LEU:HD22	2.02	0.41
78:a:365:LEU:HD12	78:a:365:LEU:HA	1.87	0.41
83:f:264:LEU:HD23	83:f:264:LEU:HA	1.84	0.41
1:1:152:C:HO2'	1:1:153:U:H6	1.65	0.41
1:1:696:C:H4'	1:1:697:A:H5'	2.02	0.41
1:1:1254:C:C5'	40:1o:115:LYS:HZ3	2.33	0.41
1:1:1612:G:H2'	1:1:1613:G:H8	1.85	0.41
1:1:2499:C:H2'	1:1:2500:U:C6	2.56	0.41
6:1F:1:MET:SD	38:1l:51:GLN:HG3	2.60	0.41
6:1F:51:LEU:HD12	6:1F:51:LEU:HA	1.79	0.41
9:1I:61:PHE:O	9:1I:65:GLU:HG2	2.21	0.41
13:1M:131:LYS:HG2	13:1M:133:HIS:NE2	2.36	0.41
19:1S:179:LEU:HD23	19:1S:193:ILE:HG22	2.02	0.41
28:1b:25:ARG:HG3	28:1b:68:MET:HA	2.01	0.41
35:1i:97:GLU:CD	35:1i:97:GLU:N	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:1u:201:VAL:O	46:1u:205:VAL:HG23	2.20	0.41
47:1v:281:LYS:HE2	47:1v:281:LYS:HB2	1.67	0.41
48:2:291:C:H2'	48:2:292:A:H8	1.84	0.41
48:2:929:C:C2	48:2:930:A:C8	3.07	0.41
54:C:46:ARG:NH2	55:D:148:SER:HB3	2.36	0.41
59:H:310:GLY:HA3	59:H:378:ALA:O	2.20	0.41
60:I:134:ILE:O	60:I:185:LYS:HA	2.21	0.41
67:P:53:ASP:HB2	67:P:76:LYS:O	2.21	0.41
71:T:74:LYS:HA	71:T:74:LYS:HD3	1.83	0.41
77:Z:112:LYS:HB2	77:Z:112:LYS:HE2	1.78	0.41
1:1:766:A:H4'	5:1E:270:ASN:ND2	2.35	0.41
1:1:778:U:C2	13:1M:136:PRO:HD2	2.56	0.41
1:1:929:G:H4'	1:1:930:G:O5'	2.20	0.41
1:1:1017:U:H2'	1:1:1018:G:C8	2.55	0.41
3:1C:204:PHE:CE2	3:1C:206:PRO:HG3	2.55	0.41
48:2:1801:A:O2'	48:2:1802:A:H5'	2.21	0.41
53:B:391:GLU:OE2	53:B:395:VAL:HG23	2.20	0.41
53:B:414:ASN:HD22	53:B:417:PHE:HD2	1.68	0.41
54:C:189:ARG:HB3	55:D:139:LEU:HD22	2.01	0.41
55:D:84:LEU:O	55:D:87:VAL:HG12	2.21	0.41
59:H:239:SER:HB2	85:i:298:LYS:NZ	2.36	0.41
61:J:311:LYS:HE3	61:J:311:LYS:HB3	1.87	0.41
65:N:359:HIS:NE2	65:N:363:VAL:HG21	2.34	0.41
74:W:190:ILE:HD12	74:W:190:ILE:HA	1.89	0.41
75:X:370:SER:HB3	75:X:373:HIS:HB3	2.02	0.41
78:a:358:GLU:HG3	78:a:362:LYS:HE3	2.03	0.41
81:d:100:LEU:HD13	81:d:100:LEU:HA	1.87	0.41
84:h:187:HIS:NE2	84:h:220:THR:HG22	2.35	0.41
85:i:175:LYS:HA	85:i:175:LYS:HD3	1.85	0.41
85:i:295:MET:HA	85:i:298:LYS:HE2	2.02	0.41
86:k:20:MET:HE2	86:k:20:MET:HA	2.02	0.41
1:1:60:U:H6	27:1a:108:PRO:HG3	1.86	0.41
1:1:136:G:H8	1:1:136:G:OP2	2.04	0.41
1:1:315:U:H2'	1:1:316:U:H6	1.85	0.41
1:1:1616:C:H2'	1:1:1617:G:O4'	2.20	0.41
1:1:2446:G:H1'	1:1:2476:A:N3	2.35	0.41
2:1B:87:LEU:HA	2:1B:87:LEU:HD23	1.75	0.41
6:1F:102:MET:HE2	6:1F:102:MET:HB3	1.86	0.41
10:1J:42:ASN:N	10:1J:73:HIS:HE1	2.18	0.41
11:1K:107:LYS:HB3	11:1K:107:LYS:HE3	1.78	0.41
18:1R:47:ARG:O	18:1R:51:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:1u:154:MET:CE	46:1u:186:ASP:HB3	2.50	0.41
46:1u:281:MET:HE3	46:1u:282:LYS:N	2.36	0.41
48:2:861:C:H2'	48:2:862:G:O4'	2.20	0.41
48:2:1506:C:H2'	48:2:1507:A:C8	2.54	0.41
54:C:302:LYS:HE2	54:C:302:LYS:HB2	1.85	0.41
55:D:196:LYS:HE2	55:D:196:LYS:HB2	1.90	0.41
56:E:24:ALA:HA	73:V:181:LEU:HD21	2.02	0.41
59:H:270:LEU:HA	59:H:273:GLU:HG2	2.02	0.41
70:S:99:ARG:NH1	86:k:26:MET:HG3	2.34	0.41
72:U:105:VAL:O	72:U:108:MET:HG3	2.20	0.41
75:X:403:ILE:HD13	78:a:365:LEU:HD23	2.03	0.41
81:d:46:LEU:O	81:d:54:GLU:HG3	2.20	0.41
83:f:208:ASP:O	83:f:212:MET:HB2	2.20	0.41
85:i:168:GLU:O	85:i:172:THR:HG23	2.20	0.41
1:1:160:U:O2'	1:1:161:U:H5'	2.21	0.41
1:1:162:U:H4'	1:1:163:G:OP1	2.21	0.41
1:1:331:A:C2'	1:1:332:A:H5'	2.51	0.41
1:1:1232:U:H2'	1:1:1233:U:O4'	2.20	0.41
1:1:1318:C:H2'	1:1:1319:U:H6	1.85	0.41
1:1:2198:U:H2'	1:1:2199:U:C6	2.55	0.41
1:1:2490:U:H2'	1:1:2491:A:C8	2.56	0.41
6:1F:36:VAL:CG1	6:1F:95:SER:HB2	2.50	0.41
9:1I:13:LYS:HD3	9:1I:53:LEU:HD11	2.02	0.41
9:1I:44:LEU:HB3	9:1I:50:THR:OG1	2.20	0.41
11:1K:59:PRO:HG3	18:1R:57:GLY:HA2	2.01	0.41
15:1O:39:LYS:HA	15:1O:94:MET:HE1	2.03	0.41
16:1P:87:ILE:N	16:1P:87:ILE:HD13	2.35	0.41
22:1V:147:THR:O	22:1V:154:LYS:HD2	2.21	0.41
43:1r:73:VAL:HB	43:1r:74:PRO:HD3	2.03	0.41
46:1u:134:LEU:HD13	46:1u:156:MET:HE1	2.03	0.41
46:1u:342:ASP:O	46:1u:345:LEU:HG	2.21	0.41
46:1u:345:LEU:O	46:1u:349:GLU:HG2	2.21	0.41
48:2:472:C:H2'	48:2:473:G:C8	2.56	0.41
48:2:714:G:H5'	61:J:304:ASN:OD1	2.21	0.41
48:2:753:U:H2'	48:2:754:G:O4'	2.21	0.41
48:2:1089:C:H2'	48:2:1090:U:C6	2.55	0.41
48:2:1110:C:H2'	48:2:1111:C:H6	1.85	0.41
48:2:1822:A:H2'	48:2:1823:G:H8	1.85	0.41
54:C:116:PHE:C	54:C:117:LEU:HD12	2.45	0.41
55:D:75:GLU:H	55:D:75:GLU:HG3	1.71	0.41
62:K:64:PHE:HB3	62:K:93:VAL:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:M:90:TYR:HB3	64:M:111:LEU:HB2	2.02	0.41
72:U:34:PRO:HA	72:U:35:PRO:HD3	1.97	0.41
73:V:47:GLU:HG3	82:e:359:GLY:HA3	2.01	0.41
84:h:117:ARG:CZ	84:h:118:LYS:HB2	2.51	0.41
1:1:19:U:H3	1:1:667:G:H1	1.67	0.41
1:1:114:C:H2'	1:1:115:G:H8	1.86	0.41
1:1:528:U:H1'	46:1u:93:ARG:NH2	2.35	0.41
1:1:561:U:H2'	1:1:562:C:H6	1.84	0.41
1:1:2416:C:H2'	1:1:2417:C:C6	2.55	0.41
5:1E:247:ILE:HG21	5:1E:263:ILE:HD12	2.03	0.41
19:1S:221:LYS:HA	19:1S:221:LYS:HD3	1.90	0.41
22:1V:68:PHE:N	22:1V:68:PHE:HD1	2.18	0.41
40:1o:91:LEU:HB3	40:1o:107:PHE:CD1	2.56	0.41
46:1u:130:LEU:HD22	46:1u:163:VAL:HG11	2.02	0.41
46:1u:363:TYR:CE1	46:1u:382:ILE:HB	2.56	0.41
46:1u:734:LYS:HE2	46:1u:734:LYS:HB2	1.92	0.41
48:2:621:G:H2'	48:2:622:G:H8	1.86	0.41
54:C:205:LYS:HE3	54:C:205:LYS:HB2	1.83	0.41
56:E:8:LEU:HB3	56:E:88:LEU:HD21	2.02	0.41
57:F:37:HIS:NE2	74:W:477:PRO:HG2	2.36	0.41
73:V:160:LYS:HE2	73:V:160:LYS:HB2	1.86	0.41
77:Z:69:MET:HG3	77:Z:81:ILE:CD1	2.47	0.41
78:a:307:HIS:CE1	78:a:309:LYS:HG3	2.55	0.41
81:d:107:ALA:O	81:d:110:ILE:HG22	2.21	0.41
84:h:235:ASP:O	84:h:239:LYS:HG2	2.21	0.41
85:i:186:MET:HA	85:i:186:MET:HE3	2.02	0.41
86:k:3:TYR:O	86:k:7:PHE:HD1	2.03	0.41
1:1:120:A:H5"	1:1:121:C:O4'	2.21	0.41
1:1:350:A:H2'	1:1:351:A:O4'	2.21	0.41
1:1:490:U:H2'	1:1:491:U:C6	2.55	0.41
1:1:566:G:H1'	1:1:567:C:C5'	2.51	0.41
1:1:587:C:H2'	1:1:588:G:O4'	2.21	0.41
1:1:746:G:H2'	1:1:747:A:C8	2.56	0.41
1:1:929:G:H5'	1:1:930:G:OP1	2.20	0.41
1:1:2066:U:H2'	1:1:2067:U:C6	2.56	0.41
1:1:2239:U:H2'	1:1:2240:G:H8	1.85	0.41
1:1:2273:U:H6	1:1:2856:U:O2	2.04	0.41
1:1:2559:G:N2	14:1N:128:GLY:HA3	2.36	0.41
7:1G:82:LYS:HB3	7:1G:82:LYS:HE2	1.64	0.41
8:1H:103:LYS:HE2	8:1H:103:LYS:HB3	1.79	0.41
15:1O:70:ASP:HA	15:1O:73:ILE:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1S:138:GLU:HA	19:1S:139:PRO:HD3	1.79	0.41
26:1Z:138:LEU:O	26:1Z:138:LEU:HD23	2.21	0.41
29:1c:3:LYS:HD3	38:1l:61:PHE:CD1	2.56	0.41
38:1l:113:LEU:HB2	38:1l:210:TRP:CZ3	2.55	0.41
44:1s:101:THR:HA	44:1s:102:PRO:HD3	1.95	0.41
46:1u:208:PHE:HE1	46:1u:222:SER:OG	2.04	0.41
46:1u:325:VAL:HG21	46:1u:356:ILE:HB	2.02	0.41
46:1u:419:LEU:O	46:1u:422:MET:HB2	2.20	0.41
46:1u:651:ASP:HA	46:1u:680:LEU:HD21	2.03	0.41
48:2:471:G:H4'	82:e:326:ARG:HH11	1.85	0.41
48:2:491:G:H2'	48:2:492:G:C4	2.56	0.41
52:A:116:PHE:CD1	52:A:116:PHE:C	2.98	0.41
52:A:152:LEU:HD23	52:A:152:LEU:HA	1.93	0.41
53:B:394:LYS:HA	53:B:394:LYS:HD3	1.71	0.41
54:C:250:LYS:HB2	54:C:250:LYS:HE2	1.77	0.41
55:D:179:GLN:HA	55:D:182:THR:HG22	2.01	0.41
55:D:218:MET:HB2	55:D:218:MET:HE2	1.77	0.41
55:D:218:MET:SD	82:e:167:LEU:HD23	2.61	0.41
55:D:236:ILE:O	55:D:240:MET:HG2	2.21	0.41
57:F:94:GLU:O	57:F:98:LYS:HG2	2.21	0.41
61:J:261:LYS:HG2	61:J:296:GLU:HB2	2.02	0.41
76:Y:44:LYS:HB3	76:Y:44:LYS:HE2	1.86	0.41
82:e:175:GLY:O	82:e:257:ARG:HG3	2.20	0.41
82:e:185:GLU:HB3	82:e:209:TYR:HE2	1.86	0.41
83:f:88:PHE:HB3	83:f:139:PRO:HB2	2.03	0.41
85:i:100:PHE:HD2	85:i:144:PHE:HE1	1.68	0.41
1:1:491:U:H2'	1:1:492:C:C6	2.56	0.41
1:1:515:C:H5"	1:1:516:G:O4'	2.19	0.41
1:1:784:A:H2'	1:1:785:A:C8	2.56	0.41
1:1:855:G:H1	1:1:865:G:N2	2.18	0.41
1:1:1000:C:H2'	1:1:1001:G:C8	2.56	0.41
1:1:1071:G:H2'	1:1:1072:G:C8	2.55	0.41
1:1:1862:A:H2'	1:1:1863:C:C6	2.55	0.41
1:1:2405:C:H2'	1:1:2406:G:H8	1.85	0.41
4:1D:195:GLY:HA2	4:1D:237:PRO:HB3	2.03	0.41
38:1l:124:SER:HB2	38:1l:126:LYS:HG2	2.02	0.41
48:2:144:U:H2'	48:2:145:U:C6	2.55	0.41
48:2:339:G:H2'	48:2:340:A:C8	2.56	0.41
48:2:401:A:H4'	73:V:70:ARG:CZ	2.51	0.41
48:2:1664:4OC:HM23	48:2:1664:4OC:H1'	1.89	0.41
53:B:375:LYS:HB2	53:B:378:GLU:OE2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:B:447:GLN:HB3	78:a:155:ASP:HA	2.02	0.41
55:D:351:LYS:HB3	55:D:351:LYS:HE3	1.93	0.41
59:H:330:VAL:HG22	59:H:365:CYS:SG	2.61	0.41
61:J:290:ASN:HD21	70:S:36:LEU:HD13	1.86	0.41
72:U:70:GLU:HB2	72:U:71:PRO:HD3	2.02	0.41
75:X:356:LEU:HD23	75:X:356:LEU:HA	1.92	0.41
83:f:111:ILE:HD11	83:f:116:THR:HG23	2.03	0.41
1:1:1190:G:H2'	1:1:1191:A:H8	1.86	0.40
1:1:2713:U:H2'	1:1:2714:G:C8	2.56	0.40
4:1D:80:ILE:H	4:1D:107:ASN:HD21	1.69	0.40
20:1T:189:ILE:HD12	20:1T:189:ILE:HA	1.83	0.40
27:1a:37:PRO:O	27:1a:40:GLU:HG3	2.22	0.40
45:1t:307:GLN:HA	45:1t:310:VAL:HG12	2.03	0.40
46:1u:735:GLN:O	46:1u:738:VAL:HG22	2.21	0.40
47:1v:147:SER:O	47:1v:150:VAL:HG12	2.21	0.40
48:2:590:A:H2'	48:2:591:U:C6	2.56	0.40
48:2:1022:G:H2'	48:2:1023:U:C6	2.56	0.40
48:2:1110:C:H2'	48:2:1111:C:C6	2.56	0.40
48:2:1703:G:OP2	48:2:1703:G:H8	2.04	0.40
53:B:246:LYS:HB3	53:B:246:LYS:HE3	1.89	0.40
69:R:187:ILE:HD12	69:R:187:ILE:N	2.36	0.40
73:V:94:GLU:HG2	73:V:97:ARG:NH2	2.31	0.40
73:V:112:GLU:HG2	73:V:115:ARG:HH21	1.86	0.40
84:h:210:LYS:HG3	84:h:210:LYS:HZ2	1.62	0.40
84:h:361:ILE:HB	84:h:362:PRO:HD3	2.04	0.40
85:i:109:ARG:HH22	85:i:121:LYS:NZ	2.18	0.40
1:1:1137:C:H2'	1:1:1138:A:O4'	2.21	0.40
1:1:2938:G:H5'	20:1T:231:LYS:HZ2	1.86	0.40
3:1C:109:PHE:HE1	8:1H:89:LEU:HD11	1.87	0.40
41:1p:85:LYS:O	41:1p:89:ILE:HG12	2.21	0.40
46:1u:363:TYR:O	46:1u:367:LEU:HG	2.21	0.40
48:2:135:A:H2'	48:2:136:A:C8	2.56	0.40
48:2:510:U:H2'	48:2:511:C:H6	1.87	0.40
48:2:513:G:H2'	48:2:514:U:H6	1.86	0.40
49:3:112:C:H2'	49:3:113:C:H6	1.87	0.40
59:H:231:ALA:HB1	72:U:77:PHE:HB3	2.03	0.40
81:d:59:ARG:HE	81:d:63:GLU:HG3	1.86	0.40
83:f:110:SER:HA	83:f:113:GLU:CD	2.47	0.40
85:i:130:LEU:O	85:i:134:LYS:HG2	2.21	0.40
1:1:83:A:C2	1:1:97:A:C5	3.10	0.40
1:1:255:U:H4'	1:1:256:U:O4'	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:492:C:H4'	1:1:493:G:OP1	2.21	0.40
1:1:1069:C:H2'	1:1:1070:A:H8	1.86	0.40
1:1:1578:A:H5'	1:1:1579:C:OP2	2.19	0.40
1:1:1922:G:N3	47:1v:157:LYS:HE3	2.37	0.40
1:1:2399:U:H2'	1:1:2400:A:H8	1.86	0.40
1:1:2606:C:O2	1:1:2606:C:H2'	2.21	0.40
1:1:2959:C:H2'	1:1:2960:C:C6	2.56	0.40
1:1:3153:A:H8	1:1:3154:U:O2	2.04	0.40
3:1C:209:ARG:NH2	46:1u:144:GLY:HA2	2.36	0.40
3:1C:243:LEU:HD12	3:1C:243:LEU:H	1.85	0.40
6:1F:60:LYS:HD2	29:1c:5:VAL:HG13	2.03	0.40
12:1L:66:MET:CE	12:1L:88:LYS:HE3	2.50	0.40
15:1O:26:VAL:HG11	15:1O:72:VAL:HG13	2.03	0.40
38:1l:213:LYS:O	38:1l:217:LEU:HD23	2.22	0.40
40:1o:60:LEU:HD23	40:1o:60:LEU:HA	1.85	0.40
46:1u:585:ILE:HG21	46:1u:617:LEU:HD13	2.02	0.40
46:1u:702:TYR:C	46:1u:702:TYR:CD1	2.99	0.40
48:2:1008:U:H2'	48:2:1009:C:C6	2.56	0.40
48:2:1702:G:H2'	48:2:1703:G:C8	2.56	0.40
53:B:293:VAL:HA	53:B:296:LEU:HG	2.03	0.40
53:B:528:THR:HG22	53:B:529:ARG:N	2.36	0.40
57:F:4:LEU:HD22	57:F:47:ILE:HD13	2.02	0.40
58:G:5:ILE:HG13	58:G:6:LEU:N	2.35	0.40
65:N:306:LYS:HD2	65:N:309:LEU:HD12	2.03	0.40
74:W:279:GLU:HB3	74:W:280:PRO:HD3	2.03	0.40
75:X:348:MET:HE3	75:X:348:MET:HB3	1.98	0.40
75:X:389:GLU:OE2	75:X:391:GLU:HB2	2.21	0.40
82:e:177:ARG:HB3	82:e:258:GLU:HB2	2.03	0.40
85:i:233:LEU:HD23	85:i:233:LEU:HA	1.94	0.40
85:i:375:LEU:HG	85:i:375:LEU:O	2.21	0.40
1:1:314:U:O4	46:1u:237:MET:HE2	2.21	0.40
1:1:795:U:H3'	1:1:796:U:H5'	2.03	0.40
1:1:2333:A:N3	30:1d:83:VAL:HG12	2.37	0.40
1:1:2575:A:H4'	1:1:2576:A:N3	2.36	0.40
3:1C:42:ARG:HD3	3:1C:62:ASP:OD1	2.22	0.40
3:1C:192:PRO:C	3:1C:195:PRO:HD2	2.46	0.40
9:1I:36:GLN:O	9:1I:39:GLU:HG3	2.22	0.40
23:1W:42:GLU:OE1	45:1t:285:ARG:HG3	2.21	0.40
36:1j:45:GLY:HA3	36:1j:54:VAL:O	2.21	0.40
47:1v:255:TRP:CE3	47:1v:255:TRP:HA	2.56	0.40
50:5:66:U:H2'	50:5:67:C:H6	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:C:54:LYS:HE3	54:C:54:LYS:HB3	1.89	0.40
54:C:160:ILE:HG13	54:C:161:ILE:N	2.35	0.40
54:C:224:MET:HE2	54:C:224:MET:HB2	1.87	0.40
55:D:231:ILE:HG22	55:D:235:LYS:HE2	2.04	0.40
78:a:225:PHE:CD1	78:a:225:PHE:C	2.99	0.40
84:h:84:GLU:HA	84:h:87:LYS:HE3	2.02	0.40
84:h:288:LEU:HG	84:h:318:TYR:CE2	2.57	0.40
1:1:307:A:H2'	1:1:308:A:C2	2.57	0.40
1:1:350:A:H2'	1:1:351:A:C8	2.56	0.40
1:1:546:A:H2'	1:1:547:A:O4'	2.21	0.40
1:1:808:U:H2'	1:1:809:A:H8	1.86	0.40
1:1:1355:U:C2	1:1:1356:U:C5	3.09	0.40
1:1:1438:G:H2'	1:1:1439:U:C6	2.57	0.40
1:1:1875:G:H2'	1:1:1876:U:C6	2.57	0.40
1:1:2025:C:H2'	1:1:2026:C:C6	2.56	0.40
1:1:2601:A:H2'	1:1:2602:G:H8	1.87	0.40
1:1:3032:C:H2'	1:1:3033:U:O4'	2.22	0.40
8:1H:43:LYS:HB3	8:1H:63:LYS:HG3	2.04	0.40
16:1P:14:ASP:N	16:1P:14:ASP:OD1	2.54	0.40
35:1i:251:ARG:HH21	63:L:101:ARG:HG2	1.86	0.40
46:1u:541:ARG:N	46:1u:541:ARG:HD3	2.36	0.40
48:2:520:C:H41	62:K:50:ARG:NH2	2.17	0.40
50:5:63:C:H2'	50:5:64:U:H6	1.86	0.40
53:B:428:SER:OG	53:B:435:THR:HG22	2.22	0.40
53:B:481:ARG:HG2	53:B:542:SER:OG	2.21	0.40
70:S:30:LYS:HD3	70:S:32:PHE:CE1	2.57	0.40
74:W:101:ARG:HD3	74:W:170:TRP:HZ3	1.85	0.40
75:X:417:LYS:HD2	75:X:417:LYS:H	1.87	0.40
78:a:92:GLU:OE2	78:a:94:ASN:HB3	2.21	0.40
83:f:310:PRO:HD3	83:f:368:TRP:HD1	1.85	0.40
84:h:256:PHE:CE2	84:h:279:ARG:HB2	2.57	0.40
85:i:137:GLU:O	85:i:140:GLU:HG3	2.22	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	
2	1B	175/217 (81%)	171 (98%)	4 (2%)	0	100	100
3	1C	203/286 (71%)	194 (96%)	8 (4%)	1 (0%)	24	53
4	1D	262/319 (82%)	256 (98%)	6 (2%)	0	100	100
5	1E	219/296 (74%)	215 (98%)	4 (2%)	0	100	100
6	1F	154/185 (83%)	147 (96%)	7 (4%)	0	100	100
7	1G	96/102 (94%)	95 (99%)	1 (1%)	0	100	100
8	1H	64/220 (29%)	63 (98%)	1 (2%)	0	100	100
9	1I	128/170 (75%)	125 (98%)	2 (2%)	1 (1%)	16	43
10	1J	145/156 (93%)	132 (91%)	13 (9%)	0	100	100
11	1K	187/204 (92%)	185 (99%)	2 (1%)	0	100	100
12	1L	125/176 (71%)	119 (95%)	6 (5%)	0	100	100
13	1M	208/281 (74%)	199 (96%)	9 (4%)	0	100	100
14	1N	146/179 (82%)	141 (97%)	5 (3%)	0	100	100
15	1O	149/160 (93%)	141 (95%)	8 (5%)	0	100	100
16	1P	111/114 (97%)	104 (94%)	7 (6%)	0	100	100
17	1Q	120/233 (52%)	115 (96%)	5 (4%)	0	100	100
18	1R	108/126 (86%)	106 (98%)	2 (2%)	0	100	100
19	1S	143/270 (53%)	140 (98%)	3 (2%)	0	100	100
20	1T	153/264 (58%)	148 (97%)	5 (3%)	0	100	100
21	1U	126/180 (70%)	123 (98%)	3 (2%)	0	100	100
22	1V	156/159 (98%)	153 (98%)	3 (2%)	0	100	100
23	1W	203/238 (85%)	198 (98%)	5 (2%)	0	100	100
24	1X	214/271 (79%)	208 (97%)	6 (3%)	0	100	100
25	1Y	96/156 (62%)	94 (98%)	2 (2%)	0	100	100
26	1Z	175/215 (81%)	173 (99%)	2 (1%)	0	100	100
27	1a	106/144 (74%)	106 (100%)	0	0	100	100
28	1b	98/109 (90%)	93 (95%)	5 (5%)	0	100	100
29	1c	57/135 (42%)	53 (93%)	4 (7%)	0	100	100
30	1d	47/139 (34%)	46 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	1e	52/106 (49%)	52 (100%)	0	0	100	100
32	1f	42/146 (29%)	42 (100%)	0	0	100	100
33	1g	89/162 (55%)	87 (98%)	2 (2%)	0	100	100
34	1h	36/103 (35%)	35 (97%)	1 (3%)	0	100	100
35	1i	181/247 (73%)	178 (98%)	3 (2%)	0	100	100
36	1j	69/90 (77%)	67 (97%)	2 (3%)	0	100	100
37	1k	116/119 (98%)	114 (98%)	2 (2%)	0	100	100
38	1l	209/239 (87%)	200 (96%)	9 (4%)	0	100	100
39	1m	120/128 (94%)	116 (97%)	4 (3%)	0	100	100
40	1o	74/125 (59%)	70 (95%)	4 (5%)	0	100	100
41	1p	115/130 (88%)	115 (100%)	0	0	100	100
42	1q	48/78 (62%)	47 (98%)	0	1 (2%)	5	20
43	1r	90/167 (54%)	85 (94%)	5 (6%)	0	100	100
44	1s	116/181 (64%)	114 (98%)	2 (2%)	0	100	100
45	1t	482/491 (98%)	466 (97%)	16 (3%)	0	100	100
46	1u	664/751 (88%)	627 (94%)	36 (5%)	1 (0%)	43	71
47	1v	429/514 (84%)	417 (97%)	12 (3%)	0	100	100
52	A	202/212 (95%)	192 (95%)	10 (5%)	0	100	100
53	B	457/554 (82%)	429 (94%)	28 (6%)	0	100	100
54	C	329/362 (91%)	322 (98%)	7 (2%)	0	100	100
55	D	413/501 (82%)	398 (96%)	15 (4%)	0	100	100
56	E	99/138 (72%)	96 (97%)	3 (3%)	0	100	100
57	F	146/157 (93%)	141 (97%)	5 (3%)	0	100	100
58	G	126/129 (98%)	121 (96%)	5 (4%)	0	100	100
59	H	209/383 (55%)	196 (94%)	12 (6%)	1 (0%)	24	53
60	I	111/228 (49%)	107 (96%)	4 (4%)	0	100	100
61	J	125/304 (41%)	123 (98%)	2 (2%)	0	100	100
62	K	122/125 (98%)	120 (98%)	2 (2%)	0	100	100
63	L	117/154 (76%)	110 (94%)	7 (6%)	0	100	100
64	M	99/155 (64%)	99 (100%)	0	0	100	100
65	N	114/414 (28%)	113 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
66	O	108/136 (79%)	104 (96%)	4 (4%)	0	100	100
67	P	89/110 (81%)	86 (97%)	3 (3%)	0	100	100
68	Q	88/237 (37%)	87 (99%)	1 (1%)	0	100	100
69	R	162/212 (76%)	155 (96%)	7 (4%)	0	100	100
70	S	73/100 (73%)	72 (99%)	1 (1%)	0	100	100
71	T	48/94 (51%)	46 (96%)	2 (4%)	0	100	100
72	U	125/192 (65%)	120 (96%)	4 (3%)	1 (1%)	16	43
73	V	162/193 (84%)	158 (98%)	4 (2%)	0	100	100
74	W	376/483 (78%)	368 (98%)	8 (2%)	0	100	100
75	X	202/496 (41%)	190 (94%)	10 (5%)	2 (1%)	12	37
76	Y	96/102 (94%)	92 (96%)	4 (4%)	0	100	100
77	Z	78/153 (51%)	75 (96%)	3 (4%)	0	100	100
78	a	311/424 (73%)	305 (98%)	6 (2%)	0	100	100
79	b	75/80 (94%)	66 (88%)	9 (12%)	0	100	100
80	c	24/128 (19%)	24 (100%)	0	0	100	100
81	d	76/110 (69%)	75 (99%)	1 (1%)	0	100	100
82	e	244/383 (64%)	234 (96%)	10 (4%)	0	100	100
83	f	375/410 (92%)	362 (96%)	13 (4%)	0	100	100
84	h	308/384 (80%)	300 (97%)	8 (3%)	0	100	100
85	i	302/725 (42%)	292 (97%)	10 (3%)	0	100	100
86	k	43/153 (28%)	40 (93%)	3 (7%)	0	100	100
All	All	13140/18602 (71%)	12693 (97%)	439 (3%)	8 (0%)	49	76

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
59	H	225	ILE
72	U	64	PRO
9	1I	133	PRO
46	1u	84	HIS
75	X	428	ILE
3	1C	187	SER
75	X	461	VAL
42	1q	64	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	1B	141/173 (82%)	137 (97%)	4 (3%)	38 70
3	1C	184/239 (77%)	179 (97%)	5 (3%)	39 71
4	1D	216/264 (82%)	208 (96%)	8 (4%)	30 63
5	1E	192/256 (75%)	189 (98%)	3 (2%)	55 81
6	1F	145/168 (86%)	139 (96%)	6 (4%)	27 60
7	1G	82/86 (95%)	82 (100%)	0	100 100
8	1H	58/196 (30%)	56 (97%)	2 (3%)	32 65
9	1I	113/143 (79%)	111 (98%)	2 (2%)	51 79
10	1J	125/131 (95%)	124 (99%)	1 (1%)	73 89
11	1K	161/170 (95%)	159 (99%)	2 (1%)	63 85
12	1L	103/140 (74%)	101 (98%)	2 (2%)	50 78
13	1M	169/235 (72%)	161 (95%)	8 (5%)	23 55
14	1N	116/146 (80%)	115 (99%)	1 (1%)	70 88
15	1O	129/139 (93%)	126 (98%)	3 (2%)	44 74
16	1P	94/95 (99%)	88 (94%)	6 (6%)	16 43
17	1Q	110/208 (53%)	105 (96%)	5 (4%)	24 56
18	1R	96/110 (87%)	94 (98%)	2 (2%)	47 76
19	1S	130/244 (53%)	128 (98%)	2 (2%)	57 82
20	1T	133/229 (58%)	131 (98%)	2 (2%)	57 82
21	1U	114/147 (78%)	114 (100%)	0	100 100
22	1V	132/133 (99%)	130 (98%)	2 (2%)	57 82
23	1W	181/204 (89%)	176 (97%)	5 (3%)	38 70
24	1X	186/235 (79%)	181 (97%)	5 (3%)	39 71
25	1Y	80/127 (63%)	80 (100%)	0	100 100
26	1Z	150/177 (85%)	148 (99%)	2 (1%)	61 84
27	1a	102/128 (80%)	99 (97%)	3 (3%)	37 69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	1b	88/95 (93%)	88 (100%)	0	100	100
29	1c	51/119 (43%)	49 (96%)	2 (4%)	28	61
30	1d	42/119 (35%)	40 (95%)	2 (5%)	23	54
31	1e	49/98 (50%)	45 (92%)	4 (8%)	10	31
32	1f	35/129 (27%)	35 (100%)	0	100	100
33	1g	84/152 (55%)	83 (99%)	1 (1%)	63	85
34	1h	36/87 (41%)	34 (94%)	2 (6%)	19	48
35	1i	152/203 (75%)	145 (95%)	7 (5%)	24	56
36	1j	64/79 (81%)	64 (100%)	0	100	100
37	1k	105/106 (99%)	99 (94%)	6 (6%)	18	48
38	1l	189/214 (88%)	184 (97%)	5 (3%)	40	72
39	1m	107/112 (96%)	104 (97%)	3 (3%)	38	70
40	1o	71/105 (68%)	71 (100%)	0	100	100
41	1p	101/108 (94%)	101 (100%)	0	100	100
42	1q	41/64 (64%)	40 (98%)	1 (2%)	43	73
43	1r	83/138 (60%)	82 (99%)	1 (1%)	63	85
44	1s	103/155 (66%)	101 (98%)	2 (2%)	50	78
45	1t	417/423 (99%)	411 (99%)	6 (1%)	59	83
46	1u	578/659 (88%)	558 (96%)	20 (4%)	32	64
47	1v	374/454 (82%)	357 (96%)	17 (4%)	24	56
52	A	177/182 (97%)	174 (98%)	3 (2%)	53	80
53	B	421/492 (86%)	406 (96%)	15 (4%)	31	63
54	C	314/343 (92%)	297 (95%)	17 (5%)	20	49
55	D	370/444 (83%)	363 (98%)	7 (2%)	50	78
56	E	90/126 (71%)	88 (98%)	2 (2%)	45	75
57	F	124/124 (100%)	122 (98%)	2 (2%)	55	81
58	G	112/113 (99%)	111 (99%)	1 (1%)	70	88
59	H	176/320 (55%)	169 (96%)	7 (4%)	28	61
60	I	104/197 (53%)	98 (94%)	6 (6%)	18	47
61	J	108/256 (42%)	105 (97%)	3 (3%)	38	70
62	K	107/108 (99%)	101 (94%)	6 (6%)	19	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
63	L	99/128 (77%)	97 (98%)	2 (2%)	48 77
64	M	90/137 (66%)	88 (98%)	2 (2%)	45 75
65	N	107/362 (30%)	106 (99%)	1 (1%)	70 88
66	O	93/117 (80%)	88 (95%)	5 (5%)	20 49
67	P	78/95 (82%)	77 (99%)	1 (1%)	61 84
68	Q	75/203 (37%)	75 (100%)	0	100 100
69	R	141/180 (78%)	139 (99%)	2 (1%)	59 83
70	S	68/90 (76%)	68 (100%)	0	100 100
71	T	44/79 (56%)	44 (100%)	0	100 100
72	U	109/170 (64%)	106 (97%)	3 (3%)	38 70
73	V	147/173 (85%)	142 (97%)	5 (3%)	32 65
74	W	328/410 (80%)	322 (98%)	6 (2%)	51 79
75	X	174/395 (44%)	166 (95%)	8 (5%)	24 56
76	Y	84/86 (98%)	77 (92%)	7 (8%)	10 30
77	Z	65/119 (55%)	63 (97%)	2 (3%)	35 67
78	a	252/374 (67%)	243 (96%)	9 (4%)	31 63
79	b	68/71 (96%)	67 (98%)	1 (2%)	57 82
80	c	25/116 (22%)	25 (100%)	0	100 100
81	d	65/93 (70%)	63 (97%)	2 (3%)	35 67
82	e	226/339 (67%)	222 (98%)	4 (2%)	51 79
83	f	321/351 (92%)	313 (98%)	8 (2%)	42 73
84	h	271/337 (80%)	266 (98%)	5 (2%)	51 79
85	i	272/629 (43%)	263 (97%)	9 (3%)	33 65
86	k	22/110 (20%)	21 (96%)	1 (4%)	24 56
All	All	11539/16011 (72%)	11227 (97%)	312 (3%)	40 71

All (312) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1B	53	MET
2	1B	70	ILE
2	1B	182	THR
2	1B	185	SER
3	1C	53	MET

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Mol	Chain	Res	Type
3	1C	55	ILE
3	1C	166	VAL
3	1C	319	LYS
3	1C	321	VAL
4	1D	115	ILE
4	1D	232	LYS
4	1D	264	VAL
4	1D	279	ASN
4	1D	285	LYS
4	1D	289	SER
4	1D	297	LEU
4	1D	317	VAL
5	1E	82	THR
5	1E	83	ILE
5	1E	89	LEU
6	1F	17	LEU
6	1F	36	VAL
6	1F	94	GLN
6	1F	107	VAL
6	1F	133	THR
6	1F	179	LYS
8	1H	62	VAL
8	1H	63	LYS
9	1I	57	ASN
9	1I	59	LEU
10	1J	68	THR
11	1K	40	GLN
11	1K	158	VAL
12	1L	111	MET
12	1L	140	THR
13	1M	106	MET
13	1M	168	ILE
13	1M	172	ILE
13	1M	215	VAL
13	1M	227	LYS
13	1M	234	LYS
13	1M	248	GLN
13	1M	250	ASP
14	1N	153	VAL
15	1O	86	ASP
15	1O	94	MET
15	1O	122	SER

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Mol	Chain	Res	Type
16	1P	33	GLN
16	1P	39	THR
16	1P	59	VAL
16	1P	92	GLU
16	1P	105	SER
16	1P	112	LYS
17	1Q	116	MET
17	1Q	125	GLU
17	1Q	145	LYS
17	1Q	176	ILE
17	1Q	209	ARG
18	1R	45	GLU
18	1R	102	SER
19	1S	210	GLU
19	1S	245	GLU
20	1T	235	LYS
20	1T	249	THR
22	1V	74	LEU
22	1V	131	THR
23	1W	81	GLN
23	1W	111	ILE
23	1W	184	LEU
23	1W	210	VAL
23	1W	220	SER
24	1X	38	GLU
24	1X	66	ILE
24	1X	109	LEU
24	1X	117	ARG
24	1X	241	GLU
26	1Z	91	VAL
26	1Z	92	LYS
27	1a	33	ILE
27	1a	100	MET
27	1a	122	THR
29	1c	24	VAL
29	1c	48	ILE
30	1d	95	ILE
30	1d	109	ILE
31	1e	10	MET
31	1e	27	ARG
31	1e	38	GLU
31	1e	48	ARG

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Mol	Chain	Res	Type
33	1g	116	SER
34	1h	5	SER
34	1h	18	LYS
35	1i	99	GLU
35	1i	119	GLN
35	1i	198	ILE
35	1i	210	LEU
35	1i	214	LEU
35	1i	227	THR
35	1i	230	ILE
37	1k	10	GLN
37	1k	50	LEU
37	1k	68	ARG
37	1k	78	ASP
37	1k	100	THR
37	1k	117	VAL
38	1l	25	ASP
38	1l	28	VAL
38	1l	80	GLU
38	1l	170	HIS
38	1l	223	GLN
39	1m	4	PHE
39	1m	8	VAL
39	1m	81	MET
42	1q	59	THR
43	1r	85	VAL
44	1s	159	MET
44	1s	175	LEU
45	1t	17	THR
45	1t	68	ARG
45	1t	201	ARG
45	1t	350	VAL
45	1t	352	LYS
45	1t	433	LEU
46	1u	85	GLU
46	1u	141	GLU
46	1u	146	ILE
46	1u	202	GLN
46	1u	277	PHE
46	1u	290	ASP
46	1u	316	MET
46	1u	383	LEU

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Mol	Chain	Res	Type
46	1u	397	SER
46	1u	399	PHE
46	1u	438	ILE
46	1u	539	VAL
46	1u	591	ASP
46	1u	602	MET
46	1u	609	VAL
46	1u	612	GLU
46	1u	615	MET
46	1u	618	ILE
46	1u	647	THR
46	1u	676	ARG
47	1v	148	PHE
47	1v	150	VAL
47	1v	153	PHE
47	1v	170	LYS
47	1v	220	LYS
47	1v	223	GLU
47	1v	245	GLU
47	1v	261	LEU
47	1v	262	ASP
47	1v	285	MET
47	1v	311	LEU
47	1v	313	MET
47	1v	314	GLU
47	1v	348	MET
47	1v	373	ILE
47	1v	414	MET
47	1v	436	MET
52	A	38	MET
52	A	81	GLU
52	A	103	MET
53	B	62	LEU
53	B	152	LYS
53	B	154	GLN
53	B	160	ASP
53	B	188	VAL
53	B	204	THR
53	B	210	PHE
53	B	252	ASP
53	B	259	HIS
53	B	285	ILE

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Mol	Chain	Res	Type
53	B	308	ASN
53	B	368	TRP
53	B	476	LYS
53	B	481	ARG
53	B	527	SER
54	C	52	ILE
54	C	54	LYS
54	C	59	SER
54	C	70	GLN
54	C	72	THR
54	C	77	LEU
54	C	85	THR
54	C	125	GLN
54	C	138	MET
54	C	180	ILE
54	C	182	LYS
54	C	218	GLN
54	C	230	GLU
54	C	234	LYS
54	C	251	ARG
54	C	289	LEU
54	C	312	ILE
55	D	82	ASP
55	D	133	LEU
55	D	139	LEU
55	D	222	LYS
55	D	234	GLN
55	D	464	MET
55	D	499	THR
56	E	13	ILE
56	E	56	ASP
57	F	93	LEU
57	F	122	ARG
58	G	103	VAL
59	H	224	VAL
59	H	242	THR
59	H	268	GLU
59	H	315	SER
59	H	322	VAL
59	H	405	THR
59	H	428	VAL
60	I	125	ILE

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Mol	Chain	Res	Type
60	I	151	SER
60	I	188	LEU
60	I	204	LEU
60	I	208	ARG
60	I	232	SER
61	J	190	GLU
61	J	246	ILE
61	J	289	GLN
62	K	13	GLU
62	K	16	ARG
62	K	31	THR
62	K	33	VAL
62	K	38	SER
62	K	41	THR
63	L	34	VAL
63	L	105	GLU
64	M	68	LYS
64	M	79	LEU
65	N	310	VAL
66	O	23	THR
66	O	51	ARG
66	O	77	LEU
66	O	89	VAL
66	O	100	THR
67	P	12	LYS
69	R	181	THR
69	R	183	VAL
72	U	25	VAL
72	U	30	MET
72	U	49	VAL
73	V	132	GLN
73	V	145	GLU
73	V	162	LYS
73	V	177	GLU
73	V	193	THR
74	W	162	ILE
74	W	247	THR
74	W	293	ILE
74	W	351	VAL
74	W	424	ARG
74	W	448	VAL
75	X	348	MET

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Mol	Chain	Res	Type
75	X	352	ILE
75	X	399	SER
75	X	430	ASP
75	X	448	MET
75	X	462	THR
75	X	475	THR
75	X	512	ASP
76	Y	18	VAL
76	Y	29	MET
76	Y	30	LEU
76	Y	33	THR
76	Y	41	ILE
76	Y	83	ARG
76	Y	90	GLN
77	Z	49	LYS
77	Z	112	LYS
78	a	152	GLU
78	a	172	PHE
78	a	175	MET
78	a	188	ILE
78	a	203	LEU
78	a	294	GLN
78	a	336	VAL
78	a	361	ARG
78	a	386	ARG
79	b	78	ASN
81	d	46	LEU
81	d	72	VAL
82	e	202	VAL
82	e	281	ILE
82	e	333	LYS
82	e	367	VAL
83	f	136	TYR
83	f	172	HIS
83	f	196	LEU
83	f	255	LEU
83	f	261	THR
83	f	264	LEU
83	f	359	LEU
83	f	398	LEU
84	h	95	ASP
84	h	109	LEU

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Mol	Chain	Res	Type
84	h	113	ILE
84	h	122	ILE
84	h	327	GLU
85	i	96	THR
85	i	169	VAL
85	i	186	MET
85	i	205	ILE
85	i	230	TYR
85	i	281	LYS
85	i	293	VAL
85	i	295	MET
85	i	356	ILE
86	k	12	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (99) such sidechains are listed below:

Mol	Chain	Res	Type
2	1B	166	HIS
3	1C	313	HIS
3	1C	314	GLN
4	1D	107	ASN
5	1E	98	ASN
5	1E	127	GLN
5	1E	162	HIS
5	1E	232	GLN
5	1E	257	ASN
5	1E	259	HIS
6	1F	7	HIS
9	1I	20	ASN
9	1I	57	ASN
10	1J	51	ASN
10	1J	73	HIS
10	1J	128	GLN
11	1K	26	ASN
11	1K	75	ASN
11	1K	187	ASN
12	1L	69	GLN
14	1N	93	HIS
14	1N	105	ASN
15	1O	28	HIS
16	1P	33	GLN
18	1R	90	HIS

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Mol	Chain	Res	Type
20	1T	156	HIS
21	1U	27	ASN
22	1V	12	HIS
23	1W	34	GLN
24	1X	100	ASN
24	1X	101	GLN
24	1X	108	HIS
25	1Y	102	HIS
26	1Z	65	ASN
26	1Z	96	HIS
26	1Z	147	ASN
27	1a	36	ASN
27	1a	98	ASN
27	1a	103	ASN
36	1j	62	ASN
37	1k	10	GLN
37	1k	55	HIS
38	1l	51	GLN
38	1l	60	GLN
38	1l	159	HIS
39	1m	93	GLN
39	1m	112	HIS
42	1q	49	GLN
45	1t	419	GLN
46	1u	381	ASN
46	1u	433	HIS
47	1v	330	ASN
52	A	9	GLN
53	B	64	HIS
53	B	282	GLN
53	B	468	HIS
53	B	507	HIS
53	B	516	ASN
53	B	517	GLN
54	C	186	GLN
54	C	322	ASN
55	D	174	HIS
55	D	410	GLN
58	G	50	GLN
60	I	139	ASN
61	J	263	ASN
63	L	41	ASN

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Mol	Chain	Res	Type
65	N	318	ASN
65	N	349	GLN
65	N	370	HIS
67	P	27	ASN
67	P	47	ASN
67	P	66	HIS
68	Q	198	GLN
70	S	60	GLN
70	S	62	HIS
70	S	63	HIS
74	W	248	HIS
74	W	307	GLN
74	W	323	GLN
74	W	327	ASN
74	W	395	HIS
75	X	383	ASN
77	Z	62	ASN
77	Z	92	HIS
77	Z	100	HIS
78	a	107	GLN
78	a	190	HIS
78	a	356	HIS
81	d	56	HIS
82	e	217	HIS
83	f	172	HIS
83	f	224	HIS
83	f	251	GLN
84	h	174	HIS
84	h	187	HIS
84	h	344	HIS
84	h	345	GLN
86	k	12	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2910/2923 (99%)	542 (18%)	29 (0%)
48	2	1555/1766 (88%)	248 (15%)	11 (0%)
49	3	117/118 (99%)	25 (21%)	1 (0%)
50	5	76/77 (98%)	19 (25%)	0
51	6	5/6 (83%)	2 (40%)	1 (20%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	4663/4890 (95%)	836 (17%)	42 (0%)

All (836) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	30	G
1	1	37	G
1	1	47	A
1	1	49	G
1	1	50	G
1	1	51	A
1	1	63	A
1	1	64	G
1	1	65	A
1	1	70	A
1	1	73	G
1	1	74	G
1	1	82	G
1	1	86	U
1	1	87	A
1	1	88	C
1	1	96	G
1	1	113	U
1	1	126	U
1	1	127	C
1	1	128	C
1	1	129	A
1	1	131	G
1	1	132	C
1	1	136	G
1	1	137	U
1	1	138	G
1	1	139	G
1	1	140	C
1	1	141	U
1	1	142	A
1	1	144	U
1	1	147	G
1	1	148	C
1	1	150	C
1	1	151	U
1	1	152	C

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Mol	Chain	Res	Type
1	1	153	U
1	1	157	G
1	1	158	A
1	1	159	C
1	1	161	U
1	1	163	G
1	1	164	A
1	1	172	G
1	1	181	A
1	1	184	A
1	1	201	A
1	1	206	A
1	1	207	A
1	1	233	G
1	1	249	U
1	1	251	G
1	1	256	U
1	1	257	U
1	1	259	A
1	1	276	A
1	1	308	A
1	1	309	A
1	1	311	A
1	1	313	U
1	1	314	U
1	1	331	A
1	1	332	A
1	1	333	A
1	1	334	A
1	1	337	A
1	1	339	A
1	1	342	A
1	1	344	A
1	1	345	A
1	1	352	A
1	1	353	A
1	1	354	A
1	1	357	A
1	1	416	U
1	1	418	U
1	1	419	U
1	1	421	A

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Mol	Chain	Res	Type
1	1	422	C
1	1	424	G
1	1	425	U
1	1	426	A
1	1	428	U
1	1	435	A
1	1	436	A
1	1	445	G
1	1	457	G
1	1	463	G
1	1	464	A
1	1	481	U
1	1	485	U
1	1	486	A
1	1	487	U
1	1	488	U
1	1	491	U
1	1	493	G
1	1	495	U
1	1	498	U
1	1	499	U
1	1	500	C
1	1	501	C
1	1	502	C
1	1	504	G
1	1	514	G
1	1	515	C
1	1	516	G
1	1	526	U
1	1	535	U
1	1	537	U
1	1	538	U
1	1	539	A
1	1	540	C
1	1	541	G
1	1	542	C
1	1	547	A
1	1	553	G
1	1	566	G
1	1	567	C
1	1	597	C
1	1	598	A

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Mol	Chain	Res	Type
1	1	599	A
1	1	620	A
1	1	623	G
1	1	633	A
1	1	646	A
1	1	649	G
1	1	650	A
1	1	651	A
1	1	652	C
1	1	670	C
1	1	671	A
1	1	672	A
1	1	673	U
1	1	674	C
1	1	675	A
1	1	676	G
1	1	687	A
1	1	689	U
1	1	690	C
1	1	691	A
1	1	692	A
1	1	693	G
1	1	694	C
1	1	695	G
1	1	696	C
1	1	697	A
1	1	698	C
1	1	700	C
1	1	701	A
1	1	714	A
1	1	724	U
1	1	725	G
1	1	726	A
1	1	737	A
1	1	754	G
1	1	771	U
1	1	779	U
1	1	780	U
1	1	781	C
1	1	785	A
1	1	789	G
1	1	790	G

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Mol	Chain	Res	Type
1	1	793	U
1	1	795	U
1	1	796	U
1	1	799	A
1	1	800	G
1	1	808	U
1	1	812	U
1	1	830	U
1	1	853	G
1	1	854	A
1	1	871	G
1	1	875	A
1	1	885	C
1	1	909	A
1	1	910	C
1	1	920	G
1	1	921	G
1	1	927	A
1	1	929	G
1	1	930	G
1	1	937	A
1	1	950	G
1	1	957	U
1	1	972	U
1	1	973	U
1	1	975	A
1	1	989	U
1	1	992	C
1	1	1004	G
1	1	1011	A
1	1	1021	C
1	1	1022	U
1	1	1023	A
1	1	1024	G
1	1	1044	A
1	1	1045	C
1	1	1046	C
1	1	1055	G
1	1	1058	A
1	1	1094	G
1	1	1098	U
1	1	1099	U

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Mol	Chain	Res	Type
1	1	1101	G
1	1	1111	G
1	1	1124	G
1	1	1146	C
1	1	1159	A
1	1	1162	C
1	1	1163	A
1	1	1172	G
1	1	1176	A
1	1	1195	A
1	1	1196	U
1	1	1197	G
1	1	1198	A
1	1	1207	A
1	1	1211	G
1	1	1218	G
1	1	1219	A
1	1	1220	A
1	1	1221	G
1	1	1234	G
1	1	1237	G
1	1	1238	A
1	1	1239	A
1	1	1240	A
1	1	1242	C
1	1	1243	G
1	1	1244	U
1	1	1262	G
1	1	1269	G
1	1	1282	U
1	1	1283	A
1	1	1285	C
1	1	1292	C
1	1	1293	A
1	1	1325	G
1	1	1327	U
1	1	1328	G
1	1	1329	C
1	1	1331	U
1	1	1332	U
1	1	1338	G
1	1	1339	U

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Mol	Chain	Res	Type
1	1	1352	A
1	1	1393	G
1	1	1395	G
1	1	1407	G
1	1	1412	U
1	1	1413	G
1	1	1428	G
1	1	1430	A
1	1	1444	A
1	1	1453	G
1	1	1457	G
1	1	1459	C
1	1	1467	G
1	1	1485	A
1	1	1487	U
1	1	1510	U
1	1	1516	A
1	1	1523	A
1	1	1531	G
1	1	1533	C
1	1	1540	U
1	1	1545	A
1	1	1546	C
1	1	1557	C
1	1	1566	U
1	1	1567	U
1	1	1572	U
1	1	1574	C
1	1	1578	A
1	1	1584	C
1	1	1587	C
1	1	1588	U
1	1	1593	U
1	1	1594	G
1	1	1595	G
1	1	1596	A
1	1	1597	G
1	1	1598	C
1	1	1599	G
1	1	1600	A
1	1	1602	U
1	1	1603	U

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Mol	Chain	Res	Type
1	1	1604	G
1	1	1605	G
1	1	1606	A
1	1	1607	U
1	1	1619	G
1	1	1620	G
1	1	1621	G
1	1	1623	A
1	1	1627	U
1	1	1629	G
1	1	1630	C
1	1	1631	G
1	1	1634	U
1	1	1635	C
1	1	1638	C
1	1	1643	C
1	1	1644	A
1	1	1645	C
1	1	1648	U
1	1	1649	C
1	1	1670	G
1	1	1671	A
1	1	1672	G
1	1	1678	A
1	1	1679	A
1	1	1681	G
1	1	1685	U
1	1	1693	C
1	1	1694	A
1	1	1699	U
1	1	1834	A
1	1	1848	A
1	1	1849	U
1	1	1850	U
1	1	1852	U
1	1	1853	A
1	1	1854	A
1	1	1858	C
1	1	1869	U
1	1	1874	A
1	1	1875	G
1	1	1876	U

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Mol	Chain	Res	Type
1	1	1877	C
1	1	1880	G
1	1	1883	G
1	1	1884	G
1	1	1889	A
1	1	1890	A
1	1	1896	A
1	1	1899	A
1	1	1903	A
1	1	1919	G
1	1	1922	G
1	1	1923	A
1	1	1924	U
1	1	1925	C
1	1	1934	G
1	1	1935	A
1	1	1936	A
1	1	1937	C
1	1	1950	A
1	1	1976	U
1	1	1988	C
1	1	1989	U
1	1	1990	U
1	1	2009	G
1	1	2016	G
1	1	2017	C
1	1	2058	U
1	1	2060	U
1	1	2062	U
1	1	2064	G
1	1	2065	A
1	1	2066	U
1	1	2067	U
1	1	2080	C
1	1	2081	A
1	1	2082	U
1	1	2088	G
1	1	2097	A
1	1	2104	A
1	1	2124	C
1	1	2125	U
1	1	2132	U

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Mol	Chain	Res	Type
1	1	2140	U
1	1	2153	A
1	1	2176	C
1	1	2182	G
1	1	2185	A
1	1	2190	U
1	1	2191	U
1	1	2192	A
1	1	2193	U
1	1	2194	A
1	1	2214	G
1	1	2224	G
1	1	2232	C
1	1	2233	U
1	1	2247	G
1	1	2248	G
1	1	2255	A
1	1	2256	A
1	1	2259	C
1	1	2273	U
1	1	2282	G
1	1	2284	A
1	1	2285	C
1	1	2288	A
1	1	2289	U
1	1	2290	G
1	1	2293	G
1	1	2309	U
1	1	2310	G
1	1	2311	U
1	1	2315	C
1	1	2341	C
1	1	2349	A
1	1	2351	A
1	1	2373	C
1	1	2374	G
1	1	2378	A
1	1	2379	G
1	1	2380	A
1	1	2387	G
1	1	2394	C
1	1	2415	A

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Mol	Chain	Res	Type
1	1	2420	G
1	1	2421	A
1	1	2423	C
1	1	2426	A
1	1	2428	G
1	1	2429	U
1	1	2430	G
1	1	2434	G
1	1	2436	U
1	1	2437	A
1	1	2438	G
1	1	2439	G
1	1	2440	U
1	1	2444	A
1	1	2445	G
1	1	2446	G
1	1	2448	C
1	1	2449	C
1	1	2450	U
1	1	2451	C
1	1	2452	A
1	1	2454	A
1	1	2455	U
1	1	2461	G
1	1	2462	A
1	1	2464	C
1	1	2465	A
1	1	2466	A
1	1	2467	U
1	1	2468	C
1	1	2470	U
1	1	2473	A
1	1	2474	A
1	1	2475	G
1	1	2476	A
1	1	2479	A
1	1	2480	C
1	1	2482	C
1	1	2483	U
1	1	2484	U
1	1	2488	U
1	1	2501	A

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Mol	Chain	Res	Type
1	1	2506	C
1	1	2534	A
1	1	2547	G
1	1	2548	G
1	1	2588	G
1	1	2592	U
1	1	2596	A
1	1	2597	A
1	1	2613	A
1	1	2618	C
1	1	2622	U
1	1	2623	C
1	1	2639	U
1	1	2640	A
1	1	2641	A
1	1	2650	G
1	1	2652	C
1	1	2688	G
1	1	2690	C
1	1	2696	G
1	1	2705	G
1	1	2711	U
1	1	2730	A
1	1	2735	A
1	1	2736	U
1	1	2740	A
1	1	2746	G
1	1	2753	A
1	1	2779	U
1	1	2781	U
1	1	2785	C
1	1	2803	OMC
1	1	2807	G
1	1	2808	2MA
1	1	2810	G
1	1	2811	U
1	1	2823	A
1	1	2825	C
1	1	2834	G
1	1	2840	G
1	1	2871	A
1	1	2872	G

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Mol	Chain	Res	Type
1	1	2877	A
1	1	2878	C
1	1	2883	G
1	1	2887	G
1	1	2907	A
1	1	2908	G
1	1	2914	U
1	1	2915	U
1	1	2918	U
1	1	2920	U
1	1	2934	U
1	1	2935	A
1	1	2936	A
1	1	2937	A
1	1	2938	G
1	1	2939	C
1	1	2954	G
1	1	2955	C
1	1	2972	G
1	1	2988	A
1	1	2998	U
1	1	2999	A
1	1	3021	G
1	1	3023	G
1	1	3026	G
1	1	3035	A
1	1	3042	A
1	1	3050	A
1	1	3053	G
1	1	3058	U
1	1	3059	U
1	1	3067	A
1	1	3080	A
1	1	3114	C
1	1	3116	A
1	1	3142	G
1	1	3148	G
1	1	3153	A
1	1	3160	A
1	1	3161	C
1	1	3164	A
1	1	3166[A]	C

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Mol	Chain	Res	Type
1	1	3169	A
48	2	6	A
48	2	12	A
48	2	17	G
48	2	30	G
48	2	40	A
48	2	47	G
48	2	55	C
48	2	56	U
48	2	59	A
48	2	76	G
48	2	79	G
48	2	82	C
48	2	83	U
48	2	150	A
48	2	151	A
48	2	152	G
48	2	153	A
48	2	154	G
48	2	156	U
48	2	157	G
48	2	162	C
48	2	163	A
48	2	164	A
48	2	183	A
48	2	184	A
48	2	185	G
48	2	194	A
48	2	195	U
48	2	203	A
48	2	208	U
48	2	214	U
48	2	215	A
48	2	225	G
48	2	226	A
48	2	228	A
48	2	233	G
48	2	245	U
48	2	259	A
48	2	264	U
48	2	266	G
48	2	270	G

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Mol	Chain	Res	Type
48	2	285	G
48	2	286	C
48	2	288	G
48	2	298	A
48	2	308	G
48	2	317	U
48	2	318	U
48	2	319	C
48	2	325	A
48	2	347	C
48	2	351	G
48	2	363	A
48	2	364	C
48	2	365	G
48	2	366	G
48	2	370	G
48	2	371	C
48	2	373	G
48	2	386	U
48	2	391	C
48	2	392	A
48	2	416	A
48	2	420	U
48	2	425	G
48	2	430	A
48	2	432	G
48	2	440	A
48	2	441	U
48	2	443	C
48	2	444	C
48	2	450	U
48	2	459	U
48	2	467	G
48	2	469	G
48	2	470	C
48	2	471	G
48	2	479	G
48	2	480	A
48	2	484	G
48	2	492	G
48	2	494	A
48	2	495	G

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Mol	Chain	Res	Type
48	2	507	A
48	2	509	C
48	2	516	C
48	2	530	A
48	2	531	A
48	2	545	A
48	2	557	A
48	2	560	G
48	2	562	C
48	2	566	G
48	2	571	A
48	2	573	G
48	2	574	G
48	2	575	G
48	2	586	G
48	2	617	A
48	2	629	G
48	2	661	A
48	2	684	G
48	2	699	G
48	2	714	G
48	2	717	A
48	2	718	A
48	2	720	A
48	2	730	G
48	2	745	A
48	2	751	G
48	2	755	G
48	2	773	A
48	2	789	U
48	2	790	A
48	2	811	A
48	2	813	C
48	2	836	A
48	2	837	U
48	2	838	U
48	2	839	C
48	2	840	U
48	2	846	G
48	2	865	A
48	2	866	A
48	2	878	G

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Mol	Chain	Res	Type
48	2	893	A
48	2	907	A
48	2	919	G
48	2	924	C
48	2	926	G
48	2	927	C
48	2	928	A
48	2	932	G
48	2	953	U
48	2	962	A
48	2	964	G
48	2	968	A
48	2	969	G
48	2	970	A
48	2	985	U
48	2	986	G
48	2	987	A
48	2	999	G
48	2	1000	A
48	2	1007	A
48	2	1029	C
48	2	1030	U
48	2	1036	A
48	2	1037	C
48	2	1057	U
48	2	1065	U
48	2	1082	U
48	2	1086	G
48	2	1093	A
48	2	1116	G
48	2	1117	U
48	2	1118	U
48	2	1123	A
48	2	1125	A
48	2	1127	A
48	2	1129	G
48	2	1133	C
48	2	1135	A
48	2	1136	A
48	2	1137	G
48	2	1138	G
48	2	1139	A

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Mol	Chain	Res	Type
48	2	1140	G
48	2	1142	A
48	2	1380	U
48	2	1381	C
48	2	1382	C
48	2	1385	A
48	2	1386	A
48	2	1387	C
48	2	1388	A
48	2	1389	A
48	2	1395	A
48	2	1399	U
48	2	1422	U
48	2	1450	G
48	2	1459	A
48	2	1460	A
48	2	1475	U
48	2	1476	A
48	2	1477	U
48	2	1490	A
48	2	1501	A
48	2	1504	G
48	2	1511	A
48	2	1516	G
48	2	1521	G
48	2	1523	A
48	2	1542	A
48	2	1543	A
48	2	1561	A
48	2	1564	U
48	2	1582	C
48	2	1602	A
48	2	1615	G
48	2	1625	A
48	2	1632	G
48	2	1643	A
48	2	1647	G
48	2	1652	C
48	2	1660	A
48	2	1701	C
48	2	1702	G
48	2	1703	G

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Mol	Chain	Res	Type
48	2	1706	C
48	2	1707	A
48	2	1714	A
48	2	1719	G
48	2	1722	C
48	2	1723	U
48	2	1725	C
48	2	1727	G
48	2	1728	U
48	2	1731	A
48	2	1732	A
48	2	1735	C
48	2	1736	U
48	2	1743	A
48	2	1744	C
48	2	1745	A
48	2	1746	A
48	2	1749	A
48	2	1751	U
48	2	1753	U
48	2	1762	U
48	2	1763	U
48	2	1764	A
48	2	1768	A
48	2	1771	C
48	2	1774	A
48	2	1784	G
48	2	1801	A
48	2	1802	A
48	2	1803	G
48	2	1806	G
48	2	1812	A
48	2	1814	G
48	2	1815	U
48	2	1826	G
48	2	1828	MA6
48	2	1838	G
48	2	1839	G
48	2	1848	C
49	3	2	A
49	3	3	A
49	3	13	A

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Mol	Chain	Res	Type
49	3	15	G
49	3	23	G
49	3	26	A
49	3	37	U
49	3	44	C
49	3	46	G
49	3	53	A
49	3	55	A
49	3	56	U
49	3	59	G
49	3	65	G
49	3	66	U
49	3	67	C
49	3	68	U
49	3	69	U
49	3	70	G
49	3	72	G
49	3	87	A
49	3	90	G
49	3	91	U
49	3	106	C
49	3	118	A
50	5	3	C
50	5	5	G
50	5	14	A
50	5	15	A
50	5	17	U
50	5	18	G
50	5	19	G
50	5	21	C
50	5	22	A
50	5	23	A
50	5	31	G
50	5	41	C
50	5	48	U
50	5	58	G
50	5	60	A
50	5	65	G
50	5	66	U
50	5	70	C
50	5	71	G
51	6	2	A

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Mol	Chain	Res	Type
51	6	3	U

All (42) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	131	G
1	1	163	G
1	1	308	A
1	1	310	A
1	1	312	A
1	1	427	A
1	1	487	U
1	1	492	C
1	1	515	C
1	1	540	C
1	1	566	G
1	1	619	A
1	1	688	G
1	1	891	PSU
1	1	929	G
1	1	991	U
1	1	1100	U
1	1	1566	U
1	1	1598	C
1	1	1642	U
1	1	1923	A
1	1	2057	A
1	1	2059	C
1	1	2445	G
1	1	2461	G
1	1	2505	G
1	1	2617	U
1	1	2935	A
1	1	2998	U
48	2	225	G
48	2	491	G
48	2	493	A
48	2	998	A
48	2	1117	U
48	2	1701	C
48	2	1705	C
48	2	1706	C

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Mol	Chain	Res	Type
48	2	1726	U
48	2	1802	A
48	2	1814	G
49	3	12	U
51	6	2	A

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

17 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
1	OMG	1	2560	88,50,1	23,26,27	2.71	8 (34%)	33,38,41	3.05	12 (36%)
1	PSU	1	2762	1	18,21,22	4.23	7 (38%)	22,30,33	1.88	6 (27%)
1	2MA	1	2808	87,1	22,25,26	3.80	7 (31%)	33,37,40	2.18	10 (30%)
1	H2U	1	2754	1	18,21,22	0.50	0	21,30,33	1.00	1 (4%)
1	OMU	1	2857	87,1	19,22,23	2.99	8 (42%)	26,31,34	1.69	5 (19%)
1	PSU	1	891	87,1	18,21,22	4.35	8 (44%)	22,30,33	1.88	5 (22%)
48	G7M	2	525	48	23,26,27	2.60	9 (39%)	35,39,42	1.74	9 (25%)
48	2MG	2	1825	48	23,26,27	0.50	0	32,38,41	0.61	0
48	UR3	2	1807	48	19,22,23	0.28	0	26,32,35	0.64	0
1	PSU	1	2885	88,1	18,21,22	4.27	8 (44%)	22,30,33	1.89	6 (27%)
48	MA6	2	1827	48	23,26,27	1.34	3 (13%)	34,38,41	3.59	11 (32%)
1	PSU	1	2910	1	18,21,22	4.28	7 (38%)	22,30,33	1.80	5 (22%)
1	PSU	1	1105	1	18,21,22	4.27	7 (38%)	22,30,33	1.83	5 (22%)
1	OMC	1	2803	87,1	19,22,23	3.67	8 (42%)	26,31,34	0.81	0
48	MA6	2	1828	48	23,26,27	1.34	3 (13%)	34,38,41	3.57	11 (32%)
48	4OC	2	1664	48	20,23,24	0.35	0	26,32,35	0.48	0
1	5MU	1	2257	88,1	19,22,23	0.46	0	28,32,35	0.49	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	1	2560	88,50,1	-	1/9/27/28	0/3/3/3
1	PSU	1	2762	1	-	0/7/25/26	0/2/2/2
1	2MA	1	2808	87,1	-	2/7/25/26	0/3/3/3
1	H2U	1	2754	1	-	0/7/38/39	0/2/2/2
1	OMU	1	2857	87,1	-	0/9/27/28	0/2/2/2
1	PSU	1	891	87,1	-	3/7/25/26	0/2/2/2
48	G7M	2	525	48	-	1/7/25/26	0/3/3/3
48	2MG	2	1825	48	-	0/9/27/28	0/3/3/3
48	UR3	2	1807	48	-	0/7/25/26	0/2/2/2
1	PSU	1	2885	88,1	-	2/7/25/26	0/2/2/2
48	MA6	2	1827	48	-	0/11/29/30	0/3/3/3
1	PSU	1	2910	1	-	0/7/25/26	0/2/2/2
1	PSU	1	1105	1	-	0/7/25/26	0/2/2/2
1	OMC	1	2803	87,1	-	2/9/27/28	0/2/2/2
48	MA6	2	1828	48	-	1/11/29/30	0/3/3/3
48	4OC	2	1664	48	-	0/9/29/30	0/2/2/2
1	5MU	1	2257	88,1	-	0/7/25/26	0/2/2/2

All (83) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2808	2MA	C4-N3	12.19	1.49	1.34
1	1	891	PSU	C6-C5	11.29	1.48	1.35
1	1	1105	PSU	C6-C5	11.07	1.48	1.35
1	1	2910	PSU	C6-C5	11.04	1.48	1.35
1	1	2885	PSU	C6-C5	10.93	1.48	1.35
1	1	2762	PSU	C6-C5	10.88	1.48	1.35
1	1	891	PSU	C2-N1	8.65	1.48	1.36
1	1	2910	PSU	C2-N1	8.52	1.48	1.36
1	1	1105	PSU	C2-N1	8.48	1.48	1.36
1	1	2885	PSU	C2-N1	8.42	1.48	1.36
1	1	2762	PSU	C2-N1	8.39	1.48	1.36
1	1	2803	OMC	C4-N4	7.61	1.51	1.33
1	1	2560	OMG	C2-N2	7.55	1.52	1.34
1	1	891	PSU	C2-N3	7.38	1.50	1.37
1	1	2885	PSU	C2-N3	7.31	1.50	1.37
1	1	2910	PSU	C2-N3	7.31	1.50	1.37
1	1	1105	PSU	C2-N3	7.29	1.50	1.37
1	1	2762	PSU	C2-N3	7.20	1.49	1.37
1	1	2803	OMC	C2-N3	6.86	1.50	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2808	2MA	C2-N3	6.85	1.46	1.34
1	1	2803	OMC	C6-C5	6.82	1.50	1.35
1	1	2857	OMU	C2-N1	6.78	1.49	1.38
1	1	2857	OMU	C2-N3	6.73	1.50	1.38
48	2	525	G7M	C4-N3	6.33	1.49	1.34
1	1	2560	OMG	C4-N3	6.09	1.48	1.34
1	1	2857	OMU	C6-C5	5.70	1.48	1.35
1	1	2803	OMC	C2-N1	5.70	1.52	1.40
1	1	2808	2MA	C2-N1	5.68	1.44	1.34
1	1	2808	2MA	C6-N1	5.66	1.43	1.35
1	1	1105	PSU	C6-N1	5.60	1.45	1.36
1	1	2910	PSU	C6-N1	5.60	1.45	1.36
1	1	2762	PSU	C6-N1	5.50	1.45	1.36
1	1	891	PSU	C6-N1	5.49	1.45	1.36
1	1	2885	PSU	C6-N1	5.44	1.45	1.36
48	2	525	G7M	C2-N3	5.30	1.46	1.33
1	1	2560	OMG	C2-N3	5.28	1.45	1.33
1	1	2803	OMC	C4-N3	4.96	1.44	1.34
48	2	525	G7M	C2-N2	4.79	1.45	1.34
48	2	525	G7M	C5-N7	-4.73	1.33	1.39
1	1	2808	2MA	C5-C6	4.49	1.53	1.41
1	1	2803	OMC	O2-C2	-4.32	1.15	1.23
1	1	2857	OMU	C4-N3	3.99	1.45	1.38
1	1	2808	2MA	C6-N6	-3.96	1.24	1.34
1	1	2762	PSU	O2-C2	-3.88	1.15	1.23
1	1	2910	PSU	O2-C2	-3.84	1.15	1.23
1	1	2885	PSU	O2-C2	-3.83	1.15	1.23
1	1	2910	PSU	C4-N3	3.82	1.45	1.38
1	1	891	PSU	C4-N3	3.80	1.45	1.38
1	1	1105	PSU	C4-N3	3.78	1.45	1.38
1	1	891	PSU	O2-C2	-3.77	1.15	1.23
1	1	2762	PSU	C4-N3	3.76	1.45	1.38
1	1	1105	PSU	O2-C2	-3.76	1.15	1.23
48	2	525	G7M	C5-C6	3.75	1.53	1.43
1	1	2885	PSU	C4-N3	3.75	1.45	1.38
1	1	2803	OMC	C5-C4	3.67	1.51	1.42
1	1	2803	OMC	C6-N1	3.56	1.46	1.38
1	1	2885	PSU	O4-C4	-3.52	1.16	1.23
1	1	2762	PSU	O4-C4	-3.49	1.16	1.23
1	1	2910	PSU	O4-C4	-3.44	1.17	1.23
1	1	1105	PSU	O4-C4	-3.43	1.17	1.23
48	2	1828	MA6	C6-N6	3.40	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2560	OMG	C2-N1	3.39	1.46	1.37
1	1	2560	OMG	C6-N1	3.39	1.45	1.38
48	2	1827	MA6	C6-N6	3.37	1.46	1.36
1	1	891	PSU	O4-C4	-3.37	1.17	1.23
1	1	2808	2MA	C5-N7	-3.17	1.33	1.39
1	1	2857	OMU	O4-C4	-2.99	1.18	1.24
1	1	2857	OMU	C6-N1	2.84	1.44	1.38
1	1	2560	OMG	C5-N7	-2.79	1.33	1.39
48	2	525	G7M	C2-N1	2.60	1.44	1.37
1	1	2885	PSU	O4'-C1'	-2.59	1.40	1.43
48	2	525	G7M	O6-C6	-2.52	1.18	1.23
48	2	525	G7M	C6-N1	2.47	1.43	1.38
1	1	2857	OMU	O2-C2	-2.44	1.18	1.23
1	1	891	PSU	O4'-C1'	-2.34	1.40	1.43
48	2	1828	MA6	C5-N7	-2.30	1.34	1.39
1	1	2560	OMG	C5-C6	2.29	1.52	1.44
1	1	2857	OMU	C5-C4	2.23	1.48	1.43
48	2	1827	MA6	C5-C4	-2.22	1.34	1.39
48	2	1827	MA6	C5-N7	-2.19	1.34	1.39
48	2	1828	MA6	C5-C4	-2.17	1.35	1.39
48	2	525	G7M	C4-N9	-2.10	1.32	1.38
1	1	2560	OMG	C4-N9	-2.03	1.32	1.38

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	2	1827	MA6	N1-C6-N6	-14.80	100.90	117.08
48	2	1828	MA6	N1-C6-N6	-14.63	101.08	117.08
1	1	2560	OMG	C1'-N9-C8	-10.46	96.92	126.70
1	1	2560	OMG	C1'-N9-C4	9.45	154.57	126.50
48	2	1827	MA6	C5-C6-N6	7.56	138.47	125.30
48	2	1828	MA6	C5-C6-N6	7.46	138.30	125.30
1	1	2808	2MA	C5-C4-N3	-6.97	119.35	127.19
48	2	1828	MA6	N1-C2-N3	-5.50	120.00	128.60
48	2	1827	MA6	N1-C2-N3	-5.50	120.01	128.60
48	2	1827	MA6	N9-C8-N7	-5.36	106.59	113.91
1	1	2857	OMU	C4-N3-C2	-5.28	119.61	126.58
48	2	1828	MA6	N9-C8-N7	-5.24	106.75	113.91
48	2	1828	MA6	C5-C4-N3	-4.96	120.27	126.75
48	2	1827	MA6	C5-C4-N3	-4.77	120.52	126.75
1	1	891	PSU	C4-N3-C2	-4.65	119.64	126.34
1	1	2808	2MA	N3-C4-N9	4.54	133.29	126.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	2910	PSU	C4-N3-C2	-4.52	119.82	126.34
1	1	2762	PSU	C4-N3-C2	-4.48	119.88	126.34
1	1	2560	OMG	C5-C4-N3	-4.45	121.25	128.46
1	1	1105	PSU	C4-N3-C2	-4.44	119.95	126.34
1	1	891	PSU	N1-C2-N3	4.41	120.12	115.13
1	1	2885	PSU	C4-N3-C2	-4.34	120.08	126.34
1	1	2560	OMG	C2-N3-C4	4.32	120.00	112.30
48	2	525	G7M	C2-N3-C4	4.28	119.93	112.30
1	1	2762	PSU	N1-C2-N3	4.23	119.92	115.13
1	1	2808	2MA	N9-C8-N7	-4.19	108.18	113.91
1	1	2885	PSU	N1-C2-N3	4.16	119.84	115.13
1	1	1105	PSU	N1-C2-N3	4.12	119.80	115.13
1	1	2910	PSU	N1-C2-N3	4.01	119.68	115.13
1	1	2857	OMU	N3-C2-N1	3.94	120.11	114.89
48	2	525	G7M	C5-C6-N1	3.90	119.94	111.79
48	2	1827	MA6	C4-N9-C8	3.88	109.93	105.73
48	2	525	G7M	C5-C4-N3	-3.80	120.86	128.15
48	2	1828	MA6	C4-N9-C8	3.67	109.70	105.73
48	2	1828	MA6	N3-C4-N9	3.49	132.84	127.08
48	2	1828	MA6	C2-N3-C4	3.46	119.93	111.75
48	2	1827	MA6	C2-N1-C6	3.44	119.88	111.75
48	2	1828	MA6	C2-N1-C6	3.42	119.83	111.75
48	2	1827	MA6	C2-N3-C4	3.40	119.78	111.75
48	2	525	G7M	O6-C6-C5	-3.38	120.42	128.06
1	1	2857	OMU	C5-C4-N3	3.36	119.87	114.84
48	2	1827	MA6	C5-N7-C8	3.36	108.28	103.51
48	2	1828	MA6	C5-N7-C8	3.35	108.27	103.51
48	2	1827	MA6	N3-C4-N9	3.35	132.60	127.08
1	1	2560	OMG	N9-C8-N7	-3.34	107.11	113.39
1	1	891	PSU	C6-C5-C4	3.33	120.52	118.20
1	1	2885	PSU	C6-N1-C2	-3.28	119.33	122.68
1	1	2762	PSU	C6-C5-C4	3.19	120.43	118.20
1	1	2754	H2U	C5-C4-N3	-3.13	113.13	116.65
1	1	2808	2MA	C5-N7-C8	3.13	107.96	103.51
48	2	1828	MA6	C4-C5-C6	3.10	119.35	115.88
1	1	2808	2MA	N3-C2-N1	-3.06	120.10	125.72
1	1	2762	PSU	C6-N1-C2	-3.04	119.58	122.68
1	1	891	PSU	C6-N1-C2	-3.03	119.58	122.68
1	1	2560	OMG	C2-N1-C6	-3.01	119.61	125.10
1	1	1105	PSU	C6-N1-C2	-2.99	119.62	122.68
48	2	525	G7M	N9-C4-N3	2.98	131.92	125.94
48	2	1827	MA6	C4-C5-C6	2.95	119.18	115.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	1105	PSU	C6-C5-C4	2.94	120.25	118.20
1	1	2885	PSU	C6-C5-C4	2.92	120.24	118.20
1	1	2808	2MA	C4-N9-C1'	-2.84	119.83	126.59
48	2	525	G7M	C2-N1-C6	-2.82	119.96	125.10
1	1	2910	PSU	C6-C5-C4	2.82	120.17	118.20
1	1	2910	PSU	C6-N1-C2	-2.76	119.86	122.68
1	1	2857	OMU	O4-C4-C5	-2.68	120.45	125.16
1	1	2560	OMG	C5-C6-N1	2.67	119.98	113.19
1	1	2885	PSU	O2-C2-N1	-2.57	119.96	122.79
1	1	2762	PSU	O2-C2-N1	-2.53	120.00	122.79
1	1	1105	PSU	O2-C2-N1	-2.48	120.06	122.79
1	1	2560	OMG	O6-C6-C5	-2.45	120.11	126.60
1	1	891	PSU	O2-C2-N1	-2.39	120.16	122.79
1	1	2808	2MA	C6-C5-C4	2.37	120.36	117.18
1	1	2560	OMG	C8-N7-C5	2.35	108.49	104.24
48	2	525	G7M	C1'-N9-C4	-2.30	119.68	126.50
1	1	2885	PSU	O4'-C1'-C2'	2.26	108.33	105.14
1	1	2910	PSU	O2-C2-N1	-2.25	120.31	122.79
1	1	2808	2MA	C4-N9-C8	2.22	108.14	105.73
1	1	2560	OMG	N2-C2-N1	2.20	121.40	116.71
1	1	2560	OMG	N9-C4-N3	2.20	130.35	125.94
48	2	525	G7M	CN7-N7-C5	2.19	129.49	126.77
1	1	2808	2MA	N6-C6-N1	2.19	120.12	117.03
1	1	2808	2MA	C1'-N9-C8	2.17	132.04	127.14
1	1	2762	PSU	O4'-C1'-C2'	2.16	108.20	105.14
48	2	525	G7M	N9-C8-N7	-2.16	106.86	112.21
1	1	2560	OMG	C4-C5-N7	-2.04	107.49	110.72
1	1	2857	OMU	O2-C2-N1	-2.03	120.08	122.79

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	891	PSU	C2'-C1'-C5-C6
1	1	2560	OMG	C1'-C2'-O2'-CM2
1	1	2808	2MA	O4'-C4'-C5'-O5'
1	1	2808	2MA	C3'-C4'-C5'-O5'
1	1	2885	PSU	O4'-C4'-C5'-O5'
1	1	2803	OMC	O4'-C4'-C5'-O5'
48	2	525	G7M	C3'-C4'-C5'-O5'
48	2	1828	MA6	C4'-C5'-O5'-P
1	1	891	PSU	O4'-C1'-C5-C4

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Mol	Chain	Res	Type	Atoms
1	1	891	PSU	O4'-C1'-C5-C6
1	1	2885	PSU	C3'-C4'-C5'-O5'
1	1	2803	OMC	C3'-C4'-C5'-O5'

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1	2560	OMG	1	0
48	2	1827	MA6	1	0
1	1	2803	OMC	1	0
48	2	1664	4OC	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 435 ligands modelled in this entry, 433 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
91	ATP	W	502	87	29,33,33	0.33	0	44,52,52	0.54	1 (2%)
89	CLM	1	3238	-	19,20,20	0.54	0	23,27,27	0.86	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
91	ATP	W	502	87	-	1/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
89	CLM	1	3238	-	-	4/20/22/22	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
89	1	3238	CLM	O5-C5-C3	2.18	113.83	107.99
91	W	502	ATP	PB-O3B-PG	2.04	139.82	132.83

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
89	1	3238	CLM	CL1-C1-C2-N2
89	1	3238	CLM	CL2-C1-C2-O2
89	1	3238	CLM	CL2-C1-C2-N2
89	1	3238	CLM	CL1-C1-C2-O2
91	W	502	ATP	PA-O3A-PB-O2B

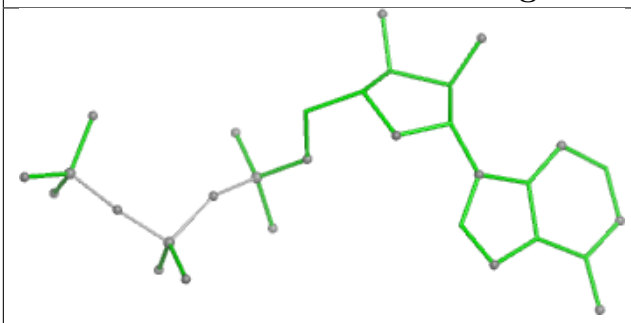
There are no ring outliers.

1 monomer is involved in 1 short contact:

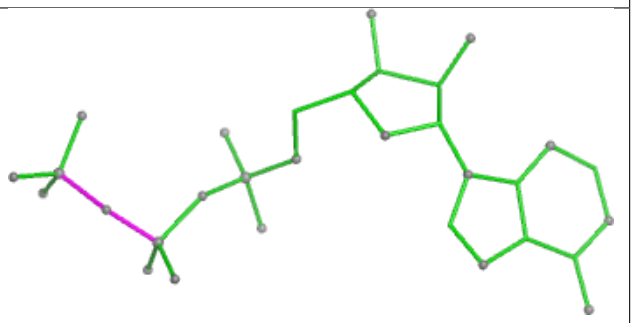
Mol	Chain	Res	Type	Clashes	Symm-Clashes
89	1	3238	CLM	1	0

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 then 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.

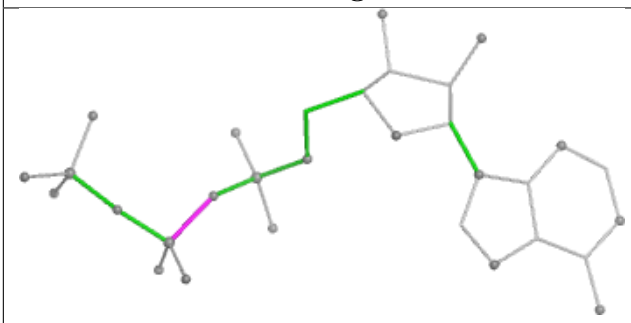
Ligand ATP W 502



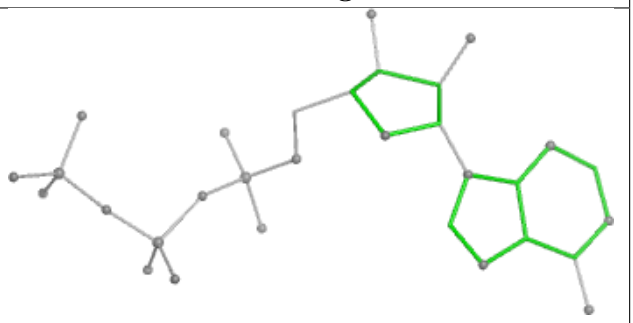
Bond lengths



Bond angles

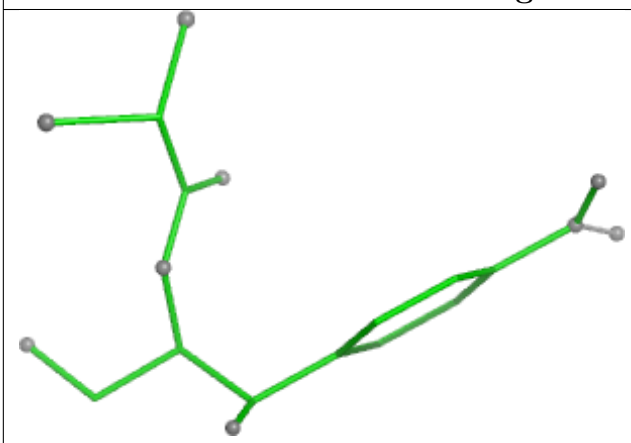


Torsions

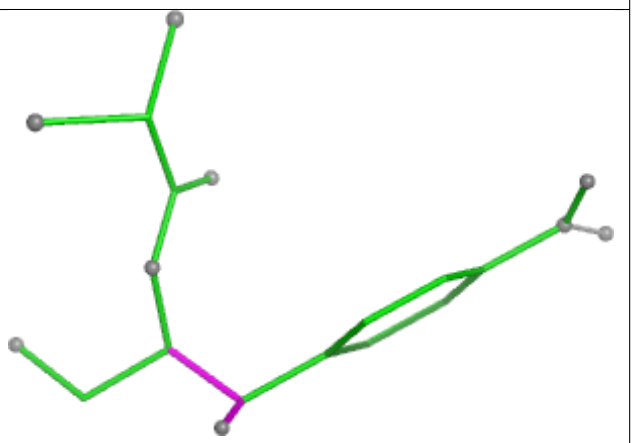


Rings

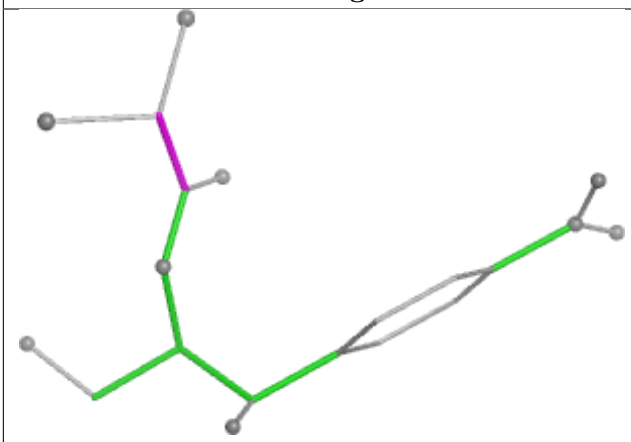
Ligand CLM 1 3238



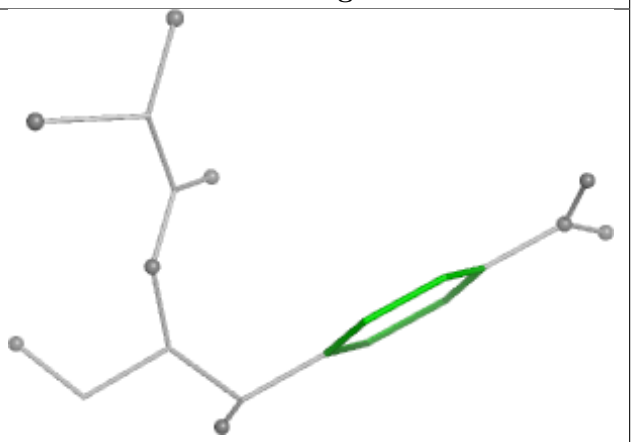
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	1	11
48	2	2
3	1C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1C	256:LEU	C	298:ALA	N	38.94
1	1	261:G	O3'	270:A	P	27.38
1	1	295:U	O3'	307:A	P	27.27
1	1	1704:U	O3'	1831:A	P	17.63
1	1	363:A	O3'	405:U	P	17.03
1	1	1028:G	O3'	1041:C	P	16.79
1	1	283:A	O3'	288:U	P	16.60
1	1	2613:A	O3'	2617:U	P	15.89
1	1	323:U	O3'	330:A	P	15.50
1	2	137:A	O3'	142:U	P	14.76
1	1	1664:A	O3'	1667:C	P	12.35
1	1	2509:C	O3'	2528:G	P	9.64
1	2	1842:U	O3'	1845:A	P	7.75
1	1	859:U	O3'	861:A	P	3.85

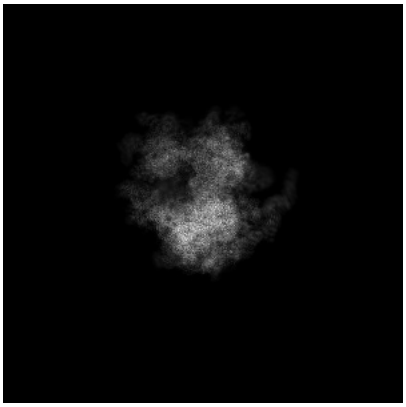
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-56210. These allow visual inspection of the internal detail of the map and identification of artifacts.

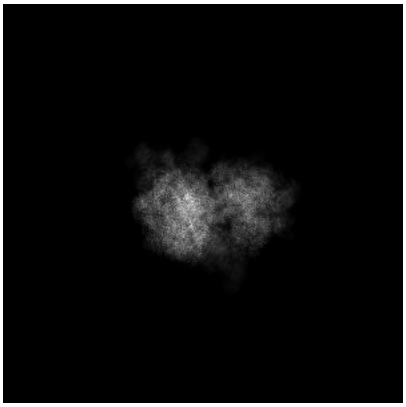
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

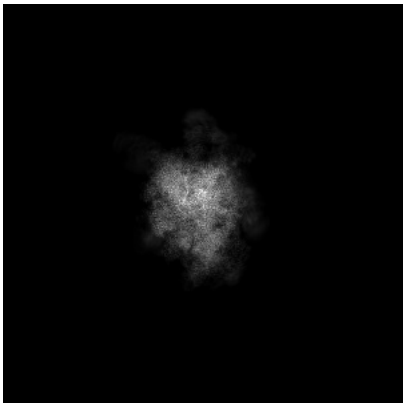
6.1.1 Primary map



X



Y



Z

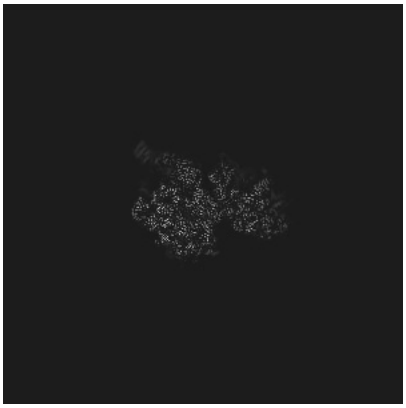
The images above show the map projected in three orthogonal directions.

6.2 Central slices

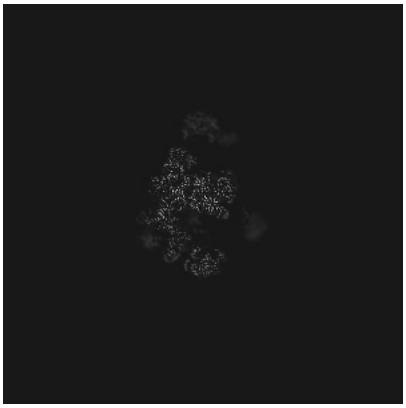
6.2.1 Primary map



X Index: 378



Y Index: 378

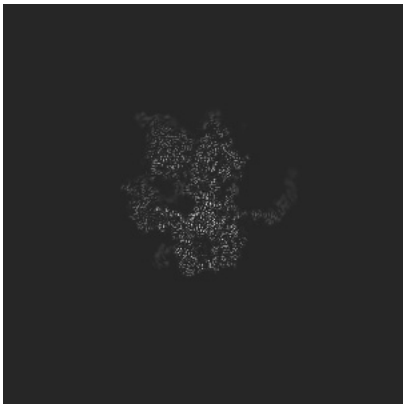


Z Index: 378

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

6.3 Largest variance slices (i)

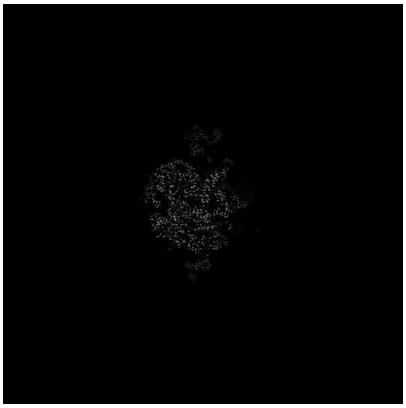
6.3.1 Primary map



X Index: 381



Y Index: 400

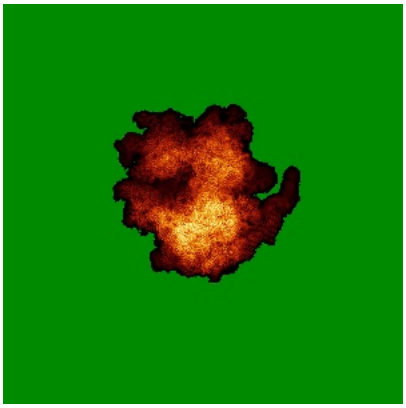


Z Index: 341

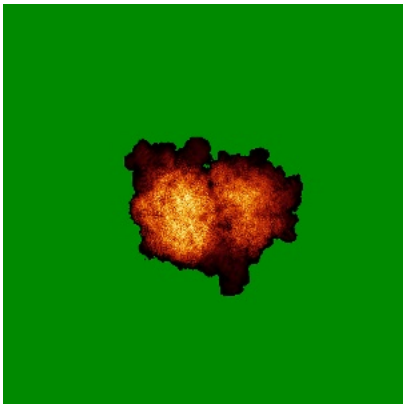
The images above show the largest variance slices of the map in three orthogonal directions.

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

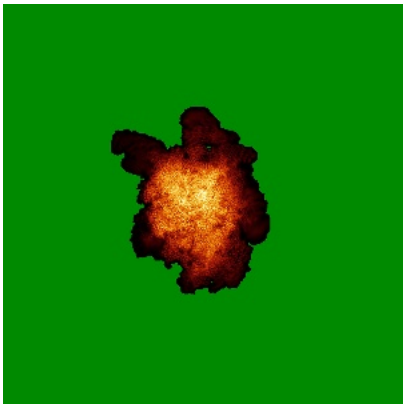
6.4.1 Primary map



X



Y

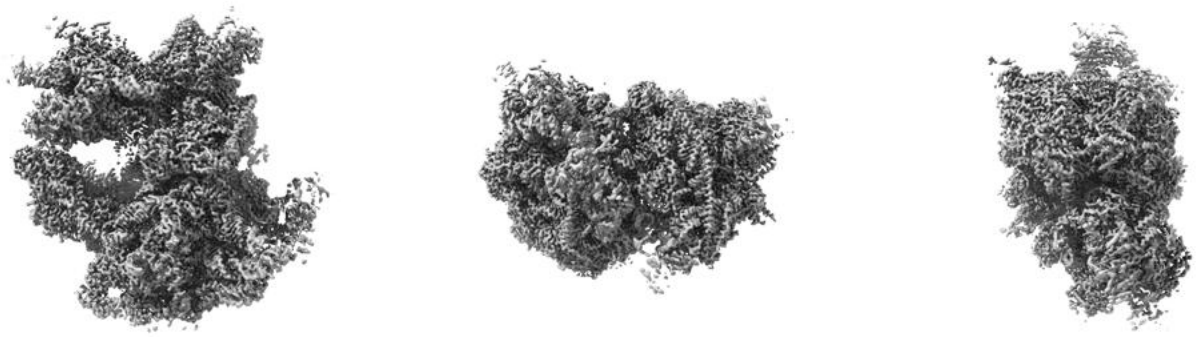


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

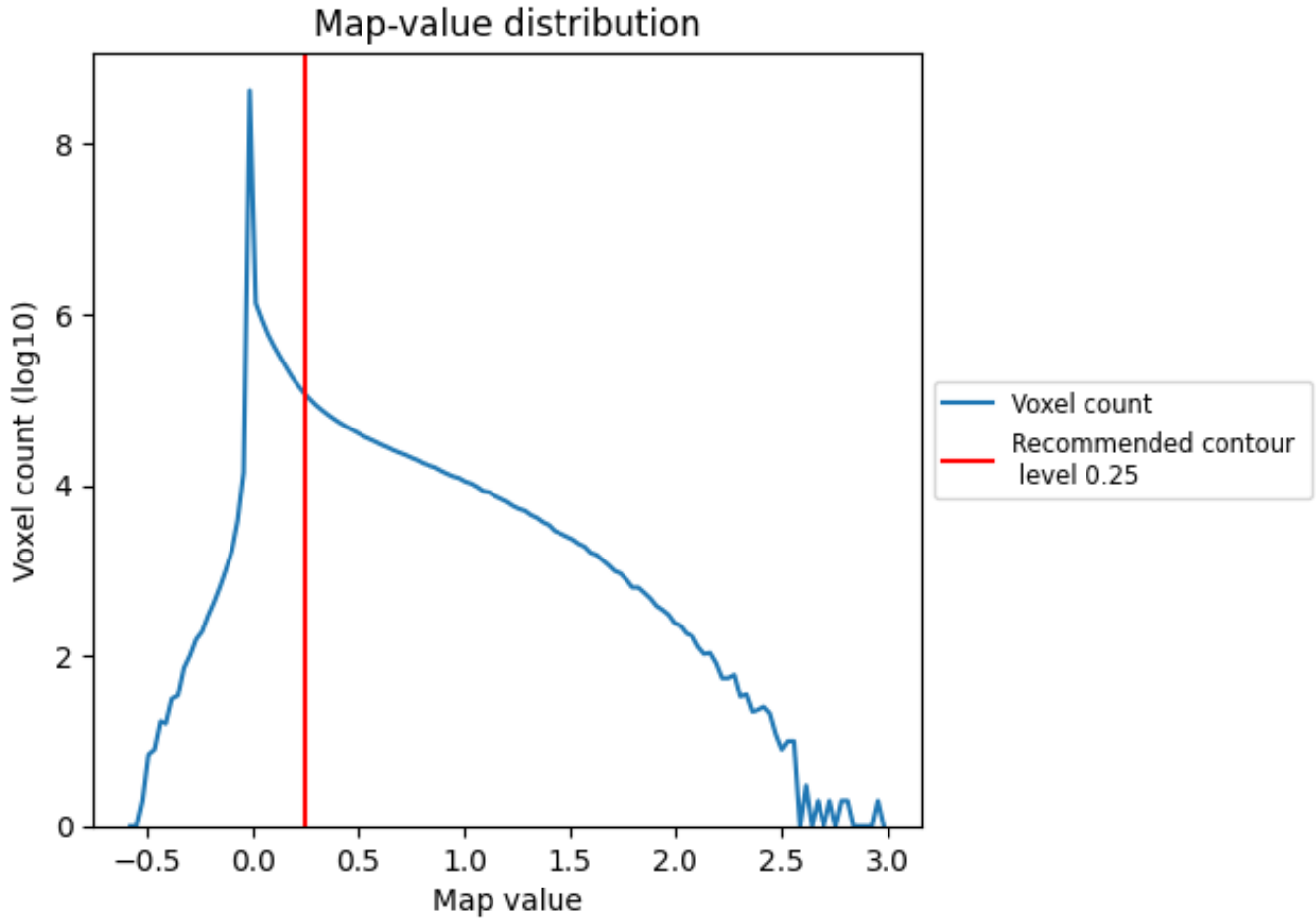
6.6 Mask visualisation (i)

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

7 Map analysis

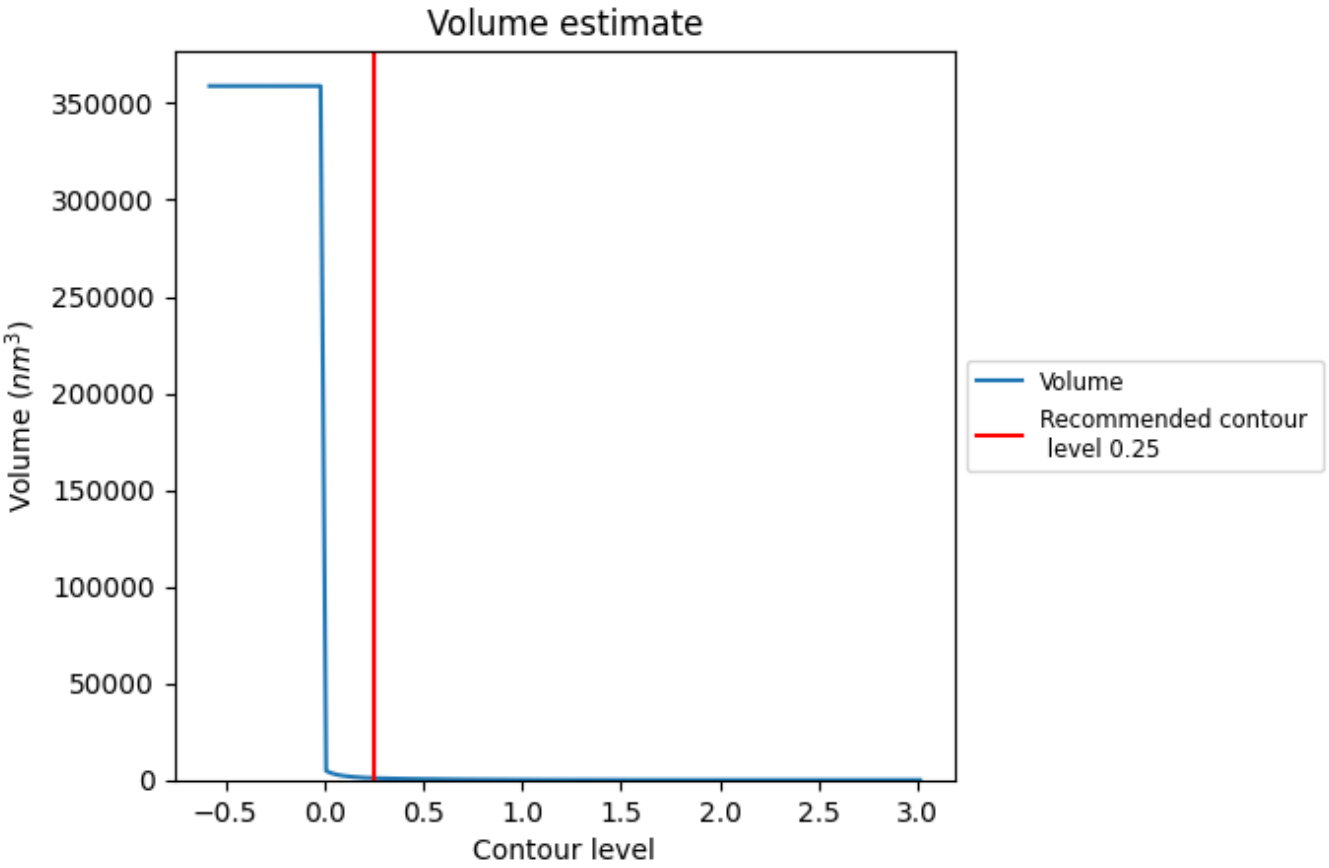
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

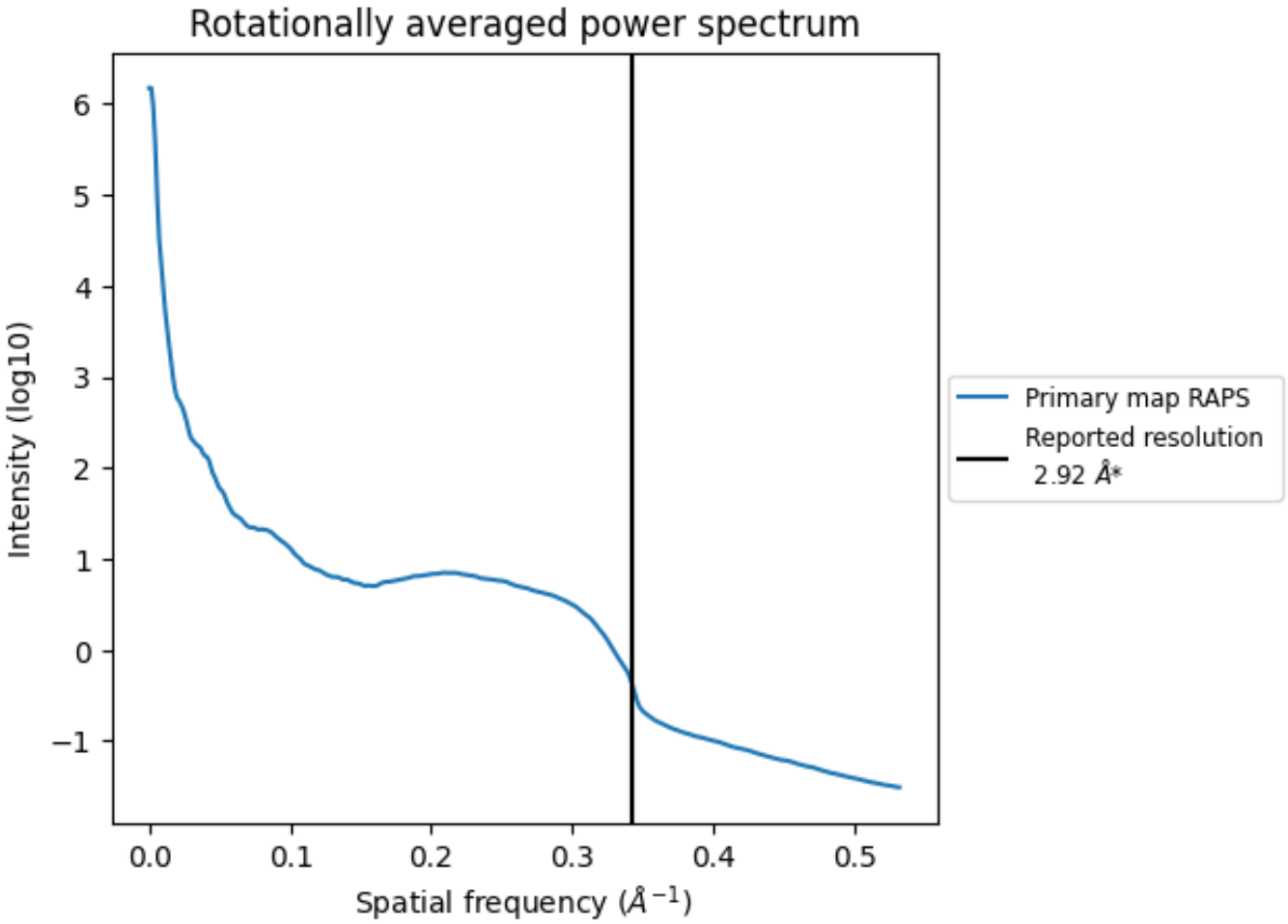
7.2 Volume estimate



The volume at the recommended contour level is 973 nm^3; this corresponds to an approximate mass of 879 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 (i)



*Reported resolution corresponds to spatial frequency of 0.342 Å^{-1}

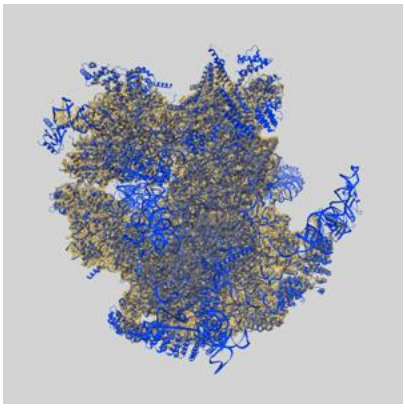
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

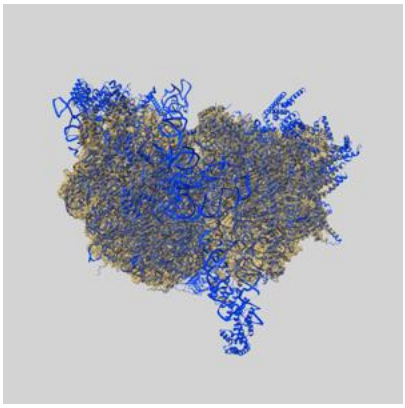
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-56210 and PDB model 9TS7. Per-residue inclusion information can be found in section 3 on page 26.

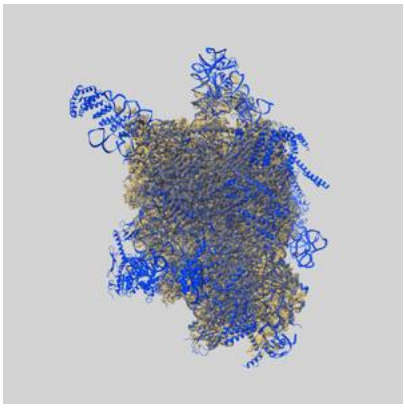
9.1 Map-model overlay



X



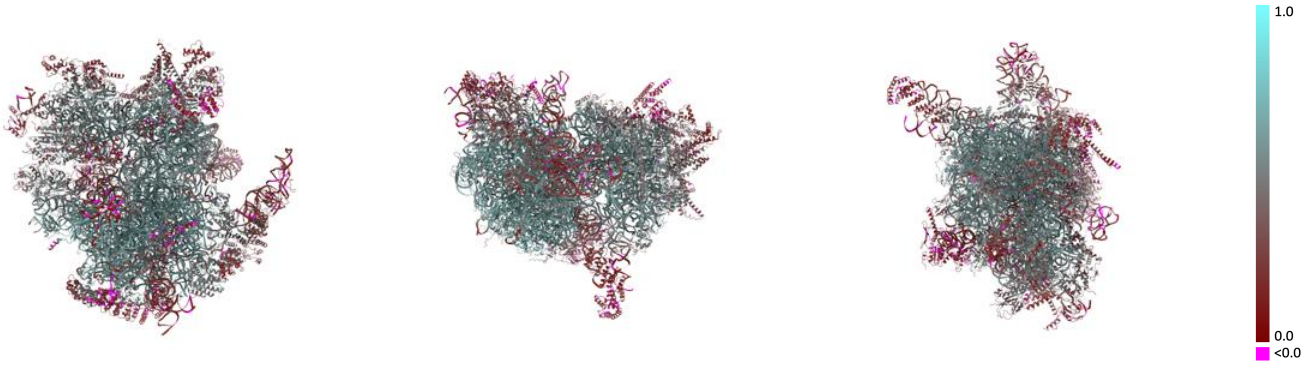
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.25 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.

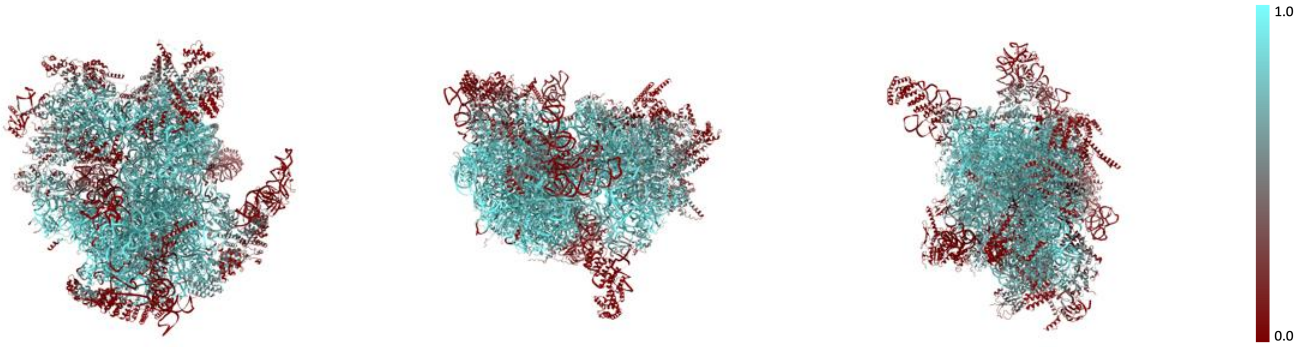
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

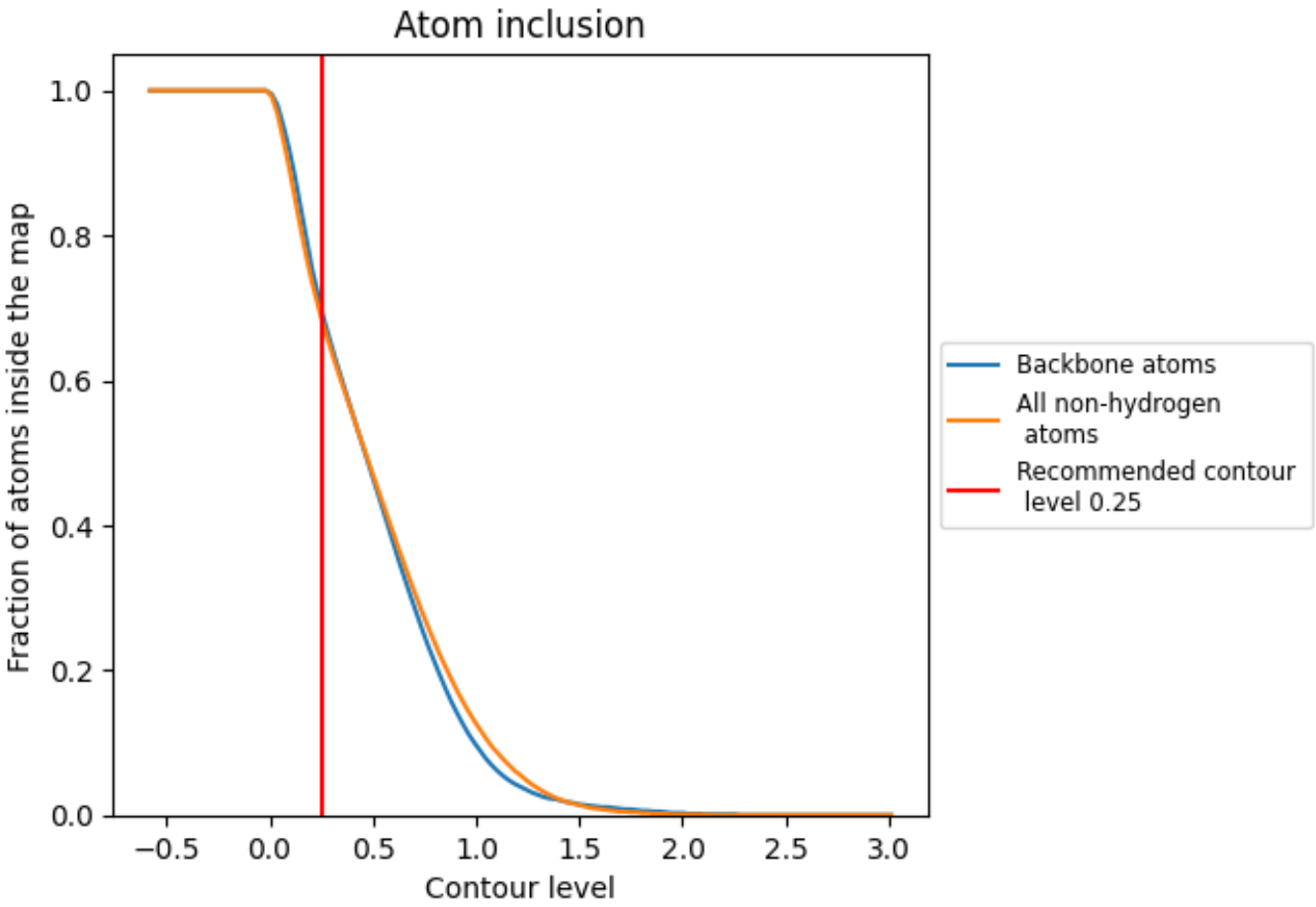
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.25).

9.4 Atom inclusion (i)



At the recommended contour level, 70% of all backbone atoms, 69% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6860	0.4890
1	0.8060	0.5440
1B	0.8580	0.5940
1C	0.4200	0.3750
1D	0.9010	0.6180
1E	0.9120	0.6130
1F	0.6170	0.4810
1G	0.0930	0.3380
1H	0.6200	0.4290
1I	0.0000	0.0750
1J	0.0000	0.0820
1K	0.8380	0.5690
1L	0.8770	0.6100
1M	0.8990	0.5970
1N	0.5710	0.4800
1O	0.9390	0.6250
1P	0.8440	0.5730
1Q	0.8600	0.5920
1R	0.9600	0.6380
1S	0.8750	0.5900
1T	0.9070	0.6120
1U	0.8070	0.5730
1V	0.8590	0.5900
1W	0.0190	0.1730
1X	0.6140	0.4820
1Y	0.8290	0.5560
1Z	0.5330	0.4220
1a	0.8860	0.6010
1b	0.8920	0.6110
1c	0.6810	0.4920
1d	0.9510	0.6330
1e	0.8040	0.5760
1f	0.9830	0.6560
1g	0.9220	0.6190
1h	0.6690	0.5430



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Chain	Atom inclusion	Q-score
1i	0.5320	0.4340
1j	0.9120	0.6130
1k	0.9110	0.6090
1l	0.4690	0.4030
1m	0.0040	0.1270
1o	0.0000	0.1090
1p	0.7810	0.5550
1q	0.8840	0.5870
1r	0.7690	0.5380
1s	0.7720	0.5460
1t	0.4160	0.3660
1u	0.1810	0.2740
1v	0.5150	0.4140
2	0.8500	0.5440
3	0.9050	0.5630
5	0.1900	0.3050
6	0.4810	0.4520
A	0.7270	0.5180
B	0.4490	0.3910
C	0.7220	0.5010
D	0.5970	0.4490
E	0.8220	0.5630
F	0.0610	0.2700
G	0.8990	0.5920
H	0.5600	0.4210
I	0.7730	0.5460
J	0.6540	0.4790
K	0.7750	0.5430
L	0.6520	0.4760
M	0.8100	0.5500
N	0.7910	0.5410
O	0.9070	0.5880
P	0.7890	0.5520
Q	0.7420	0.5210
R	0.3080	0.3070
S	0.5310	0.4400
T	0.8510	0.5750
U	0.2830	0.2860
V	0.6070	0.4510
W	0.5350	0.4350
X	0.4240	0.3610
Y	0.5960	0.4680

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Chain	Atom inclusion	Q-score
Z	0.4660	0.4040
a	0.3900	0.3640
b	0.0050	0.1870
c	0.7180	0.5490
d	0.6480	0.4830
e	0.7550	0.5150
f	0.4800	0.3950
h	0.0130	0.1620
i	0.1520	0.2030
k	0.0420	0.2250