



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 04:17 AM UTC

PDB ID : 6HCM / pdb_00006hcm
EMDB ID : EMD-0195
Title : Structure of the rabbit collided di-ribosome (stalled monosome)
Authors : Juskiewicz, S.; Chandrasekaran, V.; Lin, Z.; Kraatz, S.; Ramakrishnan, V.; Hegde, R.S.
Deposited on : 2018-08-15
Resolution : 6.80 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

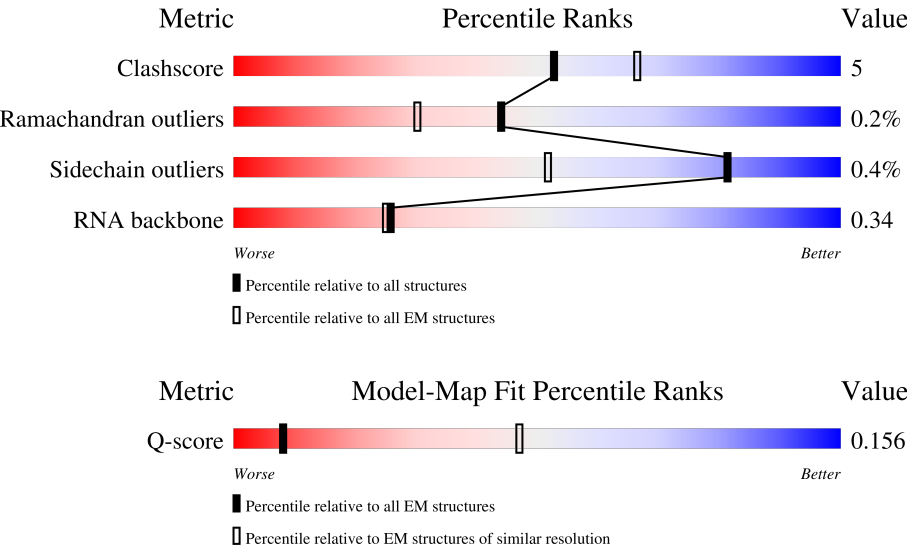
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance i

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

The reported resolution of this entry is 6.80 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	503 (6.30 - 7.30)

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

Mol	Chain	Length	Quality of chain
1	A1	1869	25% 57% 32% 7%
2	B1	295	66% 7% 26%
3	C1	264	39% 67% 14% 19%

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Mol	Chain	Length	Quality of chain
4	D1	293	
5	E1	243	
6	F1	263	
7	G1	204	
8	H1	249	
9	I1	194	
10	J1	208	
11	K1	194	
12	L1	165	
13	M1	158	
14	N1	132	
15	O1	151	
16	P1	168	
17	Q1	145	
18	R1	146	
19	S1	135	
20	T1	152	
21	U1	145	
22	V1	119	
23	W1	83	
24	X1	130	
25	Y1	143	
26	Z1	130	
27	a1	125	
28	b1	115	

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Mol	Chain	Length	Quality of chain
29	c1	84	
30	d1	69	
31	e1	56	
32	f1	133	
33	g1	156	
34	h1	317	
35	j1	439	
36	k1	599	
37	52	3634	
38	72	120	
39	82	156	
40	A3	257	
41	B3	403	
42	C3	425	
43	E3	291	
44	F3	247	
45	H3	192	
46	L3	211	
47	M3	218	
48	N3	204	
49	O3	203	
50	P3	184	
51	Q3	188	
52	R3	196	
53	S3	176	

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Mol	Chain	Length	Quality of chain
54	T3	160	
55	U3	128	
56	V3	140	
57	W3	157	
58	X3	156	
59	Y3	145	
60	Z3	136	
61	a3	148	
62	b3	245	
63	c3	115	
64	d3	125	
65	e3	134	
66	f3	110	
67	g3	117	
68	h3	123	
69	i3	105	
70	j3	97	
71	k3	70	
72	l3	51	
73	m3	102	
74	n3	25	
75	o3	106	
76	p3	92	
77	r3	137	
78	s3	318	

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Mol	Chain	Length	Quality of chain
79	t3	165	
80	23	76	
81	w3	23	
82	J3	178	
83	G3	319	
84	D3	297	
85	I3	214	
86	1	22	
87	u3	217	

2 Entry composition [i](#)

There are 91 unique types of molecules in this entry. The entry contains 226754 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 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A1	1732	Total	C	N	O	P	0	0
			36969	16502	6637	12099	1731		

- Molecule 2 is a protein called uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B1	217	Total	C	N	O	S	0	0
			1710	1086	300	316	8		

- Molecule 3 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C1	213	Total	C	N	O	S	0	0
			1729	1098	309	308	14		

- Molecule 4 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D1	221	Total	C	N	O	S	0	0
			1716	1111	295	301	9		

- Molecule 5 is a protein called uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E1	228	Total	C	N	O	S	0	0
			1768	1126	318	316	8		

- Molecule 6 is a protein called eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F1	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 7 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G1	185	Total	C	N	O	S	0	0
			1471	921	277	266	7		

- Molecule 8 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H1	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 9 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I1	185	Total	C	N	O	S	0	0
			1488	952	271	264	1		

- Molecule 10 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J1	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

- Molecule 11 is a protein called Ribosomal protein S9 (Predicted).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K1	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 12 is a protein called eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L1	96	Total	C	N	O	S	0	0
			810	530	143	131	6		

- Molecule 13 is a protein called Ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M1	143	Total	C	N	O	S	0	0
			1175	749	222	198	6		

- Molecule 14 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N1	117	Total	C	N	O	S	0	0
			908	570	161	169	8		

- Molecule 15 is a protein called uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O1	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 16 is a protein called uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P1	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

- Molecule 17 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q1	120	Total	C	N	O	S	0	0
			997	635	187	168	7		

- Molecule 18 is a protein called Ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R1	142	Total	C	N	O	S	0	0
			1128	717	213	195	3		

- Molecule 19 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S1	132	Total	C	N	O	S	0	0
			1068	670	199	195	4		

- Molecule 20 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T1	144	Total	C	N	O	S	0	0
			1190	746	241	202	1		

- Molecule 21 is a protein called eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U1	141	Total	C	N	O	S	0	0
			1097	688	211	195	3		

- Molecule 22 is a protein called uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V1	100	Total	C	N	O	S	0	0
			795	498	152	141	4		

- Molecule 23 is a protein called eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W1	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

- Molecule 24 is a protein called Ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X1	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 25 is a protein called uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y1	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 26 is a protein called eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z1	124	Total	C	N	O	S	0	0
			1011	640	198	168	5		

- Molecule 27 is a protein called eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a1	75	Total	C	N	O	S	0	0
			598	382	111	104	1		

- Molecule 28 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b1	101	Total	C	N	O	S	0	0
			814	507	170	132	5		

- Molecule 29 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c1	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 30 is a protein called Ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d1	62	Total	C	N	O	S	0	0
			488	297	97	92	2		

- Molecule 31 is a protein called uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e1	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 32 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f1	55	Total	C	N	O	S	0	0
			443	274	97	71	1		

- Molecule 33 is a protein called Ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g1	68	Total	C	N	O	S	0	0
			555	351	103	94	7		

- Molecule 34 is a protein called RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	h1	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 35 is a protein called eRF1(AAQ).

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j1	419	Total	C	N	O	S	0	0
			3309	2106	562	629	12		

- Molecule 36 is a protein called ATP binding cassette subfamily E member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k1	577	Total	C	N	O	S	0	0
			4555	2914	780	830	31		

- Molecule 37 is a RNA chain called 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	52	3634	Total	C	N	O	P	0	0
			77819	34651	14241	25293	3634		

- Molecule 38 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	72	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 39 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	82	151	Total	C	N	O	P	0	0
			3208	1432	564	1062	150		

- Molecule 40 is a protein called Ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	A3	248	Total	C	N	O	S	0	0
			1898	1189	389	314	6		

- Molecule 41 is a protein called uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	B3	394	Total	C	N	O	S	0	0
			3172	2020	597	542	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B3	1	MET	-	initiating methionine	UNP G1TL06

- Molecule 42 is a protein called uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	C3	362	Total	C	N	O	S	0	0
			2883	1812	577	480	14		

- Molecule 43 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	E3	216	Total	C	N	O	S	0	0
			1729	1115	329	282	3		

- Molecule 44 is a protein called uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	F3	225	Total	C	N	O	S	0	0
			1875	1205	358	303	9		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F3	61	ARG	GLY	conflict	UNP G1TUB1
F3	93	ARG	GLY	conflict	UNP G1TUB1
F3	131	MET	VAL	conflict	UNP G1TUB1
F3	153	ILE	VAL	conflict	UNP G1TUB1

- Molecule 45 is a protein called uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	H3	190	Total	C	N	O	S	0	0
			1516	954	284	272	6		

- Molecule 46 is a protein called eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	L3	210	Total	C	N	O	S	0	0
			1702	1065	354	279	4		

- Molecule 47 is a protein called Ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	M3	138	Total	C	N	O	S	0	0
			1137	727	221	182	7		

- Molecule 48 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	N3	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 49 is a protein called uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	O3	199	Total	C	N	O	S	0	0
			1630	1051	319	255	5		

- Molecule 50 is a protein called uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	P3	153	Total	C	N	O	S	0	0
			1242	777	241	215	9		

- Molecule 51 is a protein called eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Q3	187	Total	C	N	O	S	0	0
			1515	946	315	250	4		

- Molecule 52 is a protein called eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	R3	180	Total	C	N	O	S	0	0
			1508	933	328	238	9		

- Molecule 53 is a protein called eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	S3	176	Total	C	N	O	S	0	0
			1462	930	285	236	11		

- Molecule 54 is a protein called eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	T3	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 55 is a protein called eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	U3	99	Total	C	N	O	S	0	0
			809	519	141	147	2		

- Molecule 56 is a protein called Ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	V3	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 57 is a protein called eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	W3	106	Total	C	N	O	S	0	0
			860	538	174	144	4		

- Molecule 58 is a protein called uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	X3	118	Total	C	N	O	S	0	0
			967	618	181	167	1		

- Molecule 59 is a protein called Ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Y3	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 60 is a protein called eL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	Z3	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 61 is a protein called uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	a3	147	Total	C	N	O	S	0	0
			1162	734	239	185	4		

- Molecule 62 is a protein called eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	b3	104	Total	C	N	O	S	0	0
			848	527	189	129	3		

- Molecule 63 is a protein called eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	c3	98	Total	C	N	O	S	0	0
			761	481	134	140	6		

- Molecule 64 is a protein called eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	d3	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 65 is a protein called eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	e3	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 66 is a protein called eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	f3	109	Total	C	N	O	S	0	0
			876	555	174	143	4		

- Molecule 67 is a protein called eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	g3	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 68 is a protein called uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	h3	122	Total	C	N	O	S	0	0
			1013	640	204	168	1		

- Molecule 69 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	i3	102	Total	C	N	O	S	0	0
			830	520	176	129	5		

- Molecule 70 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	j3	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 71 is a protein called eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	k3	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 72 is a protein called eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	l3	50	Total	C	N	O	S	0	0
			447	286	96	64	1		

- Molecule 73 is a protein called eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	m3	52	Total	C	N	O	S	0	0
			429	266	90	67	6		

- Molecule 74 is a protein called eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	n3	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

- Molecule 75 is a protein called eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	o3	104	Total	C	N	O	S	0	0
			851	533	174	138	6		

- Molecule 76 is a protein called eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	p3	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 77 is a protein called eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	r3	124	Total	C	N	O	S	0	0
			994	616	205	167	6		

- Molecule 78 is a protein called uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	s3	196	Total	C	N	O	S	0	0
			1507	959	263	276	9		

- Molecule 79 is a protein called Ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	t3	153	Total	C	N	O	S	0	0
			1160	722	218	217	3		

- Molecule 80 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	23	76	Total	C	N	O	P	0	0
			1616	723	291	527	75		

- Molecule 81 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	w3	23	Total	C	N	O	P	0	0
			493	222	94	154	23		

- Molecule 82 is a protein called Ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	J3	170	Total	C	N	O	S	0	0
			1362	861	254	241	6		

- Molecule 83 is a protein called eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	G3	233	Total	C	N	O	S	0	0
			1879	1199	361	315	4		

- Molecule 84 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	D3	293	Total	C	N	O	S	0	0
			2391	1512	438	427	14		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D3	1	MET	-	initiating methionine	UNP G1SYJ6

- Molecule 85 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	I3	205	Total	C	N	O	S	0	0
			1664	1056	321	274	13		

- Molecule 86 is a protein called nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
86	1	22	Total	C	N	O	0	0
			110	66	22	22		

- Molecule 87 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	u3	217	Total	C	N	O	S	0	0
			1741	1113	312	307	9		

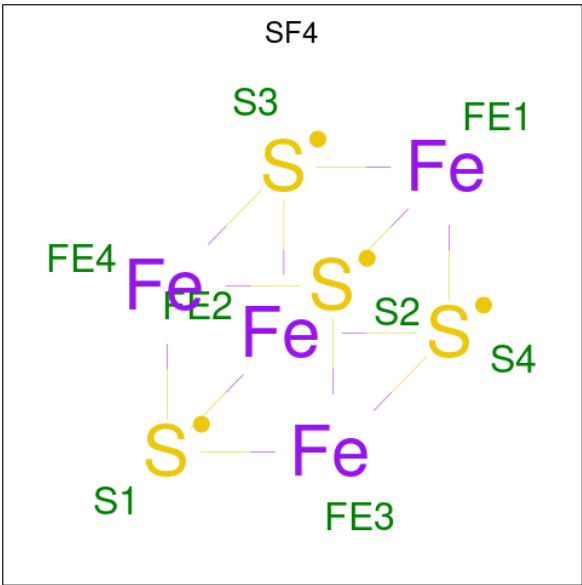
- Molecule 88 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
88	A1	77	Total 77	Mg 77	0
88	G1	1	Total 1	Mg 1	0
88	M1	1	Total 1	Mg 1	0
88	52	204	Total 204	Mg 204	0
88	72	7	Total 7	Mg 7	0
88	82	5	Total 5	Mg 5	0
88	P3	1	Total 1	Mg 1	0
88	V3	1	Total 1	Mg 1	0
88	a3	1	Total 1	Mg 1	0
88	g3	1	Total 1	Mg 1	0
88	w3	1	Total 1	Mg 1	0

- Molecule 89 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
89	b1	1	Total 1	Zn 1	0
89	e1	1	Total 1	Zn 1	0
89	g1	1	Total 1	Zn 1	0
89	g3	1	Total 1	Zn 1	0
89	j3	1	Total 1	Zn 1	0
89	m3	1	Total 1	Zn 1	0
89	o3	1	Total 1	Zn 1	0
89	p3	1	Total 1	Zn 1	0

- Molecule 90 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			AltConf
90	k1	1	Total	Fe	S	0
			8	4	4	
90	k1	1	Total	Fe	S	0
			8	4	4	

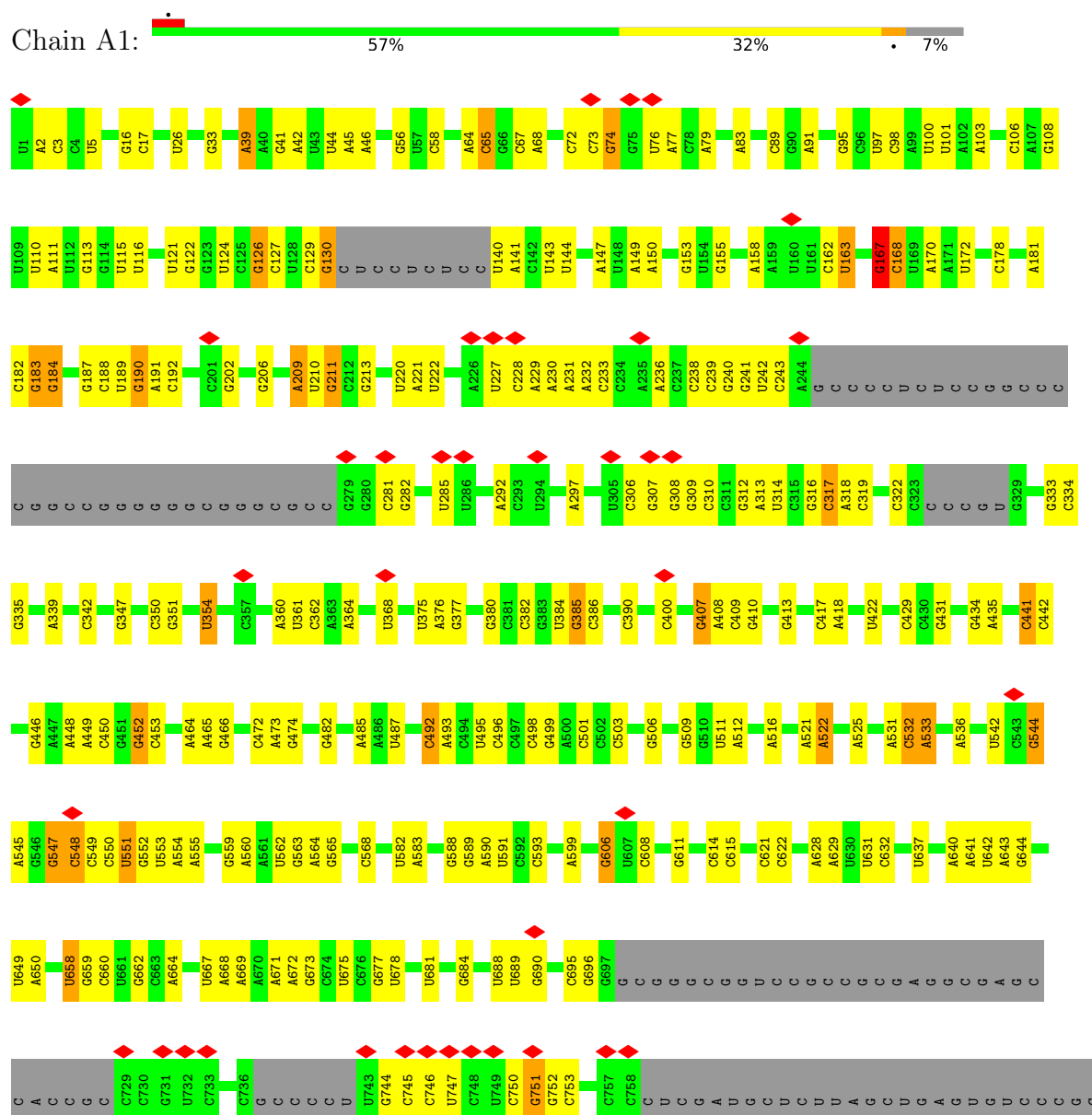
- Molecule 91 is water.

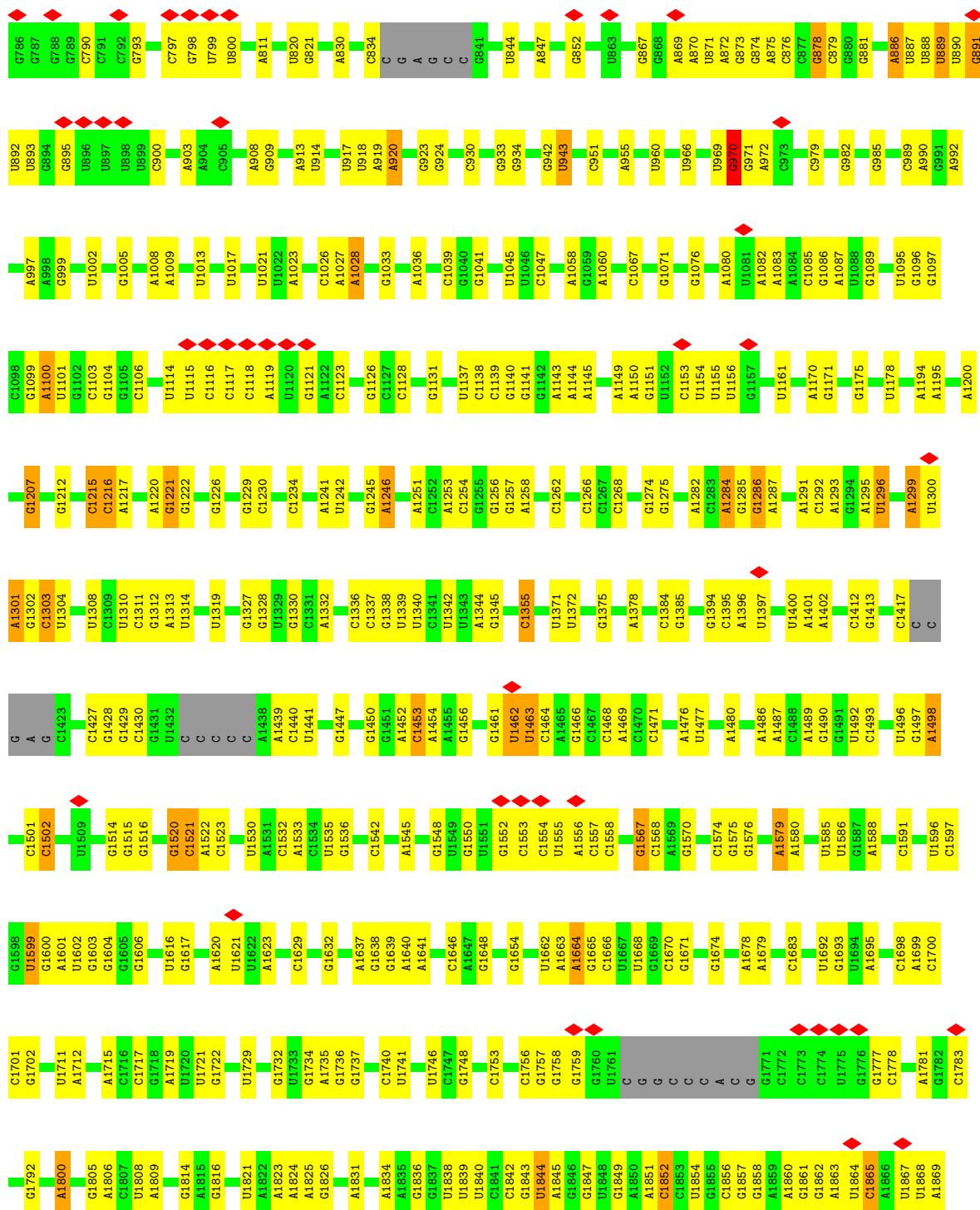
Mol	Chain	Residues	Atoms		AltConf
91	52	3	Total	O	0
			3	3	
91	1	1	Total	O	0
			1	1	

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.

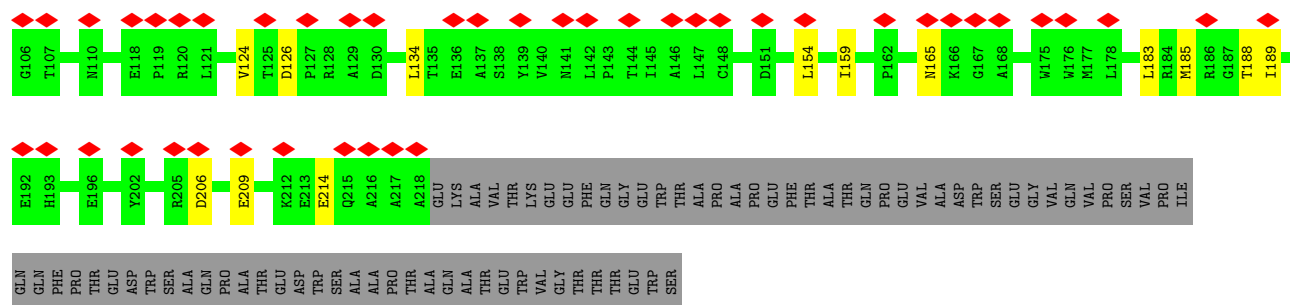
• Molecule 1: 18S ribosomal RNA



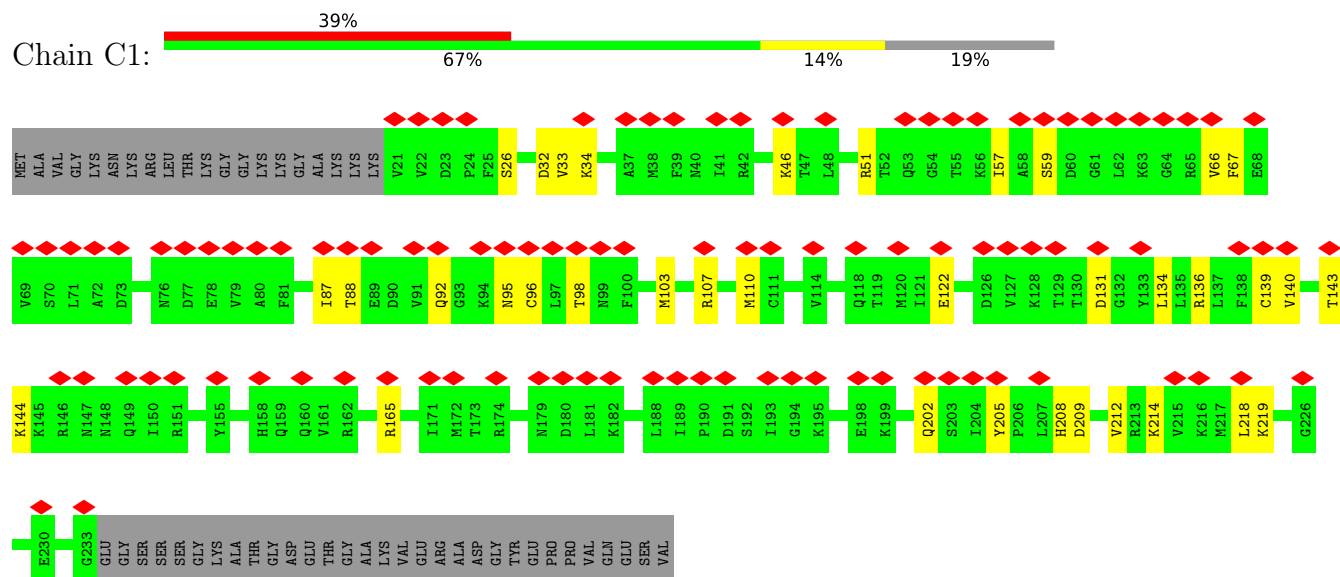


• Molecule 2: uS2

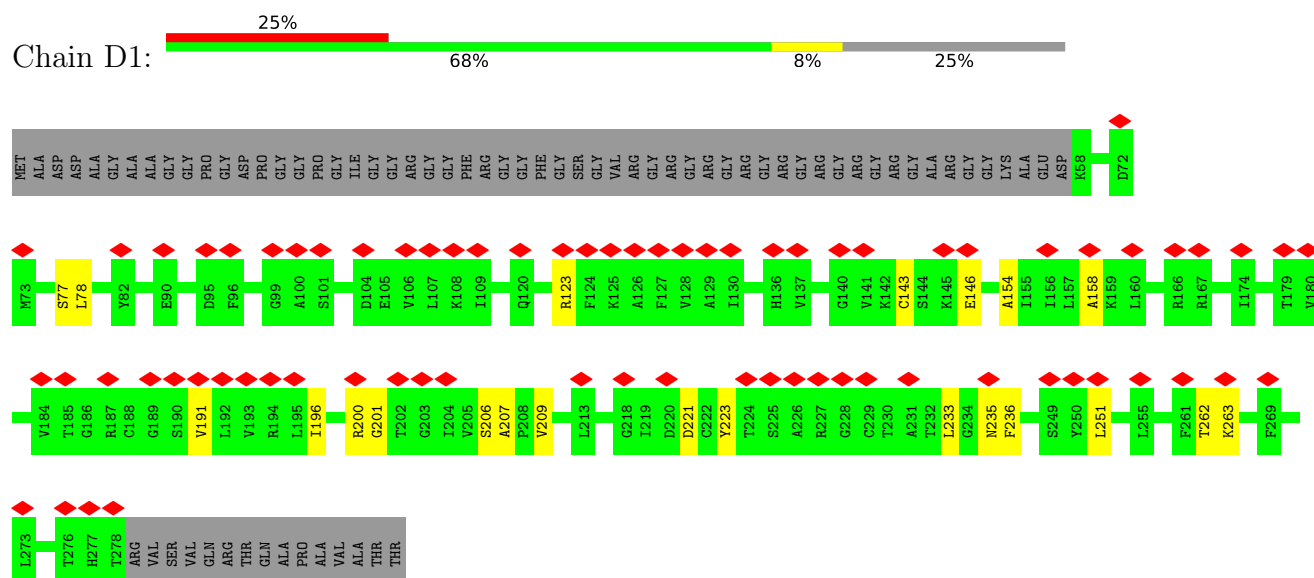




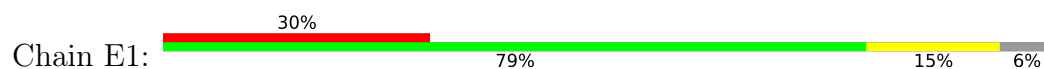
- Molecule 3: 40S ribosomal protein S3a

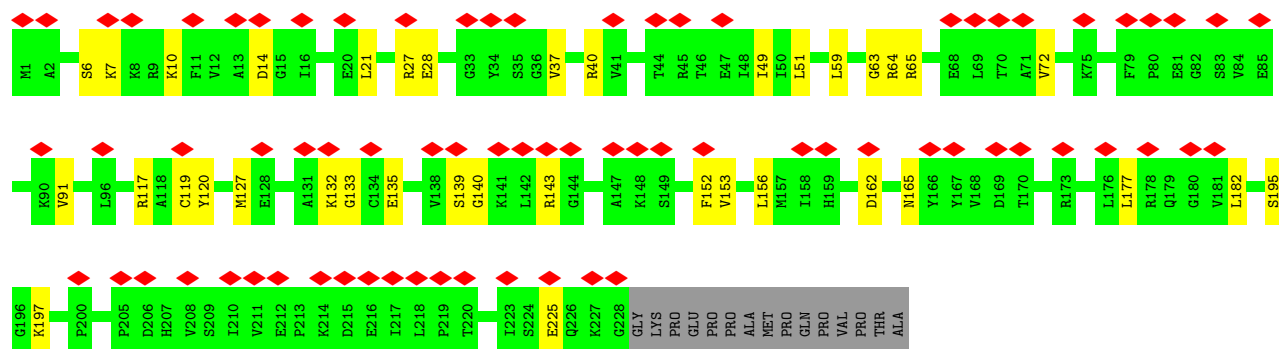


- Molecule 4: uS5

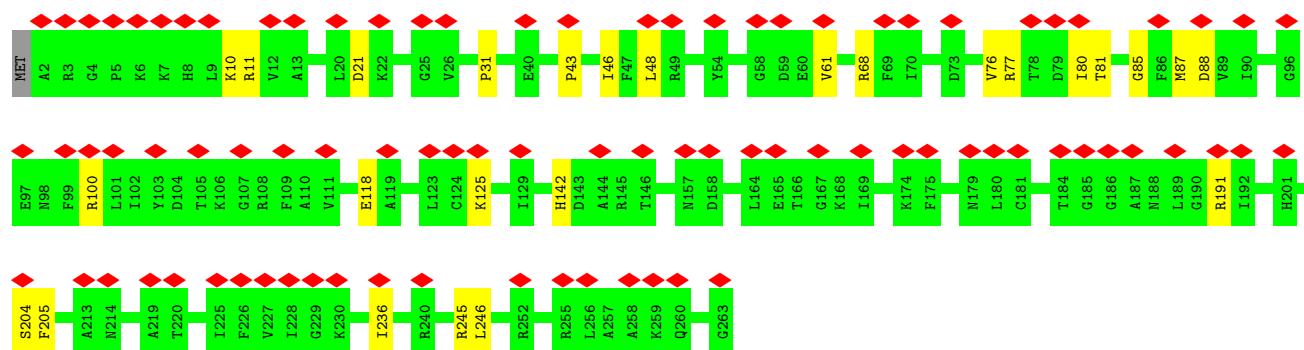


- Molecule 5: uS3

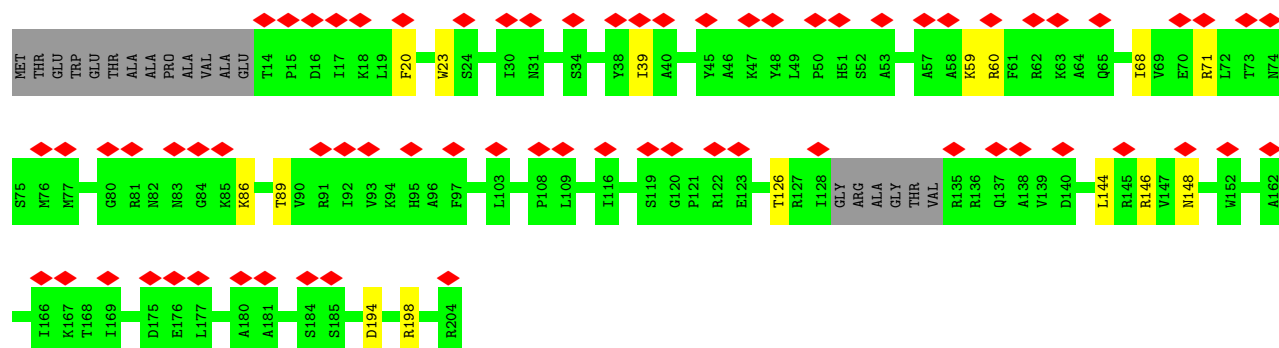
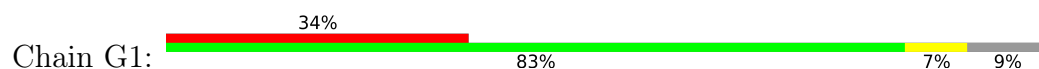




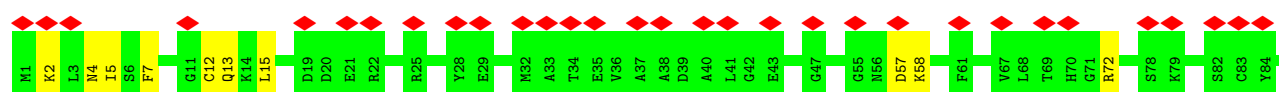
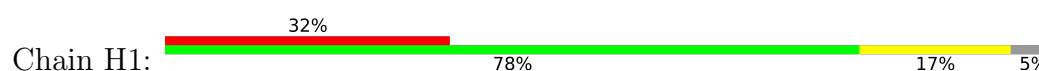
- Molecule 6: eS4

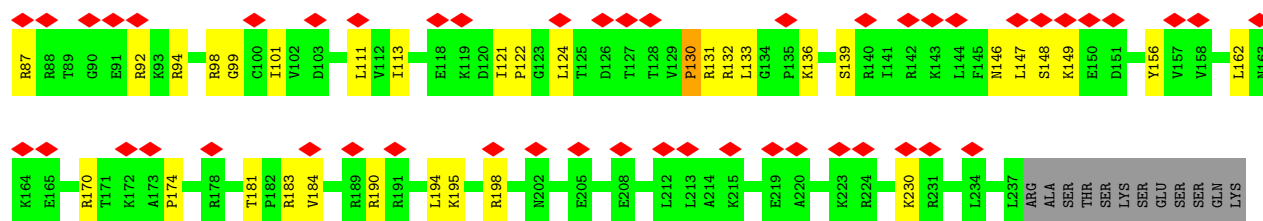


- Molecule 7: Ribosomal protein S5



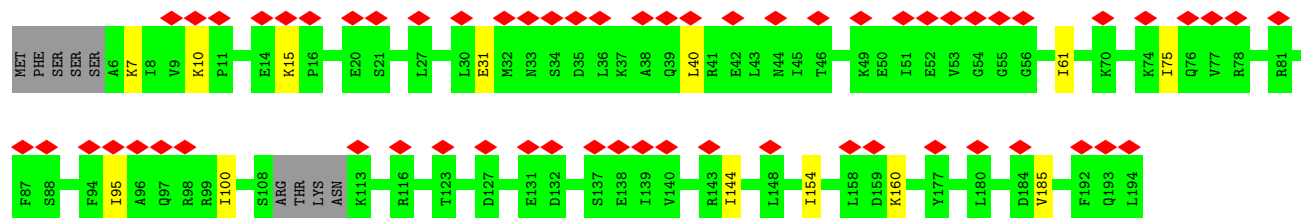
- Molecule 8: 40S ribosomal protein S6





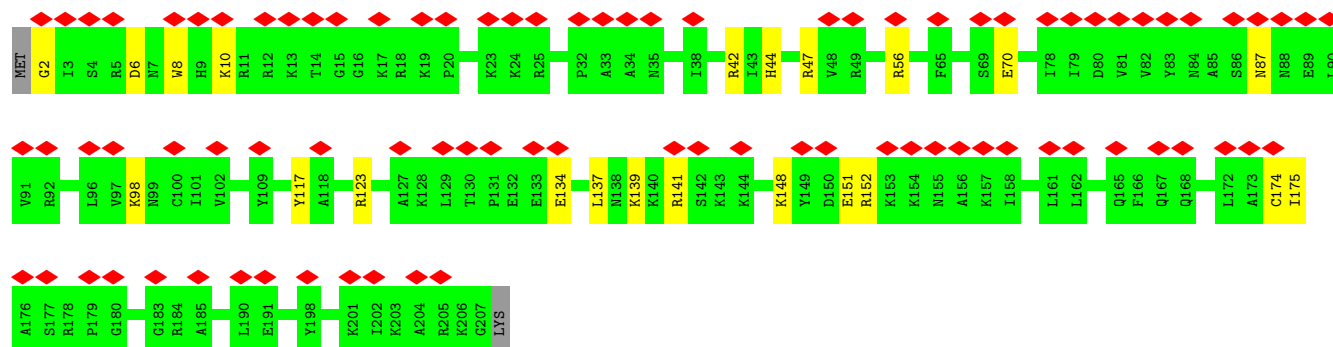
• Molecule 9: 40S ribosomal protein S7

Chain I1:



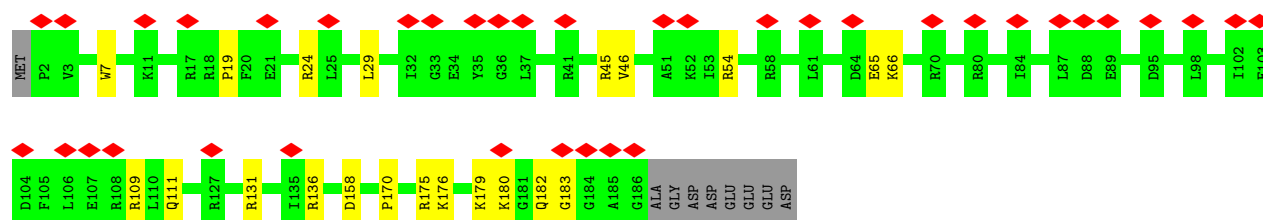
• Molecule 10: eS8

Chain J1:



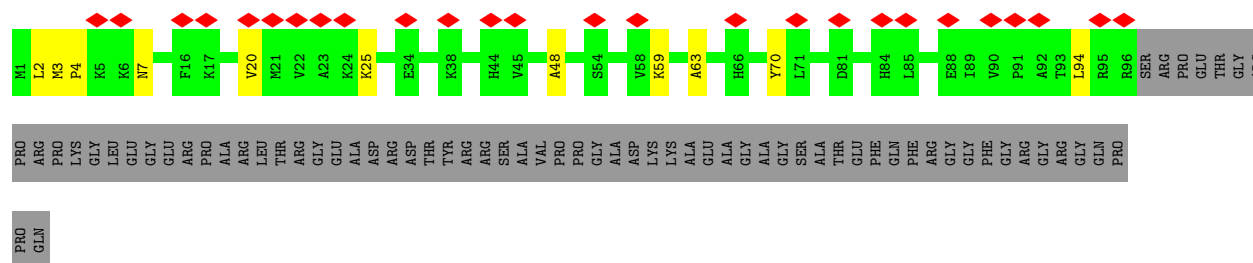
• Molecule 11: Ribosomal protein S9 (Predicted)

Chain K1:

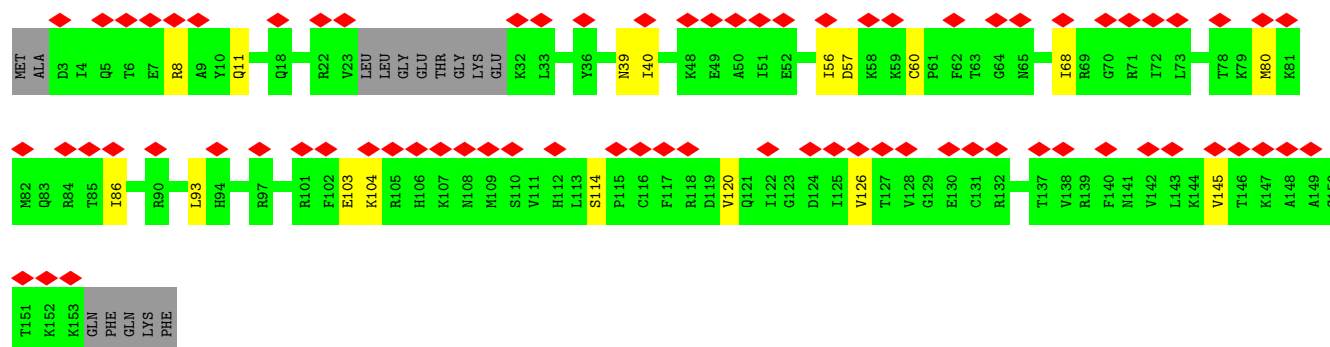
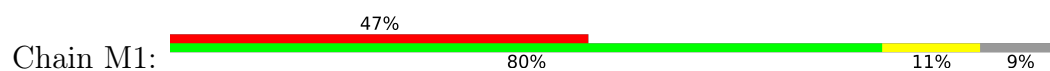


• Molecule 12: eS10

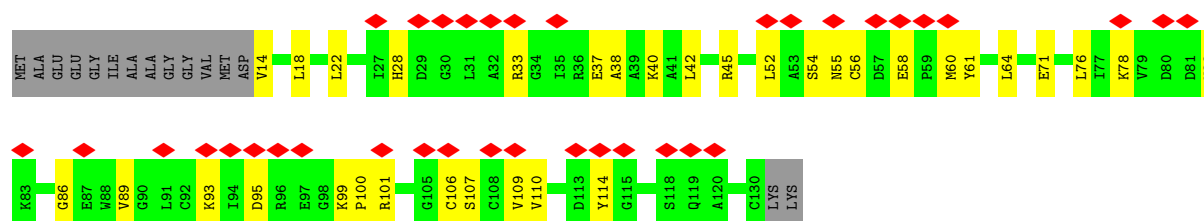
Chain L1:



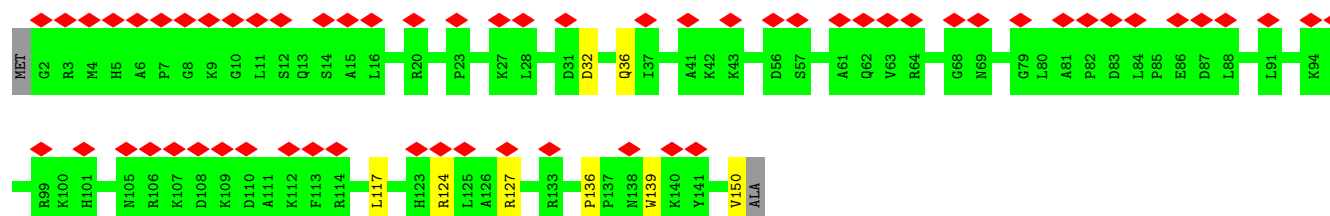
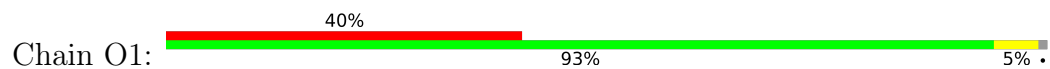
• Molecule 13: Ribosomal protein S11



• Molecule 14: 40S ribosomal protein S12

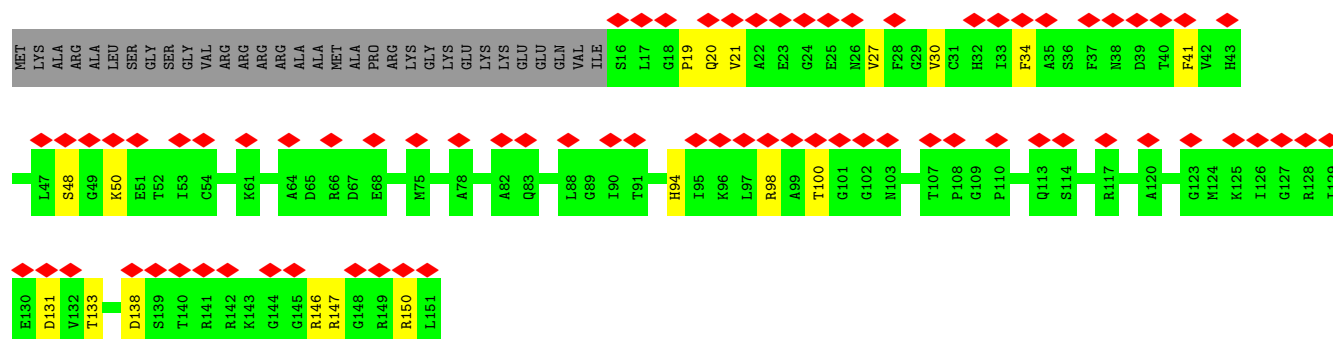


• Molecule 15: uS15

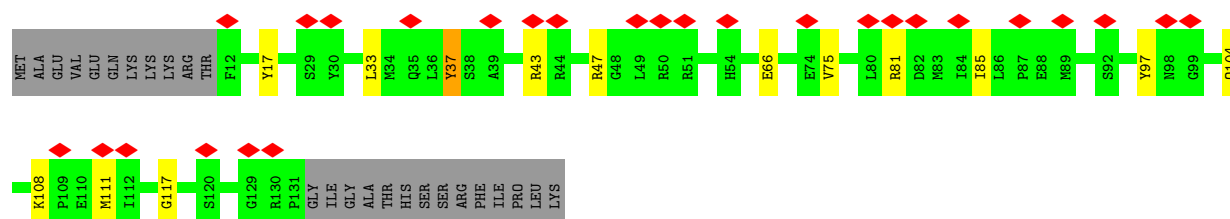
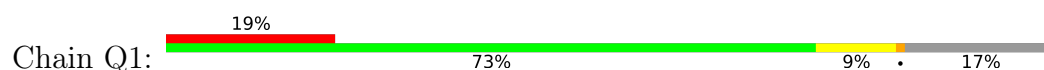


• Molecule 16: uS11

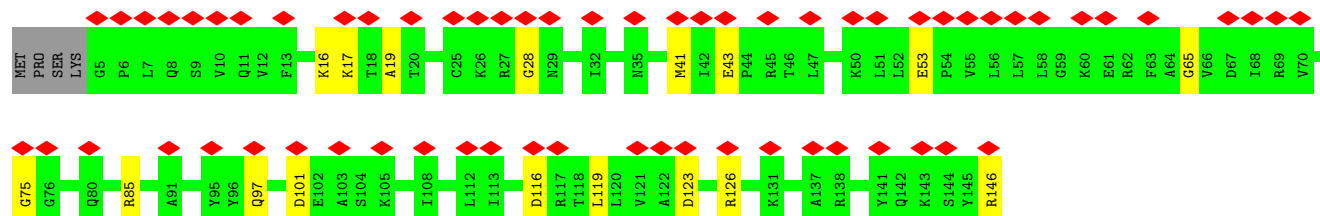
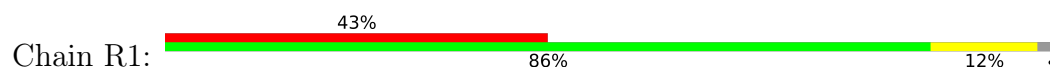




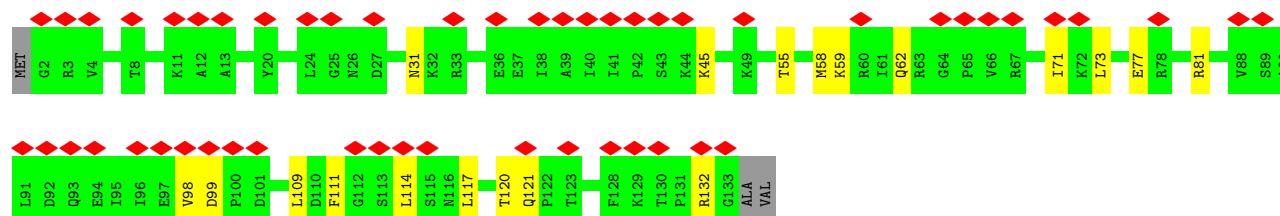
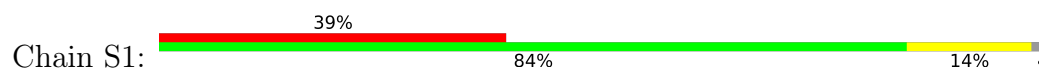
• Molecule 17: uS19



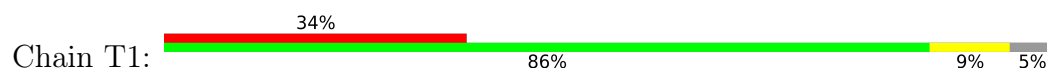
• Molecule 18: Ribosomal protein S16

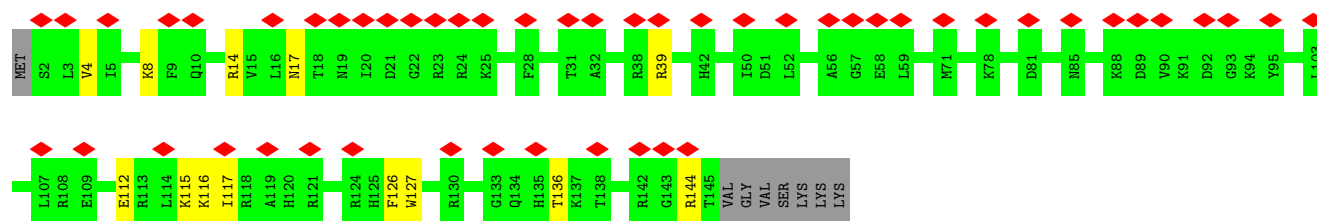


• Molecule 19: eS17

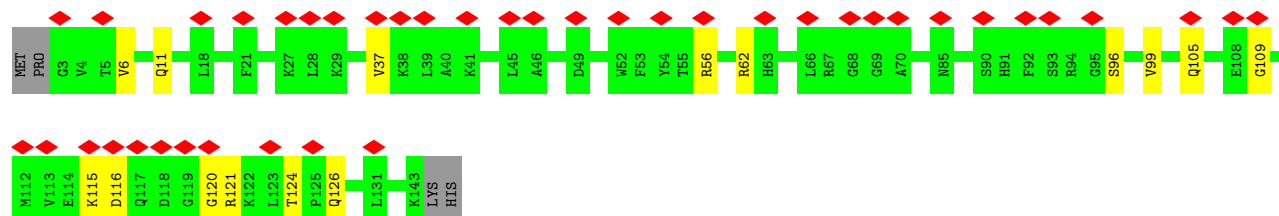


• Molecule 20: uS13

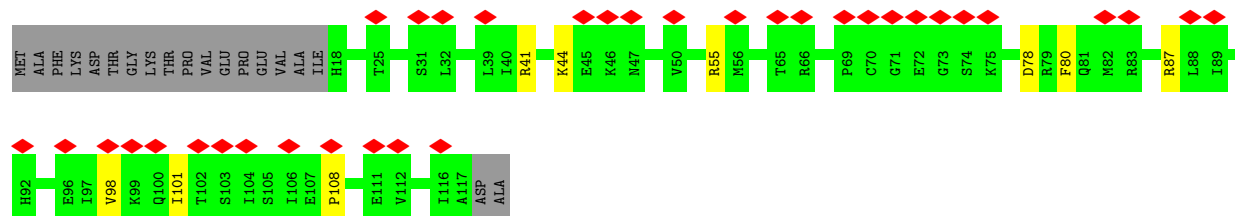
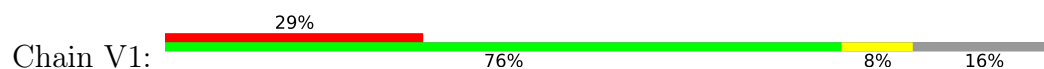




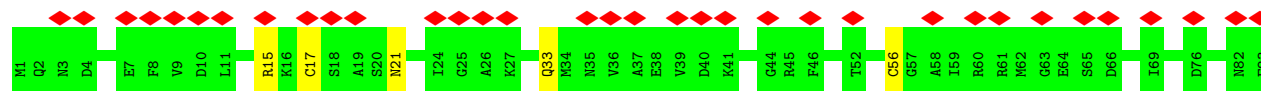
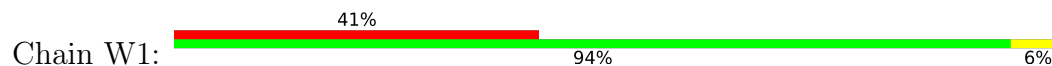
• Molecule 21: eS19



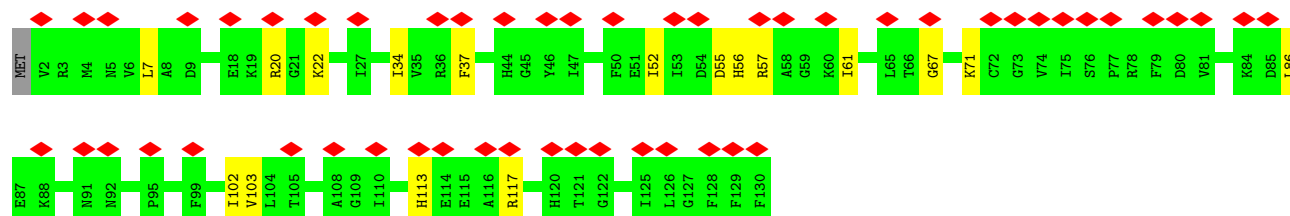
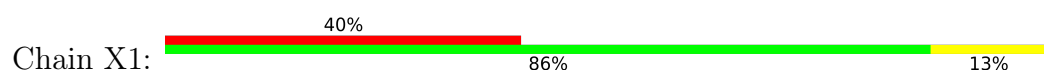
• Molecule 22: uS10



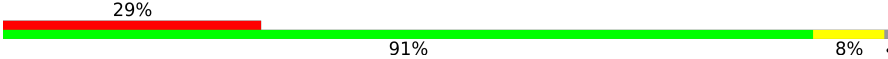
• Molecule 23: eS21

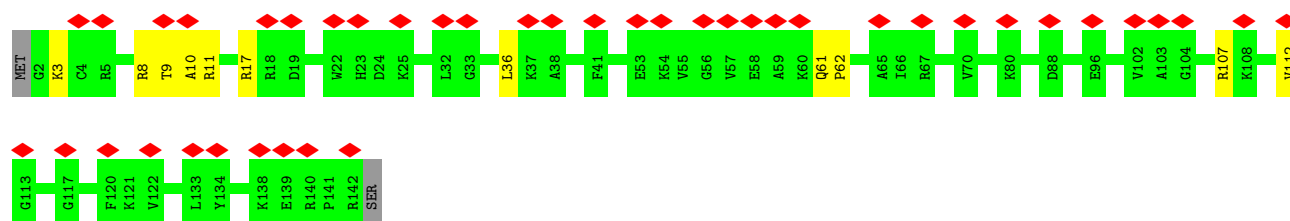


• Molecule 24: Ribosomal protein S15a



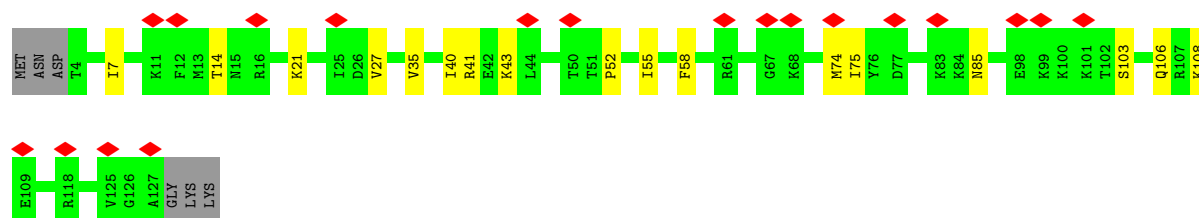
• Molecule 25: uS12

Chain Y1: 



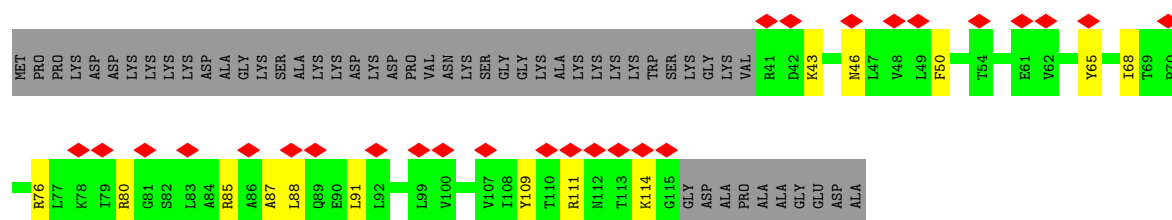
• Molecule 26: eS24

Chain Z1: 



• Molecule 27: eS25

Chain a1: 



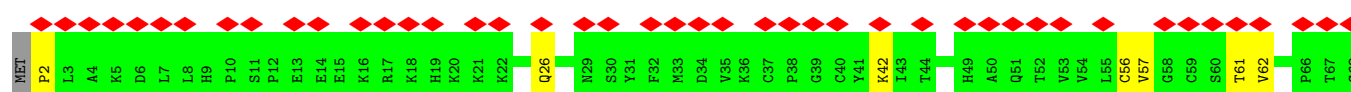
• Molecule 28: eS26

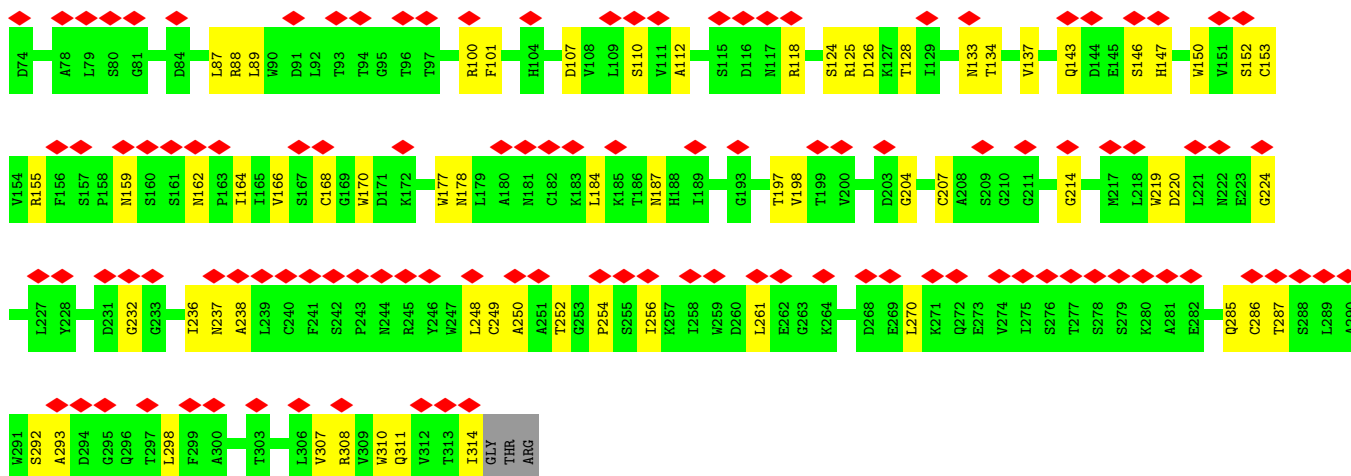
Chain b1: 



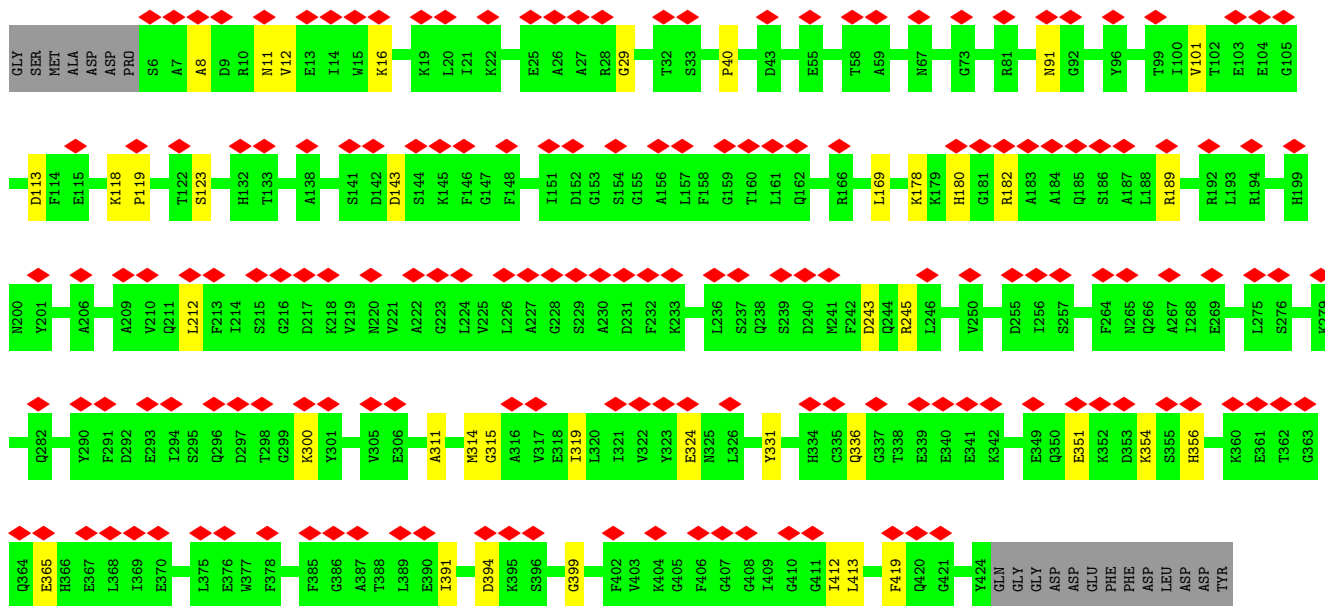
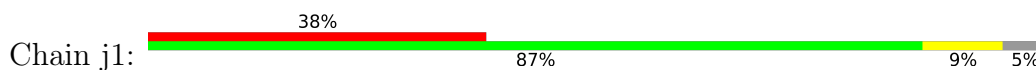
• Molecule 29: 40S ribosomal protein S27

Chain c1: 

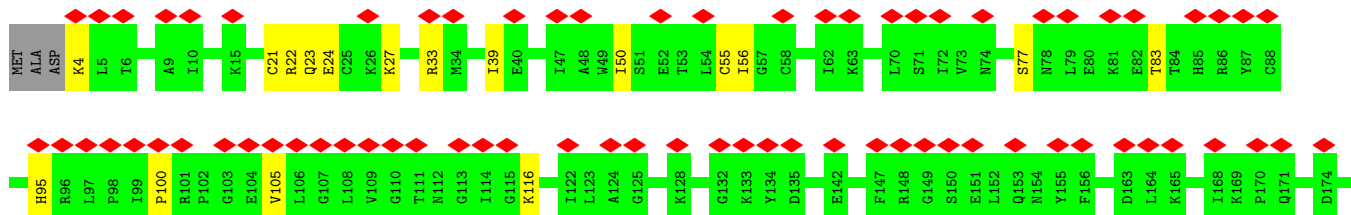
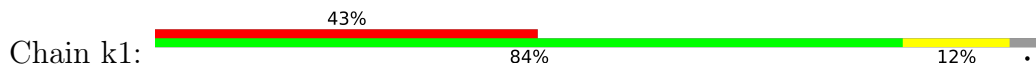


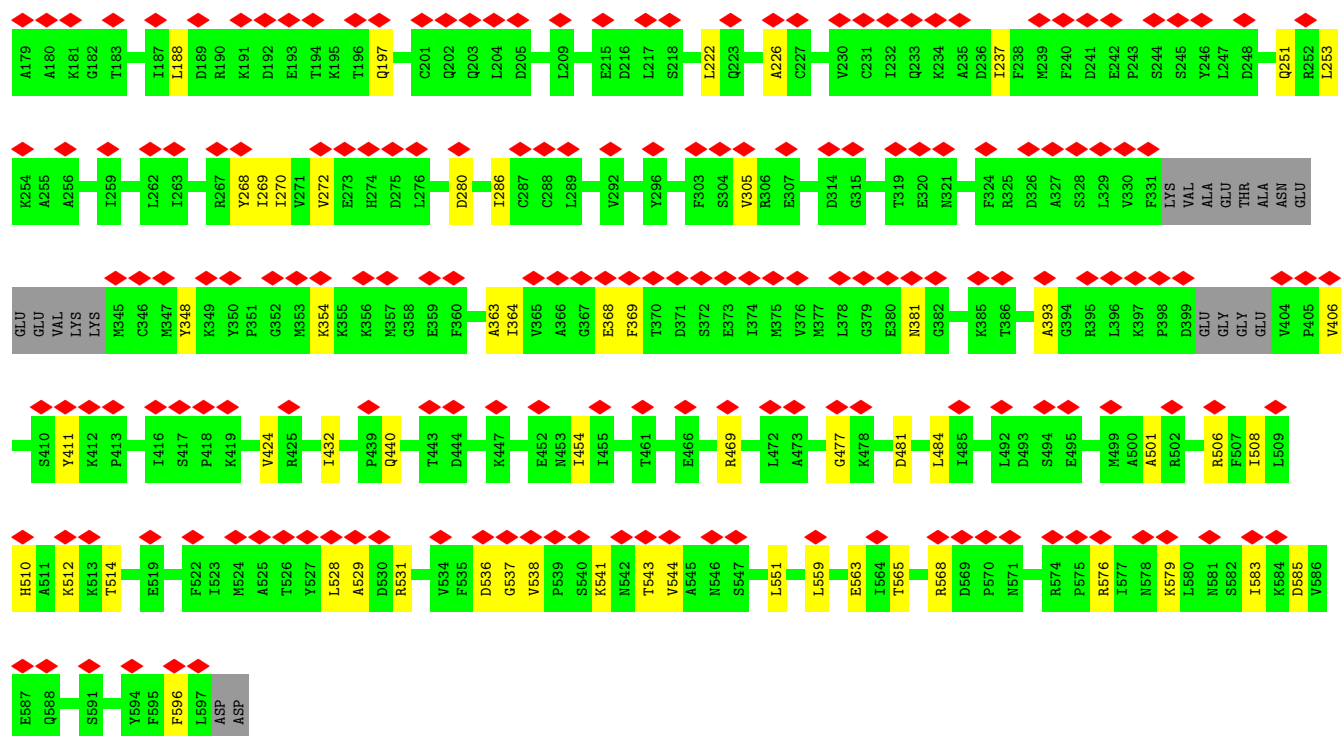


• Molecule 35: eRF1(AAQ)

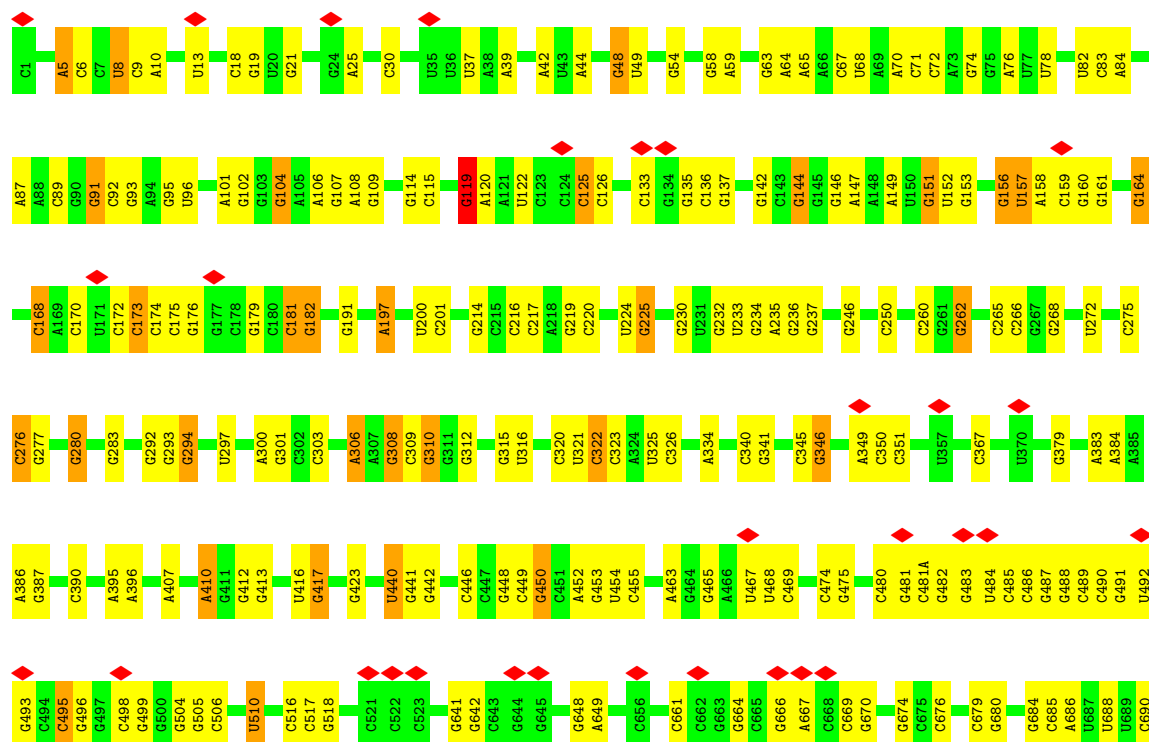


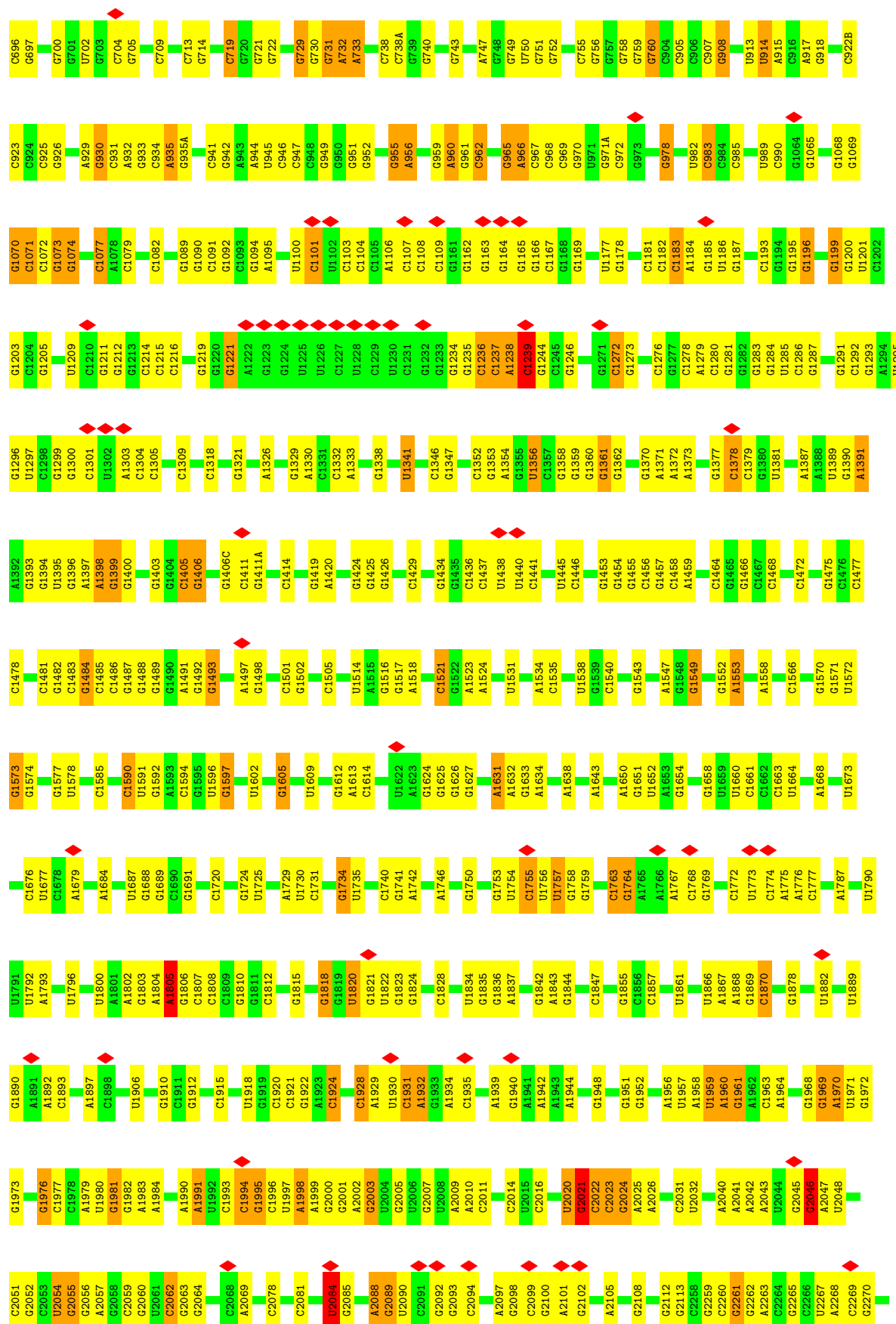
• Molecule 36: ATP binding cassette subfamily E member 1

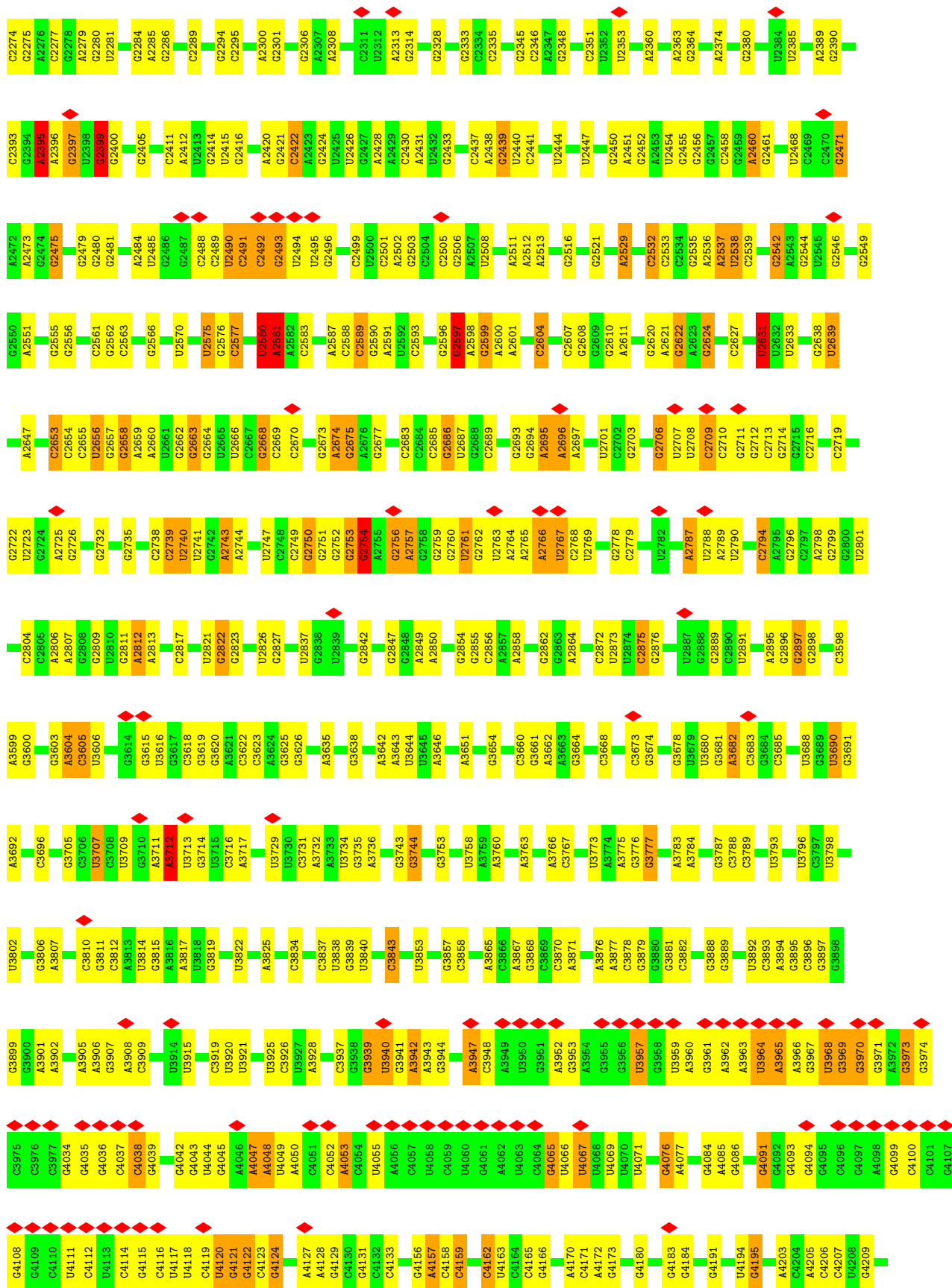


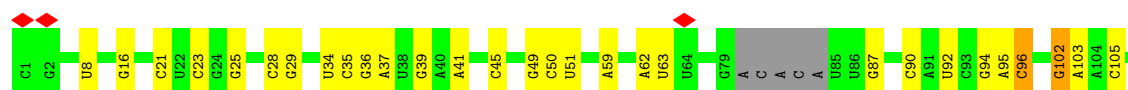


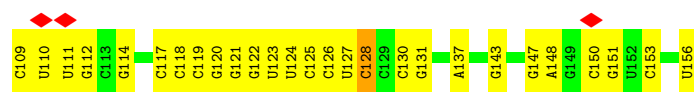
• Molecule 37: 28S ribosomal RNA



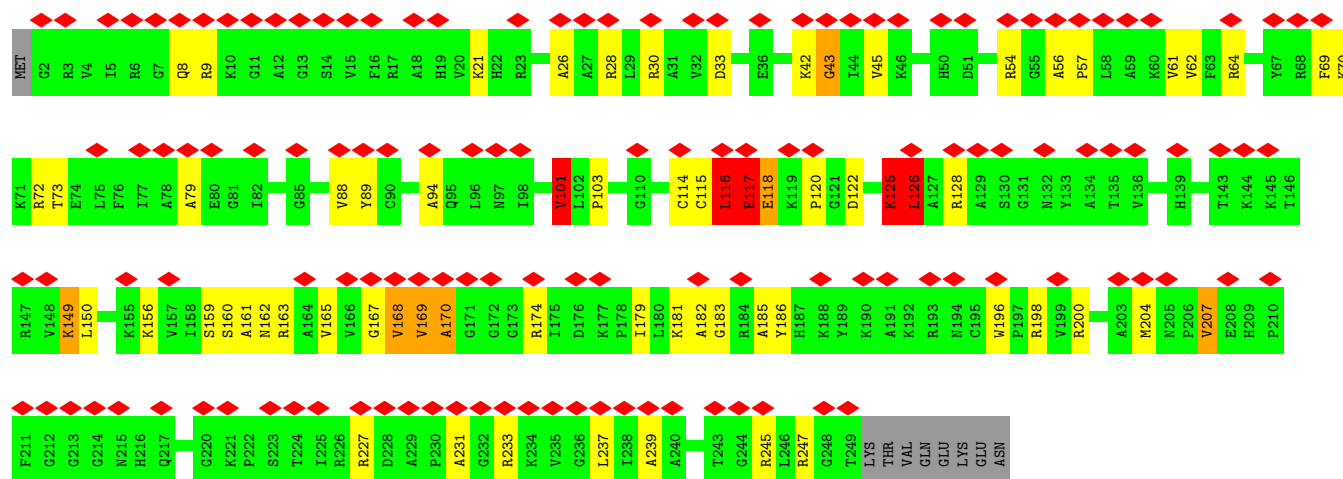




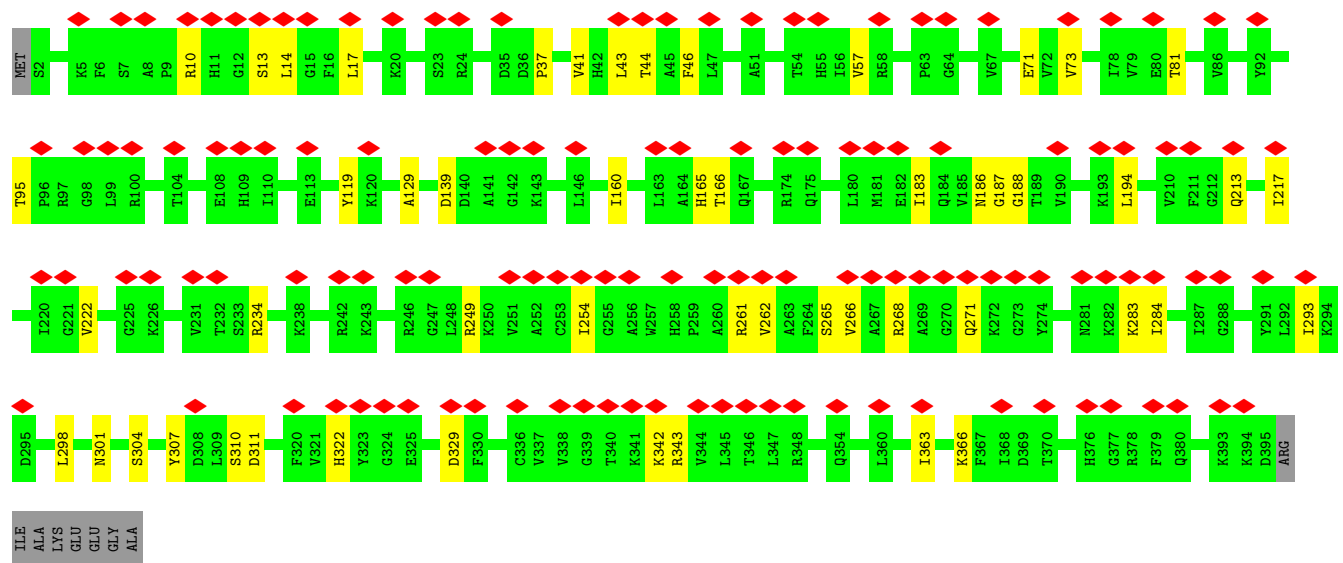
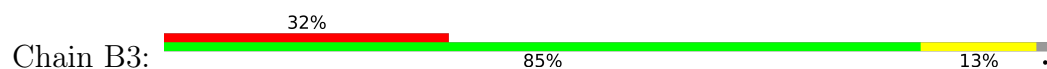




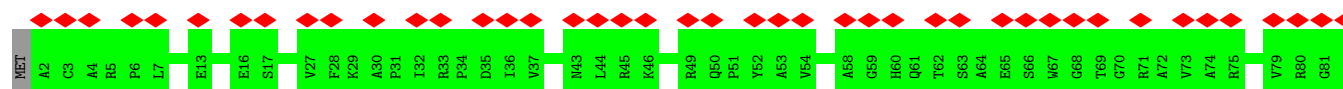
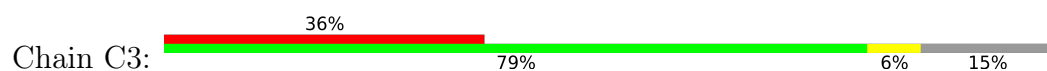
• Molecule 40: Ribosomal protein L8



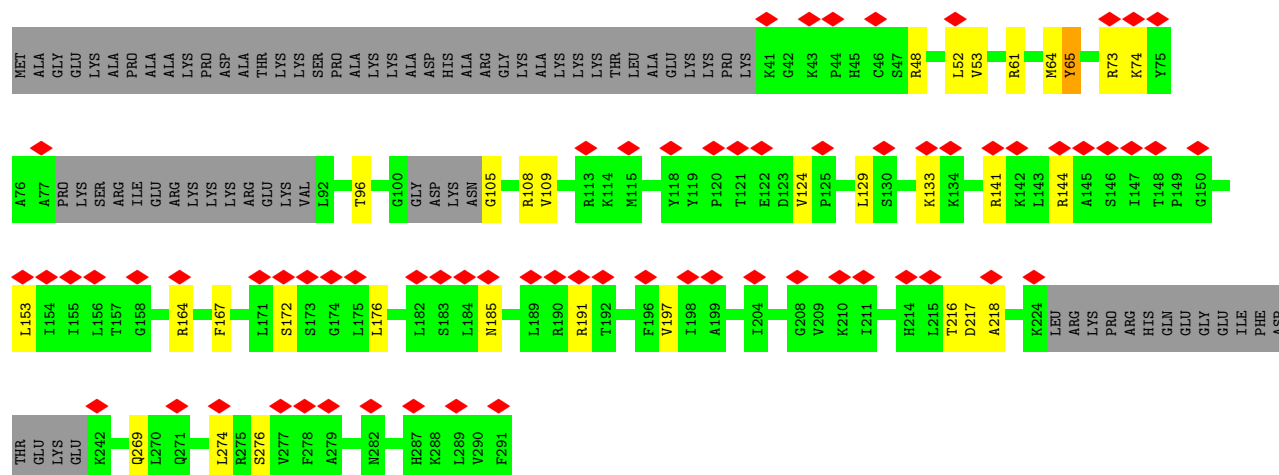
• Molecule 41: uL3



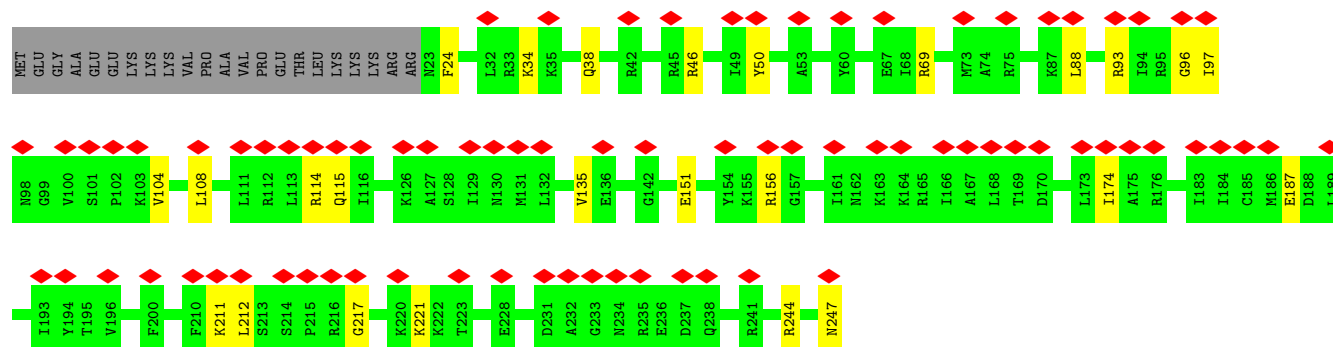
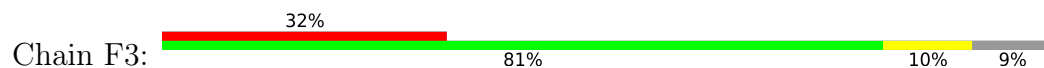
• Molecule 42: uL4



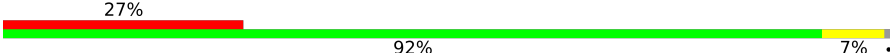
- Molecule 43: 60S ribosomal protein L6

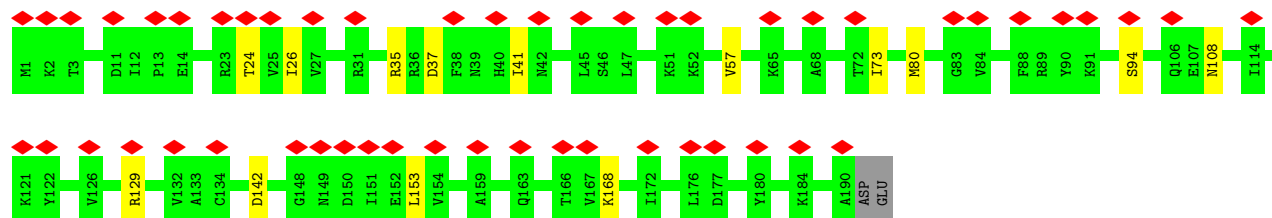


- Molecule 44: uL30

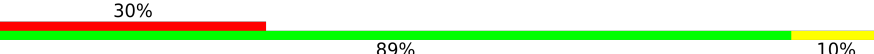


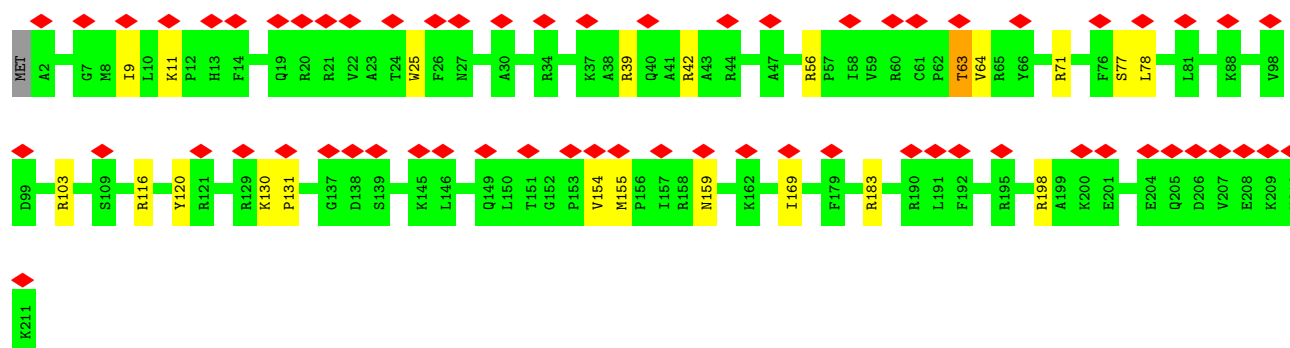
- Molecule 45: uL6

Chain H3: 



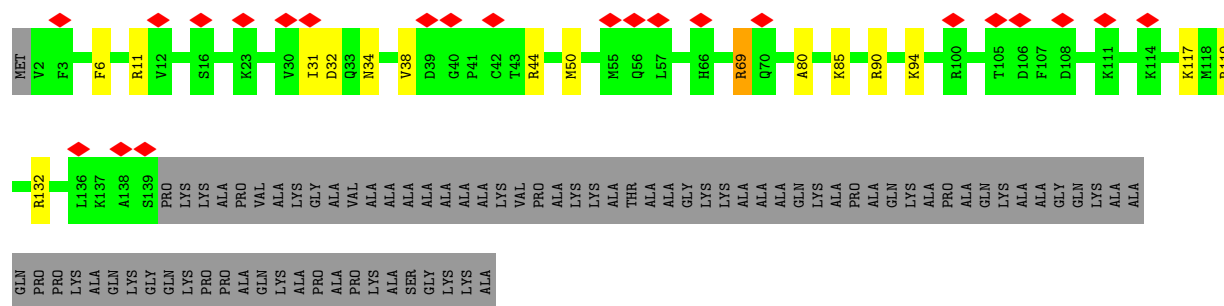
- Molecule 46: eL13

Chain L3: 



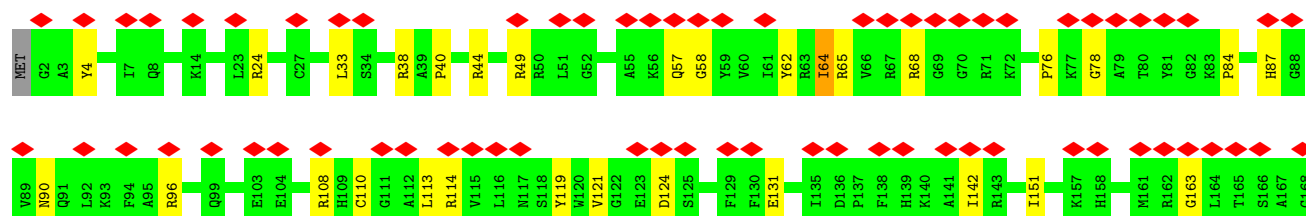
- Molecule 47: Ribosomal protein L14

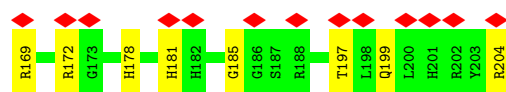
Chain M3: 



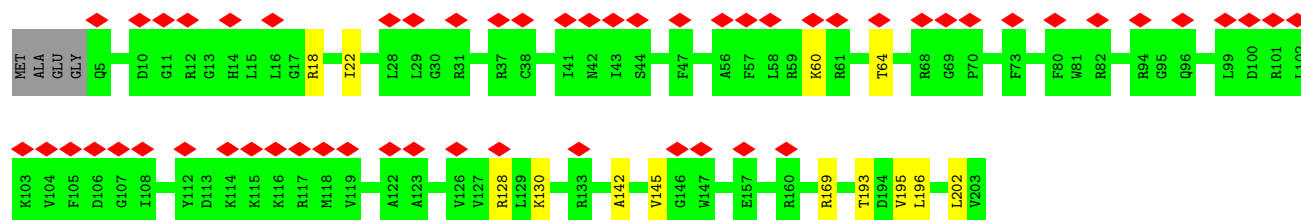
- Molecule 48: Ribosomal protein L15

Chain N3: 

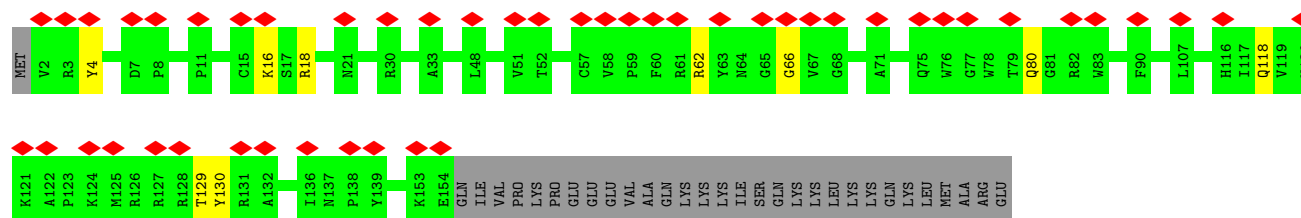
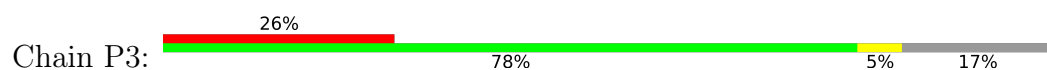




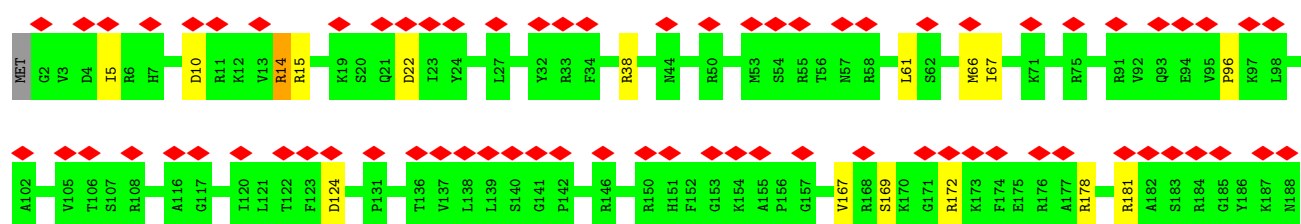
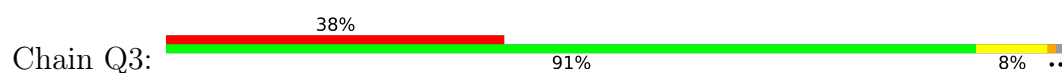
• Molecule 49: uL13



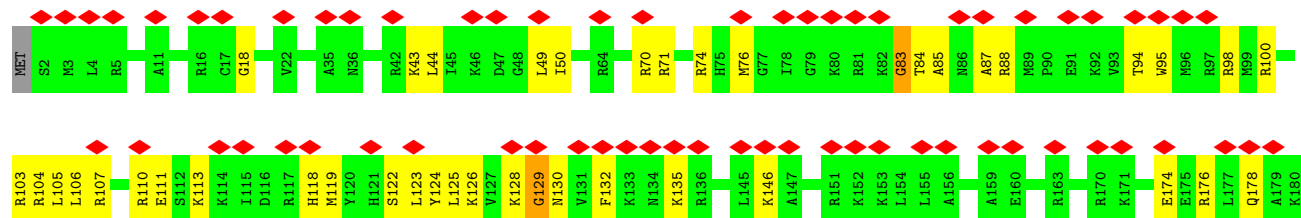
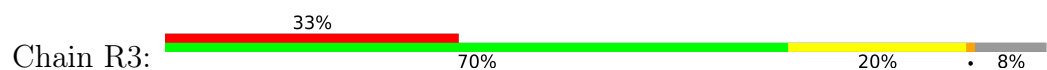
• Molecule 50: uL22

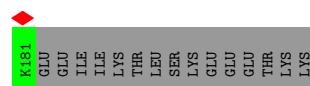


• Molecule 51: eL18

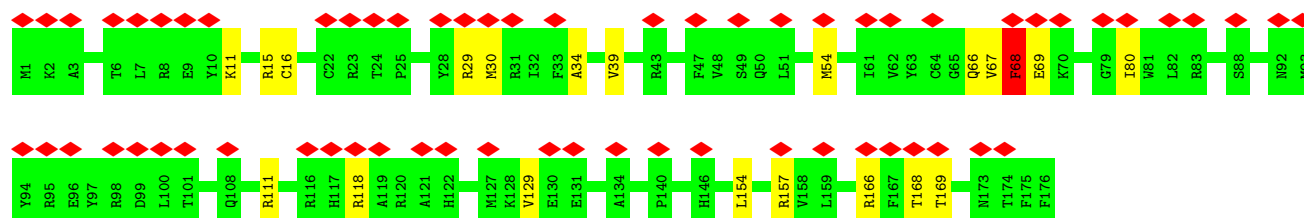
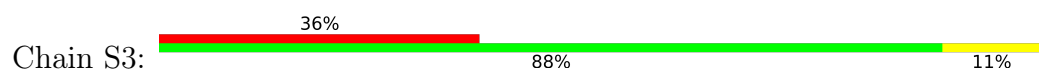


• Molecule 52: eL19

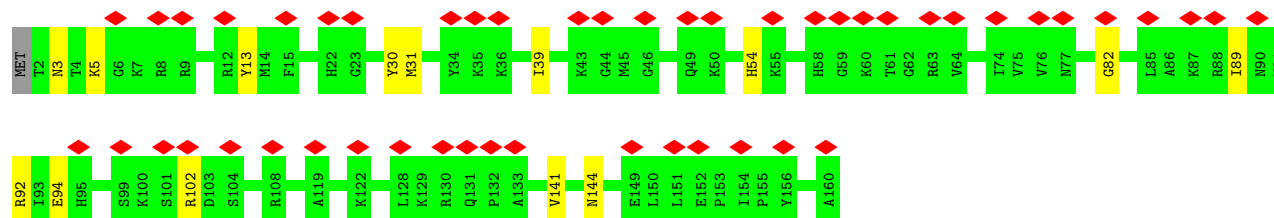




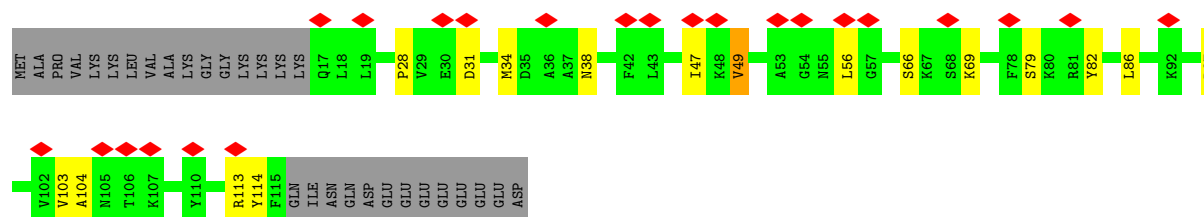
- Molecule 53: eL20



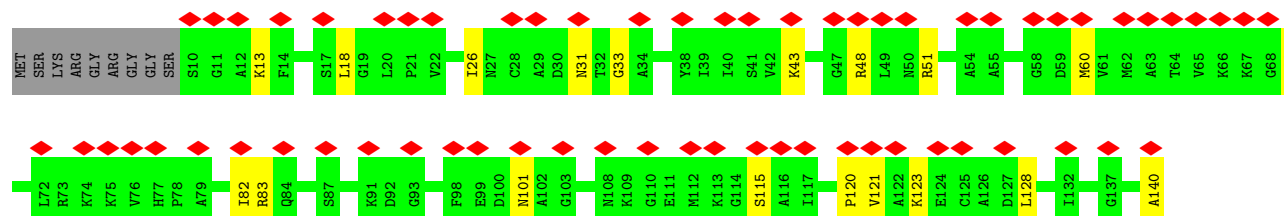
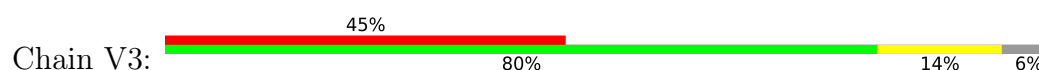
- Molecule 54: eL21



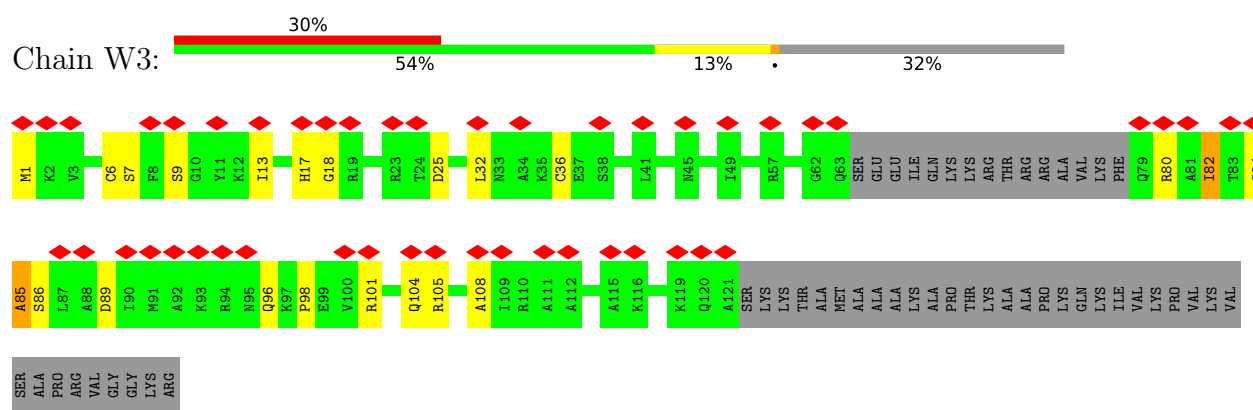
- Molecule 55: eL22



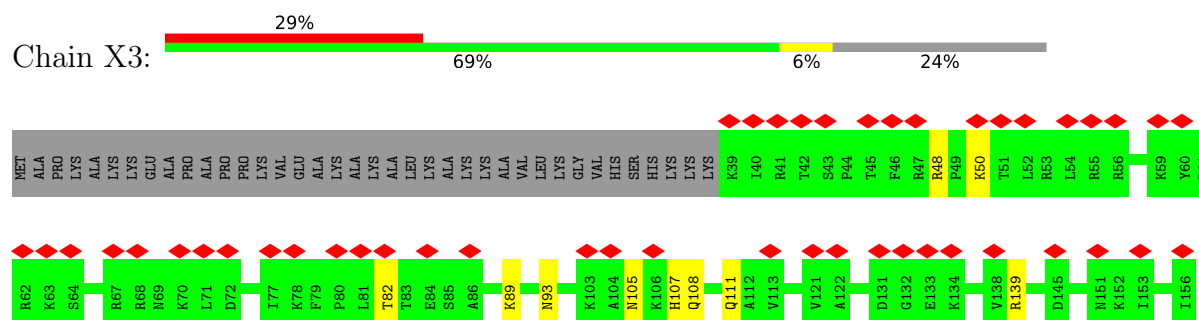
- Molecule 56: Ribosomal protein L23



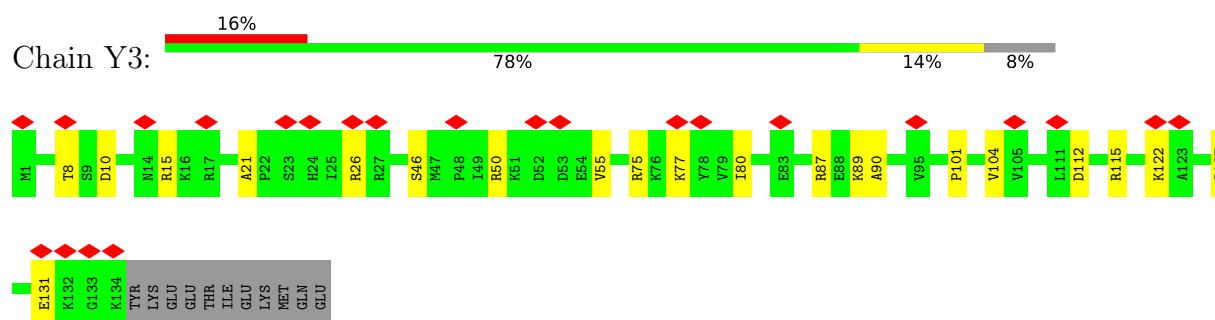
- Molecule 57: eL24



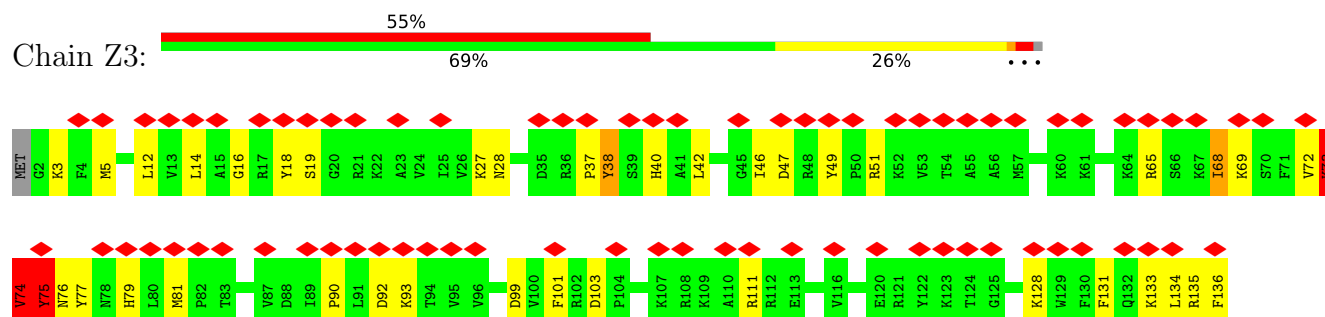
- Molecule 58: uL23



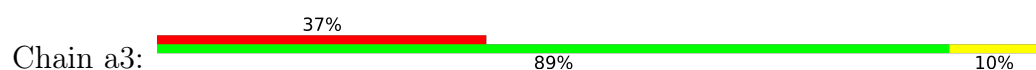
- Molecule 59: Ribosomal protein L26

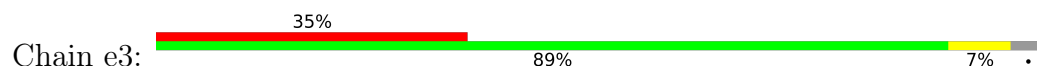


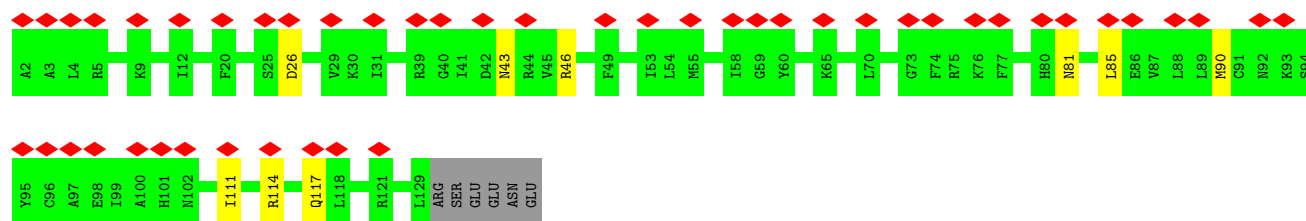
- Molecule 60: eL27



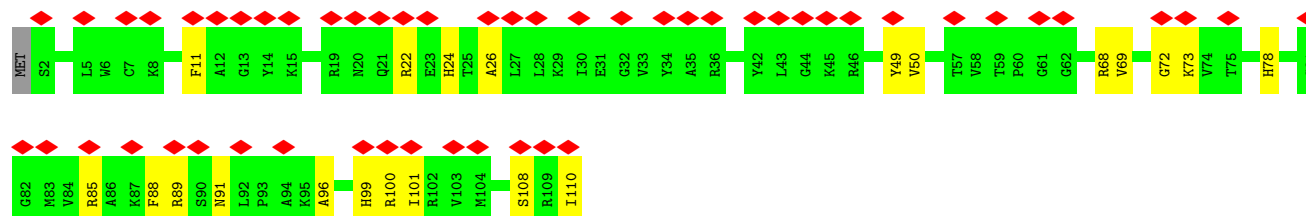
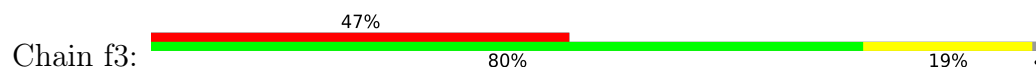
- Molecule 61: uL15



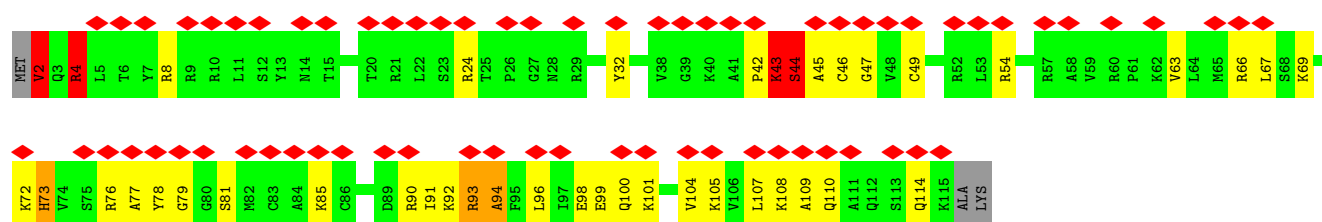




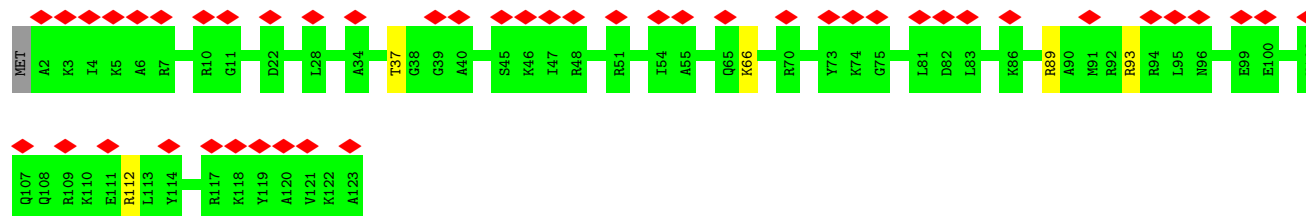
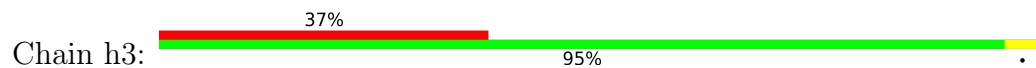
• Molecule 66: eL33



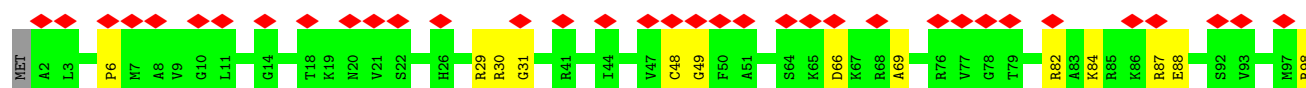
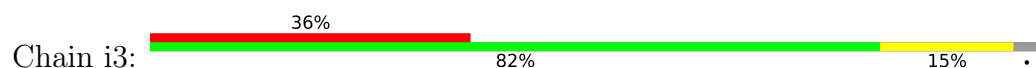
• Molecule 67: eL34

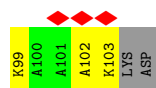


• Molecule 68: uL29

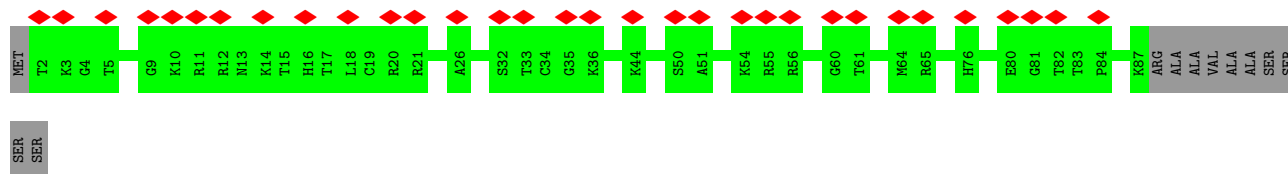
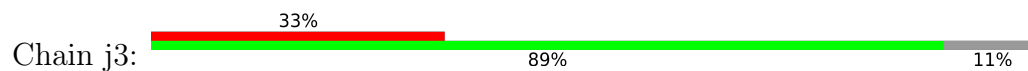


• Molecule 69: 60S ribosomal protein L36

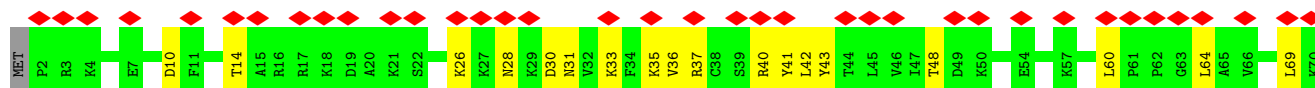
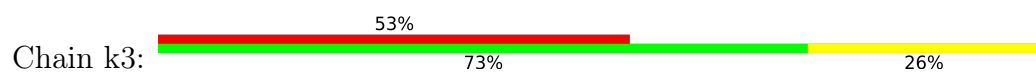




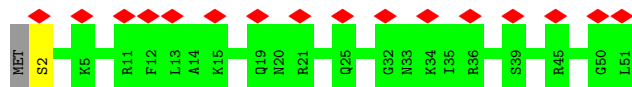
• Molecule 70: Ribosomal protein L37



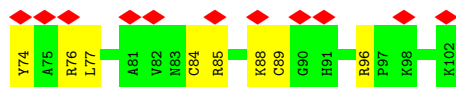
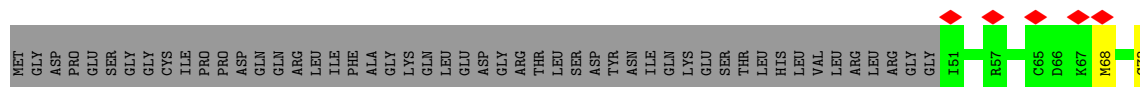
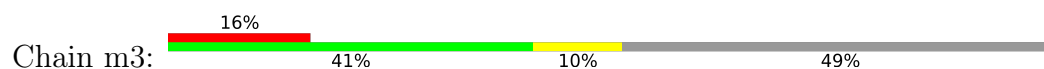
• Molecule 71: eL38



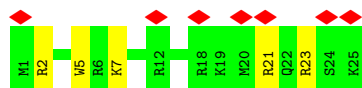
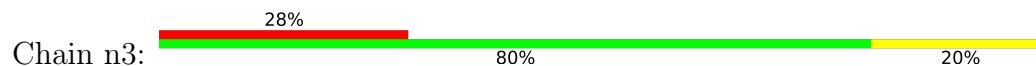
• Molecule 72: eL39



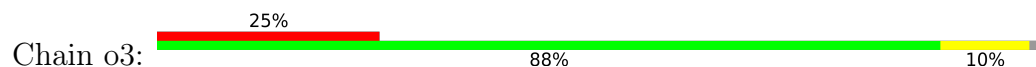
• Molecule 73: eL40

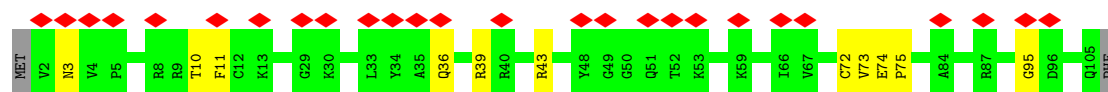


• Molecule 74: eL41

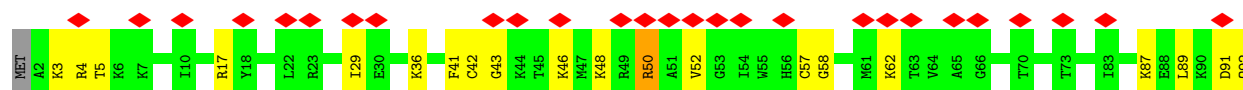
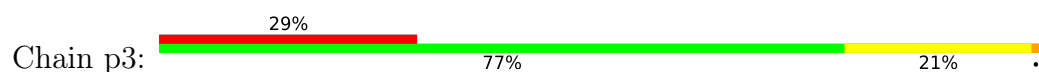


• Molecule 75: eL42

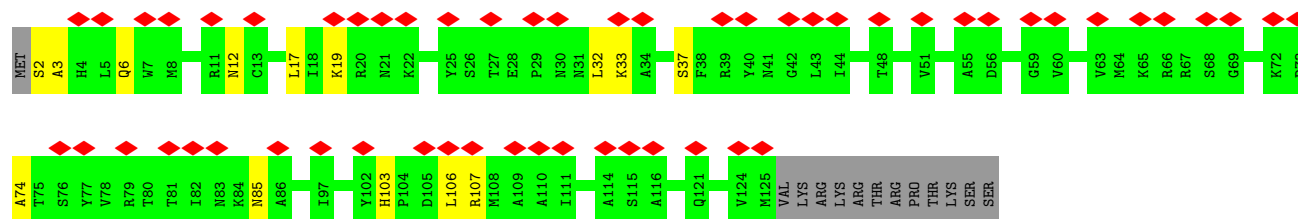
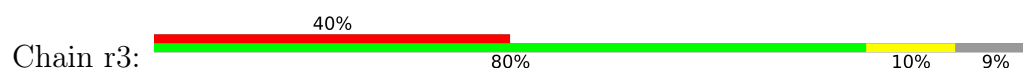




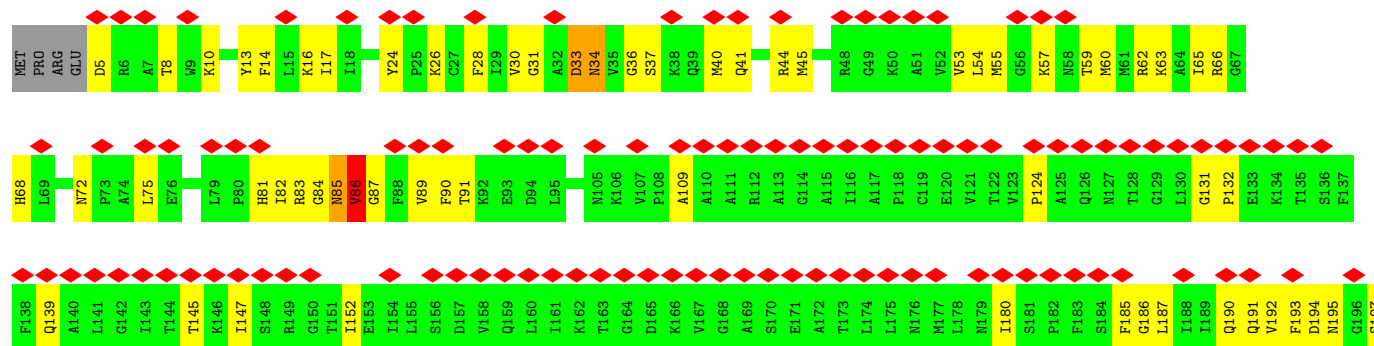
- Molecule 76: eL43



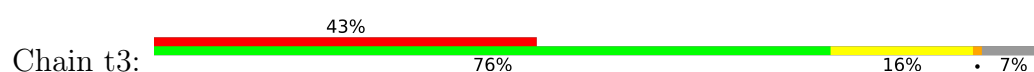
- Molecule 77: eL28

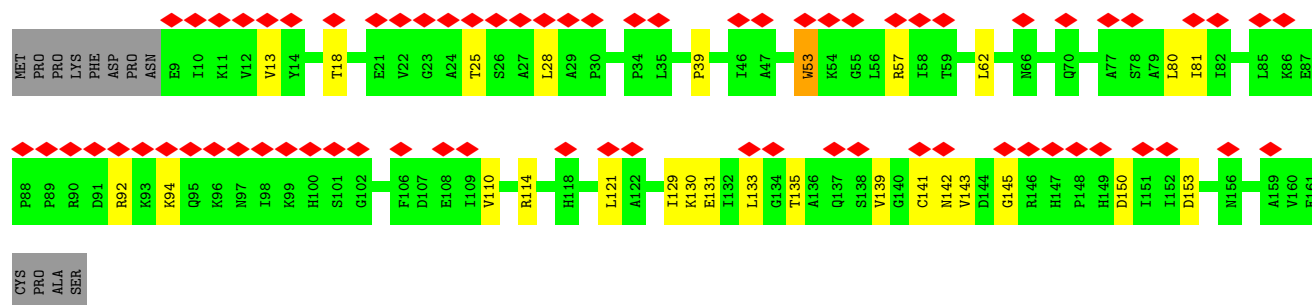


- Molecule 78: uL10

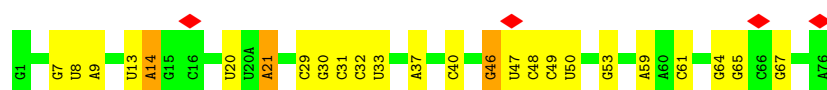


- Molecule 79: Ribosomal protein L12

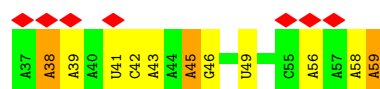




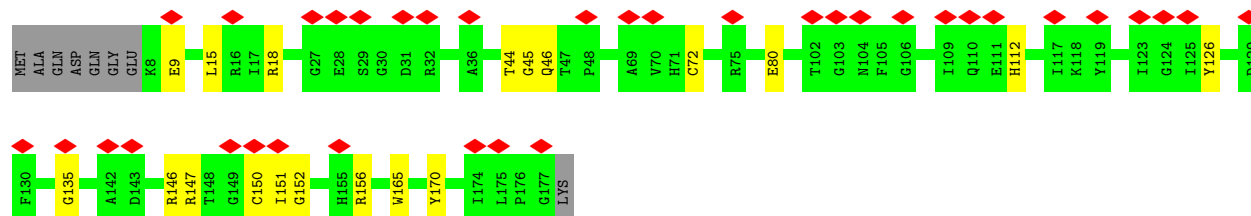
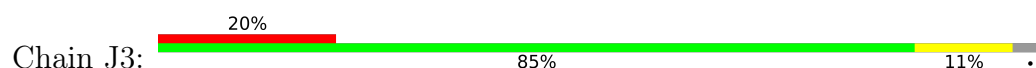
• Molecule 80: P-site tRNA



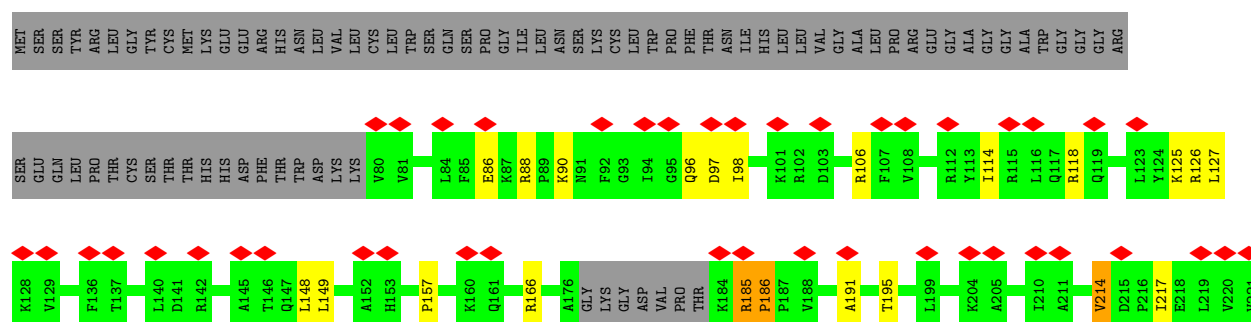
• Molecule 81: mRNA

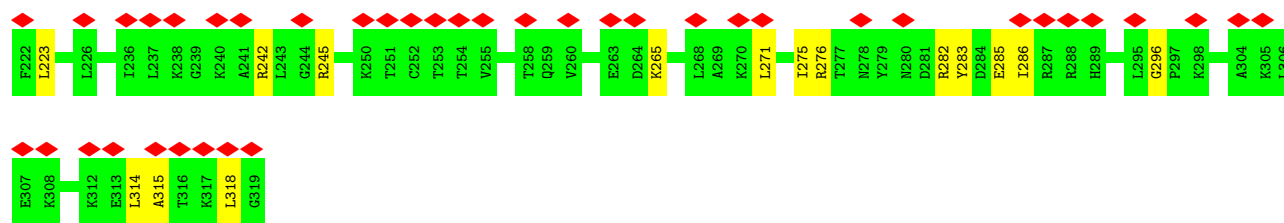


• Molecule 82: Ribosomal protein L11



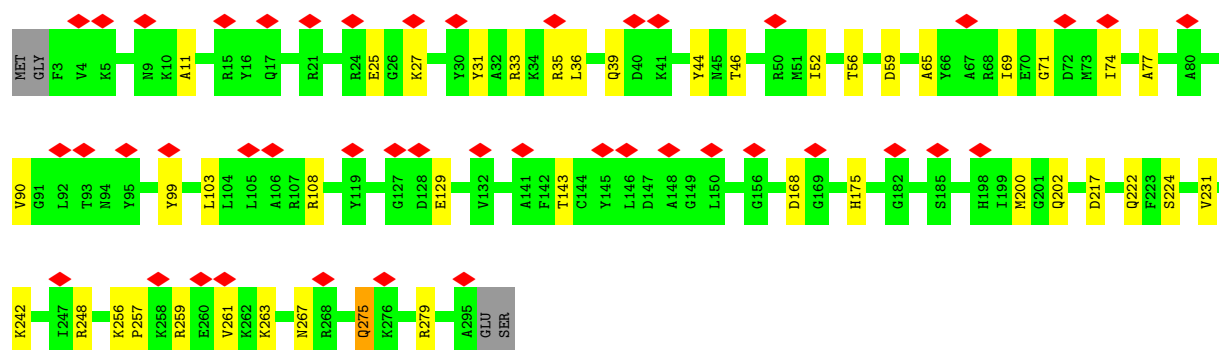
• Molecule 83: eL8





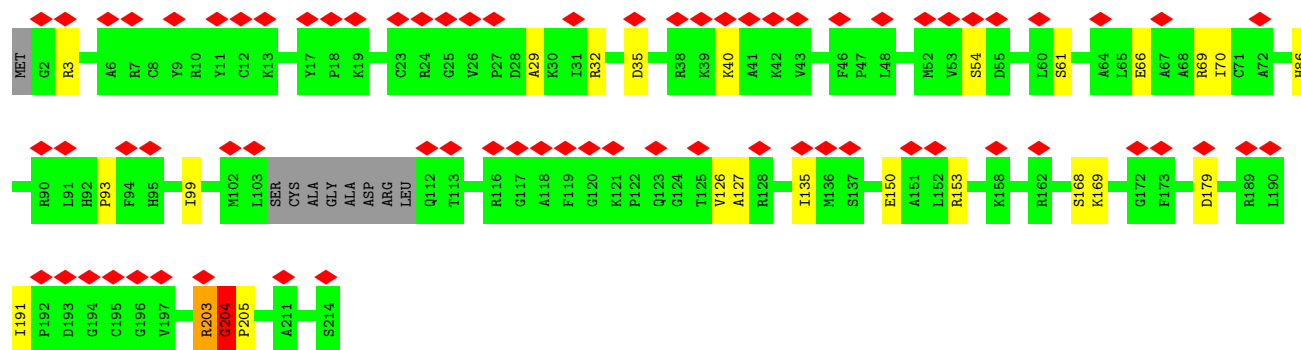
• Molecule 84: 60S ribosomal protein L5

Chain D3: 15% 85% 14% .



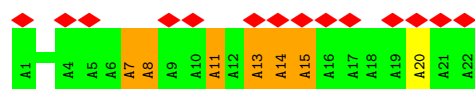
• Molecule 85: 60S ribosomal protein L10

Chain I3: 34% 84% 11% .



• Molecule 86: nascent chain

Chain 1: 64% 68% 5% 27%



• Molecule 87: Ribosomal protein

Chain u3: 90% 75% 24% .

I183	H184	L185	A186	V187	N188	F189	L190	V191	S192	L193	L194	K195	K196	N197	N198	Q199	N200	V201	R202	A203	L204	Y205	I206	K207	S208	T209	M210	G211	K212	P213	Q214	R215	L216	Y217																									
I123	L124	G125	P126	G127	L128	N129	K130	A131	G132	K133	F134	P135	S136	L137	L138	T139	H140	N141	E142	N143	M144	V145	A146	K147	V148	D149	E150	V151	K152	S153	T154	I155	K156	F157	Q158	H159	K160	K161	V162	L163	C164	L165	A166	V167	A168	V169	G170	H171	V172	K173	M174	T175	D176	D177	E178	L179	V180	N181	N182
P61	K62	F63	S64	V65	C66	V67	L68	G69	D70	Q71	Q72	H73	C74	D75	E76	A77	K78	A79	V80	D81	I82	P83	H84	H85	D86	I87	E88	A89	L90	K91	T91	L93	N94	K95	N96	K97	K98	L99	V100	K101	K102	K106	Y107	D108	A109	F110	G111	A112	S113	E114	S115	L116	I117	K118	Q119	I120	P121	R122	
M1	S2	S3	K4	V5	S6	R7	D8	T9	L10	Y11	E12	A13	V14	R15	E16	V17	L18	H19	G20	N21	Q22	K24	R25	R26	K27	F28	L29	E30	T31	V32	E33	L34	Q35	I36	S37	L38	K39	N40	Y41	D42	P43	Q44	K45	D46	K47	R48	F49	S50	G51	T52	V53	R54	L55	K56	S57	T58	P59	R60	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14634	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.79	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.373	Depositor
Minimum map value	-0.246	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	1070.0, 1070.0, 1070.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.14, 2.14, 2.14	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, SF4

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	A1	0.70	6/41324 (0.0%)	0.43	12/64370 (0.0%)
2	B1	0.35	0/1747	0.57	0/2374
3	C1	0.33	0/1756	0.61	2/2350 (0.1%)
4	D1	0.39	0/1753	0.60	2/2369 (0.1%)
5	E1	0.33	0/1796	0.62	1/2417 (0.0%)
6	F1	0.34	0/2118	0.58	0/2849
7	G1	0.34	0/1492	0.59	0/2005
8	H1	0.35	0/1946	0.71	1/2590 (0.0%)
9	I1	0.30	0/1510	0.62	1/2022 (0.0%)
10	J1	0.37	0/1715	0.62	0/2287
11	K1	0.35	0/1550	0.64	1/2069 (0.0%)
12	L1	0.31	0/834	0.64	2/1125 (0.2%)
13	M1	0.39	0/1195	0.61	0/1597
14	N1	0.27	0/918	0.68	0/1233
15	O1	0.35	0/1226	0.52	0/1649
16	P1	0.35	0/1029	0.56	0/1380
17	Q1	0.37	0/1017	0.70	2/1358 (0.1%)
18	R1	0.35	0/1146	0.64	0/1534
19	S1	0.30	0/1082	0.54	0/1452
20	T1	0.34	0/1208	0.63	0/1618
21	U1	0.35	0/1115	0.62	0/1493
22	V1	0.30	0/805	0.56	0/1081
23	W1	0.36	0/643	0.60	0/860
24	X1	0.40	0/1051	0.64	0/1406
25	Y1	0.37	0/1116	0.60	0/1490
26	Z1	0.31	0/1028	0.53	0/1366
27	a1	0.37	0/604	0.65	0/810
28	b1	0.37	0/828	0.59	0/1109
29	c1	0.32	0/665	0.62	0/891
30	d1	0.34	0/490	0.56	0/656
31	e1	0.37	0/470	0.60	0/623
32	f1	0.30	0/447	0.56	0/587

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	g1	0.22	0/567	0.57	0/753
34	h1	0.29	0/2493	0.59	0/3394
35	j1	0.29	0/3363	0.57	0/4523
36	k1	0.30	0/4640	0.61	0/6264
37	52	1.15	52/87026 (0.1%)	0.49	39/135683 (0.0%)
38	72	2.17	6/2858 (0.2%)	0.44	0/4455
39	82	0.46	0/3581	0.42	0/5577
40	A3	0.55	1/1936 (0.1%)	1.10	15/2596 (0.6%)
41	B3	0.46	0/3240	0.68	4/4339 (0.1%)
42	C3	0.51	0/2937	0.69	0/3946
43	E3	1.82	2/1762 (0.1%)	0.68	1/2362 (0.0%)
44	F3	0.53	0/1911	0.70	1/2549 (0.0%)
45	H3	0.42	0/1535	0.64	0/2063
46	L3	0.46	0/1733	0.72	2/2316 (0.1%)
47	M3	0.46	0/1158	0.65	0/1547
48	N3	0.53	0/1746	0.71	0/2338
49	O3	0.50	0/1662	0.69	0/2222
50	P3	0.50	0/1268	0.65	0/1700
51	Q3	2.37	2/1539 (0.1%)	0.90	3/2054 (0.1%)
52	R3	0.48	0/1524	0.84	1/2013 (0.0%)
53	S3	1.85	2/1501 (0.1%)	0.98	5/2012 (0.2%)
54	T3	0.46	0/1326	0.62	0/1770
55	U3	3.16	3/823 (0.4%)	1.46	8/1104 (0.7%)
56	V3	0.44	0/993	0.66	0/1332
57	W3	0.44	0/873	0.69	0/1158
58	X3	0.42	0/984	0.63	0/1323
59	Y3	0.46	0/1132	0.69	0/1504
60	Z3	0.64	0/1130	1.19	9/1507 (0.6%)
61	a3	0.50	0/1191	0.64	0/1590
62	b3	2.76	2/861 (0.2%)	1.02	6/1138 (0.5%)
63	c3	0.50	1/771 (0.1%)	1.08	5/1034 (0.5%)
64	d3	0.46	0/903	0.70	0/1216
65	e3	0.49	0/1071	0.64	0/1429
66	f3	0.54	0/895	0.69	0/1198
67	g3	4.61	4/916 (0.4%)	1.32	9/1220 (0.7%)
68	h3	0.46	0/1021	0.67	0/1348
69	i3	0.41	0/841	0.68	0/1112
70	j3	0.48	0/720	0.69	0/952
71	k3	0.45	0/575	0.91	0/761
72	l3	0.48	0/459	0.64	0/608
73	m3	0.43	0/435	0.62	0/575
74	n3	0.41	0/240	0.75	0/305
75	o3	0.38	0/864	0.62	0/1140

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	p3	0.47	0/718	0.86	0/953
77	r3	0.49	0/1010	0.72	2/1354 (0.1%)
78	s3	0.69	1/1530 (0.1%)	1.08	7/2064 (0.3%)
79	t3	0.29	0/1174	0.72	0/1582
80	23	0.28	0/1805	0.41	0/2809
81	w3	0.29	0/553	0.52	0/859
82	J3	0.37	0/1385	0.70	2/1852 (0.1%)
83	G3	1.82	2/1910 (0.1%)	1.05	9/2569 (0.4%)
84	D3	0.45	0/2437	0.79	2/3264 (0.1%)
85	I3	1.25	2/1702 (0.1%)	1.11	4/2272 (0.2%)
86	1	0.84	0/109	1.21	1/151 (0.7%)
87	u3	0.28	0/1769	0.82	0/2371
All	All	0.97	86/242730 (0.0%)	0.59	159/355150 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B1	0	1
14	N1	0	1
16	P1	0	1
17	Q1	0	2
25	Y1	0	1
35	j1	0	1
36	k1	0	1
40	A3	0	5
42	C3	0	1
47	M3	0	1
48	N3	0	2
52	R3	0	5
53	S3	0	1
55	U3	0	1
57	W3	0	1
60	Z3	0	3
63	c3	0	1
67	g3	0	8
71	k3	0	1
76	p3	0	2
78	s3	0	4
79	t3	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
83	G3	0	3
85	I3	0	1
87	u3	0	2
All	All	0	51

All (86) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	g3	2	VAL	CA-CB	114.44	4.63	1.54
51	Q3	14	ARG	CD-NE	90.52	2.73	1.46
55	U3	49	VAL	CA-CB	88.62	2.57	1.54
62	b3	28	ARG	CA-CB	79.93	2.68	1.53
83	G3	185	ARG	CD-NE	76.41	2.53	1.46
67	g3	4	ARG	CD-NE	76.34	2.53	1.46
43	E3	65	TYR	CZ-OH	73.56	2.92	1.38
53	S3	68	PHE	CA-C	68.83	2.35	1.52
1	A1	970	G	N1-C2	59.05	2.55	1.37
37	52	2631	U	N1-C2	58.15	2.54	1.38
37	52	732	A	C6-N1	57.38	2.50	1.35
1	A1	970	G	C6-N1	56.71	2.52	1.39
37	52	2631	U	N3-C4	56.71	2.51	1.38
38	72	63	C	C2-N3	56.45	2.48	1.35
37	52	2631	U	C2-N3	56.15	2.50	1.37
37	52	732	A	N1-C2	55.56	2.45	1.34
37	52	732	A	N3-C4	55.17	2.45	1.34
37	52	1805	A	C6-N1	54.94	2.45	1.35
38	72	63	C	N3-C4	53.99	2.41	1.33
37	52	1805	A	N1-C2	53.83	2.42	1.34
37	52	732	A	C2-N3	53.73	2.41	1.33
37	52	1805	A	C5-C6	53.71	2.48	1.41
37	52	1805	A	N3-C4	53.15	2.41	1.34
37	52	2631	U	N1-C6	53.12	2.44	1.38
37	52	2631	U	C4-C5	52.18	2.48	1.43
37	52	1805	A	C2-N3	51.68	2.37	1.33
37	52	119	G	C2-N3	50.16	2.33	1.32
37	52	2399	G	C2-N3	50.02	2.32	1.32
37	52	2399	G	N3-C4	49.34	2.34	1.35
37	52	119	G	N3-C4	49.26	2.33	1.35
37	52	732	A	C5-C6	49.10	2.39	1.41
37	52	2631	U	C5-C6	48.97	2.32	1.34
1	A1	970	G	C2-N3	46.35	2.25	1.32
37	52	1805	A	C5-C4	45.95	2.30	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A1	970	G	C5-C6	45.76	2.33	1.42
1	A1	970	G	N3-C4	45.68	2.26	1.35
37	52	2084	U	N3-C4	45.27	2.29	1.38
37	52	2084	U	C2-N3	44.88	2.27	1.37
37	52	732	A	C5-C4	44.87	2.28	1.38
38	72	63	C	N1-C2	44.83	2.29	1.40
37	52	2084	U	N1-C2	44.77	2.28	1.38
37	52	2084	U	N1-C6	42.81	2.23	1.38
85	I3	203	ARG	C-N	42.20	1.96	1.33
37	52	1239	C	C2-N3	41.80	2.19	1.35
37	52	1239	C	N3-C4	41.49	2.16	1.33
38	72	63	C	N1-C6	41.18	2.19	1.37
1	A1	970	G	C5-C4	41.14	2.20	1.38
38	72	63	C	C4-C5	40.75	2.24	1.43
37	52	2084	U	C4-C5	40.63	2.24	1.43
37	52	119	G	C6-N1	40.02	2.19	1.39
37	52	119	G	N1-C2	39.41	2.16	1.37
37	52	2399	G	C6-N1	39.09	2.17	1.39
37	52	2399	G	N1-C2	38.88	2.15	1.37
37	52	2084	U	C5-C6	38.53	2.11	1.34
38	72	63	C	C5-C6	37.89	2.10	1.34
37	52	3712	A	N1-C2	36.98	2.08	1.34
37	52	3712	A	C2-N3	36.77	2.07	1.33
37	52	2399	G	C5-C6	36.23	2.14	1.42
37	52	119	G	C5-C6	36.19	2.14	1.42
37	52	2399	G	C5-C4	33.17	2.04	1.38
37	52	119	G	C5-C4	32.92	2.04	1.38
37	52	1239	C	N1-C2	30.27	2.00	1.40
37	52	1239	C	N1-C6	28.02	1.93	1.37
37	52	1239	C	C4-C5	26.23	1.95	1.43
37	52	1239	C	C5-C6	24.75	1.83	1.34
85	I3	204	GLY	N-CA	23.17	1.76	1.44
37	52	3712	A	C6-N1	22.95	1.81	1.35
78	s3	186	GLY	C-N	22.74	1.66	1.33
37	52	2395	A	C6-N1	22.04	1.79	1.35
37	52	3712	A	N3-C4	21.88	1.78	1.34
37	52	2395	A	N1-C2	21.41	1.77	1.34
37	52	2395	A	N3-C4	20.41	1.75	1.34
37	52	2395	A	C2-N3	19.95	1.73	1.33
37	52	2395	A	C5-C6	19.40	1.79	1.41
37	52	2395	A	C5-C4	17.85	1.74	1.38
83	G3	185	ARG	NE-CZ	13.46	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	g3	4	ARG	NE-CZ	12.91	1.47	1.33
55	U3	49	VAL	CB-CG1	10.58	1.87	1.52
55	U3	49	VAL	CB-CG2	9.11	1.82	1.52
51	Q3	14	ARG	NE-CZ	8.28	1.42	1.33
62	b3	28	ARG	CB-CG	6.01	1.70	1.52
67	g3	4	ARG	CG-CD	5.91	1.70	1.52
40	A3	101	VAL	C-N	-5.73	1.26	1.33
63	c3	52	CYS	C-N	5.59	1.40	1.33
43	E3	133	LYS	C-N	-5.50	1.25	1.33
53	S3	68	PHE	C-N	5.29	1.41	1.33

All (159) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	52	3712	A	N1-C2-N3	-40.01	9.27	129.30
85	I3	203	ARG	CA-C-N	24.88	160.93	121.87
85	I3	203	ARG	C-N-CA	24.88	160.93	121.87
67	g3	4	ARG	CD-NE-CZ	24.40	158.55	124.40
83	G3	185	ARG	CD-NE-CZ	23.86	157.80	124.40
51	Q3	14	ARG	CD-NE-CZ	23.15	156.81	124.40
53	S3	68	PHE	O-C-N	-20.92	98.83	123.31
78	s3	186	GLY	CA-C-N	17.96	148.68	122.09
78	s3	186	GLY	C-N-CA	17.96	148.68	122.09
55	U3	49	VAL	CA-CB-CG1	17.61	140.34	110.40
62	b3	28	ARG	CA-CB-CG	17.18	148.46	114.10
53	S3	68	PHE	CB-CA-C	16.82	140.14	109.70
55	U3	49	VAL	CA-CB-CG2	16.48	138.41	110.40
55	U3	49	VAL	CB-CA-C	15.53	132.25	110.98
55	U3	49	VAL	N-CA-C	-15.38	85.53	107.99
85	I3	203	ARG	CA-C-O	-15.25	102.33	121.55
55	U3	49	VAL	CG1-CB-CG2	-15.09	77.61	110.80
37	52	3712	A	C2-N3-C4	14.68	154.63	110.60
55	U3	49	VAL	N-CA-CB	14.59	128.28	111.21
62	b3	28	ARG	CB-CA-C	14.37	131.82	110.26
78	s3	186	GLY	O-C-N	-14.27	97.33	123.16
1	A1	168	C	OP1-P-OP2	-14.13	77.22	119.60
37	52	3712	A	C6-N1-C2	13.89	160.27	118.60
53	S3	68	PHE	CA-C-O	13.18	134.94	120.32
63	c3	30	GLY	N-CA-C	12.23	129.03	114.48
51	Q3	14	ARG	CG-CD-NE	11.44	137.17	112.00
1	A1	167	G	OP2-P-O3'	-10.82	75.54	108.00
62	b3	28	ARG	N-CA-C	-10.51	94.14	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	Z3	38	TYR	N-CA-C	10.44	121.60	108.45
1	A1	168	C	O5'-P-OP1	-10.32	77.04	108.00
1	A1	167	G	OP1-P-O3'	10.25	138.75	108.00
67	g3	4	ARG	CG-CD-NE	9.62	133.16	112.00
83	G3	185	ARG	CG-CD-NE	8.98	131.75	112.00
53	S3	68	PHE	N-CA-CB	-8.71	95.73	110.80
37	52	3712	A	N3-C4-N9	8.70	153.51	127.40
83	G3	185	ARG	NE-CZ-NH1	8.65	130.15	121.50
8	H1	130	PRO	CA-C-O	-8.42	111.44	121.03
37	52	3712	A	C4-C5-C6	-8.02	92.94	117.00
85	I3	204	GLY	N-CA-C	7.83	128.31	112.34
62	b3	28	ARG	N-CA-CB	7.75	121.64	109.71
43	E3	65	TYR	CE1-CZ-CE2	-7.71	104.89	120.30
67	g3	2	VAL	CA-CB-CG1	7.66	123.42	110.40
17	Q1	66	GLU	CA-C-N	7.62	132.27	120.60
17	Q1	66	GLU	C-N-CA	7.62	132.27	120.60
37	52	2581	A	C5'-C4'-C3'	7.40	127.09	116.00
40	A3	233	ARG	N-CA-C	-7.16	105.47	114.56
37	52	2399	G	N3-C4-N9	7.14	147.42	126.00
67	g3	4	ARG	NE-CZ-NH1	7.03	128.53	121.50
40	A3	126	LEU	CA-CB-CG	6.88	140.39	116.30
67	g3	2	VAL	CA-CB-CG2	6.88	122.09	110.40
9	I1	75	ILE	N-CA-C	-6.87	106.61	113.20
37	52	119	G	N3-C4-N9	6.81	146.43	126.00
40	A3	125	LYS	CA-C-N	6.78	134.48	121.54
40	A3	125	LYS	C-N-CA	6.78	134.48	121.54
67	g3	43	LYS	CA-C-N	6.68	134.30	121.54
67	g3	43	LYS	C-N-CA	6.68	134.30	121.54
63	c3	31	TYR	CA-C-N	-6.68	112.55	122.56
63	c3	31	TYR	C-N-CA	-6.68	112.55	122.56
51	Q3	14	ARG	NE-CZ-NH1	6.64	128.14	121.50
37	52	2753	G	O3'-P-O5'	6.59	113.89	104.00
40	A3	117	GLU	CB-CA-C	-6.51	97.46	110.42
40	A3	117	GLU	N-CA-C	6.44	124.53	110.80
3	C1	34	LYS	CA-C-N	6.44	134.61	121.48
3	C1	34	LYS	C-N-CA	6.44	134.61	121.48
55	U3	49	VAL	CA-C-N	6.42	133.79	121.54
55	U3	49	VAL	C-N-CA	6.42	133.79	121.54
1	A1	168	C	O5'-P-OP2	6.40	127.19	108.00
37	52	3712	A	N3-C4-C5	-6.37	107.70	126.80
83	G3	114	ILE	N-CA-C	-6.34	107.11	113.20
60	Z3	74	VAL	CA-C-N	6.30	133.57	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	Z3	74	VAL	C-N-CA	6.30	133.57	121.54
83	G3	96	GLN	N-CA-C	-6.29	106.83	114.75
4	D1	251	LEU	CA-C-N	6.22	129.32	120.49
4	D1	251	LEU	C-N-CA	6.22	129.32	120.49
44	F3	174	ILE	N-CA-C	-6.21	106.87	111.90
60	Z3	72	VAL	CA-C-N	6.19	133.36	121.54
60	Z3	72	VAL	C-N-CA	6.19	133.36	121.54
37	52	732	A	N7-C8-N9	6.16	132.28	113.80
40	A3	43	GLY	N-CA-C	6.16	127.77	113.18
41	B3	213	GLN	CA-C-N	6.13	131.10	122.46
41	B3	213	GLN	C-N-CA	6.13	131.10	122.46
37	52	2580	U	OP2-P-O3'	-6.09	89.72	108.00
37	52	2754	G	O5'-C5'-C4'	6.09	120.84	111.70
83	G3	185	ARG	NE-CZ-NH2	-6.09	113.72	119.20
40	A3	168	VAL	CA-C-N	6.06	132.88	121.97
40	A3	168	VAL	C-N-CA	6.06	132.88	121.97
37	52	2580	U	O3'-P-O5'	6.05	113.08	104.00
86	1	11	ALA	N-CA-C	6.04	117.42	108.60
62	b3	27	GLN	CA-C-N	6.00	129.89	121.24
62	b3	27	GLN	C-N-CA	6.00	129.89	121.24
37	52	2395	A	N1-C2-N3	-6.00	111.29	129.30
67	g3	43	LYS	N-CA-C	5.88	118.98	109.40
78	s3	82	ILE	CA-CB-CG2	5.88	120.49	110.50
78	s3	85	ASN	N-CA-C	5.85	116.97	107.32
63	c3	30	GLY	CA-C-N	5.84	136.02	126.86
63	c3	30	GLY	C-N-CA	5.84	136.02	126.86
37	52	2021	G	N9-C1'-C2'	5.83	120.74	112.00
37	52	732	A	N3-C4-N9	5.82	144.87	127.40
37	52	732	A	N1-C2-N3	-5.80	111.90	129.30
37	52	1805	A	C4-C5-N7	-5.77	93.39	110.70
84	D3	275	GLN	N-CA-C	-5.75	106.81	113.88
37	52	2399	G	N1-C2-N3	-5.72	106.73	123.90
60	Z3	75	TYR	N-CA-C	5.72	122.97	110.80
37	52	119	G	N1-C2-N3	-5.69	106.82	123.90
11	K1	46	VAL	N-CA-C	-5.69	107.27	112.96
37	52	2399	G	C2-N3-C4	5.67	128.90	111.90
40	A3	126	LEU	CB-CA-C	-5.65	99.17	110.42
40	A3	126	LEU	N-CA-C	5.65	122.83	110.80
67	g3	4	ARG	NE-CZ-NH2	-5.62	114.14	119.20
83	G3	265	LYS	N-CA-C	-5.58	107.47	114.56
84	D3	11	ALA	N-CA-C	-5.58	106.83	113.97
12	L1	63	ALA	CA-C-N	5.57	132.17	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L1	63	ALA	C-N-CA	5.57	132.17	121.54
37	52	119	G	C2-N3-C4	5.55	128.56	111.90
37	52	1805	A	N7-C8-N9	5.55	130.44	113.80
1	A1	167	G	O3'-P-O5'	-5.54	95.70	104.00
53	S3	68	PHE	CA-CB-CG	5.53	119.33	113.80
37	52	1970	A	N9-C1'-C2'	5.52	120.28	112.00
83	G3	98	ILE	CA-C-N	5.52	128.72	120.83
83	G3	98	ILE	C-N-CA	5.52	128.72	120.83
1	A1	751	G	P-O3'-C3'	5.50	128.45	120.20
78	s3	33	ASP	CA-C-N	5.49	132.03	121.54
78	s3	33	ASP	C-N-CA	5.49	132.03	121.54
46	L3	63	THR	CA-C-N	5.49	131.85	121.97
46	L3	63	THR	C-N-CA	5.49	131.85	121.97
82	J3	9	GLU	CA-C-N	5.48	128.67	120.83
82	J3	9	GLU	C-N-CA	5.48	128.67	120.83
37	52	1805	A	N1-C2-N3	-5.47	112.88	129.30
37	52	2399	G	N3-C4-C5	-5.47	112.18	128.60
37	52	48	G	P-O3'-C3'	5.46	128.39	120.20
37	52	2046	G	P-O3'-C3'	5.45	128.38	120.20
37	52	732	A	C4-C5-N7	-5.44	94.38	110.70
40	A3	149	LYS	N-CA-C	5.43	117.19	111.28
77	r3	32	LEU	CA-C-N	5.42	131.90	121.54
77	r3	32	LEU	C-N-CA	5.42	131.90	121.54
60	Z3	73	LYS	CB-CA-C	5.38	121.13	110.42
37	52	2021	G	O4'-C1'-N9	5.36	116.54	108.50
1	A1	970	G	N1-C2-N3	-5.35	107.84	123.90
37	52	2395	A	C2-N3-C4	5.26	126.39	110.60
40	A3	115	CYS	CA-C-N	5.26	131.59	121.54
40	A3	115	CYS	C-N-CA	5.26	131.59	121.54
1	A1	1664	A	P-O3'-C3'	5.26	128.09	120.20
37	52	119	G	N3-C4-C5	-5.25	112.84	128.60
37	52	2875	C	P-O3'-C3'	5.24	128.05	120.20
37	52	1239	C	N1-C2-N3	-5.23	103.52	119.20
1	A1	970	G	C2-N3-C4	5.21	127.52	111.90
37	52	930	G	C2'-C3'-O3'	5.17	121.46	113.70
52	R3	85	ALA	N-CA-C	-5.16	106.39	113.30
1	A1	970	G	C4-C5-N7	-5.09	95.52	110.80
40	A3	117	GLU	CA-CB-CG	5.08	124.25	114.10
41	B3	17	LEU	CA-C-N	-5.08	113.50	119.84
41	B3	17	LEU	C-N-CA	-5.08	113.50	119.84
37	52	1805	A	N3-C4-N9	5.07	142.62	127.40
1	A1	970	G	N7-C8-N9	5.07	128.30	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	52	2597	G	O3'-P-O5'	5.06	111.58	104.00
5	E1	143	ARG	CA-CB-CG	5.05	124.21	114.10
37	52	2089	G	P-O3'-C3'	5.02	127.73	120.20
60	Z3	37	PRO	CA-C-N	-5.02	113.57	122.20
60	Z3	37	PRO	C-N-CA	-5.02	113.57	122.20

There are no chirality outliers.

All (51) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
40	A3	116	LEU	Peptide
40	A3	117	GLU	Peptide
40	A3	168	VAL	Peptide
40	A3	170	ALA	Peptide
40	A3	94	ALA	Peptide
2	B1	42	LYS	Peptide
42	C3	339	THR	Peptide
83	G3	157	PRO	Peptide
83	G3	186	PRO	Peptide
83	G3	214	VAL	Peptide
85	I3	204	GLY	Peptide
47	M3	69	ARG	Peptide
14	N1	37	GLU	Peptide
48	N3	76	PRO	Peptide
48	N3	78	GLY	Peptide
16	P1	21	VAL	Peptide
17	Q1	17	TYR	Peptide
17	Q1	37	TYR	Peptide
52	R3	106	LEU	Peptide
52	R3	113	LYS	Peptide
52	R3	123	LEU	Peptide
52	R3	129	GLY	Peptide
52	R3	83	GLY	Peptide
53	S3	68	PHE	Peptide
55	U3	86	LEU	Peptide
57	W3	85	ALA	Peptide
25	Y1	61	GLN	Peptide
60	Z3	18	TYR	Peptide
60	Z3	79	HIS	Peptide
60	Z3	92	ASP	Peptide
63	c3	87	LYS	Peptide
67	g3	2	VAL	Peptide

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Mol	Chain	Res	Type	Group
67	g3	4	ARG	Sidechain
67	g3	43	LYS	Mainchain
67	g3	44	SER	Peptide
67	g3	73	HIS	Peptide
67	g3	93	ARG	Peptide
67	g3	94	ALA	Peptide
67	g3	99	GLU	Peptide
35	j1	315	GLY	Peptide
36	k1	364	ILE	Peptide
71	k3	43	TYR	Peptide
76	p3	50	ARG	Peptide
76	p3	52	VAL	Peptide
78	s3	33	ASP	Peptide
78	s3	72	ASN	Peptide
78	s3	81	HIS	Peptide
78	s3	86	VAL	Peptide
79	t3	53	TRP	Peptide
87	u3	209	THR	Peptide
87	u3	60	ARG	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A1	36969	0	18687	200	0
2	B1	1710	0	1708	15	0
3	C1	1729	0	1803	21	0
4	D1	1716	0	1806	12	0
5	E1	1768	0	1866	23	0
6	F1	2076	0	2177	14	0
7	G1	1471	0	1522	10	0
8	H1	1923	0	2089	36	0
9	I1	1488	0	1582	8	0
10	J1	1686	0	1772	16	0
11	K1	1525	0	1640	13	0
12	L1	810	0	836	6	0
13	M1	1175	0	1249	12	0
14	N1	908	0	939	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	O1	1202	0	1289	7	0
16	P1	1016	0	1039	15	0
17	Q1	997	0	1045	8	0
18	R1	1128	0	1195	11	0
19	S1	1068	0	1121	13	0
20	T1	1190	0	1249	8	0
21	U1	1097	0	1132	9	0
22	V1	795	0	862	7	0
23	W1	636	0	637	3	0
24	X1	1034	0	1080	14	0
25	Y1	1098	0	1167	8	0
26	Z1	1011	0	1083	10	0
27	a1	598	0	656	11	0
28	b1	814	0	865	10	0
29	c1	651	0	672	5	0
30	d1	488	0	514	4	0
31	e1	459	0	449	3	0
32	f1	443	0	492	0	0
33	g1	555	0	564	5	0
34	h1	2436	0	2393	42	0
35	j1	3309	0	3350	22	0
36	k1	4555	0	4696	44	0
37	52	77819	0	39310	770	0
38	72	2558	0	1296	37	0
39	82	3208	0	1629	13	0
40	A3	1898	0	1993	49	0
41	B3	3172	0	3310	30	0
42	C3	2883	0	3053	18	0
43	E3	1729	0	1887	33	0
44	F3	1875	0	1995	19	0
45	H3	1516	0	1597	7	0
46	L3	1702	0	1820	15	0
47	M3	1137	0	1211	12	0
48	N3	1701	0	1749	27	0
49	O3	1630	0	1778	13	0
50	P3	1242	0	1274	7	0
51	Q3	1515	0	1634	31	0
52	R3	1508	0	1664	31	0
53	S3	1462	0	1508	35	0
54	T3	1298	0	1366	11	0
55	U3	809	0	833	41	0
56	V3	979	0	1039	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	W3	860	0	903	20	0
58	X3	967	0	1040	8	0
59	Y3	1115	0	1205	13	0
60	Z3	1107	0	1182	45	0
61	a3	1162	0	1209	12	0
62	b3	848	0	920	28	0
63	c3	761	0	794	25	0
64	d3	888	0	930	4	0
65	e3	1053	0	1147	6	0
66	f3	876	0	912	14	0
67	g3	906	0	1001	71	0
68	h3	1013	0	1147	5	0
69	i3	830	0	916	52	0
70	j3	705	0	737	0	0
71	k3	569	0	637	17	0
72	l3	447	0	480	1	0
73	m3	429	0	465	7	0
74	n3	239	0	289	4	0
75	o3	851	0	922	6	0
76	p3	708	0	757	15	0
77	r3	994	0	1051	11	0
78	s3	1507	0	1564	102	0
79	t3	1160	0	1218	21	0
80	23	1616	0	824	7	0
81	w3	493	0	249	4	0
82	J3	1362	0	1399	10	0
83	G3	1879	0	2027	37	0
84	D3	2391	0	2424	26	0
85	I3	1664	0	1711	29	0
86	1	110	0	112	9	0
87	u3	1741	0	1854	100	0
88	52	204	0	0	0	0
88	72	7	0	0	0	0
88	82	5	0	0	0	0
88	A1	77	0	0	0	0
88	G1	1	0	0	0	0
88	M1	1	0	0	0	0
88	P3	1	0	0	0	0
88	V3	1	0	0	0	0
88	a3	1	0	0	0	0
88	g3	1	0	0	0	0
88	w3	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
89	b1	1	0	0	0	0
89	e1	1	0	0	0	0
89	g1	1	0	0	0	0
89	g3	1	0	0	0	0
89	j3	1	0	0	0	0
89	m3	1	0	0	0	0
89	o3	1	0	0	0	0
89	p3	1	0	0	0	0
90	k1	16	0	0	0	0
91	1	1	0	0	0	0
91	52	3	0	0	0	0
All	All	226754	0	171198	1914	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (1914) 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)
37:52:2395:A:C5	37:52:2395:A:C6	1.79	1.66
37:52:1239:C:C5	37:52:1239:C:C6	1.83	1.62
55:U3:49:VAL:CB	55:U3:49:VAL:CG2	1.82	1.56
37:52:1239:C:C5	37:52:1239:C:C4	1.95	1.55
69:i3:103:LYS:CB	87:u3:7:ARG:HG2	1.36	1.54
37:52:2395:A:N3	37:52:2395:A:C2	1.73	1.53
37:52:2395:A:C2	37:52:2395:A:N1	1.77	1.53
55:U3:49:VAL:CB	55:U3:49:VAL:CG1	1.87	1.53
37:52:2395:A:N3	37:52:2395:A:C4	1.75	1.52
37:52:3712:A:C4	37:52:3712:A:N3	1.78	1.50
37:52:2395:A:C5	37:52:2395:A:C4	1.74	1.48
37:52:3712:A:C6	37:52:3712:A:N1	1.81	1.48
37:52:2395:A:C6	37:52:2395:A:N1	1.79	1.47
69:i3:103:LYS:CA	87:u3:7:ARG:NE	1.74	1.46
85:I3:204:GLY:N	85:I3:204:GLY:CA	1.76	1.46
78:s3:193:PHE:CD1	78:s3:198:ILE:CG1	2.03	1.41
69:i3:99:LYS:HA	87:u3:9:THR:CG2	1.51	1.40
37:52:2399:G:C5	37:52:2399:G:C4	2.04	1.39
38:72:63:C:C5	38:72:63:C:C6	2.10	1.39
37:52:2084:U:C6	37:52:2084:U:C5	2.11	1.38
37:52:119:G:C4	37:52:119:G:C5	2.04	1.38
78:s3:30:VAL:HB	78:s3:187:LEU:CD1	1.52	1.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:s3:193:PHE:HD1	78:s3:198:ILE:CG1	1.37	1.37
37:52:1239:C:C6	37:52:1239:C:N1	1.93	1.36
37:52:2399:G:C5	37:52:2399:G:C6	2.14	1.35
37:52:119:G:C5	37:52:119:G:C6	2.14	1.34
37:52:3712:A:C4	37:52:3712:A:N1	1.96	1.34
37:52:2399:G:N3	67:g3:4:ARG:NE	1.78	1.32
37:52:3712:A:N3	37:52:3712:A:C6	1.97	1.32
38:72:63:C:N3	85:I3:204:GLY:N	1.73	1.31
37:52:1239:C:N1	37:52:1239:C:C2	2.00	1.30
37:52:119:G:N3	83:G3:185:ARG:NE	1.78	1.29
78:s3:192:VAL:O	78:s3:198:ILE:HG23	1.22	1.29
69:i3:103:LYS:HB2	87:u3:7:ARG:CG	1.62	1.29
69:i3:99:LYS:C	87:u3:9:THR:HG21	1.56	1.28
78:s3:193:PHE:CE1	78:s3:198:ILE:HD11	1.67	1.27
38:72:63:C:C5	38:72:63:C:C4	2.24	1.24
37:52:1239:C:N3	43:E3:65:TYR:OH	1.69	1.24
85:I3:203:ARG:C	85:I3:204:GLY:N	1.96	1.24
37:52:2084:U:C5	37:52:2084:U:C4	2.24	1.24
1:A1:970:G:C4	1:A1:970:G:C5	2.20	1.23
37:52:3712:A:N3	37:52:3712:A:C2	2.07	1.22
37:52:3712:A:N1	37:52:3712:A:C2	2.08	1.21
78:s3:192:VAL:HB	78:s3:199:TYR:O	1.08	1.21
78:s3:192:VAL:O	78:s3:198:ILE:CG2	1.87	1.20
69:i3:99:LYS:O	87:u3:9:THR:HG21	1.34	1.20
37:52:3974:G:H4'	87:u3:26:ARG:NE	1.55	1.20
37:52:1805:A:C4	37:52:1805:A:C5	2.30	1.19
37:52:732:A:C4	37:52:732:A:C5	2.28	1.18
37:52:2631:U:C6	37:52:2631:U:C5	2.32	1.18
78:s3:192:VAL:CB	78:s3:199:TYR:O	1.92	1.18
37:52:3974:G:C4'	87:u3:26:ARG:NE	2.08	1.17
1:A1:970:G:N1	37:52:3712:A:N1	1.92	1.17
69:i3:103:LYS:CD	87:u3:10:LEU:HD11	1.75	1.17
1:A1:970:G:C5	1:A1:970:G:C6	2.33	1.16
69:i3:103:LYS:HD2	87:u3:10:LEU:CD1	1.75	1.16
78:s3:193:PHE:CD1	78:s3:198:ILE:HG13	1.78	1.15
69:i3:99:LYS:CA	87:u3:9:THR:HG21	1.74	1.14
37:52:2399:G:C2	37:52:2399:G:N1	2.15	1.14
78:s3:193:PHE:CD1	78:s3:198:ILE:HG12	1.75	1.13
37:52:1239:C:C4	37:52:1239:C:N3	2.16	1.13
37:52:119:G:C2	37:52:119:G:N1	2.16	1.13
37:52:2399:G:C6	37:52:2399:G:N1	2.17	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:i3:99:LYS:CA	87:u3:9:THR:CG2	2.27	1.12
78:s3:192:VAL:HG21	78:s3:200:ASN:CA	1.79	1.11
78:s3:192:VAL:CG2	78:s3:200:ASN:HA	1.81	1.11
37:52:1239:C:C2	37:52:1239:C:N3	2.19	1.11
37:52:732:A:C5	37:52:732:A:C6	2.39	1.10
38:72:63:C:C6	38:72:63:C:N1	2.19	1.10
37:52:119:G:C6	37:52:119:G:N1	2.19	1.09
69:i3:103:LYS:HA	87:u3:7:ARG:NE	0.82	1.09
78:s3:192:VAL:HG21	78:s3:200:ASN:HA	1.20	1.09
78:s3:30:VAL:HB	78:s3:187:LEU:HD13	1.12	1.08
55:U3:49:VAL:CG2	55:U3:49:VAL:CG1	2.31	1.08
69:i3:103:LYS:HD2	87:u3:10:LEU:HD11	1.07	1.06
55:U3:49:VAL:HB	55:U3:49:VAL:CA	1.86	1.06
37:52:3974:G:OP1	87:u3:27:LYS:HB3	1.54	1.06
69:i3:99:LYS:O	87:u3:9:THR:CG2	2.04	1.06
37:52:2084:U:C6	37:52:2084:U:N1	2.23	1.05
1:A1:970:G:C2	1:A1:970:G:N3	2.25	1.04
38:72:63:C:C2	85:I3:204:GLY:N	2.26	1.03
37:52:2084:U:C2	37:52:2084:U:N3	2.27	1.03
1:A1:970:G:C4	1:A1:970:G:N3	2.26	1.03
37:52:2631:U:C5	37:52:2631:U:C4	2.47	1.02
37:52:2084:U:N1	37:52:2084:U:C2	2.28	1.02
69:i3:103:LYS:CB	87:u3:7:ARG:CG	2.27	1.02
69:i3:99:LYS:HA	87:u3:9:THR:CB	1.89	1.01
37:52:1805:A:C5	37:52:1805:A:C6	2.48	1.01
69:i3:102:ALA:O	87:u3:7:ARG:NH1	1.75	1.01
37:52:2084:U:C4	37:52:2084:U:N3	2.29	1.00
55:U3:49:VAL:HG21	55:U3:49:VAL:HG11	1.38	1.00
78:s3:31:GLY:O	78:s3:187:LEU:CB	2.08	1.00
38:72:63:C:N1	38:72:63:C:C2	2.29	1.00
53:S3:68:PHE:C	53:S3:68:PHE:CA	2.35	1.00
37:52:119:G:C2	83:G3:185:ARG:NE	2.31	0.99
37:52:732:A:N1	53:S3:69:GLU:N	2.09	0.99
78:s3:30:VAL:CB	78:s3:187:LEU:HD13	1.91	0.99
69:i3:103:LYS:CA	87:u3:7:ARG:HG2	1.91	0.98
78:s3:193:PHE:HD1	78:s3:198:ILE:HG12	0.83	0.98
37:52:2399:G:C4	67:g3:4:ARG:NE	2.31	0.98
37:52:2399:G:C2	67:g3:4:ARG:NE	2.30	0.98
37:52:119:G:C4	83:G3:185:ARG:NE	2.31	0.98
37:52:4042:G:H1'	87:u3:101:LYS:NZ	1.79	0.98
37:52:2399:G:N3	37:52:2399:G:C2	2.32	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:72:63:C:C4	85:I3:204:GLY:N	2.32	0.97
37:52:119:G:C4	37:52:119:G:N3	2.34	0.96
37:52:119:G:N3	37:52:119:G:C2	2.33	0.96
37:52:4055:U:O2'	87:u3:162:VAL:HG11	1.63	0.96
37:52:2399:G:C4	37:52:2399:G:N3	2.34	0.96
37:52:2631:U:C5	55:U3:49:VAL:HA	2.01	0.95
78:s3:193:PHE:CD1	78:s3:198:ILE:CD1	2.50	0.95
69:i3:99:LYS:HA	87:u3:9:THR:OG1	1.66	0.94
78:s3:31:GLY:O	78:s3:187:LEU:HB2	1.66	0.94
37:52:732:A:N1	53:S3:68:PHE:HA	1.82	0.93
37:52:2631:U:N3	55:U3:49:VAL:HB	1.83	0.93
37:52:2631:U:C6	55:U3:49:VAL:HA	2.04	0.92
78:s3:193:PHE:CE1	78:s3:198:ILE:CD1	2.51	0.92
37:52:1805:A:C2	37:52:1805:A:N3	2.36	0.92
1:A1:970:G:N1	37:52:3712:A:N3	2.18	0.92
37:52:1805:A:C5	62:b3:28:ARG:HB3	2.05	0.92
78:s3:30:VAL:CB	78:s3:187:LEU:CD1	2.44	0.92
69:i3:99:LYS:HA	87:u3:9:THR:HG23	1.53	0.90
37:52:2084:U:C2	51:Q3:14:ARG:NE	2.40	0.90
37:52:732:A:N3	37:52:732:A:C2	2.41	0.89
37:52:1805:A:C4	37:52:1805:A:N3	2.41	0.89
37:52:3974:G:C5'	87:u3:26:ARG:NE	2.34	0.89
37:52:1239:C:C2	43:E3:65:TYR:OH	2.26	0.89
37:52:1805:A:C2	37:52:1805:A:N1	2.42	0.88
1:A1:970:G:N1	37:52:3712:A:C2	2.42	0.88
38:72:63:C:N3	38:72:63:C:C4	2.41	0.88
69:i3:103:LYS:CE	87:u3:10:LEU:HD11	2.03	0.87
69:i3:99:LYS:HA	87:u3:9:THR:HG21	1.37	0.86
37:52:732:A:N3	53:S3:68:PHE:N	2.22	0.86
37:52:4055:U:O2'	87:u3:162:VAL:CG1	2.22	0.86
37:52:2631:U:C6	37:52:2631:U:N1	2.44	0.86
37:52:3974:G:H5''	87:u3:26:ARG:NE	1.91	0.86
37:52:1805:A:C4	62:b3:28:ARG:HA	2.11	0.85
78:s3:193:PHE:CD1	78:s3:198:ILE:HD11	2.11	0.85
37:52:732:A:C4	37:52:732:A:N3	2.45	0.85
78:s3:192:VAL:HG21	78:s3:200:ASN:C	2.01	0.85
1:A1:970:G:C2	37:52:3712:A:N1	2.43	0.85
37:52:1805:A:C6	37:52:1805:A:N1	2.45	0.85
37:52:3974:G:O3'	87:u3:26:ARG:NE	2.10	0.85
69:i3:103:LYS:HD2	87:u3:10:LEU:CG	2.08	0.84
78:s3:193:PHE:HE1	78:s3:198:ILE:HD11	1.31	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:52:732:A:N1	37:52:732:A:C2	2.45	0.84
69:i3:103:LYS:HA	87:u3:7:ARG:CZ	2.02	0.84
37:52:1239:C:C4	43:E3:65:TYR:OH	2.30	0.83
55:U3:49:VAL:CG1	55:U3:49:VAL:HG21	2.02	0.83
78:s3:192:VAL:C	78:s3:198:ILE:HG23	2.03	0.83
37:52:1805:A:N3	62:b3:28:ARG:HA	1.95	0.82
37:52:4042:G:C1'	87:u3:101:LYS:HZ2	1.92	0.82
37:52:4042:G:H4'	87:u3:101:LYS:H	1.43	0.82
37:52:1805:A:N3	62:b3:28:ARG:HB2	1.94	0.82
38:72:63:C:N3	38:72:63:C:C2	2.48	0.82
1:A1:970:G:C2	37:52:3712:A:C2	2.68	0.81
55:U3:49:VAL:CB	55:U3:49:VAL:CA	2.57	0.81
37:52:4042:G:C1'	87:u3:101:LYS:NZ	2.43	0.81
1:A1:970:G:C4	37:52:3712:A:C2	2.69	0.80
37:52:2631:U:C2	55:U3:49:VAL:HB	2.16	0.80
37:52:732:A:C6	37:52:732:A:N1	2.50	0.80
37:52:732:A:C6	53:S3:68:PHE:C	2.60	0.80
37:52:2084:U:C4	51:Q3:14:ARG:NE	2.49	0.80
37:52:2399:G:C5	67:g3:4:ARG:NE	2.50	0.80
1:A1:970:G:C6	37:52:3712:A:C2	2.70	0.80
37:52:1239:C:N3	43:E3:65:TYR:CZ	2.51	0.79
37:52:2631:U:N3	37:52:2631:U:C2	2.50	0.79
37:52:2794:C:N3	86:l:11:ALA:HB3	1.97	0.79
69:i3:103:LYS:CA	87:u3:7:ARG:HE	1.66	0.79
37:52:2753:G:H2'	60:Z3:51:ARG:HH21	1.47	0.79
78:s3:5:ASP:N	78:s3:8:THR:HG1	1.81	0.79
37:52:2084:U:N1	51:Q3:14:ARG:NE	2.31	0.79
37:52:732:A:C5	53:S3:68:PHE:C	2.61	0.79
37:52:2084:U:C6	51:Q3:14:ARG:NE	2.51	0.79
55:U3:49:VAL:CG2	55:U3:49:VAL:HG11	2.05	0.78
80:23:50:U:H3	80:23:64:G:H1	1.30	0.78
37:52:1239:C:C2	43:E3:65:TYR:CZ	2.71	0.78
37:52:2631:U:C4	37:52:2631:U:N3	2.51	0.78
37:52:119:G:C5	83:G3:185:ARG:NE	2.52	0.77
37:52:4043:G:OP1	87:u3:100:VAL:HG13	1.83	0.77
1:A1:970:G:N1	1:A1:970:G:C6	2.53	0.77
37:52:732:A:C2	53:S3:68:PHE:C	2.63	0.77
37:52:2581:A:H5''	60:Z3:73:LYS:HB3	1.67	0.77
1:A1:970:G:C6	37:52:3712:A:N3	2.52	0.77
1:A1:970:G:C5	37:52:3712:A:C2	2.73	0.77
78:s3:31:GLY:C	78:s3:187:LEU:HB2	2.09	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:i3:99:LYS:CA	87:u3:9:THR:OG1	2.32	0.76
37:52:3974:G:C3'	87:u3:26:ARG:NE	2.49	0.76
1:A1:1033:G:H1	1:A1:1080:A:HO2'	1.34	0.76
37:52:2395:A:C6	67:g3:2:VAL:HB	2.20	0.76
8:H1:130:PRO:O	57:W3:84:GLY:N	2.19	0.75
37:52:1805:A:C6	62:b3:28:ARG:CB	2.70	0.75
37:52:1805:A:C4	62:b3:28:ARG:HB3	2.21	0.75
37:52:2631:U:N1	37:52:2631:U:C2	2.54	0.75
37:52:1805:A:C4	62:b3:28:ARG:CB	2.69	0.74
1:A1:970:G:N1	1:A1:970:G:C2	2.55	0.74
37:52:732:A:N1	53:S3:68:PHE:C	2.45	0.74
78:s3:31:GLY:O	78:s3:187:LEU:HB3	1.85	0.74
37:52:2084:U:N3	51:Q3:14:ARG:NE	2.35	0.74
37:52:1805:A:C5	62:b3:28:ARG:CB	2.72	0.73
37:52:2084:U:C5	51:Q3:14:ARG:NE	2.55	0.73
37:52:2399:G:C6	67:g3:4:ARG:NE	2.55	0.73
37:52:2631:U:C2	55:U3:49:VAL:CB	2.71	0.73
37:52:4042:G:O3'	87:u3:100:VAL:HA	1.88	0.73
40:A3:118:GLU:H	40:A3:162:ASN:HD22	1.35	0.73
37:52:732:A:C4	53:S3:68:PHE:C	2.67	0.72
78:s3:28:PHE:HB2	78:s3:89:VAL:HB	1.71	0.72
62:b3:28:ARG:CB	62:b3:28:ARG:CA	2.68	0.72
83:G3:185:ARG:NE	83:G3:185:ARG:CD	2.53	0.72
37:52:4124:G:N7	40:A3:64:ARG:NH2	2.37	0.72
38:72:63:C:N1	85:I3:204:GLY:N	2.38	0.71
37:52:119:G:C6	83:G3:185:ARG:NE	2.58	0.71
38:72:6:C:H42	84:D3:71:GLY:HA2	1.55	0.71
1:A1:970:G:C4	37:52:3712:A:N3	2.58	0.71
69:i3:98:ARG:C	87:u3:9:THR:OG1	2.32	0.71
37:52:2399:G:N1	67:g3:4:ARG:NE	2.39	0.71
67:g3:4:ARG:NE	67:g3:4:ARG:CD	2.53	0.71
69:i3:98:ARG:O	87:u3:9:THR:CB	2.39	0.71
1:A1:970:G:C5	37:52:3712:A:N3	2.59	0.71
37:52:4042:G:H1'	87:u3:101:LYS:HZ1	1.53	0.71
16:P1:34:PHE:HB3	16:P1:41:PHE:HB2	1.70	0.70
1:A1:970:G:C6	37:52:3712:A:N1	2.59	0.70
37:52:1805:A:C2	62:b3:28:ARG:CB	2.74	0.70
37:52:2753:G:H5''	60:Z3:51:ARG:HG2	1.74	0.70
40:A3:181:LYS:HG3	40:A3:183:GLY:H	1.55	0.70
37:52:4424:A:H5'	73:m3:96:ARG:HH12	1.55	0.70
67:g3:78:TYR:HA	67:g3:81:SER:HB3	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:s3:192:VAL:HG11	78:s3:199:TYR:C	2.17	0.69
37:52:1239:C:C4	43:E3:65:TYR:CZ	2.80	0.69
76:p3:42:CYS:SG	76:p3:43:GLY:N	2.66	0.69
78:s3:193:PHE:HA	78:s3:198:ILE:HG23	1.75	0.69
37:52:4042:G:O3'	87:u3:100:VAL:HG12	1.92	0.69
48:N3:163:GLY:O	48:N3:172:ARG:NH2	2.26	0.69
37:52:119:G:N1	83:G3:185:ARG:NE	2.40	0.69
37:52:989:U:H3	37:52:1065:G:H1	1.41	0.69
37:52:2754:G:N3	60:Z3:51:ARG:NH1	2.41	0.69
1:A1:122:G:H1	1:A1:342:C:H42	1.40	0.68
37:52:732:A:N3	53:S3:68:PHE:C	2.51	0.68
60:Z3:128:LYS:HA	60:Z3:131:PHE:HD2	1.58	0.68
69:i3:103:LYS:C	87:u3:7:ARG:NE	2.52	0.68
1:A1:1860:A:N7	28:b1:34:LYS:NZ	2.42	0.68
14:N1:58:GLU:HB3	14:N1:61:TYR:HB3	1.75	0.68
37:52:2753:G:H3'	60:Z3:51:ARG:HE	1.58	0.68
78:s3:193:PHE:CG	78:s3:198:ILE:HG13	2.28	0.68
37:52:4043:G:OP1	87:u3:100:VAL:CG1	2.42	0.68
1:A1:970:G:N3	37:52:3712:A:C2	2.62	0.68
55:U3:79:SER:HB3	55:U3:82:TYR:HB2	1.76	0.68
37:52:1758:G:H1	37:52:1774:C:H42	1.41	0.67
37:52:4745:G:H1	37:52:4955:A:H61	1.40	0.67
67:g3:67:LEU:HB2	67:g3:72:LYS:HZ1	1.59	0.67
78:s3:192:VAL:CG1	78:s3:199:TYR:C	2.67	0.67
37:52:914:U:N3	37:52:918:G:N7	2.40	0.67
37:52:4431:U:OP2	85:I3:3:ARG:NH2	2.28	0.67
84:D3:200:MET:HB3	84:D3:202:GLN:HE22	1.57	0.67
78:s3:192:VAL:CG1	78:s3:199:TYR:O	2.42	0.67
36:k1:536:ASP:HB3	36:k1:544:VAL:HB	1.76	0.67
37:52:2399:G:N2	37:52:2400:G:N3	2.43	0.67
39:82:151:G:OP2	83:G3:118:ARG:NH1	2.27	0.67
78:s3:198:ILE:HD12	78:s3:198:ILE:H	1.58	0.67
6:F1:191:ARG:HH21	6:F1:245:ARG:HD3	1.60	0.67
65:e3:90:MET:HG2	77:r3:33:LYS:HA	1.76	0.66
69:i3:103:LYS:HA	87:u3:7:ARG:HE	0.83	0.66
37:52:4212:A:N1	54:T3:3:ASN:ND2	2.42	0.66
1:A1:658:U:O2	25:Y1:17:ARG:NH2	2.28	0.66
37:52:95:G:OP2	46:L3:11:LYS:NZ	2.29	0.66
40:A3:28:ARG:HD2	40:A3:30:ARG:HE	1.59	0.66
37:52:1952:G:N2	37:52:2032:U:O2	2.28	0.66
69:i3:98:ARG:O	87:u3:9:THR:HB	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:k1:454:ILE:HD11	36:k1:469:ARG:HH11	1.61	0.66
40:A3:118:GLU:HB3	40:A3:120:PRO:HD2	1.76	0.66
34:h1:118:ARG:HH21	34:h1:134:THR:H	1.41	0.66
37:52:2575:U:O2	37:52:2589:C:N4	2.29	0.66
14:N1:33:ARG:HH12	14:N1:89:VAL:HG11	1.60	0.66
78:s3:193:PHE:HA	78:s3:198:ILE:HG13	1.77	0.66
37:52:2631:U:C2	55:U3:49:VAL:CA	2.79	0.65
78:s3:30:VAL:HB	78:s3:187:LEU:HD12	1.69	0.65
37:52:2597:G:N2	37:52:2749:C:O2	2.30	0.65
37:52:2837:U:OP1	41:B3:249:ARG:NH1	2.29	0.65
78:s3:30:VAL:HB	78:s3:187:LEU:HD11	1.70	0.65
37:52:2046:G:H5'	49:O3:60:LYS:HE2	1.79	0.65
37:52:732:A:C4	53:S3:68:PHE:O	2.50	0.65
36:k1:237:ILE:HG22	36:k1:268:TYR:HB2	1.77	0.65
38:72:63:C:C5	85:I3:204:GLY:N	2.65	0.65
69:i3:103:LYS:HB2	87:u3:7:ARG:HG2	0.67	0.65
15:O1:136:PRO:HG2	15:O1:139:TRP:HB2	1.78	0.65
37:52:2631:U:C4	55:U3:49:VAL:CB	2.80	0.65
37:52:1805:A:N1	62:b3:28:ARG:CB	2.60	0.65
45:H3:129:ARG:HG2	45:H3:153:LEU:HD22	1.80	0.64
37:52:2084:U:C2	51:Q3:14:ARG:CD	2.80	0.64
37:52:2393:C:N4	37:52:2822:G:O6	2.30	0.64
44:F3:93:ARG:HE	44:F3:108:LEU:HD13	1.61	0.64
13:M1:93:LEU:HD21	25:Y1:8:ARG:HH11	1.63	0.64
60:Z3:16:GLY:O	60:Z3:19:SER:OG	2.15	0.64
67:g3:54:ARG:H	67:g3:76:ARG:HH12	1.44	0.64
37:52:4122:G:C5	60:Z3:135:ARG:HD2	2.32	0.64
37:52:1963:C:H42	37:52:4694:G:H1	1.45	0.64
1:A1:1104:G:H1	1:A1:1128:C:H42	1.46	0.64
37:52:1805:A:N3	62:b3:28:ARG:CB	2.61	0.64
87:u3:87:ILE:HG13	87:u3:90:LEU:HD12	1.79	0.64
1:A1:1858:G:OP2	16:P1:146:ARG:NH2	2.32	0.63
37:52:3688:U:OP2	40:A3:198:ARG:NH2	2.31	0.63
71:k3:28:ASN:OD1	71:k3:31:ASN:ND2	2.30	0.63
37:52:230:G:OP1	59:Y3:15:ARG:NH1	2.31	0.63
37:52:2455:G:N2	37:52:2471:G:N7	2.46	0.63
38:72:63:C:C6	85:I3:204:GLY:N	2.66	0.63
37:52:1182:C:OP2	37:52:1183:C:N4	2.32	0.63
37:52:1280:C:O2'	42:C3:321:ASN:ND2	2.30	0.63
37:52:1332:C:H2'	37:52:1333:A:H8	1.63	0.63
36:k1:251:GLN:HE22	36:k1:381:ASN:HB2	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:52:2631:U:N3	55:U3:49:VAL:CB	2.60	0.63
37:52:2538:U:O4	71:k3:40:ARG:NH2	2.31	0.63
69:i3:102:ALA:HB3	87:u3:9:THR:HG22	1.80	0.63
13:M1:11:GLN:HB3	13:M1:56:ILE:HD11	1.79	0.63
37:52:3970:G:O2'	87:u3:33:GLU:OE2	2.16	0.63
37:52:2405:G:N7	72:l3:2:SER:N	2.47	0.62
55:U3:47:ILE:HD12	55:U3:56:LEU:HD13	1.79	0.62
42:C3:329:ASN:ND2	44:F3:187:GLU:OE2	2.32	0.62
63:c3:33:GLN:HA	63:c3:36:LYS:HB2	1.81	0.62
52:R3:126:LYS:O	52:R3:132:PHE:N	2.32	0.62
27:a1:111:ARG:HH22	27:a1:114:LYS:HD2	1.63	0.62
37:52:1805:A:C4	62:b3:28:ARG:CA	2.82	0.62
69:i3:103:LYS:HD3	87:u3:10:LEU:HD21	1.81	0.62
1:A1:970:G:C2	37:52:3712:A:N3	2.68	0.62
78:s3:68:HIS:HB2	78:s3:75:LEU:HD12	1.82	0.62
37:52:732:A:C6	53:S3:68:PHE:HA	2.34	0.62
42:C3:330:PRO:HB3	44:F3:46:ARG:HH21	1.63	0.62
37:52:2624:G:N2	37:52:2633:U:O2	2.33	0.62
37:52:2812:A:OP1	52:R3:88:ARG:NH1	2.33	0.62
37:52:3894:A:H61	37:52:4566:U:H3	1.48	0.62
41:B3:322:HIS:O	41:B3:342:LYS:NZ	2.31	0.62
43:E3:191:ARG:NH2	43:E3:217:ASP:OD1	2.33	0.62
1:A1:522:A:O3'	11:K1:131:ARG:NH2	2.33	0.62
20:T1:127:TRP:O	20:T1:144:ARG:NH2	2.33	0.62
63:c3:47:ILE:HG12	63:c3:72:HIS:HB3	1.82	0.62
37:52:1552:G:O2'	37:52:1574:G:N2	2.30	0.61
38:72:85:G:OP1	44:F3:221:LYS:NZ	2.32	0.61
1:A1:39:A:H5'	11:K1:7:TRP:HE1	1.65	0.61
37:52:1577:G:OP1	76:p3:17:ARG:NH1	2.33	0.61
37:52:1969:G:H21	78:s3:40:MET:HE2	1.64	0.61
40:A3:122:ASP:OD1	40:A3:122:ASP:N	2.30	0.61
45:H3:94:SER:HB3	45:H3:142:ASP:HB3	1.83	0.61
10:J1:123:ARG:NH1	10:J1:134:GLU:OE1	2.33	0.61
37:52:3939:G:HO2'	37:52:4076:G:H1	1.49	0.61
37:52:3940:U:OP2	48:N3:24:ARG:NH2	2.34	0.61
1:A1:377:G:OP1	10:J1:98:LYS:NZ	2.34	0.61
37:52:2262:G:OP2	77:r3:107:ARG:NH1	2.34	0.61
37:52:2654:C:O3'	60:Z3:76:ASN:ND2	2.32	0.61
37:52:3896:C:O2'	41:B3:268:ARG:NH1	2.34	0.61
53:S3:34:ALA:HB1	53:S3:39:VAL:HG23	1.82	0.61
80:23:14:A:N6	80:23:21:A:O2'	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:52:3892:U:O2'	50:P3:80:GLN:NE2	2.34	0.61
78:s3:192:VAL:CB	78:s3:199:TYR:C	2.73	0.61
14:N1:33:ARG:HA	14:N1:110:VAL:HB	1.83	0.61
40:A3:162:ASN:OD1	40:A3:162:ASN:N	2.32	0.61
59:Y3:50:ARG:HB2	59:Y3:115:ARG:HH22	1.66	0.61
37:52:312:G:N2	37:52:326:C:O2	2.34	0.61
44:F3:114:ARG:HD3	51:Q3:5:ILE:HD11	1.83	0.61
56:V3:31:ASN:HD21	56:V3:115:SER:HB2	1.66	0.61
8:H1:131:ARG:O	57:W3:85:ALA:N	2.34	0.61
37:52:2598:A:H5''	67:g3:43:LYS:HG3	1.82	0.61
37:52:1187:G:H1'	84:D3:275:GLN:HE21	1.65	0.60
37:52:3787:G:H21	37:52:3789:C:H42	1.47	0.60
37:52:1969:G:OP2	78:s3:34:ASN:ND2	2.35	0.60
37:52:2631:U:C4	55:U3:49:VAL:CA	2.84	0.60
58:X3:48:ARG:HH12	58:X3:50:LYS:HG3	1.66	0.60
67:g3:100:GLN:O	67:g3:104:VAL:N	2.33	0.60
26:Z1:7:ILE:HD12	26:Z1:43:LYS:HD2	1.84	0.60
69:i3:99:LYS:N	87:u3:9:THR:OG1	2.33	0.60
69:i3:103:LYS:CA	87:u3:7:ARG:CZ	2.73	0.60
8:H1:146:ASN:O	57:W3:101:ARG:NH1	2.34	0.60
37:52:732:A:C4	53:S3:68:PHE:CA	2.83	0.60
37:52:1999:A:H61	78:s3:40:MET:HB3	1.66	0.60
37:52:713:C:H2'	37:52:714:G:H8	1.67	0.60
37:52:2663:G:OP2	52:R3:118:HIS:NE2	2.35	0.60
1:A1:678:U:H5''	15:O1:127:ARG:HH12	1.67	0.60
37:52:732:A:C6	53:S3:68:PHE:CA	2.84	0.60
37:52:732:A:C6	53:S3:69:GLU:N	2.69	0.60
30:d1:66:ARG:NH2	81:w3:41:U:OP1	2.33	0.60
37:52:982:U:OP2	37:52:983:C:N4	2.35	0.60
1:A1:1096:G:OP1	24:X1:20:ARG:NH1	2.35	0.60
37:52:2658:G:N2	37:52:2675:G:O2'	2.33	0.60
39:82:21:C:OP1	42:C3:195:LYS:NZ	2.34	0.60
43:E3:185:ASN:ND2	43:E3:274:LEU:O	2.34	0.60
1:A1:943:U:OP1	3:C1:214:LYS:NZ	2.34	0.59
1:A1:1567:G:H1'	21:U1:37:VAL:HG21	1.84	0.59
59:Y3:46:SER:O	59:Y3:122:LYS:NZ	2.35	0.59
82:J3:46:GLN:NE2	82:J3:72:CYS:SG	2.74	0.59
1:A1:1284:A:N6	1:A1:1313:A:O2'	2.34	0.59
1:A1:1854:U:OP1	16:P1:150:ARG:NH1	2.35	0.59
36:k1:55:CYS:SG	36:k1:56:ILE:N	2.75	0.59
37:52:1805:A:C2	62:b3:28:ARG:HB2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:M3:80:ALA:O	47:M3:85:LYS:NZ	2.35	0.59
6:F1:43:PRO:HD2	6:F1:46:ILE:HD12	1.84	0.59
35:j1:336:GLN:NE2	35:j1:365:GLU:O	2.35	0.59
4:D1:209:VAL:HG11	4:D1:233:LEU:HD11	1.84	0.59
38:72:63:C:N3	85:I3:203:ARG:C	2.59	0.59
67:g3:63:VAL:HG13	67:g3:66:ARG:HE	1.66	0.59
67:g3:104:VAL:O	67:g3:108:LYS:N	2.35	0.59
69:i3:103:LYS:CD	87:u3:10:LEU:HD21	2.32	0.59
37:52:2577:C:OP1	60:Z3:111:ARG:NE	2.36	0.59
45:H3:26:ILE:HG22	45:H3:35:ARG:HG2	1.84	0.59
47:M3:119:ARG:NH2	49:O3:193:THR:OG1	2.35	0.59
59:Y3:21:ALA:O	59:Y3:26:ARG:NH2	2.35	0.59
1:A1:521:A:OP1	11:K1:45:ARG:NH1	2.35	0.59
37:52:4162:C:N3	83:G3:125:LYS:NZ	2.48	0.59
42:C3:232:VAL:HG21	42:C3:256:ALA:HB1	1.84	0.59
52:R3:84:THR:OG1	52:R3:87:ALA:N	2.35	0.59
24:X1:22:LYS:NZ	29:c1:2:PRO:O	2.35	0.59
37:52:1970:A:N6	37:52:2016:C:OP2	2.36	0.59
37:52:3707:U:O2	37:52:3744:G:N2	2.35	0.59
60:Z3:38:TYR:OH	60:Z3:74:VAL:O	2.18	0.59
1:A1:506:G:OP1	26:Z1:108:LYS:NZ	2.36	0.59
37:52:1857:C:N3	37:52:1878:G:N2	2.50	0.59
79:t3:150:ASP:HA	79:t3:153:ASP:HB3	1.85	0.59
82:J3:152:GLY:O	82:J3:156:ARG:NH1	2.36	0.59
37:52:1906:U:OP1	44:F3:217:GLY:N	2.35	0.59
63:c3:33:GLN:O	63:c3:37:MET:N	2.35	0.59
1:A1:659:G:HO2'	1:A1:662:G:HO2'	1.42	0.59
6:F1:11:ARG:NH2	6:F1:21:ASP:OD1	2.35	0.59
37:52:2658:G:N3	37:52:2675:G:N2	2.51	0.59
37:52:2794:C:H42	86:1:11:ALA:HB3	1.67	0.59
83:G3:90:LYS:NZ	83:G3:97:ASP:OD2	2.36	0.59
1:A1:942:G:N2	16:P1:138:ASP:OD2	2.35	0.58
7:G1:71:ARG:NH1	7:G1:148:ASN:OD1	2.37	0.58
24:X1:102:ILE:H	24:X1:113:HIS:HD2	1.50	0.58
35:j1:118:LYS:NZ	35:j1:143:ASP:OD1	2.36	0.58
37:52:1239:C:N1	43:E3:65:TYR:OH	2.36	0.58
37:52:1764:G:O2'	37:52:1767:A:N7	2.35	0.58
12:L1:59:LYS:HB3	12:L1:70:TYR:HB2	1.85	0.58
37:52:732:A:C2	53:S3:68:PHE:CA	2.86	0.58
37:52:2084:U:C4	51:Q3:14:ARG:CD	2.87	0.58
37:52:4661:G:N2	37:52:5005:G:OP1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:A3:149:LYS:HD2	40:A3:156:LYS:HE2	1.85	0.58
2:B1:188:THR:HG22	2:B1:189:ILE:HG13	1.86	0.58
57:W3:6:CYS:SG	57:W3:7:SER:N	2.77	0.58
73:m3:84:CYS:SG	73:m3:85:ARG:N	2.77	0.58
37:52:3711:A:N6	37:52:3736:A:OP2	2.36	0.58
37:52:3973:G:H1	37:52:4038:C:H42	1.51	0.58
46:L3:25:TRP:HE1	48:N3:199:GLN:HB3	1.67	0.58
48:N3:114:ARG:NH1	48:N3:151:ILE:O	2.36	0.58
60:Z3:47:ASP:HB3	60:Z3:69:LYS:HB3	1.86	0.58
80:23:21:A:N6	80:23:46:G:O2'	2.36	0.58
37:52:2023:C:OP1	78:s3:83:ARG:NH1	2.36	0.58
21:U1:11:GLN:OE1	21:U1:62:ARG:NH1	2.37	0.58
37:52:2709:C:OP2	52:R3:43:LYS:NZ	2.36	0.58
37:52:191:G:O6	37:52:250:C:N4	2.36	0.58
24:X1:52:ILE:HG22	24:X1:61:ILE:HG12	1.85	0.58
37:52:1079:C:N4	37:52:1221:G:O6	2.37	0.58
37:52:3939:G:O2'	37:52:4076:G:N1	2.37	0.58
37:52:3965:A:N6	37:52:4048:A:N3	2.52	0.58
51:Q3:178:ARG:H	61:a3:51:GLY:HA2	1.68	0.58
11:K1:170:PRO:O	11:K1:175:ARG:NH1	2.37	0.57
36:k1:568:ARG:HD2	36:k1:596:PHE:HB2	1.85	0.57
37:52:1590:C:O2	37:52:1605:G:N2	2.37	0.57
37:52:3968:U:H3	37:52:4053:A:H61	1.49	0.57
41:B3:165:HIS:ND1	41:B3:166:THR:O	2.36	0.57
85:I3:93:PRO:HA	85:I3:127:ALA:HB2	1.86	0.57
87:u3:37:SER:HB3	87:u3:203:ALA:HB3	1.86	0.57
1:A1:1514:G:H2'	1:A1:1515:G:H8	1.69	0.57
3:C1:66:VAL:HG22	3:C1:87:ILE:HG22	1.86	0.57
36:k1:501:ALA:HB1	36:k1:528:LEU:HD21	1.85	0.57
44:F3:151:GLU:O	44:F3:247:ASN:ND2	2.35	0.57
75:o3:72:CYS:SG	75:o3:73:VAL:N	2.77	0.57
1:A1:64:A:H2	1:A1:83:A:H62	1.51	0.57
1:A1:1629:C:OP1	20:T1:39:ARG:NH2	2.37	0.57
26:Z1:14:THR:HG22	26:Z1:21:LYS:HG3	1.86	0.57
36:k1:21:CYS:SG	36:k1:22:ARG:N	2.77	0.57
36:k1:22:ARG:HB3	36:k1:24:GLU:HG3	1.86	0.57
36:k1:39:ILE:HG12	36:k1:50:ILE:HG12	1.87	0.57
37:52:1177:U:H2'	37:52:1178:G:H8	1.70	0.57
37:52:1239:C:C6	43:E3:65:TYR:OH	2.57	0.57
37:52:4389:C:H2'	37:52:4390:A:H8	1.69	0.57
67:g3:105:LYS:HD3	67:g3:108:LYS:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:I3:61:SER:HA	85:I3:126:VAL:HG23	1.86	0.57
5:E1:28:GLU:OE2	5:E1:65:ARG:NH2	2.38	0.57
34:h1:249:CYS:SG	34:h1:250:ALA:N	2.78	0.57
37:52:2059:C:O2	53:S3:118:ARG:NH1	2.37	0.57
37:52:2420:A:N6	37:52:2424:G:N7	2.52	0.57
37:52:4772:C:N4	37:52:4864:U:O2	2.37	0.57
10:J1:174:CYS:SG	10:J1:175:ILE:N	2.77	0.57
79:t3:143:VAL:N	79:t3:145:GLY:O	2.37	0.57
5:E1:133:GLY:HA3	5:E1:156:LEU:H	1.69	0.57
37:52:1553:A:O4'	76:p3:4:ARG:NH1	2.37	0.57
1:A1:1292:C:O2	33:g1:138:ARG:NH1	2.37	0.57
37:52:1805:A:C6	62:b3:28:ARG:CA	2.87	0.57
37:52:2779:C:H5'	58:X3:105:ASN:HD22	1.69	0.57
53:S3:11:LYS:HD2	53:S3:29:ARG:HD2	1.86	0.57
58:X3:107:HIS:O	58:X3:111:GLN:NE2	2.37	0.57
63:c3:51:ASN:O	76:p3:62:LYS:NZ	2.37	0.57
1:A1:442:C:N3	1:A1:452:G:N2	2.52	0.57
24:X1:37:PHE:HE1	24:X1:103:VAL:HG11	1.70	0.57
34:h1:298:LEU:HB3	34:h1:310:TRP:HB2	1.87	0.57
37:52:1239:C:C6	43:E3:65:TYR:CZ	2.92	0.57
37:52:1516:G:OP2	61:a3:32:ARG:NH1	2.38	0.57
37:52:2581:A:O5'	60:Z3:75:TYR:N	2.37	0.57
59:Y3:50:ARG:NH1	59:Y3:112:ASP:OD2	2.38	0.57
63:c3:47:ILE:HG22	63:c3:74:TYR:HB2	1.86	0.57
1:A1:121:U:O3'	6:F1:77:ARG:NH1	2.38	0.57
27:a1:68:ILE:HB	27:a1:109:TYR:HB2	1.87	0.57
37:52:1805:A:C6	62:b3:28:ARG:N	2.73	0.57
37:52:1823:G:O2'	84:D3:44:TYR:O	2.23	0.57
37:52:2596:G:O2'	67:g3:81:SER:O	2.22	0.57
7:G1:20:PHE:HB3	7:G1:23:TRP:HB2	1.86	0.57
37:52:1997:U:O2'	78:s3:44:ARG:NH1	2.37	0.57
34:h1:118:ARG:NH2	34:h1:134:THR:OG1	2.38	0.56
37:52:1763:C:H2'	37:52:1769:G:H22	1.69	0.56
43:E3:144:ARG:NH2	66:f3:108:SER:OG	2.35	0.56
43:E3:164:ARG:NH1	43:E3:276:SER:OG	2.38	0.56
37:52:1755:C:O2'	37:52:1757:U:OP2	2.23	0.56
44:F3:104:VAL:HG13	44:F3:135:VAL:HG12	1.87	0.56
83:G3:148:LEU:HD23	83:G3:271:LEU:HD21	1.87	0.56
1:A1:1095:U:O2	1:A1:1151:G:N2	2.38	0.56
37:52:102:G:O2'	37:52:1381:U:O2'	2.20	0.56
37:52:386:A:O2'	59:Y3:87:ARG:NH2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:52:960:A:H62	43:E3:129:LEU:H	1.52	0.56
37:52:1995:G:H8	79:t3:130:LYS:HD3	1.70	0.56
37:52:2631:U:N1	55:U3:49:VAL:CA	2.68	0.56
37:52:4122:G:O6	67:g3:98:GLU:N	2.33	0.56
87:u3:18:LEU:HD13	87:u3:176:ASP:HB3	1.86	0.56
87:u3:157:PHE:HB2	87:u3:165:LEU:HD11	1.86	0.56
1:A1:1229:G:N2	1:A1:1530:U:O2	2.39	0.56
8:H1:162:LEU:HD22	8:H1:170:ARG:HB2	1.87	0.56
37:52:8:U:H5'	48:N3:40:PRO:HG3	1.86	0.56
37:52:679:C:H2'	37:52:680:G:H8	1.71	0.56
37:52:1239:C:C6	37:52:1239:C:C1'	2.88	0.56
37:52:3974:G:H5''	87:u3:26:ARG:CD	2.34	0.56
37:52:4970:C:N4	37:52:5063:G:O6	2.38	0.56
39:82:36:G:H3'	68:h3:89:ARG:HD2	1.87	0.56
41:B3:57:VAL:HG22	41:B3:73:VAL:HG12	1.86	0.56
83:G3:282:ARG:NH1	83:G3:285:GLU:OE2	2.38	0.56
1:A1:611:G:H1	1:A1:632:C:H42	1.51	0.56
1:A1:1497:G:N7	12:L1:25:LYS:NZ	2.49	0.56
3:C1:57:ILE:HG22	3:C1:59:SER:H	1.69	0.56
87:u3:144:MET:HG3	87:u3:145:VAL:HG23	1.87	0.56
37:52:1239:C:C5	43:E3:65:TYR:OH	2.58	0.56
39:82:147:G:H2'	39:82:148:A:H8	1.70	0.56
55:U3:103:VAL:HG21	55:U3:113:ARG:HE	1.71	0.56
77:r3:17:LEU:HD21	77:r3:19:LYS:HE3	1.87	0.56
1:A1:599:A:H2'	1:A1:606:G:H21	1.71	0.56
36:k1:116:LYS:HE3	36:k1:272:VAL:HG11	1.87	0.56
37:52:2756:G:O6	60:Z3:65:ARG:NH2	2.38	0.56
34:h1:10:THR:HG22	34:h1:308:ARG:HG2	1.87	0.56
37:52:2590:G:H21	60:Z3:65:ARG:HH21	1.54	0.56
48:N3:68:ARG:NH1	48:N3:124:ASP:O	2.38	0.56
6:F1:48:LEU:HD23	6:F1:61:VAL:HG13	1.88	0.56
6:F1:100:ARG:HH21	6:F1:118:GLU:HG2	1.71	0.56
37:52:4633:G:O2'	37:52:4635:A:OP2	2.23	0.56
41:B3:254:ILE:HG23	41:B3:266:VAL:HG11	1.88	0.56
2:B1:50:ASN:OD1	2:B1:53:ARG:NH1	2.39	0.56
21:U1:56:ARG:NH2	21:U1:99:VAL:O	2.39	0.56
37:52:119:G:C6	83:G3:185:ARG:CD	2.89	0.55
37:52:181:C:N4	37:52:182:G:O6	2.39	0.55
37:52:2750:G:O2'	67:g3:79:GLY:O	2.24	0.55
37:52:4872:G:OP2	47:M3:94:LYS:NZ	2.39	0.55
37:52:4949:G:H4'	37:52:4950:U:H5'	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:878:G:H22	1:A1:908:A:H2	1.55	0.55
63:c3:102:SER:OG	63:c3:103:ASP:N	2.39	0.55
71:k3:37:ARG:NH2	71:k3:41:TYR:O	2.39	0.55
2:B1:41:ARG:HE	2:B1:45:GLY:HA2	1.69	0.55
34:h1:107:ASP:HB2	34:h1:125:ARG:HD2	1.89	0.55
37:52:442:G:OP1	66:f3:68:ARG:NH1	2.39	0.55
37:52:1818:G:O2'	37:52:1820:U:OP2	2.24	0.55
37:52:2100:G:H1	42:C3:310:HIS:HA	1.71	0.55
37:52:2400:G:H1	37:52:2804:C:H42	1.54	0.55
75:o3:36:GLN:OE1	75:o3:39:ARG:NH2	2.39	0.55
78:s3:30:VAL:CG2	78:s3:187:LEU:HD13	2.35	0.55
1:A1:316:G:H3'	8:H1:183:ARG:HH22	1.72	0.55
37:52:2084:U:N3	51:Q3:14:ARG:CD	2.69	0.55
37:52:2756:G:C2	37:52:2757:A:H1'	2.41	0.55
37:52:3965:A:H61	37:52:4045:G:H21	1.53	0.55
10:J1:148:LYS:HA	10:J1:151:GLU:HB2	1.88	0.55
36:k1:188:LEU:O	36:k1:197:GLN:NE2	2.39	0.55
40:A3:160:SER:OG	40:A3:161:ALA:N	2.40	0.55
60:Z3:136:PHE:HB2	67:g3:90:ARG:HD3	1.87	0.55
8:H1:12:CYS:SG	8:H1:13:GLN:N	2.79	0.55
21:U1:115:LYS:HA	21:U1:121:ARG:HA	1.87	0.55
34:h1:254:PRO:HA	34:h1:285:GLN:HA	1.87	0.55
37:52:1239:C:C5	43:E3:65:TYR:CZ	2.95	0.55
37:52:2754:G:C4	60:Z3:51:ARG:HD3	2.42	0.55
38:72:77:A:H62	38:72:99:G:H21	1.54	0.55
58:X3:82:THR:HG21	68:h3:37:THR:HG22	1.89	0.55
26:Z1:103:SER:OG	26:Z1:106:GLN:OE1	2.25	0.55
37:52:322:C:N4	37:52:4355:G:O6	2.40	0.55
37:52:1720:C:OP1	37:52:1835:G:N2	2.40	0.55
37:52:2631:U:C6	55:U3:49:VAL:CA	2.86	0.55
37:52:4882:U:OP1	47:M3:117:LYS:NZ	2.39	0.55
37:52:2631:U:C6	55:U3:49:VAL:CB	2.89	0.55
37:52:2794:C:C4	86:1:11:ALA:HB3	2.42	0.55
37:52:4459:U:O2'	41:B3:265:SER:OG	2.25	0.55
38:72:105:C:OP2	85:I3:203:ARG:NH2	2.39	0.55
37:52:495:C:N4	37:52:496:G:O6	2.40	0.55
37:52:956:A:H62	37:52:1283:G:H1'	1.71	0.55
37:52:1805:A:C5	62:b3:28:ARG:CA	2.90	0.55
37:52:2022:C:H4'	78:s3:83:ARG:HA	1.89	0.55
37:52:4735:G:H1	37:52:4964:C:H42	1.55	0.55
53:S3:16:CYS:HB2	53:S3:54:MET:HE2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:V3:83:ARG:NH1	56:V3:120:PRO:O	2.35	0.55
63:c3:29:LEU:HD22	63:c3:94:LEU:HA	1.88	0.55
1:A1:678:U:OP1	15:O1:127:ARG:NH2	2.41	0.55
24:X1:57:ARG:NH1	29:c1:26:GLN:OE1	2.40	0.55
27:a1:88:LEU:HD23	27:a1:91:LEU:HD12	1.88	0.55
37:52:2631:U:N3	55:U3:49:VAL:CA	2.70	0.55
37:52:2631:U:N1	55:U3:49:VAL:CB	2.70	0.55
43:E3:96:THR:HG22	43:E3:109:VAL:HG22	1.89	0.55
52:R3:70:ARG:HD2	52:R3:76:MET:HE2	1.89	0.55
1:A1:453:C:O2'	8:H1:92:ARG:O	2.24	0.54
37:52:2439:G:N2	37:52:2539:C:O2	2.40	0.54
37:52:2794:C:N4	86:1:11:ALA:HB3	2.22	0.54
37:52:3928:A:OP1	48:N3:90:ASN:ND2	2.39	0.54
38:72:62:U:OP1	84:D3:279:ARG:NH2	2.40	0.54
76:p3:89:LEU:O	76:p3:92:GLN:NE2	2.39	0.54
1:A1:140:U:O2'	8:H1:149:LYS:NZ	2.39	0.54
1:A1:380:G:OP1	10:J1:56:ARG:NH2	2.41	0.54
1:A1:1520:G:N2	1:A1:1521:C:N3	2.56	0.54
18:R1:19:ALA:HB2	18:R1:75:GLY:HA3	1.89	0.54
36:k1:100:PRO:HB3	36:k1:270:ILE:HD11	1.89	0.54
37:52:104:G:HO2'	37:52:1361:G:HO2'	1.56	0.54
37:52:1424:G:O2'	62:b3:28:ARG:NH2	2.40	0.54
37:52:2045:G:N2	37:52:2046:G:N7	2.56	0.54
38:72:5:A:H4'	84:D3:52:ILE:HD13	1.88	0.54
28:b1:46:GLU:HB2	81:w3:38:A:H5''	1.89	0.54
37:52:1928:C:N4	37:52:2054:U:O2	2.39	0.54
37:52:1981:G:H4'	79:t3:25:THR:HG21	1.89	0.54
37:52:2739:C:O2	40:A3:174:ARG:NH1	2.39	0.54
37:52:3942:A:N6	37:52:4067:U:O4	2.35	0.54
8:H1:98:ARG:NH1	8:H1:99:GLY:O	2.40	0.54
14:N1:99:LYS:H	14:N1:101:ARG:HH12	1.54	0.54
34:h1:87:LEU:HB2	34:h1:101:PHE:HB2	1.89	0.54
34:h1:162:ASN:HB3	34:h1:164:ILE:HB	1.89	0.54
37:52:1398:A:N6	37:52:1399:G:N3	2.56	0.54
37:52:3806:G:O3'	74:n3:23:ARG:NH1	2.40	0.54
38:72:63:C:C4	85:I3:203:ARG:C	2.86	0.54
40:A3:159:SER:OG	40:A3:160:SER:N	2.39	0.54
13:M1:120:VAL:HG22	13:M1:145:VAL:HG11	1.89	0.54
34:h1:220:ASP:HB3	34:h1:224:GLY:HA2	1.90	0.54
37:52:1689:G:O6	37:52:1847:C:N4	2.40	0.54
37:52:1759:G:H1	37:52:1773:U:H3	1.54	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:N3:33:LEU:O	48:N3:65:ARG:NH1	2.41	0.54
84:D3:39:GLN:NE2	84:D3:46:THR:O	2.40	0.54
1:A1:232:A:OP2	1:A1:889:U:O2'	2.25	0.54
36:k1:4:LYS:HB3	36:k1:77:SER:HB3	1.88	0.54
37:52:119:G:C2	83:G3:185:ARG:CD	2.91	0.54
37:52:2399:G:N3	67:g3:4:ARG:CD	2.71	0.54
37:52:4055:U:O2'	87:u3:162:VAL:HG12	2.07	0.54
39:82:130:C:H2'	39:82:131:G:H8	1.72	0.54
1:A1:970:G:N3	37:52:3712:A:N3	2.56	0.54
14:N1:82:ASN:O	14:N1:86:GLY:N	2.41	0.54
19:S1:31:ASN:HD21	19:S1:55:THR:HG22	1.72	0.54
30:d1:31:ARG:HD2	30:d1:43:ILE:HG12	1.89	0.54
37:52:175:C:O2	37:52:262:G:N2	2.41	0.54
37:52:2395:A:C6	67:g3:2:VAL:CA	2.91	0.54
37:52:2395:A:C6	67:g3:2:VAL:CB	2.91	0.54
18:R1:123:ASP:O	18:R1:126:ARG:NH2	2.40	0.54
37:52:2597:G:H3'	67:g3:44:SER:N	2.22	0.54
37:52:2794:C:N3	86:1:11:ALA:CB	2.69	0.54
1:A1:167:G:O3'	57:W3:80:ARG:NH2	2.41	0.54
14:N1:38:ALA:HA	14:N1:42:LEU:HD13	1.90	0.54
17:Q1:85:ILE:HD13	17:Q1:111:MET:HB3	1.90	0.54
37:52:738(A):C:O2'	37:52:740:G:OP2	2.26	0.54
1:A1:1082:A:HO2'	1:A1:1842:C:HO2'	1.50	0.54
10:J1:6:ASP:OD1	10:J1:6:ASP:N	2.40	0.54
35:j1:324:GLU:HB3	35:j1:391:ILE:HG23	1.90	0.54
37:52:1103:C:N4	37:52:1195:G:O2'	2.41	0.54
37:52:1996:C:H42	37:52:2000:G:H1	1.56	0.54
37:52:2490:U:O2'	37:52:2491:C:O4'	2.24	0.54
37:52:2749:C:H2'	37:52:2750:G:H8	1.72	0.54
37:52:4039:G:H1'	37:52:4050:A:H1'	1.90	0.54
40:A3:179:ILE:HG21	40:A3:185:ALA:HB2	1.90	0.54
52:R3:103:ARG:HH21	52:R3:128:LYS:HB2	1.72	0.54
82:J3:146:ARG:HG2	82:J3:147:ARG:HG2	1.90	0.54
6:F1:204:SER:OG	6:F1:205:PHE:N	2.40	0.53
37:52:4485:C:O2'	73:m3:88:LYS:NZ	2.40	0.53
4:D1:196:ILE:HB	4:D1:223:TYR:HB2	1.89	0.53
9:I1:7:LYS:NZ	9:I1:40:LEU:O	2.38	0.53
37:52:732:A:C5	53:S3:68:PHE:CA	2.91	0.53
84:D3:261:VAL:HG12	84:D3:263:LYS:H	1.72	0.53
37:52:119:G:O6	83:G3:166:ARG:NH1	2.41	0.53
37:52:2399:G:C2	67:g3:4:ARG:CD	2.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:52:4704:C:H2'	37:52:4705:A:H8	1.73	0.53
55:U3:49:VAL:CB	55:U3:49:VAL:HA	2.37	0.53
78:s3:45:MET:HE2	79:t3:121:LEU:HA	1.90	0.53
87:u3:67:VAL:H	87:u3:82:ILE:HD11	1.72	0.53
1:A1:951:C:O2'	16:P1:50:LYS:NZ	2.41	0.53
28:b1:23:CYS:SG	28:b1:24:THR:N	2.81	0.53
34:h1:70:VAL:HG11	34:h1:112:ALA:HA	1.90	0.53
37:52:417:G:O2'	39:82:16:G:N2	2.34	0.53
37:52:1570:G:N2	52:R3:129:GLY:O	2.42	0.53
37:52:2787:A:H2	37:52:2801:U:H3	1.56	0.53
37:52:3717:A:OP2	37:52:3735:G:N2	2.41	0.53
37:52:3961:G:H1	37:52:3964:U:H5''	1.72	0.53
37:52:4240:G:N2	37:52:4285:U:O2	2.41	0.53
78:s3:10:LYS:O	78:s3:14:PHE:N	2.41	0.53
1:A1:1568:C:OP1	21:U1:96:SER:OG	2.26	0.53
37:52:3605:C:OP2	52:R3:71:ARG:NH1	2.41	0.53
78:s3:28:PHE:N	78:s3:89:VAL:O	2.39	0.53
1:A1:492:C:N3	1:A1:509:G:N2	2.57	0.53
37:52:2653:C:H1'	67:g3:54:ARG:HH12	1.72	0.53
40:A3:26:ALA:HB3	40:A3:28:ARG:HE	1.73	0.53
8:H1:181:THR:HG22	8:H1:184:VAL:HG23	1.89	0.53
8:H1:194:LEU:O	8:H1:198:ARG:NH2	2.42	0.53
37:52:308:G:O2'	69:i3:31:GLY:O	2.25	0.53
37:52:942:G:OP1	44:F3:244:ARG:NH1	2.40	0.53
44:F3:156:ARG:NH2	44:F3:211:LYS:O	2.42	0.53
1:A1:970:G:H22	37:52:3709:U:H6	1.55	0.53
1:A1:1327:G:H1	1:A1:1502:C:H42	1.56	0.53
12:L1:4:PRO:HD2	12:L1:7:ASN:HD22	1.73	0.53
26:Z1:41:ARG:NH2	26:Z1:52:PRO:O	2.40	0.53
37:52:2475:G:C5	58:X3:50:LYS:HD2	2.44	0.53
78:s3:193:PHE:CA	78:s3:198:ILE:HG23	2.39	0.53
37:52:346:G:OP1	59:Y3:8:THR:OG1	2.26	0.53
37:52:729:G:C6	37:52:732:A:H1'	2.44	0.53
37:52:1186:U:H2'	37:52:1187:G:C8	2.44	0.53
1:A1:1617:G:N1	1:A1:1620:A:OP2	2.42	0.53
14:N1:95:ASP:HB3	14:N1:101:ARG:HH11	1.73	0.53
37:52:1485:C:H2'	46:L3:198:ARG:HH12	1.73	0.53
37:52:2430:C:H2'	37:52:2431:A:H8	1.74	0.53
38:72:20:U:O2	38:72:59:G:N2	2.42	0.53
63:c3:28:VAL:HG12	63:c3:34:SER:HB3	1.90	0.53
80:23:30:G:H1	80:23:40:C:H42	1.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:106:C:H4'	1:A1:410:G:H21	1.74	0.52
37:52:1805:A:C2	62:b3:28:ARG:CA	2.92	0.52
41:B3:41:VAL:HG12	41:B3:187:GLY:HA3	1.91	0.52
80:23:21:A:N6	80:23:48:C:OP2	2.42	0.52
1:A1:1262:C:O2'	31:e1:12:ARG:NH1	2.42	0.52
4:D1:191:VAL:HG11	4:D1:236:PHE:HD1	1.74	0.52
14:N1:93:LYS:HG2	14:N1:100:PRO:HG3	1.90	0.52
34:h1:237:ASN:ND2	34:h1:286:CYS:O	2.42	0.52
37:52:1239:C:N1	43:E3:65:TYR:CZ	2.77	0.52
37:52:1668:A:OP2	37:52:2280:G:N2	2.41	0.52
37:52:2631:U:C2	55:U3:49:VAL:N	2.78	0.52
43:E3:48:ARG:HB2	43:E3:64:MET:HE1	1.90	0.52
85:I3:35:ASP:OD1	85:I3:86:HIS:NE2	2.40	0.52
1:A1:1299:A:N6	1:A1:1301:A:N7	2.57	0.52
34:h1:214:GLY:O	34:h1:232:GLY:N	2.43	0.52
37:52:1805:A:C5	62:b3:28:ARG:N	2.77	0.52
37:52:2399:G:C6	67:g3:4:ARG:CD	2.92	0.52
37:52:2533:C:OP1	58:X3:139:ARG:NH2	2.43	0.52
37:52:2581:A:H8	60:Z3:73:LYS:HG3	1.73	0.52
37:52:2647:A:H62	37:52:2686:G:H8	1.55	0.52
37:52:3681:G:N3	40:A3:125:LYS:HD3	2.25	0.52
40:A3:57:PRO:HD2	40:A3:170:ALA:HB3	1.91	0.52
69:i3:48:CYS:SG	69:i3:49:GLY:N	2.82	0.52
78:s3:124:PRO:HD2	78:s3:180:ILE:HD13	1.91	0.52
1:A1:1036:A:N3	1:A1:1844:U:O2'	2.43	0.52
3:C1:134:LEU:HD13	3:C1:219:LYS:HD2	1.91	0.52
5:E1:162:ASP:OD1	5:E1:165:ASN:ND2	2.42	0.52
37:52:1169:G:O6	37:52:1193:C:N4	2.42	0.52
1:A1:1400:U:OP1	34:h1:100:ARG:NH1	2.42	0.52
3:C1:92:GLN:HB3	3:C1:95:ASN:HB2	1.91	0.52
11:K1:179:LYS:O	11:K1:183:GLY:N	2.36	0.52
36:k1:368:GLU:HB2	36:k1:531:ARG:HH12	1.75	0.52
36:k1:440:GLN:HE21	36:k1:510:HIS:HB3	1.73	0.52
37:52:119:G:N3	83:G3:185:ARG:CD	2.72	0.52
37:52:2703:G:OP1	55:U3:113:ARG:NH1	2.42	0.52
37:52:4633:G:N2	37:52:4664:A:OP2	2.38	0.52
43:E3:105:GLY:HA2	43:E3:108:ARG:HH22	1.73	0.52
60:Z3:12:LEU:HB2	60:Z3:81:MET:HB3	1.91	0.52
87:u3:33:GLU:HA	87:u3:168:ALA:HA	1.92	0.52
1:A1:1121:G:N2	3:C1:202:GLN:O	2.38	0.52
17:Q1:75:VAL:HG21	17:Q1:104:GLN:HE22	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R1:41:MET:N	18:R1:41:MET:SD	2.82	0.52
37:52:1973:G:H22	79:t3:135:THR:HG21	1.73	0.52
37:52:1998:A:N7	78:s3:44:ARG:NH2	2.57	0.52
37:52:2041:A:N7	37:52:4434:C:O2'	2.41	0.52
59:Y3:26:ARG:NH1	59:Y3:75:ARG:O	2.42	0.52
63:c3:50:ASN:O	63:c3:57:LYS:NZ	2.43	0.52
76:p3:3:LYS:HG2	76:p3:5:THR:H	1.74	0.52
17:Q1:81:ARG:NH2	17:Q1:117:GLY:O	2.43	0.52
37:52:732:A:N3	53:S3:68:PHE:CA	2.72	0.52
37:52:1805:A:N1	62:b3:28:ARG:CA	2.73	0.52
37:52:2399:G:C6	67:g3:4:ARG:CZ	2.93	0.52
37:52:2743:A:O2'	40:A3:21:LYS:NZ	2.42	0.52
52:R3:125:LEU:HA	52:R3:129:GLY:H	1.75	0.52
65:e3:26:ASP:OD1	65:e3:26:ASP:N	2.39	0.52
1:A1:681:U:H4'	25:Y1:9:THR:HG22	1.92	0.52
37:52:2395:A:C4	67:g3:2:VAL:CA	2.92	0.52
37:52:4128:A:O2'	83:G3:88:ARG:NH1	2.43	0.52
37:52:4735:G:N2	37:52:4736:C:N3	2.57	0.52
44:F3:34:LYS:O	44:F3:38:GLN:NE2	2.43	0.52
5:E1:139:SER:OG	5:E1:140:GLY:N	2.42	0.52
37:52:54:G:HO2'	48:N3:108:ARG:HH22	1.57	0.52
37:52:450:G:H1	37:52:1297:U:H3	1.58	0.52
37:52:2666:U:H5''	52:R3:107:ARG:HH21	1.75	0.52
37:52:4195:G:OP2	37:52:4195:G:N2	2.40	0.52
51:Q3:14:ARG:NE	51:Q3:14:ARG:CD	2.73	0.52
78:s3:198:ILE:HD12	78:s3:198:ILE:N	2.23	0.52
41:B3:222:VAL:O	41:B3:343:ARG:NH1	2.43	0.52
79:t3:92:ARG:HA	79:t3:94:LYS:HE3	1.92	0.52
3:C1:122:GLU:O	3:C1:165:ARG:NH2	2.43	0.51
36:k1:393:ALA:HB1	36:k1:406:VAL:HA	1.92	0.51
37:52:423:G:OP1	50:P3:62:ARG:NH2	2.41	0.51
41:B3:307:TYR:HD2	41:B3:366:LYS:HG2	1.76	0.51
71:k3:60:LEU:HD12	71:k3:64:LEU:HD23	1.92	0.51
1:A1:1328:G:N2	1:A1:1502:C:O2	2.43	0.51
20:T1:115:LYS:HE2	20:T1:126:PHE:HB2	1.90	0.51
37:52:1356:U:O2'	37:52:1505:C:O2	2.28	0.51
37:52:2400:G:N7	67:g3:4:ARG:NH2	2.58	0.51
75:o3:3:ASN:ND2	75:o3:95:GLY:O	2.43	0.51
75:o3:10:THR:OG1	75:o3:11:PHE:N	2.41	0.51
1:A1:1679:A:OP1	7:G1:60:ARG:NH2	2.44	0.51
1:A1:1711:U:H2'	1:A1:1712:A:H8	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M1:104:LYS:O	25:Y1:11:ARG:NH2	2.42	0.51
34:h1:153:CYS:SG	34:h1:155:ARG:NH1	2.84	0.51
36:k1:251:GLN:OE1	36:k1:381:ASN:ND2	2.42	0.51
37:52:63:G:OP2	48:N3:169:ARG:NH1	2.38	0.51
37:52:4122:G:C2	60:Z3:135:ARG:HB3	2.45	0.51
1:A1:678:U:OP2	1:A1:1026:C:N4	2.43	0.51
1:A1:970:G:C2	37:52:3712:A:C6	2.98	0.51
24:X1:86:LEU:HD23	24:X1:117:ARG:HE	1.76	0.51
34:h1:152:SER:OG	34:h1:168:CYS:SG	2.67	0.51
37:52:2395:A:C2	67:g3:2:VAL:CA	2.93	0.51
37:52:2751:G:H4'	67:g3:77:ALA:HA	1.92	0.51
37:52:4254:G:H22	37:52:4257:A:H2	1.56	0.51
59:Y3:89:LYS:HG2	59:Y3:90:ALA:H	1.76	0.51
61:a3:82:VAL:HG21	61:a3:101:ILE:HG12	1.91	0.51
1:A1:1296:U:O2	1:A1:1303:C:N4	2.44	0.51
3:C1:32:ASP:OD1	3:C1:46:LYS:NZ	2.37	0.51
36:k1:506:ARG:O	36:k1:510:HIS:ND1	2.41	0.51
37:52:2631:U:C5	55:U3:49:VAL:CB	2.93	0.51
42:C3:169:LEU:HD12	42:C3:172:LYS:HG3	1.92	0.51
87:u3:50:SER:HA	87:u3:158:GLN:HA	1.91	0.51
1:A1:1741:U:OP1	10:J1:42:ARG:NH2	2.44	0.51
78:s3:53:VAL:HG13	78:s3:89:VAL:HG22	1.92	0.51
1:A1:190:G:O2'	1:A1:209:A:N6	2.43	0.51
1:A1:970:G:N3	37:52:3712:A:N1	2.58	0.51
5:E1:6:SER:OG	5:E1:7:LYS:N	2.42	0.51
37:52:219:G:C2	42:C3:172:LYS:HD3	2.45	0.51
37:52:2422:C:O2'	37:52:3857:G:O2'	2.25	0.51
37:52:2659:A:N7	37:52:2675:G:N2	2.59	0.51
56:V3:123:LYS:HB3	56:V3:140:ALA:HB2	1.92	0.51
10:J1:139:LYS:O	10:J1:141:ARG:NH2	2.44	0.51
34:h1:177:TRP:HA	34:h1:184:LEU:HA	1.91	0.51
37:52:1970:A:H1'	78:s3:37:SER:H	1.76	0.51
41:B3:283:LYS:HD3	41:B3:363:ILE:HD11	1.92	0.51
47:M3:31:ILE:HG22	47:M3:32:ASP:HB2	1.92	0.51
48:N3:38:ARG:HG2	48:N3:62:TYR:HE1	1.76	0.51
3:C1:136:ARG:HE	3:C1:218:LEU:HD11	1.76	0.51
4:D1:146:GLU:OE2	5:E1:120:TYR:OH	2.29	0.51
37:52:1991:A:N6	37:52:2003:G:OP1	2.44	0.51
37:52:4680:G:N2	37:52:4711:C:O2	2.44	0.51
37:52:4908:G:H21	37:52:4913:G:H1	1.57	0.51
84:D3:99:TYR:OH	84:D3:168:ASP:OD2	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:52:2638:G:O3'	67:g3:24:ARG:NH1	2.40	0.51
57:W3:9:SER:OG	57:W3:36:CYS:SG	2.62	0.51
67:g3:101:LYS:HA	67:g3:104:VAL:HB	1.93	0.51
87:u3:160:LYS:HD3	87:u3:162:VAL:H	1.76	0.51
37:52:91:G:H5'	37:52:92:C:H5''	1.93	0.50
37:52:2452:G:N2	37:52:2508:U:O4	2.44	0.50
41:B3:234:ARG:NH1	41:B3:271:GLN:O	2.40	0.50
78:s3:193:PHE:HA	78:s3:198:ILE:CG1	2.40	0.50
87:u3:57:SER:OG	87:u3:182:ASN:ND2	2.42	0.50
1:A1:1286:G:N3	1:A1:1312:G:N2	2.59	0.50
5:E1:40:ARG:HH12	5:E1:49:ILE:HD11	1.75	0.50
37:52:119:G:C5	83:G3:185:ARG:HD3	2.46	0.50
37:52:235:A:O2'	37:52:237:G:OP2	2.28	0.50
37:52:292:G:O6	48:N3:181:HIS:ND1	2.41	0.50
37:52:721:G:H1	37:52:947:C:H42	1.58	0.50
37:52:1952:G:H1	37:52:2031:C:H42	1.58	0.50
37:52:2395:A:C4	67:g3:2:VAL:CB	2.94	0.50
37:52:2822:G:H5'	52:R3:18:GLY:HA3	1.92	0.50
41:B3:71:GLU:OE1	57:W3:1:MET:N	2.42	0.50
2:B1:183:LEU:HD22	2:B1:188:THR:HG21	1.93	0.50
13:M1:103:GLU:HB3	25:Y1:10:ALA:HB3	1.92	0.50
38:72:63:C:C6	85:I3:203:ARG:C	2.89	0.50
52:R3:95:TRP:HH2	52:R3:103:ARG:HH22	1.58	0.50
57:W3:96:GLN:HB3	57:W3:101:ARG:HH21	1.76	0.50
1:A1:970:G:N1	37:52:3712:A:C6	2.79	0.50
35:j1:394:ASP:HA	35:j1:399:GLY:HA3	1.94	0.50
37:52:83:C:H1'	37:52:101:A:H61	1.76	0.50
37:52:732:A:C8	37:52:733:A:H1'	2.46	0.50
37:52:1968:G:H22	37:52:2020:U:H3	1.59	0.50
37:52:2696:A:C8	71:k3:26:LYS:HE2	2.46	0.50
63:c3:51:ASN:HB2	76:p3:41:PHE:HD1	1.77	0.50
73:m3:68:MET:HB2	73:m3:77:LEU:HB2	1.93	0.50
37:52:1077:C:O2	37:52:1234:G:N2	2.45	0.50
37:52:2021:G:N3	78:s3:85:ASN:N	2.59	0.50
43:E3:52:LEU:HD13	43:E3:53:VAL:HG23	1.93	0.50
1:A1:65:C:H41	8:H1:136:LYS:HB2	1.75	0.50
37:52:2624:G:OP2	55:U3:97:ARG:NH2	2.45	0.50
37:52:2631:U:C4	55:U3:49:VAL:C	2.90	0.50
79:t3:110:VAL:O	79:t3:114:ARG:N	2.43	0.50
6:F1:80:ILE:HG13	6:F1:81:THR:HG23	1.94	0.50
14:N1:52:LEU:HB2	14:N1:76:LEU:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:b1:22:ARG:HH21	28:b1:27:ALA:HB1	1.76	0.50
33:g1:134:SER:HA	33:g1:139:HIS:HD2	1.77	0.50
35;j1:169:LEU:HD13	35;j1:212:LEU:HD12	1.94	0.50
36:k1:481:ASP:O	36:k1:514:THR:OG1	2.27	0.50
37:52:1969:G:N7	78:s3:36:GLY:N	2.59	0.50
37:52:2081:C:O2'	51:Q3:10:ASP:O	2.27	0.50
37:52:2738:C:O2'	37:52:2740:U:O2	2.28	0.50
37:52:3942:A:O2'	37:52:3943:A:OP2	2.30	0.50
37:52:4522:G:O2'	37:52:4525:C:OP2	2.26	0.50
38:72:63:C:C2	85:I3:203:ARG:C	2.89	0.50
44:F3:156:ARG:HH22	44:F3:212:LEU:HA	1.77	0.50
76:p3:36:LYS:HD3	76:p3:46:LYS:HA	1.93	0.50
1:A1:108:G:N2	1:A1:354:U:O2	2.44	0.50
37:52:280:G:N2	37:52:306:A:OP2	2.42	0.50
37:52:1272:C:H3'	62:b3:117:ARG:HH21	1.76	0.50
37:52:2460:A:O2'	48:N3:96:ARG:NH1	2.44	0.50
41:B3:310:SER:OG	41:B3:311:ASP:N	2.45	0.50
42:C3:84:THR:HG23	42:C3:86:ARG:H	1.77	0.50
87:u3:143:ASN:HB3	87:u3:147:LYS:HB2	1.93	0.50
1:A1:1599:U:OP1	27:a1:80:ARG:NH2	2.45	0.50
37:52:68:U:OP1	48:N3:178:HIS:ND1	2.38	0.50
37:52:517:C:H2'	37:52:518:G:H8	1.76	0.50
37:52:3619:G:N2	37:52:3623:C:N3	2.60	0.50
1:A1:1498:A:OP2	5:E1:27:ARG:NH2	2.44	0.49
8:H1:58:LYS:HB2	36:k1:583:ILE:HD13	1.94	0.49
34:h1:61:GLY:O	34:h1:88:ARG:NH2	2.46	0.49
37:52:2395:A:C5	67:g3:2:VAL:CB	2.95	0.49
37:52:2580:U:H5	60:Z3:38:TYR:CZ	2.30	0.49
37:52:2580:U:H3'	60:Z3:74:VAL:HA	1.93	0.49
40:A3:45:VAL:HG22	40:A3:61:VAL:HG12	1.94	0.49
63:c3:32:LYS:O	63:c3:36:LYS:N	2.44	0.49
35;j1:311:ALA:HB2	35;j1:419:PHE:HZ	1.76	0.49
36:k1:424:VAL:HG21	36:k1:454:ILE:HG22	1.93	0.49
37:52:1487:G:H2'	37:52:1488:G:H8	1.77	0.49
37:52:1492:G:O2'	62:b3:41:ARG:NH1	2.45	0.49
37:52:4042:G:C5'	87:u3:101:LYS:H	2.25	0.49
37:52:4042:G:C4'	87:u3:101:LYS:H	2.18	0.49
41:B3:160:ILE:HD13	41:B3:194:LEU:HD13	1.95	0.49
53:S3:68:PHE:C	53:S3:68:PHE:HA	2.31	0.49
1:A1:144:U:OP2	8:H1:139:SER:OG	2.31	0.49
35;j1:40:PRO:HD3	35;j1:123:SER:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:k1:348:TYR:HB2	36:k1:369:PHE:HB3	1.94	0.49
40:A3:182:ALA:O	40:A3:186:TYR:N	2.41	0.49
43:E3:216:THR:HG23	43:E3:218:ALA:H	1.77	0.49
69:i3:102:ALA:HB3	87:u3:9:THR:CG2	2.42	0.49
84:D3:25:GLU:OE1	84:D3:27:LYS:NZ	2.38	0.49
1:A1:1805:G:H2'	1:A1:1806:A:H8	1.77	0.49
37:52:119:G:N2	83:G3:186:PRO:O	2.45	0.49
37:52:1100:U:O2'	37:52:1101:C:O4'	2.31	0.49
37:52:3919:C:H4'	40:A3:207:VAL:HG12	1.94	0.49
37:52:4091:G:N2	37:52:4159:C:O2	2.45	0.49
40:A3:8:GLN:NE2	40:A3:231:ALA:O	2.46	0.49
77:r3:103:HIS:CD2	77:r3:106:LEU:HD23	2.47	0.49
1:A1:1843:G:OP1	74:n3:7:LYS:NZ	2.43	0.49
7:G1:126:THR:OG1	30:d1:26:GLN:NE2	2.45	0.49
8:H1:131:ARG:N	57:W3:85:ALA:O	2.45	0.49
14:N1:14:VAL:HG23	14:N1:18:LEU:HB2	1.94	0.49
34:h1:3:GLU:HA	34:h1:314:ILE:HG13	1.95	0.49
37:52:1882:U:OP1	37:52:2280:G:O2'	2.29	0.49
37:52:1961:G:N2	37:52:2024:G:O2'	2.45	0.49
37:52:1976:G:O6	37:52:1990:A:N6	2.38	0.49
43:E3:141:ARG:NH1	43:E3:172:SER:O	2.45	0.49
52:R3:110:ARG:HD3	52:R3:111:GLU:HG3	1.94	0.49
60:Z3:46:ILE:HA	60:Z3:68:ILE:HG23	1.93	0.49
69:i3:103:LYS:NZ	87:u3:10:LEU:HD11	2.26	0.49
78:s3:195:ASN:C	78:s3:197:SER:H	2.20	0.49
37:52:1398:A:H62	37:52:1419:G:H21	1.58	0.49
39:82:96:C:H5'	68:h3:66:LYS:HD3	1.95	0.49
42:C3:286:ASN:N	51:Q3:124:ASP:OD2	2.44	0.49
67:g3:46:CYS:SG	67:g3:47:GLY:N	2.85	0.49
78:s3:139:GLN:NE2	78:s3:145:THR:O	2.46	0.49
84:D3:77:ALA:O	84:D3:108:ARG:NH2	2.45	0.49
1:A1:441:C:OP2	10:J1:2:GLY:N	2.46	0.49
37:52:164:G:N2	37:52:272:U:O2	2.46	0.49
37:52:1982:G:N2	37:52:2009:A:O2'	2.41	0.49
37:52:2468:U:N3	37:52:2471:G:O6	2.46	0.49
53:S3:168:THR:OG1	53:S3:169:THR:N	2.45	0.49
87:u3:120:ILE:HG13	87:u3:124:LEU:HB2	1.94	0.49
1:A1:677:G:H21	1:A1:1028:A:H62	1.61	0.49
8:H1:7:PHE:HD1	8:H1:113:ILE:HB	1.78	0.49
14:N1:52:LEU:HD23	14:N1:78:LYS:HG2	1.93	0.49
16:P1:30:VAL:HG23	16:P1:94:HIS:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:j1:180:HIS:HB2	35:j1:182:ARG:HG3	1.94	0.49
37:52:119:G:C4	83:G3:185:ARG:CD	2.95	0.49
37:52:2479:G:H1	37:52:2499:C:H42	1.61	0.49
37:52:2599:G:N2	37:52:2747:U:O4	2.45	0.49
37:52:3971:G:H21	37:52:4050:A:H62	1.60	0.49
37:52:4042:G:H4'	87:u3:101:LYS:N	2.21	0.49
48:N3:58:GLY:HA3	48:N3:142:ILE:HD11	1.95	0.49
52:R3:119:MET:HE1	52:R3:146:LYS:HZ3	1.77	0.49
69:i3:98:ARG:O	87:u3:9:THR:OG1	2.31	0.49
78:s3:63:LYS:HA	78:s3:66:ARG:HB2	1.93	0.49
83:G3:86:GLU:O	83:G3:88:ARG:NH1	2.46	0.49
1:A1:498:C:N4	1:A1:499:G:O6	2.46	0.49
1:A1:909:G:OP2	52:R3:176:ARG:NH1	2.43	0.49
1:A1:1616:U:OP2	17:Q1:43:ARG:NH2	2.46	0.49
16:P1:131:ASP:HB3	16:P1:133:THR:HG23	1.95	0.49
37:52:1073:G:H2'	37:52:1074:G:H8	1.78	0.49
37:52:2604:C:H42	37:52:2735:G:H1	1.60	0.49
37:52:2897:G:N3	37:52:3603:G:N1	2.61	0.49
48:N3:110:CYS:HB3	48:N3:113:LEU:HD12	1.95	0.49
63:c3:79:ILE:O	63:c3:83:THR:OG1	2.26	0.49
8:H1:132:ARG:HG3	8:H1:133:LEU:HD12	1.95	0.49
33:g1:134:SER:HA	33:g1:139:HIS:CD2	2.47	0.49
37:52:2695:A:O5'	71:k3:33:LYS:NZ	2.35	0.49
86:1:13:ALA:O	86:1:14:ALA:HB2	2.12	0.49
4:D1:206:SER:OG	4:D1:207:ALA:N	2.46	0.48
34:h1:110:SER:HB3	34:h1:153:CYS:HA	1.95	0.48
37:52:1553:A:O5'	76:p3:4:ARG:NH1	2.46	0.48
37:52:2891:U:OP2	52:R3:74:ARG:NH2	2.46	0.48
39:82:41:A:N6	39:82:102:G:O2'	2.46	0.48
63:c3:55:LEU:O	63:c3:59:GLU:N	2.45	0.48
78:s3:59:THR:HG22	78:s3:62:ARG:HE	1.77	0.48
84:D3:90:VAL:HG21	84:D3:231:VAL:HG21	1.95	0.48
1:A1:282:G:H5''	1:A1:891:G:H4'	1.95	0.48
1:A1:970:G:C5	37:52:3712:A:C4	3.00	0.48
1:A1:1401:A:N6	1:A1:1441:U:O2'	2.46	0.48
37:52:1069:G:H2'	37:52:1070:G:H4'	1.96	0.48
37:52:1237:C:N3	43:E3:61:ARG:NH2	2.61	0.48
37:52:1395:U:OP1	46:L3:183:ARG:NH1	2.44	0.48
37:52:2756:G:N1	37:52:2757:A:N3	2.60	0.48
37:52:4121:G:N3	67:g3:93:ARG:NH2	2.60	0.48
47:M3:6:PHE:O	47:M3:11:ARG:NE	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:P3:4:TYR:HE2	50:P3:16:LYS:HB3	1.78	0.48
83:G3:314:LEU:O	83:G3:318:LEU:N	2.44	0.48
87:u3:58:THR:HA	87:u3:153:SER:HB2	1.95	0.48
36:k1:538:VAL:HG23	36:k1:541:LYS:HB2	1.94	0.48
37:52:709:C:H1'	37:52:4942:C:H5	1.77	0.48
37:52:962:C:H42	37:52:970:G:H1	1.60	0.48
37:52:1960:A:H8	78:s3:63:LYS:HD3	1.79	0.48
37:52:1964:A:N7	37:52:4694:G:N2	2.61	0.48
37:52:1994:C:H1'	79:t3:130:LYS:HD2	1.94	0.48
37:52:2395:A:C2	67:g3:4:ARG:HG3	2.48	0.48
37:52:2631:U:C4	55:U3:49:VAL:HB	2.48	0.48
37:52:4384:U:O2'	37:52:4386:C:OP1	2.30	0.48
37:52:4993:G:N2	37:52:5059:C:O2	2.42	0.48
2:B1:63:ARG:HD3	2:B1:185:MET:HE1	1.94	0.48
8:H1:146:ASN:HB3	57:W3:101:ARG:HH12	1.77	0.48
37:52:2631:U:C5	55:U3:49:VAL:CA	2.88	0.48
37:52:4045:G:H22	37:52:4048:A:H5''	1.77	0.48
59:Y3:55:VAL:HG13	59:Y3:104:VAL:HG13	1.95	0.48
82:J3:18:ARG:HG3	82:J3:135:GLY:HA3	1.95	0.48
23:W1:15:ARG:HH11	23:W1:33:GLN:HE21	1.61	0.48
36:k1:536:ASP:N	36:k1:544:VAL:O	2.47	0.48
37:52:488:G:N2	37:52:489:C:O2	2.47	0.48
37:52:978:G:N2	37:52:1278:C:N3	2.57	0.48
37:52:4425:G:OP1	73:m3:74:TYR:OH	2.31	0.48
38:72:47:G:H21	84:D3:222:GLN:HE22	1.61	0.48
57:W3:13:ILE:HG12	57:W3:32:LEU:HD13	1.94	0.48
60:Z3:28:ASN:N	60:Z3:28:ASN:OD1	2.41	0.48
79:t3:141:CYS:SG	79:t3:142:ASN:N	2.87	0.48
8:H1:132:ARG:H	57:W3:82:ILE:HB	1.78	0.48
8:H1:132:ARG:N	57:W3:82:ILE:HB	2.28	0.48
19:S1:58:MET:O	19:S1:62:GLN:NE2	2.46	0.48
21:U1:116:ASP:N	21:U1:120:GLY:O	2.46	0.48
37:52:1100:U:H3	37:52:1195:G:H22	1.61	0.48
37:52:4165:C:OP1	83:G3:106:ARG:NH2	2.46	0.48
36:k1:27:LYS:O	36:k1:33:ARG:NH1	2.47	0.48
37:52:280:G:OP2	48:N3:44:ARG:NH2	2.38	0.48
37:52:283:G:H1'	69:i3:82:ARG:HH12	1.78	0.48
37:52:1100:U:O2	37:52:1196:G:N2	2.46	0.48
37:52:5047:C:O2'	37:52:5050:C:OP2	2.32	0.48
55:U3:47:ILE:H	55:U3:56:LEU:HD22	1.79	0.48
83:G3:315:ALA:HA	83:G3:318:LEU:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P1:34:PHE:HD1	16:P1:98:ARG:HD2	1.79	0.48
36:k1:529:ALA:HB3	36:k1:551:LEU:HD12	1.94	0.48
37:52:119:G:C6	83:G3:185:ARG:CZ	2.97	0.48
37:52:2021:G:H2'	78:s3:83:ARG:H	1.79	0.48
37:52:2529:A:N6	37:52:2532:C:O2	2.47	0.48
37:52:4471:U:OP2	45:H3:168:LYS:NZ	2.47	0.48
1:A1:744:G:O2'	1:A1:746:C:N4	2.47	0.48
3:C1:103:MET:HE1	3:C1:212:VAL:HG23	1.96	0.48
5:E1:21:LEU:HD23	5:E1:37:VAL:HG21	1.96	0.48
5:E1:127:MET:HE1	5:E1:133:GLY:HA2	1.96	0.48
5:E1:177:LEU:HD13	5:E1:182:LEU:HD13	1.96	0.48
18:R1:16:LYS:HG3	18:R1:17:LYS:H	1.79	0.48
27:a1:68:ILE:N	27:a1:109:TYR:O	2.47	0.48
37:52:119:G:C5	83:G3:185:ARG:CD	2.97	0.48
37:52:3660:C:H2'	37:52:3682:A:H61	1.78	0.48
67:g3:49:CYS:HB3	67:g3:85:LYS:HD3	1.96	0.48
1:A1:677:G:OP1	15:O1:124:ARG:NH2	2.47	0.48
16:P1:20:GLN:HG2	16:P1:27:VAL:HG23	1.96	0.48
17:Q1:33:LEU:HG	17:Q1:37:TYR:HE1	1.79	0.48
36:k1:222:LEU:O	36:k1:226:ALA:N	2.44	0.48
36:k1:537:GLY:HA3	36:k1:543:THR:HG22	1.94	0.48
37:52:125:C:O2	37:52:144:G:N2	2.40	0.48
37:52:2389:A:H2'	37:52:2390:G:H8	1.78	0.48
37:52:2395:A:C5	67:g3:2:VAL:CA	2.97	0.48
60:Z3:40:HIS:O	60:Z3:77:TYR:OH	2.26	0.48
60:Z3:134:LEU:HD21	67:g3:91:ILE:HD13	1.94	0.48
85:I3:179:ASP:OD1	85:I3:179:ASP:N	2.47	0.48
1:A1:429:C:OP1	6:F1:10:LYS:NZ	2.35	0.47
5:E1:132:LYS:HG3	5:E1:156:LEU:HB3	1.95	0.47
9:I1:61:ILE:HD11	9:I1:95:ILE:HD12	1.96	0.47
19:S1:77:GLU:OE2	19:S1:81:ARG:NH1	2.46	0.47
37:52:2284:G:H2'	37:52:2285:A:H8	1.79	0.47
37:52:2399:G:C4	67:g3:4:ARG:CD	2.97	0.47
37:52:4992:G:N2	37:52:5060:A:N3	2.62	0.47
39:82:131:G:H5''	58:X3:108:GLN:HE21	1.78	0.47
46:L3:77:SER:OG	46:L3:78:LEU:N	2.47	0.47
1:A1:1662:U:O4	1:A1:1663:A:N6	2.47	0.47
1:A1:1737:G:OP1	8:H1:94:ARG:NH2	2.47	0.47
13:M1:40:ILE:HD11	13:M1:68:ILE:HG13	1.95	0.47
18:R1:97:GLN:HE21	34:h1:58:ALA:HB3	1.79	0.47
23:W1:17:CYS:HB2	23:W1:56:CYS:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:h1:248:LEU:HB3	34:h1:261:LEU:HD21	1.96	0.47
37:52:119:G:H22	83:G3:186:PRO:HG2	1.79	0.47
37:52:759:G:N2	37:52:760:G:O2'	2.47	0.47
37:52:1968:G:H21	78:s3:85:ASN:HD21	1.62	0.47
37:52:3690:U:OP2	40:A3:200:ARG:NH1	2.47	0.47
37:52:4910:A:H4'	41:B3:95:THR:HG22	1.96	0.47
37:52:5057:C:O2'	64:d3:23:ARG:NH2	2.47	0.47
40:A3:101:VAL:HB	40:A3:165:VAL:HG12	1.96	0.47
73:m3:73:CYS:HB3	73:m3:89:CYS:HB3	1.96	0.47
1:A1:511:U:H2'	1:A1:512:A:H8	1.79	0.47
1:A1:1462:U:OP2	1:A1:1463:U:N3	2.42	0.47
1:A1:1692:U:H2'	1:A1:1693:G:C8	2.48	0.47
22:V1:41:ARG:HA	22:V1:44:LYS:HB2	1.96	0.47
26:Z1:55:ILE:HG12	26:Z1:75:ILE:HG12	1.95	0.47
37:52:325:U:OP1	46:L3:103:ARG:NH1	2.46	0.47
37:52:1184:A:H2'	37:52:1185:G:C5	2.49	0.47
37:52:1406(C):G:H1	37:52:1411:C:H42	1.61	0.47
55:U3:47:ILE:HB	55:U3:56:LEU:HD22	1.96	0.47
1:A1:163:U:OP2	8:H1:87:ARG:NH2	2.48	0.47
1:A1:1355:C:O2	4:D1:235:ASN:ND2	2.46	0.47
26:Z1:85:ASN:OD1	26:Z1:85:ASN:N	2.46	0.47
27:a1:65:TYR:OH	27:a1:76:ARG:NH2	2.47	0.47
37:52:106:A:OP1	46:L3:39:ARG:NH2	2.43	0.47
37:52:156:G:N2	37:52:157:U:O4	2.47	0.47
37:52:1332:C:H2'	37:52:1333:A:C8	2.48	0.47
38:72:120:U:H3'	84:D3:259:ARG:HH12	1.79	0.47
40:A3:43:GLY:HA3	40:A3:88:VAL:H	1.79	0.47
59:Y3:127:GLN:O	59:Y3:131:GLU:N	2.47	0.47
78:s3:65:ILE:HG23	78:s3:75:LEU:HB3	1.94	0.47
87:u3:65:VAL:HB	87:u3:147:LYS:HE2	1.96	0.47
5:E1:225:GLU:HB3	34:h1:187:ASN:HB2	1.95	0.47
35:j1:319:ILE:HB	35:j1:412:ILE:HD12	1.96	0.47
37:52:152:U:OP2	48:N3:49:ARG:NH2	2.38	0.47
37:52:731:G:H21	53:S3:68:PHE:HE2	1.62	0.47
37:52:2395:A:C2	67:g3:2:VAL:CB	2.96	0.47
54:T3:31:MET:HG3	84:D3:69:ILE:HG22	1.97	0.47
63:c3:35:LEU:O	63:c3:39:ARG:N	2.40	0.47
65:e3:114:ARG:NH1	65:e3:117:GLN:OE1	2.47	0.47
87:u3:33:GLU:N	87:u3:207:LYS:O	2.35	0.47
1:A1:334:C:H5	8:H1:190:ARG:HH12	1.62	0.47
1:A1:1515:G:H2'	1:A1:1516:G:H8	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:1692:U:H2'	1:A1:1693:G:H8	1.79	0.47
3:C1:33:VAL:HA	3:C1:96:CYS:HB2	1.97	0.47
3:C1:139:CYS:SG	3:C1:140:VAL:N	2.88	0.47
36:k1:506:ARG:NH1	37:52:4600:G:OP1	2.38	0.47
37:52:115:C:O2'	37:52:276:C:OP1	2.33	0.47
37:52:709:C:OP1	66:f3:89:ARG:NH1	2.48	0.47
37:52:4043:G:P	87:u3:100:VAL:HG12	2.54	0.47
37:52:4300:U:H4'	54:T3:89:ILE:HG22	1.95	0.47
50:P3:4:TYR:HE1	50:P3:18:ARG:HD3	1.79	0.47
78:s3:26:LYS:HG2	78:s3:91:THR:HG23	1.96	0.47
1:A1:316:G:H1	1:A1:334:C:H42	1.63	0.47
1:A1:667:U:O4	1:A1:1143:A:N6	2.48	0.47
5:E1:72:VAL:HG22	12:L1:20:VAL:HG21	1.96	0.47
9:I1:144:ILE:HD12	24:X1:52:ILE:HD11	1.97	0.47
16:P1:98:ARG:NH1	16:P1:100:THR:O	2.48	0.47
36:k1:508:ILE:HA	36:k1:512:LYS:H	1.79	0.47
37:52:351:C:N3	39:82:25:G:N2	2.63	0.47
37:52:1998:A:C4	78:s3:55:MET:HG3	2.50	0.47
37:52:1998:A:C6	78:s3:55:MET:HE3	2.49	0.47
37:52:3777:G:O2'	37:52:3815:G:O6	2.31	0.47
38:72:6:C:H3'	38:72:7:G:H4'	1.95	0.47
53:S3:154:LEU:HB3	53:S3:157:ARG:HD3	1.97	0.47
86:1:14:ALA:O	86:1:15:ALA:HB2	2.14	0.47
87:u3:23:ARG:HG2	87:u3:212:LYS:HD2	1.97	0.47
8:H1:5:ILE:HG12	8:H1:111:LEU:HB2	1.96	0.47
20:T1:14:ARG:HE	20:T1:17:ASN:HA	1.80	0.47
37:52:714:G:N3	37:52:955:G:N2	2.62	0.47
37:52:732:A:N1	53:S3:68:PHE:CA	2.69	0.47
37:52:1073:G:H2'	37:52:1074:G:C8	2.49	0.47
37:52:1868:A:N6	37:52:1870:C:O2	2.48	0.47
37:52:1959:U:OP1	37:52:1960:A:O2'	2.28	0.47
1:A1:1216:C:H5''	1:A1:1217:A:H5''	1.97	0.47
1:A1:1808:U:H2'	1:A1:1809:A:H8	1.80	0.47
2:B1:124:VAL:HG21	2:B1:134:LEU:HD21	1.97	0.47
5:E1:195:SER:HB2	5:E1:197:LYS:HE2	1.97	0.47
10:J1:148:LYS:O	10:J1:152:ARG:N	2.45	0.47
18:R1:116:ASP:HB3	18:R1:119:LEU:HD23	1.97	0.47
20:T1:112:GLU:O	20:T1:116:LYS:N	2.47	0.47
38:72:19:C:O2	38:72:60:G:N2	2.48	0.47
79:t3:28:LEU:HD13	79:t3:39:PRO:HB2	1.96	0.47
1:A1:969:U:OP1	1:A1:970:G:O2'	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K1:176:LYS:O	11:K1:180:LYS:N	2.41	0.47
37:52:2084:U:C6	51:Q3:14:ARG:CD	2.98	0.47
37:52:2084:U:N3	51:Q3:14:ARG:HD3	2.29	0.47
37:52:4313:A:OP1	54:T3:92:ARG:NH2	2.44	0.47
37:52:4729:A:OP2	37:52:5068:G:N2	2.48	0.47
37:52:4740:G:H22	37:52:4959:U:H3	1.63	0.47
60:Z3:99:ASP:O	60:Z3:103:ASP:N	2.42	0.47
1:A1:1719:A:N6	1:A1:1814:G:O2'	2.48	0.46
11:K1:179:LYS:HA	11:K1:182:GLN:HB2	1.97	0.46
15:O1:32:ASP:O	15:O1:36:GLN:N	2.46	0.46
37:52:1441:C:H42	37:52:2113:G:H1	1.63	0.46
37:52:2749:C:H2'	37:52:2750:G:C8	2.50	0.46
63:c3:78:ASN:HD21	76:p3:43:GLY:HA2	1.79	0.46
65:e3:85:LEU:HD11	65:e3:111:ILE:HG23	1.96	0.46
1:A1:149:A:H2'	1:A1:150:A:H8	1.80	0.46
1:A1:970:G:N7	37:52:3712:A:H1'	2.30	0.46
1:A1:1600:G:H5'	27:a1:43:LYS:HG3	1.96	0.46
11:K1:19:PRO:O	11:K1:24:ARG:NH2	2.47	0.46
37:52:173:C:O2	68:h3:112:ARG:NH1	2.49	0.46
37:52:2021:G:O4'	78:s3:86:VAL:HB	2.15	0.46
37:52:2581:A:P	60:Z3:75:TYR:H	2.38	0.46
37:52:2583:C:C2	60:Z3:73:LYS:HG2	2.51	0.46
67:g3:43:LYS:HG2	67:g3:44:SER:N	2.30	0.46
9:I1:31:GLU:HB2	9:I1:40:LEU:HB2	1.97	0.46
34:h1:292:SER:OG	34:h1:293:ALA:N	2.46	0.46
35:j1:300:LYS:HA	35:j1:413:LEU:HD12	1.97	0.46
37:52:300:A:H2'	37:52:301:G:H8	1.80	0.46
37:52:983:C:N3	43:E3:73:ARG:NE	2.63	0.46
37:52:1790:U:OP2	54:T3:13:TYR:OH	2.32	0.46
37:52:2084:U:N1	51:Q3:14:ARG:CD	2.77	0.46
37:52:2537:A:H5''	71:k3:41:TYR:HD1	1.81	0.46
83:G3:282:ARG:HG3	83:G3:283:TYR:H	1.80	0.46
84:D3:65:ALA:HB2	84:D3:74:ILE:HD13	1.96	0.46
1:A1:74:G:N2	1:A1:77:A:OP2	2.49	0.46
1:A1:77:A:O2'	8:H1:174:PRO:O	2.33	0.46
1:A1:1310:U:H3'	14:N1:40:LYS:HZ1	1.80	0.46
34:h1:150:TRP:HB2	34:h1:170:TRP:CD1	2.51	0.46
37:52:2696:A:C8	71:k3:69:LEU:HB3	2.50	0.46
13:M1:57:ASP:OD2	13:M1:60:CYS:N	2.49	0.46
37:52:107:G:OP2	46:L3:42:ARG:NH1	2.45	0.46
85:I3:29:ALA:HB3	85:I3:32:ARG:HH22	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:446:G:OP2	10:J1:47:ARG:NH1	2.48	0.46
1:A1:532:C:H2'	1:A1:533:A:C8	2.51	0.46
1:A1:1468:C:H2'	1:A1:1469:A:H8	1.79	0.46
34:h1:207:CYS:HB3	34:h1:219:TRP:HB2	1.98	0.46
37:52:5:A:O2'	83:G3:245:ARG:NH2	2.39	0.46
37:52:1805:A:N3	62:b3:28:ARG:CA	2.74	0.46
37:52:3920:U:O2	37:52:4382:G:N2	2.48	0.46
37:52:3969:G:H1	37:52:4052:C:H42	1.62	0.46
49:O3:18:ARG:HH22	49:O3:128:ARG:CZ	2.28	0.46
57:W3:86:SER:OG	57:W3:89:ASP:N	2.48	0.46
69:i3:99:LYS:HG3	87:u3:10:LEU:HD23	1.98	0.46
1:A1:1284:A:N6	1:A1:1313:A:HO2'	2.14	0.46
2:B1:126:ASP:OD1	2:B1:165:ASN:ND2	2.49	0.46
4:D1:201:GLY:N	4:D1:221:ASP:OD2	2.48	0.46
13:M1:80:MET:HG2	13:M1:86:ILE:HG22	1.98	0.46
25:Y1:107:ARG:HD3	25:Y1:112:VAL:HG22	1.98	0.46
37:52:147:A:H1'	48:N3:57:GLN:HE21	1.80	0.46
37:52:690:C:H4'	77:r3:85:ASN:HD22	1.80	0.46
37:52:2399:G:C6	67:g3:4:ARG:HD2	2.51	0.46
63:c3:51:ASN:OD1	63:c3:52:CYS:N	2.47	0.46
65:e3:43:ASN:HB3	65:e3:46:ARG:HG2	1.97	0.46
78:s3:193:PHE:CA	78:s3:198:ILE:HG13	2.43	0.46
84:D3:256:LYS:HD3	84:D3:257:PRO:HD2	1.97	0.46
35:j1:113:ASP:N	35:j1:113:ASP:OD1	2.47	0.46
37:52:1209:U:O3'	44:F3:69:ARG:NH1	2.48	0.46
37:52:4045:G:H22	37:52:4047:A:H3'	1.79	0.46
43:E3:153:LEU:HD13	43:E3:197:VAL:HG11	1.98	0.46
1:A1:210:U:H2'	1:A1:211:G:C8	2.51	0.46
29:c1:42:LYS:HD2	29:c1:57:VAL:HG11	1.96	0.46
34:h1:39:THR:HG22	34:h1:60:ARG:HG2	1.98	0.46
35:j1:178:LYS:NZ	37:52:3788:C:O2'	2.49	0.46
37:52:2399:G:C5	67:g3:4:ARG:CD	2.99	0.46
37:52:3947:A:H61	37:52:4065:G:H22	1.62	0.46
37:52:4156:G:H5''	37:52:4157:A:H3'	1.98	0.46
38:72:63:C:N1	85:I3:203:ARG:C	2.74	0.46
46:L3:169:ILE:HD13	61:a3:142:GLY:HA2	1.97	0.46
55:U3:31:ASP:OD2	55:U3:114:TYR:OH	2.31	0.46
55:U3:66:SER:HB2	55:U3:69:LYS:HB3	1.98	0.46
1:A1:1856:C:N4	1:A1:1857:G:O6	2.49	0.46
6:F1:125:LYS:H	6:F1:142:HIS:HD2	1.62	0.46
10:J1:137:LEU:O	10:J1:141:ARG:NH1	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z1:35:VAL:HG21	26:Z1:40:ILE:HD11	1.98	0.46
34:h1:24:THR:HG21	34:h1:30:MET:HE3	1.98	0.46
37:52:2411:C:H2'	37:52:2412:A:H8	1.80	0.46
37:52:2673:G:N1	63:c3:87:LYS:HD2	2.31	0.46
52:R3:83:GLY:H	52:R3:88:ARG:HH21	1.63	0.46
53:S3:66:GLN:HG2	53:S3:68:PHE:HB3	1.97	0.46
1:A1:97:U:H2'	1:A1:98:C:H6	1.81	0.45
1:A1:918:U:O2'	24:X1:56:HIS:O	2.33	0.45
1:A1:1207:G:N2	81:w3:45:A:O2'	2.49	0.45
1:A1:1575:G:H2'	1:A1:1576:G:H8	1.81	0.45
1:A1:1734:G:O2'	1:A1:1800:A:N6	2.48	0.45
7:G1:86:LYS:HA	7:G1:89:THR:HG22	1.97	0.45
18:R1:53:GLU:OE1	18:R1:85:ARG:NH2	2.49	0.45
28:b1:2:THR:OG1	28:b1:3:LYS:N	2.47	0.45
28:b1:44:ILE:HD12	28:b1:45:VAL:HG13	1.97	0.45
36:k1:559:LEU:O	36:k1:563:GLU:N	2.46	0.45
37:52:1484:G:O2'	37:52:1486:C:OP2	2.33	0.45
37:52:1572:U:H4'	52:R3:95:TRP:CZ3	2.50	0.45
53:S3:80:ILE:HG12	53:S3:129:VAL:HG22	1.98	0.45
86:1:7:ALA:O	86:1:8:ALA:HB3	2.16	0.45
1:A1:1245:G:O2'	1:A1:1492:U:OP1	2.30	0.45
18:R1:146:ARG:HH22	80:23:33:U:H5	1.63	0.45
24:X1:7:LEU:HD23	24:X1:34:ILE:HG12	1.97	0.45
37:52:303:C:OP2	48:N3:68:ARG:NH2	2.49	0.45
37:52:1477:C:O2	37:52:1489:G:N2	2.50	0.45
37:52:1549:G:H4'	52:R3:87:ALA:HA	1.97	0.45
37:52:2084:U:C4	51:Q3:14:ARG:CZ	3.00	0.45
37:52:2411:C:H2'	37:52:2412:A:C8	2.52	0.45
43:E3:144:ARG:NH1	66:f3:110:ILE:OXT	2.49	0.45
51:Q3:61:LEU:HD21	51:Q3:66:MET:HB2	1.97	0.45
37:52:119:G:N1	83:G3:185:ARG:CD	2.79	0.45
37:52:146:G:H2'	37:52:147:A:H8	1.81	0.45
37:52:2597:G:N3	67:g3:42:PRO:HB2	2.32	0.45
37:52:3661:G:H1'	40:A3:125:LYS:HZ1	1.81	0.45
37:52:3908:A:N6	86:1:20:ALA:HA	2.31	0.45
37:52:4052:C:H1'	87:u3:210:MET:HA	1.98	0.45
51:Q3:167:VAL:HG12	51:Q3:169:SER:H	1.80	0.45
52:R3:174:GLU:O	52:R3:178:GLN:NE2	2.49	0.45
79:t3:142:ASN:HB2	79:t3:145:GLY:H	1.82	0.45
1:A1:375:U:H2'	1:A1:376:A:H8	1.81	0.45
1:A1:547:G:H21	1:A1:548:C:H5	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C1:131:ASP:OD1	3:C1:131:ASP:N	2.48	0.45
8:H1:2:LYS:HD3	8:H1:15:LEU:HD21	1.97	0.45
37:52:729:G:C8	37:52:732:A:H4'	2.50	0.45
37:52:1068:G:H2'	37:52:1069:G:H8	1.82	0.45
37:52:2639:U:P	67:g3:24:ARG:HH12	2.40	0.45
45:H3:41:ILE:HG12	45:H3:73:ILE:HD11	1.99	0.45
78:s3:13:TYR:HA	78:s3:16:LYS:HB2	1.96	0.45
78:s3:192:VAL:O	78:s3:198:ILE:HG22	2.02	0.45
87:u3:64:SER:O	87:u3:108:ASP:N	2.40	0.45
1:A1:1156:U:OP1	24:X1:71:LYS:NZ	2.42	0.45
29:c1:56:CYS:SG	29:c1:57:VAL:N	2.90	0.45
35:j1:331:TYR:OH	35:j1:351:GLU:OE1	2.34	0.45
37:52:101:A:H2'	37:52:102:G:H8	1.82	0.45
37:52:2597:G:H5''	67:g3:44:SER:HB3	1.99	0.45
37:52:3758:U:H3	37:52:3767:C:H42	1.64	0.45
38:72:8:G:O6	38:72:111:C:N4	2.49	0.45
41:B3:261:ARG:HB2	49:O3:64:THR:HG21	1.99	0.45
82:J3:151:ILE:H	82:J3:151:ILE:HG13	1.69	0.45
8:H1:121:ILE:HG23	8:H1:124:LEU:HB2	1.99	0.45
37:52:151:G:OP2	48:N3:4:TYR:OH	2.34	0.45
37:52:469:C:OP2	37:52:684:G:N1	2.45	0.45
37:52:2021:G:N3	78:s3:84:GLY:HA3	2.31	0.45
37:52:4896:G:N2	37:52:4925:U:O2	2.50	0.45
40:A3:227:ARG:HG3	40:A3:239:ALA:HB2	1.98	0.45
44:F3:93:ARG:NH1	44:F3:96:GLY:O	2.50	0.45
60:Z3:42:LEU:HD21	60:Z3:101:PHE:HZ	1.82	0.45
1:A1:317:C:H42	1:A1:333:G:H1	1.63	0.45
36:k1:411:TYR:HA	36:k1:484:LEU:HB2	1.97	0.45
37:52:648:G:H2'	37:52:649:A:H8	1.82	0.45
37:52:719:C:H42	37:52:949:G:H1	1.65	0.45
37:52:1968:G:H2'	78:s3:34:ASN:H	1.81	0.45
37:52:1969:G:H5''	78:s3:34:ASN:HD21	1.81	0.45
56:V3:13:LYS:HD2	56:V3:128:LEU:HD22	1.99	0.45
66:f3:96:ALA:HA	66:f3:99:HIS:HD2	1.80	0.45
2:B1:42:LYS:NZ	19:S1:99:ASP:OD2	2.35	0.45
8:H1:148:SER:OG	57:W3:105:ARG:NH2	2.45	0.45
14:N1:45:ARG:NH1	14:N1:71:GLU:OE2	2.49	0.45
27:a1:85:ARG:HA	27:a1:88:LEU:HD12	1.98	0.45
37:52:1972:G:N1	79:t3:131:GLU:OE2	2.49	0.45
37:52:2084:U:C2	51:Q3:14:ARG:HD3	2.51	0.45
37:52:3839:G:N2	37:52:3843:C:O2	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:A3:116:LEU:HA	40:A3:116:LEU:HD23	1.62	0.45
55:U3:34:MET:HB2	55:U3:38:ASN:HD22	1.81	0.45
62:b3:36:ASP:N	62:b3:36:ASP:OD1	2.46	0.45
67:g3:104:VAL:HG22	67:g3:107:LEU:HD12	1.97	0.45
82:J3:80:GLU:OE2	82:J3:170:TYR:OH	2.32	0.45
87:u3:59:PRO:O	87:u3:171:HIS:ND1	2.50	0.45
1:A1:970:G:C4	37:52:3712:A:N1	2.85	0.45
8:H1:147:LEU:HD11	8:H1:156:TYR:HD2	1.82	0.45
21:U1:6:VAL:O	21:U1:11:GLN:NE2	2.42	0.45
37:52:119:G:N1	83:G3:185:ARG:HD2	2.30	0.45
37:52:2265:G:OP2	77:r3:33:LYS:NZ	2.49	0.45
37:52:4699:U:H1'	37:52:4700:A:H5''	1.98	0.45
37:52:4898:G:N2	37:52:4923:U:O2'	2.50	0.45
42:C3:266:THR:OG1	42:C3:267:TRP:N	2.50	0.45
61:a3:19:HIS:HB3	61:a3:25:HIS:HB2	1.99	0.45
61:a3:89:ASN:O	61:a3:93:ASN:ND2	2.50	0.45
1:A1:385:G:O2'	10:J1:10:LYS:NZ	2.49	0.45
8:H1:57:ASP:OD2	8:H1:72:ARG:NH1	2.50	0.45
37:52:74:G:O3'	46:L3:71:ARG:NH2	2.50	0.45
37:52:907:C:H2'	37:52:908:G:C8	2.52	0.45
37:52:1094:G:H2'	37:52:1095:A:C8	2.52	0.45
37:52:4055:U:HO2'	87:u3:162:VAL:HG11	1.76	0.45
1:A1:1161:U:O4	25:Y1:3:LYS:NZ	2.48	0.44
1:A1:1215:C:H42	1:A1:1220:A:H61	1.65	0.44
3:C1:67:PHE:HE1	16:P1:48:SER:HB2	1.81	0.44
27:a1:87:ALA:O	27:a1:91:LEU:N	2.50	0.44
37:52:19:G:OP2	68:h3:93:ARG:NH2	2.50	0.44
37:52:294:G:OP1	75:o3:43:ARG:NH1	2.50	0.44
37:52:1411:C:H2'	37:52:1411(A):G:C8	2.52	0.44
37:52:2753:G:C3'	60:Z3:51:ARG:HE	2.29	0.44
37:52:2759:G:H21	37:52:2765:A:H2	1.63	0.44
37:52:4122:G:N3	67:g3:94:ALA:HB1	2.31	0.44
37:52:4492:U:O2'	37:52:4512:U:O2	2.32	0.44
42:C3:284:MET:HE3	51:Q3:124:ASP:HB3	1.99	0.44
78:s3:194:ASP:H	78:s3:198:ILE:HA	1.82	0.44
79:t3:18:THR:HA	79:t3:57:ARG:HG2	1.99	0.44
1:A1:551:U:H2'	1:A1:552:G:H8	1.82	0.44
3:C1:144:LYS:HB2	3:C1:208:HIS:HB3	1.99	0.44
6:F1:85:GLY:N	6:F1:88:ASP:OD2	2.50	0.44
37:52:1577:G:N7	40:A3:181:LYS:HE3	2.33	0.44
37:52:1687:U:H2'	37:52:1688:G:H8	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:52:1970:A:N3	78:s3:36:GLY:HA2	2.32	0.44
37:52:2492:C:H2'	37:52:2493:G:H4'	1.99	0.44
37:52:2597:G:H2'	67:g3:42:PRO:C	2.42	0.44
37:52:2694:G:OP2	71:k3:35:LYS:NZ	2.40	0.44
83:G3:149:LEU:HD13	83:G3:242:ARG:HH11	1.82	0.44
36:k1:565:THR:OG1	36:k1:585:ASP:OD1	2.35	0.44
37:52:89:C:O2'	37:52:293:G:OP1	2.35	0.44
37:52:935:A:H1'	47:M3:44:ARG:HB3	2.00	0.44
37:52:1931:C:N4	37:52:2040:A:O2'	2.48	0.44
37:52:2062:C:O2'	53:S3:111:ARG:NH1	2.50	0.44
37:52:2664:G:H4'	37:52:2677:G:H4'	1.99	0.44
37:52:2674:A:P	63:c3:32:LYS:H	2.40	0.44
41:B3:37:PRO:HA	41:B3:188:GLY:HA2	2.00	0.44
41:B3:261:ARG:HE	49:O3:64:THR:HG21	1.82	0.44
53:S3:15:ARG:HH21	54:T3:141:VAL:HG22	1.82	0.44
5:E1:10:LYS:NZ	5:E1:14:ASP:OD2	2.50	0.44
14:N1:28:HIS:CG	14:N1:114:TYR:HB3	2.52	0.44
34:h1:256:ILE:HB	34:h1:270:LEU:HB2	2.00	0.44
35:j1:8:ALA:HA	35:j1:11:ASN:HD22	1.80	0.44
36:k1:280:ASP:OD2	36:k1:576:ARG:NE	2.49	0.44
37:52:176:G:N2	37:52:260:C:O2	2.51	0.44
37:52:1341:U:O3'	48:N3:204:ARG:NH1	2.51	0.44
37:52:2608:G:P	52:R3:100:ARG:HH22	2.40	0.44
60:Z3:27:LYS:HG2	60:Z3:93:LYS:HD3	1.99	0.44
78:s3:193:PHE:HA	78:s3:198:ILE:CG2	2.44	0.44
83:G3:126:ARG:HH12	83:G3:296:GLY:N	2.15	0.44
3:C1:88:THR:HG22	3:C1:98:THR:HG22	1.98	0.44
9:I1:10:LYS:NZ	9:I1:15:LYS:O	2.50	0.44
37:52:1199:G:H2'	37:52:1200:G:C8	2.52	0.44
37:52:1573:G:OP1	52:R3:95:TRP:NE1	2.51	0.44
37:52:1691:G:OP1	51:Q3:15:ARG:NE	2.44	0.44
37:52:3853:U:O2'	37:52:4979:A:N3	2.49	0.44
40:A3:54:ARG:HG3	40:A3:56:ALA:H	1.82	0.44
44:F3:93:ARG:NH2	44:F3:115:GLN:O	2.49	0.44
1:A1:106:C:OP1	1:A1:431:G:O2'	2.36	0.44
1:A1:1599:U:OP2	27:a1:46:ASN:ND2	2.51	0.44
22:V1:98:VAL:HA	22:V1:101:ILE:HB	2.00	0.44
35:j1:311:ALA:HA	35:j1:314:MET:HG2	1.99	0.44
37:52:350:C:OP1	37:52:2294:G:O2'	2.34	0.44
37:52:1378:C:N4	46:L3:159:ASN:O	2.48	0.44
37:52:1805:A:C2	62:b3:28:ARG:C	2.96	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:52:2084:U:C5	51:Q3:14:ARG:CD	3.01	0.44
56:V3:26:ILE:HG22	56:V3:101:ASN:HB3	2.00	0.44
87:u3:209:THR:O	87:u3:211:GLY:N	2.51	0.44
1:A1:1867:U:H4'	1:A1:1868:U:H5'	1.99	0.44
5:E1:40:ARG:HG2	22:V1:108:PRO:HG3	1.99	0.44
6:F1:87:MET:HE1	6:F1:236:ILE:HD13	1.99	0.44
17:Q1:108:LYS:HD2	20:T1:117:ILE:HG22	1.99	0.44
19:S1:71:ILE:HG22	19:S1:73:LEU:H	1.83	0.44
37:52:1664:U:O2	37:52:2286:G:N2	2.50	0.44
37:52:1995:G:O6	78:s3:41:GLN:NE2	2.50	0.44
37:52:2444:U:HO2'	39:82:112:G:HO2'	1.65	0.44
37:52:2484:A:N1	37:52:2495:U:N3	2.65	0.44
37:52:3605:C:OP1	52:R3:71:ARG:NH2	2.45	0.44
38:72:59:G:O2'	84:D3:267:ASN:ND2	2.51	0.44
52:R3:44:LEU:HD22	52:R3:49:LEU:HD12	2.00	0.44
57:W3:98:PRO:HA	57:W3:101:ARG:HB2	2.00	0.44
78:s3:198:ILE:CD1	78:s3:198:ILE:H	2.30	0.44
85:I3:150:GLU:OE2	85:I3:153:ARG:NH1	2.49	0.44
1:A1:1100:A:O5'	19:S1:132:ARG:NH2	2.51	0.44
37:52:755:C:H2'	37:52:756:G:H8	1.83	0.44
37:52:1244:G:O6	62:b3:117:ARG:N	2.51	0.44
37:52:2084:U:N1	51:Q3:14:ARG:HD2	2.33	0.44
37:52:3974:G:OP1	87:u3:27:LYS:CB	2.45	0.44
52:R3:94:THR:HG23	52:R3:98:ARG:HH22	1.82	0.44
37:52:37:U:H4'	61:a3:32:ARG:HD2	2.00	0.44
37:52:2580:U:H6	37:52:2580:U:H2'	1.54	0.44
37:52:2631:U:N1	55:U3:49:VAL:N	2.66	0.44
66:f3:78:HIS:HB2	66:f3:85:ARG:HG3	1.99	0.44
67:g3:110:GLN:O	67:g3:114:GLN:NE2	2.51	0.44
69:i3:103:LYS:C	87:u3:7:ARG:CZ	2.90	0.44
22:V1:80:PHE:HB3	31:e1:52:PHE:HB3	1.99	0.43
34:h1:166:VAL:HG11	34:h1:198:VAL:HG11	2.00	0.43
37:52:2399:G:N1	67:g3:4:ARG:CD	2.81	0.43
37:52:4099:G:H22	37:52:4108:G:H1	1.66	0.43
37:52:4120:U:H3	67:g3:100:GLN:HB2	1.83	0.43
37:52:4906:C:H2'	37:52:4907:G:C8	2.53	0.43
38:72:7:G:OP1	84:D3:33:ARG:NH2	2.51	0.43
38:72:63:C:C6	85:I3:204:GLY:HA2	2.53	0.43
39:82:28:C:H2'	39:82:29:G:H8	1.83	0.43
60:Z3:5:MET:HE3	60:Z3:28:ASN:HD22	1.82	0.43
87:u3:39:LYS:HB2	87:u3:198:TRP:HZ3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C1:143:THR:HB	3:C1:205:TYR:HE2	1.83	0.43
5:E1:59:LEU:HB2	5:E1:63:GLY:HA2	1.99	0.43
7:G1:194:ASP:OD2	7:G1:198:ARG:NH2	2.50	0.43
8:H1:4:ASN:O	8:H1:111:LEU:N	2.48	0.43
12:L1:3:MET:HE1	12:L1:48:ALA:HB2	2.00	0.43
13:M1:126:VAL:HG23	13:M1:145:VAL:HG22	1.99	0.43
34:h1:197:THR:HG21	34:h1:238:ALA:HA	1.99	0.43
37:52:2581:A:OP2	60:Z3:73:LYS:N	2.33	0.43
37:52:4930:C:H5'	43:E3:269:GLN:HG2	2.00	0.43
40:A3:118:GLU:N	40:A3:162:ASN:HD22	2.09	0.43
41:B3:329:ASP:OD1	41:B3:329:ASP:N	2.51	0.43
42:C3:341:LEU:O	42:C3:345:ARG:NH1	2.52	0.43
51:Q3:172:ARG:NH2	61:a3:58:MET:O	2.51	0.43
85:I3:66:GLU:OE2	85:I3:69:ARG:NH1	2.52	0.43
5:E1:117:ARG:NH1	81:w3:59:A:O2'	2.51	0.43
7:G1:39:ILE:HG23	7:G1:68:ILE:HG21	1.98	0.43
10:J1:70:GLU:OE1	10:J1:117:TYR:OH	2.30	0.43
16:P1:150:ARG:HD3	16:P1:150:ARG:H	1.84	0.43
37:52:423:G:H21	50:P3:118:GLN:HE22	1.65	0.43
37:52:2622:G:OP2	55:U3:104:ALA:HB3	2.18	0.43
37:52:2660:A:H62	63:c3:88:TYR:HD2	1.65	0.43
37:52:3716:C:H3'	37:52:3735:G:H22	1.82	0.43
37:52:3893:C:H5''	50:P3:66:GLY:HA2	2.00	0.43
37:52:4123:C:O4'	60:Z3:135:ARG:HG3	2.19	0.43
40:A3:79:ALA:HB1	40:A3:167:GLY:HA3	2.00	0.43
49:O3:22:ILE:HG23	53:S3:166:ARG:HH11	1.83	0.43
56:V3:48:ARG:HB3	56:V3:51:ARG:HG3	2.00	0.43
78:s3:24:TYR:CG	78:s3:90:PHE:HB3	2.53	0.43
1:A1:1114:U:H3	1:A1:1119:A:H61	1.67	0.43
1:A1:1384:C:H2'	1:A1:1385:G:H8	1.83	0.43
11:K1:65:GLU:HG3	11:K1:66:LYS:HD2	2.01	0.43
37:52:168:C:H1'	37:52:268:G:H1	1.84	0.43
37:52:966:A:C8	44:F3:24:PHE:HB2	2.53	0.43
37:52:2542:G:O2'	39:82:128:C:O2	2.24	0.43
37:52:4476:C:O2'	37:52:4478:G:OP2	2.30	0.43
38:72:63:C:C5	85:I3:203:ARG:O	2.72	0.43
44:F3:97:ILE:HD12	44:F3:97:ILE:HA	1.85	0.43
69:i3:66:ASP:HA	69:i3:69:ALA:HB3	2.01	0.43
74:n3:2:ARG:HB3	74:n3:5:TRP:HD1	1.82	0.43
85:I3:54:SER:HB2	85:I3:135:ILE:HD11	1.99	0.43
1:A1:1103:C:N4	1:A1:1104:G:O6	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:1332:A:H62	1:A1:1493:C:H42	1.66	0.43
6:F1:31:PRO:HG3	6:F1:43:PRO:HG3	1.99	0.43
37:52:440:U:H2'	37:52:441:G:H8	1.82	0.43
37:52:2656:U:H3'	37:52:2657:G:C8	2.54	0.43
38:72:49:A:H5''	84:D3:224:SER:HB3	1.99	0.43
47:M3:38:VAL:HG21	47:M3:50:MET:HE2	2.00	0.43
60:Z3:134:LEU:HD21	67:g3:91:ILE:HG21	1.99	0.43
83:G3:214:VAL:HG13	83:G3:217:ILE:HA	1.99	0.43
87:u3:78:LYS:NZ	87:u3:84:HIS:O	2.48	0.43
1:A1:1226:G:N1	1:A1:1639:G:OP2	2.46	0.43
5:E1:64:ARG:HH21	12:L1:94:LEU:HD11	1.84	0.43
37:52:78:U:H5''	48:N3:185:GLY:HA2	2.00	0.43
42:C3:94:ASN:OD1	42:C3:94:ASN:N	2.47	0.43
49:O3:18:ARG:HH12	49:O3:128:ARG:HH11	1.65	0.43
63:c3:47:ILE:HB	63:c3:94:LEU:HB3	2.01	0.43
1:A1:1086:G:OP2	28:b1:12:LYS:NZ	2.51	0.43
1:A1:1234:C:H4'	1:A1:1246:A:H61	1.82	0.43
1:A1:1337:C:H2'	1:A1:1338:G:C8	2.54	0.43
8:H1:230:LYS:HE2	8:H1:230:LYS:HB3	1.91	0.43
10:J1:6:ASP:OD2	10:J1:8:TRP:NE1	2.52	0.43
14:N1:60:MET:O	14:N1:64:LEU:N	2.49	0.43
37:52:114:G:H22	37:52:158:A:H61	1.66	0.43
37:52:440:U:O2'	66:f3:91:ASN:O	2.35	0.43
37:52:3974:G:H5'	87:u3:28:PHE:CD1	2.54	0.43
46:L3:120:TYR:HB2	46:L3:155:MET:HE1	2.00	0.43
55:U3:28:PRO:HB2	55:U3:34:MET:HG2	2.00	0.43
56:V3:33:GLY:HA3	56:V3:69:LYS:HD2	2.01	0.43
60:Z3:38:TYR:O	60:Z3:40:HIS:ND1	2.51	0.43
67:g3:73:HIS:ND1	67:g3:73:HIS:O	2.51	0.43
1:A1:1008:A:H2'	1:A1:1009:A:H8	1.84	0.43
3:C1:107:ARG:HA	3:C1:110:MET:HB3	2.01	0.43
29:c1:61:THR:OG1	29:c1:62:VAL:N	2.51	0.43
36:k1:83:THR:HG22	36:k1:95:HIS:CE1	2.53	0.43
37:52:1073:G:H22	37:52:1239:C:H1'	1.84	0.43
37:52:2575:U:O4	37:52:2759:G:N1	2.41	0.43
37:52:4921:C:O2'	37:52:4922:C:O4'	2.36	0.43
41:B3:44:THR:HG21	41:B3:186:ASN:HD22	1.83	0.43
41:B3:119:TYR:OH	41:B3:129:ALA:N	2.51	0.43
49:O3:142:ALA:HA	49:O3:145:VAL:HG12	2.00	0.43
67:g3:105:LYS:O	67:g3:109:ALA:N	2.44	0.43
78:s3:17:ILE:HD12	78:s3:17:ILE:HA	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:1339:U:H2'	1:A1:1340:U:H6	1.84	0.43
1:A1:1550:G:H3'	1:A1:1579:A:H61	1.84	0.43
4:D1:123:ARG:NH2	4:D1:143:CYS:SG	2.92	0.43
37:52:510:U:H5'	61:a3:86:THR:HG22	2.00	0.43
37:52:2591:A:N6	60:Z3:51:ARG:HH22	2.16	0.43
37:52:4114:C:H2'	37:52:4115:G:H8	1.83	0.43
37:52:4275:G:N2	37:52:4334:U:O2	2.51	0.43
37:52:4277:G:N2	37:52:4332:C:N3	2.67	0.43
37:52:4301:U:H4'	54:T3:54:HIS:CD2	2.54	0.43
37:52:4620:U:OP2	37:52:4670:C:N4	2.51	0.43
87:u3:29:LEU:HD22	87:u3:29:LEU:HA	1.88	0.43
1:A1:65:C:C4	8:H1:133:LEU:HD23	2.54	0.43
34:h1:286:CYS:SG	34:h1:287:THR:N	2.92	0.43
37:52:320:C:OP1	69:i3:84:LYS:NZ	2.33	0.43
37:52:732:A:C5	53:S3:68:PHE:CG	3.07	0.43
37:52:4753:U:OP2	66:f3:100:ARG:NH1	2.52	0.43
45:H3:80:MET:HE3	45:H3:80:MET:HB2	1.86	0.43
49:O3:18:ARG:HH22	49:O3:128:ARG:NH1	2.17	0.43
66:f3:49:TYR:HD1	66:f3:101:ILE:HG22	1.83	0.43
85:I3:168:SER:OG	85:I3:169:LYS:N	2.52	0.43
1:A1:677:G:N1	1:A1:1027:A:OP2	2.45	0.42
37:52:1631:A:C6	40:A3:204:MET:HE2	2.54	0.42
52:R3:100:ARG:HH21	52:R3:104:ARG:NH2	2.17	0.42
53:S3:30:MET:HE2	53:S3:30:MET:HB3	1.92	0.42
1:A1:1717:C:O3'	74:n3:21:ARG:NH1	2.52	0.42
1:A1:1740:C:OP1	10:J1:44:HIS:ND1	2.42	0.42
19:S1:98:VAL:HG21	19:S1:117:LEU:HD22	2.01	0.42
20:T1:4:VAL:HA	27:a1:50:PHE:HB2	2.00	0.42
23:W1:21:ASN:HB3	24:X1:67:GLY:HA3	2.01	0.42
34:h1:11:LEU:HB2	34:h1:307:VAL:HB	2.01	0.42
37:52:1912:G:H1	37:52:2051:C:H42	1.66	0.42
37:52:2021:G:H3'	78:s3:84:GLY:N	2.34	0.42
37:52:4291:G:H8	37:52:4328:G:H2'	1.85	0.42
40:A3:79:ALA:HA	40:A3:169:VAL:HA	2.01	0.42
57:W3:17:HIS:HB3	57:W3:18:GLY:H	1.67	0.42
71:k3:30:ASP:O	71:k3:48:THR:OG1	2.27	0.42
78:s3:55:MET:HA	78:s3:87:GLY:HA3	2.01	0.42
79:t3:13:VAL:HG12	79:t3:62:LEU:H	1.84	0.42
79:t3:18:THR:HA	79:t3:57:ARG:HA	2.01	0.42
7:G1:144:LEU:O	7:G1:148:ASN:ND2	2.52	0.42
18:R1:28:GLY:N	18:R1:65:GLY:O	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U1:124:THR:HG23	21:U1:126:GLN:H	1.84	0.42
37:52:732:A:H3'	37:52:733:A:H4'	2.01	0.42
37:52:4459:U:H5'	41:B3:10:ARG:HG2	2.01	0.42
37:52:4704:C:H2'	37:52:4705:A:C8	2.52	0.42
40:A3:70:LYS:HD3	40:A3:72:ARG:HH12	1.83	0.42
42:C3:148:PRO:HA	77:r3:74:ALA:HB2	2.01	0.42
76:p3:87:LYS:HD3	76:p3:91:ASP:HB3	2.00	0.42
78:s3:57:LYS:N	78:s3:60:MET:HB3	2.34	0.42
78:s3:131:GLY:HA3	78:s3:132:PRO:HD3	1.89	0.42
82:J3:112:HIS:CE1	82:J3:126:TYR:H	2.37	0.42
84:D3:56:THR:OG1	84:D3:59:ASP:O	2.36	0.42
84:D3:103:LEU:HD11	84:D3:248:ARG:HH21	1.84	0.42
1:A1:640:A:H2'	1:A1:641:A:C8	2.54	0.42
1:A1:695:C:H2'	1:A1:696:G:C8	2.54	0.42
1:A1:1221:G:H2'	1:A1:1222:G:C8	2.55	0.42
4:D1:154:ALA:O	4:D1:158:ALA:N	2.50	0.42
36:k1:286:ILE:HD12	36:k1:305:VAL:HA	2.00	0.42
36:k1:354:LYS:HG2	36:k1:363:ALA:HA	2.02	0.42
37:52:197:A:N1	37:52:225:G:O2'	2.39	0.42
37:52:2267:U:OP1	77:r3:37:SER:OG	2.33	0.42
67:g3:105:LYS:HA	67:g3:108:LYS:HB3	2.01	0.42
69:i3:87:ARG:NE	69:i3:88:GLU:OE2	2.50	0.42
87:u3:67:VAL:HG12	87:u3:84:HIS:CE1	2.54	0.42
1:A1:1453:C:OP2	19:S1:45:LYS:NZ	2.52	0.42
1:A1:1865:C:OP1	28:b1:87:ARG:NH1	2.52	0.42
2:B1:59:LEU:O	2:B1:63:ARG:N	2.50	0.42
6:F1:68:ARG:HG3	6:F1:76:VAL:HG11	2.02	0.42
21:U1:105:GLN:O	21:U1:109:GLY:N	2.53	0.42
34:h1:133:ASN:HD22	34:h1:137:VAL:HB	1.84	0.42
34:h1:146:SER:OG	34:h1:147:HIS:N	2.53	0.42
35:j1:91:ASN:HA	35:j1:119:PRO:HA	2.02	0.42
37:52:1391:A:P	51:Q3:181:ARG:HH12	2.42	0.42
37:52:1403:G:O6	37:52:1414:C:N4	2.52	0.42
37:52:1405:C:H2'	37:52:1406:G:C8	2.55	0.42
37:52:2703:G:H1	37:52:2713:C:H42	1.67	0.42
37:52:4489:G:N1	37:52:4708:A:N7	2.67	0.42
37:52:4868:G:O3'	47:M3:90:ARG:NH1	2.52	0.42
37:52:4895:C:H1'	47:M3:132:ARG:HH22	1.83	0.42
51:Q3:67:ILE:HD12	51:Q3:96:PRO:HD2	2.02	0.42
64:d3:47:LYS:O	64:d3:51:LYS:N	2.45	0.42
78:s3:10:LYS:HA	78:s3:13:TYR:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:s3:109:ALA:H	78:s3:185:PHE:HD2	1.67	0.42
1:A1:544:G:H2'	1:A1:545:A:H8	1.84	0.42
2:B1:50:ASN:HD21	19:S1:109:LEU:HD11	1.85	0.42
4:D1:262:THR:OG1	4:D1:263:LYS:N	2.51	0.42
16:P1:34:PHE:CD1	16:P1:98:ARG:HD2	2.55	0.42
26:Z1:58:PHE:HE1	26:Z1:74:MET:HE1	1.83	0.42
37:52:2261:G:N7	37:52:2262:G:N1	2.67	0.42
37:52:2395:A:N1	67:g3:2:VAL:CB	2.82	0.42
37:52:2598:A:N9	67:g3:43:LYS:HB2	2.34	0.42
37:52:3651:A:OP1	40:A3:200:ARG:HG2	2.20	0.42
41:B3:13:SER:OG	41:B3:14:LEU:N	2.52	0.42
46:L3:56:ARG:O	46:L3:116:ARG:NH2	2.52	0.42
78:s3:190:GLN:HG2	78:s3:191:GLN:HG2	2.00	0.42
1:A1:744:G:H2'	1:A1:745:C:C2	2.55	0.42
37:52:1285:U:H2'	37:52:1286:C:H6	1.83	0.42
37:52:1890:G:N2	37:52:1939:A:H61	2.18	0.42
37:52:2581:A:C5	60:Z3:74:VAL:HB	2.55	0.42
37:52:2696:A:C8	71:k3:26:LYS:HG3	2.55	0.42
41:B3:301:ASN:HB2	41:B3:304:SER:HB2	2.02	0.42
63:c3:53:PRO:HG3	76:p3:62:LYS:HD2	2.01	0.42
63:c3:81:LEU:HD13	63:c3:92:CYS:HA	2.01	0.42
75:o3:74:GLU:HA	75:o3:75:PRO:HD3	1.90	0.42
1:A1:126:G:OP2	8:H1:195:LYS:NZ	2.53	0.42
1:A1:982:G:N2	1:A1:1045:U:O2	2.44	0.42
5:E1:119:CYS:HB2	5:E1:152:PHE:HE2	1.84	0.42
37:52:310:G:H22	69:i3:30:ARG:CZ	2.33	0.42
37:52:407:A:O2'	37:52:410:A:OP1	2.31	0.42
37:52:965:G:H5'	44:F3:24:PHE:CE1	2.55	0.42
37:52:1304:C:H2'	37:52:1305:C:H6	1.83	0.42
37:52:1594:C:O2'	37:52:1597:G:O2'	2.34	0.42
37:52:2761:U:O5'	37:52:2762:G:N2	2.52	0.42
37:52:4325:A:N3	84:D3:36:LEU:HB3	2.35	0.42
51:Q3:178:ARG:NH2	61:a3:46:ASP:OD1	2.52	0.42
54:T3:39:ILE:HD12	54:T3:102:ARG:HB2	2.02	0.42
63:c3:23:LYS:HE2	63:c3:23:LYS:HB3	1.87	0.42
79:t3:81:ILE:HD12	79:t3:139:VAL:HG21	2.01	0.42
33:g1:110:GLU:OE2	33:g1:111:ASN:ND2	2.52	0.42
34:h1:128:THR:HG22	34:h1:143:GLN:HG2	2.02	0.42
37:52:1472:C:O2	37:52:1493:G:N1	2.53	0.42
37:52:1968:G:C5	78:s3:34:ASN:HA	2.55	0.42
37:52:5058:A:H4'	64:d3:23:ARG:HH12	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:72:3:C:O2	38:72:116:G:N2	2.53	0.42
40:A3:196:TRP:O	40:A3:198:ARG:N	2.53	0.42
41:B3:46:PHE:HE2	41:B3:81:THR:HB	1.84	0.42
41:B3:217:ILE:HD13	41:B3:284:ILE:HD11	2.01	0.42
69:i3:99:LYS:CA	87:u3:9:THR:CB	2.78	0.42
69:i3:103:LYS:HD2	87:u3:10:LEU:CD2	2.49	0.42
79:t3:53:TRP:HH2	79:t3:80:LEU:HD23	1.85	0.42
79:t3:129:ILE:HG22	79:t3:133:LEU:HB2	2.01	0.42
1:A1:920:A:OP1	24:X1:57:ARG:NH2	2.53	0.42
1:A1:1456:G:OP1	19:S1:59:LYS:NZ	2.45	0.42
9:I1:100:ILE:HA	9:I1:100:ILE:HD12	1.85	0.42
14:N1:56:CYS:SG	14:N1:82:ASN:ND2	2.92	0.42
28:b1:33:ASP:OD1	28:b1:33:ASP:N	2.53	0.42
34:h1:126:ASP:O	34:h1:128:THR:N	2.53	0.42
34:h1:159:ASN:HB2	34:h1:204:GLY:HA3	2.02	0.42
37:52:738(A):C:H4'	47:M3:69:ARG:HH21	1.85	0.42
37:52:1464:C:H5''	62:b3:32:LEU:HD12	2.02	0.42
37:52:3661:G:N2	37:52:3682:A:OP2	2.43	0.42
37:52:3957:U:N3	37:52:3964:U:H5'	2.35	0.42
67:g3:8:ARG:NH2	67:g3:32:TYR:O	2.53	0.42
82:J3:15:LEU:HD22	82:J3:165:TRP:CG	2.55	0.42
87:u3:65:VAL:HG22	87:u3:109:ALA:HB3	2.01	0.42
13:M1:60:CYS:HG	13:M1:114:SER:HG	1.64	0.41
15:O1:150:VAL:N	63:c3:19:GLN:OE1	2.53	0.41
28:b1:45:VAL:HB	28:b1:49:ALA:HB3	2.01	0.41
35:j1:354:LYS:HG3	35:j1:356:HIS:H	1.85	0.41
37:52:1346:C:H2'	37:52:1347:G:C8	2.55	0.41
37:52:1996:C:H42	37:52:2000:G:H22	1.67	0.41
37:52:2021:G:O5'	78:s3:86:VAL:N	2.46	0.41
37:52:2722:G:N2	37:52:2723:U:O2	2.53	0.41
40:A3:42:LYS:HD2	40:A3:89:TYR:HE1	1.85	0.41
43:E3:167:PHE:HE1	43:E3:176:LEU:HD22	1.85	0.41
59:Y3:80:ILE:HG23	59:Y3:101:PRO:HG3	2.02	0.41
61:a3:148:ALA:HB2	69:i3:6:PRO:HB2	2.01	0.41
77:r3:106:LEU:HD13	77:r3:106:LEU:HA	1.93	0.41
78:s3:147:ILE:HA	78:s3:152:ILE:HG12	2.02	0.41
83:G3:127:LEU:HD13	83:G3:127:LEU:HA	1.88	0.41
87:u3:29:LEU:HG	87:u3:173:LYS:HE3	2.02	0.41
2:B1:214:GLU:OE2	19:S1:81:ARG:NH1	2.53	0.41
7:G1:146:ARG:HH22	30:d1:57:THR:HB	1.84	0.41
14:N1:54:SER:OG	14:N1:55:ASN:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:h1:8:ARG:HE	34:h1:311:GLN:HB2	1.85	0.41
35:j1:12:VAL:O	35:j1:16:LYS:N	2.42	0.41
35:j1:29:GLY:HA2	35:j1:101:VAL:HG12	2.02	0.41
36:k1:253:LEU:HD23	36:k1:253:LEU:HA	1.88	0.41
37:52:1109:C:O2	37:52:1162:G:N2	2.52	0.41
37:52:1426:G:N1	37:52:1458:C:OP2	2.39	0.41
37:52:1802:A:H5''	37:52:1803:G:H5'	2.01	0.41
37:52:2597:G:OP2	67:g3:45:ALA:N	2.51	0.41
37:52:3870:C:H2'	37:52:3871:A:C8	2.55	0.41
37:52:3974:G:H5''	87:u3:26:ARG:HD2	2.03	0.41
37:52:4122:G:N3	60:Z3:135:ARG:HB3	2.35	0.41
37:52:4302:U:H4'	54:T3:5:LYS:HD2	2.01	0.41
40:A3:62:VAL:HG12	40:A3:73:THR:HG22	2.02	0.41
41:B3:139:ASP:OD1	41:B3:139:ASP:N	2.53	0.41
45:H3:24:THR:OG1	45:H3:37:ASP:OD1	2.30	0.41
67:g3:69:LYS:HA	67:g3:69:LYS:HD2	1.83	0.41
69:i3:99:LYS:CA	87:u3:9:THR:HG23	2.25	0.41
78:s3:53:VAL:HA	78:s3:89:VAL:HA	2.02	0.41
1:A1:1039:C:H42	1:A1:1076:G:H1	1.68	0.41
3:C1:208:HIS:CD2	3:C1:209:ASP:HB2	2.54	0.41
19:S1:120:THR:OG1	19:S1:121:GLN:N	2.51	0.41
34:h1:89:LEU:HB2	34:h1:101:PHE:HE2	1.85	0.41
37:52:1961:G:C5	78:s3:59:THR:HG21	2.56	0.41
37:52:2088:A:OP1	51:Q3:38:ARG:NH2	2.40	0.41
37:52:2395:A:H1'	37:52:2806:A:H1'	2.02	0.41
40:A3:103:PRO:HG3	40:A3:163:ARG:CZ	2.51	0.41
54:T3:30:TYR:HE1	54:T3:94:GLU:HG3	1.85	0.41
1:A1:544:G:H2'	1:A1:545:A:C8	2.56	0.41
1:A1:1847:G:O6	1:A1:1852:C:N4	2.48	0.41
8:H1:131:ARG:HA	57:W3:82:ILE:H	1.85	0.41
13:M1:39:ASN:OD1	13:M1:39:ASN:N	2.54	0.41
37:52:2590:G:N2	60:Z3:65:ARG:HH21	2.18	0.41
37:52:3654:G:O6	37:52:3691:G:N2	2.53	0.41
38:72:63:C:C5	85:I3:203:ARG:C	2.99	0.41
46:L3:9:ILE:HD12	46:L3:9:ILE:HA	1.96	0.41
49:O3:196:LEU:HB3	49:O3:202:LEU:HD13	2.02	0.41
56:V3:43:LYS:HD3	56:V3:60:MET:HG2	2.02	0.41
66:f3:11:PHE:HE1	66:f3:26:ALA:HB1	1.84	0.41
2:B1:159:ILE:HD12	2:B1:159:ILE:HA	1.90	0.41
16:P1:147:ARG:HH21	16:P1:150:ARG:NH1	2.18	0.41
22:V1:55:ARG:HG2	22:V1:87:ARG:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:52:1239:C:C4	43:E3:65:TYR:CE1	3.08	0.41
37:52:1687:U:H2'	37:52:1688:G:C8	2.56	0.41
37:52:1924:C:H42	37:52:2060:G:H1	1.67	0.41
37:52:1956:A:N6	37:52:1957:U:O4	2.53	0.41
37:52:1995:G:H2'	37:52:1996:C:C6	2.56	0.41
37:52:2395:A:N1	67:g3:2:VAL:CA	2.83	0.41
37:52:3681:G:OP2	40:A3:128:ARG:NH2	2.54	0.41
37:52:4237:C:O2	37:52:4321:U:O2'	2.36	0.41
40:A3:9:ARG:HH11	40:A3:9:ARG:HD2	1.74	0.41
48:N3:64:ILE:H	48:N3:64:ILE:HG13	1.80	0.41
57:W3:104:GLN:O	57:W3:108:ALA:N	2.53	0.41
64:d3:112:THR:OG1	64:d3:113:THR:N	2.54	0.41
84:D3:31:TYR:O	84:D3:35:ARG:NH1	2.53	0.41
87:u3:146:ALA:O	87:u3:150:GLU:N	2.48	0.41
1:A1:183:G:O2'	1:A1:184:G:O4'	2.35	0.41
2:B1:5:LEU:HD12	2:B1:5:LEU:HA	1.92	0.41
2:B1:33:GLN:HB3	2:B1:154:LEU:HD12	2.03	0.41
11:K1:109:ARG:HG2	11:K1:111:GLN:H	1.85	0.41
36:k1:83:THR:HG22	36:k1:95:HIS:HE1	1.85	0.41
37:52:3947:A:N6	37:52:3948:C:O3'	2.53	0.41
37:52:4473:A:P	73:m3:76:ARG:HH21	2.43	0.41
56:V3:82:ILE:HG23	56:V3:121:VAL:HG13	2.01	0.41
66:f3:50:VAL:HG22	66:f3:69:VAL:HG12	2.02	0.41
71:k3:10:ASP:O	71:k3:14:THR:N	2.53	0.41
84:D3:129:GLU:OE1	84:D3:175:HIS:NE2	2.53	0.41
1:A1:1805:G:H2'	1:A1:1806:A:C8	2.55	0.41
4:D1:200:ARG:O	11:K1:54:ARG:NH1	2.39	0.41
5:E1:135:GLU:HG3	5:E1:153:VAL:HG22	2.01	0.41
9:I1:154:ILE:HB	9:I1:185:VAL:HG22	2.02	0.41
11:K1:136:ARG:NE	11:K1:158:ASP:OD1	2.47	0.41
35:j1:245:ARG:H	35:j1:245:ARG:HD3	1.85	0.41
37:52:1071:C:H41	43:E3:48:ARG:HH22	1.68	0.41
37:52:1924:C:H5'	47:M3:34:ASN:HD21	1.86	0.41
37:52:2610:G:H2'	37:52:2611:A:H8	1.85	0.41
37:52:2668:G:OP2	52:R3:124:TYR:OH	2.25	0.41
37:52:3965:A:H61	37:52:4045:G:N2	2.17	0.41
48:N3:84:PRO:HA	48:N3:87:HIS:ND1	2.35	0.41
67:g3:91:ILE:HA	67:g3:94:ALA:HB2	2.03	0.41
67:g3:96:LEU:O	67:g3:100:GLN:N	2.53	0.41
1:A1:158:A:H4'	36:k1:579:LYS:HD2	2.02	0.41
1:A1:220:U:H2'	1:A1:221:A:H8	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:521:A:H5''	11:K1:45:ARG:HH12	1.85	0.41
17:Q1:43:ARG:NH1	17:Q1:47:ARG:HH21	2.19	0.41
37:52:416:U:H5	37:52:417:G:C5	2.39	0.41
37:52:2055:G:C5	49:O3:130:LYS:HG2	2.56	0.41
40:A3:125:LYS:HZ2	40:A3:126:LEU:HD22	1.86	0.41
63:c3:35:LEU:HA	63:c3:38:ILE:HB	2.02	0.41
66:f3:22:ARG:HB3	66:f3:24:HIS:CE1	2.56	0.41
67:g3:101:LYS:O	67:g3:105:LYS:N	2.53	0.41
76:p3:48:LYS:HE2	76:p3:50:ARG:HA	2.02	0.41
78:s3:62:ARG:O	78:s3:66:ARG:N	2.47	0.41
1:A1:407:G:C2	25:Y1:36:LEU:HD23	2.56	0.41
1:A1:970:G:C5	37:52:3712:A:H1'	2.55	0.41
1:A1:1140:G:H2'	1:A1:1141:G:C8	2.55	0.41
7:G1:59:LYS:HG2	7:G1:60:ARG:H	1.85	0.41
8:H1:121:ILE:HD12	8:H1:122:PRO:HD2	2.03	0.41
14:N1:106:CYS:SG	14:N1:107:SER:N	2.94	0.41
15:O1:117:LEU:HD23	15:O1:117:LEU:HA	1.92	0.41
19:S1:111:PHE:HB3	19:S1:114:LEU:HD21	2.02	0.41
22:V1:78:ASP:OD2	31:e1:44:ARG:NH1	2.54	0.41
34:h1:124:SER:OG	34:h1:125:ARG:N	2.53	0.41
34:h1:236:ILE:HG12	34:h1:252:THR:HG22	2.02	0.41
35:j1:189:ARG:HG3	37:52:4439:U:H5'	2.02	0.41
37:52:732:A:C2	53:S3:69:GLU:N	2.88	0.41
37:52:1390:G:N2	37:52:1393:G:OP2	2.54	0.41
37:52:1521:C:OP1	42:C3:100:ARG:NH2	2.51	0.41
37:52:2022:C:O4'	78:s3:84:GLY:N	2.53	0.41
37:52:2754:G:C8	60:Z3:51:ARG:HB2	2.55	0.41
37:52:2766:A:C5	37:52:2767:U:H1'	2.56	0.41
37:52:4860:G:H5''	49:O3:169:ARG:NH2	2.36	0.41
41:B3:43:LEU:HD23	41:B3:183:ILE:HG21	2.03	0.41
41:B3:293:ILE:HG12	41:B3:298:LEU:HB3	2.02	0.41
57:W3:25:ASP:OD1	57:W3:25:ASP:N	2.54	0.41
60:Z3:14:LEU:HD21	67:g3:92:LYS:HG3	2.03	0.41
77:r3:2:SER:OG	77:r3:3:ALA:N	2.53	0.41
83:G3:275:ILE:HG22	83:G3:276:ARG:H	1.85	0.41
85:I3:40:LYS:HE2	85:I3:40:LYS:HB2	1.88	0.41
85:I3:99:ILE:HD12	85:I3:99:ILE:HA	1.96	0.41
1:A1:1268:C:O2	17:Q1:97:TYR:OH	2.36	0.41
22:V1:55:ARG:HE	22:V1:87:ARG:NH1	2.19	0.41
35:j1:243:ASP:OD2	35:j1:245:ARG:NE	2.42	0.41
37:52:3690:U:OP1	40:A3:200:ARG:NH2	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:72:31:G:H2'	38:72:32:A:H8	1.86	0.41
40:A3:33:ASP:N	40:A3:33:ASP:OD1	2.54	0.41
46:L3:130:LYS:HA	46:L3:131:PRO:HD3	1.92	0.41
48:N3:197:THR:OG1	48:N3:199:GLN:NE2	2.54	0.41
49:O3:195:VAL:HG23	49:O3:196:LEU:HD12	2.02	0.41
52:R3:122:SER:HA	52:R3:125:LEU:HB2	2.03	0.41
60:Z3:49:TYR:CD2	60:Z3:133:LYS:HA	2.57	0.41
65:e3:81:ASN:OD1	65:e3:81:ASN:N	2.54	0.41
80:23:29:C:H2'	80:23:30:G:H8	1.85	0.41
1:A1:886:A:N6	1:A1:900:C:N3	2.69	0.40
1:A1:1304:U:H5'	33:g1:93:HIS:HB2	2.02	0.40
3:C1:26:SER:O	3:C1:51:ARG:NH2	2.44	0.40
18:R1:101:ASP:OD1	18:R1:101:ASP:N	2.54	0.40
26:Z1:7:ILE:HG12	26:Z1:27:VAL:HG22	2.03	0.40
36:k1:105:VAL:HG22	36:k1:269:ILE:HB	2.04	0.40
37:52:489:C:N3	37:52:664:G:N1	2.62	0.40
37:52:1237:C:H5''	44:F3:50:TYR:CE2	2.55	0.40
37:52:1995:G:H5''	79:t3:130:LYS:HB2	2.03	0.40
37:52:1996:C:N4	37:52:2000:G:H22	2.19	0.40
37:52:2706:G:H21	37:52:2709:C:H5	1.69	0.40
37:52:2754:G:O5'	60:Z3:51:ARG:HB3	2.21	0.40
37:52:4223:C:H2'	37:52:4224:A:H8	1.85	0.40
40:A3:237:LEU:HD23	40:A3:237:LEU:H	1.86	0.40
42:C3:275:SER:OG	42:C3:276:ASN:N	2.54	0.40
48:N3:119:TYR:CZ	48:N3:131:GLU:HG3	2.56	0.40
66:f3:72:GLY:HA3	66:f3:88:PHE:CD1	2.56	0.40
77:r3:2:SER:O	77:r3:6:GLN:NE2	2.54	0.40
1:A1:130:G:O6	1:A1:181:A:N6	2.53	0.40
1:A1:390:C:O2'	13:M1:8:ARG:NH2	2.54	0.40
1:A1:970:G:C5	37:52:3712:A:N1	2.88	0.40
1:A1:1521:C:OP2	20:T1:136:THR:OG1	2.29	0.40
2:B1:206:ASP:HB3	2:B1:209:GLU:HB2	2.03	0.40
9:I1:160:LYS:HA	9:I1:160:LYS:HD2	1.91	0.40
14:N1:22:LEU:HD21	14:N1:109:VAL:HG11	2.02	0.40
36:k1:22:ARG:HG2	36:k1:23:GLN:H	1.86	0.40
37:52:702:U:H5'	43:E3:124:VAL:HG21	2.03	0.40
37:52:1929:A:N7	37:52:1932:A:H1'	2.37	0.40
37:52:2666:U:H5''	52:R3:107:ARG:NH2	2.36	0.40
37:52:2673:G:H8	37:52:2675:G:C6	2.39	0.40
40:A3:245:ARG:HD3	40:A3:247:ARG:HH12	1.86	0.40
84:D3:217:ASP:OD1	84:D3:217:ASP:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:649:U:H2'	1:A1:650:A:C8	2.56	0.40
1:A1:923:G:H2'	1:A1:924:G:H8	1.86	0.40
1:A1:1542:C:O2'	18:R1:43:GLU:OE2	2.39	0.40
3:C1:46:LYS:HE3	16:P1:19:PRO:HG2	2.03	0.40
4:D1:77:SER:OG	4:D1:78:LEU:N	2.54	0.40
36:k1:432:ILE:HG21	36:k1:477:GLY:HA3	2.03	0.40
37:52:2896:G:O6	37:52:3604:A:N6	2.54	0.40
37:52:3952:A:H2'	37:52:3953:G:C8	2.57	0.40
40:A3:114:CYS:HB3	40:A3:165:VAL:HG23	2.03	0.40
42:C3:198:ASN:HD21	59:Y3:10:ASP:CG	2.30	0.40
50:P3:129:THR:OG1	50:P3:130:TYR:N	2.54	0.40
61:a3:117:LEU:HD23	61:a3:140:VAL:HG21	2.02	0.40
71:k3:10:ASP:O	71:k3:14:THR:OG1	2.37	0.40
71:k3:33:LYS:O	71:k3:35:LYS:N	2.54	0.40
71:k3:33:LYS:HD3	71:k3:35:LYS:HE2	2.03	0.40
78:s3:65:ILE:HA	78:s3:75:LEU:HD13	2.03	0.40
79:t3:135:THR:O	79:t3:139:VAL:N	2.52	0.40
82:J3:44:THR:OG1	82:J3:45:GLY:N	2.54	0.40
1:A1:955:A:N7	1:A1:972:A:N6	2.69	0.40
37:52:952:G:H5''	66:f3:73:LYS:HD3	2.02	0.40
37:52:1734:G:O2'	37:52:1793:A:N6	2.54	0.40
37:52:2397:G:O6	67:g3:2:VAL:HG21	2.22	0.40
37:52:4124:G:H5''	40:A3:69:PHE:HE1	1.86	0.40
40:A3:182:ALA:HA	40:A3:185:ALA:HB3	2.03	0.40
54:T3:144:ASN:OD1	54:T3:144:ASN:N	2.54	0.40
78:s3:193:PHE:HA	78:s3:198:ILE:HA	2.03	0.40
82:J3:150:CYS:SG	82:J3:151:ILE:N	2.94	0.40
1:A1:1606:G:H22	1:A1:1632:G:H1'	1.87	0.40
1:A1:1736:G:H2'	1:A1:1737:G:C8	2.56	0.40
5:E1:51:LEU:HG	5:E1:91:VAL:HG22	2.03	0.40
24:X1:55:ASP:OD1	24:X1:55:ASP:N	2.55	0.40
37:52:1091:C:H2'	37:52:1092:G:C8	2.57	0.40
37:52:1236:C:O2'	37:52:1238:A:OP1	2.38	0.40
37:52:1244:G:H8	43:E3:74:LYS:HZ3	1.69	0.40
37:52:1403:G:N1	37:52:1414:C:N3	2.69	0.40
37:52:1998:A:H5'	78:s3:54:LEU:HD12	2.03	0.40
37:52:2537:A:H3'	71:k3:41:TYR:CE1	2.57	0.40
37:52:2537:A:OP2	71:k3:42:LEU:N	2.45	0.40
37:52:2897:G:OP1	52:R3:135:LYS:HG2	2.21	0.40
37:52:3899:G:O6	37:52:4562:C:N4	2.50	0.40
37:52:4034:G:H2'	37:52:4035:G:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:Q3:22:ASP:N	51:Q3:22:ASP:OD1	2.46	0.40
58:X3:89:LYS:HD3	58:X3:93:ASN:HD22	1.85	0.40
76:p3:3:LYS:HG2	76:p3:5:THR:N	2.34	0.40
76:p3:57:CYS:SG	76:p3:58:GLY:N	2.95	0.40
78:s3:13:TYR:O	78:s3:17:ILE:N	2.54	0.40
83:G3:191:ALA:O	83:G3:195:THR:OG1	2.39	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	B1	215/295 (73%)	199 (93%)	16 (7%)	0	100	100
3	C1	211/264 (80%)	191 (90%)	20 (10%)	0	100	100
4	D1	219/293 (75%)	206 (94%)	13 (6%)	0	100	100
5	E1	226/243 (93%)	211 (93%)	15 (7%)	0	100	100
6	F1	260/263 (99%)	227 (87%)	33 (13%)	0	100	100
7	G1	181/204 (89%)	167 (92%)	14 (8%)	0	100	100
8	H1	235/249 (94%)	218 (93%)	17 (7%)	0	100	100
9	I1	181/194 (93%)	165 (91%)	16 (9%)	0	100	100
10	J1	204/208 (98%)	184 (90%)	20 (10%)	0	100	100
11	K1	183/194 (94%)	173 (94%)	10 (6%)	0	100	100
12	L1	94/165 (57%)	83 (88%)	11 (12%)	0	100	100
13	M1	139/158 (88%)	128 (92%)	11 (8%)	0	100	100
14	N1	115/132 (87%)	101 (88%)	14 (12%)	0	100	100
15	O1	147/151 (97%)	139 (95%)	8 (5%)	0	100	100
16	P1	134/168 (80%)	123 (92%)	11 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	Q1	118/145 (81%)	106 (90%)	12 (10%)	0	100	100
18	R1	140/146 (96%)	126 (90%)	14 (10%)	0	100	100
19	S1	130/135 (96%)	122 (94%)	8 (6%)	0	100	100
20	T1	142/152 (93%)	128 (90%)	14 (10%)	0	100	100
21	U1	139/145 (96%)	128 (92%)	11 (8%)	0	100	100
22	V1	98/119 (82%)	94 (96%)	4 (4%)	0	100	100
23	W1	81/83 (98%)	72 (89%)	9 (11%)	0	100	100
24	X1	127/130 (98%)	119 (94%)	8 (6%)	0	100	100
25	Y1	139/143 (97%)	124 (89%)	14 (10%)	1 (1%)	18	56
26	Z1	122/130 (94%)	109 (89%)	13 (11%)	0	100	100
27	a1	73/125 (58%)	65 (89%)	8 (11%)	0	100	100
28	b1	99/115 (86%)	92 (93%)	7 (7%)	0	100	100
29	c1	81/84 (96%)	74 (91%)	7 (9%)	0	100	100
30	d1	60/69 (87%)	57 (95%)	3 (5%)	0	100	100
31	e1	53/56 (95%)	50 (94%)	3 (6%)	0	100	100
32	f1	53/133 (40%)	49 (92%)	4 (8%)	0	100	100
33	g1	66/156 (42%)	58 (88%)	8 (12%)	0	100	100
34	h1	311/317 (98%)	268 (86%)	43 (14%)	0	100	100
35	j1	417/439 (95%)	388 (93%)	29 (7%)	0	100	100
36	k1	571/599 (95%)	517 (90%)	54 (10%)	0	100	100
40	A3	246/257 (96%)	185 (75%)	54 (22%)	7 (3%)	4	24
41	B3	392/403 (97%)	355 (91%)	37 (9%)	0	100	100
42	C3	360/425 (85%)	325 (90%)	35 (10%)	0	100	100
43	E3	208/291 (72%)	191 (92%)	17 (8%)	0	100	100
44	F3	223/247 (90%)	205 (92%)	18 (8%)	0	100	100
45	H3	188/192 (98%)	174 (93%)	13 (7%)	1 (0%)	24	63
46	L3	208/211 (99%)	194 (93%)	12 (6%)	2 (1%)	12	48
47	M3	136/218 (62%)	121 (89%)	15 (11%)	0	100	100
48	N3	201/204 (98%)	181 (90%)	20 (10%)	0	100	100
49	O3	197/203 (97%)	185 (94%)	12 (6%)	0	100	100
50	P3	151/184 (82%)	143 (95%)	8 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	Q3	185/188 (98%)	167 (90%)	18 (10%)	0	100	100
52	R3	178/196 (91%)	161 (90%)	17 (10%)	0	100	100
53	S3	174/176 (99%)	154 (88%)	20 (12%)	0	100	100
54	T3	157/160 (98%)	144 (92%)	12 (8%)	1 (1%)	21	59
55	U3	97/128 (76%)	79 (81%)	18 (19%)	0	100	100
56	V3	129/140 (92%)	119 (92%)	10 (8%)	0	100	100
57	W3	102/157 (65%)	92 (90%)	10 (10%)	0	100	100
58	X3	116/156 (74%)	109 (94%)	7 (6%)	0	100	100
59	Y3	132/145 (91%)	120 (91%)	12 (9%)	0	100	100
60	Z3	133/136 (98%)	105 (79%)	25 (19%)	3 (2%)	5	28
61	a3	145/148 (98%)	134 (92%)	11 (8%)	0	100	100
62	b3	100/245 (41%)	94 (94%)	6 (6%)	0	100	100
63	c3	96/115 (84%)	81 (84%)	15 (16%)	0	100	100
64	d3	105/125 (84%)	90 (86%)	15 (14%)	0	100	100
65	e3	126/134 (94%)	115 (91%)	11 (9%)	0	100	100
66	f3	107/110 (97%)	96 (90%)	11 (10%)	0	100	100
67	g3	112/117 (96%)	98 (88%)	13 (12%)	1 (1%)	14	51
68	h3	120/123 (98%)	113 (94%)	7 (6%)	0	100	100
69	i3	100/105 (95%)	96 (96%)	4 (4%)	0	100	100
70	j3	84/97 (87%)	75 (89%)	9 (11%)	0	100	100
71	k3	67/70 (96%)	59 (88%)	8 (12%)	0	100	100
72	l3	48/51 (94%)	41 (85%)	7 (15%)	0	100	100
73	m3	50/102 (49%)	48 (96%)	2 (4%)	0	100	100
74	n3	23/25 (92%)	23 (100%)	0	0	100	100
75	o3	102/106 (96%)	96 (94%)	6 (6%)	0	100	100
76	p3	89/92 (97%)	77 (86%)	12 (14%)	0	100	100
77	r3	122/137 (89%)	110 (90%)	12 (10%)	0	100	100
78	s3	194/318 (61%)	156 (80%)	37 (19%)	1 (0%)	24	63
79	t3	151/165 (92%)	127 (84%)	24 (16%)	0	100	100
82	J3	168/178 (94%)	158 (94%)	10 (6%)	0	100	100
83	G3	229/319 (72%)	195 (85%)	34 (15%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
84	D3	291/297 (98%)	253 (87%)	38 (13%)	0	100	100
85	I3	201/214 (94%)	167 (83%)	33 (16%)	1 (0%)	24	63
86	1	20/22 (91%)	11 (55%)	4 (20%)	5 (25%)	0	1
87	u3	215/217 (99%)	183 (85%)	30 (14%)	2 (1%)	14	51
All	All	12742/14651 (87%)	11466 (90%)	1251 (10%)	25 (0%)	44	78

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
40	A3	116	LEU
40	A3	118	GLU
40	A3	126	LEU
46	L3	64	VAL
60	Z3	73	LYS
86	1	15	ALA
87	u3	101	LYS
40	A3	169	VAL
78	s3	34	ASN
86	1	7	ALA
87	u3	210	MET
46	L3	63	THR
60	Z3	75	TYR
67	g3	44	SER
86	1	13	ALA
86	1	14	ALA
40	A3	117	GLU
86	1	8	ALA
40	A3	125	LYS
45	H3	108	ASN
40	A3	150	LEU
25	Y1	62	PRO
85	I3	205	PRO
54	T3	82	GLY
60	Z3	90	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B1	180/245 (74%)	180 (100%)	0	100	100
3	C1	194/231 (84%)	194 (100%)	0	100	100
4	D1	187/225 (83%)	187 (100%)	0	100	100
5	E1	190/202 (94%)	190 (100%)	0	100	100
6	F1	224/225 (100%)	223 (100%)	1 (0%)	84	84
7	G1	158/170 (93%)	158 (100%)	0	100	100
8	H1	207/218 (95%)	206 (100%)	1 (0%)	81	83
9	I1	165/174 (95%)	165 (100%)	0	100	100
10	J1	178/180 (99%)	177 (99%)	1 (1%)	78	83
11	K1	161/168 (96%)	160 (99%)	1 (1%)	78	83
12	L1	87/136 (64%)	86 (99%)	1 (1%)	65	76
13	M1	130/142 (92%)	130 (100%)	0	100	100
14	N1	99/108 (92%)	99 (100%)	0	100	100
15	O1	130/131 (99%)	130 (100%)	0	100	100
16	P1	106/130 (82%)	106 (100%)	0	100	100
17	Q1	109/130 (84%)	109 (100%)	0	100	100
18	R1	117/121 (97%)	117 (100%)	0	100	100
19	S1	119/121 (98%)	119 (100%)	0	100	100
20	T1	125/132 (95%)	124 (99%)	1 (1%)	73	80
21	U1	111/115 (96%)	111 (100%)	0	100	100
22	V1	92/107 (86%)	92 (100%)	0	100	100
23	W1	67/67 (100%)	67 (100%)	0	100	100
24	X1	112/113 (99%)	112 (100%)	0	100	100
25	Y1	113/115 (98%)	113 (100%)	0	100	100
26	Z1	107/112 (96%)	107 (100%)	0	100	100
27	a1	66/103 (64%)	66 (100%)	0	100	100
28	b1	88/98 (90%)	88 (100%)	0	100	100
29	c1	75/76 (99%)	75 (100%)	0	100	100
30	d1	55/62 (89%)	55 (100%)	0	100	100
31	e1	48/49 (98%)	48 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	f1	46/106 (43%)	46 (100%)	0	100	100
33	g1	61/140 (44%)	61 (100%)	0	100	100
34	h1	272/275 (99%)	271 (100%)	1 (0%)	84	84
35	j1	361/377 (96%)	361 (100%)	0	100	100
36	k1	509/526 (97%)	509 (100%)	0	100	100
40	A3	190/199 (96%)	188 (99%)	2 (1%)	65	76
41	B3	342/348 (98%)	341 (100%)	1 (0%)	86	86
42	C3	302/347 (87%)	300 (99%)	2 (1%)	76	81
43	E3	190/251 (76%)	190 (100%)	0	100	100
44	F3	196/215 (91%)	195 (100%)	1 (0%)	81	83
45	H3	169/171 (99%)	168 (99%)	1 (1%)	78	83
46	L3	175/176 (99%)	174 (99%)	1 (1%)	78	83
47	M3	117/161 (73%)	117 (100%)	0	100	100
48	N3	171/172 (99%)	169 (99%)	2 (1%)	63	75
49	O3	171/173 (99%)	171 (100%)	0	100	100
50	P3	134/163 (82%)	134 (100%)	0	100	100
51	Q3	164/165 (99%)	164 (100%)	0	100	100
52	R3	159/175 (91%)	156 (98%)	3 (2%)	50	67
53	S3	157/157 (100%)	156 (99%)	1 (1%)	78	83
54	T3	139/140 (99%)	139 (100%)	0	100	100
55	U3	89/114 (78%)	89 (100%)	0	100	100
56	V3	101/107 (94%)	100 (99%)	1 (1%)	68	78
57	W3	86/126 (68%)	85 (99%)	1 (1%)	63	75
58	X3	106/134 (79%)	106 (100%)	0	100	100
59	Y3	124/135 (92%)	123 (99%)	1 (1%)	73	80
60	Z3	117/118 (99%)	113 (97%)	4 (3%)	32	54
61	a3	119/120 (99%)	119 (100%)	0	100	100
62	b3	84/184 (46%)	84 (100%)	0	100	100
63	c3	84/98 (86%)	83 (99%)	1 (1%)	63	75
64	d3	98/110 (89%)	98 (100%)	0	100	100
65	e3	114/120 (95%)	114 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
66	f3	88/89 (99%)	88 (100%)	0	100	100
67	g3	98/100 (98%)	98 (100%)	0	100	100
68	h3	109/110 (99%)	109 (100%)	0	100	100
69	i3	86/89 (97%)	85 (99%)	1 (1%)	63	75
70	j3	73/80 (91%)	73 (100%)	0	100	100
71	k3	64/65 (98%)	63 (98%)	1 (2%)	55	70
72	l3	47/48 (98%)	47 (100%)	0	100	100
73	m3	48/90 (53%)	48 (100%)	0	100	100
74	n3	24/24 (100%)	24 (100%)	0	100	100
75	o3	92/94 (98%)	92 (100%)	0	100	100
76	p3	74/75 (99%)	73 (99%)	1 (1%)	59	72
77	r3	108/121 (89%)	107 (99%)	1 (1%)	70	79
78	s3	164/258 (64%)	162 (99%)	2 (1%)	63	75
79	t3	126/137 (92%)	126 (100%)	0	100	100
82	J3	143/149 (96%)	143 (100%)	0	100	100
83	G3	200/272 (74%)	198 (99%)	2 (1%)	68	78
84	D3	247/250 (99%)	245 (99%)	2 (1%)	73	80
85	I3	175/181 (97%)	173 (99%)	2 (1%)	65	76
87	u3	195/196 (100%)	194 (100%)	1 (0%)	81	83
All	All	11108/12437 (89%)	11066 (100%)	42 (0%)	81	84

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	F1	246	LEU
8	H1	101	ILE
10	J1	87	ASN
11	K1	29	LEU
12	L1	2	LEU
20	T1	8	LYS
34	h1	178	ASN
40	A3	101	VAL
40	A3	207	VAL
41	B3	262	VAL
42	C3	227	ILE

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Mol	Chain	Res	Type
42	C3	321	ASN
44	F3	88	LEU
45	H3	57	VAL
46	L3	154	VAL
48	N3	64	ILE
48	N3	121	VAL
52	R3	50	ILE
52	R3	105	LEU
52	R3	130	ASN
53	S3	67	VAL
56	V3	18	LEU
57	W3	82	ILE
59	Y3	77	LYS
60	Z3	3	LYS
60	Z3	68	ILE
60	Z3	74	VAL
60	Z3	75	TYR
63	c3	55	LEU
69	i3	29	ARG
71	k3	36	VAL
76	p3	29	ILE
77	r3	12	ASN
78	s3	86	VAL
78	s3	200	ASN
83	G3	223	LEU
83	G3	286	ILE
84	D3	143	THR
84	D3	242	LYS
85	I3	70	ILE
85	I3	191	ILE
87	u3	29	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (175) such sidechains are listed below:

Mol	Chain	Res	Type
2	B1	113	GLN
2	B1	141	ASN
3	C1	40	ASN
3	C1	147	ASN
4	D1	113	GLN
5	E1	22	ASN
6	F1	50	ASN

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Mol	Chain	Res	Type
6	F1	112	HIS
6	F1	138	HIS
6	F1	142	HIS
6	F1	188	ASN
6	F1	201	HIS
6	F1	209	HIS
6	F1	232	ASN
7	G1	79	HIS
7	G1	83	ASN
7	G1	101	HIS
7	G1	114	ASN
7	G1	149	GLN
8	H1	56	ASN
8	H1	81	HIS
8	H1	177	GLN
8	H1	186	GLN
8	H1	202	ASN
9	I1	33	ASN
9	I1	73	GLN
9	I1	186	ASN
9	I1	193	GLN
10	J1	84	ASN
10	J1	87	ASN
10	J1	146	GLN
11	K1	111	GLN
11	K1	134	HIS
12	L1	7	ASN
12	L1	44	HIS
13	M1	83	GLN
13	M1	94	HIS
13	M1	106	HIS
13	M1	121	GLN
14	N1	19	GLN
14	N1	28	HIS
14	N1	55	ASN
14	N1	72	HIS
14	N1	82	ASN
15	O1	5	HIS
15	O1	105	ASN
17	Q1	104	GLN
18	R1	77	HIS
18	R1	97	GLN

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Mol	Chain	Res	Type
19	S1	31	ASN
19	S1	121	GLN
20	T1	19	ASN
20	T1	72	GLN
20	T1	97	GLN
20	T1	120	HIS
21	U1	91	HIS
22	V1	47	ASN
23	W1	29	HIS
24	X1	113	HIS
25	Y1	61	GLN
25	Y1	77	ASN
26	Z1	112	ASN
30	d1	26	GLN
30	d1	29	GLN
31	e1	28	HIS
32	f1	110	GLN
33	g1	111	ASN
33	g1	135	HIS
34	h1	26	GLN
34	h1	133	ASN
34	h1	159	ASN
34	h1	178	ASN
34	h1	187	ASN
34	h1	196	ASN
34	h1	215	GLN
34	h1	226	HIS
35	j1	11	ASN
35	j1	91	ASN
35	j1	121	ASN
35	j1	185	GLN
35	j1	211	GLN
35	j1	380	ASN
36	k1	90	ASN
36	k1	171	GLN
36	k1	208	HIS
36	k1	251	GLN
36	k1	274	HIS
36	k1	321	ASN
36	k1	381	ASN
36	k1	440	GLN
36	k1	496	GLN

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Mol	Chain	Res	Type
36	k1	520	HIS
40	A3	22	HIS
40	A3	38	HIS
40	A3	139	HIS
40	A3	187	HIS
40	A3	194	ASN
40	A3	205	ASN
41	B3	179	HIS
41	B3	203	GLN
41	B3	245	HIS
41	B3	328	ASN
42	C3	38	ASN
42	C3	112	HIS
42	C3	142	HIS
42	C3	245	HIS
42	C3	282	HIS
42	C3	321	ASN
42	C3	329	ASN
42	C3	347	HIS
43	E3	160	HIS
44	F3	38	GLN
44	F3	57	HIS
44	F3	130	ASN
44	F3	205	ASN
45	H3	8	GLN
45	H3	15	ASN
45	H3	102	ASN
47	M3	20	HIS
48	N3	57	GLN
48	N3	182	HIS
48	N3	199	GLN
49	O3	14	HIS
49	O3	50	ASN
50	P3	25	HIS
50	P3	34	GLN
50	P3	56	GLN
50	P3	80	GLN
50	P3	118	GLN
51	Q3	7	HIS
52	R3	36	ASN
52	R3	178	GLN
53	S3	156	HIS

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Mol	Chain	Res	Type
53	S3	163	HIS
54	T3	22	HIS
57	W3	30	GLN
57	W3	59	HIS
57	W3	120	GLN
58	X3	57	GLN
58	X3	93	ASN
58	X3	105	ASN
58	X3	107	HIS
58	X3	108	GLN
58	X3	111	GLN
60	Z3	127	ASN
61	a3	120	GLN
62	b3	101	HIS
64	d3	18	ASN
64	d3	30	HIS
65	e3	57	ASN
65	e3	107	ASN
66	f3	99	HIS
67	g3	14	ASN
67	g3	114	GLN
70	j3	76	HIS
72	l3	4	HIS
73	m3	83	ASN
73	m3	94	ASN
77	r3	12	ASN
77	r3	45	HIS
78	s3	85	ASN
78	s3	126	GLN
83	G3	119	GLN
83	G3	134	ASN
83	G3	206	GLN
83	G3	280	ASN
83	G3	293	ASN
84	D3	122	GLN
84	D3	202	GLN
84	D3	222	GLN
84	D3	275	GLN
85	I3	51	HIS
85	I3	95	HIS
85	I3	100	ASN
87	u3	188	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A1	1712/1869 (91%)	477 (27%)	23 (1%)
37	52	3596/3634 (98%)	1141 (31%)	45 (1%)
38	72	119/120 (99%)	34 (28%)	0
39	82	149/156 (95%)	43 (28%)	0
80	23	74/76 (97%)	18 (24%)	0
81	w3	22/23 (95%)	10 (45%)	0
All	All	5672/5878 (96%)	1723 (30%)	68 (1%)

All (1723) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A1	2	A
1	A1	3	C
1	A1	5	U
1	A1	16	G
1	A1	17	C
1	A1	26	U
1	A1	33	G
1	A1	39	A
1	A1	41	G
1	A1	42	A
1	A1	44	U
1	A1	45	A
1	A1	46	A
1	A1	56	G
1	A1	58	C
1	A1	65	C
1	A1	67	C
1	A1	68	A
1	A1	72	C
1	A1	73	C
1	A1	74	G
1	A1	76	U
1	A1	79	A
1	A1	89	C
1	A1	91	A
1	A1	95	G
1	A1	100	U
1	A1	101	U
1	A1	103	A
1	A1	111	A

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Mol	Chain	Res	Type
1	A1	113	G
1	A1	115	U
1	A1	116	U
1	A1	124	U
1	A1	126	G
1	A1	127	C
1	A1	129	C
1	A1	130	G
1	A1	141	A
1	A1	143	U
1	A1	147	A
1	A1	153	G
1	A1	155	G
1	A1	162	C
1	A1	163	U
1	A1	167	G
1	A1	168	C
1	A1	170	A
1	A1	172	U
1	A1	178	C
1	A1	182	C
1	A1	183	G
1	A1	184	G
1	A1	187	G
1	A1	188	C
1	A1	189	U
1	A1	190	G
1	A1	191	A
1	A1	192	C
1	A1	202	G
1	A1	206	G
1	A1	209	A
1	A1	211	G
1	A1	213	G
1	A1	222	U
1	A1	227	U
1	A1	228	C
1	A1	229	A
1	A1	230	A
1	A1	231	A
1	A1	233	C
1	A1	236	A

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Mol	Chain	Res	Type
1	A1	238	C
1	A1	239	C
1	A1	240	G
1	A1	241	G
1	A1	242	U
1	A1	243	C
1	A1	281	C
1	A1	285	U
1	A1	292	A
1	A1	297	A
1	A1	306	C
1	A1	307	G
1	A1	308	G
1	A1	309	G
1	A1	310	C
1	A1	312	G
1	A1	313	A
1	A1	314	U
1	A1	317	C
1	A1	318	A
1	A1	319	C
1	A1	322	C
1	A1	335	G
1	A1	339	A
1	A1	347	G
1	A1	350	C
1	A1	351	G
1	A1	354	U
1	A1	360	A
1	A1	361	U
1	A1	362	C
1	A1	364	A
1	A1	368	U
1	A1	382	C
1	A1	384	U
1	A1	385	G
1	A1	386	C
1	A1	400	C
1	A1	407	G
1	A1	408	A
1	A1	409	C
1	A1	413	G

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Mol	Chain	Res	Type
1	A1	417	C
1	A1	418	A
1	A1	422	U
1	A1	435	A
1	A1	441	C
1	A1	448	A
1	A1	449	A
1	A1	450	C
1	A1	452	G
1	A1	464	A
1	A1	465	A
1	A1	466	G
1	A1	472	C
1	A1	473	A
1	A1	474	G
1	A1	482	G
1	A1	485	A
1	A1	487	U
1	A1	492	C
1	A1	493	A
1	A1	495	U
1	A1	496	C
1	A1	501	C
1	A1	503	C
1	A1	516	A
1	A1	522	A
1	A1	525	A
1	A1	531	A
1	A1	532	C
1	A1	533	A
1	A1	536	A
1	A1	542	U
1	A1	544	G
1	A1	547	G
1	A1	548	C
1	A1	549	C
1	A1	550	C
1	A1	551	U
1	A1	554	A
1	A1	555	A
1	A1	559	G
1	A1	560	A

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Mol	Chain	Res	Type
1	A1	562	U
1	A1	563	G
1	A1	564	A
1	A1	565	G
1	A1	568	C
1	A1	582	U
1	A1	583	A
1	A1	588	G
1	A1	589	G
1	A1	590	A
1	A1	591	U
1	A1	593	C
1	A1	606	G
1	A1	608	C
1	A1	614	C
1	A1	615	C
1	A1	621	C
1	A1	622	C
1	A1	628	A
1	A1	629	A
1	A1	631	U
1	A1	637	U
1	A1	642	U
1	A1	643	A
1	A1	644	G
1	A1	658	U
1	A1	660	C
1	A1	664	A
1	A1	668	A
1	A1	669	A
1	A1	671	A
1	A1	672	A
1	A1	673	G
1	A1	675	U
1	A1	684	G
1	A1	688	U
1	A1	689	U
1	A1	690	G
1	A1	747	U
1	A1	750	C
1	A1	752	G
1	A1	753	C

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Mol	Chain	Res	Type
1	A1	790	C
1	A1	793	G
1	A1	797	C
1	A1	798	G
1	A1	799	U
1	A1	800	U
1	A1	811	A
1	A1	820	U
1	A1	821	G
1	A1	830	A
1	A1	834	C
1	A1	844	U
1	A1	847	A
1	A1	852	G
1	A1	867	G
1	A1	869	A
1	A1	870	A
1	A1	871	U
1	A1	872	A
1	A1	873	G
1	A1	874	G
1	A1	875	A
1	A1	876	C
1	A1	878	G
1	A1	879	C
1	A1	881	G
1	A1	886	A
1	A1	887	U
1	A1	888	U
1	A1	889	U
1	A1	890	U
1	A1	891	G
1	A1	892	U
1	A1	893	U
1	A1	895	G
1	A1	903	A
1	A1	913	A
1	A1	914	U
1	A1	917	U
1	A1	919	A
1	A1	920	A
1	A1	930	C

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Mol	Chain	Res	Type
1	A1	933	G
1	A1	934	G
1	A1	943	U
1	A1	960	U
1	A1	966	U
1	A1	970	G
1	A1	971	G
1	A1	979	C
1	A1	985	G
1	A1	989	C
1	A1	990	A
1	A1	992	A
1	A1	997	A
1	A1	999	G
1	A1	1002	U
1	A1	1005	G
1	A1	1013	U
1	A1	1017	U
1	A1	1021	U
1	A1	1023	A
1	A1	1028	A
1	A1	1041	G
1	A1	1047	C
1	A1	1058	A
1	A1	1060	A
1	A1	1067	C
1	A1	1071	G
1	A1	1083	A
1	A1	1085	C
1	A1	1087	A
1	A1	1089	G
1	A1	1097	G
1	A1	1099	G
1	A1	1100	A
1	A1	1101	U
1	A1	1106	C
1	A1	1115	U
1	A1	1116	C
1	A1	1117	C
1	A1	1118	C
1	A1	1123	C
1	A1	1126	G

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Mol	Chain	Res	Type
1	A1	1131	G
1	A1	1138	C
1	A1	1139	C
1	A1	1144	A
1	A1	1145	A
1	A1	1149	A
1	A1	1150	A
1	A1	1153	C
1	A1	1154	U
1	A1	1155	U
1	A1	1170	A
1	A1	1171	G
1	A1	1175	G
1	A1	1178	U
1	A1	1194	A
1	A1	1195	A
1	A1	1200	A
1	A1	1207	G
1	A1	1212	G
1	A1	1215	C
1	A1	1216	C
1	A1	1221	G
1	A1	1230	C
1	A1	1241	A
1	A1	1242	U
1	A1	1246	A
1	A1	1251	A
1	A1	1253	A
1	A1	1254	C
1	A1	1256	G
1	A1	1257	G
1	A1	1258	A
1	A1	1266	C
1	A1	1274	G
1	A1	1275	G
1	A1	1282	A
1	A1	1284	A
1	A1	1285	G
1	A1	1286	G
1	A1	1287	A
1	A1	1291	A
1	A1	1293	A

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Mol	Chain	Res	Type
1	A1	1295	A
1	A1	1296	U
1	A1	1299	A
1	A1	1300	U
1	A1	1301	A
1	A1	1302	G
1	A1	1303	C
1	A1	1308	U
1	A1	1311	C
1	A1	1314	U
1	A1	1319	U
1	A1	1330	G
1	A1	1336	C
1	A1	1342	U
1	A1	1344	A
1	A1	1345	G
1	A1	1355	C
1	A1	1371	U
1	A1	1372	U
1	A1	1375	G
1	A1	1378	A
1	A1	1395	C
1	A1	1396	A
1	A1	1397	U
1	A1	1402	A
1	A1	1412	C
1	A1	1413	G
1	A1	1417	C
1	A1	1427	C
1	A1	1428	G
1	A1	1429	G
1	A1	1430	C
1	A1	1439	A
1	A1	1440	C
1	A1	1447	G
1	A1	1450	G
1	A1	1452	A
1	A1	1453	C
1	A1	1454	A
1	A1	1461	G
1	A1	1462	U
1	A1	1463	U

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Mol	Chain	Res	Type
1	A1	1464	C
1	A1	1466	G
1	A1	1471	C
1	A1	1476	A
1	A1	1477	U
1	A1	1480	A
1	A1	1486	A
1	A1	1487	A
1	A1	1489	A
1	A1	1490	G
1	A1	1496	U
1	A1	1498	A
1	A1	1501	C
1	A1	1502	C
1	A1	1521	C
1	A1	1522	A
1	A1	1523	C
1	A1	1532	C
1	A1	1533	A
1	A1	1535	U
1	A1	1536	G
1	A1	1545	A
1	A1	1548	G
1	A1	1552	G
1	A1	1553	C
1	A1	1554	C
1	A1	1555	U
1	A1	1556	A
1	A1	1557	C
1	A1	1558	C
1	A1	1567	G
1	A1	1570	G
1	A1	1574	C
1	A1	1579	A
1	A1	1580	A
1	A1	1585	U
1	A1	1586	U
1	A1	1588	A
1	A1	1591	C
1	A1	1596	U
1	A1	1597	C
1	A1	1599	U

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Mol	Chain	Res	Type
1	A1	1601	A
1	A1	1602	U
1	A1	1603	G
1	A1	1604	G
1	A1	1621	U
1	A1	1623	A
1	A1	1637	A
1	A1	1638	G
1	A1	1640	A
1	A1	1641	A
1	A1	1646	C
1	A1	1648	G
1	A1	1654	G
1	A1	1665	G
1	A1	1666	C
1	A1	1668	U
1	A1	1670	C
1	A1	1671	G
1	A1	1674	G
1	A1	1678	A
1	A1	1683	C
1	A1	1695	A
1	A1	1698	C
1	A1	1699	A
1	A1	1700	C
1	A1	1701	C
1	A1	1702	G
1	A1	1715	A
1	A1	1721	U
1	A1	1722	G
1	A1	1729	U
1	A1	1732	G
1	A1	1735	A
1	A1	1746	U
1	A1	1748	G
1	A1	1753	C
1	A1	1756	C
1	A1	1757	G
1	A1	1758	G
1	A1	1759	G
1	A1	1777	G
1	A1	1778	C

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Mol	Chain	Res	Type
1	A1	1781	A
1	A1	1783	C
1	A1	1792	G
1	A1	1800	A
1	A1	1816	G
1	A1	1821	U
1	A1	1823	A
1	A1	1824	A
1	A1	1825	A
1	A1	1826	G
1	A1	1831	A
1	A1	1834	A
1	A1	1836	G
1	A1	1838	U
1	A1	1839	U
1	A1	1840	U
1	A1	1844	U
1	A1	1845	A
1	A1	1849	G
1	A1	1851	A
1	A1	1852	C
1	A1	1861	G
1	A1	1862	G
1	A1	1863	A
1	A1	1864	U
1	A1	1865	C
1	A1	1869	A
37	52	5	A
37	52	6	C
37	52	8	U
37	52	9	C
37	52	10	A
37	52	13	U
37	52	18	C
37	52	21	G
37	52	25	A
37	52	30	C
37	52	39	A
37	52	42	A
37	52	44	A
37	52	48	G
37	52	49	U

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Mol	Chain	Res	Type
37	52	58	G
37	52	59	A
37	52	64	A
37	52	65	A
37	52	67	C
37	52	70	A
37	52	71	C
37	52	72	C
37	52	76	A
37	52	82	U
37	52	84	A
37	52	87	A
37	52	91	G
37	52	93	G
37	52	96	U
37	52	104	G
37	52	108	A
37	52	109	G
37	52	119	G
37	52	120	A
37	52	122	U
37	52	126	C
37	52	133	C
37	52	135	G
37	52	136	C
37	52	137	G
37	52	142	G
37	52	144	G
37	52	149	A
37	52	151	G
37	52	153	G
37	52	156	G
37	52	157	U
37	52	159	C
37	52	160	G
37	52	161	G
37	52	164	G
37	52	168	C
37	52	170	C
37	52	172	C
37	52	173	C
37	52	174	C

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Mol	Chain	Res	Type
37	52	179	G
37	52	181	C
37	52	182	G
37	52	197	A
37	52	200	U
37	52	201	C
37	52	214	G
37	52	216	C
37	52	217	C
37	52	220	C
37	52	224	U
37	52	225	G
37	52	232	G
37	52	233	U
37	52	234	G
37	52	236	G
37	52	246	G
37	52	262	G
37	52	265	C
37	52	266	C
37	52	276	C
37	52	277	G
37	52	280	G
37	52	294	G
37	52	297	U
37	52	306	A
37	52	308	G
37	52	309	C
37	52	310	G
37	52	315	G
37	52	316	U
37	52	321	U
37	52	322	C
37	52	323	C
37	52	334	A
37	52	340	C
37	52	341	G
37	52	345	C
37	52	346	G
37	52	349	A
37	52	367	C
37	52	379	G

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Mol	Chain	Res	Type
37	52	383	A
37	52	384	A
37	52	387	G
37	52	390	C
37	52	395	A
37	52	396	A
37	52	410	A
37	52	412	G
37	52	413	G
37	52	417	G
37	52	440	U
37	52	446	C
37	52	448	G
37	52	449	C
37	52	450	G
37	52	452	A
37	52	453	G
37	52	454	U
37	52	455	C
37	52	463	A
37	52	465	G
37	52	467	U
37	52	468	U
37	52	474	C
37	52	475	G
37	52	481	G
37	52	481(A)	C
37	52	482	G
37	52	483	G
37	52	484	U
37	52	485	C
37	52	486	C
37	52	487	G
37	52	490	C
37	52	491	G
37	52	492	U
37	52	493	G
37	52	495	C
37	52	498	C
37	52	499	G
37	52	505	G
37	52	506	C

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Mol	Chain	Res	Type
37	52	510	U
37	52	516	C
37	52	641	G
37	52	642	G
37	52	661	C
37	52	666	G
37	52	667	A
37	52	669	C
37	52	670	G
37	52	674	G
37	52	676	C
37	52	685	C
37	52	686	A
37	52	688	U
37	52	691	C
37	52	696	C
37	52	697	G
37	52	700	G
37	52	704	C
37	52	705	G
37	52	719	C
37	52	722	G
37	52	729	G
37	52	730	G
37	52	731	G
37	52	733	A
37	52	738	C
37	52	743	G
37	52	747	A
37	52	749	G
37	52	750	U
37	52	751	G
37	52	752	G
37	52	758	G
37	52	760	G
37	52	905	C
37	52	908	G
37	52	913	U
37	52	914	U
37	52	915	A
37	52	917	A
37	52	922(B)	C

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Mol	Chain	Res	Type
37	52	923	C
37	52	925	C
37	52	926	G
37	52	929	A
37	52	930	G
37	52	931	C
37	52	932	A
37	52	933	G
37	52	934	C
37	52	935	A
37	52	935(A)	G
37	52	941	C
37	52	944	A
37	52	945	U
37	52	946	C
37	52	951	G
37	52	955	G
37	52	956	A
37	52	959	G
37	52	960	A
37	52	961	G
37	52	962	C
37	52	965	G
37	52	966	A
37	52	967	C
37	52	968	C
37	52	969	C
37	52	972	C
37	52	978	G
37	52	983	C
37	52	985	C
37	52	990	C
37	52	1070	G
37	52	1071	C
37	52	1072	C
37	52	1073	G
37	52	1074	G
37	52	1077	C
37	52	1082	C
37	52	1089	G
37	52	1090	G
37	52	1101	C

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Mol	Chain	Res	Type
37	52	1104	C
37	52	1107	C
37	52	1108	C
37	52	1163	G
37	52	1164	G
37	52	1165	G
37	52	1166	G
37	52	1167	C
37	52	1181	C
37	52	1183	C
37	52	1196	G
37	52	1199	G
37	52	1201	U
37	52	1203	G
37	52	1205	G
37	52	1211	G
37	52	1212	G
37	52	1214	C
37	52	1215	C
37	52	1216	C
37	52	1219	G
37	52	1221	G
37	52	1235	G
37	52	1236	C
37	52	1237	C
37	52	1238	A
37	52	1239	C
37	52	1246	G
37	52	1272	C
37	52	1273	G
37	52	1276	C
37	52	1279	A
37	52	1281	G
37	52	1284	G
37	52	1287	G
37	52	1292	C
37	52	1293	G
37	52	1295	U
37	52	1296	G
37	52	1299	G
37	52	1300	G
37	52	1301	C

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Mol	Chain	Res	Type
37	52	1303	A
37	52	1309	C
37	52	1318	C
37	52	1321	G
37	52	1326	A
37	52	1330	A
37	52	1338	G
37	52	1341	U
37	52	1352	C
37	52	1353	G
37	52	1354	A
37	52	1356	U
37	52	1358	G
37	52	1359	G
37	52	1360	G
37	52	1361	G
37	52	1362	G
37	52	1370	G
37	52	1371	A
37	52	1372	A
37	52	1373	A
37	52	1377	G
37	52	1378	C
37	52	1379	C
37	52	1387	A
37	52	1389	U
37	52	1391	A
37	52	1394	G
37	52	1396	G
37	52	1397	A
37	52	1398	A
37	52	1399	G
37	52	1400	G
37	52	1405	C
37	52	1406	G
37	52	1420	A
37	52	1425	G
37	52	1429	C
37	52	1434	G
37	52	1436	C
37	52	1437	C
37	52	1438	U

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Mol	Chain	Res	Type
37	52	1440	U
37	52	1445	U
37	52	1446	C
37	52	1453	G
37	52	1454	G
37	52	1456	C
37	52	1457	G
37	52	1459	A
37	52	1466	G
37	52	1468	C
37	52	1475	G
37	52	1478	C
37	52	1481	C
37	52	1482	G
37	52	1483	C
37	52	1484	G
37	52	1491	A
37	52	1493	G
37	52	1497	A
37	52	1498	G
37	52	1501	C
37	52	1502	G
37	52	1514	U
37	52	1517	G
37	52	1518	A
37	52	1521	C
37	52	1523	A
37	52	1524	A
37	52	1531	U
37	52	1534	A
37	52	1535	C
37	52	1538	U
37	52	1540	C
37	52	1543	G
37	52	1547	A
37	52	1549	G
37	52	1553	A
37	52	1558	A
37	52	1566	C
37	52	1571	G
37	52	1573	G
37	52	1578	U

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Mol	Chain	Res	Type
37	52	1585	C
37	52	1590	C
37	52	1591	U
37	52	1592	G
37	52	1596	U
37	52	1597	G
37	52	1602	U
37	52	1605	G
37	52	1609	U
37	52	1612	G
37	52	1613	A
37	52	1614	C
37	52	1624	G
37	52	1625	G
37	52	1626	G
37	52	1627	G
37	52	1631	A
37	52	1632	A
37	52	1633	G
37	52	1634	A
37	52	1638	A
37	52	1643	A
37	52	1650	A
37	52	1651	G
37	52	1652	U
37	52	1654	G
37	52	1658	G
37	52	1660	U
37	52	1661	C
37	52	1663	C
37	52	1673	U
37	52	1676	C
37	52	1677	U
37	52	1679	A
37	52	1684	A
37	52	1724	G
37	52	1725	U
37	52	1729	A
37	52	1730	U
37	52	1731	C
37	52	1734	G
37	52	1735	U

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Mol	Chain	Res	Type
37	52	1740	C
37	52	1741	G
37	52	1742	A
37	52	1746	A
37	52	1750	G
37	52	1753	G
37	52	1754	U
37	52	1755	C
37	52	1756	U
37	52	1757	U
37	52	1763	C
37	52	1764	G
37	52	1768	C
37	52	1772	C
37	52	1775	A
37	52	1776	A
37	52	1777	C
37	52	1787	A
37	52	1792	U
37	52	1796	U
37	52	1800	U
37	52	1804	A
37	52	1805	A
37	52	1806	G
37	52	1807	C
37	52	1808	C
37	52	1810	G
37	52	1812	C
37	52	1815	G
37	52	1818	G
37	52	1820	U
37	52	1821	G
37	52	1822	U
37	52	1824	G
37	52	1828	C
37	52	1834	U
37	52	1836	G
37	52	1837	A
37	52	1842	G
37	52	1843	A
37	52	1844	G
37	52	1855	G

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Mol	Chain	Res	Type
37	52	1861	U
37	52	1866	U
37	52	1867	A
37	52	1869	G
37	52	1870	C
37	52	1889	U
37	52	1892	A
37	52	1893	C
37	52	1897	A
37	52	1910	G
37	52	1915	C
37	52	1918	U
37	52	1920	C
37	52	1921	C
37	52	1922	G
37	52	1924	C
37	52	1928	C
37	52	1930	U
37	52	1931	C
37	52	1932	A
37	52	1934	A
37	52	1935	C
37	52	1940	G
37	52	1942	A
37	52	1944	A
37	52	1948	G
37	52	1951	G
37	52	1958	A
37	52	1959	U
37	52	1960	A
37	52	1961	G
37	52	1969	G
37	52	1971	U
37	52	1976	G
37	52	1977	C
37	52	1979	A
37	52	1980	U
37	52	1981	G
37	52	1983	A
37	52	1984	A
37	52	1991	A
37	52	1993	C

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Mol	Chain	Res	Type
37	52	1994	C
37	52	1995	G
37	52	1998	A
37	52	2001	G
37	52	2002	A
37	52	2003	G
37	52	2005	G
37	52	2007	G
37	52	2010	A
37	52	2011	C
37	52	2014	C
37	52	2020	U
37	52	2021	G
37	52	2022	C
37	52	2023	C
37	52	2024	G
37	52	2025	A
37	52	2026	A
37	52	2042	A
37	52	2043	A
37	52	2046	G
37	52	2047	A
37	52	2048	U
37	52	2052	G
37	52	2054	U
37	52	2055	G
37	52	2056	G
37	52	2057	A
37	52	2062	C
37	52	2063	G
37	52	2064	G
37	52	2069	A
37	52	2078	C
37	52	2084	U
37	52	2085	G
37	52	2088	A
37	52	2089	G
37	52	2090	U
37	52	2092	G
37	52	2093	G
37	52	2094	C
37	52	2097	A

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Mol	Chain	Res	Type
37	52	2098	G
37	52	2099	C
37	52	2101	A
37	52	2102	G
37	52	2105	A
37	52	2108	G
37	52	2112	G
37	52	2259	G
37	52	2260	C
37	52	2261	G
37	52	2263	A
37	52	2268	A
37	52	2269	C
37	52	2270	G
37	52	2274	C
37	52	2275	G
37	52	2277	C
37	52	2279	A
37	52	2281	U
37	52	2289	C
37	52	2295	C
37	52	2300	A
37	52	2301	G
37	52	2306	G
37	52	2308	A
37	52	2313	A
37	52	2314	G
37	52	2328	G
37	52	2333	G
37	52	2335	C
37	52	2345	G
37	52	2346	C
37	52	2348	G
37	52	2351	C
37	52	2353	U
37	52	2360	A
37	52	2363	A
37	52	2364	G
37	52	2374	A
37	52	2380	G
37	52	2385	U
37	52	2395	A

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Mol	Chain	Res	Type
37	52	2396	A
37	52	2397	G
37	52	2399	G
37	52	2414	G
37	52	2415	U
37	52	2416	G
37	52	2421	G
37	52	2422	C
37	52	2426	U
37	52	2428	A
37	52	2433	G
37	52	2437	C
37	52	2438	A
37	52	2439	G
37	52	2440	U
37	52	2441	C
37	52	2447	U
37	52	2450	G
37	52	2451	A
37	52	2454	U
37	52	2456	G
37	52	2458	C
37	52	2460	A
37	52	2461	G
37	52	2471	G
37	52	2473	A
37	52	2475	G
37	52	2480	G
37	52	2481	G
37	52	2485	U
37	52	2488	C
37	52	2489	C
37	52	2490	U
37	52	2491	C
37	52	2492	C
37	52	2493	G
37	52	2494	U
37	52	2496	G
37	52	2501	C
37	52	2503	G
37	52	2505	C
37	52	2506	G

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Mol	Chain	Res	Type
37	52	2511	A
37	52	2512	A
37	52	2513	A
37	52	2516	G
37	52	2521	G
37	52	2529	A
37	52	2532	C
37	52	2535	G
37	52	2536	A
37	52	2537	A
37	52	2538	U
37	52	2542	G
37	52	2544	G
37	52	2546	G
37	52	2549	G
37	52	2551	A
37	52	2555	G
37	52	2556	G
37	52	2561	C
37	52	2562	G
37	52	2563	C
37	52	2566	G
37	52	2570	U
37	52	2575	U
37	52	2576	G
37	52	2577	C
37	52	2580	U
37	52	2581	A
37	52	2587	A
37	52	2588	C
37	52	2589	C
37	52	2593	C
37	52	2597	G
37	52	2599	G
37	52	2600	A
37	52	2601	A
37	52	2604	C
37	52	2607	C
37	52	2620	G
37	52	2621	A
37	52	2622	G
37	52	2624	G

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Mol	Chain	Res	Type
37	52	2627	C
37	52	2631	U
37	52	2639	U
37	52	2653	C
37	52	2655	C
37	52	2656	U
37	52	2658	G
37	52	2662	G
37	52	2663	G
37	52	2668	G
37	52	2669	C
37	52	2670	C
37	52	2674	A
37	52	2675	G
37	52	2683	C
37	52	2685	C
37	52	2686	G
37	52	2687	U
37	52	2689	C
37	52	2693	G
37	52	2695	A
37	52	2696	A
37	52	2697	A
37	52	2701	U
37	52	2706	G
37	52	2707	U
37	52	2708	U
37	52	2709	C
37	52	2710	C
37	52	2711	G
37	52	2712	G
37	52	2714	G
37	52	2716	C
37	52	2719	C
37	52	2725	A
37	52	2726	G
37	52	2732	G
37	52	2739	C
37	52	2740	U
37	52	2741	U
37	52	2743	A
37	52	2744	A

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Mol	Chain	Res	Type
37	52	2750	G
37	52	2752	G
37	52	2754	G
37	52	2756	G
37	52	2757	A
37	52	2760	G
37	52	2761	U
37	52	2763	U
37	52	2764	A
37	52	2766	A
37	52	2767	U
37	52	2768	C
37	52	2769	U
37	52	2778	G
37	52	2787	A
37	52	2788	U
37	52	2789	A
37	52	2790	U
37	52	2794	C
37	52	2796	G
37	52	2798	A
37	52	2799	G
37	52	2807	A
37	52	2809	G
37	52	2811	G
37	52	2812	A
37	52	2813	A
37	52	2817	C
37	52	2821	U
37	52	2822	G
37	52	2823	G
37	52	2826	U
37	52	2827	G
37	52	2842	G
37	52	2847	G
37	52	2849	A
37	52	2850	A
37	52	2854	G
37	52	2855	G
37	52	2856	C
37	52	2858	A
37	52	2862	G

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Mol	Chain	Res	Type
37	52	2864	A
37	52	2872	C
37	52	2873	U
37	52	2875	C
37	52	2876	G
37	52	2889	G
37	52	2895	A
37	52	2897	G
37	52	2898	G
37	52	3598	C
37	52	3599	A
37	52	3600	G
37	52	3604	A
37	52	3605	C
37	52	3606	U
37	52	3615	G
37	52	3616	U
37	52	3618	C
37	52	3620	G
37	52	3622	C
37	52	3625	G
37	52	3626	G
37	52	3635	A
37	52	3638	G
37	52	3642	A
37	52	3643	A
37	52	3644	U
37	52	3646	A
37	52	3662	A
37	52	3664	G
37	52	3668	C
37	52	3673	C
37	52	3674	G
37	52	3678	G
37	52	3680	U
37	52	3682	A
37	52	3683	C
37	52	3685	C
37	52	3690	U
37	52	3692	A
37	52	3696	C
37	52	3705	G

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Mol	Chain	Res	Type
37	52	3707	U
37	52	3712	A
37	52	3713	U
37	52	3714	G
37	52	3729	U
37	52	3731	C
37	52	3732	A
37	52	3734	U
37	52	3743	G
37	52	3744	G
37	52	3753	G
37	52	3760	A
37	52	3763	A
37	52	3766	A
37	52	3773	U
37	52	3775	A
37	52	3776	G
37	52	3777	G
37	52	3783	A
37	52	3784	A
37	52	3793	U
37	52	3796	U
37	52	3798	U
37	52	3802	U
37	52	3807	A
37	52	3810	C
37	52	3811	G
37	52	3812	C
37	52	3814	U
37	52	3817	A
37	52	3819	G
37	52	3822	U
37	52	3825	A
37	52	3834	C
37	52	3837	C
37	52	3838	U
37	52	3840	U
37	52	3843	C
37	52	3858	C
37	52	3865	A
37	52	3867	A
37	52	3868	G

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Mol	Chain	Res	Type
37	52	3876	A
37	52	3877	A
37	52	3878	C
37	52	3879	G
37	52	3881	G
37	52	3882	C
37	52	3889	G
37	52	3895	G
37	52	3897	G
37	52	3901	A
37	52	3902	A
37	52	3905	A
37	52	3906	A
37	52	3907	G
37	52	3909	C
37	52	3915	U
37	52	3921	U
37	52	3925	U
37	52	3926	C
37	52	3937	C
37	52	3940	U
37	52	3941	G
37	52	3942	A
37	52	3944	G
37	52	3947	A
37	52	3957	U
37	52	3959	U
37	52	3960	A
37	52	3962	A
37	52	3963	A
37	52	3964	U
37	52	3965	A
37	52	3966	A
37	52	3967	G
37	52	3969	G
37	52	3970	G
37	52	3973	G
37	52	4037	C
37	52	4038	C
37	52	4044	U
37	52	4047	A
37	52	4048	A

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Mol	Chain	Res	Type
37	52	4049	U
37	52	4053	A
37	52	4065	G
37	52	4066	U
37	52	4067	U
37	52	4069	U
37	52	4071	U
37	52	4076	G
37	52	4077	A
37	52	4084	G
37	52	4085	A
37	52	4086	G
37	52	4091	G
37	52	4093	G
37	52	4094	G
37	52	4100	C
37	52	4111	U
37	52	4112	C
37	52	4116	C
37	52	4117	U
37	52	4118	U
37	52	4119	C
37	52	4120	U
37	52	4121	G
37	52	4122	G
37	52	4124	G
37	52	4127	A
37	52	4129	G
37	52	4131	G
37	52	4133	C
37	52	4157	A
37	52	4158	C
37	52	4159	C
37	52	4162	C
37	52	4163	U
37	52	4166	G
37	52	4170	A
37	52	4171	C
37	52	4172	A
37	52	4173	G
37	52	4180	G
37	52	4183	G

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Mol	Chain	Res	Type
37	52	4184	G
37	52	4191	G
37	52	4194	U
37	52	4195	G
37	52	4203	A
37	52	4205	A
37	52	4206	C
37	52	4207	C
37	52	4209	G
37	52	4212	A
37	52	4215	C
37	52	4229	U
37	52	4233	A
37	52	4234	A
37	52	4251	A
37	52	4254	G
37	52	4255	A
37	52	4257	A
37	52	4265	U
37	52	4266	G
37	52	4268	A
37	52	4271	A
37	52	4273	A
37	52	4275	G
37	52	4280	A
37	52	4281	A
37	52	4282	A
37	52	4285	U
37	52	4290	U
37	52	4291	G
37	52	4293	U
37	52	4305	G
37	52	4306	U
37	52	4317	A
37	52	4318	C
37	52	4322	G
37	52	4329	G
37	52	4330	G
37	52	4335	C
37	52	4336	A
37	52	4339	A
37	52	4348	A

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Mol	Chain	Res	Type
37	52	4349	C
37	52	4350	C
37	52	4351	U
37	52	4355	G
37	52	4359	U
37	52	4366	A
37	52	4374	U
37	52	4377	G
37	52	4378	A
37	52	4379	A
37	52	4380	A
37	52	4386	C
37	52	4387	C
37	52	4393	G
37	52	4394	A
37	52	4395	U
37	52	4396	A
37	52	4398	C
37	52	4405	G
37	52	4417	C
37	52	4419	U
37	52	4420	U
37	52	4422	A
37	52	4424	A
37	52	4426	C
37	52	4430	G
37	52	4431	U
37	52	4433	G
37	52	4435	U
37	52	4437	U
37	52	4440	G
37	52	4444	C
37	52	4448	G
37	52	4449	A
37	52	4450	U
37	52	4452	U
37	52	4453	C
37	52	4464	A
37	52	4466	C
37	52	4472	G
37	52	4475	G
37	52	4476	C

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Mol	Chain	Res	Type
37	52	4477	A
37	52	4480	A
37	52	4481	U
37	52	4482	U
37	52	4497	U
37	52	4499	G
37	52	4500	U
37	52	4501	U
37	52	4507	A
37	52	4511	A
37	52	4512	U
37	52	4513	A
37	52	4519	C
37	52	4522	G
37	52	4524	G
37	52	4530	U
37	52	4531	U
37	52	4532	U
37	52	4548	A
37	52	4549	G
37	52	4552	U
37	52	4553	A
37	52	4554	G
37	52	4567	G
37	52	4570	G
37	52	4573	G
37	52	4575	G
37	52	4589	A
37	52	4590	A
37	52	4599	A
37	52	4604	G
37	52	4606	G
37	52	4634	U
37	52	4635	A
37	52	4636	U
37	52	4637	G
37	52	4639	G
37	52	4652	G
37	52	4654	C
37	52	4656	A
37	52	4657	U
37	52	4662	C

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Mol	Chain	Res	Type
37	52	4670	C
37	52	4672	A
37	52	4673	U
37	52	4677	U
37	52	4693	C
37	52	4694	G
37	52	4695	C
37	52	4700	A
37	52	4709	U
37	52	4716	C
37	52	4719	G
37	52	4720	C
37	52	4721	G
37	52	4726	G
37	52	4728	U
37	52	4738	C
37	52	4739	C
37	52	4740	G
37	52	4750	G
37	52	4751	G
37	52	4753	U
37	52	4754	G
37	52	4757	C
37	52	4759	C
37	52	4761	G
37	52	4764	A
37	52	4765	G
37	52	4766	C
37	52	4771	C
37	52	4772	C
37	52	4860	G
37	52	4862	G
37	52	4868	G
37	52	4870	G
37	52	4871	C
37	52	4872	G
37	52	4873	G
37	52	4874	A
37	52	4875	G
37	52	4876	A
37	52	4877	G
37	52	4882	U

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Mol	Chain	Res	Type
37	52	4883	C
37	52	4885	U
37	52	4893	A
37	52	4894	A
37	52	4895	C
37	52	4898	G
37	52	4904	G
37	52	4905	C
37	52	4906	C
37	52	4907	G
37	52	4908	G
37	52	4909	A
37	52	4910	A
37	52	4911	A
37	52	4912	G
37	52	4913	G
37	52	4914	G
37	52	4915	G
37	52	4918	C
37	52	4920	C
37	52	4921	C
37	52	4922	C
37	52	4923	U
37	52	4924	C
37	52	4926	C
37	52	4927	G
37	52	4928	C
37	52	4930	C
37	52	4931	G
37	52	4933	C
37	52	4935	C
37	52	4937	C
37	52	4938	A
37	52	4940	C
37	52	4943	A
37	52	4944	C
37	52	4945	G
37	52	4947	U
37	52	4949	G
37	52	4950	U
37	52	4951	G
37	52	4955	A

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Mol	Chain	Res	Type
37	52	4956	A
37	52	4958	C
37	52	4959	U
37	52	4964	C
37	52	4965	U
37	52	4966	A
37	52	4967	A
37	52	4976	U
37	52	4980	C
37	52	4988	U
37	52	4989	U
37	52	4990	C
37	52	5005	G
37	52	5009	G
37	52	5017	G
37	52	5018	C
37	52	5019	A
37	52	5022	U
37	52	5035	U
37	52	5040	U
37	52	5041	G
37	52	5043	A
37	52	5047	C
37	52	5048	A
37	52	5050	C
37	52	5053	U
37	52	5054	C
37	52	5055	G
37	52	5056	A
37	52	5058	A
37	52	5059	C
37	52	5061	A
37	52	5062	G
37	52	5069	U
38	72	2	U
38	72	3	C
38	72	6	C
38	72	7	G
38	72	11	A
38	72	17	C
38	72	21	G
38	72	22	A

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Mol	Chain	Res	Type
38	72	23	A
38	72	24	C
38	72	25	G
38	72	28	C
38	72	30	C
38	72	42	A
38	72	45	U
38	72	48	G
38	72	50	A
38	72	53	U
38	72	54	A
38	72	55	A
38	72	60	G
38	72	61	G
38	72	63	C
38	72	64	G
38	72	78	C
38	72	90	A
38	72	97	G
38	72	100	A
38	72	102	U
38	72	103	A
38	72	106	G
38	72	110	G
38	72	117	G
38	72	120	U
39	82	8	U
39	82	23	C
39	82	34	U
39	82	35	C
39	82	37	A
39	82	39	G
39	82	45	C
39	82	49	G
39	82	50	C
39	82	51	U
39	82	59	A
39	82	62	A
39	82	63	U
39	82	87	G
39	82	90	C
39	82	92	U

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Mol	Chain	Res	Type
39	82	94	G
39	82	95	A
39	82	96	C
39	82	102	G
39	82	103	A
39	82	105	C
39	82	109	C
39	82	110	U
39	82	111	U
39	82	114	G
39	82	117	C
39	82	118	C
39	82	119	C
39	82	120	G
39	82	121	G
39	82	122	G
39	82	123	U
39	82	124	U
39	82	125	C
39	82	126	C
39	82	127	U
39	82	128	C
39	82	137	A
39	82	143	G
39	82	150	C
39	82	153	C
39	82	156	U
80	23	7	G
80	23	8	U
80	23	9	A
80	23	13	U
80	23	14	A
80	23	20	U
80	23	21	A
80	23	31	C
80	23	32	C
80	23	37	A
80	23	46	G
80	23	47	U
80	23	49	C
80	23	53	G
80	23	59	A

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Mol	Chain	Res	Type
80	23	61	C
80	23	65	G
80	23	67	G
81	w3	38	A
81	w3	39	A
81	w3	42	C
81	w3	43	A
81	w3	45	A
81	w3	46	G
81	w3	49	U
81	w3	56	A
81	w3	58	A
81	w3	59	A

All (68) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A1	110	U
1	A1	182	C
1	A1	228	C
1	A1	241	G
1	A1	434	G
1	A1	465	A
1	A1	532	C
1	A1	553	U
1	A1	642	U
1	A1	688	U
1	A1	751	G
1	A1	870	A
1	A1	874	G
1	A1	1137	U
1	A1	1253	A
1	A1	1394	G
1	A1	1395	C
1	A1	1396	A
1	A1	1489	A
1	A1	1520	G
1	A1	1637	A
1	A1	1664	A
1	A1	1824	A
37	52	48	G
37	52	125	C

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Mol	Chain	Res	Type
37	52	265	C
37	52	275	C
37	52	449	C
37	52	480	C
37	52	498	C
37	52	504	G
37	52	930	G
37	52	959	G
37	52	966	A
37	52	971(A)	G
37	52	1106	A
37	52	1211	G
37	52	1238	A
37	52	1291	G
37	52	1329	G
37	52	1370	G
37	52	1445	U
37	52	1455	G
37	52	1979	A
37	52	1994	C
37	52	2046	G
37	52	2089	G
37	52	2502	A
37	52	2536	A
37	52	2875	C
37	52	3625	G
37	52	3876	A
37	52	3888	G
37	52	3939	G
37	52	3940	U
37	52	3959	U
37	52	3965	A
37	52	3968	U
37	52	4036	G
37	52	4157	A
37	52	4232	U
37	52	4448	G
37	52	4699	U
37	52	4719	G
37	52	4859	C
37	52	4884	G
37	52	4925	U

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Mol	Chain	Res	Type
37	52	4936	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 310 ligands modelled in this entry, 308 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	$\# Z > 2$
90	SF4	k1	600	-	0,12,12	-	-	-		
90	SF4	k1	601	-	0,12,12	-	-	-		

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
90	SF4	k1	600	-	-	-	0/6/5/5
90	SF4	k1	601	-	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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
37	52	37
1	A1	12
80	23	1
85	I3	1
78	s3	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	52	2113:G	O3'	2258:C	P	42.99
1	52	1252:C	O3'	1271:G	P	36.84
1	52	1406(C):G	O3'	1411:C	P	19.26
1	52	1109:C	O3'	1161:G	P	17.69
1	52	3977:C	O3'	4034:G	P	16.37
1	52	1696:C	O3'	1720:C	P	16.22
1	52	4101:C	O3'	4107:G	P	15.99
1	52	990:C	O3'	1064:G	P	15.06
1	52	5022:U	O3'	5028:G	P	14.93
1	52	4777:C	O3'	4859:C	P	14.91
1	52	523:C	O3'	638:G	P	14.66
1	52	1364:U	O3'	1368:A	P	14.61
1	52	2901:G	O3'	3597:G	P	13.74
1	52	4138:C	O3'	4146:G	P	13.54
1	52	760:G	O3'	904:C	P	12.47
1	52	4729:A	O3'	4735:G	P	9.89
1	52	182:G	O3'	189:G	P	9.08
1	52	500:G	O3'	504:G	P	7.93
1	A1	745:C	O3'	746:C	P	7.34
1	52	512:U	O3'	515:C	P	7.27
1	52	3938:G	O3'	3939:G	P	6.79
1	52	3937:C	O3'	3938:G	P	6.76

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	52	4740:G	O3'	4743:G	P	6.72
1	A1	787:G	O3'	788:G	P	6.10
1	52	3948:C	O3'	3949:A	P	5.77
1	52	4899:G	O3'	4902:C	P	5.75
1	52	1222:A	O3'	1223:G	P	5.52
1	23	16:C	O3'	18:G	P	5.52
1	52	3942:A	O3'	3943:A	P	5.07
1	52	1219:G	O3'	1220:G	P	4.89
1	A1	225:G	O3'	226:A	P	4.57
1	52	1221:G	O3'	1222:A	P	4.51
1	52	3947:A	O3'	3948:C	P	4.39
1	52	170:C	O3'	171:U	P	4.17
1	52	5020:G	O3'	5021:C	P	4.08
1	A1	748:C	O3'	749:U	P	4.02
1	A1	322:C	O3'	323:C	P	3.93
1	A1	747:U	O3'	748:C	P	3.87
1	A1	286:U	O3'	287:U	P	3.86
1	A1	304:C	O3'	305:U	P	3.66
1	A1	903:A	O3'	904:A	P	3.65
1	52	1239:C	O3'	1244:G	P	3.53
1	52	1088:C	O3'	1089:G	P	3.45
1	A1	309:G	O3'	310:C	P	3.43
1	A1	902:G	O3'	903:A	P	3.29
1	52	1438:U	O3'	1440:U	P	3.24
1	52	751:G	O3'	752:G	P	3.23
1	A1	1295:A	O3'	1296:U	P	3.20
1	52	267:G	O3'	268:G	P	3.20
1	52	4076:G	O3'	4077:A	P	3.11
1	I3	203:ARG	C	204:GLY	N	1.96
1	s3	186:GLY	C	187:LEU	N	1.66

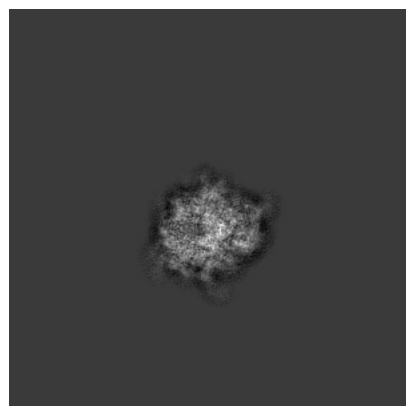
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0195. These allow visual inspection of the internal detail of the map and identification of artifacts.

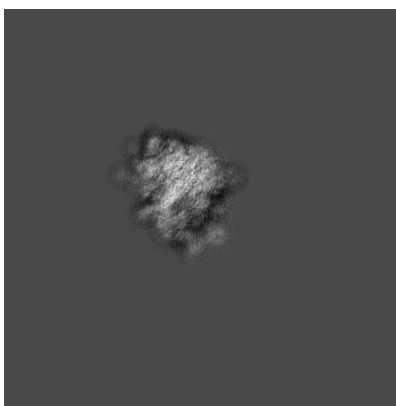
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

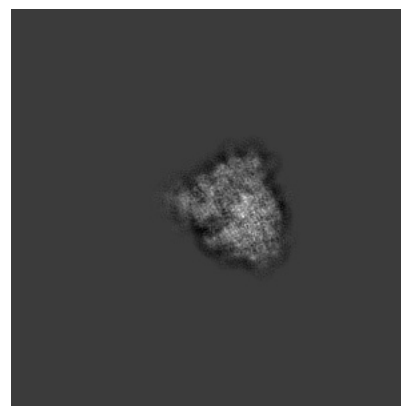
6.1.1 Primary map



X

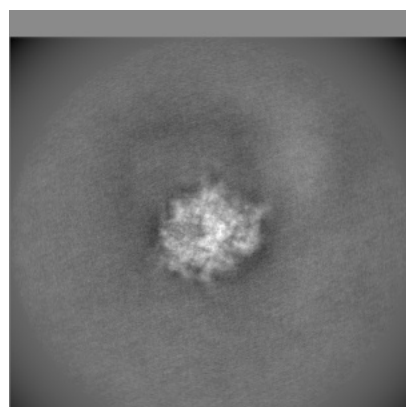


Y

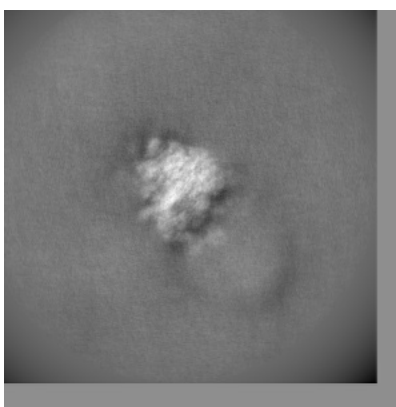


Z

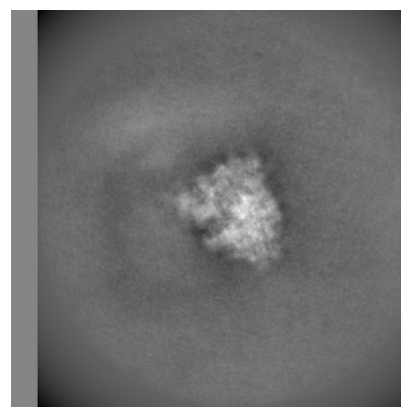
6.1.2 Raw map



X



Y

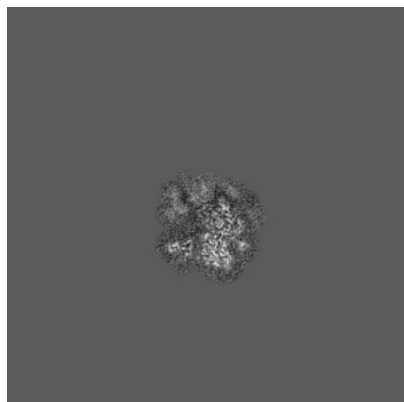


Z

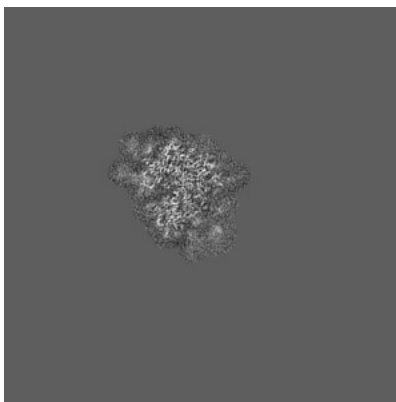
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

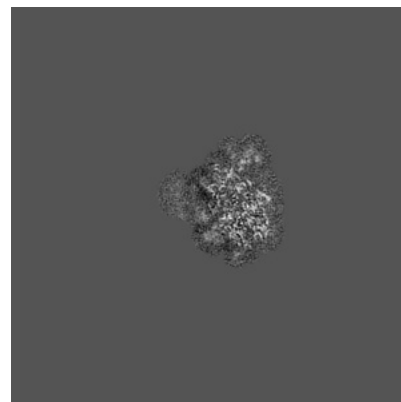
6.2.1 Primary map



X Index: 250

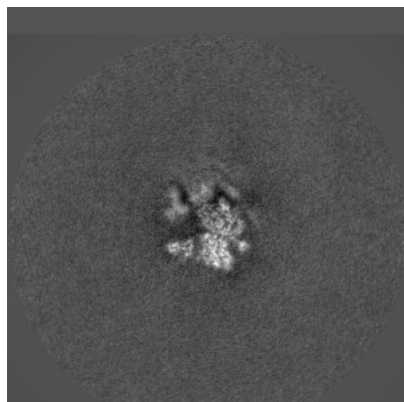


Y Index: 250

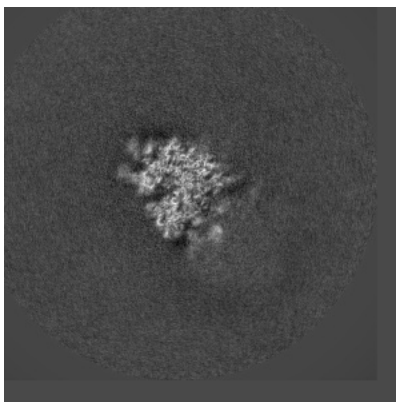


Z Index: 250

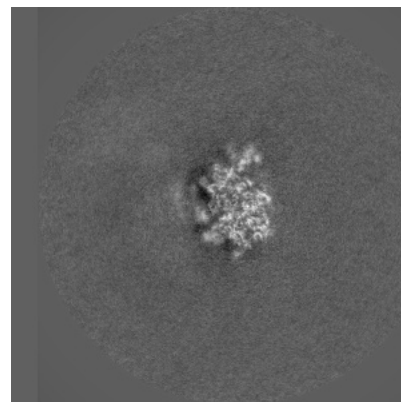
6.2.2 Raw map



X Index: 250



Y Index: 250

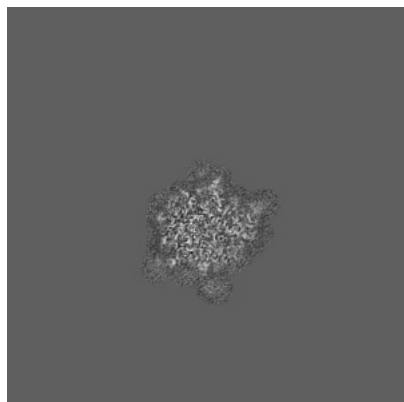


Z Index: 250

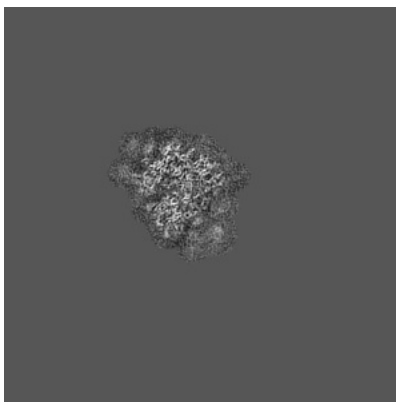
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

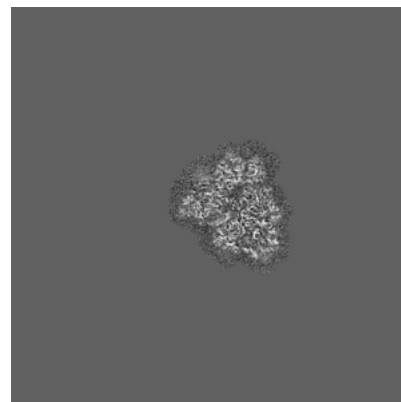
6.3.1 Primary map



X Index: 293

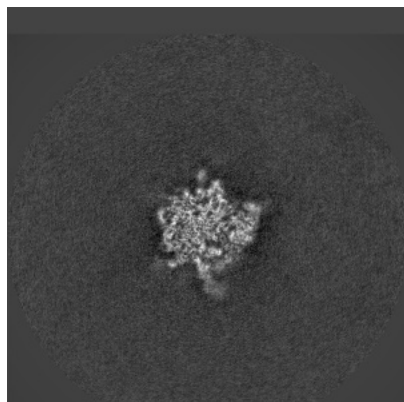


Y Index: 251

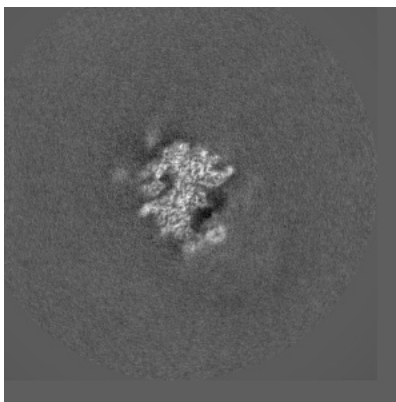


Z Index: 208

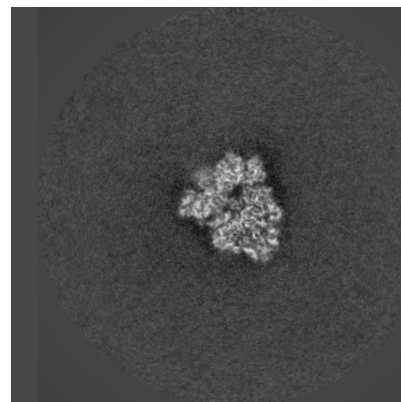
6.3.2 Raw map



X Index: 290



Y Index: 264

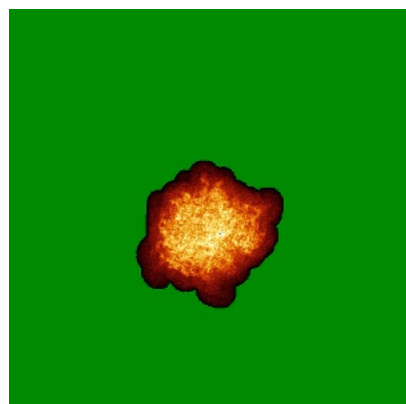


Z Index: 207

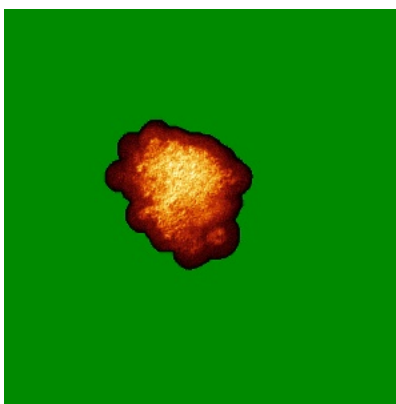
The images above show the largest variance slices of the map in three orthogonal directions.

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

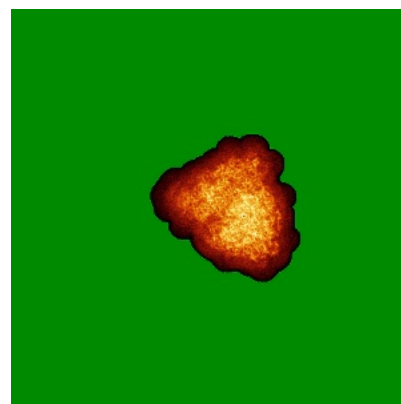
6.4.1 Primary map



X

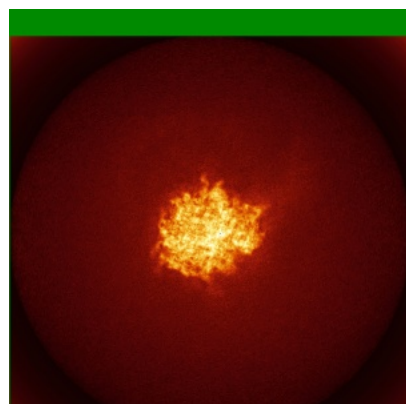


Y

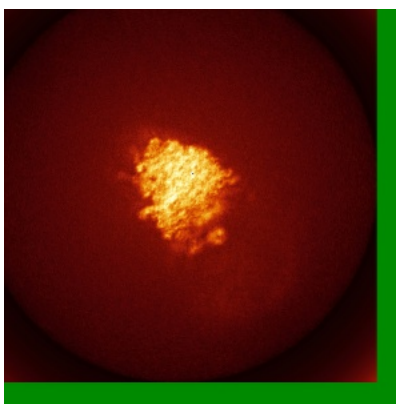


Z

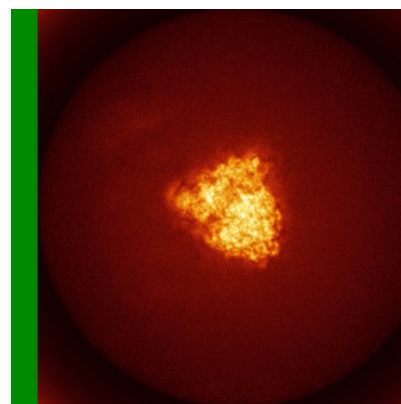
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

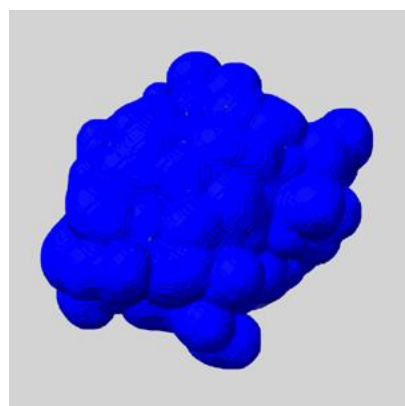
6.6 Mask visualisation [i](#)

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

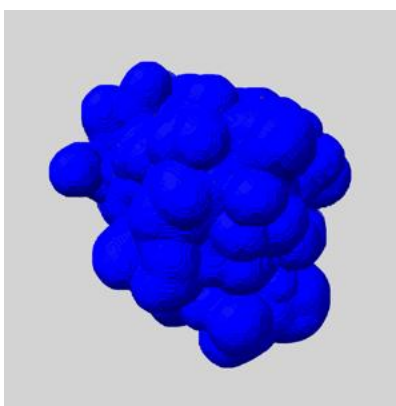
A mask typically either:

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

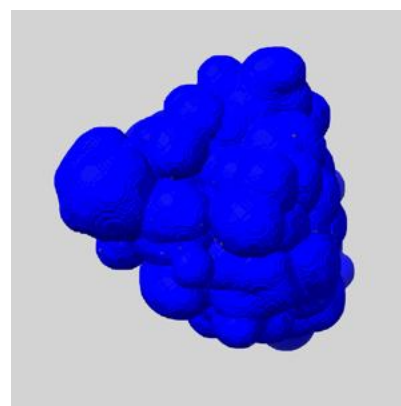
6.6.1 emd_0195_msk_1.map [i](#)



X



Y

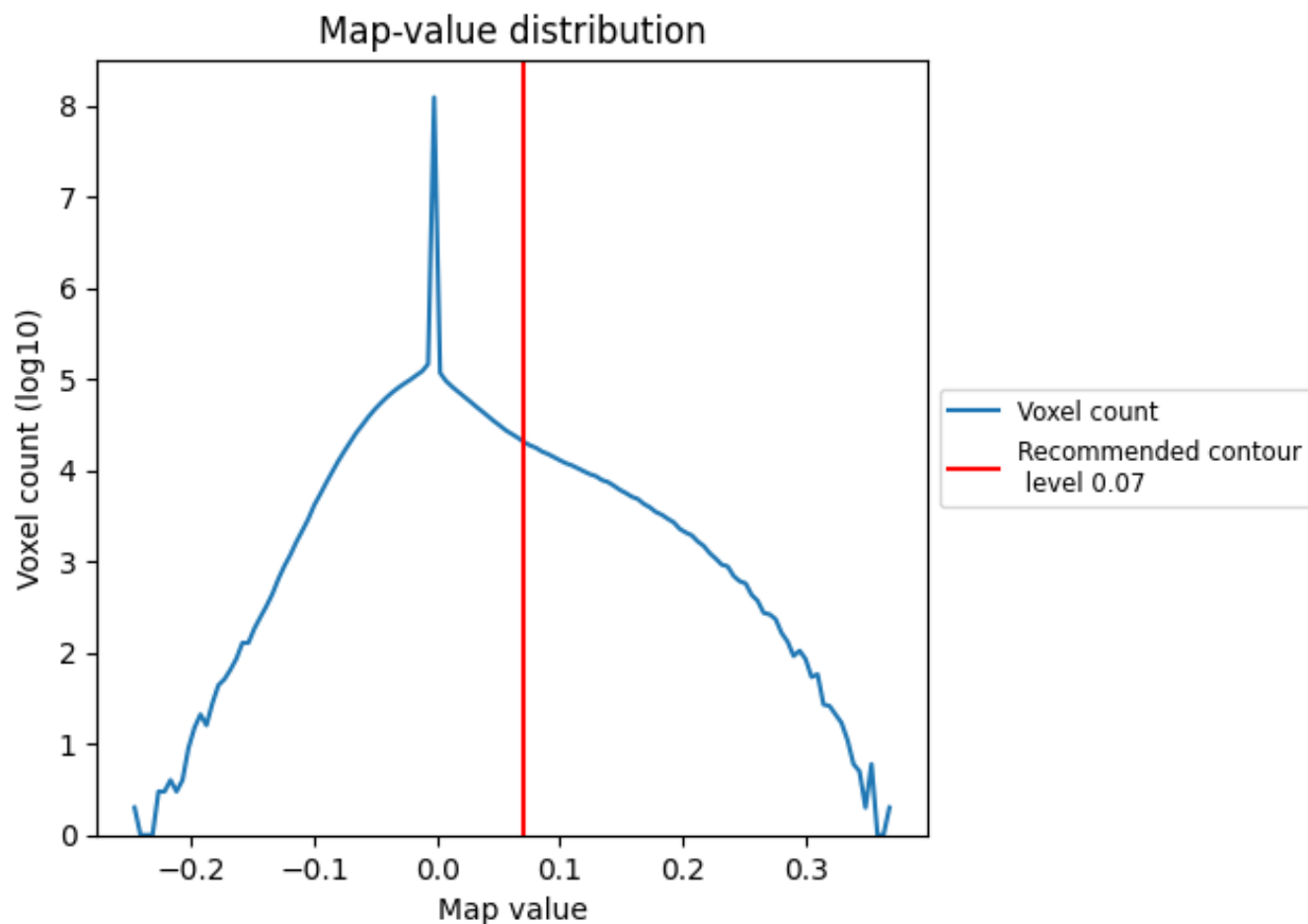


Z

7 Map analysis [i](#)

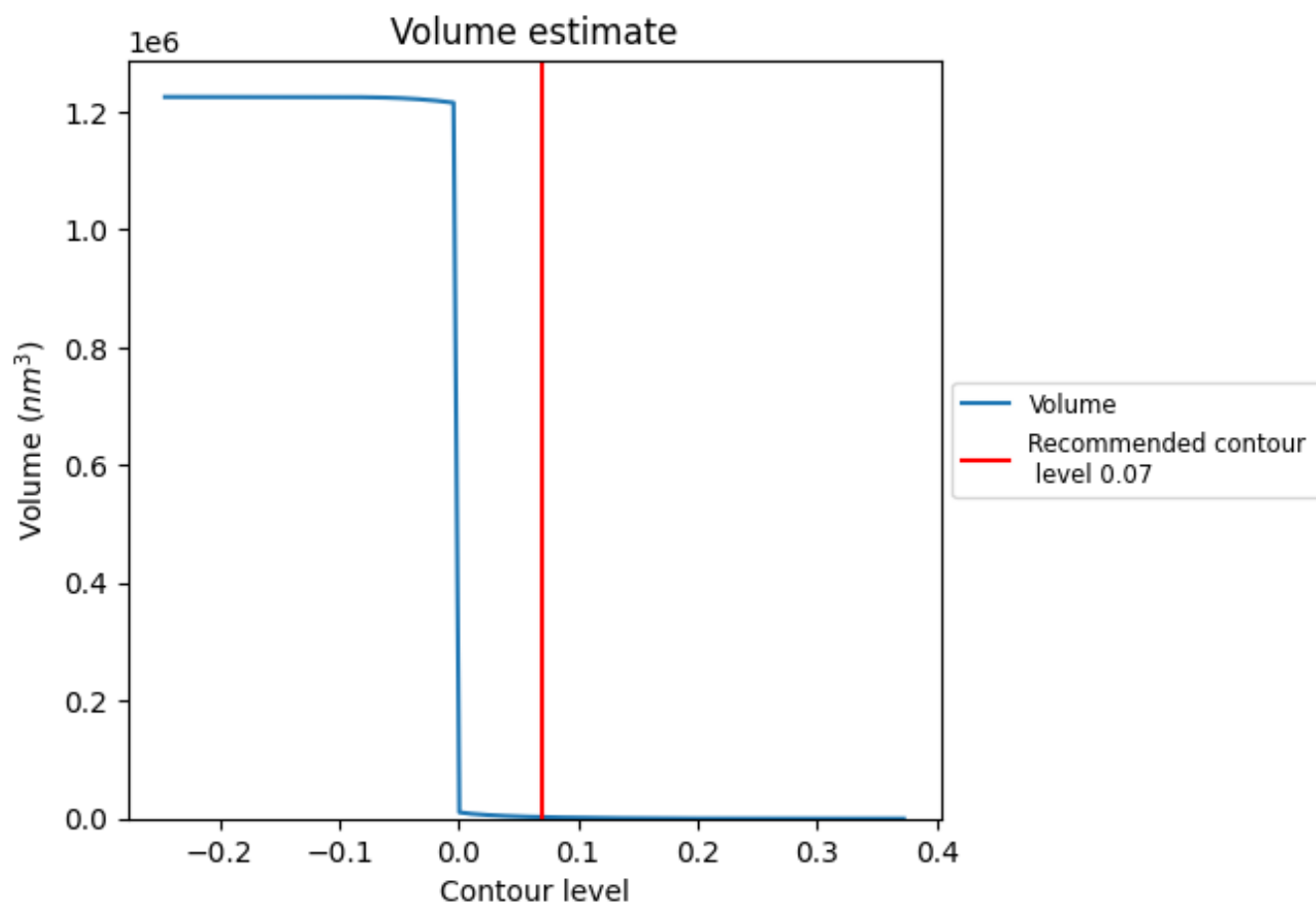
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

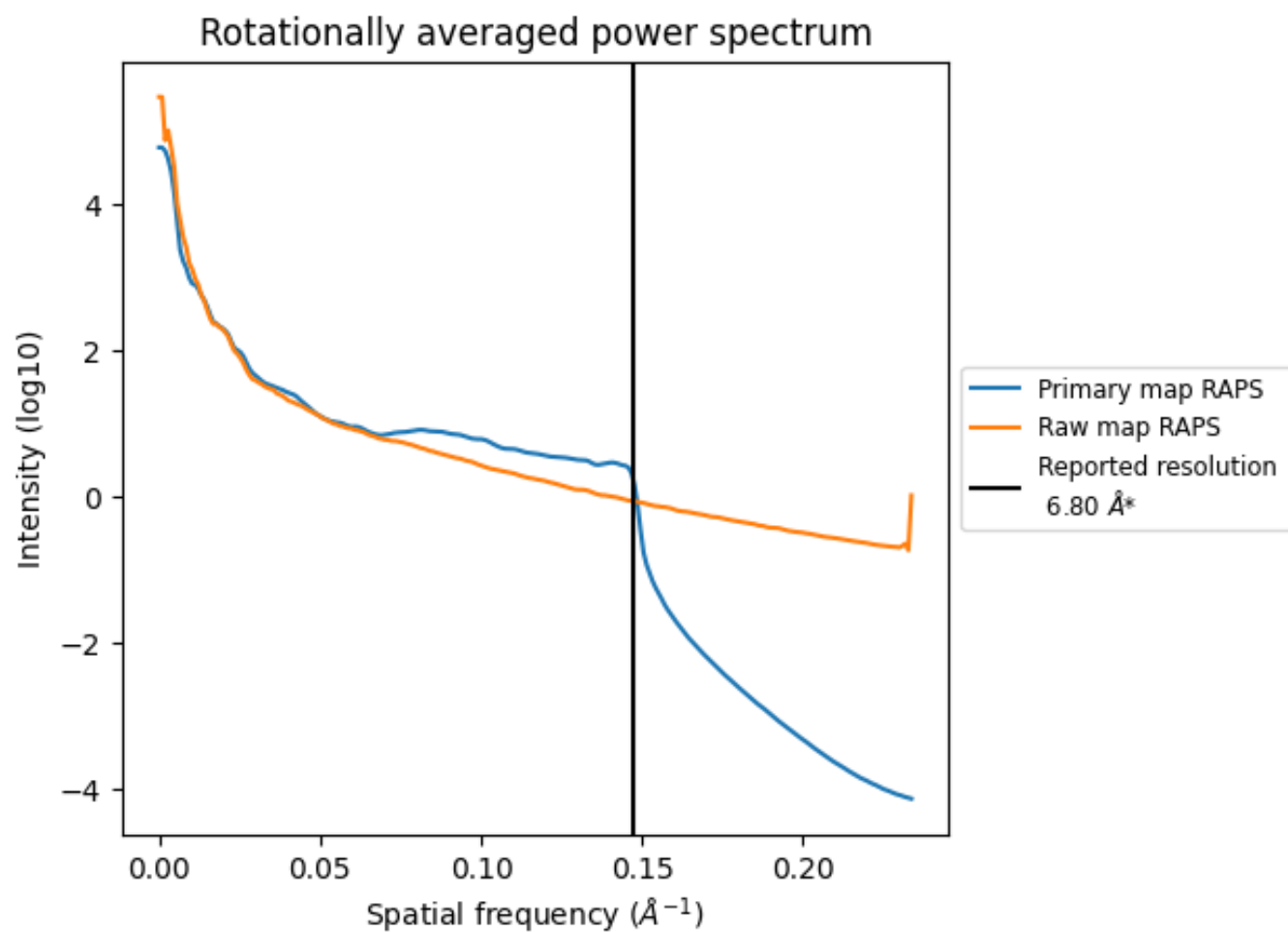
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2563 nm^3 ; this corresponds to an approximate mass of 2315 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

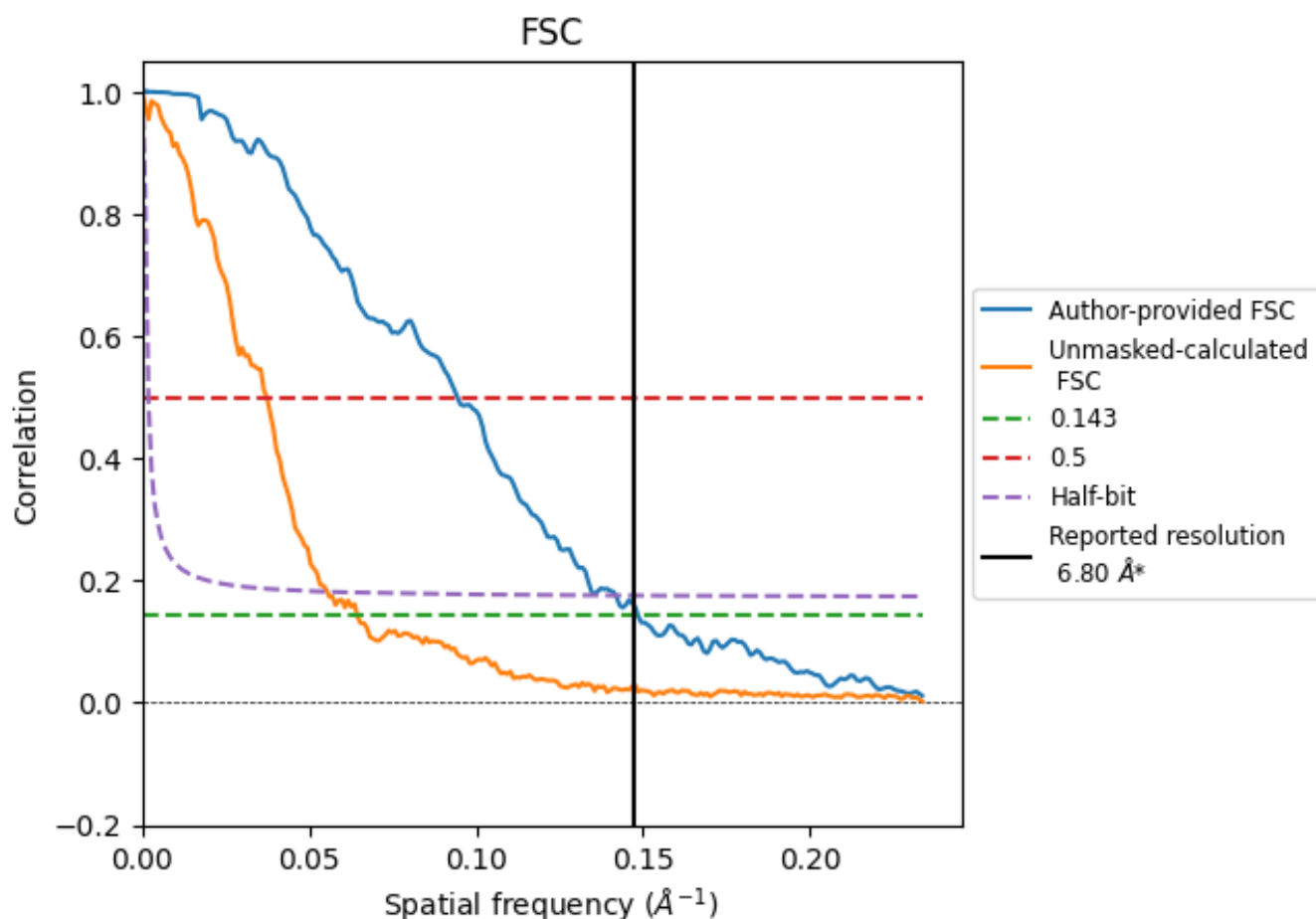


*Reported resolution corresponds to spatial frequency of 0.147 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.147 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

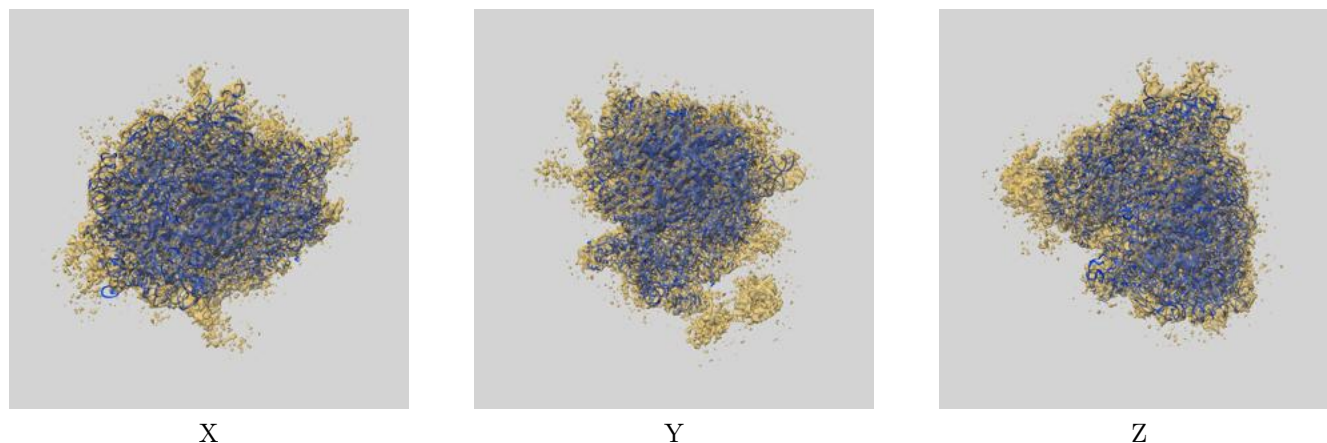
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.80	-	-
Author-provided FSC curve	6.73	10.59	7.05
Unmasked-calculated*	15.53	26.81	18.05

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 15.53 differs from the reported value 6.8 by more than 10 %

9 Map-model fit [i](#)

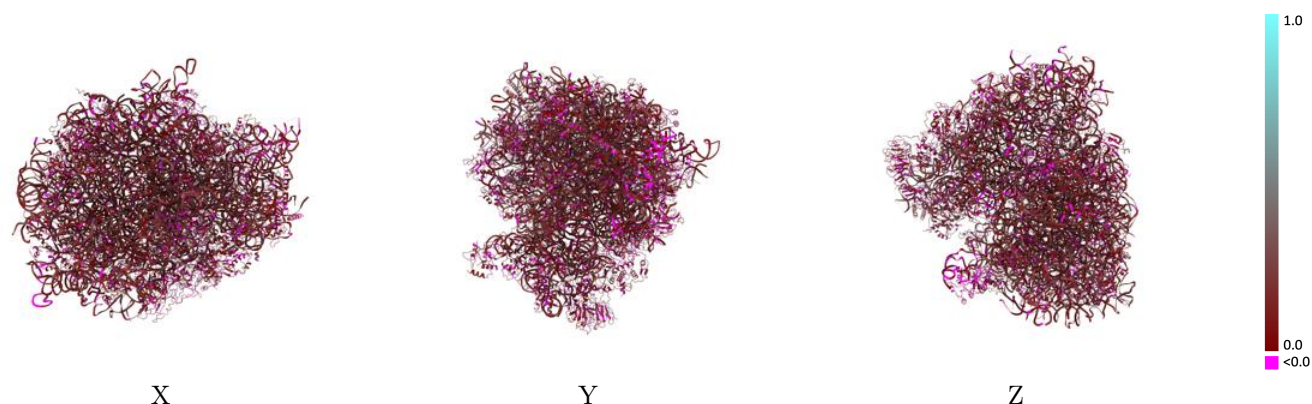
This section contains information regarding the fit between EMDB map EMD-0195 and PDB model 6HCM. Per-residue inclusion information can be found in [section 3](#) on [page 22](#).

9.1 Map-model overlay [i](#)



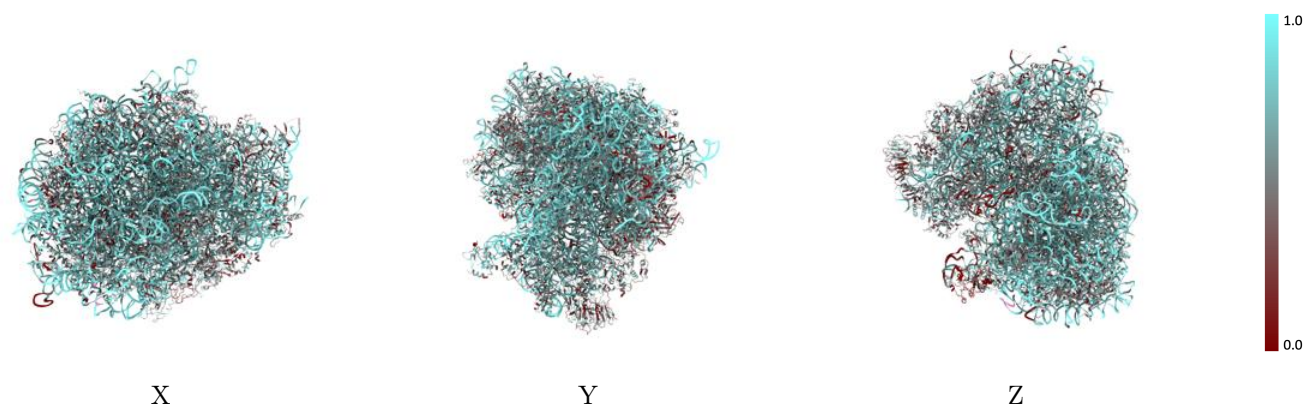
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



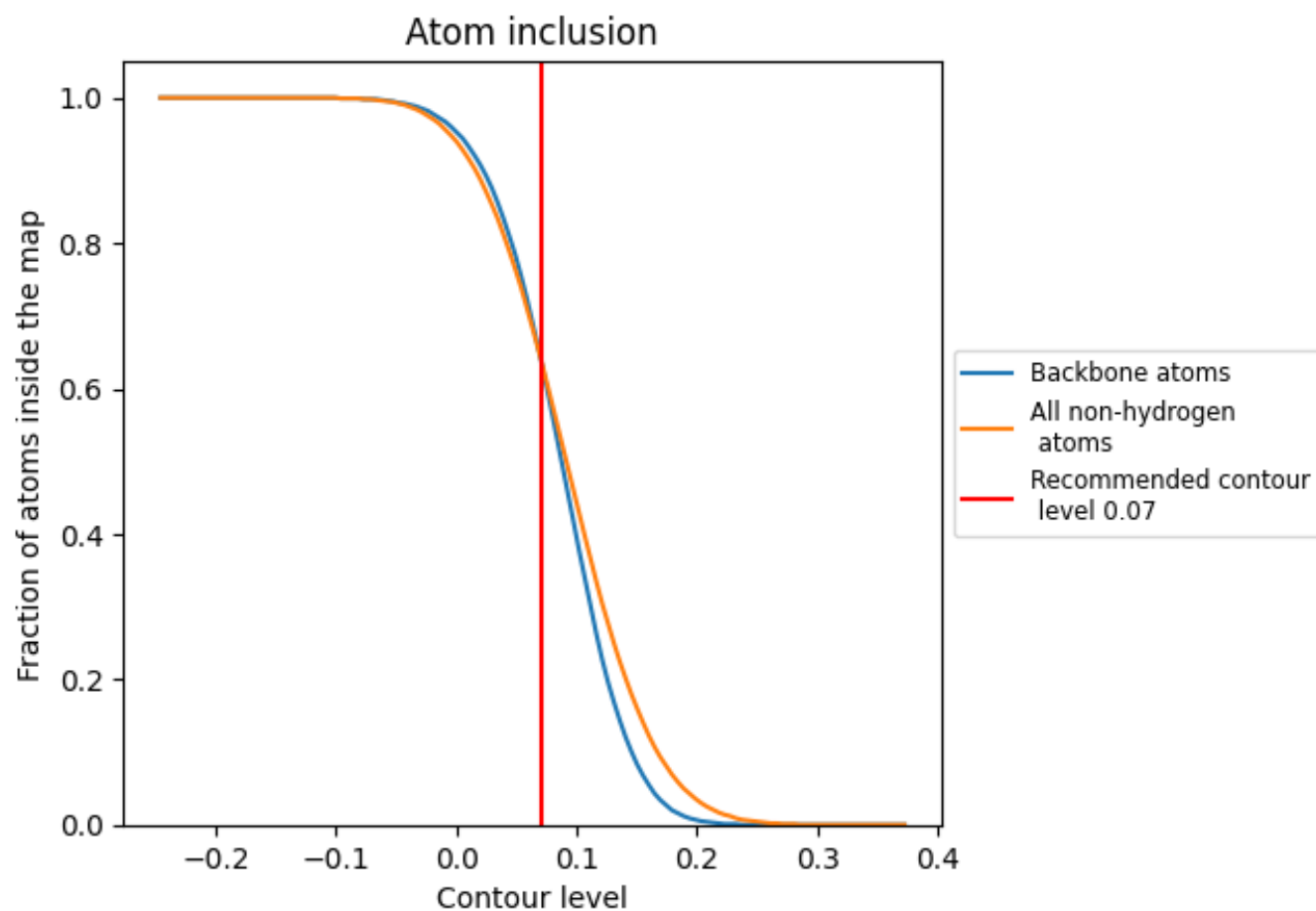
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.07).

9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 64% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6430	 0.1560
1	 0.3820	 0.2540
23	 0.8380	 0.1860
52	 0.7750	 0.1840
72	 0.8570	 0.1930
82	 0.7810	 0.1910
A1	 0.8010	 0.1860
A3	 0.4000	 0.1180
B1	 0.5040	 0.1410
B3	 0.5100	 0.1250
C1	 0.3840	 0.1360
C3	 0.4490	 0.1210
D1	 0.5040	 0.1390
D3	 0.6500	 0.1380
E1	 0.5010	 0.1310
E3	 0.5310	 0.1480
F1	 0.5090	 0.1320
F3	 0.4770	 0.1160
G1	 0.4840	 0.1100
G3	 0.4950	 0.1370
H1	 0.5170	 0.1190
H3	 0.5210	 0.1440
I1	 0.4930	 0.1200
I3	 0.5110	 0.1390
J1	 0.4680	 0.1170
J3	 0.5990	 0.1310
K1	 0.5900	 0.1370
L1	 0.5420	 0.1290
L3	 0.5190	 0.1400
M1	 0.3740	 0.1340
M3	 0.6010	 0.1400
N1	 0.5390	 0.1050
N3	 0.4740	 0.1140
O1	 0.4680	 0.1380
O3	 0.5240	 0.1390



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Chain	Atom inclusion	Q-score
P1	 0.3760	 0.1270
P3	 0.4850	 0.1130
Q1	 0.5750	 0.1100
Q3	 0.4550	 0.1380
R1	 0.4510	 0.1160
R3	 0.4980	 0.0900
S1	 0.4370	 0.1370
S3	 0.5060	 0.1360
T1	 0.5150	 0.1230
T3	 0.5050	 0.1470
U1	 0.5330	 0.1170
U3	 0.5840	 0.1060
V1	 0.4880	 0.1300
V3	 0.4030	 0.1360
W1	 0.4370	 0.1090
W3	 0.4680	 0.0970
X1	 0.4540	 0.1250
X3	 0.4770	 0.1340
Y1	 0.5110	 0.1410
Y3	 0.6080	 0.1250
Z1	 0.6340	 0.1340
Z3	 0.3850	 0.0220
a1	 0.4430	 0.1270
a3	 0.4970	 0.1220
b1	 0.4460	 0.1270
b3	 0.4630	 0.1180
c1	 0.3520	 0.1230
c3	 0.3700	 0.0290
d1	 0.5060	 0.1370
d3	 0.5230	 0.1210
e1	 0.5270	 0.1260
e3	 0.4710	 0.1410
f1	 0.5420	 0.1390
f3	 0.4330	 0.1350
g1	 0.6580	 0.1120
g3	 0.3670	 0.0690
h1	 0.4140	 0.1270
h3	 0.5120	 0.1120
i3	 0.4890	 0.1140
j1	 0.4510	 0.1310
j3	 0.5070	 0.1090
k1	 0.4340	 0.1300

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Chain	Atom inclusion	Q-score
k3	 0.4070	 0.0340
l3	 0.5180	 0.1500
m3	 0.5430	 0.1360
n3	 0.4910	 0.1060
o3	 0.5750	 0.1300
p3	 0.5180	 0.1170
r3	 0.4460	 0.1340
s3	 0.3870	 0.0720
t3	 0.4490	 0.1160
u3	 0.1270	 0.0230
w3	 0.5850	 0.1600