



## Full wwPDB EM Validation Report ⓘ

Apr 21, 2026 – 02:35 pm BST

PDB ID : 9QWT / pdb\_00009qwt  
EMDB ID : EMD-53427  
Title : Mouse Ribosome RPS15 (uS19) P131S rotated-2 PRE state  
Authors : Santo, P.E.; Astier, A.; Plisson-Chastang, C.  
Deposited on : 2025-04-15  
Resolution : 3.10 Å(reported)  
Based on initial model : 7LS1

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

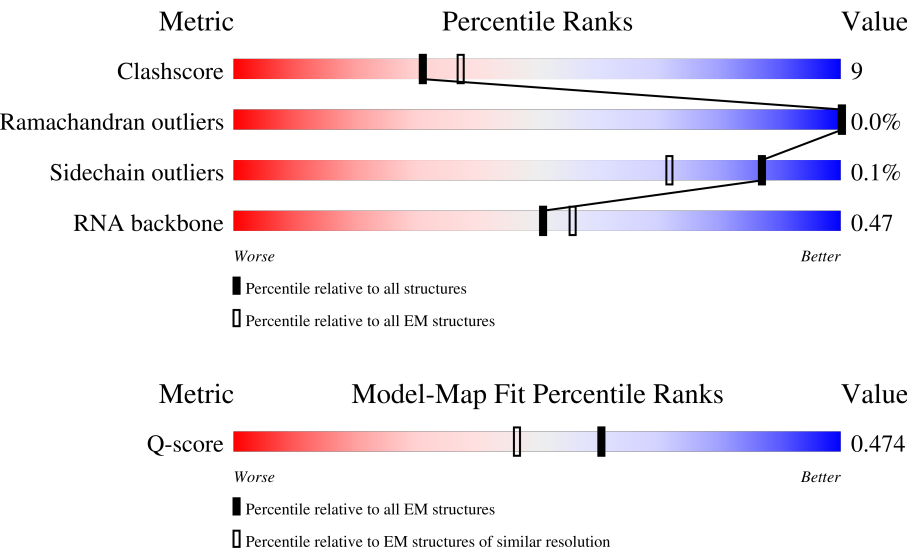
EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.10 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.





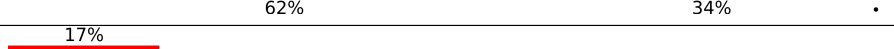




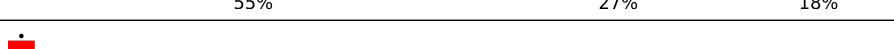



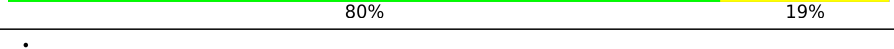

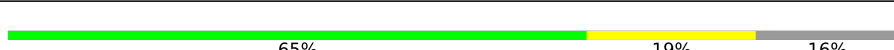

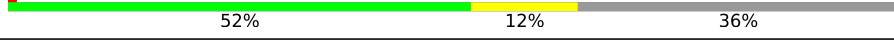
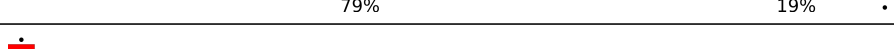







Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14724 ( 2.60 - 3.60 )

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  $\geq 3$ , 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	270	<div><div></div><div>59%</div><div>23%</div><div>18%</div></div>
2	A2	3615	<div><div>7%</div><div>55%</div><div>36%</div><div>6%</div></div>
3	A3	152	<div><div>5%</div><div>57%</div><div>34%</div><div>9%</div></div>

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Mol	Chain	Length	Quality of chain
4	B1	266	
5	B2	121	
6	B3	145	
7	Bv	76	
8	Bx	10	
9	By	22	
10	C1	192	
11	C2	156	
12	C3	119	
13	D1	214	
14	D2	257	
15	D3	83	
16	E1	178	
17	E2	403	
18	E3	142	
19	F1	211	
20	F2	419	
21	F3	114	
22	G1	217	
23	G2	297	
24	G3	69	
25	H1	204	
26	H2	296	
27	H3	56	
28	I2	203	



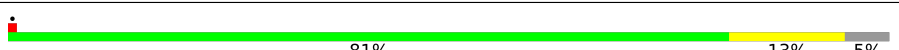
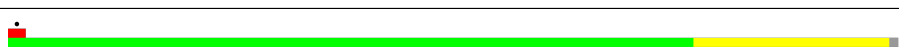

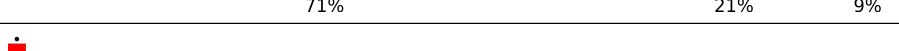
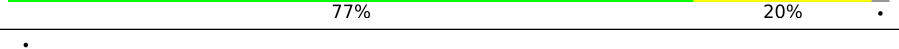





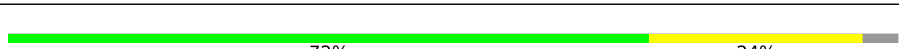


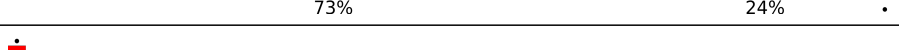

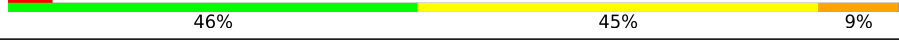






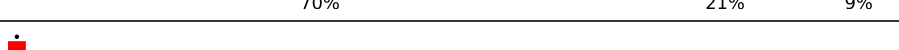
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Mol	Chain	Length	Quality of chain
29	I3	317	
30	J2	184	
31	J3	293	
32	K2	188	
33	K3	249	
34	L2	196	
35	L3	194	
36	M2	176	
37	M3	132	
38	N2	160	
39	N3	151	
40	O2	128	
41	O3	151	
42	P2	140	
43	P3	130	
44	Q2	157	
45	Q3	133	
46	R2	156	
47	R3	125	
48	S2	145	
49	S3	84	
50	T2	136	
51	T3	133	
52	U2	148	
53	V2	160	

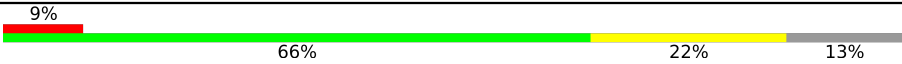
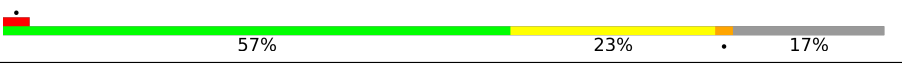
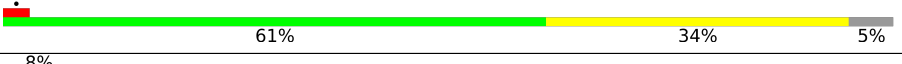

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Mol	Chain	Length	Quality of chain
54	W2	115	
55	X2	125	
56	Y2	135	
57	Z2	110	
58	a2	117	
59	b2	123	
60	c2	105	
61	d2	97	
62	e2	70	
63	f2	51	
64	g2	128	
65	h2	25	
66	i2	105	
67	j2	92	
68	k2	137	
69	m2	1633	
70	n2	73	
71	o2	295	
72	p2	264	
73	q2	242	
74	r2	257	
75	s2	204	
76	t2	194	
77	u2	208	
78	v2	165	

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Mol	Chain	Length	Quality of chain
79	w2	158	
80	x2	145	
81	y2	146	
82	z2	135	

## 2 Entry composition

There are 87 unique types of molecules in this entry. The entry contains 206855 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A1	222	Total	C	N	O	S	0	0
			1843	1185	353	297	8		

- Molecule 2 is a RNA chain called 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A2	3512	Total	C	N	O	P	0	0
			75341	33588	13744	24498	3511		

- Molecule 3 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A3	139	Total	C	N	O	S	0	0
			1154	725	233	195	1		

- Molecule 4 is a protein called Large ribosomal subunit protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B1	217	Total	C	N	O	S	1	0
			1764	1127	340	293	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B2	119	Total	C	N	O	P	0	0
			2538	1132	454	834	118		

- Molecule 6 is a protein called Small ribosomal subunit protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B3	140	Total	C	N	O	S	0	0
			1091	686	210	192	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B3	88	MET	ARG	conflict	UNP Q9CZX8

- Molecule 7 is a RNA chain called transfer RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Bv	66	Total	C	N	O	P	0	0
			1412	629	255	462	66		

- Molecule 8 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Bx	10	Total	C	N	O	P	0	0
			200	90	20	80	10		

- Molecule 9 is a protein called Nascent protein chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	By	22	Total	C	N	O	0	0
			110	66	22	22		

- Molecule 10 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C1	190	Total	C	N	O	S	0	0
			1519	956	284	273	6		

- Molecule 11 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C2	156	Total	C	N	O	P	0	0
			3315	1481	585	1094	155		

- Molecule 12 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	C3	97	Total	C	N	O	S	0	0
			769	483	144	138	4		

- Molecule 13 is a protein called Large ribosomal subunit protein uL16.



Mol	Chain	Residues	Atoms					AltConf	Trace
13	D1	204	Total	C	N	O	S	0	0
			1656	1052	319	272	13		

- Molecule 14 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	D2	245	Total	C	N	O	S	0	0
			1876	1177	383	310	6		

- Molecule 15 is a protein called Small ribosomal subunit protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	D3	83	Total	C	N	O	S	0	0
			589	369	111	104	5		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D3	25	GLY	ALA	conflict	UNP Q9CQR2
D3	41	LYS	ARG	conflict	UNP Q9CQR2
D3	42	VAL	THR	conflict	UNP Q9CQR2
D3	54	ALA	GLY	conflict	UNP Q9CQR2

- Molecule 16 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	E1	174	Total	C	N	O	S	0	0
			1397	880	260	251	6		

- Molecule 17 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	E2	402	Total	C	N	O	S	0	0
			3238	2060	609	555	14		

- Molecule 18 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	E3	139	Total	C	N	O	S	0	0
			1080	682	214	181	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E3	?	-	PRO	deletion	UNP P62267

- Molecule 19 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	F1	203	Total	C	N	O	S	0	0
			1643	1029	339	271	4		

- Molecule 20 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	F2	352	Total	C	N	O	S	0	0
			2823	1776	566	466	15		

- Molecule 21 is a protein called Small ribosomal subunit protein eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	F3	97	Total	C	N	O	S	0	0
			774	481	160	128	5		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F3	?	-	PRO	deletion	UNP P62855
F3	101	PRO	ARG	conflict	UNP P62855

- Molecule 22 is a protein called Large ribosomal subunit protein eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	G1	139	Total	C	N	O	S	0	0
			1143	732	221	183	7		

- Molecule 23 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	G2	293	Total	C	N	O	S	0	0
			2389	1509	441	425	14		

- Molecule 24 is a protein called Small ribosomal subunit protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	G3	56	Total	C	N	O	S	0	0
			435	267	85	81	2		

- Molecule 25 is a protein called Large ribosomal subunit protein eL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	H1	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 26 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	H2	218	Total	C	N	O	S	0	0
			1766	1130	337	295	4		

- Molecule 27 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	H3	51	Total	C	N	O	S	0	0
			427	269	87	66	5		

- Molecule 28 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	I2	198	Total	C	N	O	S	0	0
			1618	1043	316	253	6		

- Molecule 29 is a protein called Small ribosomal subunit protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	I3	234	Total	C	N	O	S	0	0
			1800	1135	318	337	10		

- Molecule 30 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	J2	153	Total	C	N	O	S	0	0
			1242	777	241	215	9		

- Molecule 31 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	J3	217	Total	C	N	O	S	0	0
			1590	1039	276	266	9		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J3	61	MET	ILE	conflict	UNP P25444

- Molecule 32 is a protein called Large ribosomal subunit protein eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	K2	186	Total	C	N	O	S	0	0
			1511	946	313	248	4		

- Molecule 33 is a protein called Small ribosomal subunit protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	K3	211	Total	C	N	O	S	0	0
			1708	1073	342	286	7		

- Molecule 34 is a protein called Large ribosomal subunit protein eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	L2	169	Total	C	N	O	S	0	0
			1408	873	304	222	9		

- Molecule 35 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	L3	179	Total	C	N	O	S	0	0
			1495	953	299	241	2		

- Molecule 36 is a protein called Large ribosomal subunit protein eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	M2	175	Total	C	N	O	S	0	0
			1450	924	283	233	10		

- Molecule 37 is a protein called Small ribosomal subunit protein eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	M3	84	Total	C	N	O	S	0	0
			525	332	97	91	5		

- Molecule 38 is a protein called Large ribosomal subunit protein eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	N2	159	Total	C	N	O	S	0	0
			1299	824	252	217	6		

- Molecule 39 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	N3	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 40 is a protein called Large ribosomal subunit protein eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	O2	101	Total	C	N	O	S	0	0
			825	529	144	150	2		

- Molecule 41 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	O3	135	Total	C	N	O	S	0	0
			1003	615	198	184	6		

- Molecule 42 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	P2	129	Total	C	N	O	S	0	0
			969	613	182	169	5		

- Molecule 43 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	P3	129	Total	C	N	O	S	0	0
			1027	655	192	174	6		

- Molecule 44 is a protein called Large ribosomal subunit protein eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Q2	62	Total	C	N	O	S	0	0
			519	332	101	83	3		

- Molecule 45 is a protein called Small ribosomal subunit protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Q3	121	Total	C	N	O	S	0	0
			981	620	192	164	5		

- Molecule 46 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	R2	118	Total	C	N	O	S	0	0
			967	618	181	167	1		

- Molecule 47 is a protein called Small ribosomal subunit protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	R3	73	Total	C	N	O	S	0	0
			585	374	108	102	1		

- Molecule 48 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	S2	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 49 is a protein called Small ribosomal subunit protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	S3	79	Total	C	N	O	S	0	0
			618	386	115	110	7		

- Molecule 50 is a protein called Large ribosomal subunit protein eL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	T2	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 51 is a protein called Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	T3	44	Total	C	N	O	S	0	0
			355	218	81	55	1		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T3	55	PRO	ASN	conflict	UNP P62862
T3	56	ASN	VAL	conflict	UNP P62862
T3	57	ALA	VAL	conflict	UNP P62862

- Molecule 52 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	U2	147	Total	C	N	O	S	0	0
			1164	736	239	185	4		

- Molecule 53 is a protein called Large ribosomal subunit protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	V2	117	Total	C	N	O	S	0	0
			945	596	198	146	5		

- Molecule 54 is a protein called Large ribosomal subunit protein eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	W2	94	Total	C	N	O	S	0	0
			732	465	130	131	6		

- Molecule 55 is a protein called Large ribosomal subunit protein eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	X2	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 56 is a protein called Large ribosomal subunit protein eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	Y2	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 57 is a protein called Large ribosomal subunit protein eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Z2	109	Total	C	N	O	S	0	0
			876	555	174	143	4		

- Molecule 58 is a protein called Large ribosomal subunit protein eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	a2	107	Total	C	N	O	S	0	0
			854	535	176	137	6		

- Molecule 59 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	b2	120	Total	C	N	O	S	0	0
			1001	634	201	165	1		

- Molecule 60 is a protein called Large ribosomal subunit protein eL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	c2	102	Total	C	N	O	S	0	0
			832	521	177	129	5		

- Molecule 61 is a protein called Large ribosomal subunit protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	d2	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 62 is a protein called Large ribosomal subunit protein eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	e2	69	Total	C	N	O	S	0	0
			568	365	103	99	1		

- Molecule 63 is a protein called Large ribosomal subunit protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	f2	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 64 is a protein called Ubiquitin-ribosomal protein eL40 fusion protein.



Mol	Chain	Residues	Atoms					AltConf	Trace
64	g2	52	Total	C	N	O	S	0	0
			429	266	90	67	6		

- Molecule 65 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	h2	24	Total	C	N	O	S	0	0
			230	139	62	26	3		

- Molecule 66 is a protein called Large ribosomal subunit protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	i2	103	Total	C	N	O	S	0	0
			842	528	172	136	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
i2	?	-	GLN	deletion	UNP P83882

- Molecule 67 is a protein called Large ribosomal subunit protein eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	j2	89	Total	C	N	O	S	0	0
			694	436	133	118	7		

- Molecule 68 is a protein called Large ribosomal subunit protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	k2	125	Total	C	N	O	S	0	0
			1001	621	207	168	5		

- Molecule 69 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	m2	1623	Total	C	N	O	P	0	0
			34685	15498	6234	11330	1623		

- Molecule 70 is a RNA chain called transfer RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	n2	73	Total	C	N	O	P	0	0
			1562	698	291	501	72		

- Molecule 71 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	o2	215	Total	C	N	O	S	0	0
			1704	1083	298	315	8		

- Molecule 72 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	p2	212	Total	C	N	O	S	0	0
			1722	1093	308	307	14		

- Molecule 73 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	q2	213	Total	C	N	O	S	0	0
			1655	1056	301	291	7		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
q2	195	THR	SER	conflict	UNP P62908
q2	?	-	ASP	deletion	UNP P62908

- Molecule 74 is a protein called Small ribosomal subunit protein eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	r2	257	Total	C	N	O	S	0	0
			2031	1298	381	344	8		

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
r2	46	VAL	ILE	conflict	UNP P62702
r2	78	VAL	THR	conflict	UNP P62702
r2	80	VAL	ILE	conflict	UNP P62702
r2	93	GLU	ASP	conflict	UNP P62702
r2	98	HIS	ASN	conflict	UNP P62702
r2	102	VAL	ILE	conflict	UNP P62702

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Chain	Residue	Modelled	Actual	Comment	Reference
r2	116	VAL	PRO	conflict	UNP P62702
r2	130	THR	PHE	conflict	UNP P62702
r2	133	VAL	THR	conflict	UNP P62702
r2	153	VAL	LEU	conflict	UNP P62702
r2	160	VAL	ILE	conflict	UNP P62702
r2	165	GLY	GLU	conflict	UNP P62702
r2	170	ILE	THR	conflict	UNP P62702
r2	171	ASN	ASP	conflict	UNP P62702
r2	184	ILE	THR	conflict	UNP P62702
r2	192	VAL	ILE	conflict	UNP P62702
r2	230	ASN	LYS	conflict	UNP P62702
r2	248	VAL	ILE	conflict	UNP P62702
r2	258	THR	ALA	conflict	UNP P62702

- Molecule 75 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	s2	185	Total	C	N	O	S	0	0
			1468	919	277	265	7		

- Molecule 76 is a protein called Small ribosomal subunit protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	t2	174	Total	C	N	O	S	0	0
			1322	857	246	218	1		

- Molecule 77 is a protein called Small ribosomal subunit protein eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	u2	179	Total	C	N	O	S	0	0
			1397	879	274	239	5		

- Molecule 78 is a protein called Small ribosomal subunit protein eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	v2	83	Total	C	N	O	S	0	0
			705	462	122	115	6		

- Molecule 79 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	w2	138	Total	C	N	O	S	0	0
			1134	722	214	192	6		

- Molecule 80 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	x2	120	Total	C	N	O	S	0	0
			999	635	188	169	7		

- Molecule 81 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	y2	139	Total	C	N	O	S	0	0
			1109	704	210	192	3		

- Molecule 82 is a protein called Small ribosomal subunit protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	z2	125	Total	C	N	O	S	0	0
			1011	634	187	186	4		

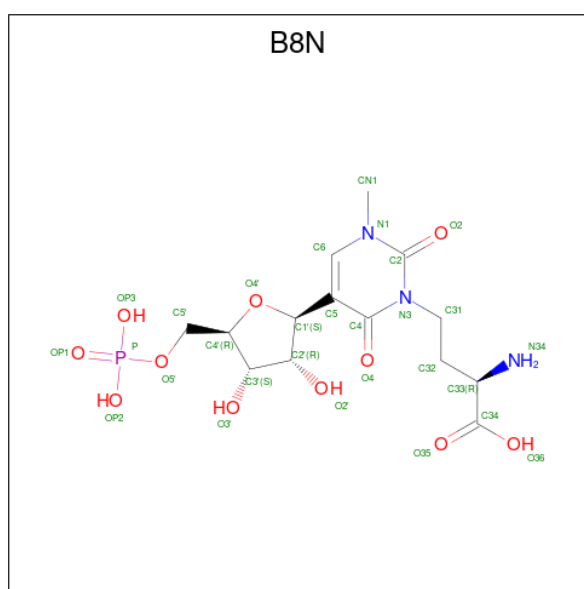
- Molecule 83 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
83	A2	84	Total	Mg	0
			84	84	
83	E3	1	Total	Mg	0
			1	1	
83	H1	1	Total	Mg	0
			1	1	
83	P2	1	Total	Mg	0
			1	1	
83	d2	1	Total	Mg	0
			1	1	
83	m2	35	Total	Mg	0
			35	35	

- Molecule 84 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

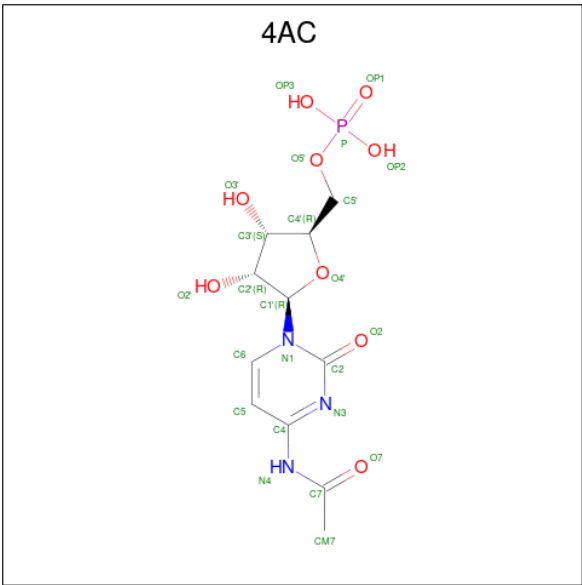
Mol	Chain	Residues	Atoms		AltConf
84	F3	1	Total	Zn	0
			1	1	
84	H3	1	Total	Zn	0
			1	1	
84	d2	1	Total	Zn	0
			1	1	
84	g2	1	Total	Zn	0
			1	1	
84	i2	1	Total	Zn	0
			1	1	
84	j2	1	Total	Zn	0
			1	1	

- Molecule 85 is (2 {R})-2-azanyl-4-[5-[(2 {S},3 {R},4 {S},5 {R})-3,4-bis(oxidanyl)-5-(phosphonoxymethyl)oxolan-2-yl]-3-methyl-2,6-bis(oxidanylidene)pyrimidin-1-yl]butanoic acid (CCD ID: B8N) (formula: C<sub>14</sub>H<sub>22</sub>N<sub>3</sub>O<sub>11</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
85	m2	1	Total	C	N	O	P	0
			28	14	3	10	1	

- Molecule 86 is N(4)-ACETILCYTIDINE-5'-MONOPHOSPHATE (CCD ID: 4AC) (formula: C<sub>11</sub>H<sub>16</sub>N<sub>3</sub>O<sub>9</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
86	m2	1	Total	C	N	O	P	0
			23	11	3	8	1	

- Molecule 87 is water.

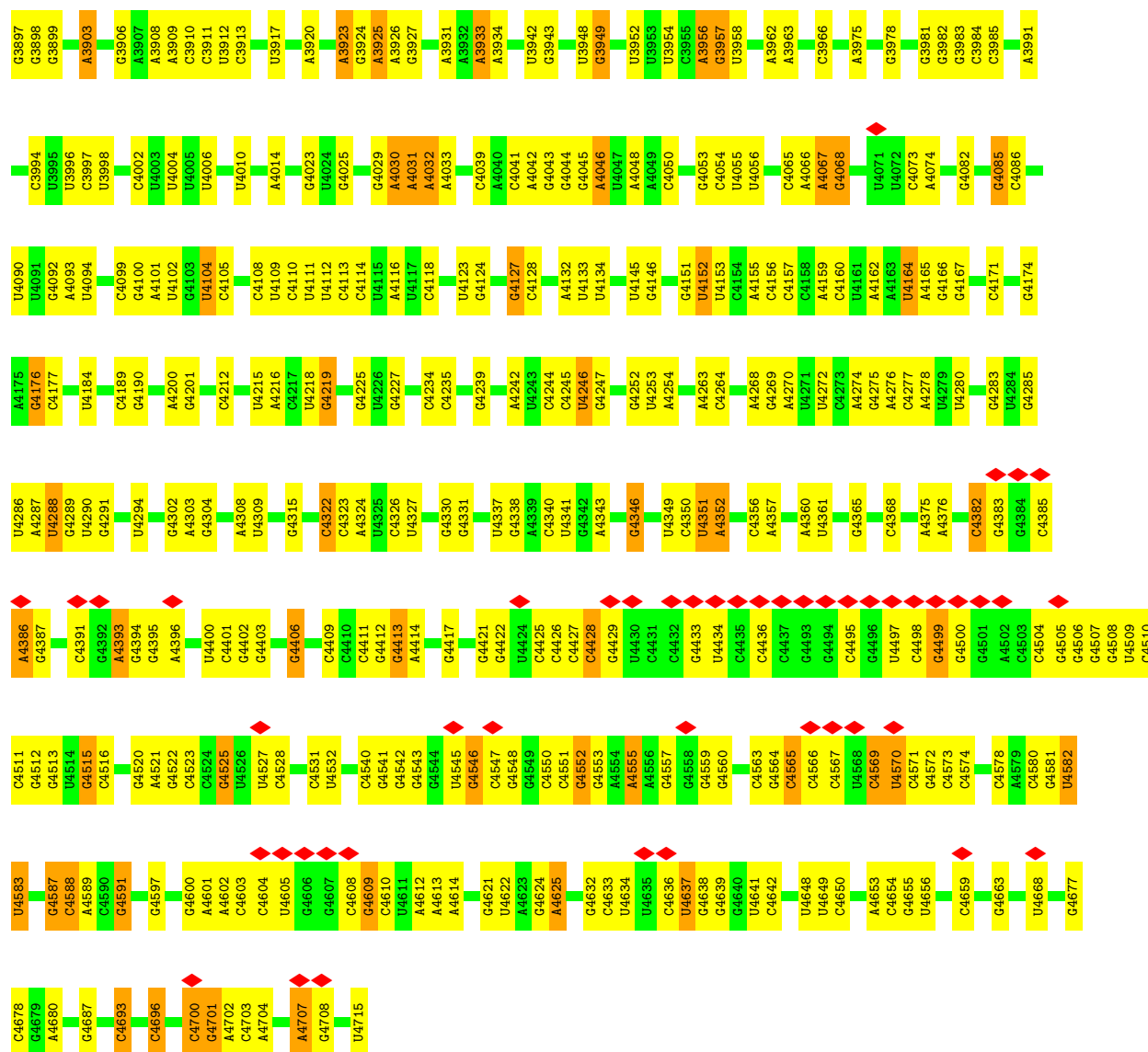
Mol	Chain	Residues	Atoms		AltConf
87	B1	1	Total	O	0
			1	1	



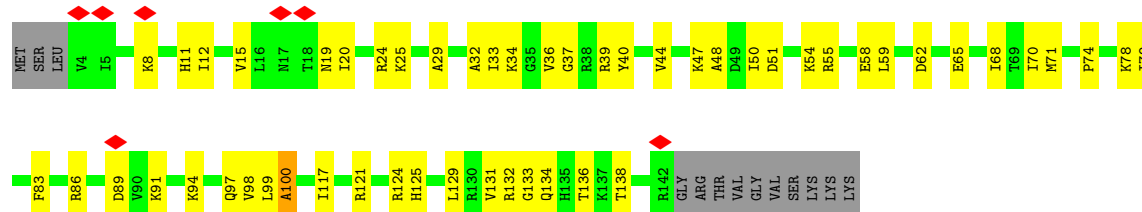




G	A3712	A3713	G	G3715	U3719	U3720	U3721	C3722	A3723	G3726	G3731	G3732	A3735	G3736	G3737	G3738	G3739	G3740	G3743	G3744	G3745	G3746	G3747	A	G	C	C	C	C	G	A3864	A3865	A3866	A3871	A3872	A3873	G3874	U3881	A3885	A3886	G3887	G3888	G3889	A3891	G3892	C3893	U3894	A3895																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
G	A3712	U3713	C	G3715	U3719	U3720	U3721	C3722	A3723	G3726	G3731	G3732	A3735	G3736	G3737	G3738	G3739	G3740	G3743	G3744	G3745	G3746	G3747	A	G	C	C	C	C	G	A3864	A3865	A3866	A3871	A3872	A3873	G3874	U3881	A3885	A3886	G3887	G3888	G3889	A3891	G3892	C3893	U3894	A3895																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
G3600	A3601	C3604	A3605	U3606	G3607	A3608	G3609	A3610	G3611	G3612	U3613	U3614	A	A	A	U	A	A	A	U	U	G	G	G	G	G	G	G	C	G	A3699	U3700	A3706	C3707	U3708	C3709	U3710	C3711	A3605	A3606	A3607	A3608	A3609	A3610	A3611	A3612	A3613	A3614	A3615																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
A3527	A3528	G3529	G3530	G3531	A3532	A3533	G3534	G3535	G3536	G3537	C3543	G3544	U3548	C3549	G3552	G3553	G3556	A3557	G3560	A3561	A3562	G3563	A3564	G3565	G3566	G3567	U3568	G3569	U3570	U3571	G3572	A3573	G3574	C3575	U3576	U3577	G3578	A3579	C3580	G3585	U3586	C3587	U3588	G3589	G3590	C3591	A3592	C3593	G3594	G3595	A3598	A3599																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
A3422	C3423	U3424	C3425	U3426	U3429	A3430	A3431	G3432	G3433	A3439	A3440	A3441	U3442	A3455	U3458	G3466	G3467	U3470	A3473	U3474	G3475	U3478	G3479	U3494	G3495	U3496	C3499	U3500	A3501	C3502	C3503	U3504	A3505	C3506	U3507	A3508	A3512	G3515	A3516	A3517	A3518	A3521	C3522	A3523	G3524	A3527	A3528	A3529	A3530	A3531	A3532	A3533	A3534	A3535	A3536	A3537	A3538	A3539	A3540	A3541	A3542	A3543	A3544	A3545	A3546	A3547	A3548	A3549	A3550	A3551	A3552	A3553	A3554	A3555	A3556	A3557	A3558	A3559	A3560	A3561	A3562	A3563	A3564	A3565	A3566	A3567	A3568	A3569	A3570	A3571	A3572	A3573	A3574	A3575	A3576	A3577	A3578	A3579	A3580	A3581	A3582	A3583	A3584	A3585	A3586	A3587	A3588	A3589	A3590	A3591	A3592	A3593	A3594	A3595	A3596	A3597	A3598	A3599	A3600	A3601	A3602	A3603	A3604	A3605	A3606	A3607	A3608	A3609	A3610	A3611	A3612	A3613	A3614	A3615	A3616	A3617	A3618	A3619	A3620	A3621	A3622	A3623	A3624	A3625	A3626	A3627	A3628	A3629	A3630	A3631	A3632	A3633	A3634	A3635	A3636	A3637	A3638	A3639	A3640	A3641	A3642	A3643	A3644	A3645	A3646	A3647	A3648	A3649	A3650	A3651	A3652	A3653	A3654	A3655	A3656	A3657	A3658	A3659	A3660	A3661	A3662	A3663	A3664	A3665	A3666	A3667	A3668	A3669	A3670	A3671	A3672	A3673	A3674	A3675	A3676	A3677	A3678	A3679	A3680	A3681	A3682	A3683	A3684	A3685	A3686	A3687	A3688	A3689	A3690	A3691	A3692	A3693	A3694	A3695	A3696	A3697	A3698	A3699	A3700	A3701	A3702	A3703	A3704	A3705	A3706	A3707	A3708	A3709	A3710	A3711	A3712	A3713	A3714	A3715	A3716	A3717	A3718	A3719	A3720	A3721	A3722	A3723	A3724	A3725	A3726	A3727	A3728	A3729	A3730	A3731	A3732	A3733	A3734	A3735	A3736	A3737	A3738	A3739	A3740	A3741	A3742	A3743	A3744	A3745	A3746	A3747	A3748	A3749	A3750	A3751	A3752	A3753	A3754	A3755	A3756	A3757	A3758	A3759	A3760	A3761	A3762	A3763	A3764	A3765	A3766	A3767	A3768	A3769	A3770	A3771	A3772	A3773	A3774	A3775	A3776	A3777	A3778	A3779	A3780	A3781	A3782	A3783	A3784	A3785	A3786	A3787	A3788	A3789	A3790	A3791	A3792	A3793	A3794	A3795	A3796	A3797	A3798	A3799	A3800	A3801	A3802	A3803	A3804	A3805	A3806	A3807	A3808	A3809	A3810	A3811	A3812	A3813	A3814	A3815	A3816	A3817	A3818	A3819	A3820	A3821	A3822	A3823	A3824	A3825	A3826	A3827	A3828	A3829	A3830	A3831	A3832	A3833	A3834	A3835	A3836	A3837	A3838	A3839	A3840	A3841	A3842	A3843	A3844	A3845	A3846	A3847	A3848	A3849	A3850	A3851	A3852	A3853	A3854	A3855	A3856	A3857	A3858	A3859	A3860	A3861	A3862	A3863	A3864	A3865	A3866	A3867	A3868	A3869	A3870	A3871	A3872	A3873	A3874	A3875	A3876	A3877	A3878	A3879	A3880	A3881	A3882	A3883	A3884	A3885	A3886	A3887	A3888	A3889	A3890	A3891	A3892	A3893	A3894	A3895	A3896	A3897	A3898	A3899	A3900	A3901	A3902	A3903	A3904	A3905	A3906	A3907	A3908	A3909	A3910	A3911	A3912	A3913	A3914	A3915	A3916	A3917	A3918	A3919	A3920	A3921	A3922	A3923	A3924	A3925	A3926	A3927	A3928	A3929	A3930	A3931	A3932	A3933	A3934	A3935	A3936	A3937	A3938	A3939	A3940	A3941	A3942	A3943	A3944	A3945	A3946	A3947	A3948	A3949	A3950	A3951	A3952	A3953	A3954	A3955	A3956	A3957	A3958	A3959	A3960	A3961	A3962	A3963	A3964	A3965	A3966	A3967	A3968	A3969	A3970	A3971	A3972	A3973	A3974	A3975	A3976	A3977	A3978	A3979	A3980	A3981	A3982	A3983	A3984	A3985	A3986	A3987	A3988	A3989	A3990	A3991	A3992	A3993	A3994	A3995	A3996	A3997	A3998	A3999	A4000	A4001	A4002	A4003	A4004	A4005	A4006	A4007	A4008	A4009	A4010	A4011	A4012	A4013	A4014	A4015	A4016	A4017	A4018	A4019	A4020	A4021	A4022	A4023	A4024	A4025	A4026	A4027	A4028	A4029	A4030	A4031	A4032	A4033	A4034	A4035	A4036	A4037	A4038	A4039	A4040	A4041	A4042	A4043	A4044	A4045	A4046	A4047	A4048	A4049	A4050	A4051	A4052	A4053	A4054	A4055	A4056	A4057	A4058	A4059	A4060	A4061	A4062	A4063	A4064	A4065	A4066	A4067	A4068	A4069	A4070	A4071	A4072	A4073	A4074	A4075	A4076	A4077	A4078	A4079	A4080	A4081	A4082	A4083	A4084	A4085	A4086	A4087	A4088	A4089	A4090	A4091	A4092	A4093	A4094	A4095	A4096	A4097	A4098	A4099	A4100	A4101	A4102	A4103	A4104	A4105	A4106	A4107	A4108	A4109	A4110	A4111	A4112	A4113	A4114	A4115	A4116	A4117	A4118	A4119	A4120	A4121	A4122	A4123	A4124	A4125	A4126	A4127	A4128	A4129	A4130	A4131	A4132	A4133	A4134	A4135	A4136	A4137	A4138	A4139	A4140	A4141	A4142	A4143	A4144	A4145	A4146	A4147	A4148	A4149	A4150	A4151	A4152	A4153	A4154	A4155	A4156	A4157	A4158	A4159	A4160	A4161	A4162	A4163	A4164	A4165	A4166	A4167	A4168	A4169	A4170	A4171	A4172	A4173	A4174	A4175	A4176	A4177	A4178	A4179	A4180	A4181	A4182	A4183	A4184	A4185	A4186	A4187	A4188	A4189	A4190	A4191	A4192	A4193	A4194	A4195	A4196	A4197	A4198	A4199	A4200	A4201	A4202	A4203	A4204	A4205	A4206	A4207	A4208	A4209	A4210	A4211	A4212	A4213	A4214	A4215	A4216	A4217	A4218	A4219	A4220	A4221	A4222	A4223	A4224	A4225	A4226	A4227	A4228	A4229	A4230	A4231	A4232	A4233	A4234	A4235	A4236	A4237	A4238	A4239	A4240	A4241	A4242	A4243	A4244	A4245	A4246	A4247	A4248	A4249	A4250	A4251	A4252	A4253	A4254	A4255	A4256	A4257	A4258	A4259	A4260	A4261	A4262	A4263	A4264	A4265	A4266	A4267	A4268	A4269	A4270	A4271	A4272	A4273	A4274	A4275	A4276	A4277	A4278	A4279	A4280	A4281	A4282	A4283	A4284	A4285	A4286	A4287	A4288	A4289	A4290	A4291	A4292	A4293	A4294	A4295	A4296	A4297	A4298	A4299	A4300	A4301	A4302	A4303	A4304	A4305	A4306	A4307	A4308	A4309	A4310	A4311	A4312	A4313	A4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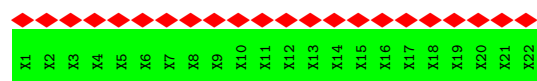
- Molecule 3: Small ribosomal subunit protein uS13



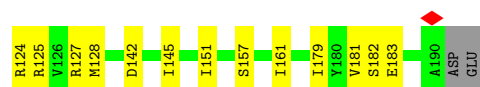
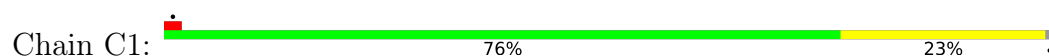
- Molecule 4: Large ribosomal subunit protein eL8



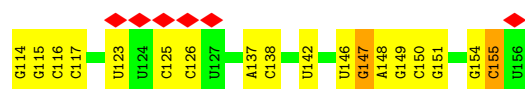
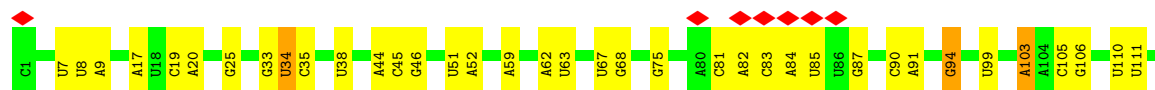




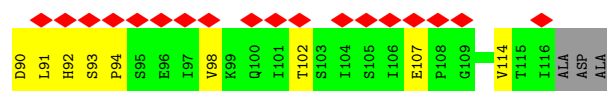
- Molecule 10: Large ribosomal subunit protein uL6



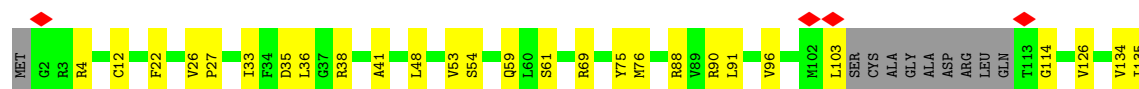
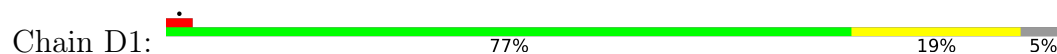
- Molecule 11: 5.8S ribosomal RNA




- Molecule 12: Small ribosomal subunit protein uS10

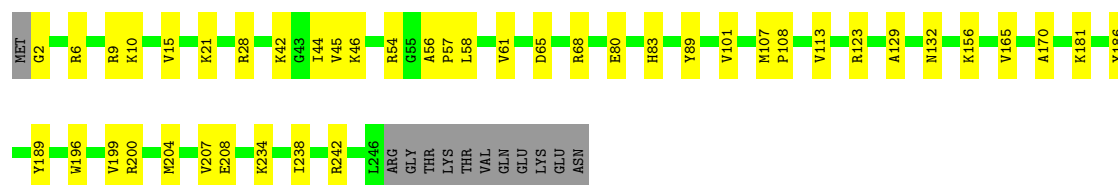


- Molecule 13: Large ribosomal subunit protein uL16




- Molecule 14: Large ribosomal subunit protein uL2

Chain D2:  79% 17% 5%




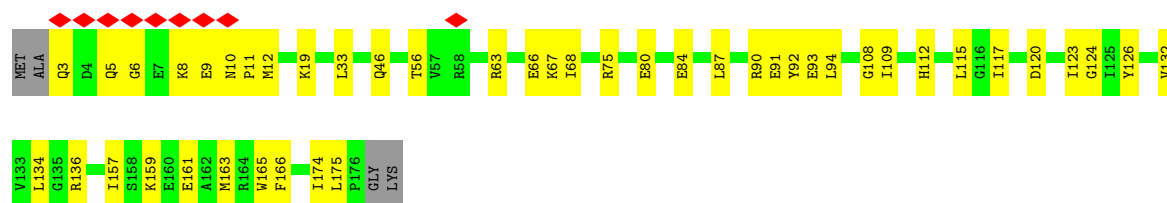
- Molecule 15: Small ribosomal subunit protein eS21

Chain D3:  78% 22%




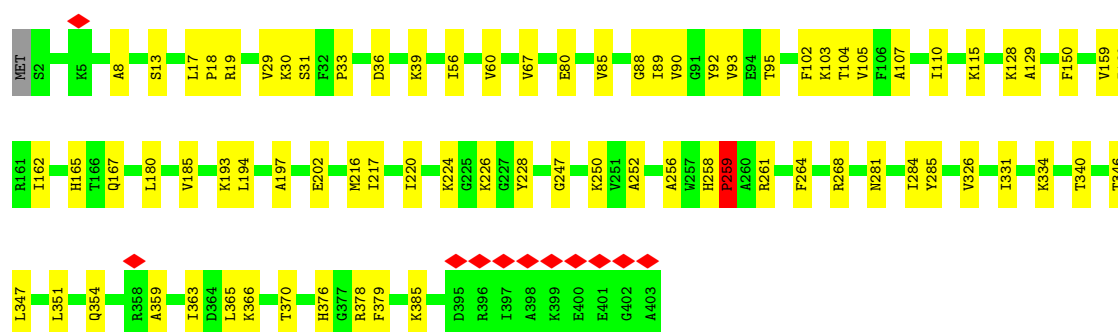
- Molecule 16: Large ribosomal subunit protein uL5

Chain E1:  5% 72% 25% .




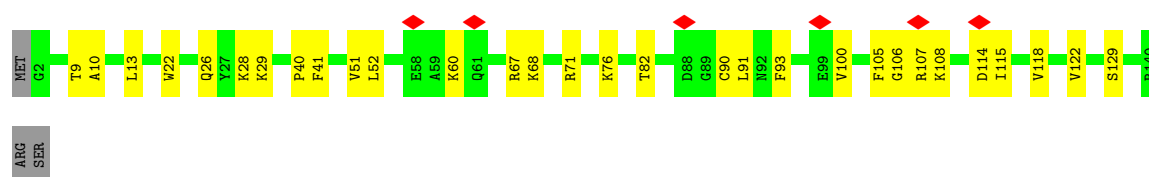
- Molecule 17: Large ribosomal subunit protein uL3

Chain E2:  80% 19%

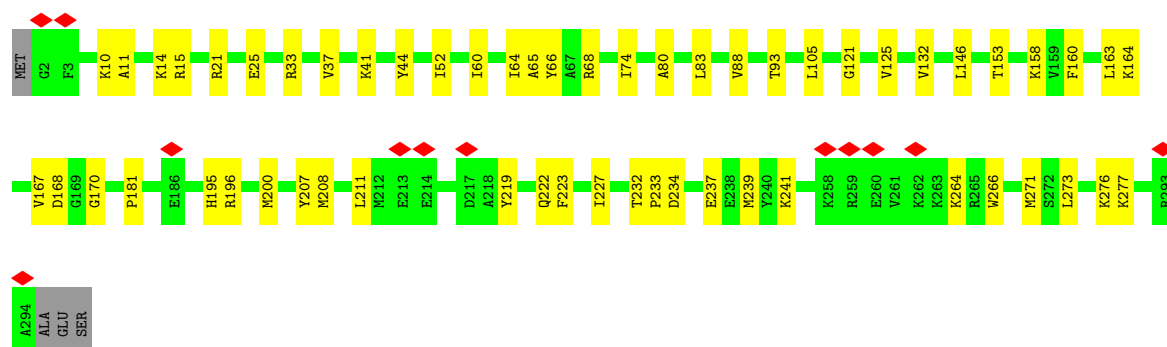


- Molecule 18: Small ribosomal subunit protein uS12

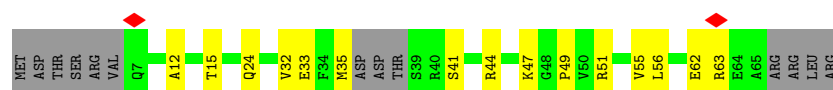
Chain E3:  77% 21% .



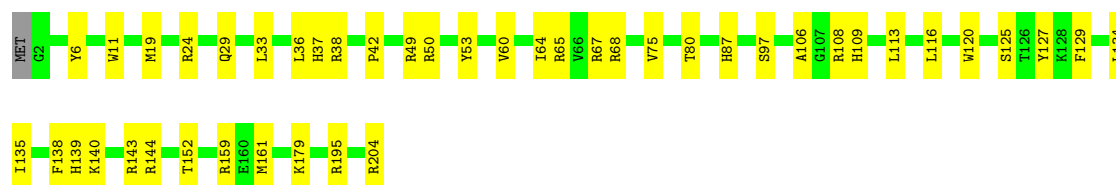
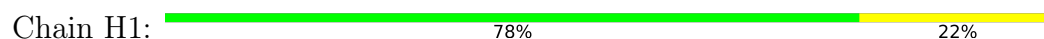
- Chain G2:  79% 19%



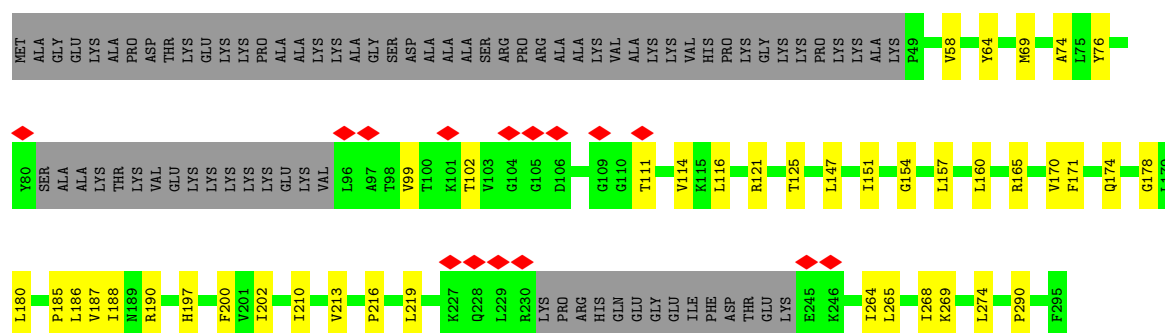
- Molecule 24: Small ribosomal subunit protein eS28



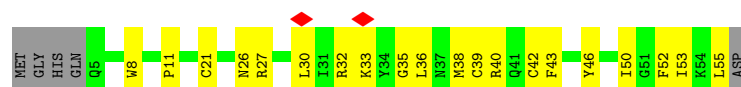
- Molecule 25: Large ribosomal subunit protein eL15



- Molecule 26: Large ribosomal subunit protein eL6

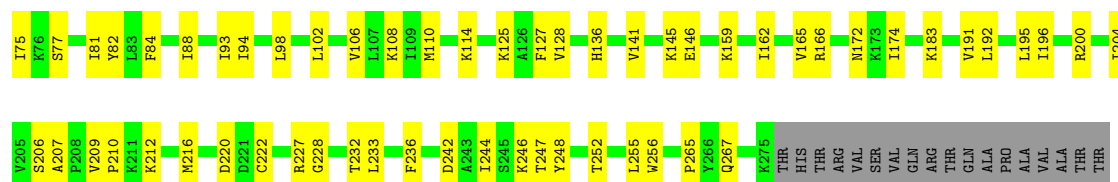


- Molecule 27: Small ribosomal subunit protein uS14



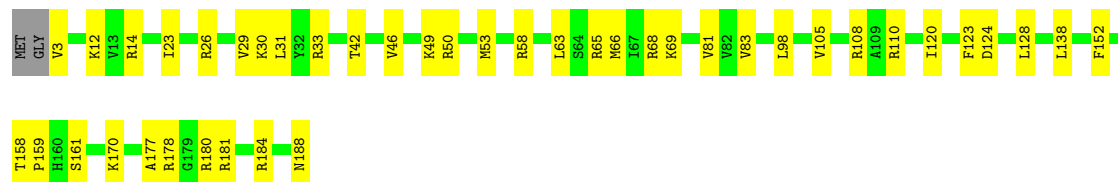
- |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | ASP | ASP | ASP | ALA | ALA | ALA | GLY | GLY | PRO | GLY | GLY | PRO | GLY | PRO | GLY | GLY | LEU | GLY | GLY | ARG | GLY | GLY | PHE | ARG | GLY | GLY | PHE | GLY | SER | GLY | LEU | ARG | GLY | ARG | GLY | GLY | ARG | GLY | ARG | GLY | ARG | GLY | ALA | ARG | GLY | GLY | LYS | ALA | GLU | ASP | ASP | E59 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|





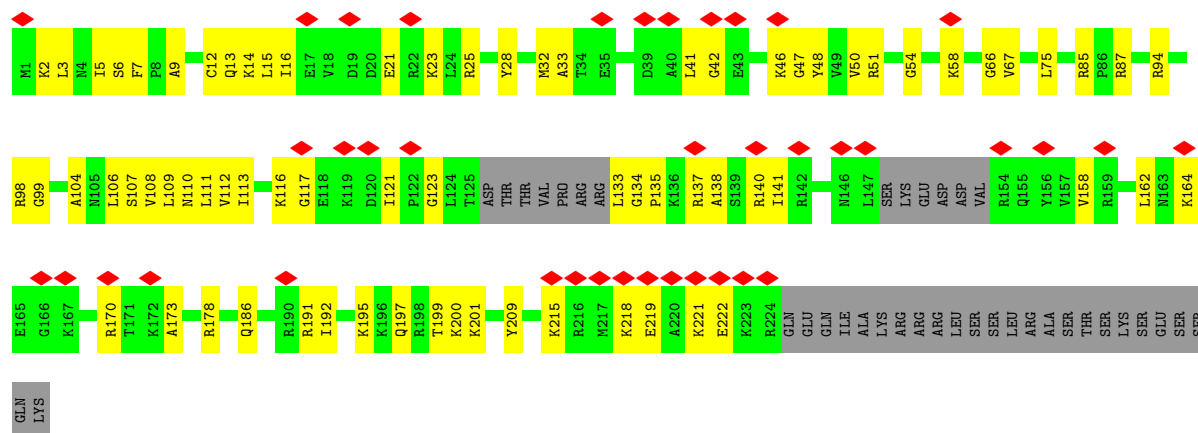
• Molecule 32: Large ribosomal subunit protein eL18

Chain K2: 77% 22%



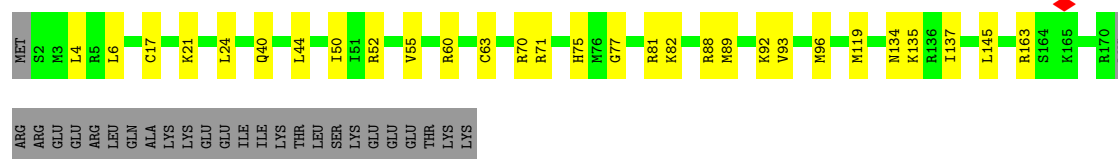
• Molecule 33: Small ribosomal subunit protein eS6

Chain K3: 16% 55% 30% 15%



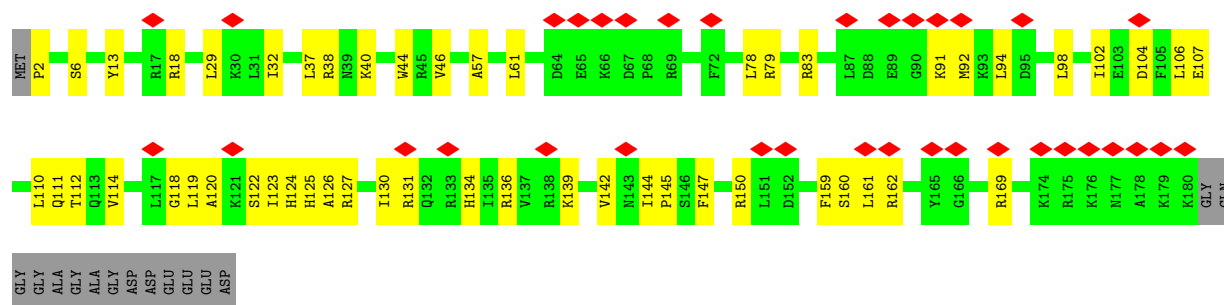
• Molecule 34: Large ribosomal subunit protein eL19

Chain L2: 71% 15% 14%



• Molecule 35: Small ribosomal subunit protein uS4

Chain L3: 18% 65% 27% 8%



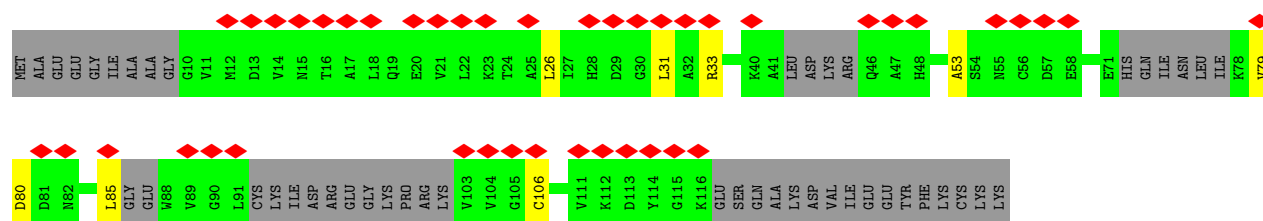
- Molecule 36: Large ribosomal subunit protein eL20

Chain M2: 79% 20%



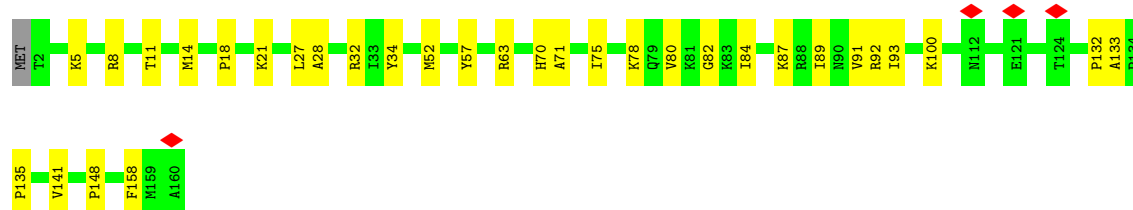
- Molecule 37: Small ribosomal subunit protein eS12

Chain M3: 33% 58% 6% 36%



- Molecule 38: Large ribosomal subunit protein eL21

Chain N2: 79% 20%



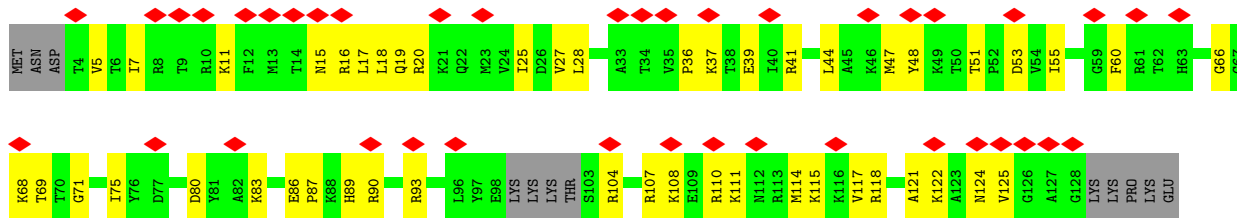
- Molecule 39: Small ribosomal subunit protein uS15

Chain N3: 72% 26%

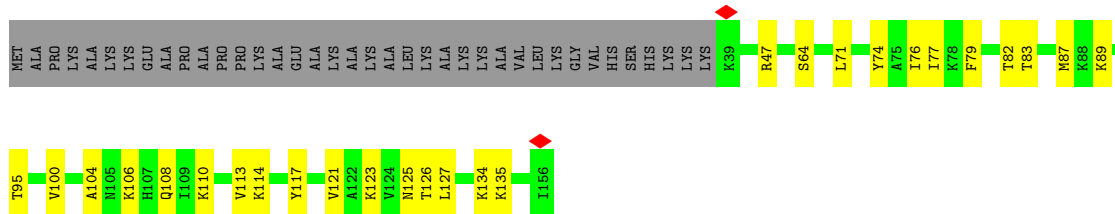




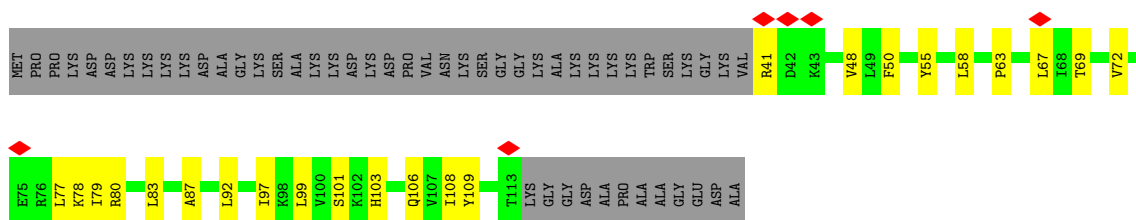
- Molecule 45: Small ribosomal subunit protein eS24



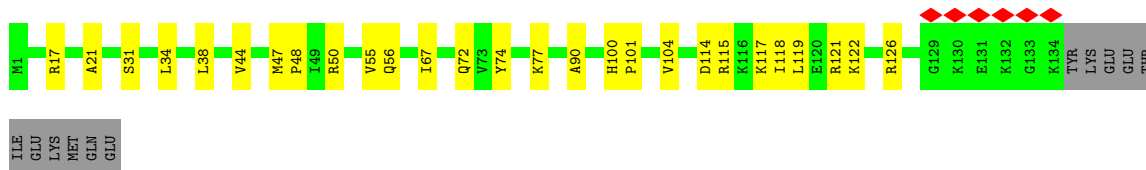
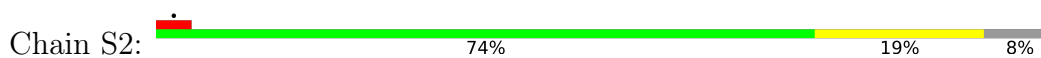
- Molecule 46: Large ribosomal subunit protein uL23



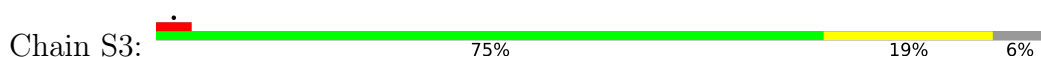
- Molecule 47: Small ribosomal subunit protein eS25

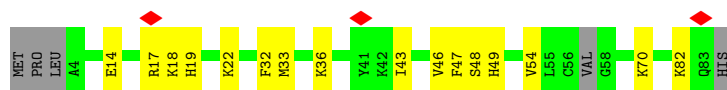


- Molecule 48: Large ribosomal subunit protein uL24

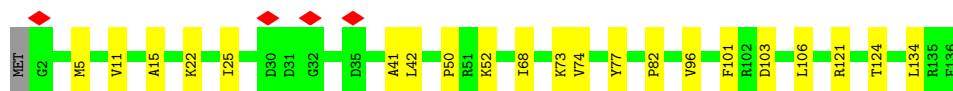
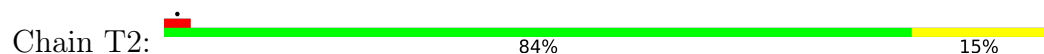


- Molecule 49: Small ribosomal subunit protein eS27

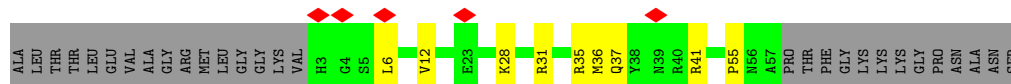
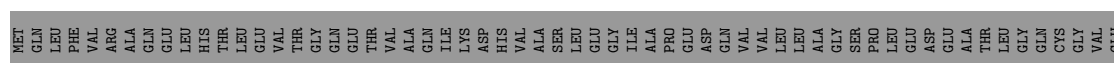




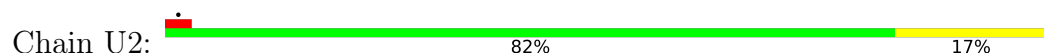
- Molecule 50: Large ribosomal subunit protein eL27



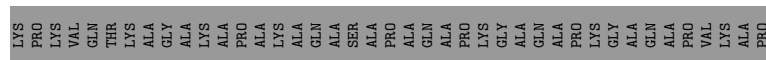
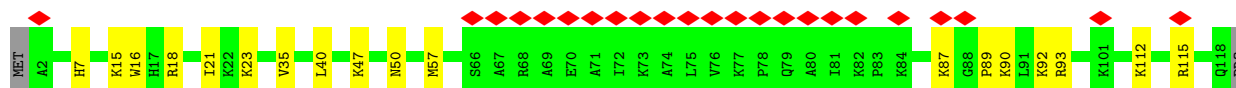
- Molecule 51: Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein



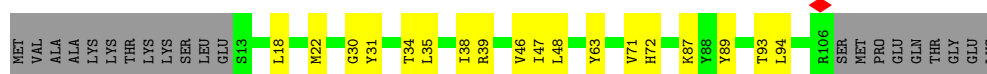
- Molecule 52: Large ribosomal subunit protein uL15



- Molecule 53: Large ribosomal subunit protein eL29

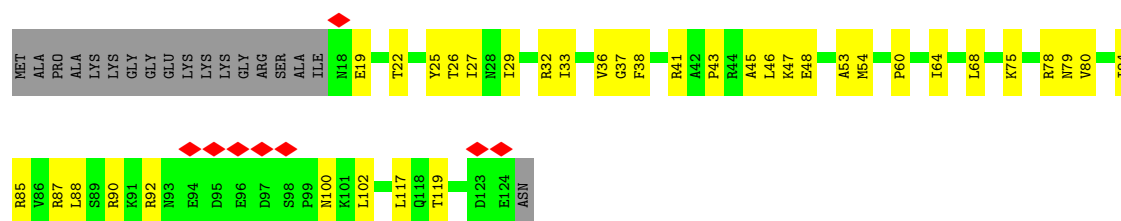


- Molecule 54: Large ribosomal subunit protein eL30

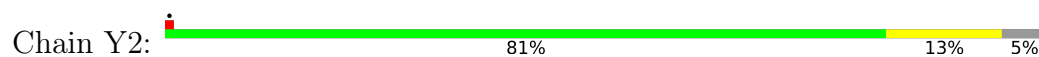


- Molecule 55: Large ribosomal subunit protein eL31

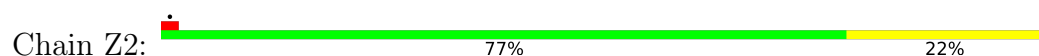




- Molecule 56: Large ribosomal subunit protein eL32



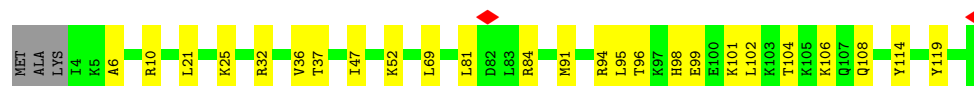
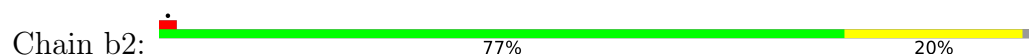
- Molecule 57: Large ribosomal subunit protein eL33



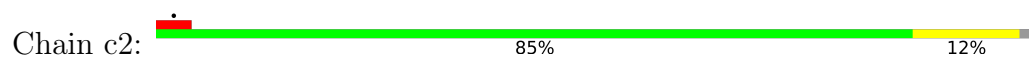
- Molecule 58: Large ribosomal subunit protein eL34



- Molecule 59: Large ribosomal subunit protein uL29

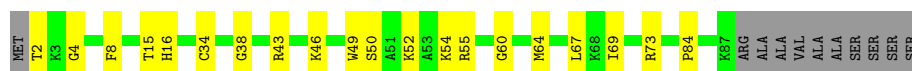


- Molecule 60: Large ribosomal subunit protein eL36

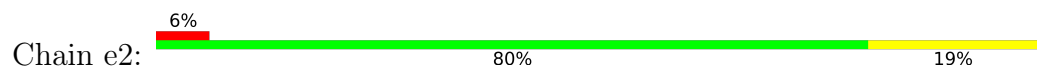


- Molecule 61: Large ribosomal subunit protein eL37

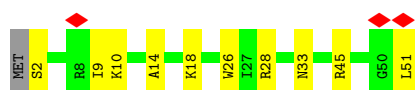
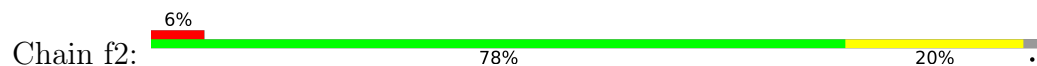




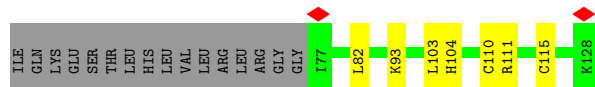
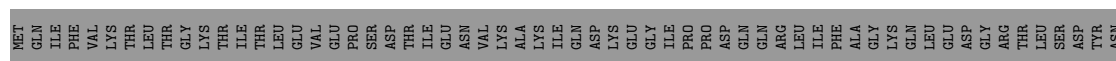
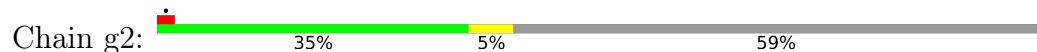
- Molecule 62: Large ribosomal subunit protein eL38



- Molecule 63: Large ribosomal subunit protein eL39



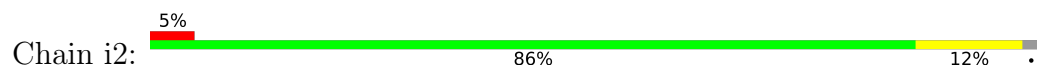
- Molecule 64: Ubiquitin-ribosomal protein eL40 fusion protein



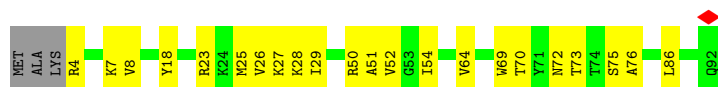
- Molecule 65: 60S ribosomal protein L41



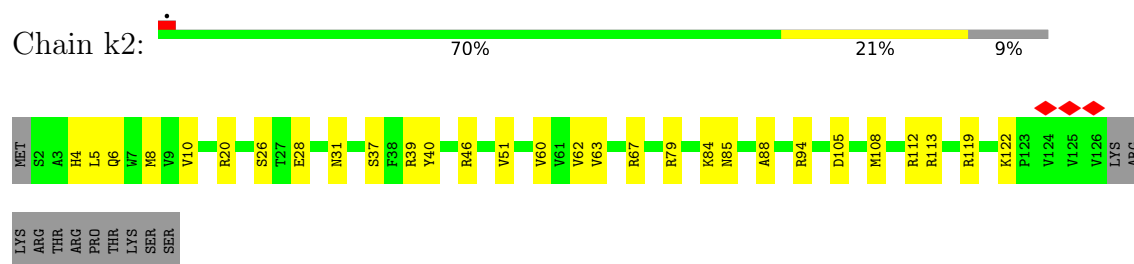
- Molecule 66: Large ribosomal subunit protein eL42



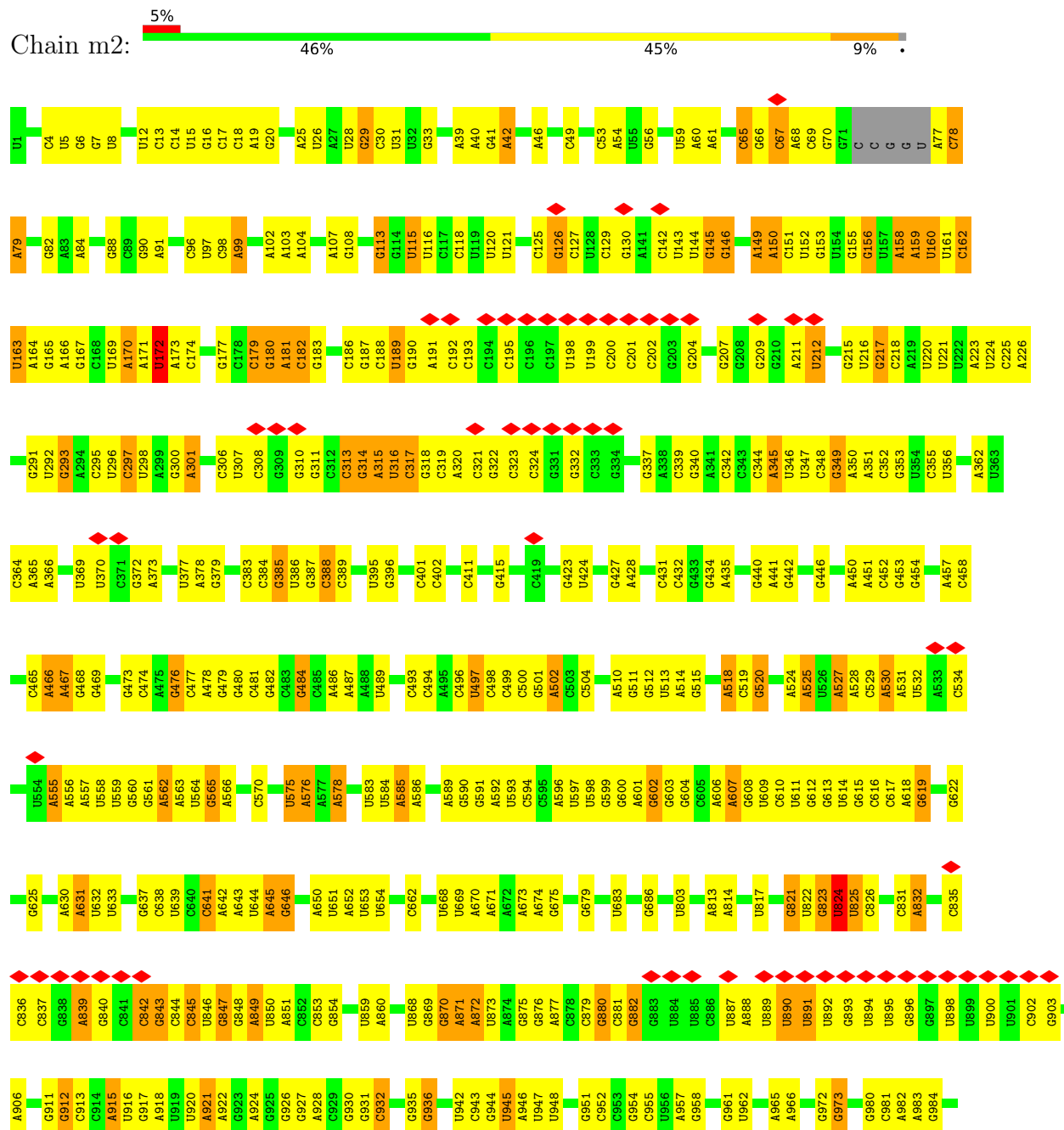
- Molecule 67: Large ribosomal subunit protein eL43



- Molecule 68: Large ribosomal subunit protein eL28

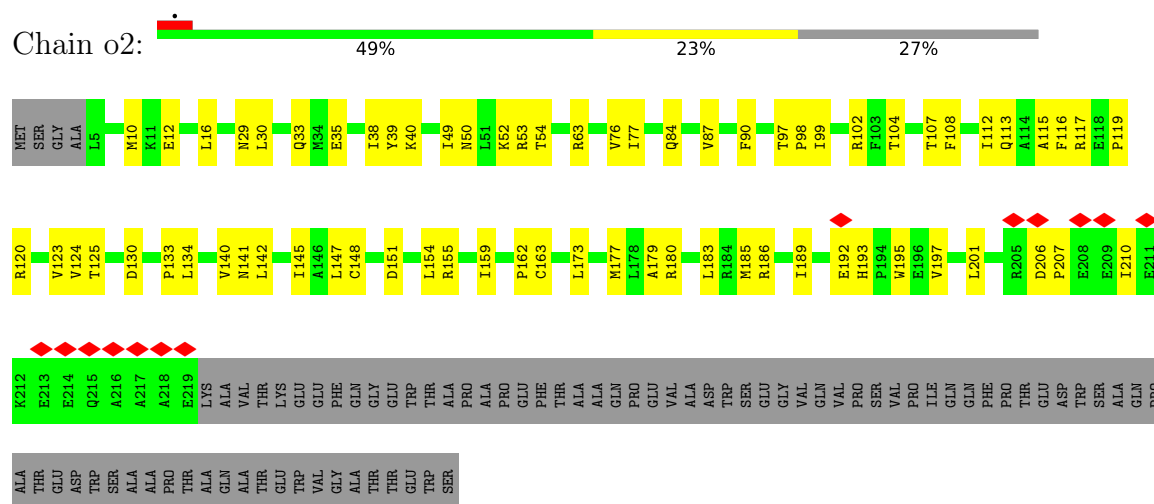


- Molecule 69: 18S ribosomal RNA





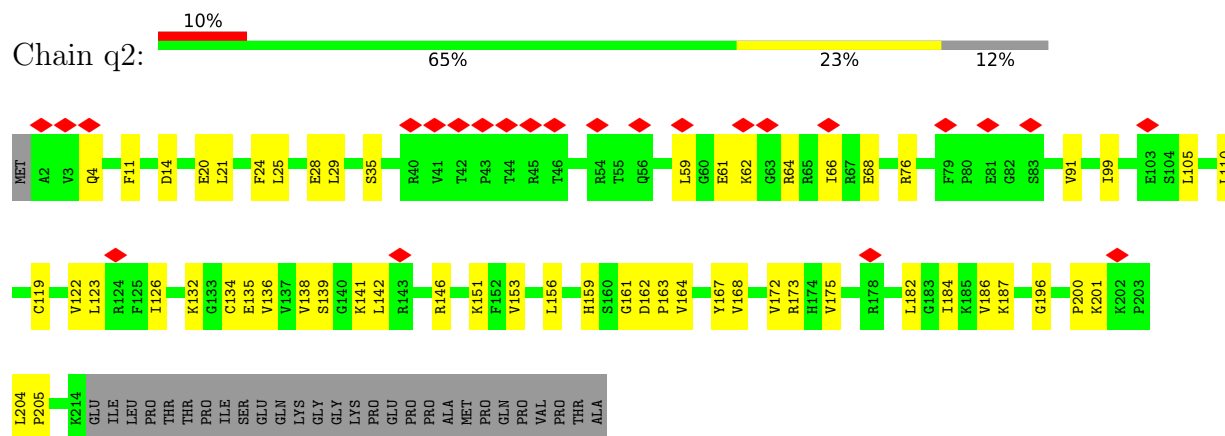




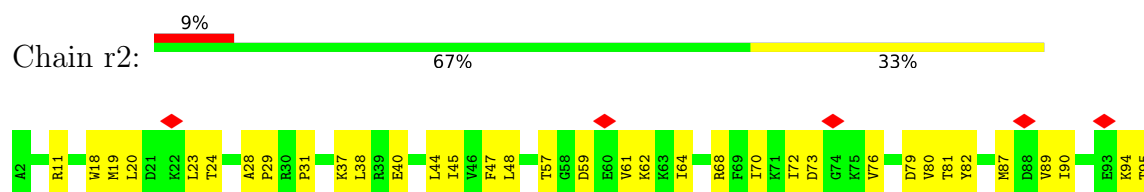
• Molecule 72: 40S ribosomal protein S3a

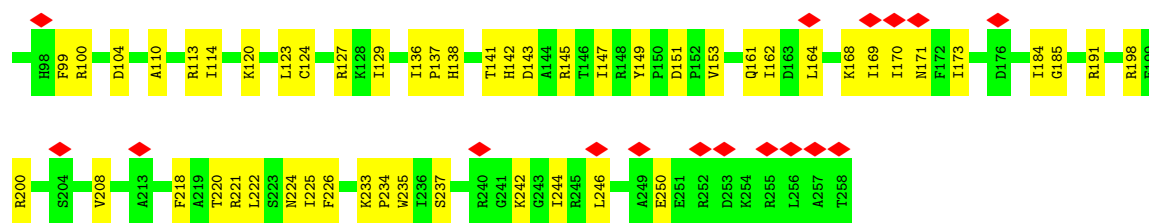


• Molecule 73: Small ribosomal subunit protein uS3



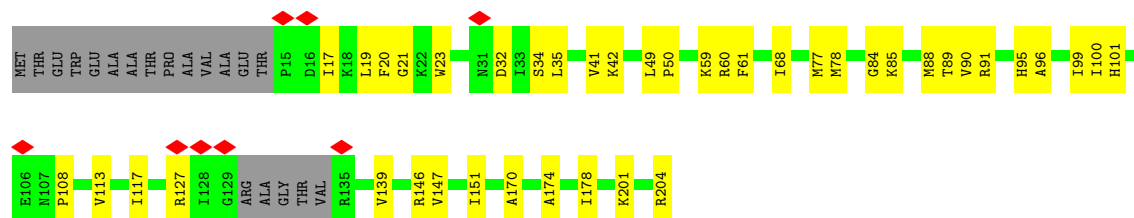
• Molecule 74: Small ribosomal subunit protein eS4





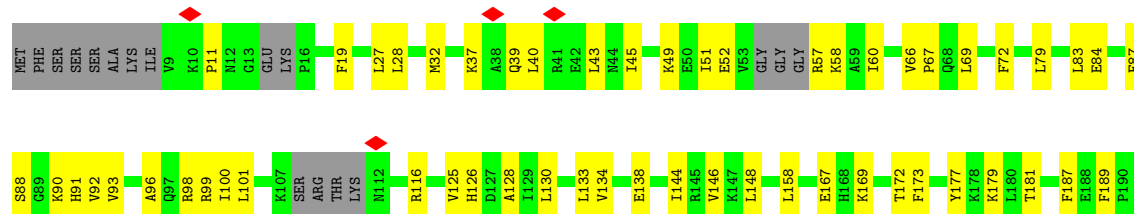
- Molecule 75: Small ribosomal subunit protein uS7

Chain s2: 70% 21% 9%



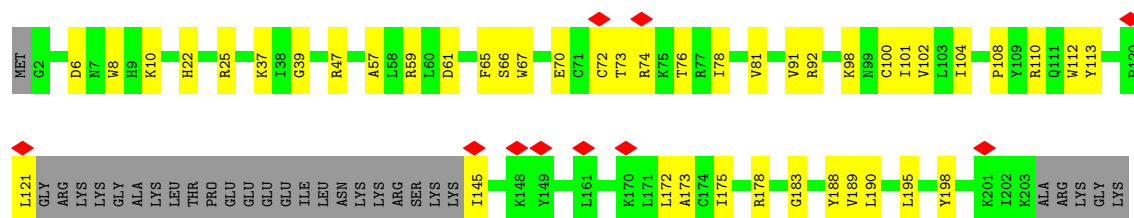
- Molecule 76: Small ribosomal subunit protein eS7

Chain t2: 61% 28% 10%



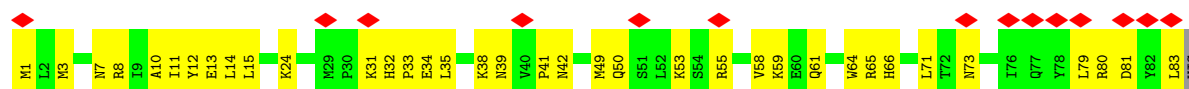
- Molecule 77: Small ribosomal subunit protein eS8

Chain u2: 5% 65% 21% 14%

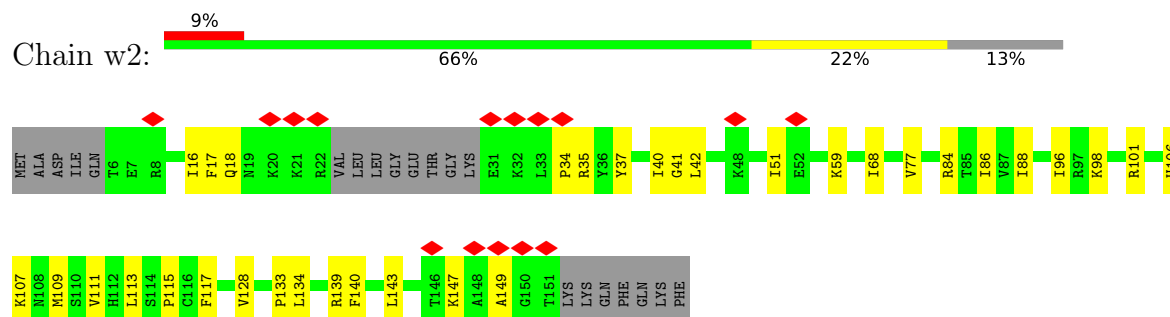


- Molecule 78: Small ribosomal subunit protein eS10

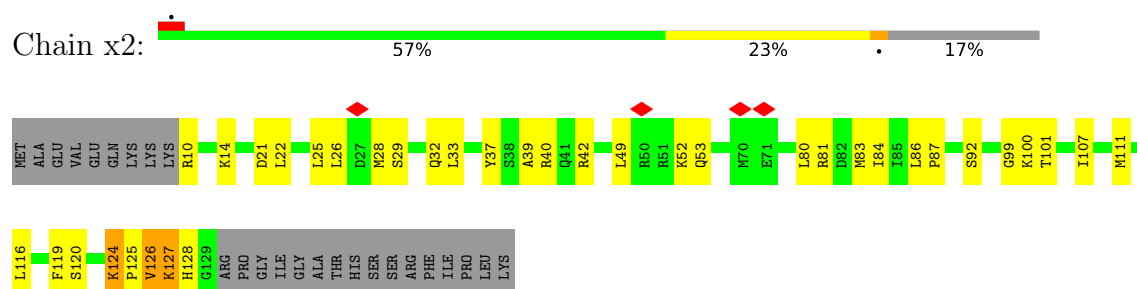
Chain v2: 8% 28% 22% 50%



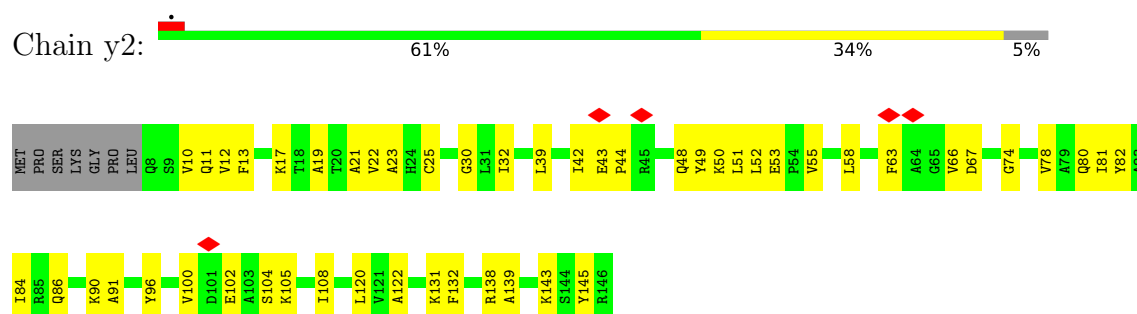
- Molecule 79: Small ribosomal subunit protein uS17



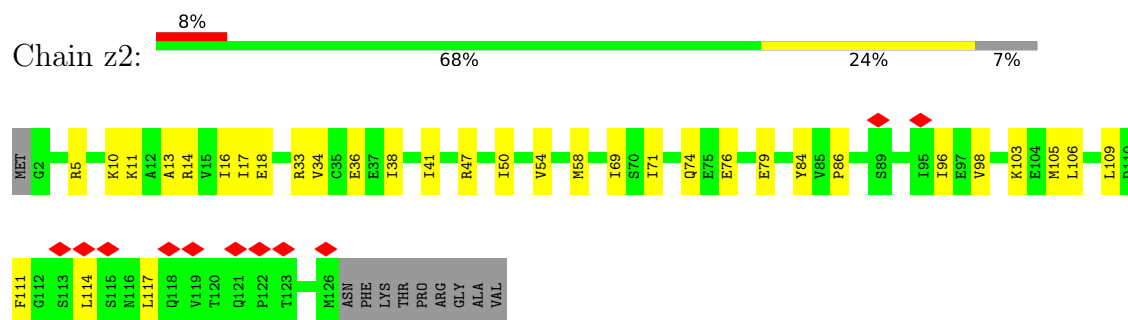
- Molecule 80: Small ribosomal subunit protein uS19



- Molecule 81: Small ribosomal subunit protein uS9



- Molecule 82: Small ribosomal subunit protein eS17



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	134861	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	45	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2900	Depositor
Magnification	100000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	2.353	Depositor
Minimum map value	-0.049	Depositor
Average map value	0.014	Depositor
Map value standard deviation	0.085	Depositor
Recommended contour level	0.0823	Depositor
Map size ( $\text{\AA}$ )	315.12, 315.12, 315.12	wwPDB
Map dimensions	312, 312, 312	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.01, 1.01, 1.01	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 4AC, ZN, 5MC, B8N, OMC, B8T, PSU, MG, OMG, UR3, OMU, 2MG, 1MA, A2M

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	0.37	0/1877	0.38	0/2502
2	A2	0.44	0/82439	0.34	0/128559
3	A3	0.30	0/1172	0.45	1/1570 (0.1%)
4	B1	0.32	0/1799	0.44	0/2424
5	B2	0.45	0/2836	0.32	0/4421
6	B3	0.27	0/1109	0.46	0/1484
7	Bv	0.20	0/1576	0.29	0/2451
8	Bx	0.36	0/219	0.40	0/336
10	C1	0.32	0/1537	0.39	0/2065
11	C2	0.45	0/3675	0.32	0/5725
12	C3	0.23	0/778	0.35	0/1045
13	D1	0.34	0/1694	0.36	0/2261
14	D2	0.39	0/1914	0.39	0/2567
15	D3	0.30	0/596	0.38	0/800
16	E1	0.29	0/1420	0.43	0/1899
17	E2	0.36	0/3305	0.43	1/4422 (0.0%)
18	E3	0.29	0/1097	0.40	0/1464
19	F1	0.34	0/1674	0.39	0/2241
20	F2	0.37	0/2877	0.42	0/3860
21	F3	0.37	0/786	0.45	0/1053
22	G1	0.32	0/1165	0.40	0/1558
23	G2	0.32	0/2435	0.38	0/3260
24	G3	0.25	0/436	0.33	0/582
25	H1	0.45	0/1746	0.39	0/2338
26	H2	0.28	0/1799	0.37	0/2413
27	H3	0.35	0/437	0.47	0/580
28	I2	0.39	0/1648	0.40	0/2203
29	I3	0.21	0/1827	0.43	0/2467
30	J2	0.37	0/1268	0.41	0/1700
31	J3	0.31	0/1626	0.46	0/2211
32	K2	0.40	0/1535	0.41	0/2048
33	K3	0.20	0/1728	0.39	0/2295

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
34	L2	0.33	0/1424	0.33	0/1884
35	L3	0.22	0/1520	0.40	0/2030
36	M2	0.38	0/1490	0.43	0/2000
37	M3	0.12	0/527	0.34	0/718
38	N2	0.35	0/1327	0.35	0/1771
39	N3	0.30	0/1226	0.40	0/1649
40	O2	0.21	0/839	0.32	0/1126
41	O3	0.31	0/1016	0.43	0/1363
42	P2	0.36	0/983	0.40	0/1319
43	P3	0.33	0/1044	0.42	0/1398
44	Q2	0.36	0/532	0.34	0/708
45	Q3	0.16	0/997	0.42	0/1325
46	R2	0.34	0/984	0.38	0/1323
47	R3	0.23	0/591	0.38	0/794
48	S2	0.32	0/1132	0.37	0/1504
49	S3	0.24	0/629	0.36	0/841
50	T2	0.31	0/1130	0.33	0/1507
51	T3	0.18	0/358	0.31	0/467
52	U2	0.38	0/1193	0.39	0/1593
53	V2	0.31	0/963	0.36	0/1275
54	W2	0.31	0/742	0.34	0/996
55	X2	0.35	0/903	0.37	0/1216
56	Y2	0.39	0/1071	0.36	0/1429
57	Z2	0.39	0/895	0.42	0/1198
58	a2	0.39	0/864	0.44	0/1152
59	b2	0.30	0/1009	0.37	0/1332
60	c2	0.28	0/843	0.33	0/1115
61	d2	0.41	0/720	0.44	0/952
62	e2	0.26	0/574	0.30	0/760
63	f2	0.36	0/454	0.29	0/599
64	g2	0.32	0/435	0.32	0/575
65	h2	0.39	0/231	0.52	0/294
66	i2	0.34	0/855	0.39	0/1128
67	j2	0.39	0/704	0.37	0/935
68	k2	0.38	0/1016	0.40	0/1363
69	m2	0.41	0/38048	0.33	0/59291
70	n2	0.26	0/1746	0.23	0/2717
71	o2	0.31	0/1741	0.46	0/2366
72	p2	0.30	0/1749	0.40	0/2340
73	q2	0.24	0/1681	0.40	0/2261
74	r2	0.24	0/2072	0.42	0/2793
75	s2	0.27	0/1489	0.44	0/1999
76	t2	0.27	0/1341	0.48	0/1803

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
77	u2	0.25	0/1424	0.38	0/1918
78	v2	0.24	0/725	0.55	0/974
79	w2	0.29	0/1154	0.36	0/1543
80	x2	0.34	0/1018	0.48	0/1359
81	y2	0.29	0/1126	0.46	0/1506
82	z2	0.24	0/1023	0.39	0/1373
All	All	0.39	0/219588	0.36	2/322686 (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
17	E2	0	2
60	c2	0	1
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A3	100	ALA	CB-CA-C	-5.38	109.91	117.23
17	E2	259	PRO	N-CA-C	-5.07	102.03	112.47

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	E2	258	HIS	Peptide
17	E2	259	PRO	Peptide
60	c2	63	VAL	Peptide

## 5.2 Too-close contacts ⓘ

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A1	1843	0	1975	52	0
2	A2	75341	0	38147	864	0
3	A3	1154	0	1210	43	0
4	B1	1764	0	1892	46	0
5	B2	2538	0	1286	20	0
6	B3	1091	0	1130	42	0
7	Bv	1412	0	716	22	0
8	Bx	200	0	101	3	0
9	By	110	0	31	0	0
10	C1	1519	0	1603	30	0
11	C2	3315	0	1685	23	0
12	C3	769	0	837	21	0
13	D1	1656	0	1706	29	0
14	D2	1876	0	1970	33	0
15	D3	589	0	566	16	0
16	E1	1397	0	1425	30	0
17	E2	3238	0	3380	61	0
18	E3	1080	0	1147	23	0
19	F1	1643	0	1750	36	0
20	F2	2823	0	2996	56	0
21	F3	774	0	821	16	0
22	G1	1143	0	1219	20	0
23	G2	2389	0	2420	48	0
24	G3	435	0	461	12	0
25	H1	1701	0	1749	41	0
26	H2	1766	0	1902	30	0
27	H3	427	0	426	22	0
28	I2	1618	0	1775	31	0
29	I3	1800	0	1770	64	0
30	J2	1242	0	1274	27	0
31	J3	1590	0	1606	43	0
32	K2	1511	0	1636	35	0
33	K3	1708	0	1864	63	0
34	L2	1408	0	1550	22	0
35	L3	1495	0	1615	57	0
36	M2	1450	0	1488	29	0
37	M3	525	0	439	8	0
38	N2	1299	0	1368	30	0
39	N3	1202	0	1289	31	0
40	O2	825	0	850	8	0
41	O3	1003	0	1028	31	0
42	P2	969	0	1031	22	0
43	P3	1027	0	1067	23	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	Q2	519	0	533	8	0
45	Q3	981	0	1039	42	0
46	R2	967	0	1040	21	0
47	R3	585	0	640	19	0
48	S2	1115	0	1205	25	0
49	S3	618	0	634	9	0
50	T2	1107	0	1182	16	0
51	T3	355	0	391	10	0
52	U2	1164	0	1213	23	0
53	V2	945	0	1037	14	0
54	W2	732	0	769	14	0
55	X2	888	0	930	26	0
56	Y2	1053	0	1147	14	0
57	Z2	876	0	912	14	0
58	a2	854	0	945	23	0
59	b2	1001	0	1138	19	0
60	c2	832	0	917	10	0
61	d2	705	0	737	13	0
62	e2	568	0	635	10	0
63	f2	444	0	483	10	0
64	g2	429	0	465	6	0
65	h2	230	0	276	5	0
66	i2	842	0	912	12	0
67	j2	694	0	738	18	0
68	k2	1001	0	1066	21	0
69	m2	34685	0	17531	556	0
70	n2	1562	0	797	15	0
71	o2	1704	0	1702	60	0
72	p2	1722	0	1794	41	0
73	q2	1655	0	1750	42	0
74	r2	2031	0	2138	60	0
75	s2	1468	0	1519	35	0
76	t2	1322	0	1365	39	0
77	u2	1397	0	1378	35	0
78	v2	705	0	722	31	0
79	w2	1134	0	1197	27	0
80	x2	999	0	1046	37	0
81	y2	1109	0	1174	39	0
82	z2	1011	0	1063	25	0
83	A2	84	0	0	0	0
83	E3	1	0	0	0	0
83	H1	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
83	P2	1	0	0	0	0
83	d2	1	0	0	0	0
83	m2	35	0	0	0	0
84	F3	1	0	0	0	0
84	H3	1	0	0	0	0
84	d2	1	0	0	0	0
84	g2	1	0	0	0	0
84	i2	1	0	0	0	0
84	j2	1	0	0	0	0
85	m2	28	0	0	1	0
86	m2	23	0	13	2	0
87	B1	1	0	0	0	0
All	All	206855	0	152374	3151	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 9.

All (3151) 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)
2:A2:3348:A:H62	2:A2:3479:G:N2	1.34	1.24
2:A2:3348:A:N6	2:A2:3479:G:H21	1.35	1.23
2:A2:444:G:H1	2:A2:1117:A:N6	1.59	1.00
69:m2:153:G:H1	69:m2:165:G:H22	1.08	0.99
69:m2:1731:U:H3	69:m2:1807:G:H1	1.11	0.95
69:m2:887:U:H3	69:m2:903:G:H1	1.16	0.94
2:A2:1022:C:N4	2:A2:1023:C:N4	2.14	0.94
2:A2:740:A:H62	2:A2:828:G:H21	1.09	0.93
6:B3:64:LEU:HD21	6:B3:121:ARG:HH21	1.33	0.91
58:a2:63:VAL:HG23	58:a2:66:ARG:HE	1.35	0.91
69:m2:1398:A:H2	69:m2:1451:G:H1	1.06	0.90
69:m2:385:G:H21	79:w2:133:PRO:HG2	1.34	0.90
81:y2:19:ALA:HA	81:y2:74:GLY:HA3	1.53	0.88
39:N3:16:LEU:HD12	39:N3:17:PRO:HD2	1.55	0.88
2:A2:1022:C:N4	2:A2:1023:C:H41	1.72	0.88
2:A2:1022:C:C4	2:A2:1023:C:N4	2.43	0.87
74:r2:141:THR:HG22	74:r2:143:ASP:H	1.40	0.87
2:A2:37:U:H4'	52:U2:32:ARG:HD2	1.57	0.86
2:A2:3600:G:H1	2:A2:3719:U:H3	1.21	0.86
69:m2:153:G:H1	69:m2:165:G:N2	1.74	0.86
69:m2:1398:A:C2	69:m2:1451:G:N1	2.42	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:m2:1398:A:H2	69:m2:1451:G:N1	1.72	0.86
2:A2:1007:A:H2	2:A2:1017:G:H1	1.25	0.85
23:G2:181:PRO:HD2	23:G2:195:HIS:HD1	1.42	0.84
2:A2:2312:G:H1	2:A2:2325:U:H3	1.26	0.84
69:m2:1523:C:H5'	80:x2:126:VAL:CG1	2.08	0.84
4:B1:59:ARG:HG2	4:B1:62:ARG:HH21	1.43	0.83
69:m2:1523:C:H5'	80:x2:126:VAL:HG12	1.61	0.83
35:L3:83:ARG:HG2	35:L3:150:ARG:HD2	1.60	0.82
2:A2:697:C:H4'	68:k2:85:ASN:HD22	1.45	0.82
69:m2:190:G:H21	69:m2:192:C:H42	1.28	0.81
39:N3:46:THR:HG23	39:N3:86:GLU:HG2	1.64	0.80
25:H1:64:ILE:HD11	25:H1:106:ALA:HB2	1.62	0.80
82:z2:18:GLU:HB2	82:z2:69:ILE:HG12	1.63	0.80
10:C1:18:ILE:HD11	10:C1:81:ILE:HD11	1.63	0.79
31:J3:98:LEU:HB3	31:J3:102:LEU:HD11	1.64	0.79
16:E1:120:ASP:HB3	16:E1:123:ILE:HG12	1.65	0.79
27:H3:30:LEU:HD13	69:m2:1661:U:H5'	1.62	0.79
68:k2:63:VAL:HG12	68:k2:79:ARG:HG2	1.65	0.79
2:A2:1006:G:H1	2:A2:1018:U:H3	1.30	0.79
2:A2:740:A:H62	2:A2:828:G:N2	1.80	0.79
71:o2:10:MET:HE1	71:o2:52:LYS:HA	1.65	0.79
2:A2:2302:G:H1	2:A2:2527:C:H5	1.29	0.78
3:A3:37:GLY:H	69:m2:1632:A:H5''	1.49	0.78
5:B2:6:C:H4'	23:G2:52:ILE:HD13	1.65	0.78
69:m2:1523:C:O4'	80:x2:126:VAL:HG11	1.83	0.78
69:m2:1398:A:N1	69:m2:1451:G:O6	2.16	0.78
72:p2:49:VAL:HG21	72:p2:62:LEU:HD22	1.65	0.78
74:r2:94:LYS:HD3	74:r2:95:THR:HG23	1.64	0.78
2:A2:3711:C:H2'	2:A2:3712:A:C8	2.18	0.77
3:A3:124:ARG:HH11	3:A3:129:LEU:HB3	1.49	0.77
58:a2:82:MET:HE2	58:a2:86:CYS:HB3	1.66	0.77
53:V2:89:PRO:HG2	53:V2:92:LYS:HD3	1.66	0.77
69:m2:514:A2M:H2'	69:m2:515:G:H8	1.50	0.77
74:r2:45:ILE:HG13	74:r2:61:VAL:HG11	1.65	0.77
71:o2:173:LEU:HD11	71:o2:177:MET:HE3	1.66	0.77
29:I3:87:LEU:HB2	29:I3:101:PHE:HB2	1.66	0.77
2:A2:2240:U:H3	2:A2:2248:G:H1	1.29	0.77
33:K3:121:ILE:HG22	33:K3:123:GLY:H	1.47	0.77
71:o2:124:VAL:HG21	71:o2:134:LEU:HD11	1.66	0.77
33:K3:5:ILE:HD11	33:K3:113:ILE:HG13	1.65	0.76
42:P2:16:ILE:HD11	42:P2:124:GLU:HG2	1.65	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A2:3524:G:H22	2:A2:3556:G:H1'	1.50	0.76
33:K3:2:LYS:HD2	33:K3:15:LEU:HD21	1.66	0.76
2:A2:2224:C:H5	2:A2:2226:G:H1	1.30	0.75
2:A2:3894:U:H3	2:A2:3933:A:H2	1.33	0.75
41:O3:52:THR:HG21	69:m2:954:G:H21	1.49	0.75
61:d2:46:LYS:HD3	61:d2:54:LYS:HE3	1.68	0.75
39:N3:40:LEU:HD23	39:N3:43:LYS:HZ1	1.50	0.74
3:A3:47:LYS:HE3	3:A3:78:LYS:HB2	1.66	0.74
10:C1:92:MET:HE2	10:C1:179:ILE:HG22	1.69	0.74
72:p2:127:VAL:HG11	72:p2:176:VAL:HG11	1.69	0.74
69:m2:555:A:H2'	69:m2:556:A:H8	1.52	0.73
31:J3:191:VAL:HG11	31:J3:236:PHE:HA	1.70	0.73
81:y2:58:LEU:HD11	81:y2:108:ILE:HG22	1.70	0.73
7:Bv:51:U:H3	7:Bv:63:G:H1	1.36	0.73
2:A2:3933:A:H2'	2:A2:3934:A:H2'	1.70	0.73
77:u2:190:LEU:HD21	77:u2:198:TYR:HD2	1.53	0.73
10:C1:94:SER:HB2	10:C1:142:ASP:HB2	1.68	0.73
60:c2:67:LYS:HE2	60:c2:71:LYS:HE2	1.69	0.73
73:q2:204:LEU:HD12	73:q2:205:PRO:HD2	1.70	0.73
33:K3:58:LYS:HA	33:K3:107:SER:HB3	1.71	0.73
36:M2:15:ARG:HB3	36:M2:27:LEU:HD23	1.71	0.73
68:k2:119:ARG:HA	68:k2:122:LYS:HE3	1.71	0.72
73:q2:122:VAL:O	73:q2:126:ILE:HD12	1.88	0.72
3:A3:51:ASP:HB3	3:A3:54:LYS:HE2	1.70	0.72
69:m2:159:A:H2	69:m2:469:G:H21	1.37	0.72
2:A2:4216:A:H5''	28:I2:68:ARG:HH12	1.54	0.72
3:A3:19:ASN:HD22	3:A3:33:ILE:HG13	1.54	0.72
34:L2:119:MET:HE1	34:L2:145:LEU:HD23	1.70	0.72
78:v2:71:LEU:HD23	78:v2:73:ASN:H	1.55	0.71
72:p2:163:GLN:HB3	72:p2:204:ILE:HD13	1.72	0.71
52:U2:88:VAL:HG12	52:U2:92:LYS:NZ	2.05	0.71
2:A2:98:A:H5'	25:H1:195:ARG:HD2	1.72	0.71
7:Bv:34:G:H1	8:Bx:51:U:H3	1.39	0.71
74:r2:137:PRO:HG2	74:r2:149:TYR:HA	1.73	0.71
81:y2:42:ILE:HD13	81:y2:51:LEU:HD21	1.73	0.70
45:Q3:60:PHE:HD1	45:Q3:71:GLY:HA3	1.56	0.70
26:H2:216:PRO:HG2	26:H2:219:LEU:HG	1.73	0.70
2:A2:265:U:H5''	2:A2:266:C:H5'	1.73	0.70
2:A2:740:A:N6	2:A2:828:G:H21	1.89	0.70
2:A2:1361:G:HO2'	2:A2:2567:A:H8	1.37	0.70
32:K2:110:ARG:HG3	32:K2:120:ILE:HD12	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:C3:80:PHE:HB3	27:H3:52:PHE:HB3	1.74	0.70
2:A2:129:C:H2'	2:A2:130:G:C8	2.26	0.70
2:A2:1354:U:H3	2:A2:1431:G:H1	1.38	0.70
2:A2:1914:C:H1'	2:A2:2004:G:H1	1.57	0.70
58:a2:82:MET:HE1	58:a2:90:ARG:HD2	1.74	0.70
70:n2:52:G:H2'	70:n2:53:A:C8	2.27	0.70
12:C3:56:MET:HB2	12:C3:86:LYS:HG3	1.73	0.69
65:h2:10:MET:HE2	69:m2:1174:U:H5'	1.73	0.69
68:k2:108:MET:O	68:k2:112:ARG:HG3	1.92	0.69
81:y2:25:CYS:HB2	81:y2:91:ALA:HB1	1.72	0.69
2:A2:444:G:H1	2:A2:1117:A:H61	1.40	0.69
2:A2:3325:G:H21	2:A2:3328:G:N2	1.90	0.69
69:m2:96:C:H1'	69:m2:476:G:H5'	1.74	0.69
11:C2:83:C:H42	48:S2:50:ARG:HH22	1.41	0.69
41:O3:31:CYS:HB2	41:O3:93:LEU:HD13	1.72	0.69
80:x2:49:LEU:HD23	80:x2:53:GLN:HG3	1.72	0.69
3:A3:34:LYS:HB2	3:A3:100:ALA:HA	1.74	0.69
29:I3:39:THR:HG22	29:I3:60:ARG:HG3	1.75	0.69
4:B1:33:GLU:HG2	4:B1:35:ARG:HH21	1.57	0.69
6:B3:64:LEU:HD21	6:B3:121:ARG:NH2	2.07	0.69
27:H3:30:LEU:HG	69:m2:1258:G:C2	2.27	0.69
79:w2:147:LYS:HG2	79:w2:149:ALA:H	1.56	0.69
29:I3:259:TRP:HA	29:I3:266:ILE:HA	1.75	0.69
47:R3:63:PRO:HA	47:R3:97:ILE:HD11	1.74	0.69
2:A2:2600:A:H61	2:A2:3499:C:H42	1.41	0.69
10:C1:128:MET:HE1	10:C1:161:ILE:HD11	1.73	0.69
70:n2:68:U:H2'	70:n2:69:G:H8	1.58	0.69
3:A3:15:VAL:HG13	3:A3:68:ILE:HD11	1.73	0.69
2:A2:2651:G:H5''	34:L2:134:ASN:ND2	2.08	0.68
69:m2:107:A:H2'	69:m2:108:G:C8	2.28	0.68
69:m2:1139:U:H4'	71:o2:155:ARG:HH22	1.57	0.68
75:s2:95:HIS:O	75:s2:99:ILE:HG12	1.93	0.68
2:A2:444:G:N1	2:A2:1117:A:N6	2.37	0.68
2:A2:4343:A:H4'	10:C1:71:ARG:HD3	1.76	0.68
69:m2:983:A:H2'	69:m2:984:G:C8	2.28	0.68
49:S3:19:HIS:HB3	49:S3:22:LYS:HG2	1.75	0.68
69:m2:1571:A:H8	69:m2:1615:G:H21	1.41	0.68
70:n2:61:C:H2'	70:n2:62:A:H8	1.57	0.68
40:O2:63:ILE:HG12	40:O2:72:VAL:HG22	1.74	0.68
65:h2:1:MET:HG3	69:m2:1708:G:H5'	1.74	0.68
69:m2:225:C:H2'	69:m2:226:A:C8	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:r2:79:ASP:HB3	74:r2:82:TYR:HB2	1.74	0.68
14:D2:28:ARG:HB2	14:D2:123:ARG:HB2	1.76	0.68
34:L2:17:CYS:HB3	34:L2:52:ARG:HE	1.58	0.68
45:Q3:27:VAL:HB	45:Q3:69:THR:HB	1.75	0.68
6:B3:41:LYS:HD3	6:B3:43:LYS:HE3	1.74	0.68
23:G2:125:VAL:HG11	23:G2:200:MET:HE2	1.76	0.68
57:Z2:7:CYS:HB2	57:Z2:103:VAL:HB	1.75	0.68
2:A2:1084:G:H1'	2:A2:1909:G:H21	1.57	0.68
33:K3:137:ARG:HB2	33:K3:140:ARG:HB2	1.76	0.68
71:o2:52:LYS:HB2	82:z2:109:LEU:HD11	1.75	0.68
72:p2:30:TRP:CE2	72:p2:48:LEU:HD21	2.29	0.68
51:T3:28:LYS:HD2	51:T3:36:MET:HB2	1.76	0.67
80:x2:107:ILE:HA	80:x2:111:MET:SD	2.34	0.67
69:m2:369:U:H4'	69:m2:373:A:C8	2.30	0.67
75:s2:50:PRO:HG2	75:s2:90:VAL:HG22	1.75	0.67
2:A2:1008:C:H42	2:A2:1016:A:H61	1.42	0.67
19:F1:64:VAL:HA	19:F1:67:HIS:CD2	2.30	0.67
31:J3:88:ILE:HG23	31:J3:93:ILE:HD11	1.77	0.67
58:a2:63:VAL:HG23	58:a2:66:ARG:NE	2.09	0.67
20:F2:10:VAL:HG13	20:F2:153:VAL:HG12	1.77	0.67
20:F2:143:ARG:HD3	20:F2:182:LYS:HD2	1.76	0.67
55:X2:64:ILE:HG23	55:X2:68:LEU:HD23	1.76	0.67
55:X2:90:ARG:HD3	55:X2:102:LEU:HD13	1.77	0.67
33:K3:67:VAL:HG23	33:K3:99:GLY:HA2	1.77	0.67
77:u2:81:VAL:HG12	77:u2:91:VAL:HG23	1.75	0.67
2:A2:3379:A:H2'	2:A2:3380:A2M:H8	1.77	0.67
69:m2:1230:A:H2'	69:m2:1231:G:H8	1.60	0.67
69:m2:1538:G:H2'	69:m2:1539:A:H8	1.60	0.67
2:A2:2500:A:H2'	2:A2:2501:A:H8	1.59	0.67
69:m2:88:G:H21	69:m2:502:A:H5'	1.59	0.67
78:v2:53:LYS:HD3	78:v2:64:TRP:HB3	1.75	0.67
3:A3:36:VAL:HG13	3:A3:40:TYR:HD2	1.59	0.67
48:S2:74:TYR:CD2	48:S2:77:LYS:HG2	2.29	0.67
69:m2:942:U:H3	69:m2:1004:U:H3	1.43	0.67
50:T2:11:VAL:HG12	50:T2:82:PRO:HA	1.77	0.66
69:m2:153:G:H22	69:m2:165:G:H21	1.39	0.66
26:H2:187:VAL:HG21	26:H2:265:LEU:HD11	1.77	0.66
29:I3:251:ALA:HB2	29:I3:289:LEU:HD21	1.77	0.66
33:K3:32:MET:HE1	33:K3:54:GLY:HA2	1.77	0.66
27:H3:8:TRP:HE1	69:m2:1514:C:H5'	1.60	0.66
73:q2:24:PHE:HB2	78:v2:58:VAL:HG11	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:y2:102:GLU:HG3	81:y2:105:LYS:HE3	1.77	0.66
2:A2:175:C:H2'	2:A2:176:G:H8	1.60	0.66
57:Z2:33:VAL:HG23	57:Z2:38:GLU:HB2	1.78	0.66
69:m2:529:C:H2'	69:m2:530:A:H8	1.59	0.66
69:m2:1230:A:H2'	69:m2:1231:G:C8	2.30	0.66
2:A2:184:U:H5''	2:A2:254:G:H22	1.60	0.66
69:m2:876:G:H2'	69:m2:877:A:H8	1.59	0.66
2:A2:139:G:H2'	2:A2:140:G:C8	2.31	0.66
2:A2:2500:A:H2'	2:A2:2501:A:C8	2.31	0.66
14:D2:44:ILE:HG23	14:D2:46:LYS:HD3	1.75	0.66
35:L3:111:GLN:HE21	35:L3:145:PRO:HB3	1.61	0.66
36:M2:19:THR:HG23	36:M2:22:CYS:H	1.60	0.66
80:x2:22:LEU:HD23	80:x2:26:LEU:HD23	1.78	0.66
2:A2:3353:U:H5''	2:A2:3354:G:H5'	1.77	0.66
23:G2:60:ILE:H	23:G2:80:ALA:HB3	1.61	0.66
30:J2:128:ARG:HH21	30:J2:136:ILE:HD13	1.59	0.66
29:I3:121:VAL:HG12	29:I3:131:LEU:HG	1.77	0.66
35:L3:114:VAL:HG22	35:L3:120:ALA:HB2	1.78	0.66
82:z2:98:VAL:HB	82:z2:114:LEU:HD12	1.78	0.66
2:A2:4603:C:H2'	2:A2:4604:C:C6	2.31	0.65
6:B3:9:VAL:HG21	6:B3:138:VAL:HG13	1.77	0.65
12:C3:31:SER:HB3	12:C3:107:GLU:HG2	1.76	0.65
27:H3:32:ARG:HH22	27:H3:38:MET:HB2	1.61	0.65
29:I3:240:CYS:H	29:I3:249:CYS:HB2	1.61	0.65
81:y2:43:GLU:HG3	81:y2:44:PRO:HD3	1.78	0.65
4:B1:58:PRO:HD2	4:B1:61:ILE:HD12	1.78	0.65
73:q2:136:VAL:HG22	73:q2:186:VAL:HG22	1.77	0.65
2:A2:3430:A:H2'	2:A2:3431:A:C8	2.32	0.65
31:J3:81:ILE:HG21	31:J3:88:ILE:HD11	1.79	0.65
2:A2:744:C:H3'	2:A2:746:G:H5''	1.79	0.65
23:G2:65:ALA:HB2	23:G2:74:ILE:HD13	1.78	0.65
63:f2:28:ARG:HA	63:f2:33:ASN:HD22	1.60	0.65
76:t2:28:LEU:HD23	76:t2:32:MET:HE1	1.79	0.65
13:D1:91:LEU:HD12	13:D1:135:ILE:HG23	1.79	0.65
69:m2:930:G:H1	69:m2:1015:U:H3	1.42	0.65
74:r2:170:ILE:HG12	74:r2:171:ASN:HD22	1.62	0.65
2:A2:1011:U:H3'	2:A2:1012:C:H5''	1.77	0.64
20:F2:287:THR:HG21	68:k2:5:LEU:HB2	1.78	0.64
33:K3:195:LYS:HB3	69:m2:126:G:H5''	1.79	0.64
38:N2:8:ARG:HE	38:N2:52:MET:HE1	1.62	0.64
2:A2:453:G:H4'	2:A2:454:U:H5'	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:m2:190:G:H5''	77:u2:145:ILE:HD12	1.79	0.64
2:A2:4563:C:H2'	2:A2:4564:G:H8	1.62	0.64
3:A3:117:ILE:HD11	80:x2:111:MET:HG3	1.79	0.64
45:Q3:17:LEU:HD12	45:Q3:18:LEU:HD12	1.79	0.64
69:m2:1654:G:H1	69:m2:1674:U:H3	1.44	0.64
71:o2:77:ILE:HG13	71:o2:99:ILE:HG13	1.79	0.64
2:A2:1040:C:H2'	2:A2:1041:G:H8	1.61	0.64
12:C3:55:ARG:HG2	12:C3:87:ARG:HD3	1.78	0.64
66:i2:23:VAL:HG12	66:i2:70:LEU:HD23	1.80	0.64
21:F3:65:PRO:HG3	41:O3:129:ILE:HB	1.79	0.64
7:Bv:26:A:H61	7:Bv:43:C:H42	1.45	0.64
23:G2:207:TYR:HE2	23:G2:222:GLN:HG2	1.62	0.64
2:A2:6:C:H5''	4:B1:197:LYS:HB3	1.80	0.64
69:m2:641:C:H2'	69:m2:642:A:H8	1.63	0.64
14:D2:54:ARG:HH11	14:D2:58:LEU:HD21	1.63	0.64
3:A3:36:VAL:HG21	3:A3:71:MET:HE3	1.79	0.64
69:m2:641:C:H2'	69:m2:642:A:C8	2.33	0.64
56:Y2:35:TRP:CZ2	56:Y2:56:PRO:HD2	2.33	0.63
35:L3:124:HIS:CD2	69:m2:528:A:H5''	2.33	0.63
69:m2:28:U:H2'	69:m2:29:G:H8	1.63	0.63
42:P2:13:LYS:HB2	42:P2:128:LEU:HD21	1.80	0.63
69:m2:1608:G:N2	69:m2:1634:G:H2'	2.12	0.63
2:A2:1722:C:H3'	2:A2:1723:C:H5''	1.80	0.63
52:U2:88:VAL:HG12	52:U2:92:LYS:HZ3	1.64	0.63
2:A2:1146:C:H2'	2:A2:1147:A:H8	1.63	0.63
6:B3:6:VAL:HG12	6:B3:135:ALA:HB2	1.80	0.63
69:m2:1523:C:C4'	80:x2:126:VAL:CG1	2.76	0.63
69:m2:1681:A:H2'	75:s2:60:ARG:HD3	1.81	0.63
76:t2:57:ARG:HH22	76:t2:172:THR:HB	1.63	0.63
2:A2:1754:G:H4'	36:M2:93:MET:HG2	1.80	0.63
69:m2:1279:C:H2'	69:m2:1280:A:H8	1.62	0.63
69:m2:1538:G:H2'	69:m2:1539:A:C8	2.34	0.63
23:G2:153:THR:HG23	23:G2:160:PHE:CZ	2.34	0.63
24:G3:44:ARG:HH12	24:G3:63:ARG:HB2	1.64	0.63
27:H3:30:LEU:HG	69:m2:1258:G:N2	2.13	0.63
54:W2:35:LEU:HD22	54:W2:63:TYR:HD2	1.64	0.63
58:a2:46:CYS:HB3	58:a2:82:MET:HE3	1.81	0.63
2:A2:1190:C:H3'	2:A2:1191:G:C8	2.34	0.62
23:G2:33:ARG:HH11	38:N2:27:LEU:HD22	1.64	0.62
69:m2:1409:U:H2'	69:m2:1410:U:C6	2.34	0.62
17:E2:89:ILE:HD12	17:E2:197:ALA:HB1	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:r2:242:LYS:HG3	74:r2:244:ILE:HG12	1.79	0.62
2:A2:223:G:H4'	2:A2:225:G:N7	2.14	0.62
2:A2:1744:A:H2'	2:A2:1745:A:C8	2.33	0.62
2:A2:3903:A:H5''	16:E1:108:GLY:HA3	1.80	0.62
28:I2:118:MET:HE3	36:M2:167:PHE:HB3	1.81	0.62
45:Q3:51:THR:HG22	45:Q3:53:ASP:H	1.64	0.62
60:c2:80:HIS:CD2	60:c2:84:LYS:HD2	2.34	0.62
71:o2:54:THR:HA	71:o2:162:PRO:HG2	1.81	0.62
17:E2:379:PHE:CD2	17:E2:385:LYS:HG3	2.35	0.62
42:P2:13:LYS:HD2	42:P2:128:LEU:HD11	1.81	0.62
68:k2:51:VAL:HG22	68:k2:62:VAL:HG22	1.80	0.62
74:r2:124:CYS:HB3	74:r2:141:THR:HG23	1.82	0.62
77:u2:100:CYS:HB3	77:u2:175:ILE:HD13	1.82	0.62
2:A2:318:A:H2'	2:A2:319:A:C8	2.34	0.62
14:D2:45:VAL:HG22	14:D2:61:VAL:HG22	1.80	0.62
23:G2:273:LEU:O	23:G2:277:LYS:HG2	2.00	0.62
33:K3:66:GLY:HA2	69:m2:1747:A:H1'	1.81	0.62
81:y2:42:ILE:HG22	81:y2:44:PRO:HD2	1.81	0.62
29:I3:72:SER:HB2	29:I3:75:GLY:HA2	1.80	0.62
45:Q3:114:MET:HB3	45:Q3:122:LYS:HD2	1.82	0.62
48:S2:31:SER:HA	48:S2:48:PRO:HA	1.82	0.62
41:O3:62:VAL:HG12	41:O3:64:ALA:H	1.65	0.62
69:m2:597:U:H2'	69:m2:598:U:C6	2.35	0.62
80:x2:81:ARG:HH21	80:x2:120:SER:HB3	1.63	0.62
7:Bv:6:G:HO2'	7:Bv:7:A:H8	1.47	0.61
27:H3:53:ILE:HG13	27:H3:55:LEU:HD12	1.82	0.61
69:m2:1523:C:C5'	80:x2:126:VAL:CG1	2.77	0.61
14:D2:129:ALA:HB3	14:D2:132:ASN:HD22	1.66	0.61
74:r2:11:ARG:HH11	74:r2:20:LEU:HB3	1.65	0.61
17:E2:56:ILE:HD12	17:E2:365:LEU:HD22	1.82	0.61
29:I3:17:TRP:HB2	29:I3:36:ARG:HD2	1.81	0.61
31:J3:166:ARG:HB3	31:J3:247:THR:HB	1.81	0.61
69:m2:930:G:H2'	69:m2:931:G:C8	2.35	0.61
69:m2:1397:C:H2'	69:m2:1398:A:C8	2.35	0.61
6:B3:107:LEU:HA	6:B3:110:LEU:HG	1.82	0.61
2:A2:1628:G:H21	53:V2:50:ASN:HD21	1.49	0.61
2:A2:4395:G:H2'	2:A2:4396:A:C8	2.35	0.61
27:H3:32:ARG:HH22	27:H3:43:PHE:HB2	1.65	0.61
31:J3:106:VAL:HG12	31:J3:128:VAL:HG22	1.81	0.61
69:m2:604:G:H1	69:m2:622:G:N2	1.98	0.61
69:m2:1201:A:H2'	69:m2:1202:A:C8	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:m2:1205:G:H2'	69:m2:1206:A:C8	2.34	0.61
46:R2:127:LEU:HD22	46:R2:135:LYS:HE2	1.83	0.61
61:d2:69:ILE:HG22	61:d2:73:ARG:HD2	1.82	0.61
69:m2:1580:U:H2'	73:q2:4:GLN:HE22	1.64	0.61
76:t2:87:PHE:HD2	76:t2:90:LYS:HZ1	1.49	0.61
51:T3:55:PRO:HG2	69:m2:607:A:H5''	1.83	0.61
69:m2:564:U:H2'	69:m2:565:G:C8	2.36	0.61
69:m2:1390:A:H61	73:q2:161:GLY:HA3	1.65	0.61
10:C1:92:MET:HG2	10:C1:181:VAL:HA	1.82	0.61
19:F1:28:GLN:O	19:F1:32:LYS:HG3	2.00	0.61
45:Q3:5:VAL:HG23	45:Q3:27:VAL:HG13	1.83	0.61
69:m2:651:U:H2'	69:m2:652:A:H8	1.66	0.61
79:w2:37:TYR:OH	79:w2:51:ILE:HA	2.01	0.61
2:A2:1140:A2M:H2'	2:A2:1141:C:C6	2.36	0.60
26:H2:151:ILE:HG12	26:H2:157:LEU:HD21	1.82	0.60
69:m2:116:OMU:HN3	69:m2:349:G:H1	1.48	0.60
69:m2:1738:G:H2'	69:m2:1739:G:C8	2.36	0.60
2:A2:718:A:H2'	2:A2:719:C:C6	2.36	0.60
2:A2:2106:OMC:HM22	20:F2:95:MET:HG3	1.83	0.60
2:A2:4264:C:C2	10:C1:120:GLU:HB2	2.36	0.60
20:F2:254:GLU:O	20:F2:258:ARG:HG3	2.00	0.60
2:A2:3926:A:H2'	2:A2:3927:G:C8	2.35	0.60
54:W2:47:ILE:HD13	54:W2:94:LEU:HD11	1.82	0.60
55:X2:36:VAL:HG23	55:X2:41:ARG:HG2	1.83	0.60
22:G1:130:LEU:HB3	28:I2:177:LEU:HD23	1.83	0.60
69:m2:1219:A:H2'	69:m2:1220:C:C6	2.37	0.60
2:A2:129:C:H2'	2:A2:130:G:H8	1.64	0.60
2:A2:140:G:H2'	2:A2:141:C:C6	2.37	0.60
73:q2:132:LYS:HE3	73:q2:156:LEU:HD23	1.82	0.60
20:F2:230:LEU:HD21	20:F2:239:LYS:HD2	1.83	0.60
35:L3:13:TYR:HE1	35:L3:44:TRP:HE3	1.50	0.60
45:Q3:16:ARG:HB2	74:r2:94:LYS:HE3	1.82	0.60
66:i2:33:LEU:HA	66:i2:38:LYS:HG2	1.83	0.60
69:m2:1590:A:H2'	69:m2:1591:A:C8	2.36	0.60
69:m2:1608:G:H22	69:m2:1634:G:H2'	1.67	0.60
2:A2:1441:C:H5''	14:D2:15:VAL:HG21	1.82	0.60
3:A3:39:ARG:HD2	6:B3:39:LEU:HD23	1.84	0.60
41:O3:53:ILE:HG23	41:O3:88:LEU:HD22	1.83	0.60
48:S2:44:VAL:HG11	48:S2:47:MET:HE2	1.82	0.60
69:m2:31:U:H3	69:m2:518:A:H2	1.48	0.60
20:F2:289:LEU:HD11	32:K2:31:LEU:HB2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:m2:529:C:H2'	69:m2:530:A:C8	2.37	0.60
72:p2:185:VAL:O	72:p2:189:ILE:HG12	2.02	0.60
2:A2:113:A:H4'	25:H1:49:ARG:HG2	1.84	0.60
4:B1:147:VAL:HG22	4:B1:179:VAL:HG21	1.84	0.60
2:A2:2294:C:H5''	58:a2:66:ARG:HH11	1.67	0.60
15:D3:14:PRO:HG2	15:D3:23:ILE:HD12	1.82	0.60
20:F2:36:ILE:HD12	20:F2:122:TYR:CE2	2.37	0.60
21:F3:22:ARG:NH1	41:O3:141:ARG:HE	1.99	0.60
23:G2:264:LYS:HD3	23:G2:266:TRP:CZ2	2.36	0.60
69:m2:853:C:H5''	69:m2:854:G:H5'	1.84	0.60
74:r2:11:ARG:HA	74:r2:28:ALA:HB2	1.82	0.60
2:A2:4109:U:H1'	17:E2:252:ALA:HB3	1.84	0.59
6:B3:71:GLY:H	6:B3:74:SER:HB3	1.66	0.59
29:I3:195:LEU:HA	29:I3:211:GLY:HA3	1.83	0.59
39:N3:129:TYR:HB3	39:N3:135:LEU:HD13	1.83	0.59
69:m2:1738:G:H2'	69:m2:1739:G:H8	1.67	0.59
73:q2:20:GLU:HG3	78:v2:59:LYS:HG3	1.84	0.59
73:q2:105:LEU:HD12	73:q2:122:VAL:HG21	1.84	0.59
2:A2:3268:C:H5'	77:u2:92:ARG:HH22	1.66	0.59
4:B1:35:ARG:HH12	50:T2:52:LYS:HE3	1.67	0.59
68:k2:28:GLU:HG3	68:k2:31:ASN:HB2	1.83	0.59
2:A2:4041:C:H2'	2:A2:4042:A:H8	1.67	0.59
69:m2:1523:C:C4'	80:x2:126:VAL:HG11	2.32	0.59
81:y2:43:GLU:CG	81:y2:44:PRO:HD3	2.33	0.59
2:A2:4044:OMG:HM21	2:A2:4046:A:H2'	1.83	0.59
14:D2:108:PRO:HG2	67:j2:86:LEU:HD23	1.83	0.59
29:I3:238:ALA:H	29:I3:251:ALA:HB3	1.67	0.59
2:A2:3912:U:H2'	2:A2:3913:C:C6	2.38	0.59
18:E3:67:ARG:HG3	18:E3:115:ILE:HG12	1.84	0.59
19:F1:59:VAL:HG21	19:F1:73:GLY:HA3	1.83	0.59
59:b2:6:ALA:O	59:b2:10:ARG:HG2	2.02	0.59
69:m2:846:U:H2'	69:m2:847:G:C8	2.38	0.59
2:A2:1068:C:H42	2:A2:1082:A:H61	1.50	0.59
42:P2:70:PRO:HA	42:P2:73:ARG:HB2	1.85	0.59
69:m2:602:G:H2'	69:m2:603:OMG:H8	1.66	0.59
2:A2:3743:G:H2'	2:A2:3744:G:C8	2.37	0.59
2:A2:3975:A:C8	23:G2:153:THR:HG21	2.37	0.59
20:F2:163:LYS:HB2	20:F2:166:GLU:HG3	1.85	0.59
29:I3:195:LEU:HD12	29:I3:209:SER:HB2	1.85	0.59
69:m2:954:G:H2'	69:m2:955:C:C6	2.37	0.59
4:B1:137[A]:ARG:HD2	4:B1:146:LEU:HD11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B1:209:SER:HA	4:B1:212:LYS:HG3	1.85	0.59
10:C1:110:SER:HB3	10:C1:127:ARG:HH12	1.68	0.59
15:D3:83:PHE:CZ	71:o2:53:ARG:HG2	2.37	0.59
29:I3:230:LEU:HD13	29:I3:259:TRP:CD2	2.38	0.59
72:p2:121:ILE:HG12	72:p2:161:VAL:HG13	1.83	0.59
75:s2:35:LEU:HD21	75:s2:146:ARG:HD3	1.85	0.59
2:A2:163:A:H2'	2:A2:164:G:H8	1.68	0.59
2:A2:4509:U:H2'	2:A2:4510:C:H6	1.67	0.59
69:m2:1223:G:H2'	69:m2:1224:G:H8	1.67	0.59
29:I3:199:THR:HG22	29:I3:208:ALA:HB3	1.85	0.59
30:J2:36:ILE:HA	30:J2:39:MET:HE2	1.84	0.59
31:J3:227:ARG:HG3	31:J3:228:GLY:H	1.66	0.59
39:N3:40:LEU:HA	39:N3:43:LYS:HZ3	1.68	0.59
72:p2:97:LEU:HB3	72:p2:232:HIS:CE1	2.38	0.59
2:A2:1430:G:H1'	2:A2:2268:A:N6	2.18	0.58
57:Z2:36:ARG:HB2	57:Z2:80:ASN:HA	1.83	0.58
76:t2:126:HIS:CD2	76:t2:181:THR:HB	2.38	0.58
1:A1:234:LYS:HB3	2:A2:1875:C:H5''	1.84	0.58
2:A2:845:C:H5''	26:H2:58:VAL:HG11	1.85	0.58
1:A1:127:VAL:HG13	1:A1:158:VAL:HG12	1.83	0.58
1:A1:242:MET:HB3	1:A1:254:ASP:OD2	2.03	0.58
2:A2:1831:A:H2'	2:A2:1832:A:C8	2.38	0.58
2:A2:4604:C:H2'	2:A2:4605:U:C6	2.38	0.58
31:J3:75:ILE:HD13	31:J3:81:ILE:HD11	1.84	0.58
62:e2:23:VAL:HG22	62:e2:36:VAL:HG22	1.83	0.58
69:m2:434:G:H2'	69:m2:435:A:C8	2.38	0.58
71:o2:39:TYR:CE2	71:o2:40:LYS:HE3	2.37	0.58
72:p2:97:LEU:HD22	72:p2:232:HIS:CD2	2.38	0.58
2:A2:175:C:H2'	2:A2:176:G:C8	2.38	0.58
2:A2:2494:C:H4'	67:j2:52:VAL:HG11	1.84	0.58
11:C2:67:U:H2'	11:C2:68:G:H8	1.68	0.58
26:H2:197:HIS:HB3	26:H2:200:PHE:HD2	1.67	0.58
69:m2:642:A:H2'	69:m2:643:A:C8	2.38	0.58
2:A2:1672:C:H2'	2:A2:1673:A2M:H8	1.84	0.58
2:A2:1893:C:C4	2:A2:1896:A:H4'	2.38	0.58
2:A2:4041:C:H2'	2:A2:4042:A:C8	2.39	0.58
2:A2:4555:A:H4'	17:E2:95:THR:HG22	1.86	0.58
6:B3:41:LYS:HB3	6:B3:95:GLY:HA2	1.86	0.58
20:F2:209:ILE:HB	20:F2:229:LEU:HD13	1.85	0.58
2:A2:3607:G:H2'	2:A2:3608:A:H8	1.67	0.58
18:E3:106:GLY:O	18:E3:108:LYS:HG2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:u2:57:ALA:HB2	77:u2:183:GLY:HA2	1.86	0.58
82:z2:71:ILE:HB	82:z2:74:GLN:HG2	1.85	0.58
2:A2:1115:C:H2'	2:A2:1117:A:C5	2.38	0.58
2:A2:4155:A:H2'	2:A2:4156:C:C6	2.39	0.58
7:Bv:45:U:H2'	7:Bv:46:G:O4'	2.04	0.58
69:m2:1398:A:N1	69:m2:1451:G:C6	2.72	0.58
23:G2:181:PRO:HD2	23:G2:195:HIS:ND1	2.17	0.58
66:i2:44:LYS:NZ	66:i2:52:THR:HB	2.19	0.58
69:m2:186:C:H2'	69:m2:187:G:C8	2.39	0.58
16:E1:136:ARG:NH1	16:E1:157:ILE:HD13	2.19	0.58
29:I3:252:THR:HG21	29:I3:257:LYS:HD3	1.86	0.58
46:R2:110:LYS:HG2	46:R2:114:LYS:HE2	1.86	0.58
69:m2:911:G:H2'	69:m2:912:G:H8	1.67	0.58
2:A2:163:A:H2'	2:A2:164:G:C8	2.39	0.58
25:H1:65:ARG:HG3	25:H1:129:PHE:CE1	2.38	0.58
45:Q3:15:ASN:HD21	45:Q3:18:LEU:HD13	1.69	0.58
2:A2:1354:U:H5''	14:D2:21:LYS:HG2	1.85	0.57
39:N3:99:ARG:HH21	39:N3:115:LEU:HD21	1.69	0.57
41:O3:64:ALA:HB3	41:O3:67:ASP:HB2	1.85	0.57
61:d2:52:LYS:HG3	61:d2:55:ARG:HH21	1.69	0.57
69:m2:186:C:H2'	69:m2:187:G:H8	1.68	0.57
2:A2:1509:C:H2'	2:A2:1510:G:C8	2.40	0.57
5:B2:110:G:H2'	5:B2:111:C:C6	2.39	0.57
14:D2:83:HIS:HB3	67:j2:64:VAL:HG22	1.85	0.57
14:D2:101:VAL:HG22	14:D2:165:VAL:HG22	1.86	0.57
43:P3:86:LEU:O	43:P3:90:GLN:HG3	2.04	0.57
77:u2:22:HIS:HB2	77:u2:25:ARG:HH21	1.68	0.57
2:A2:453:G:H1	2:A2:1107:G:N2	2.02	0.57
48:S2:117:LYS:O	48:S2:121:ARG:HG3	2.03	0.57
2:A2:1893:C:H4'	2:A2:1894:G:H5'	1.85	0.57
2:A2:2275:C:H2'	2:A2:2276:G:H8	1.69	0.57
2:A2:4612:A:H5''	17:E2:128:LYS:HG3	1.86	0.57
3:A3:25:LYS:O	3:A3:29:ALA:HB2	2.04	0.57
69:m2:936:G:H1	69:m2:1010:A:H2	1.47	0.57
1:A1:96:MET:HE1	2:A2:943:C:O2	2.04	0.57
2:A2:162:A:H2'	2:A2:163:A:H8	1.69	0.57
2:A2:3338:A:H5''	14:D2:132:ASN:ND2	2.20	0.57
2:A2:3784:C:H2'	2:A2:3785:G:H8	1.68	0.57
31:J3:114:LYS:HE2	69:m2:1204:U:H4'	1.86	0.57
82:z2:41:ILE:HD12	82:z2:47:ARG:HG3	1.85	0.57
2:A2:1628:G:H21	53:V2:50:ASN:ND2	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A2:3711:C:H2'	2:A2:3712:A:H8	1.69	0.57
2:A2:4045:G:O4'	2:A2:4099:5MC:HM52	2.05	0.57
10:C1:12:ILE:HG12	10:C1:18:ILE:HD12	1.85	0.57
12:C3:51:LYS:HE3	69:m2:1404:A:H4'	1.85	0.57
46:R2:64:SER:HB2	59:b2:69:LEU:HD23	1.87	0.57
69:m2:120:U:H2'	69:m2:121:OMU:H6	1.86	0.57
71:o2:112:ILE:HG22	71:o2:113:GLN:HG3	1.86	0.57
81:y2:143:LYS:HE2	81:y2:145:TYR:HE1	1.70	0.57
2:A2:260:C:H2'	2:A2:261:G:H8	1.68	0.57
2:A2:418:A:C2	11:C2:17:A:H1'	2.38	0.57
2:A2:4531:C:H42	2:A2:4578:C:H42	1.52	0.57
26:H2:186:LEU:HD12	26:H2:190:ARG:HA	1.86	0.57
41:O3:42:VAL:HG23	41:O3:43:HIS:H	1.69	0.57
71:o2:50:ASN:HD21	71:o2:53:ARG:HD2	1.69	0.57
17:E2:105:VAL:HG11	17:E2:150:PHE:CE1	2.39	0.57
24:G3:51:ARG:HG3	75:s2:61:PHE:CE2	2.40	0.57
55:X2:53:ALA:HA	55:X2:88:LEU:HD21	1.86	0.57
80:x2:52:LYS:HB2	80:x2:80:LEU:HD11	1.86	0.57
2:A2:2166:C:H2'	2:A2:2167:A:H8	1.69	0.57
2:A2:4395:G:H2'	2:A2:4396:A:H8	1.68	0.57
25:H1:108:ARG:HE	25:H1:161:MET:HE2	1.70	0.57
69:m2:29:G:H2'	69:m2:30:C:C6	2.40	0.57
81:y2:51:LEU:HD22	81:y2:81:ILE:HG23	1.87	0.57
2:A2:196:C:H4'	48:S2:126:ARG:HG2	1.86	0.57
2:A2:2166:C:H2'	2:A2:2167:A:C8	2.40	0.57
35:L3:18:ARG:HH22	69:m2:4:C:H1'	1.70	0.57
2:A2:2599:A:O2'	2:A2:4283:G:H4'	2.05	0.56
10:C1:128:MET:SD	10:C1:157:SER:HB3	2.45	0.56
23:G2:33:ARG:O	23:G2:37:VAL:HG22	2.05	0.56
28:I2:8:VAL:HG12	28:I2:117:ARG:HG3	1.86	0.56
29:I3:42:MET:HE2	29:I3:57:ARG:HB3	1.88	0.56
39:N3:141:TYR:HE1	39:N3:146:ALA:HB2	1.69	0.56
69:m2:1564:C:H2'	69:m2:1565:G:H8	1.70	0.56
78:v2:3:MET:HG3	78:v2:41:PRO:HB2	1.86	0.56
2:A2:1763:G:H2'	2:A2:1826:G:H22	1.68	0.56
2:A2:4030:A:O2'	2:A2:4031:A:H2'	2.04	0.56
2:A2:4505:G:H2'	2:A2:4506:G:C8	2.40	0.56
13:D1:48:LEU:HD11	13:D1:167:ILE:HD12	1.88	0.56
48:S2:101:PRO:O	48:S2:104:VAL:HG22	2.05	0.56
69:m2:16:G:H2'	69:m2:17:C:C6	2.40	0.56
2:A2:318:A:H2'	2:A2:319:A:H8	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A2:2203:G:H2'	2:A2:2204:A:C8	2.41	0.56
2:A2:3586:U:H3	2:A2:3832:G:H1	1.51	0.56
18:E3:129:SER:HB3	69:m2:29:G:H4'	1.87	0.56
30:J2:119:VAL:HG12	30:J2:146:ILE:HG12	1.87	0.56
31:J3:183:LYS:HG2	31:J3:196:ILE:HG12	1.87	0.56
40:O2:42:PHE:CE2	40:O2:90:TYR:HB2	2.40	0.56
69:m2:152:U:H2'	69:m2:153:G:C8	2.41	0.56
69:m2:1006:U:H2'	69:m2:1007:G:H8	1.69	0.56
69:m2:1223:G:H2'	69:m2:1224:G:C8	2.40	0.56
79:w2:111:VAL:HG12	79:w2:140:PHE:HB2	1.86	0.56
1:A1:147:LEU:HD22	1:A1:152:ILE:HD11	1.87	0.56
2:A2:1613:G:H21	53:V2:57:MET:HE3	1.70	0.56
6:B3:76:THR:HG21	6:B3:97:LYS:HG2	1.86	0.56
31:J3:88:ILE:HG21	31:J3:94:ILE:HD11	1.88	0.56
42:P2:82:ILE:HD12	42:P2:121:VAL:HG22	1.87	0.56
2:A2:300:A:H2'	2:A2:301:G:H8	1.69	0.56
2:A2:878:G:H2'	2:A2:879:C:H6	1.70	0.56
2:A2:3608:A:H2'	2:A2:3609:G:C8	2.40	0.56
19:F1:80:GLU:HA	19:F1:83:VAL:HG12	1.87	0.56
69:m2:1094:G:H2'	69:m2:1095:A:H8	1.71	0.56
74:r2:161:GLN:HB3	74:r2:170:ILE:O	2.05	0.56
1:A1:138:GLN:HB3	1:A1:141:ASN:OD1	2.05	0.56
2:A2:1122:C:H2'	2:A2:1123:C:C6	2.40	0.56
21:F3:22:ARG:HH12	41:O3:141:ARG:HE	1.52	0.56
50:T2:22:LYS:NZ	50:T2:134:LEU:HB2	2.20	0.56
54:W2:35:LEU:HD22	54:W2:63:TYR:CD2	2.40	0.56
69:m2:28:U:H2'	69:m2:29:G:C8	2.40	0.56
69:m2:121:OMU:HN3	69:m2:345:A:H61	1.51	0.56
2:A2:1332:C:HO2'	20:F2:102:PHE:HE1	1.54	0.56
2:A2:3910:C:H2'	2:A2:3911:C:H6	1.70	0.56
6:B3:122:LYS:HD2	6:B3:123:LEU:O	2.05	0.56
17:E2:285:TYR:OH	17:E2:334:LYS:HD2	2.05	0.56
42:P2:90:ARG:HH21	42:P2:123:LYS:HD2	1.71	0.56
72:p2:144:LYS:HG2	72:p2:146:ARG:HH21	1.71	0.56
2:A2:207:G:H2'	2:A2:208:A:C8	2.41	0.56
2:A2:1214:G:H2'	2:A2:1215:G:H8	1.69	0.56
6:B3:11:GLN:OE1	6:B3:62:ARG:HD2	2.06	0.56
7:Bv:34:G:H2'	7:Bv:35:A:C8	2.41	0.56
17:E2:89:ILE:HD12	17:E2:162:ILE:HG22	1.88	0.56
69:m2:1146:A:H5'	69:m2:1357:C:H41	1.71	0.56
70:n2:71:U:H2'	70:n2:72:A:H8	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:254:ASP:HA	1:A1:258:ARG:HH21	1.70	0.56
2:A2:938:U:H3	2:A2:1049:C:H42	1.53	0.56
39:N3:142:GLU:HG2	39:N3:143:SER:H	1.70	0.56
43:P3:52:ILE:HG12	43:P3:61:ILE:HG12	1.87	0.56
45:Q3:17:LEU:HB3	74:r2:94:LYS:HD2	1.88	0.56
69:m2:510:A:H3'	69:m2:511:OMG:H8	1.71	0.56
69:m2:564:U:H3	69:m2:589:A:H2	1.53	0.56
69:m2:1799:U:H2'	69:m2:1800:C:C6	2.41	0.56
81:y2:44:PRO:HD2	81:y2:81:ILE:HD11	1.88	0.56
2:A2:268:G:H2'	2:A2:269:G:H8	1.71	0.56
2:A2:2482:C:H2'	2:A2:2483:U:C6	2.41	0.56
2:A2:3931:A:H5'	2:A2:3933:A:H1'	1.88	0.56
27:H3:38:MET:HE3	27:H3:43:PHE:HA	1.87	0.56
36:M2:11:LYS:HD3	36:M2:63:TYR:HE2	1.71	0.56
66:i2:61:LYS:HE3	66:i2:87:ARG:HH12	1.70	0.56
2:A2:1626:G:H4'	23:G2:44:TYR:CD2	2.41	0.55
2:A2:1709:A:H2'	2:A2:1710:A:C8	2.41	0.55
2:A2:3277:A:C8	2:A2:4294:U:H1'	2.41	0.55
2:A2:4391:C:H3'	2:A2:4393:A:H5''	1.89	0.55
2:A2:4509:U:H2'	2:A2:4510:C:C6	2.41	0.55
18:E3:10:ALA:HB1	79:w2:96:ILE:HD12	1.87	0.55
27:H3:30:LEU:HD22	69:m2:1661:U:H4'	1.88	0.55
69:m2:850:U:H2'	69:m2:851:A:H8	1.71	0.55
70:n2:69:G:H2'	70:n2:70:C:H6	1.71	0.55
74:r2:44:LEU:HD11	74:r2:72:ILE:HD11	1.87	0.55
2:A2:162:A:H2'	2:A2:163:A:C8	2.42	0.55
4:B1:34:LYS:HE3	4:B1:36:PRO:HG3	1.87	0.55
38:N2:8:ARG:NE	38:N2:52:MET:HE1	2.19	0.55
69:m2:457:A:H2'	69:m2:458:C:C6	2.41	0.55
69:m2:1716:U:H2'	69:m2:1717:A:C8	2.42	0.55
1:A1:238:PRO:HG3	1:A1:242:MET:HG3	1.89	0.55
2:A2:2370:U:H3	2:A2:2477:G:H1	1.53	0.55
22:G1:117:LYS:O	22:G1:121:ARG:HG2	2.05	0.55
35:L3:159:PHE:HA	35:L3:162:ARG:HH21	1.71	0.55
69:m2:427:G:H5''	69:m2:428:A:H2	1.71	0.55
77:u2:74:ARG:HG2	77:u2:108:PRO:CB	2.36	0.55
77:u2:98:LYS:HD2	77:u2:178:ARG:HG2	1.87	0.55
2:A2:4044:OMG:H2'	2:A2:4099:5MC:HM51	1.88	0.55
29:I3:253:GLY:HA2	29:I3:285:GLN:HG3	1.89	0.55
40:O2:56:LEU:HD12	40:O2:61:VAL:HG13	1.89	0.55
73:q2:135:GLU:HG3	73:q2:153:VAL:HG12	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:z2:17:ILE:HD11	82:z2:54:VAL:HA	1.89	0.55
2:A2:1314:C:H2'	32:K2:68:ARG:NH2	2.21	0.55
2:A2:4638:G:H2'	2:A2:4639:G:C8	2.42	0.55
28:I2:125:LYS:HG3	28:I2:129:LEU:HD12	1.89	0.55
2:A2:3912:U:H2'	2:A2:3913:C:H6	1.72	0.55
16:E1:109:ILE:HG21	16:E1:115:LEU:HD11	1.88	0.55
19:F1:81:LEU:HD11	19:F1:98:VAL:HG22	1.89	0.55
23:G2:200:MET:HB3	23:G2:237:GLU:HG2	1.89	0.55
28:I2:157:GLU:O	28:I2:161:LYS:HG3	2.06	0.55
30:J2:64:ASN:HB2	30:J2:80:GLN:OE1	2.06	0.55
33:K3:2:LYS:HB2	33:K3:108:VAL:HG22	1.89	0.55
2:A2:1333:C:H5'	20:F2:102:PHE:CE1	2.42	0.55
11:C2:154:G:H2'	11:C2:155:C:C6	2.41	0.55
21:F3:75:VAL:HG11	69:m2:1866:U:C2	2.42	0.55
28:I2:141:LEU:O	28:I2:145:VAL:HG22	2.07	0.55
28:I2:168:TYR:CE2	28:I2:172:LYS:HD2	2.41	0.55
45:Q3:15:ASN:ND2	45:Q3:18:LEU:HD13	2.21	0.55
69:m2:486:A2M:H8	69:m2:486:A2M:O5'	2.07	0.55
69:m2:831:C:H4'	69:m2:832:A:H5'	1.89	0.55
71:o2:201:LEU:HD23	71:o2:201:LEU:H	1.72	0.55
2:A2:33:A:H5''	2:A2:47:A:H61	1.72	0.55
2:A2:1068:C:H2'	2:A2:1069:G:C8	2.42	0.55
4:B1:159:HIS:ND1	4:B1:185:LYS:HA	2.22	0.55
16:E1:93:GLU:HG3	16:E1:175:LEU:HD23	1.88	0.55
48:S2:74:TYR:CE2	48:S2:77:LYS:HE3	2.42	0.55
69:m2:530:A:H2'	69:m2:531:A:C8	2.42	0.55
71:o2:12:GLU:O	71:o2:16:LEU:HD23	2.07	0.55
71:o2:123:VAL:HA	71:o2:145:ILE:O	2.07	0.55
2:A2:2357:G:H2'	2:A2:2358:C:C6	2.42	0.55
2:A2:2512:A:O2'	2:A2:2513:G:H5'	2.07	0.55
2:A2:3312:A:H2'	2:A2:3313:U:C6	2.41	0.55
2:A2:3975:A:N7	23:G2:153:THR:HG21	2.22	0.55
29:I3:250:ALA:HB3	29:I3:257:LYS:O	2.06	0.55
43:P3:6:VAL:HG23	43:P3:29:PRO:HG2	1.88	0.55
69:m2:1379:U:H3'	71:o2:102:ARG:HH22	1.72	0.55
70:n2:69:G:H2'	70:n2:70:C:C6	2.42	0.55
2:A2:3926:A:H2'	2:A2:3927:G:H8	1.70	0.55
2:A2:4111:U:H2'	2:A2:4112:U:C6	2.42	0.55
6:B3:28:LEU:HD21	6:B3:53:PHE:CD2	2.42	0.55
13:D1:61:SER:HA	13:D1:126:VAL:HG12	1.88	0.55
17:E2:88:GLY:O	17:E2:89:ILE:HD13	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:G1:10:GLY:HA2	22:G1:64:PHE:CE1	2.41	0.55
71:o2:30:LEU:HD21	71:o2:35:GLU:HB3	1.88	0.55
71:o2:38:ILE:HG22	71:o2:49:ILE:HG12	1.89	0.55
76:t2:83:LEU:HB3	76:t2:92:VAL:HG21	1.89	0.55
2:A2:302:C:OP1	25:H1:68:ARG:HB2	2.07	0.54
2:A2:2366:A:H2'	2:A2:2367:G:C8	2.42	0.54
3:A3:121:ARG:HG3	3:A3:131:VAL:HB	1.87	0.54
6:B3:43:LYS:HB3	69:m2:1541:U:OP1	2.07	0.54
23:G2:207:TYR:CE2	23:G2:222:GLN:HG2	2.42	0.54
26:H2:290:PRO:HG2	57:Z2:7:CYS:SG	2.47	0.54
35:L3:111:GLN:NE2	35:L3:127:ARG:HA	2.22	0.54
69:m2:679:G:H21	69:m2:1030:A:H62	1.54	0.54
76:t2:51:ILE:HG12	76:t2:179:LYS:HG3	1.89	0.54
2:A2:2096:A:H5''	20:F2:46:LYS:HE2	1.89	0.54
2:A2:3744:G:H22	2:A2:3765:G:N2	2.05	0.54
2:A2:4010:U:H5''	19:F1:194:ILE:HD13	1.89	0.54
2:A2:4145:U:H2'	2:A2:4146:OMG:H8	1.72	0.54
6:B3:30:VAL:HB	6:B3:34:VAL:HG11	1.88	0.54
11:C2:83:C:N4	48:S2:50:ARG:HH22	2.04	0.54
35:L3:6:SER:HB3	74:r2:23:LEU:HD21	1.88	0.54
43:P3:52:ILE:HB	76:t2:144:ILE:CG2	2.37	0.54
47:R3:69:THR:H	47:R3:72:VAL:HG12	1.72	0.54
52:U2:71:PRO:HG2	52:U2:108:TYR:HA	1.89	0.54
69:m2:511:OMG:H2'	69:m2:512:G:H8	1.72	0.54
1:A1:245:LYS:HD2	2:A2:1709:A:H4'	1.89	0.54
2:A2:151:G:H3'	25:H1:49:ARG:HH21	1.72	0.54
2:A2:444:G:H2'	2:A2:445:U:C6	2.42	0.54
2:A2:1170:U:H2'	2:A2:1171:C:C6	2.43	0.54
2:A2:4253:U:H2'	2:A2:4254:A:H8	1.71	0.54
4:B1:59:ARG:HG2	4:B1:62:ARG:NH2	2.18	0.54
17:E2:8:ALA:HB1	42:P2:48:ARG:HH12	1.72	0.54
34:L2:163:ARG:HH21	69:m2:873:U:H3	1.55	0.54
37:M3:85:LEU:HG	37:M3:106:CYS:HB3	1.88	0.54
69:m2:560:G:H2'	69:m2:561:G:C8	2.42	0.54
69:m2:651:U:H2'	69:m2:652:A:C8	2.41	0.54
69:m2:842:C:H4'	69:m2:843:G:O5'	2.07	0.54
71:o2:206:ASP:HB3	71:o2:210:ILE:HG21	1.89	0.54
80:x2:111:MET:HG2	80:x2:119:PHE:CE2	2.42	0.54
2:A2:943:C:H2'	2:A2:944:G:C8	2.41	0.54
2:A2:3923:A:H62	2:A2:3983:G:N2	2.05	0.54
29:I3:212:LYS:HA	29:I3:235:ILE:HG22	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:K3:106:LEU:HD22	33:K3:109:LEU:HD12	1.90	0.54
43:P3:42:MET:SD	76:t2:148:LEU:HA	2.47	0.54
69:m2:188:C:C4	69:m2:189:U:C4	2.96	0.54
69:m2:881:C:H2'	69:m2:882:G:H8	1.73	0.54
70:n2:71:U:H2'	70:n2:72:A:C8	2.42	0.54
75:s2:17:ILE:HG23	75:s2:19:LEU:HD13	1.88	0.54
76:t2:60:ILE:HD11	76:t2:92:VAL:HG22	1.89	0.54
78:v2:14:LEU:HD11	78:v2:34:GLU:HG3	1.90	0.54
2:A2:2275:C:H5''	58:a2:33:LEU:HD22	1.90	0.54
2:A2:3600:G:H2'	2:A2:3601:A:C8	2.43	0.54
17:E2:217:ILE:HD12	17:E2:347:LEU:HB3	1.90	0.54
20:F2:94:ASN:HB3	20:F2:100:ARG:HH12	1.73	0.54
32:K2:177:ALA:O	32:K2:184:ARG:HB2	2.07	0.54
39:N3:46:THR:HG22	39:N3:48:SER:H	1.72	0.54
69:m2:1410:U:H2'	69:m2:1411:A:C8	2.43	0.54
2:A2:943:C:H2'	2:A2:944:G:H8	1.72	0.54
2:A2:1310:A:H8	32:K2:180:ARG:HH22	1.51	0.54
2:A2:3382:A:H2'	2:A2:3383:A:C8	2.43	0.54
16:E1:159:LYS:O	16:E1:163:MET:HG3	2.07	0.54
35:L3:145:PRO:HD2	69:m2:524:A:H5'	1.89	0.54
35:L3:160:SER:H	35:L3:162:ARG:NH2	2.05	0.54
75:s2:68:ILE:HD11	75:s2:151:ILE:HD11	1.90	0.54
2:A2:1068:C:N4	2:A2:1082:A:H61	2.05	0.54
2:A2:3260:A:H8	34:L2:71:ARG:HH12	1.55	0.54
2:A2:4433:G:H22	2:A2:4499:G:H1	1.55	0.54
2:A2:4637:U:H2'	2:A2:4638:G:H8	1.73	0.54
13:D1:33:ILE:HB	13:D1:69:ARG:HH12	1.72	0.54
40:O2:36:ALA:HB1	40:O2:65:ARG:HD2	1.89	0.54
59:b2:81:LEU:HA	59:b2:84:ARG:HG2	1.89	0.54
69:m2:1704:G:H2'	69:m2:1705:OMC:O4'	2.08	0.54
71:o2:145:ILE:HG13	71:o2:159:ILE:HB	1.89	0.54
73:q2:110:LEU:HD22	73:q2:175:VAL:HG13	1.88	0.54
2:A2:1333:C:H5'	20:F2:102:PHE:HE1	1.72	0.54
2:A2:2235:G:H2'	2:A2:2236:G:C8	2.43	0.54
27:H3:21:CYS:HB3	27:H3:26:ASN:H	1.73	0.54
69:m2:612:G:H2'	69:m2:613:G:H8	1.73	0.54
72:p2:160:GLN:O	72:p2:164:ILE:HD12	2.07	0.54
80:x2:111:MET:HE3	80:x2:119:PHE:CD2	2.42	0.54
2:A2:1490:PSU:H4'	2:A2:1493:G:C2	2.43	0.54
17:E2:256:ALA:HB3	17:E2:259:PRO:HD2	1.89	0.54
29:I3:240:CYS:N	29:I3:249:CYS:HB2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:L3:46:VAL:HG12	35:L3:102:ILE:HD11	1.90	0.54
35:L3:142:VAL:HA	69:m2:825:PSU:O4	2.08	0.54
56:Y2:24:GLN:HG3	56:Y2:27:ARG:HD3	1.90	0.54
69:m2:5:U:H2'	69:m2:6:G:H8	1.72	0.54
69:m2:1326:G:H1	69:m2:1506:U:H3	1.55	0.54
69:m2:1523:C:H1'	80:x2:128:HIS:HE1	1.73	0.54
71:o2:10:MET:HG3	82:z2:111:PHE:HZ	1.73	0.54
74:r2:80:VAL:HG13	74:r2:81:THR:HG23	1.90	0.54
2:A2:54:G:H5''	61:d2:43:ARG:HH12	1.73	0.54
2:A2:1648:G:H2'	2:A2:1649:C:C6	2.43	0.54
2:A2:3957:G:O6	38:N2:78:LYS:HE2	2.08	0.54
2:A2:4707:A:H4'	2:A2:4708:G:H5''	1.89	0.54
4:B1:215:LEU:O	4:B1:219:VAL:HG23	2.07	0.54
33:K3:197:GLN:HG2	33:K3:200:LYS:HE3	1.89	0.54
35:L3:169:ARG:O	35:L3:169:ARG:HG2	2.08	0.54
42:P2:20:LEU:HD21	42:P2:101:ASN:OD1	2.08	0.54
47:R3:103:HIS:CE1	75:s2:91:ARG:HH11	2.25	0.54
69:m2:180:G:H3'	69:m2:181:A:C8	2.43	0.54
2:A2:1482:A:H4'	2:A2:1498:G:N2	2.23	0.53
2:A2:4421:G:H5'	28:I2:176:ARG:HD3	1.90	0.53
12:C3:36:CYS:O	12:C3:40:ILE:HG12	2.08	0.53
15:D3:35:ASN:OD1	15:D3:52:THR:HG22	2.08	0.53
34:L2:24:LEU:HD23	34:L2:50:ILE:HG12	1.90	0.53
35:L3:134:HIS:HE1	69:m2:564:U:H5'	1.73	0.53
56:Y2:78:LEU:HB3	68:k2:20:ARG:HD3	1.90	0.53
66:i2:44:LYS:HZ3	66:i2:52:THR:HB	1.73	0.53
81:y2:30:GLY:H	81:y2:67:ASP:HB3	1.72	0.53
81:y2:51:LEU:HD23	81:y2:51:LEU:H	1.73	0.53
1:A1:98:ARG:HD2	2:A2:736:G:H5''	1.90	0.53
2:A2:1441:C:OP2	14:D2:9:ARG:HD2	2.09	0.53
4:B1:137[A]:ARG:HG2	4:B1:142:THR:HG21	1.89	0.53
6:B3:87:VAL:HG21	69:m2:1609:A:H5'	1.89	0.53
69:m2:1229:G:C2	69:m2:1230:A:C8	2.96	0.53
1:A1:108:GLU:HG3	38:N2:135:PRO:HB3	1.89	0.53
2:A2:878:G:H2'	2:A2:879:C:C6	2.43	0.53
2:A2:3925:A:H2'	2:A2:3926:A:C8	2.44	0.53
2:A2:4587:G:O2'	2:A2:4588:C:H5'	2.08	0.53
2:A2:4632:G:H2'	2:A2:4633:C:C6	2.44	0.53
6:B3:18:LEU:HD23	6:B3:58:ALA:HA	1.90	0.53
38:N2:11:THR:HA	38:N2:14:MET:HG2	1.90	0.53
39:N3:19:ARG:HD2	76:t2:138:GLU:OE2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:X2:43:PRO:O	55:X2:47:LYS:HG3	2.08	0.53
69:m2:15:U:H2'	69:m2:16:G:O4'	2.09	0.53
77:u2:47:ARG:HG2	77:u2:47:ARG:HH11	1.74	0.53
77:u2:172:LEU:HG	77:u2:190:LEU:HD22	1.89	0.53
1:A1:190:ALA:HB1	20:F2:315:LYS:HD2	1.88	0.53
2:A2:1316:A:H4'	2:A2:1317:G:H5'	1.88	0.53
2:A2:3263:U:H2'	2:A2:3264:A:C8	2.42	0.53
2:A2:3312:A:H2'	2:A2:3313:U:H6	1.73	0.53
2:A2:4113:C:H2'	2:A2:4114:C:H6	1.73	0.53
25:H1:116:LEU:HD12	25:H1:135:ILE:HD11	1.89	0.53
69:m2:1281:C:H2'	69:m2:1282:G:H8	1.74	0.53
71:o2:183:LEU:HD23	71:o2:186:ARG:HD3	1.89	0.53
79:w2:59:LYS:HD3	79:w2:134:LEU:HB3	1.90	0.53
2:A2:93:G:H2'	2:A2:94:A:C8	2.44	0.53
2:A2:399:G:H4'	30:J2:18:ARG:HG2	1.91	0.53
2:A2:3726:G:H21	25:H1:24:ARG:NH2	2.07	0.53
3:A3:86:ARG:HD3	3:A3:98:VAL:HG11	1.89	0.53
31:J3:108:LYS:HB2	31:J3:233:LEU:HD21	1.91	0.53
38:N2:63:ARG:HH12	38:N2:75:ILE:HD12	1.73	0.53
45:Q3:11:LYS:HG2	69:m2:844:C:N4	2.22	0.53
46:R2:79:PHE:CD1	59:b2:36:VAL:HG11	2.43	0.53
48:S2:74:TYR:CE2	48:S2:77:LYS:HG2	2.43	0.53
50:T2:15:ALA:HB2	58:a2:88:ARG:HH12	1.73	0.53
77:u2:74:ARG:HG2	77:u2:108:PRO:HB2	1.91	0.53
2:A2:271:C:H2'	2:A2:272:U:C6	2.44	0.53
2:A2:1695:C:H1'	2:A2:1739:C:O2	2.07	0.53
2:A2:4573:C:O2	22:G1:118:MET:HE1	2.09	0.53
4:B1:177:MET:HA	4:B1:177:MET:HE3	1.90	0.53
20:F2:24:LEU:HD21	20:F2:28:PHE:HB2	1.91	0.53
46:R2:100:VAL:HG23	46:R2:134:LYS:HB3	1.89	0.53
69:m2:1530:G:H2'	69:m2:1531:C:C6	2.44	0.53
2:A2:114:G:H21	2:A2:276:C:H4'	1.74	0.53
2:A2:3521:A:H2'	2:A2:3522:C:H6	1.74	0.53
18:E3:22:TRP:O	18:E3:28:LYS:HE2	2.09	0.53
75:s2:49:LEU:HB2	81:y2:50:LYS:NZ	2.24	0.53
82:z2:36:GLU:HB3	82:z2:47:ARG:HD2	1.89	0.53
2:A2:3784:C:H2'	2:A2:3785:G:C8	2.44	0.53
5:B2:102:U:H3'	5:B2:103:A:H8	1.74	0.53
10:C1:95:VAL:HG22	64:g2:82:LEU:HB3	1.91	0.53
17:E2:60:VAL:HG21	17:E2:67:VAL:HG23	1.90	0.53
22:G1:40:GLY:HA3	22:G1:45:VAL:HB	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:m2:1652:A:H5''	81:y2:139:ALA:HB2	1.90	0.53
70:n2:68:U:H2'	70:n2:69:G:C8	2.41	0.53
73:q2:64:ARG:HE	78:v2:83:LEU:HD23	1.74	0.53
74:r2:11:ARG:NH1	74:r2:20:LEU:HB3	2.24	0.53
2:A2:304:C:H2'	2:A2:305:A:O4'	2.09	0.53
2:A2:2235:G:H2'	2:A2:2236:G:H8	1.74	0.53
23:G2:232:THR:HG22	23:G2:234:ASP:H	1.73	0.53
37:M3:53:ALA:HA	37:M3:79:VAL:HA	1.90	0.53
41:O3:34:PHE:HA	41:O3:98:ARG:HB3	1.91	0.53
2:A2:108:A:H4'	2:A2:109:G:OP1	2.09	0.53
2:A2:665:C:H2'	2:A2:666:G:H8	1.73	0.53
2:A2:1667:G:N2	2:A2:1669:A:H3'	2.24	0.53
2:A2:3383:A:H2'	2:A2:3384:A:C8	2.44	0.53
39:N3:141:TYR:CE1	39:N3:146:ALA:HB2	2.44	0.53
52:U2:132:ARG:HG3	52:U2:132:ARG:HH11	1.73	0.53
2:A2:1092:C:H2'	2:A2:1093:A:O4'	2.09	0.52
2:A2:1411:C:H2'	2:A2:1412:A:H8	1.74	0.52
2:A2:1911:G:H2'	2:A2:1912:A:C8	2.44	0.52
2:A2:2387:U:H2'	2:A2:2388:U:C6	2.44	0.52
58:a2:82:MET:CE	58:a2:90:ARG:HD2	2.39	0.52
69:m2:166:A:H2'	69:m2:167:G:H8	1.74	0.52
69:m2:589:A:H2'	69:m2:589:A:N3	2.24	0.52
71:o2:115:ALA:O	71:o2:117:ARG:HG2	2.09	0.52
76:t2:100:ILE:HD13	76:t2:125:VAL:HG21	1.91	0.52
81:y2:25:CYS:SG	81:y2:66:VAL:HG11	2.49	0.52
2:A2:467:U:H2'	2:A2:468:U:C6	2.43	0.52
2:A2:2498:A:H2'	2:A2:2499:A:C8	2.44	0.52
29:I3:47:ARG:HA	29:I3:52:TYR:HD1	1.75	0.52
41:O3:57:THR:HG23	41:O3:60:MET:HE3	1.91	0.52
56:Y2:108:ARG:O	56:Y2:112:VAL:HG23	2.09	0.52
69:m2:1139:U:H3	69:m2:1150:A:H2	1.56	0.52
71:o2:29:ASN:HB2	71:o2:151:ASP:HB3	1.91	0.52
71:o2:97:THR:HG22	71:o2:99:ILE:HG23	1.91	0.52
2:A2:3298:A:H1'	61:d2:2:THR:HB	1.90	0.52
2:A2:4637:U:H2'	2:A2:4638:G:C8	2.45	0.52
10:C1:18:ILE:HG12	10:C1:27:VAL:HG22	1.91	0.52
15:D3:29:HIS:HA	71:o2:141:ASN:HD21	1.75	0.52
18:E3:106:GLY:HA2	69:m2:650:A:OP1	2.09	0.52
32:K2:49:LYS:O	32:K2:53:MET:HG3	2.09	0.52
69:m2:1689:C:H2'	69:m2:1690:C:H6	1.74	0.52
2:A2:1562:G:H2'	2:A2:1563:G:C8	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:G2:237:GLU:OE2	23:G2:241:LYS:HE2	2.09	0.52
29:I3:250:ALA:O	29:I3:256:ILE:HD12	2.09	0.52
30:J2:128:ARG:NH2	30:J2:136:ILE:HD13	2.23	0.52
33:K3:192:ILE:HD12	69:m2:126:G:N2	2.25	0.52
45:Q3:55:ILE:HD12	45:Q3:75:ILE:HG13	1.92	0.52
69:m2:107:A:H2'	69:m2:108:G:H8	1.72	0.52
72:p2:36:PRO:HG2	72:p2:39:PHE:HE2	1.74	0.52
2:A2:444:G:H2'	2:A2:445:U:H6	1.73	0.52
2:A2:665:C:H2'	2:A2:666:G:C8	2.44	0.52
2:A2:1590:A:H2'	13:D1:22:PHE:CE2	2.45	0.52
2:A2:2213:C:H5''	25:H1:67:ARG:HD2	1.92	0.52
2:A2:3778:A:H2	4:B1:34:LYS:HD2	1.74	0.52
3:A3:40:TYR:HA	3:A3:83:PHE:HE2	1.74	0.52
35:L3:123:ILE:HA	35:L3:126:ALA:HB3	1.91	0.52
2:A2:1417:G:H2'	2:A2:1418:G:C8	2.44	0.52
10:C1:114:ILE:HB	10:C1:124:ARG:HB2	1.91	0.52
12:C3:39:LEU:HD11	12:C3:102:THR:HG22	1.90	0.52
17:E2:378:ARG:HG2	44:Q2:32:LEU:HD21	1.91	0.52
28:I2:170:LYS:O	28:I2:174:ILE:HG12	2.10	0.52
45:Q3:37:LYS:HZ3	45:Q3:41:ARG:HD2	1.75	0.52
59:b2:21:LEU:O	59:b2:25:LYS:HG3	2.09	0.52
69:m2:181:A:C8	69:m2:182:C:H2'	2.44	0.52
69:m2:1407:A:H2'	69:m2:1408:G:O4'	2.08	0.52
73:q2:167:TYR:CD1	73:q2:200:PRO:HG2	2.45	0.52
2:A2:2465:C:H2'	2:A2:2467:G:H4'	1.91	0.52
29:I3:32:LEU:HD11	29:I3:71:ILE:HD12	1.92	0.52
69:m2:1388:A:H2'	69:m2:1389:G:O4'	2.09	0.52
2:A2:175:C:H5''	59:b2:101:LYS:HE3	1.91	0.52
2:A2:3536:G:H2'	2:A2:3537:G:C8	2.44	0.52
5:B2:33:U:C2	23:G2:207:TYR:CD1	2.97	0.52
22:G1:118:MET:O	22:G1:122:ILE:HD12	2.09	0.52
26:H2:210:ILE:O	26:H2:213:VAL:HG22	2.10	0.52
28:I2:81:TRP:HB2	28:I2:104:VAL:HG21	1.92	0.52
29:I3:149:GLU:HB2	29:I3:171:ASP:HB3	1.92	0.52
30:J2:29:THR:HG22	30:J2:119:VAL:HG11	1.92	0.52
52:U2:77:LYS:O	52:U2:80:THR:HG22	2.10	0.52
69:m2:944:G:H2'	69:m2:945:U:C6	2.45	0.52
71:o2:210:ILE:HD12	71:o2:210:ILE:H	1.74	0.52
74:r2:73:ASP:OD1	74:r2:164:LEU:HD22	2.10	0.52
2:A2:1214:G:H2'	2:A2:1215:G:C8	2.45	0.52
2:A2:4351:U:H1'	2:A2:4352:A:H5''	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B1:244:PRO:HA	4:B1:247:VAL:HG22	1.92	0.52
35:L3:144:ILE:HG13	35:L3:144:ILE:O	2.10	0.52
46:R2:83:THR:O	46:R2:87:MET:HG2	2.09	0.52
69:m2:70:G:H21	69:m2:79:A:H62	1.58	0.52
69:m2:887:U:O2	69:m2:903:G:N2	2.37	0.52
2:A2:1040:C:H2'	2:A2:1041:G:C8	2.41	0.52
2:A2:1577:A:H2'	2:A2:1578:A:C8	2.44	0.52
2:A2:2475:C:H2'	2:A2:2476:G:O4'	2.10	0.52
3:A3:25:LYS:O	3:A3:29:ALA:CB	2.58	0.52
43:P3:50:PHE:HB3	43:P3:63:VAL:HG12	1.91	0.52
47:R3:55:TYR:O	47:R3:58:LEU:HG	2.10	0.52
69:m2:597:U:H2'	69:m2:598:U:H6	1.75	0.52
72:p2:172:MET:O	72:p2:176:VAL:HG12	2.10	0.52
1:A1:179:ARG:HD2	1:A1:235:LEU:HD23	1.91	0.51
2:A2:4160:C:N3	2:A2:4164:U:H5	2.08	0.51
7:Bv:23:A:H61	7:Bv:46:G:H22	1.58	0.51
12:C3:69:PRO:HA	27:H3:40:ARG:HH12	1.73	0.51
19:F1:18:TRP:CD1	19:F1:18:TRP:H	2.28	0.51
23:G2:21:ARG:O	23:G2:25:GLU:HG3	2.10	0.51
33:K3:48:TYR:CZ	33:K3:117:GLY:HA2	2.45	0.51
35:L3:78:LEU:HB3	35:L3:92:MET:HE3	1.92	0.51
64:g2:103:LEU:HD11	64:g2:110:CYS:HA	1.91	0.51
76:t2:66:VAL:N	76:t2:67:PRO:HD2	2.25	0.51
82:z2:13:ALA:O	82:z2:17:ILE:HG13	2.10	0.51
1:A1:114:VAL:O	1:A1:142:GLY:HA2	2.10	0.51
3:A3:133:GLY:HA3	69:m2:1625:A:H5''	1.92	0.51
19:F1:182:LEU:HD11	52:U2:146:LEU:HD21	1.92	0.51
50:T2:77:TYR:HD2	54:W2:39:ARG:HD2	1.75	0.51
69:m2:351:A:H2'	69:m2:352:C:C6	2.45	0.51
69:m2:1374:U:H2'	69:m2:1375:C:O4'	2.09	0.51
71:o2:108:PHE:HB3	71:o2:140:VAL:HG21	1.93	0.51
2:A2:184:U:H5''	2:A2:254:G:N2	2.26	0.51
2:A2:3268:C:H5'	77:u2:92:ARG:NH2	2.25	0.51
29:I3:77:PHE:HB3	29:I3:89:LEU:HD11	1.93	0.51
33:K3:170:ARG:HG3	69:m2:67:C:H41	1.76	0.51
48:S2:74:TYR:HD2	48:S2:77:LYS:HG2	1.72	0.51
50:T2:41:ALA:HB2	50:T2:77:TYR:HE1	1.75	0.51
53:V2:47:LYS:HA	53:V2:50:ASN:OD1	2.09	0.51
59:b2:98:HIS:CE1	59:b2:102:LEU:HD21	2.45	0.51
69:m2:316:U:H2'	69:m2:317:C:C6	2.45	0.51
69:m2:1039:G:H4'	69:m2:1847:A:H4'	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:m2:1790:A:H2'	69:m2:1791:G:O4'	2.10	0.51
76:t2:43:LEU:HD23	76:t2:72:PHE:CD2	2.46	0.51
2:A2:2279:U:H3	2:A2:2284:A:H2	1.59	0.51
2:A2:2395:G:H2'	2:A2:2396:A:C8	2.45	0.51
2:A2:2424:C:H2'	2:A2:2425:C:O4'	2.10	0.51
2:A2:3573:A:H2'	2:A2:3574:G:H8	1.74	0.51
2:A2:4113:C:H2'	2:A2:4114:C:C6	2.46	0.51
2:A2:4375:A:H2'	2:A2:4376:A:C8	2.45	0.51
2:A2:4566:C:H2'	2:A2:4567:C:C6	2.45	0.51
29:I3:168:CYS:SG	29:I3:198:VAL:HG23	2.51	0.51
30:J2:32:THR:O	30:J2:36:ILE:HG12	2.10	0.51
31:J3:209:VAL:HA	31:J3:212:LYS:HE3	1.90	0.51
38:N2:82:GLY:HA2	53:V2:21:ILE:HD12	1.91	0.51
45:Q3:25:ILE:HG21	45:Q3:44:LEU:HD11	1.93	0.51
62:e2:5:ILE:HD11	62:e2:11:PHE:HD1	1.74	0.51
69:m2:1535:A:H2	69:m2:1538:G:N3	2.07	0.51
2:A2:181:C:H2'	2:A2:182:G:C8	2.45	0.51
2:A2:768:G:H2'	2:A2:769:G:C8	2.45	0.51
2:A2:1211:A:C8	52:U2:114:LYS:HD2	2.45	0.51
2:A2:2600:A:H61	2:A2:3499:C:N4	2.07	0.51
2:A2:3898:G:H2'	2:A2:3899:G:H8	1.76	0.51
2:A2:4582:U:H4'	2:A2:4583:U:OP1	2.09	0.51
2:A2:4642:C:H4'	55:X2:26:THR:HG23	1.92	0.51
14:D2:2:GLY:HA2	14:D2:207:VAL:HG23	1.92	0.51
23:G2:153:THR:HG23	23:G2:160:PHE:HZ	1.73	0.51
38:N2:28:ALA:O	38:N2:32:ARG:HG2	2.10	0.51
61:d2:52:LYS:HG3	61:d2:55:ARG:NH2	2.26	0.51
69:m2:498:C:H2'	69:m2:499:C:H6	1.75	0.51
71:o2:115:ALA:HB1	71:o2:117:ARG:NH1	2.25	0.51
71:o2:148:CYS:SG	71:o2:163:CYS:N	2.83	0.51
2:A2:1881:G:H2'	2:A2:1882:U:C6	2.46	0.51
2:A2:3607:G:H2'	2:A2:3608:A:C8	2.44	0.51
2:A2:4542:G:H2'	2:A2:4543:G:C8	2.45	0.51
10:C1:107:GLU:HB2	10:C1:110:SER:HB2	1.92	0.51
21:F3:92:ARG:HD3	69:m2:1867:C:OP2	2.10	0.51
32:K2:66:MET:HE3	32:K2:98:LEU:HD22	1.92	0.51
40:O2:100:LEU:HD23	40:O2:112:LEU:HD23	1.92	0.51
41:O3:103:ASN:O	41:O3:142:ARG:HD2	2.11	0.51
54:W2:87:LYS:HD2	54:W2:89:TYR:OH	2.11	0.51
77:u2:37:LYS:HB2	77:u2:59:ARG:HG3	1.92	0.51
80:x2:83:MET:HB3	80:x2:116:LEU:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A2:425:U:H4'	30:J2:6:LEU:HD21	1.93	0.51
2:A2:3262:U:H2'	2:A2:3263:U:C6	2.46	0.51
2:A2:3527:A:H2'	2:A2:3528:A:C8	2.45	0.51
2:A2:4340:C:H2'	2:A2:4341:U:C6	2.45	0.51
6:B3:60:THR:HG23	6:B3:75:MET:HE2	1.92	0.51
11:C2:67:U:H2'	11:C2:68:G:C8	2.45	0.51
25:H1:108:ARG:HE	25:H1:161:MET:CE	2.23	0.51
26:H2:170:VAL:HG21	26:H2:268:ILE:HD11	1.93	0.51
29:I3:64:HIS:HD2	29:I3:83:TRP:HB2	1.76	0.51
31:J3:165:VAL:HG13	31:J3:244:ILE:HG23	1.92	0.51
33:K3:7:PHE:HD1	33:K3:113:ILE:HB	1.76	0.51
33:K3:23:LYS:HG2	33:K3:41:LEU:HA	1.93	0.51
46:R2:71:LEU:HG	46:R2:76:ILE:HD11	1.93	0.51
47:R3:50:PHE:HE2	47:R3:87:ALA:HB2	1.75	0.51
69:m2:1434:U:H2'	69:m2:1440:A:C8	2.46	0.51
76:t2:52:GLU:HA	76:t2:58:LYS:HA	1.93	0.51
2:A2:262:G:H2'	2:A2:263:G:H8	1.76	0.51
2:A2:433:A:C2	2:A2:3523:A:H4'	2.45	0.51
2:A2:1367:A:OP2	67:j2:4:ARG:HD2	2.11	0.51
2:A2:3383:A:OP1	60:c2:67:LYS:HE3	2.10	0.51
21:F3:85:ARG:H	69:m2:1868:A:H61	1.59	0.51
33:K3:173:ALA:H	69:m2:77:A:H62	1.58	0.51
37:M3:33:ARG:HB2	69:m2:1286:A:C8	2.46	0.51
69:m2:145:G:H1	69:m2:174:OMC:H5	1.59	0.51
69:m2:377:U:H2'	69:m2:378:A:C8	2.45	0.51
69:m2:457:A:H2'	69:m2:458:C:H6	1.76	0.51
69:m2:610:C:H2'	69:m2:611:U:H6	1.76	0.51
69:m2:1007:G:H2'	69:m2:1008:C:H6	1.75	0.51
69:m2:1460:G:H2'	69:m2:1461:G:H8	1.76	0.51
69:m2:1843:C:H2'	86:m2:1936:4AC:H6	1.93	0.51
2:A2:2567:A:H2	34:L2:82:LYS:HB3	1.76	0.51
14:D2:57:PRO:HD2	14:D2:170:ALA:HB3	1.92	0.51
15:D3:82:ASN:HD21	71:o2:52:LYS:HE2	1.76	0.51
20:F2:134:PRO:HA	20:F2:150:LEU:HD22	1.93	0.51
27:H3:38:MET:HE2	27:H3:50:ILE:HD11	1.92	0.51
29:I3:195:LEU:H	29:I3:195:LEU:HD23	1.75	0.51
69:m2:611:U:H2'	69:m2:612:G:H8	1.75	0.51
77:u2:67:TRP:CD1	77:u2:70:GLU:H	2.29	0.51
81:y2:51:LEU:C	81:y2:53:GLU:H	2.19	0.51
2:A2:1153:U:H2'	2:A2:1154:OMC:C6	2.45	0.51
2:A2:2167:A:H5''	34:L2:6:LEU:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A2:3562:A:H2'	20:F2:69:THR:HG21	1.92	0.51
2:A2:4189:C:H2'	2:A2:4190:G:C8	2.46	0.51
35:L3:111:GLN:HE22	35:L3:127:ARG:HA	1.76	0.51
50:T2:50:PRO:HD3	50:T2:68:ILE:HG12	1.92	0.51
69:m2:1279:C:H2'	69:m2:1280:A:C8	2.45	0.51
72:p2:171:ILE:HD13	72:p2:174:ARG:HH22	1.75	0.51
2:A2:1146:C:H2'	2:A2:1147:A:C8	2.45	0.50
2:A2:1873:A:H2'	2:A2:1874:C:C6	2.46	0.50
2:A2:1899:G:H5'	2:A2:1900:G:H4'	1.93	0.50
2:A2:3840:U:H2'	2:A2:3841:U:C6	2.45	0.50
2:A2:4288:PSU:C2	55:X2:78:ARG:HD2	2.46	0.50
3:A3:37:GLY:N	69:m2:1632:A:H5''	2.23	0.50
7:Bv:47:C:H1'	7:Bv:48:C:C4	2.45	0.50
18:E3:40:PRO:O	18:E3:41:PHE:HB2	2.12	0.50
35:L3:2:PRO:O	69:m2:511:OMG:H5''	2.11	0.50
38:N2:71:ALA:HA	38:N2:92:ARG:HA	1.93	0.50
69:m2:102:A:H4'	69:m2:104:A:C8	2.45	0.50
79:w2:111:VAL:HG11	79:w2:128:VAL:HG11	1.92	0.50
2:A2:878:G:OP1	26:H2:69:MET:HG2	2.11	0.50
14:D2:6:ARG:HG2	14:D2:10:LYS:NZ	2.26	0.50
15:D3:32:ILE:O	15:D3:54:ALA:HA	2.11	0.50
32:K2:178:ARG:H	52:U2:51:GLY:HA2	1.77	0.50
35:L3:120:ALA:HB1	35:L3:126:ALA:HB2	1.93	0.50
35:L3:125:HIS:HB2	69:m2:529:C:H5'	1.92	0.50
39:N3:40:LEU:HA	39:N3:43:LYS:NZ	2.26	0.50
68:k2:4:HIS:O	68:k2:8:MET:HG2	2.11	0.50
69:m2:1116:U:H3'	69:m2:1117:U:H2'	1.93	0.50
69:m2:1305:C:H2'	69:m2:1306:U:C6	2.47	0.50
2:A2:181:C:H2'	2:A2:182:G:H8	1.76	0.50
2:A2:2220:C:H2'	2:A2:2221:G:O4'	2.11	0.50
6:B3:37:VAL:HG12	6:B3:46:ALA:HB1	1.94	0.50
15:D3:1:MET:HE1	31:J3:255:LEU:HD12	1.93	0.50
16:E1:56:THR:HG23	16:E1:63:ARG:HA	1.93	0.50
17:E2:33:PRO:HA	17:E2:351:LEU:HD23	1.93	0.50
38:N2:18:PRO:HG2	38:N2:21:LYS:HD2	1.92	0.50
69:m2:1705:OMC:H2'	69:m2:1706:C:O4'	2.12	0.50
75:s2:35:LEU:HD12	75:s2:147:VAL:HG23	1.92	0.50
75:s2:41:VAL:O	75:s2:42:LYS:HE2	2.11	0.50
2:A2:2068:A:H5''	11:C2:9:A:H5'	1.93	0.50
2:A2:3886:A:N7	2:A2:3923:A:N1	2.60	0.50
5:B2:110:G:H2'	5:B2:111:C:H6	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:D1:12:CYS:SG	13:D1:59:GLN:HB3	2.52	0.50
15:D3:11:LEU:HD12	15:D3:12:TYR:HD1	1.76	0.50
29:I3:85:GLY:HA2	29:I3:108:VAL:HG23	1.93	0.50
31:J3:94:ILE:HG21	31:J3:162:ILE:HD12	1.92	0.50
31:J3:166:ARG:HB2	31:J3:248:TYR:CE1	2.46	0.50
33:K3:7:PHE:CE2	33:K3:9:ALA:HB3	2.46	0.50
33:K3:21:GLU:O	33:K3:25:ARG:HG3	2.12	0.50
35:L3:142:VAL:HG13	35:L3:144:ILE:HG12	1.93	0.50
42:P2:42:VAL:HG23	42:P2:61:VAL:HG12	1.92	0.50
59:b2:32:ARG:HH12	59:b2:47:ILE:HG23	1.77	0.50
69:m2:12:U:H2'	69:m2:13:C:C6	2.47	0.50
69:m2:163:U:H2'	69:m2:164:A:H8	1.76	0.50
69:m2:318:G:H2'	69:m2:319:C:C6	2.47	0.50
69:m2:1685:C:H2'	69:m2:1686:C:H6	1.76	0.50
74:r2:45:ILE:HB	74:r2:80:VAL:HG22	1.92	0.50
74:r2:89:VAL:HG22	74:r2:100:ARG:HH21	1.77	0.50
74:r2:222:LEU:HA	74:r2:225:ILE:HD12	1.93	0.50
2:A2:663:C:H5'	20:F2:269:LYS:HD2	1.93	0.50
3:A3:50:ILE:HD13	3:A3:59:LEU:HD11	1.93	0.50
25:H1:80:THR:OG1	25:H1:87:HIS:HA	2.12	0.50
39:N3:5:HIS:HB2	39:N3:121:ARG:HH12	1.75	0.50
58:a2:59:VAL:HB	58:a2:63:VAL:HG13	1.93	0.50
69:m2:1568:G:H21	69:m2:1571:A:H2	1.60	0.50
72:p2:122:GLU:HG2	72:p2:140:VAL:HG12	1.92	0.50
74:r2:162:ILE:HG22	74:r2:169:ILE:HD13	1.92	0.50
74:r2:191:ARG:NH2	74:r2:218:PHE:HB2	2.27	0.50
81:y2:13:PHE:HA	81:y2:21:ALA:O	2.12	0.50
18:E3:68:LYS:HE2	69:m2:619:G:OP2	2.10	0.50
23:G2:80:ALA:HA	23:G2:83:LEU:HD23	1.93	0.50
37:M3:31:LEU:O	37:M3:33:ARG:HD3	2.11	0.50
69:m2:65:C:H5'	69:m2:78:C:N4	2.27	0.50
69:m2:293:G:H1'	79:w2:42:LEU:H	1.77	0.50
69:m2:477:C:C2	69:m2:478:A:C8	2.99	0.50
69:m2:622:G:H2'	69:m2:622:G:N3	2.26	0.50
69:m2:1459:U:H2'	69:m2:1460:G:H8	1.75	0.50
74:r2:104:ASP:HB2	74:r2:110:ALA:HB2	1.93	0.50
82:z2:10:LYS:O	82:z2:14:ARG:HG3	2.12	0.50
1:A1:204:PHE:CZ	1:A1:225:GLU:HG2	2.46	0.50
2:A2:462:G:H2'	2:A2:463:A:C8	2.47	0.50
2:A2:2311:G:H2'	2:A2:2312:G:C8	2.47	0.50
2:A2:3576:U:H2'	2:A2:3577:U:C6	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A2:3738:C:H2'	2:A2:3739:G:H8	1.77	0.50
17:E2:88:GLY:C	17:E2:89:ILE:HD13	2.36	0.50
18:E3:105:PHE:HE2	18:E3:118:VAL:HG12	1.77	0.50
26:H2:210:ILE:HD12	26:H2:264:ILE:HD13	1.93	0.50
29:I3:270:LEU:HD23	29:I3:310:TRP:CE3	2.47	0.50
34:L2:88:ARG:O	34:L2:89:MET:HE2	2.11	0.50
47:R3:103:HIS:HE1	75:s2:91:ARG:HH11	1.58	0.50
69:m2:998:A:H2'	69:m2:999:A:C8	2.47	0.50
69:m2:1027:U:H2'	69:m2:1028:C:O4'	2.12	0.50
69:m2:1380:A:H4'	69:m2:1381:A:O5'	2.12	0.50
69:m2:1410:U:H2'	69:m2:1411:A:H8	1.75	0.50
2:A2:1147:A:H2'	2:A2:1148:A:C8	2.47	0.50
2:A2:2458:G:C6	2:A2:2469:G:C6	2.99	0.50
2:A2:4246:U:H2'	2:A2:4247:G:H8	1.75	0.50
16:E1:66:GLU:O	16:E1:68:ILE:HG12	2.12	0.50
35:L3:147:PHE:HE1	69:m2:826:C:H5'	1.76	0.50
69:m2:610:C:H2'	69:m2:611:U:C6	2.47	0.50
69:m2:1007:G:H2'	69:m2:1008:C:C6	2.47	0.50
69:m2:1460:G:H2'	69:m2:1461:G:C8	2.47	0.50
71:o2:50:ASN:HA	82:z2:105:MET:SD	2.52	0.50
74:r2:18:TRP:HE3	74:r2:20:LEU:HD11	1.75	0.50
2:A2:1281:C:H2'	2:A2:1282:C:H6	1.76	0.50
2:A2:1894:G:H2'	2:A2:2017:G:C6	2.47	0.50
45:Q3:111:LYS:O	45:Q3:115:LYS:HG3	2.12	0.50
69:m2:993:G:C6	69:m2:1136:G:H4'	2.46	0.50
69:m2:1006:U:H2'	69:m2:1007:G:C8	2.46	0.50
69:m2:1708:G:H2'	69:m2:1709:U:H6	1.76	0.50
1:A1:112:ALA:HB2	1:A1:147:LEU:HD21	1.94	0.49
1:A1:117:ILE:O	1:A1:245:LYS:HE3	2.11	0.49
28:I2:181:ALA:O	28:I2:185:VAL:HG22	2.11	0.49
32:K2:159:PRO:HA	32:K2:188:ASN:HB2	1.93	0.49
33:K3:13:GLN:HG3	69:m2:153:G:H21	1.77	0.49
33:K3:164:LYS:HE3	69:m2:67:C:C5	2.47	0.49
62:e2:8:ILE:HG23	62:e2:56:LEU:HD12	1.93	0.49
2:A2:1067:A:C6	2:A2:1082:A:C6	3.00	0.49
2:A2:3340:G:H2'	2:A2:3341:C:C6	2.47	0.49
2:A2:3860:U:H2'	2:A2:3861:G:C8	2.47	0.49
3:A3:39:ARG:HD3	69:m2:1631:C:OP1	2.12	0.49
5:B2:47:G:H21	23:G2:222:GLN:HE22	1.59	0.49
6:B3:104:LEU:HD11	6:B3:121:ARG:NH1	2.27	0.49
22:G1:85:LYS:O	22:G1:89:THR:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:H3:8:TRP:NE1	69:m2:1514:C:H5'	2.27	0.49
35:L3:78:LEU:HD21	35:L3:94:LEU:HA	1.94	0.49
69:m2:1032:A:H2'	69:m2:1033:A2M:H8	1.95	0.49
69:m2:1219:A:H2'	69:m2:1220:C:H6	1.75	0.49
69:m2:1560:C:H2'	69:m2:1561:C:C6	2.46	0.49
80:x2:33:LEU:H	80:x2:33:LEU:HD23	1.77	0.49
2:A2:300:A:H5''	25:H1:97:SER:HB3	1.93	0.49
2:A2:1506:U:H2'	2:A2:1507:C:O4'	2.12	0.49
2:A2:3860:U:H2'	2:A2:3861:G:H8	1.76	0.49
2:A2:4133:U:H2'	2:A2:4134:U:C6	2.47	0.49
6:B3:60:THR:O	6:B3:64:LEU:HD23	2.12	0.49
6:B3:71:GLY:O	6:B3:75:MET:HG2	2.11	0.49
20:F2:154:VAL:HG11	20:F2:174:LEU:HD11	1.93	0.49
27:H3:26:ASN:HB3	27:H3:39:CYS:SG	2.53	0.49
30:J2:29:THR:HG21	30:J2:146:ILE:HD11	1.93	0.49
32:K2:12:LYS:HB2	32:K2:14:ARG:NH1	2.28	0.49
39:N3:134:VAL:HG23	39:N3:135:LEU:HD12	1.94	0.49
69:m2:25:A:O2'	69:m2:26:U:H5''	2.12	0.49
81:y2:12:VAL:O	81:y2:22:VAL:HA	2.12	0.49
2:A2:1190:C:H5''	2:A2:1191:G:C8	2.46	0.49
2:A2:1281:C:H2'	2:A2:1282:C:C6	2.47	0.49
29:I3:52:TYR:HE2	29:I3:309:VAL:HG21	1.77	0.49
30:J2:22:LEU:HD12	30:J2:146:ILE:HD12	1.93	0.49
42:P2:70:PRO:HB2	69:m2:1726:A:OP2	2.11	0.49
52:U2:89:ASN:HA	52:U2:92:LYS:HE2	1.93	0.49
69:m2:172:OMU:H6	69:m2:172:OMU:H5''	1.94	0.49
73:q2:99:ILE:HD11	73:q2:173:ARG:CZ	2.42	0.49
74:r2:184:ILE:HD13	74:r2:226:PHE:HE1	1.77	0.49
74:r2:185:GLY:H	74:r2:224:ASN:HB3	1.77	0.49
77:u2:72:CYS:HG	77:u2:112:TRP:CG	2.31	0.49
77:u2:81:VAL:HG22	77:u2:102:VAL:HG12	1.95	0.49
77:u2:190:LEU:HD21	77:u2:198:TYR:CD2	2.40	0.49
2:A2:1018:U:H2'	2:A2:1019:G:C8	2.48	0.49
2:A2:2162:G:H22	63:f2:51:LEU:HD23	1.77	0.49
2:A2:3256:G:H2'	2:A2:3257:C:C6	2.47	0.49
2:A2:3409:G:C8	2:A2:3432:G:C8	3.01	0.49
2:A2:3512:A:H5''	30:J2:83:TRP:O	2.11	0.49
35:L3:136:ARG:HD2	35:L3:162:ARG:HH22	1.77	0.49
36:M2:27:LEU:HD21	38:N2:141:VAL:HG11	1.94	0.49
70:n2:61:C:H2'	70:n2:62:A:C8	2.44	0.49
70:n2:65:C:H2'	70:n2:66:U:H6	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:p2:59:SER:O	72:p2:63:LYS:HG2	2.12	0.49
78:v2:79:LEU:HD23	78:v2:81:ASP:H	1.77	0.49
2:A2:151:G:P	25:H1:49:ARG:HH22	2.36	0.49
2:A2:4234:C:H2'	2:A2:4235:C:O4'	2.13	0.49
3:A3:89:ASP:HB3	69:m2:1613:G:O3'	2.12	0.49
4:B1:187:LYS:HD2	4:B1:198:THR:HG23	1.94	0.49
12:C3:46:LYS:HB2	12:C3:48:LEU:HD22	1.95	0.49
32:K2:178:ARG:N	52:U2:51:GLY:HA2	2.27	0.49
42:P2:24:ALA:HB3	42:P2:39:ILE:HD12	1.94	0.49
45:Q3:89:HIS:O	45:Q3:93:ARG:HG2	2.13	0.49
47:R3:50:PHE:CE2	47:R3:87:ALA:HB2	2.47	0.49
52:U2:88:VAL:HG12	52:U2:92:LYS:HZ2	1.77	0.49
69:m2:313:C:H5'	69:m2:314:G:OP1	2.13	0.49
78:v2:79:LEU:HD23	78:v2:81:ASP:N	2.28	0.49
79:w2:37:TYR:OH	79:w2:51:ILE:HD13	2.12	0.49
1:A1:109:PRO:HG3	1:A1:166:TYR:CE2	2.47	0.49
2:A2:2216:G:H4'	25:H1:108:ARG:HH22	1.78	0.49
2:A2:3549:C:H5'	30:J2:80:GLN:NE2	2.28	0.49
2:A2:4189:C:H2'	2:A2:4190:G:H8	1.75	0.49
5:B2:27:G:H21	5:B2:55:A:N6	2.10	0.49
10:C1:20:LEU:HD12	10:C1:47:LEU:HG	1.95	0.49
11:C2:44:A:H2'	11:C2:45:C:C6	2.47	0.49
33:K3:191:ARG:O	33:K3:195:LYS:HG3	2.12	0.49
45:Q3:28:LEU:HD12	45:Q3:68:LYS:HE3	1.95	0.49
69:m2:1136:G:H2'	69:m2:1137:C:C6	2.48	0.49
69:m2:1750:G:H2'	69:m2:1751:G:H8	1.77	0.49
79:w2:88:ILE:HD11	79:w2:109:MET:HE2	1.92	0.49
2:A2:262:G:H2'	2:A2:263:G:C8	2.48	0.49
2:A2:2431:A:OP2	2:A2:2431:A:H8	1.95	0.49
2:A2:2619:A:H2'	2:A2:2620:U:C6	2.48	0.49
2:A2:3439:A:H4'	2:A2:3440:A:H5''	1.94	0.49
2:A2:3521:A:H2'	2:A2:3522:C:C6	2.46	0.49
2:A2:4677:G:H2'	2:A2:4678:C:C6	2.47	0.49
19:F1:36:ARG:HG2	19:F1:36:ARG:HH11	1.77	0.49
19:F1:60:ARG:HD2	19:F1:67:HIS:O	2.13	0.49
20:F2:212:ASN:HD22	20:F2:255:SER:HB3	1.77	0.49
23:G2:88:VAL:HA	23:G2:239:MET:HE1	1.95	0.49
26:H2:74:ALA:HA	26:H2:76:TYR:CE2	2.47	0.49
30:J2:84:PRO:HB2	30:J2:87:SER:HB2	1.95	0.49
69:m2:1232:C:H2'	69:m2:1233:C:C6	2.48	0.49
74:r2:246:LEU:O	74:r2:250:GLU:HB2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:s2:23:TRP:HZ3	75:s2:101:HIS:HD2	1.61	0.49
2:A2:1034:U:H2'	2:A2:1035:C:C6	2.48	0.49
2:A2:1323:G:H2'	2:A2:1324:C:C6	2.48	0.49
14:D2:189:TYR:CD2	14:D2:196:TRP:HB2	2.48	0.49
17:E2:29:VAL:HG23	17:E2:346:THR:HG21	1.95	0.49
20:F2:8:ILE:HD11	20:F2:257:PHE:CZ	2.48	0.49
23:G2:164:LYS:HG2	23:G2:195:HIS:NE2	2.28	0.49
56:Y2:35:TRP:CE2	56:Y2:56:PRO:HD2	2.48	0.49
69:m2:957:A:H61	69:m2:973:G:H1'	1.76	0.49
74:r2:31:PRO:HD2	74:r2:38:LEU:HD11	1.95	0.49
82:z2:76:GLU:O	82:z2:79:GLU:HG3	2.12	0.49
2:A2:279:A:N1	2:A2:306:A:H5''	2.28	0.49
2:A2:2438:C:H2'	2:A2:2439:C:C6	2.48	0.49
15:D3:17:CYS:HB2	15:D3:56:CYS:SG	2.53	0.49
29:I3:109:LEU:HD23	29:I3:152:SER:HA	1.95	0.49
38:N2:70:HIS:O	38:N2:93:ILE:HG12	2.12	0.49
50:T2:74:VAL:HG23	50:T2:101:PHE:CE2	2.48	0.49
50:T2:82:PRO:HD2	54:W2:63:TYR:CE1	2.48	0.49
51:T3:37:GLN:O	51:T3:41:ARG:HG2	2.13	0.49
61:d2:15:THR:HG23	61:d2:16:HIS:ND1	2.28	0.49
69:m2:1201:A:H2'	69:m2:1202:A:H8	1.76	0.49
74:r2:61:VAL:HA	74:r2:64:ILE:HG12	1.95	0.49
74:r2:120:LYS:HA	74:r2:164:LEU:HG	1.95	0.49
76:t2:28:LEU:CD2	76:t2:32:MET:HE1	2.42	0.49
2:A2:1673:A2M:HM'2	2:A2:1674:G:H5'	1.95	0.48
2:A2:2294:C:H2'	2:A2:2295:C:C6	2.48	0.48
2:A2:3255:A:H2'	2:A2:3256:G:C8	2.48	0.48
2:A2:3304:A:H1'	2:A2:3441:A2M:N6	2.28	0.48
2:A2:4531:C:H2'	2:A2:4532:U:H6	1.77	0.48
2:A2:4580:C:H2'	2:A2:4581:G:C8	2.49	0.48
22:G1:24:LEU:HD11	22:G1:86:TRP:CG	2.48	0.48
35:L3:136:ARG:NH2	35:L3:139:LYS:HA	2.28	0.48
44:Q2:45:ASN:ND2	44:Q2:47:ARG:HB2	2.28	0.48
62:e2:11:PHE:CE2	62:e2:56:LEU:HD21	2.49	0.48
69:m2:615:G:H22	69:m2:631:A:H5'	1.78	0.48
69:m2:847:G:H3'	69:m2:848:G:C8	2.47	0.48
73:q2:167:TYR:HD1	73:q2:200:PRO:HG2	1.77	0.48
2:A2:325:U:H2'	2:A2:326:C:C6	2.48	0.48
2:A2:1596:A:H5''	2:A2:3866:A:H61	1.77	0.48
2:A2:3777:A:C2	4:B1:37:LYS:HG2	2.48	0.48
2:A2:3807:C:H2'	2:A2:3808:G:O4'	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B1:157:ILE:HB	4:B1:183:ILE:HD13	1.94	0.48
69:m2:377:U:H2'	69:m2:378:A:H8	1.78	0.48
69:m2:668:U:H2'	69:m2:669:U:C6	2.48	0.48
69:m2:1472:C:H2'	69:m2:1473:C:H6	1.77	0.48
69:m2:1581:A:H4'	69:m2:1583:C:H5	1.78	0.48
72:p2:173:THR:O	72:p2:177:GLN:HB2	2.13	0.48
2:A2:4613:A:H2'	2:A2:4614:A:C8	2.47	0.48
18:E3:13:LEU:HD12	79:w2:101:ARG:HD2	1.94	0.48
28:I2:37:ARG:HD2	28:I2:108:ILE:HD11	1.95	0.48
47:R3:92:LEU:HD11	47:R3:99:LEU:HD23	1.95	0.48
48:S2:34:LEU:HD23	48:S2:38:LEU:HB3	1.95	0.48
48:S2:114:ASP:O	48:S2:117:LYS:HG2	2.14	0.48
55:X2:27:ILE:HB	55:X2:84:ILE:HG22	1.95	0.48
59:b2:104:THR:O	59:b2:108:GLN:HG3	2.12	0.48
81:y2:11:GLN:HA	81:y2:23:ALA:O	2.14	0.48
1:A1:247:THR:HG22	1:A1:251:GLU:HG3	1.94	0.48
2:A2:1371:A:H2'	2:A2:1372:G:H8	1.78	0.48
2:A2:2619:A:H2'	2:A2:2620:U:H6	1.78	0.48
2:A2:3366:G:C2	2:A2:3367:A:H1'	2.48	0.48
2:A2:3430:A:H2'	2:A2:3431:A:H8	1.78	0.48
14:D2:80:GLU:HG2	67:j2:76:ALA:HB2	1.95	0.48
35:L3:57:ALA:O	35:L3:61:LEU:HG	2.13	0.48
36:M2:29:ARG:HB2	38:N2:148:PRO:HB2	1.95	0.48
47:R3:48:VAL:HG22	47:R3:80:ARG:HE	1.78	0.48
69:m2:849:A:H3'	69:m2:850:U:H6	1.78	0.48
82:z2:5:ARG:HB2	82:z2:10:LYS:HE3	1.96	0.48
2:A2:1260:C:C2	2:A2:1261:G:C8	3.01	0.48
2:A2:1371:A:H2'	2:A2:1372:G:C8	2.49	0.48
2:A2:1744:A:H2'	2:A2:1745:A:H8	1.77	0.48
2:A2:1836:G:OP1	36:M2:87:ARG:HG3	2.13	0.48
2:A2:2367:G:H2'	2:A2:2368:C:O4'	2.13	0.48
2:A2:3501:A:H2'	2:A2:3502:C:C6	2.49	0.48
2:A2:3593:C:H1'	25:H1:125:SER:HB3	1.95	0.48
2:A2:4572:G:P	2:A2:4573:C:H41	2.37	0.48
2:A2:4603:C:H2'	2:A2:4604:C:H6	1.78	0.48
4:B1:207:VAL:HG21	4:B1:215:LEU:HD22	1.94	0.48
6:B3:104:LEU:HD21	6:B3:121:ARG:CZ	2.43	0.48
15:D3:16:LYS:NZ	31:J3:256:TRP:HA	2.29	0.48
17:E2:80:GLU:HG3	17:E2:326:VAL:HG13	1.95	0.48
29:I3:79:LEU:HD22	29:I3:111:VAL:HG11	1.95	0.48
45:Q3:16:ARG:C	45:Q3:19:GLN:H	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:j2:25:MET:SD	69:m2:1042:G:H5''	2.54	0.48
69:m2:355:OMC:H1'	69:m2:355:OMC:HM23	1.66	0.48
69:m2:821:G:H2'	69:m2:822:U:C6	2.49	0.48
69:m2:832:A:C5	69:m2:847:G:C2	3.01	0.48
69:m2:1162:U:H2'	69:m2:1163:U:H6	1.79	0.48
69:m2:1712:C:H2'	69:m2:1713:U:C6	2.49	0.48
73:q2:138:VAL:HG12	73:q2:142:LEU:HD11	1.95	0.48
74:r2:29:PRO:HB3	74:r2:45:ILE:HG21	1.96	0.48
77:u2:39:GLY:O	77:u2:61:ASP:HB2	2.13	0.48
77:u2:66:SER:HA	77:u2:73:THR:HA	1.95	0.48
80:x2:37:TYR:OH	80:x2:87:PRO:HD3	2.13	0.48
82:z2:96:ILE:HG13	82:z2:96:ILE:O	2.13	0.48
2:A2:2506:G:H2'	2:A2:2507:G:H8	1.79	0.48
2:A2:3738:C:H2'	2:A2:3739:G:C8	2.49	0.48
4:B1:162:ASP:HB2	4:B1:163:PRO:HD3	1.95	0.48
10:C1:91:LYS:HB3	10:C1:183:GLU:HG2	1.96	0.48
14:D2:42:LYS:HD3	14:D2:89:TYR:CE2	2.49	0.48
18:E3:68:LYS:HD2	51:T3:6:LEU:HD13	1.95	0.48
23:G2:66:TYR:CE2	23:G2:68:ARG:HD3	2.48	0.48
23:G2:132:VAL:HG11	23:G2:170:GLY:O	2.14	0.48
25:H1:113:LEU:HB2	25:H1:134:LEU:HD12	1.96	0.48
48:S2:47:MET:HE1	48:S2:122:LYS:HD2	1.95	0.48
55:X2:41:ARG:HD3	55:X2:78:ARG:O	2.12	0.48
55:X2:92:ARG:HD3	55:X2:102:LEU:HD21	1.96	0.48
69:m2:19:A:H2'	69:m2:20:G:O4'	2.14	0.48
69:m2:1597:U:H2'	69:m2:1598:U:C6	2.48	0.48
2:A2:3720:U:H2'	2:A2:3721:U:C6	2.48	0.48
2:A2:3871:A:H2'	2:A2:3872:A:C8	2.48	0.48
4:B1:176:LYS:HG2	60:c2:43:MET:HE1	1.96	0.48
26:H2:185:PRO:HG2	26:H2:188:ILE:HD12	1.95	0.48
34:L2:77:GLY:O	34:L2:81:ARG:HG3	2.14	0.48
36:M2:47:PHE:HE1	36:M2:125:GLN:HG2	1.78	0.48
50:T2:5:MET:HG2	50:T2:77:TYR:CZ	2.49	0.48
58:a2:18:ASN:OD1	58:a2:34:TYR:HE2	1.96	0.48
69:m2:54:A:H3'	69:m2:453:G:H22	1.79	0.48
69:m2:844:C:H2'	69:m2:845:C:C6	2.48	0.48
69:m2:1724:G:C2	69:m2:1725:G:H1'	2.48	0.48
74:r2:87:MET:SD	74:r2:123:LEU:HB2	2.54	0.48
79:w2:84:ARG:NH1	79:w2:115:PRO:HG3	2.28	0.48
2:A2:3588:U:H2'	2:A2:3589:G:C8	2.49	0.48
18:E3:90:CYS:HA	18:E3:93:PHE:CD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:m2:54:A:N6	69:m2:453:G:H1'	2.29	0.48
74:r2:151:ASP:OD2	74:r2:153:VAL:HG12	2.14	0.48
2:A2:1156:A:OP1	25:H1:204:ARG:HD2	2.14	0.48
2:A2:3721:U:H2'	2:A2:3722:C:H6	1.79	0.48
2:A2:4436:C:H42	2:A2:4495:C:N4	2.10	0.48
14:D2:234:LYS:HG2	14:D2:238:ILE:HG12	1.94	0.48
71:o2:189:ILE:HG13	71:o2:195:TRP:CZ3	2.49	0.48
75:s2:96:ALA:O	75:s2:100:ILE:HG12	2.14	0.48
76:t2:27:LEU:HD21	76:t2:40:LEU:HD22	1.96	0.48
2:A2:221:C:H2'	2:A2:222:C:C6	2.49	0.48
2:A2:807:G:H2'	2:A2:808:A:H8	1.79	0.48
2:A2:1024:C:H2'	2:A2:1025:C:C6	2.49	0.48
2:A2:1763:G:H21	2:A2:1827:A:H62	1.62	0.48
2:A2:2016:G:H5''	68:k2:94:ARG:HD2	1.96	0.48
2:A2:3291:A:C8	2:A2:3348:A:C8	3.02	0.48
16:E1:157:ILE:HA	16:E1:161:GLU:OE2	2.14	0.48
17:E2:216:MET:HE2	17:E2:281:ASN:HB3	1.95	0.48
22:G1:101:LYS:HG2	22:G1:104:MET:HE2	1.96	0.48
33:K3:215:LYS:O	33:K3:218:LYS:HG2	2.14	0.48
34:L2:134:ASN:HB3	34:L2:137:ILE:HG12	1.96	0.48
53:V2:35:VAL:HG23	53:V2:40:LEU:HG	1.96	0.48
55:X2:54:MET:HE2	55:X2:60:PRO:HA	1.96	0.48
69:m2:1317:U:H5''	78:v2:1:MET:HB3	1.94	0.48
69:m2:1599:C:H4'	69:m2:1605:G:C6	2.48	0.48
71:o2:195:TRP:CD1	71:o2:197:VAL:HB	2.49	0.48
73:q2:59:LEU:HD23	73:q2:66:ILE:HG21	1.96	0.48
78:v2:7:ASN:ND2	78:v2:38:LYS:HB2	2.29	0.48
2:A2:465:G:H2'	2:A2:466:A:C8	2.49	0.47
2:A2:928:G:H1	2:A2:1064:G:H22	1.62	0.47
2:A2:1577:A:H2'	2:A2:1578:A:H8	1.79	0.47
2:A2:1743:A:C2	2:A2:4086:C:H5'	2.48	0.47
2:A2:3507:U:H2'	2:A2:3508:A:O4'	2.14	0.47
2:A2:3552:C:H1'	17:E2:268:ARG:NH2	2.29	0.47
2:A2:3565:C:H5	2:A2:4048:A:H61	1.61	0.47
2:A2:3567:C:H2'	2:A2:3568:U:H6	1.78	0.47
3:A3:11:HIS:HB3	3:A3:12:ILE:HD12	1.96	0.47
3:A3:39:ARG:HH22	6:B3:38:LYS:HA	1.78	0.47
13:D1:184:MET:HE2	13:D1:190:LEU:HG	1.95	0.47
17:E2:107:ALA:HB1	17:E2:202:GLU:HG2	1.96	0.47
19:F1:47:ALA:O	19:F1:149:GLN:HB2	2.14	0.47
20:F2:297:GLU:HG3	32:K2:128:LEU:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:K3:137:ARG:HE	33:K3:178:ARG:HG3	1.79	0.47
48:S2:56:GLN:HB3	48:S2:67:ILE:HD13	1.96	0.47
68:k2:46:ARG:HH22	68:k2:67:ARG:HG3	1.77	0.47
69:m2:121:OMU:HN3	69:m2:345:A:N6	2.12	0.47
69:m2:434:G:H2'	69:m2:435:A:H8	1.79	0.47
69:m2:911:G:H2'	69:m2:912:G:C8	2.47	0.47
69:m2:936:G:O6	69:m2:1010:A:N1	2.47	0.47
69:m2:1630:C:H2'	69:m2:1631:C:C6	2.48	0.47
72:p2:137:LEU:HG	72:p2:215:VAL:HG22	1.96	0.47
74:r2:147:ILE:HG21	74:r2:169:ILE:HG12	1.95	0.47
75:s2:77:MET:HB2	75:s2:89:THR:HG21	1.96	0.47
80:x2:111:MET:HE3	80:x2:119:PHE:CE2	2.49	0.47
2:A2:233:U:H4'	2:A2:234:G:OP1	2.15	0.47
2:A2:1116:U:H4'	56:Y2:18:LYS:HA	1.95	0.47
2:A2:2030:G:H2'	2:A2:2031:A:C8	2.49	0.47
2:A2:2451:A:H62	62:e2:35:LYS:NZ	2.12	0.47
2:A2:3524:G:N2	2:A2:3556:G:H1'	2.26	0.47
3:A3:55:ARG:HE	47:R3:48:VAL:CG1	2.27	0.47
6:B3:127:GLY:O	6:B3:131:LEU:HD23	2.15	0.47
17:E2:93:VAL:HG23	17:E2:102:PHE:HB2	1.97	0.47
33:K3:85:ARG:HH12	45:Q3:118:ARG:HD2	1.78	0.47
55:X2:37:GLY:O	55:X2:41:ARG:HG3	2.13	0.47
69:m2:1427:G:H2'	69:m2:1428:U:C6	2.49	0.47
69:m2:1535:A:C8	69:m2:1606:G:H1'	2.49	0.47
79:w2:84:ARG:HH12	79:w2:115:PRO:HG3	1.79	0.47
1:A1:170:LYS:HD3	1:A1:267:ARG:HH21	1.79	0.47
2:A2:1141:C:H2'	2:A2:1142:G:C8	2.50	0.47
2:A2:1352:G:O4'	14:D2:15:VAL:HG13	2.14	0.47
2:A2:1381:C:H2'	2:A2:1382:U:C6	2.50	0.47
2:A2:1668:G:H21	2:A2:4056:U:C4'	2.27	0.47
2:A2:1911:G:H2'	2:A2:1912:A:H8	1.80	0.47
2:A2:3985:C:O2'	38:N2:8:ARG:HD2	2.14	0.47
6:B3:33:TRP:CH2	6:B3:99:VAL:HG22	2.50	0.47
12:C3:22:ILE:HD12	12:C3:114:VAL:HG12	1.96	0.47
17:E2:85:VAL:HG23	17:E2:167:GLN:HE21	1.79	0.47
19:F1:124:LEU:HD11	59:b2:119:TYR:HB2	1.95	0.47
22:G1:6:TYR:CG	36:M2:151:LYS:HE3	2.49	0.47
23:G2:60:ILE:HD11	23:G2:93:THR:HA	1.95	0.47
27:H3:55:LEU:HD23	69:m2:1393:C:H4'	1.95	0.47
32:K2:58:ARG:HD2	32:K2:83:VAL:HG12	1.95	0.47
32:K2:105:VAL:HB	32:K2:110:ARG:HH21	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:P2:69:LYS:HB3	42:P2:71:GLU:OE1	2.14	0.47
50:T2:5:MET:HG3	50:T2:25:ILE:HD13	1.96	0.47
69:m2:5:U:H2'	69:m2:6:G:C8	2.49	0.47
69:m2:496:C:H5''	74:r2:57:THR:OG1	2.15	0.47
76:t2:84:GLU:O	76:t2:88:SER:HA	2.14	0.47
76:t2:177:TYR:CZ	76:t2:181:THR:HG21	2.48	0.47
2:A2:1430:G:H1'	2:A2:2268:A:H61	1.79	0.47
2:A2:3341:C:H2'	2:A2:3342:G:O4'	2.14	0.47
2:A2:4159:A:H2'	2:A2:4160:C:C6	2.49	0.47
4:B1:154:LEU:HD11	4:B1:222:ILE:HD13	1.97	0.47
7:Bv:68:C:H2'	7:Bv:69:G:C8	2.50	0.47
22:G1:6:TYR:HB3	36:M2:151:LYS:HG3	1.96	0.47
33:K3:23:LYS:HG2	33:K3:42:GLY:H	1.80	0.47
33:K3:134:GLY:HA3	33:K3:158:VAL:HG11	1.95	0.47
69:m2:1334:A:O2'	73:q2:141:LYS:HD3	2.14	0.47
69:m2:1472:C:H2'	69:m2:1473:C:C6	2.49	0.47
1:A1:65:ARG:O	1:A1:69:ARG:HG2	2.15	0.47
2:A2:116:G:H2'	2:A2:117:C:C6	2.49	0.47
2:A2:259:C:H2'	2:A2:260:C:C6	2.49	0.47
2:A2:1168:A:H5'	32:K2:108:ARG:HH21	1.79	0.47
2:A2:1263:C:H2'	2:A2:1264:G:O4'	2.14	0.47
7:Bv:6:G:O2'	7:Bv:7:A:H8	1.98	0.47
19:F1:96:ILE:HD13	19:F1:117:LEU:HD22	1.95	0.47
20:F2:221:PHE:HB2	20:F2:229:LEU:HD21	1.96	0.47
33:K3:137:ARG:HG2	69:m2:170:A:O5'	2.14	0.47
45:Q3:121:ALA:HA	45:Q3:124:ASN:ND2	2.29	0.47
58:a2:40:LYS:HE3	58:a2:52:ARG:NH2	2.29	0.47
72:p2:189:ILE:HB	72:p2:190:PRO:HD3	1.96	0.47
74:r2:68:ARG:HE	74:r2:76:VAL:HG11	1.79	0.47
2:A2:385:A:N3	2:A2:387:G:H5''	2.30	0.47
2:A2:2131:A:H2'	2:A2:2132:C:C6	2.50	0.47
31:J3:232:THR:HG21	69:m2:13:C:H5''	1.95	0.47
32:K2:83:VAL:HG22	32:K2:123:PHE:CZ	2.49	0.47
33:K3:7:PHE:HB3	33:K3:12:CYS:SG	2.55	0.47
33:K3:197:GLN:O	33:K3:200:LYS:HG3	2.14	0.47
38:N2:34:TYR:HE2	38:N2:93:ILE:HG23	1.79	0.47
69:m2:500:C:H2'	69:m2:501:G:C8	2.49	0.47
69:m2:1382:C:H2'	69:m2:1383:G:C8	2.50	0.47
69:m2:1648:C:H5''	81:y2:138:ARG:HD2	1.95	0.47
71:o2:125:THR:O	71:o2:147:LEU:HB2	2.14	0.47
73:q2:61:GLU:HB3	73:q2:62:LYS:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:v2:10:ALA:O	78:v2:13:GLU:HG3	2.14	0.47
1:A1:141:ASN:HD21	1:A1:234:LYS:HD3	1.79	0.47
2:A2:423:G:H5'	30:J2:26:PHE:HZ	1.80	0.47
2:A2:952:C:H2'	2:A2:953:G:H8	1.79	0.47
2:A2:1521:A:H62	2:A2:1643:C:N4	2.12	0.47
2:A2:1553:A:H2'	2:A2:1554:G:H8	1.80	0.47
2:A2:1643:C:H2'	2:A2:1644:G:H4'	1.97	0.47
2:A2:1893:C:N3	2:A2:1896:A:H4'	2.30	0.47
2:A2:4067:1MA:H2'	2:A2:4068:G:O4'	2.14	0.47
2:A2:4176:G:N3	17:E2:252:ALA:HB1	2.29	0.47
2:A2:4337:U:H2'	2:A2:4338:G:C8	2.49	0.47
2:A2:4515:G:H5''	22:G1:91:TRP:CD2	2.50	0.47
2:A2:4581:G:C5	26:H2:190:ARG:HD2	2.49	0.47
4:B1:63:LEU:HD21	25:H1:29:GLN:HE21	1.80	0.47
20:F2:144:ILE:O	20:F2:144:ILE:HG13	2.14	0.47
31:J3:145:LYS:HG3	31:J3:146:GLU:HG2	1.96	0.47
36:M2:2:LYS:O	36:M2:121:ALA:HB3	2.14	0.47
36:M2:107:THR:O	36:M2:111:ARG:HG2	2.14	0.47
39:N3:91:LEU:HD21	69:m2:927:G:H5''	1.97	0.47
43:P3:115:GLU:HG2	43:P3:119:LYS:HD2	1.97	0.47
45:Q3:7:ILE:HD11	45:Q3:47:MET:HE1	1.96	0.47
48:S2:74:TYR:HE2	48:S2:77:LYS:HE3	1.78	0.47
49:S3:14:GLU:HG3	49:S3:18:LYS:HE2	1.96	0.47
49:S3:36:LYS:HA	49:S3:43:ILE:HG12	1.96	0.47
50:T2:73:LYS:HB3	50:T2:73:LYS:HE3	1.65	0.47
56:Y2:28:TYR:HB2	56:Y2:31:ILE:HD12	1.96	0.47
56:Y2:90:MET:HE1	68:k2:112:ARG:HB2	1.97	0.47
67:j2:70:THR:HG23	67:j2:72:ASN:O	2.15	0.47
69:m2:339:C:H2'	69:m2:340:G:H8	1.80	0.47
69:m2:859:U:H2'	69:m2:860:A:C8	2.49	0.47
69:m2:1353:G:C6	69:m2:1354:G:N7	2.82	0.47
69:m2:1564:C:H2'	69:m2:1565:G:C8	2.49	0.47
73:q2:99:ILE:HD11	73:q2:173:ARG:NE	2.29	0.47
78:v2:15:LEU:HD11	78:v2:66:HIS:HB2	1.96	0.47
80:x2:14:LYS:HE2	80:x2:21:ASP:HB2	1.97	0.47
81:y2:80:GLN:O	81:y2:84:ILE:HG13	2.14	0.47
81:y2:104:SER:O	81:y2:108:ILE:HG12	2.14	0.47
1:A1:120:ILE:HG21	32:K2:3:VAL:HG12	1.97	0.47
2:A2:1766:A:H1'	2:A2:4346:G:N2	2.30	0.47
2:A2:2513:G:H2'	2:A2:2514:G:C8	2.50	0.47
2:A2:4552:G:H2'	2:A2:4559:G:H22	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:E1:10:ASN:N	16:E1:11:PRO:HD2	2.29	0.47
20:F2:73:VAL:HG22	20:F2:78:ARG:NH2	2.30	0.47
29:I3:208:ALA:N	29:I3:218:LEU:HD13	2.29	0.47
36:M2:165:PRO:C	36:M2:167:PHE:H	2.22	0.47
69:m2:190:G:H21	69:m2:192:C:N4	2.07	0.47
69:m2:596:A:C6	69:m2:645:A:C8	3.02	0.47
69:m2:879:C:H2'	69:m2:880:G:C8	2.49	0.47
69:m2:928:A:H61	69:m2:1017:U:H3	1.63	0.47
69:m2:981:C:H2'	69:m2:982:A:C8	2.49	0.47
69:m2:1391:C:O2'	73:q2:162:ASP:HB3	2.15	0.47
69:m2:1523:C:C1'	80:x2:128:HIS:HE1	2.26	0.47
76:t2:11:PRO:HD2	76:t2:45:ILE:O	2.13	0.47
2:A2:724:U:H2'	2:A2:725:C:C6	2.50	0.47
2:A2:2463:U:C2	34:L2:40:GLN:HG2	2.50	0.47
2:A2:3364:C:H2'	2:A2:3365:U:H5''	1.96	0.47
2:A2:3517:A:H2'	2:A2:3518:A:C8	2.49	0.47
2:A2:4350:C:H3'	64:g2:111:ARG:NH1	2.28	0.47
2:A2:4648:U:H2'	2:A2:4649:U:C6	2.50	0.47
7:Bv:44:G:N3	7:Bv:44:G:H2'	2.29	0.47
35:L3:111:GLN:CD	35:L3:127:ARG:HD2	2.40	0.47
45:Q3:66:GLY:H	69:m2:583:U:H5''	1.80	0.47
69:m2:159:A:O2'	69:m2:160:U:H5''	2.14	0.47
69:m2:1376:C:H2'	69:m2:1377:G:O4'	2.14	0.47
69:m2:1726:A:H2'	69:m2:1727:U:C6	2.49	0.47
77:u2:76:THR:HG23	77:u2:104:ILE:HD12	1.97	0.47
1:A1:170:LYS:O	1:A1:174:GLU:HG2	2.14	0.47
2:A2:358:C:H2'	2:A2:359:A:C8	2.50	0.47
2:A2:952:C:H2'	2:A2:953:G:C8	2.50	0.47
2:A2:1523:G:H2'	2:A2:1524:C:C6	2.50	0.47
2:A2:3816:C:H2'	2:A2:3817:C:C6	2.50	0.47
2:A2:4315:G:OP1	44:Q2:34:ALA:HB3	2.14	0.47
18:E3:9:THR:HG22	69:m2:683:U:H4'	1.97	0.47
33:K3:209:TYR:CD1	74:r2:149:TYR:HB3	2.49	0.47
34:L2:40:GLN:O	34:L2:44:LEU:HG	2.15	0.47
39:N3:3:ARG:HB3	39:N3:6:ALA:HB3	1.97	0.47
39:N3:71:ILE:O	39:N3:75:LEU:HD23	2.15	0.47
41:O3:42:VAL:CG2	41:O3:81:VAL:HG21	2.44	0.47
69:m2:1672:C:H2'	69:m2:1673:G:C8	2.50	0.47
69:m2:1860:G:H2'	69:m2:1861:A:H8	1.80	0.47
71:o2:33:GLN:HB3	71:o2:154:LEU:HD12	1.98	0.47
71:o2:130:ASP:C	71:o2:133:PRO:HD2	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:p2:105:LEU:HD11	72:p2:211:PHE:HD2	1.80	0.47
72:p2:222:LYS:HD3	72:p2:223:PHE:N	2.30	0.47
74:r2:37:LYS:HB2	74:r2:40:GLU:CD	2.40	0.47
79:w2:113:LEU:HD11	79:w2:117:PHE:HB2	1.96	0.47
2:A2:10:A:H2'	2:A2:11:G:H8	1.80	0.46
2:A2:138:C:H2'	2:A2:139:G:C8	2.50	0.46
2:A2:1114:G:H2'	2:A2:1115:C:C6	2.50	0.46
2:A2:1244:C:H2'	2:A2:1245:G:O4'	2.14	0.46
2:A2:4703:C:H2'	2:A2:4704:A:C8	2.50	0.46
17:E2:165:HIS:HB3	17:E2:180:LEU:HD12	1.97	0.46
21:F3:45:VAL:HG23	21:F3:50:VAL:HG12	1.97	0.46
22:G1:126:GLU:HB3	28:I2:181:ALA:HB1	1.97	0.46
25:H1:33:LEU:HD13	25:H1:37:HIS:CD2	2.50	0.46
42:P2:87:SER:HA	42:P2:97:TYR:HB3	1.97	0.46
47:R3:106:GLN:HE21	75:s2:170:ALA:HB3	1.79	0.46
69:m2:291:G:H2'	69:m2:292:U:C6	2.50	0.46
69:m2:1540:C:H2'	69:m2:1541:U:C6	2.50	0.46
76:t2:167:GLU:HA	76:t2:189:PHE:HZ	1.80	0.46
77:u2:190:LEU:HD23	77:u2:195:LEU:HA	1.95	0.46
2:A2:278:G:H2'	2:A2:329:A:N7	2.30	0.46
2:A2:927:C:H2'	2:A2:928:G:C8	2.51	0.46
2:A2:2366:A:H5'	2:A2:2443:G:H4'	1.98	0.46
2:A2:3374:A2M:H2	2:A2:3590:G:O4'	2.15	0.46
2:A2:3504:U:H2'	2:A2:3505:A:C8	2.50	0.46
2:A2:3567:C:H2'	2:A2:3568:U:C6	2.51	0.46
3:A3:71:MET:HB3	3:A3:99:LEU:HD21	1.97	0.46
7:Bv:53:G:H2'	7:Bv:62:C:H41	1.80	0.46
22:G1:108:ASP:O	22:G1:112:VAL:HG23	2.16	0.46
25:H1:38:ARG:HH21	25:H1:60:VAL:HG12	1.79	0.46
32:K2:158:THR:HB	32:K2:161:SER:HB3	1.96	0.46
69:m2:7:G:H2'	69:m2:8:U:H5''	1.97	0.46
69:m2:868:U:H2'	69:m2:869:OMG:C8	2.50	0.46
69:m2:1523:C:H4'	80:x2:126:VAL:HG13	1.96	0.46
81:y2:96:TYR:HA	81:y2:100:VAL:HG22	1.97	0.46
1:A1:147:LEU:HD22	1:A1:152:ILE:CD1	2.45	0.46
2:A2:461:G:H2'	2:A2:462:G:H8	1.80	0.46
2:A2:1765:C:N3	2:A2:1766:A:C8	2.83	0.46
2:A2:3957:G:C2	38:N2:80:VAL:HG21	2.50	0.46
3:A3:8:LYS:HD3	3:A3:58:GLU:HA	1.97	0.46
4:B1:37:LYS:HB2	4:B1:44:ASP:OD2	2.16	0.46
33:K3:28:TYR:CE1	33:K3:104:ALA:HB2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:K3:33:ALA:HA	33:K3:51:ARG:HG3	1.96	0.46
33:K3:110:ASN:C	33:K3:111:LEU:HD12	2.41	0.46
35:L3:134:HIS:HA	35:L3:162:ARG:HD2	1.96	0.46
67:j2:8:VAL:O	67:j2:27:LYS:HE3	2.15	0.46
71:o2:206:ASP:OD1	71:o2:207:PRO:HD2	2.15	0.46
73:q2:196:GLY:N	73:q2:201:LYS:HZ1	2.14	0.46
75:s2:100:ILE:HB	75:s2:108:PRO:HB3	1.98	0.46
1:A1:204:PHE:HB3	1:A1:222:ARG:HG3	1.97	0.46
2:A2:131:C:H2'	2:A2:132:G:C8	2.51	0.46
2:A2:1310:A:C2	32:K2:170:LYS:HE2	2.50	0.46
2:A2:2013:C:H5	2:A2:2014:G:H21	1.62	0.46
2:A2:4653:A:H2'	2:A2:4654:C:H6	1.80	0.46
5:B2:39:C:O2'	16:E1:46:GLN:HB3	2.15	0.46
29:I3:259:TRP:CZ3	29:I3:266:ILE:HG12	2.51	0.46
30:J2:15:CYS:SG	30:J2:150:LEU:HB2	2.55	0.46
35:L3:32:ILE:HD11	35:L3:40:LYS:HG2	1.96	0.46
37:M3:31:LEU:O	37:M3:31:LEU:HD23	2.16	0.46
41:O3:124:MET:HE3	41:O3:124:MET:HB3	1.73	0.46
41:O3:138:ASP:HB2	69:m2:944:G:N2	2.29	0.46
47:R3:101:SER:O	47:R3:108:ILE:HG22	2.15	0.46
54:W2:34:THR:HG21	54:W2:93:THR:HG22	1.96	0.46
69:m2:223:A:H2'	69:m2:224:U:H6	1.81	0.46
69:m2:555:A:H2'	69:m2:556:A:C8	2.41	0.46
69:m2:1714:A:H2'	69:m2:1715:C:C6	2.50	0.46
2:A2:301:G:H2'	2:A2:302:C:C6	2.50	0.46
2:A2:488:G:H2'	2:A2:489:G:H8	1.80	0.46
2:A2:2297:G:H2'	2:A2:2298:A:C8	2.51	0.46
2:A2:2393:G:H22	2:A2:2474:C:P	2.39	0.46
2:A2:2534:C:OP2	46:R2:106:LYS:HD2	2.15	0.46
2:A2:4285:G:O3'	2:A2:4286:U:H3'	2.16	0.46
19:F1:46:ILE:HB	19:F1:49:ARG:HD2	1.98	0.46
19:F1:91:ALA:HB1	19:F1:96:ILE:HB	1.97	0.46
19:F1:179:PHE:CD2	52:U2:131:ARG:HB2	2.51	0.46
21:F3:63:VAL:HG11	41:O3:128:ARG:HA	1.98	0.46
23:G2:11:ALA:O	23:G2:15:ARG:HG3	2.15	0.46
29:I3:64:HIS:HE1	69:m2:1453:G:H5'	1.81	0.46
30:J2:16:LYS:HG2	30:J2:149:ILE:CD1	2.46	0.46
35:L3:136:ARG:HB3	35:L3:162:ARG:HH22	1.81	0.46
69:m2:166:A:H2'	69:m2:167:G:C8	2.51	0.46
69:m2:563:A:H2'	69:m2:564:U:C6	2.50	0.46
69:m2:1224:G:H5''	75:s2:78:MET:HE3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:m2:1734:G:H2'	69:m2:1735:U:H6	1.81	0.46
2:A2:260:C:H2'	2:A2:261:G:C8	2.49	0.46
2:A2:1660:A:H2'	2:A2:1661:C:H6	1.80	0.46
2:A2:2129:A:H2'	2:A2:2130:A:C8	2.50	0.46
2:A2:2587:A:H2'	2:A2:2588:A:C8	2.51	0.46
2:A2:3515:G:H4'	30:J2:139:TYR:CE1	2.50	0.46
2:A2:4218:U:H2'	2:A2:4219:G:O4'	2.16	0.46
7:Bv:9:A:H1'	7:Bv:46:G:H21	1.81	0.46
8:Bx:49:U:HO2'	8:Bx:50:U:H6	1.59	0.46
17:E2:370:THR:HG22	17:E2:370:THR:O	2.16	0.46
27:H3:42:CYS:O	27:H3:46:TYR:HD1	1.97	0.46
33:K3:50:VAL:HG21	33:K3:111:LEU:HD23	1.97	0.46
35:L3:40:LYS:HD2	69:m2:643:A:P	2.55	0.46
39:N3:16:LEU:HD21	39:N3:65:PHE:HZ	1.79	0.46
53:V2:16:TRP:HB3	53:V2:21:ILE:HD11	1.98	0.46
69:m2:602:G:H2'	69:m2:603:OMG:C8	2.50	0.46
71:o2:76:VAL:HG23	71:o2:98:PRO:HA	1.97	0.46
2:A2:659:C:O2'	2:A2:660:G:H5'	2.16	0.46
2:A2:951:C:H2'	2:A2:952:C:H6	1.81	0.46
2:A2:1034:U:H2'	2:A2:1035:C:H6	1.81	0.46
2:A2:2240:U:H2'	2:A2:2241:G:C8	2.51	0.46
2:A2:2293:U:H2'	2:A2:2294:C:C6	2.50	0.46
2:A2:2579:OMC:HM23	2:A2:2579:OMC:H1'	1.66	0.46
2:A2:3366:G:N3	2:A2:3368:A:N6	2.63	0.46
2:A2:3421:G:HO2'	2:A2:3422:A:H2	1.64	0.46
2:A2:3566:C:H2'	2:A2:3567:C:C6	2.51	0.46
2:A2:3608:A:H2'	2:A2:3609:G:H8	1.79	0.46
2:A2:4356:C:H2'	2:A2:4357:A:C8	2.50	0.46
5:B2:54:A:C6	16:E1:12:MET:HG2	2.51	0.46
13:D1:156:LYS:HE3	13:D1:163:GLN:H	1.81	0.46
35:L3:40:LYS:HD2	69:m2:643:A:OP1	2.16	0.46
41:O3:138:ASP:HB2	69:m2:944:G:H21	1.80	0.46
47:R3:58:LEU:HB3	47:R3:77:LEU:HD21	1.98	0.46
55:X2:33:ILE:O	55:X2:36:VAL:HG22	2.15	0.46
61:d2:60:GLY:HA2	61:d2:64:MET:SD	2.55	0.46
62:e2:47:ILE:HG22	62:e2:49:ASP:H	1.80	0.46
63:f2:26:TRP:CD1	63:f2:26:TRP:H	2.31	0.46
69:m2:1310:U:H2'	69:m2:1311:C:C6	2.51	0.46
72:p2:149:GLN:HE22	72:p2:154:SER:HB2	1.80	0.46
74:r2:233:LYS:HD3	74:r2:234:PRO:HD2	1.97	0.46
79:w2:35:ARG:HD2	79:w2:35:ARG:HA	1.71	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:x2:92:SER:HB2	80:x2:107:ILE:HD12	1.97	0.46
2:A2:821:U:H2'	2:A2:822:C:C6	2.50	0.46
2:A2:1285:C:H2'	2:A2:1286:U:C6	2.50	0.46
2:A2:1668:G:H8	2:A2:1668:G:O5'	1.99	0.46
2:A2:2168:U:H2'	2:A2:2169:G:H8	1.80	0.46
2:A2:2275:C:H2'	2:A2:2276:G:C8	2.49	0.46
6:B3:28:LEU:HD21	6:B3:53:PHE:HD2	1.80	0.46
13:D1:38:ARG:HG2	13:D1:41:ALA:HB2	1.98	0.46
17:E2:89:ILE:CD1	17:E2:197:ALA:HB1	2.45	0.46
25:H1:64:ILE:CD1	25:H1:106:ALA:HB2	2.40	0.46
45:Q3:104:ARG:HG2	69:m2:493:C:OP2	2.16	0.46
48:S2:72:GLN:HE21	48:S2:74:TYR:HD1	1.64	0.46
50:T2:121:ARG:O	50:T2:124:THR:HG22	2.15	0.46
64:g2:93:LYS:HD2	64:g2:103:LEU:O	2.16	0.46
69:m2:480:G:H2'	69:m2:481:C:C6	2.50	0.46
69:m2:497:U:H2'	69:m2:498:C:O4'	2.15	0.46
69:m2:1104:G:H2'	69:m2:1105:C:C6	2.51	0.46
69:m2:1427:G:H2'	69:m2:1428:U:H6	1.81	0.46
69:m2:1708:G:H2'	69:m2:1709:U:C6	2.51	0.46
73:q2:28:GLU:HG2	78:v2:65:ARG:HH22	1.80	0.46
80:x2:52:LYS:HD2	80:x2:53:GLN:N	2.30	0.46
81:y2:10:VAL:HG23	81:y2:25:CYS:HB3	1.97	0.46
82:z2:41:ILE:HD13	82:z2:50:ILE:HD12	1.98	0.46
2:A2:1881:G:H2'	2:A2:1882:U:H6	1.81	0.46
2:A2:2162:G:N2	63:f2:51:LEU:HD23	2.31	0.46
2:A2:2311:G:H2'	2:A2:2312:G:H8	1.80	0.46
2:A2:4613:A:H2'	2:A2:4614:A:H8	1.81	0.46
3:A3:74:PRO:HB3	3:A3:79:ILE:HD12	1.98	0.46
3:A3:138:THR:HG21	69:m2:1235:G:O6	2.15	0.46
4:B1:182:CYS:HB3	4:B1:222:ILE:HG12	1.98	0.46
10:C1:101:ILE:HG23	10:C1:114:ILE:HG23	1.97	0.46
18:E3:90:CYS:HA	18:E3:93:PHE:HD2	1.81	0.46
21:F3:39:PHE:CD2	21:F3:41:ILE:HD11	2.51	0.46
35:L3:104:ASP:O	35:L3:107:GLU:HG3	2.16	0.46
43:P3:19:LYS:NZ	69:m2:1154:U:H4'	2.31	0.46
46:R2:47:ARG:HA	46:R2:47:ARG:HD2	1.69	0.46
57:Z2:6:TRP:CE3	57:Z2:102:ARG:HG2	2.51	0.46
69:m2:39:A:H2'	69:m2:40:A:O4'	2.15	0.46
1:A1:166:TYR:CE2	1:A1:259:GLU:HB2	2.51	0.46
1:A1:206:ILE:HD11	1:A1:215:GLU:HG2	1.98	0.46
1:A1:254:ASP:HA	1:A1:258:ARG:NH2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A2:119:G:H3'	2:A2:120:A:H5''	1.97	0.46
2:A2:811:G:H8	2:A2:811:G:OP2	1.99	0.46
2:A2:1064:G:H2'	2:A2:1065:U:H5''	1.98	0.46
2:A2:1187:A:H2	20:F2:234:LYS:HD3	1.80	0.46
2:A2:1331:A:H5'	52:U2:27:LYS:NZ	2.31	0.46
2:A2:2536:G:OP1	63:f2:10:LYS:HD3	2.16	0.46
2:A2:4700:C:H4'	2:A2:4701:G:C8	2.51	0.46
5:B2:46:C:OP1	23:G2:158:LYS:HG3	2.15	0.46
10:C1:91:LYS:HA	10:C1:145:ILE:HD13	1.98	0.46
18:E3:68:LYS:HB3	18:E3:91:LEU:HD22	1.97	0.46
28:I2:197:LYS:HG3	28:I2:203:VAL:HG22	1.97	0.46
30:J2:36:ILE:HA	30:J2:39:MET:CE	2.46	0.46
33:K3:162:LEU:HB3	33:K3:164:LYS:HZ3	1.80	0.46
33:K3:199:THR:HG21	69:m2:126:G:H2'	1.96	0.46
34:L2:92:LYS:HG2	34:L2:96:MET:HE2	1.98	0.46
43:P3:50:PHE:CZ	76:t2:146:VAL:HG21	2.51	0.46
48:S2:115:ARG:HD3	48:S2:118:ILE:HD11	1.98	0.46
49:S3:33:MET:HE2	49:S3:48:SER:HA	1.98	0.46
53:V2:15:LYS:HA	53:V2:18:ARG:HH11	1.79	0.46
69:m2:1641:G:H2'	69:m2:1642:A:C8	2.51	0.46
76:t2:100:ILE:CD1	76:t2:125:VAL:HG21	2.45	0.46
80:x2:39:ALA:HA	80:x2:42:ARG:HH11	1.81	0.46
2:A2:151:G:H3'	25:H1:49:ARG:NH2	2.30	0.45
2:A2:1136:A:H1'	2:A2:1138:A:OP2	2.17	0.45
2:A2:2440:C:H2'	2:A2:2441:G:O4'	2.16	0.45
2:A2:4290:U:H2'	2:A2:4291:G:N3	2.30	0.45
2:A2:4653:A:H2'	2:A2:4654:C:C6	2.50	0.45
4:B1:232:GLU:O	4:B1:236:HIS:HB2	2.15	0.45
12:C3:79:ARG:HH12	81:y2:132:PHE:HD2	1.63	0.45
18:E3:107:ARG:HD2	69:m2:20:G:OP1	2.16	0.45
35:L3:134:HIS:CE1	69:m2:564:U:H5'	2.51	0.45
43:P3:52:ILE:HB	76:t2:144:ILE:HG22	1.98	0.45
69:m2:149:A:H5'	69:m2:150:A:OP2	2.16	0.45
69:m2:947:U:H2'	69:m2:948:U:C6	2.51	0.45
69:m2:1115:A:H2'	69:m2:1116:U:C6	2.51	0.45
69:m2:1463:G:H2'	69:m2:1466:C:H41	1.82	0.45
71:o2:90:PHE:HD1	71:o2:179:ALA:HB2	1.81	0.45
71:o2:192:GLU:HG2	71:o2:193:HIS:N	2.32	0.45
79:w2:133:PRO:HB3	79:w2:139:ARG:NH1	2.31	0.45
2:A2:668:C:H2'	2:A2:669:C:C6	2.52	0.45
2:A2:1379:C:H2'	2:A2:1380:U:H6	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A2:1590:A:H2'	13:D1:22:PHE:CZ	2.51	0.45
2:A2:3719:U:H2'	2:A2:3720:U:C6	2.51	0.45
2:A2:3962:A:H2'	2:A2:3963:A:O4'	2.16	0.45
2:A2:4110:C:H2'	2:A2:4111:U:C6	2.51	0.45
4:B1:87:LEU:HD13	4:B1:91:THR:HG22	1.98	0.45
13:D1:175:LYS:O	13:D1:175:LYS:HG3	2.15	0.45
16:E1:80:GLU:O	16:E1:84:GLU:HG2	2.16	0.45
17:E2:185:VAL:HG12	17:E2:193:LYS:HG2	1.97	0.45
28:I2:14:HIS:CD2	28:I2:19:LEU:HD13	2.51	0.45
29:I3:256:ILE:HG23	29:I3:270:LEU:HB2	1.98	0.45
33:K3:98:ARG:HD2	33:K3:99:GLY:H	1.82	0.45
52:U2:102:ASP:HB3	52:U2:105:ARG:HB3	1.97	0.45
68:k2:6:GLN:O	68:k2:10:VAL:HG22	2.15	0.45
69:m2:1447:U:H1'	69:m2:1582:A:N6	2.31	0.45
69:m2:1742:C:H2'	69:m2:1743:U:C6	2.51	0.45
73:q2:25:LEU:HD12	73:q2:29:LEU:HD12	1.99	0.45
74:r2:99:PHE:CE1	74:r2:113:ARG:HG2	2.51	0.45
78:v2:11:ILE:HG22	78:v2:35:LEU:HD11	1.97	0.45
2:A2:1112:C:H2'	2:A2:1113:G:C8	2.51	0.45
2:A2:1118:C:H2'	2:A2:1119:C:C6	2.52	0.45
2:A2:1511:C:H2'	2:A2:1512:U:C4	2.51	0.45
2:A2:1560:G:H2'	2:A2:1561:G:C8	2.52	0.45
2:A2:2422:C:O4'	34:L2:96:MET:HG2	2.15	0.45
2:A2:3844:A:H2'	2:A2:3845:C:H6	1.82	0.45
17:E2:31:SER:OG	17:E2:351:LEU:HD11	2.15	0.45
17:E2:247:GLY:HA3	17:E2:250:LYS:HD2	1.97	0.45
17:E2:285:TYR:CD1	17:E2:363:ILE:HD13	2.52	0.45
20:F2:76:ILE:HG12	20:F2:96:CYS:SG	2.56	0.45
21:F3:47:ALA:O	21:F3:50:VAL:HG22	2.16	0.45
26:H2:265:LEU:O	26:H2:269:LYS:HG3	2.16	0.45
28:I2:192:PHE:HA	28:I2:195:VAL:HG12	1.98	0.45
41:O3:138:ASP:OD2	69:m2:987:G:H1'	2.15	0.45
48:S2:55:VAL:CG2	48:S2:104:VAL:HB	2.47	0.45
69:m2:17:C:H2'	69:m2:18:C:C6	2.51	0.45
69:m2:70:G:N2	69:m2:79:A:H62	2.14	0.45
69:m2:981:C:H2'	69:m2:982:A:H8	1.82	0.45
69:m2:1215:C:H2'	69:m2:1216:A:C8	2.51	0.45
69:m2:1334:A:C2	69:m2:1502:G:C4	3.05	0.45
73:q2:151:LYS:HB2	73:q2:151:LYS:HE3	1.78	0.45
78:v2:31:LYS:HA	78:v2:39:ASN:HB3	1.97	0.45
2:A2:1381:C:H2'	2:A2:1382:U:H6	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A2:1429:U:H2'	2:A2:1430:G:H8	1.81	0.45
2:A2:2284:A:H2'	2:A2:2284:A:N3	2.32	0.45
2:A2:2520:A:H2'	2:A2:2521:A:C8	2.51	0.45
4:B1:229:ARG:HH21	4:B1:232:GLU:CD	2.24	0.45
12:C3:48:LEU:HD12	12:C3:93:SER:HB2	1.97	0.45
12:C3:52:GLY:HA3	69:m2:1403:A:H4'	1.97	0.45
18:E3:52:LEU:HD12	18:E3:71:ARG:HG2	1.98	0.45
19:F1:16:LYS:O	19:F1:16:LYS:HG2	2.17	0.45
29:I3:150:TRP:O	29:I3:170:TRP:HB3	2.16	0.45
35:L3:107:GLU:HA	35:L3:112:THR:HG21	1.98	0.45
45:Q3:108:LYS:HD3	69:m2:53:C:H4'	1.99	0.45
46:R2:77:ILE:HD13	46:R2:100:VAL:HG12	1.98	0.45
51:T3:12:VAL:HG23	69:m2:618:A:H1'	1.98	0.45
57:Z2:25:THR:HG21	57:Z2:85:ARG:HD3	1.97	0.45
60:c2:29:ARG:HA	60:c2:32:ARG:HD2	1.99	0.45
67:j2:51:ALA:HB3	67:j2:54:ILE:HD12	1.98	0.45
69:m2:1734:G:H2'	69:m2:1735:U:C6	2.51	0.45
75:s2:23:TRP:CZ3	75:s2:101:HIS:HD2	2.35	0.45
78:v2:3:MET:HG3	78:v2:41:PRO:CB	2.45	0.45
2:A2:76:A:H5'	19:F1:101:ARG:NH1	2.32	0.45
2:A2:1210:G:H5''	52:U2:132:ARG:NH1	2.32	0.45
2:A2:1734:A:H2'	2:A2:1735:G:C8	2.51	0.45
2:A2:3409:G:H2'	2:A2:3410:G:O4'	2.16	0.45
2:A2:3504:U:H2'	2:A2:3505:A:H8	1.80	0.45
2:A2:4268:A:H2'	2:A2:4269:G:O4'	2.17	0.45
2:A2:4275:OMG:HM23	2:A2:4275:OMG:H1'	1.82	0.45
2:A2:4427:C:H2'	2:A2:4428:C:C6	2.51	0.45
2:A2:4499:G:H2'	2:A2:4500:G:C8	2.51	0.45
6:B3:31:PRO:O	6:B3:34:VAL:HG12	2.16	0.45
19:F1:42:LYS:O	19:F1:46:ILE:HG12	2.16	0.45
23:G2:64:ILE:HG12	23:G2:105:LEU:HD11	1.99	0.45
24:G3:32:VAL:HG11	24:G3:56:LEU:HD21	1.98	0.45
31:J3:267:GLN:HB3	71:o2:120:ARG:CZ	2.47	0.45
36:M2:43:ARG:HD2	36:M2:43:ARG:HA	1.69	0.45
42:P2:69:LYS:HA	42:P2:70:PRO:HD3	1.82	0.45
57:Z2:40:GLU:HA	57:Z2:43:LEU:HD13	1.98	0.45
69:m2:96:C:H2'	69:m2:97:U:C6	2.52	0.45
69:m2:973:G:H8	69:m2:973:G:OP2	2.00	0.45
70:n2:22:C:H2'	70:n2:23:G:H8	1.82	0.45
74:r2:136:ILE:HG13	74:r2:138:HIS:NE2	2.30	0.45
82:z2:54:VAL:O	82:z2:58:MET:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A2:176:G:H2'	2:A2:177:G:C8	2.52	0.45
2:A2:398:A2M:H8	2:A2:398:A2M:O5'	2.17	0.45
2:A2:687:G:H2'	2:A2:688:G:C8	2.52	0.45
2:A2:1820:C:H2'	2:A2:1821:C:C6	2.51	0.45
2:A2:4649:U:H2'	2:A2:4650:C:C6	2.52	0.45
2:A2:4693:C:O2'	2:A2:4696:C:H5'	2.17	0.45
5:B2:118:C:H2'	5:B2:119:U:C6	2.52	0.45
7:Bv:37:A:H2'	7:Bv:38:A:O4'	2.16	0.45
17:E2:115:LYS:HE3	17:E2:129:ALA:HB3	1.99	0.45
17:E2:378:ARG:CG	44:Q2:32:LEU:HD21	2.47	0.45
25:H1:116:LEU:HA	25:H1:159:ARG:HH21	1.81	0.45
30:J2:54:LYS:HA	30:J2:83:TRP:CD1	2.51	0.45
31:J3:209:VAL:CG1	31:J3:210:PRO:HD3	2.47	0.45
32:K2:12:LYS:HB2	32:K2:14:ARG:HH11	1.81	0.45
45:Q3:117:VAL:HG11	45:Q3:125:VAL:HG11	1.99	0.45
48:S2:50:ARG:HD2	48:S2:115:ARG:NH2	2.31	0.45
63:f2:9:ILE:HD12	63:f2:51:LEU:HD22	1.99	0.45
69:m2:890:U:H2'	69:m2:891:U:C6	2.51	0.45
69:m2:972:G:H4'	69:m2:973:G:OP2	2.16	0.45
69:m2:1630:C:H2'	69:m2:1631:C:H6	1.80	0.45
71:o2:99:ILE:HG13	71:o2:99:ILE:O	2.17	0.45
71:o2:107:THR:O	71:o2:116:PHE:HA	2.17	0.45
78:v2:24:LYS:HG2	78:v2:61:GLN:OE1	2.16	0.45
2:A2:1486:U:H2'	2:A2:1487:C:C6	2.52	0.45
2:A2:1541:G:H2'	2:A2:1542:C:C6	2.51	0.45
2:A2:1697:G:H2'	2:A2:1698:A:O4'	2.17	0.45
2:A2:2177:OMC:HM23	2:A2:2177:OMC:H1'	1.67	0.45
2:A2:4239:G:OP1	28:I2:61:ARG:HD2	2.16	0.45
2:A2:4600:G:H2'	2:A2:4601:A:C8	2.51	0.45
10:C1:111:LEU:HD21	10:C1:125:ARG:HG2	1.97	0.45
16:E1:92:TYR:HD2	80:x2:10:ARG:HD2	1.82	0.45
30:J2:131:ARG:HG3	30:J2:137:ASN:HB2	1.99	0.45
34:L2:70:ARG:HE	34:L2:75:HIS:HB2	1.80	0.45
36:M2:96:GLU:HB3	36:M2:142:VAL:HG21	1.99	0.45
42:P2:126:ALA:HA	42:P2:133:ALA:HB2	1.99	0.45
45:Q3:60:PHE:HB3	45:Q3:69:THR:HG22	1.99	0.45
58:a2:95:PHE:HD2	58:a2:96:LEU:HD22	1.82	0.45
72:p2:171:ILE:HD13	72:p2:174:ARG:HH12	1.81	0.45
76:t2:93:VAL:HG21	76:t2:133:LEU:HD12	1.98	0.45
78:v2:32:HIS:CD2	78:v2:33:PRO:HD2	2.52	0.45
2:A2:112:C:C2	2:A2:113:A:C8	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A2:1478:C:H2'	2:A2:1479:C:C6	2.51	0.45
2:A2:1478:C:H2'	2:A2:1479:C:H6	1.82	0.45
2:A2:1648:G:H2'	2:A2:1649:C:H6	1.80	0.45
2:A2:1668:G:H1	2:A2:4092:G:N2	2.14	0.45
2:A2:1677:C:H2'	2:A2:1678:U:C6	2.52	0.45
2:A2:2544:A:H1'	63:f2:45:ARG:HH22	1.82	0.45
2:A2:4555:A:C8	28:I2:156:LEU:HD12	2.52	0.45
10:C1:4:ILE:HG12	10:C1:61:TRP:CH2	2.52	0.45
18:E3:51:VAL:HG23	18:E3:100:VAL:HG21	1.98	0.45
20:F2:284:MET:HE3	32:K2:124:ASP:HB3	1.99	0.45
23:G2:41:LYS:HG3	38:N2:93:ILE:HG13	1.98	0.45
23:G2:153:THR:HG23	23:G2:160:PHE:CE2	2.51	0.45
23:G2:219:TYR:CE2	23:G2:227:ILE:HD11	2.52	0.45
31:J3:94:ILE:HD13	31:J3:159:LYS:O	2.17	0.45
47:R3:69:THR:H	47:R3:72:VAL:CG1	2.30	0.45
51:T3:12:VAL:HG21	69:m2:618:A:N3	2.31	0.45
69:m2:223:A:H2'	69:m2:224:U:C6	2.52	0.45
69:m2:585:A:C4	69:m2:586:A:C8	3.05	0.45
69:m2:823:G:H1'	69:m2:826:C:OP1	2.17	0.45
69:m2:1103:U:OP1	72:p2:151:ARG:HG2	2.17	0.45
69:m2:1493:G:H2'	69:m2:1494:U:C6	2.51	0.45
69:m2:1661:U:H5''	69:m2:1662:C:OP2	2.17	0.45
69:m2:1819:G:H2'	69:m2:1820:A:C8	2.52	0.45
78:v2:80:ARG:HD2	78:v2:83:LEU:HB3	1.99	0.45
79:w2:40:ILE:HG23	79:w2:68:ILE:HD12	1.98	0.45
82:z2:103:LYS:HD3	82:z2:117:LEU:HD13	1.99	0.45
2:A2:1154:OMC:HM21	20:F2:106:LYS:HB2	1.99	0.45
2:A2:2570:A2M:H2	2:A2:3279:C:O4'	2.16	0.45
6:B3:37:VAL:HG12	6:B3:47:PRO:HD2	1.99	0.45
11:C2:33:G:H5''	11:C2:34:U:OP1	2.17	0.45
14:D2:200:ARG:O	14:D2:204:MET:HG3	2.17	0.45
15:D3:70:LEU:HD21	15:D3:74:LYS:NZ	2.32	0.45
22:G1:110:PHE:O	22:G1:114:LYS:HG2	2.16	0.45
24:G3:15:THR:HG21	24:G3:33:GLU:HG3	1.98	0.45
24:G3:24:GLN:HE22	75:s2:127:ARG:NH2	2.15	0.45
29:I3:289:LEU:HA	29:I3:299:PHE:O	2.17	0.45
31:J3:252:THR:HG22	31:J3:255:LEU:H	1.81	0.45
32:K2:26:ARG:O	32:K2:30:LYS:HG3	2.16	0.45
33:K3:47:GLY:HA3	33:K3:116:LYS:HD3	1.98	0.45
39:N3:25:TRP:CE2	49:S3:82:LYS:HE2	2.52	0.45
56:Y2:82:VAL:O	56:Y2:86:GLU:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:m2:164:A:H2'	69:m2:165:G:C8	2.51	0.45
69:m2:401:C:O2'	79:w2:106:HIS:CE1	2.69	0.45
69:m2:1313:C:H2'	69:m2:1314:G:O4'	2.16	0.45
69:m2:1650:G:N7	81:y2:17:LYS:HE2	2.32	0.45
71:o2:50:ASN:OD1	71:o2:53:ARG:HB2	2.17	0.45
78:v2:53:LYS:HE2	78:v2:53:LYS:HA	1.99	0.45
79:w2:16:ILE:HG13	79:w2:17:PHE:H	1.81	0.45
2:A2:1023:C:H2'	2:A2:1024:C:C6	2.52	0.45
2:A2:1862:G:N2	36:M2:115:ALA:HB2	2.31	0.45
2:A2:2168:U:C2	2:A2:2169:G:C8	3.04	0.45
2:A2:3297:U:H5	2:A2:3302:A:N7	2.13	0.45
2:A2:4349:U:H4'	64:g2:104:HIS:CE1	2.52	0.45
2:A2:4425:C:H2'	2:A2:4426:C:H6	1.83	0.45
8:Bx:50:U:H2'	8:Bx:51:U:C6	2.51	0.45
12:C3:67:LYS:HE2	12:C3:78:ASP:OD1	2.17	0.45
29:I3:269:GLU:C	29:I3:270:LEU:HD12	2.42	0.45
39:N3:120:SER:O	39:N3:124:ARG:HG3	2.17	0.45
50:T2:42:LEU:HD21	50:T2:96:VAL:HG12	1.99	0.45
62:e2:51:GLU:HG2	62:e2:52:LYS:N	2.31	0.45
69:m2:498:C:OP1	74:r2:29:PRO:HG3	2.17	0.45
69:m2:575:U:O2	69:m2:578:A2M:H8	2.17	0.45
69:m2:1597:U:H2'	69:m2:1598:U:H6	1.81	0.45
71:o2:148:CYS:N	71:o2:163:CYS:SG	2.89	0.45
75:s2:77:MET:HG3	75:s2:84:GLY:O	2.18	0.45
2:A2:398:A2M:HM'3	2:A2:398:A2M:H1'	1.78	0.44
2:A2:1067:A:C5	2:A2:1082:A:C6	3.06	0.44
2:A2:1168:A:H5'	32:K2:108:ARG:NH2	2.32	0.44
2:A2:1391:U:H2'	2:A2:1392:C:H6	1.81	0.44
2:A2:1639:A:O2'	38:N2:132:PRO:HD3	2.17	0.44
2:A2:1831:A:H2'	2:A2:1832:A:H8	1.80	0.44
2:A2:2451:A:C8	62:e2:26:LYS:HE3	2.52	0.44
2:A2:2470:G:H2'	2:A2:2471:C:H6	1.82	0.44
4:B1:153:GLN:HG3	4:B1:205:THR:O	2.16	0.44
14:D2:107:MET:SD	14:D2:113:VAL:HG11	2.57	0.44
19:F1:89:LYS:HD3	59:b2:114:TYR:CE2	2.51	0.44
22:G1:100:ARG:HH21	28:I2:203:VAL:HG21	1.81	0.44
30:J2:67:VAL:HG22	30:J2:82:ARG:HD2	1.99	0.44
34:L2:4:LEU:HD13	34:L2:24:LEU:HD13	1.99	0.44
35:L3:124:HIS:CD2	51:T3:35:ARG:HD2	2.51	0.44
69:m2:350:A:H2'	69:m2:351:A:H8	1.82	0.44
69:m2:583:U:H2'	69:m2:584:U:C6	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:p2:71:LEU:HD13	72:p2:84:PHE:CE1	2.52	0.44
72:p2:136:ARG:HB2	72:p2:218:LEU:HD11	1.98	0.44
72:p2:141:GLY:HA3	72:p2:207:LEU:HD23	1.99	0.44
1:A1:146:LYS:HB2	1:A1:223:PHE:CE2	2.53	0.44
1:A1:169:LEU:HA	1:A1:172:VAL:HG12	1.99	0.44
2:A2:91:G:OP1	66:i2:44:LYS:HE3	2.17	0.44
2:A2:2089:C:C5	20:F2:191:ALA:HB2	2.51	0.44
2:A2:2178:A:H2'	2:A2:2179:OMG:O4'	2.18	0.44
2:A2:2324:G:H2'	2:A2:2325:U:H6	1.82	0.44
2:A2:2375:G:OP2	40:O2:79:SER:HB2	2.17	0.44
2:A2:2389:C:H2'	2:A2:2390:U:C6	2.52	0.44
2:A2:2631:G:OP1	67:j2:8:VAL:HG23	2.18	0.44
2:A2:3720:U:H2'	2:A2:3721:U:H6	1.82	0.44
2:A2:4123:U:H2'	2:A2:4124:G:H8	1.80	0.44
2:A2:4322:C:O3'	2:A2:4323:C:H3'	2.17	0.44
11:C2:146:U:H2'	11:C2:147:G:O4'	2.16	0.44
23:G2:196:ARG:HH12	23:G2:200:MET:HG3	1.83	0.44
28:I2:55:LEU:HD23	28:I2:58:LEU:HD12	1.98	0.44
29:I3:44:LYS:HG2	29:I3:56:GLN:HB2	2.00	0.44
45:Q3:18:LEU:HD22	45:Q3:20:ARG:CZ	2.46	0.44
69:m2:150:A:H5''	69:m2:151:C:OP2	2.18	0.44
69:m2:177:G:H1'	69:m2:315:A:N6	2.32	0.44
69:m2:350:A:H2'	69:m2:351:A:C8	2.52	0.44
69:m2:530:A:H2'	69:m2:531:A:H8	1.80	0.44
69:m2:1743:U:H2'	69:m2:1744:C:O4'	2.17	0.44
71:o2:84:GLN:HA	71:o2:87:VAL:HG12	2.00	0.44
71:o2:180:ARG:HG3	71:o2:195:TRP:CE3	2.52	0.44
2:A2:298:G:H5'	25:H1:179:LYS:O	2.17	0.44
2:A2:1873:A:H2'	2:A2:1874:C:H6	1.81	0.44
2:A2:2022:U:C6	2:A2:2025:G:H4'	2.53	0.44
2:A2:2568:A:O2'	2:A2:2569:C:H5'	2.17	0.44
2:A2:4511:C:C2	2:A2:4512:G:C8	3.05	0.44
3:A3:48:ALA:HB2	3:A3:70:ILE:HD12	1.98	0.44
11:C2:7:U:H2'	11:C2:8:U:C6	2.52	0.44
17:E2:216:MET:SD	17:E2:359:ALA:HA	2.57	0.44
17:E2:224:LYS:HB2	17:E2:226:LYS:NZ	2.32	0.44
17:E2:376:HIS:O	17:E2:378:ARG:HD2	2.18	0.44
18:E3:82:THR:O	18:E3:118:VAL:HG13	2.17	0.44
33:K3:14:LYS:HZ2	33:K3:16:ILE:HG12	1.82	0.44
33:K3:87:ARG:HH22	69:m2:162:C:H5''	1.83	0.44
35:L3:83:ARG:CG	35:L3:150:ARG:HD2	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:R2:126:THR:HG21	46:R2:134:LYS:HE2	1.99	0.44
69:m2:653:U:H2'	69:m2:654:U:C6	2.53	0.44
69:m2:813:A:H2'	69:m2:814:A:O4'	2.17	0.44
69:m2:920:U:H3'	69:m2:921:A:C8	2.52	0.44
72:p2:164:ILE:HG23	72:p2:201:CYS:SG	2.57	0.44
77:u2:78:ILE:HG13	77:u2:104:ILE:HD11	1.99	0.44
77:u2:110:ARG:NH1	77:u2:121:LEU:HB3	2.31	0.44
81:y2:143:LYS:HE2	81:y2:145:TYR:CE1	2.52	0.44
2:A2:270:U:H2'	2:A2:271:C:H6	1.83	0.44
2:A2:821:U:H2'	2:A2:822:C:H6	1.82	0.44
2:A2:1112:C:H2'	2:A2:1113:G:H8	1.83	0.44
2:A2:1588:A:H2'	2:A2:1591:C:C5	2.52	0.44
2:A2:3777:A:O2'	2:A2:3778:A:H8	2.00	0.44
2:A2:3948:U:H2'	2:A2:3949:G:O4'	2.16	0.44
6:B3:38:LYS:HD2	69:m2:1569:G:H4'	2.00	0.44
14:D2:181:LYS:HG2	67:j2:18:TYR:OH	2.18	0.44
14:D2:204:MET:HB3	14:D2:208:GLU:HG3	1.99	0.44
16:E1:134:LEU:HD21	16:E1:165:TRP:CE3	2.53	0.44
19:F1:107:THR:HG22	60:c2:20:ASN:HB3	1.98	0.44
20:F2:281:MET:HE3	20:F2:281:MET:HB3	1.87	0.44
29:I3:33:SER:HB2	29:I3:43:TRP:HE1	1.81	0.44
33:K3:138:ALA:H	33:K3:178:ARG:HB2	1.82	0.44
45:Q3:47:MET:HE2	45:Q3:48:TYR:CE1	2.53	0.44
47:R3:79:ILE:HB	47:R3:83:LEU:HD23	1.98	0.44
57:Z2:24:HIS:O	57:Z2:87:LYS:HD2	2.17	0.44
69:m2:153:G:H22	69:m2:165:G:N2	2.12	0.44
69:m2:373:A:OP2	77:u2:10:LYS:HB2	2.16	0.44
69:m2:824:PSU:H5''	69:m2:825:PSU:H5'	1.99	0.44
69:m2:1166:G:O2'	69:m2:1167:G:H5'	2.16	0.44
71:o2:195:TRP:HD1	71:o2:197:VAL:O	2.01	0.44
74:r2:198:ARG:NH1	74:r2:200:ARG:HD2	2.33	0.44
1:A1:154:MET:O	1:A1:158:VAL:HG22	2.16	0.44
2:A2:678:G:H2'	2:A2:679:C:C6	2.52	0.44
2:A2:1458:C:H2'	2:A2:1459:A:C8	2.52	0.44
2:A2:1553:A:H2'	2:A2:1554:G:C8	2.53	0.44
2:A2:1626:G:H2'	2:A2:1627:A:C8	2.53	0.44
2:A2:1834:U:O2'	2:A2:1835:A:H5'	2.18	0.44
2:A2:2090:C:H2'	2:A2:2091:G:H8	1.83	0.44
2:A2:2324:G:H2'	2:A2:2325:U:C6	2.53	0.44
2:A2:3898:G:H2'	2:A2:3899:G:C8	2.52	0.44
2:A2:3956:A:C2	52:U2:43:ILE:HG23	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A2:4093:A:H5''	13:D1:114:GLY:HA2	2.00	0.44
7:Bv:23:A:H2'	7:Bv:24:G:O4'	2.17	0.44
10:C1:12:ILE:HD12	10:C1:53:LYS:HB2	1.99	0.44
20:F2:214:ASP:OD2	20:F2:218:ILE:HD12	2.18	0.44
20:F2:298:ILE:O	20:F2:302:LEU:HG	2.17	0.44
25:H1:6:TYR:CZ	60:c2:40:VAL:HG22	2.52	0.44
26:H2:99:VAL:HG13	26:H2:116:LEU:HD21	2.00	0.44
29:I3:59:LEU:HD11	29:I3:92:LEU:HD23	2.00	0.44
29:I3:195:LEU:CD1	29:I3:209:SER:HB2	2.46	0.44
30:J2:60:PHE:CE1	30:J2:82:ARG:HB2	2.52	0.44
36:M2:69:GLU:HG2	36:M2:101:THR:HG22	1.98	0.44
36:M2:93:MET:HE1	36:M2:117:HIS:CE1	2.52	0.44
43:P3:28:ARG:HB3	43:P3:29:PRO:HD3	1.99	0.44
59:b2:96:THR:OG1	59:b2:99:GLU:HG2	2.17	0.44
69:m2:155:G:H2'	69:m2:156:G:C8	2.53	0.44
69:m2:951:G:H2'	69:m2:952:C:C6	2.53	0.44
69:m2:1020:U:H2'	69:m2:1021:C:C6	2.53	0.44
69:m2:1503:C:H2'	69:m2:1504:C:H6	1.83	0.44
72:p2:32:ASP:OD1	72:p2:95:ASN:HA	2.18	0.44
73:q2:172:VAL:HA	73:q2:184:ILE:O	2.16	0.44
76:t2:126:HIS:NE2	76:t2:181:THR:HB	2.33	0.44
2:A2:381:U:H2'	2:A2:382:G:O4'	2.17	0.44
2:A2:1227:G:H2'	2:A2:1228:G:H8	1.83	0.44
2:A2:1468:C:H3'	52:U2:26:ARG:HH12	1.82	0.44
2:A2:1668:G:H8	13:D1:4:ARG:HH12	1.66	0.44
2:A2:2470:G:H2'	2:A2:2471:C:C6	2.52	0.44
2:A2:2570:A2M:HM'3	2:A2:2570:A2M:H1'	1.88	0.44
2:A2:2630:C:H2'	67:j2:7:LYS:NZ	2.32	0.44
3:A3:132:ARG:HB2	3:A3:134:GLN:HE22	1.81	0.44
4:B1:138:ALA:HB2	4:B1:194:VAL:HG11	1.99	0.44
19:F1:155:MET:HE2	19:F1:155:MET:HB3	1.79	0.44
36:M2:74:ARG:O	36:M2:76:LYS:HE2	2.18	0.44
39:N3:55:ARG:HD3	69:m2:1019:U:H5'	2.00	0.44
53:V2:112:LYS:HA	53:V2:115:ARG:HD3	1.99	0.44
55:X2:22:THR:HG21	55:X2:87:ARG:NH1	2.32	0.44
64:g2:110:CYS:HB3	64:g2:115:CYS:SG	2.57	0.44
67:j2:23:ARG:HA	67:j2:26:VAL:HG12	1.98	0.44
69:m2:931:G:H2'	69:m2:932:C:O4'	2.18	0.44
69:m2:1401:C:H2'	69:m2:1402:U:C6	2.53	0.44
69:m2:1456:A:H3'	82:z2:5:ARG:HH21	1.83	0.44
77:u2:172:LEU:H	77:u2:172:LEU:HD23	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A2:723:C:H2'	2:A2:724:U:O4'	2.18	0.44
2:A2:939:C:H2'	2:A2:940:C:C6	2.52	0.44
2:A2:1028:G:H2'	2:A2:1029:C:C6	2.52	0.44
2:A2:1285:C:H2'	2:A2:1286:U:H6	1.82	0.44
2:A2:2382:C:C2	2:A2:2383:U:C5	3.06	0.44
2:A2:2438:C:H2'	2:A2:2439:C:H6	1.82	0.44
2:A2:2567:A:H2'	2:A2:2568:A:N3	2.33	0.44
2:A2:4053:G:H2'	2:A2:4054:C:H6	1.83	0.44
2:A2:4400:U:H2'	2:A2:4401:C:C6	2.53	0.44
6:B3:27:LYS:O	6:B3:110:LEU:HD22	2.17	0.44
16:E1:19:LYS:HB3	16:E1:75:ARG:NH1	2.32	0.44
17:E2:366:LYS:HE2	17:E2:366:LYS:HB2	1.82	0.44
25:H1:19:MET:HE3	25:H1:19:MET:HB3	1.74	0.44
25:H1:60:VAL:CG2	25:H1:134:LEU:HB2	2.47	0.44
30:J2:47:TYR:O	30:J2:51:VAL:HG23	2.18	0.44
31:J3:82:TYR:HE2	31:J3:136:HIS:CD2	2.35	0.44
31:J3:108:LYS:HD2	31:J3:233:LEU:HD21	1.99	0.44
31:J3:255:LEU:HD23	31:J3:255:LEU:HA	1.81	0.44
38:N2:57:TYR:OH	38:N2:87:LYS:HE2	2.18	0.44
47:R3:67:LEU:HD11	75:s2:99:ILE:HG23	1.99	0.44
65:h2:20:MET:O	65:h2:23:ARG:HG2	2.17	0.44
69:m2:220:U:H2'	69:m2:221:U:C6	2.53	0.44
69:m2:1513:U:H2'	69:m2:1514:C:C6	2.53	0.44
71:o2:195:TRP:NE1	71:o2:197:VAL:HB	2.33	0.44
82:z2:84:TYR:CE2	82:z2:86:PRO:HG3	2.51	0.44
2:A2:25:A:H4'	2:A2:340:C:H2'	2.00	0.44
2:A2:444:G:N2	2:A2:1117:A:N1	2.66	0.44
2:A2:1020:C:H2'	2:A2:1021:G:C8	2.52	0.44
2:A2:1035:C:H2'	2:A2:1036:G:O4'	2.17	0.44
2:A2:1446:G:H5'	2:A2:1447:A:OP1	2.17	0.44
2:A2:2240:U:O4	2:A2:2248:G:O6	2.35	0.44
2:A2:3566:C:H2'	2:A2:3567:C:H6	1.82	0.44
2:A2:4245:C:H2'	2:A2:4246:U:C6	2.53	0.44
13:D1:35:ASP:OD1	13:D1:88:ARG:HG3	2.18	0.44
20:F2:155:GLU:HG3	20:F2:157:LYS:HG2	1.99	0.44
26:H2:160:LEU:HD11	26:H2:202:ILE:HG13	1.99	0.44
26:H2:174:GLN:HE21	26:H2:178:GLY:HA2	1.82	0.44
28:I2:85:ARG:HD3	28:I2:90:HIS:ND1	2.33	0.44
29:I3:11:LEU:HB2	29:I3:307:VAL:HB	1.99	0.44
29:I3:173:LEU:HG	29:I3:175:LYS:HE2	2.00	0.44
33:K3:134:GLY:O	69:m2:169:U:H4'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:L2:21:LYS:HE3	34:L2:55:VAL:HA	2.00	0.44
47:R3:97:ILE:CG2	47:R3:109:TYR:HB3	2.48	0.44
49:S3:14:GLU:HA	49:S3:17:ARG:HG2	2.00	0.44
66:i2:26:TYR:CG	66:i2:82:MET:HE1	2.53	0.44
69:m2:561:G:O2'	69:m2:562:A:H8	2.00	0.44
69:m2:599:G:N1	69:m2:642:A:C6	2.86	0.44
69:m2:848:G:N3	74:r2:19:MET:HE1	2.32	0.44
69:m2:1566:C:C2	69:m2:1567:C:C5	3.06	0.44
73:q2:11:PHE:HA	73:q2:14:ASP:OD2	2.17	0.44
73:q2:196:GLY:C	73:q2:201:LYS:HZ1	2.26	0.44
74:r2:129:ILE:HD12	74:r2:138:HIS:O	2.18	0.44
74:r2:185:GLY:N	74:r2:224:ASN:HB3	2.32	0.44
74:r2:220:THR:HG22	74:r2:221:ARG:O	2.18	0.44
75:s2:49:LEU:HD12	81:y2:50:LYS:HE2	1.99	0.44
75:s2:59:LYS:HG3	75:s2:60:ARG:H	1.82	0.44
79:w2:77:VAL:HG22	79:w2:86:ILE:HD12	2.00	0.44
2:A2:283:G:H1'	60:c2:82:ARG:NH1	2.32	0.44
2:A2:1611:C:H2'	2:A2:1612:G:H8	1.82	0.44
2:A2:2216:G:H2'	2:A2:2217:U:H6	1.83	0.44
2:A2:2481:G:H2'	2:A2:2482:C:C6	2.53	0.44
2:A2:2587:A:H2'	2:A2:2588:A:H8	1.83	0.44
2:A2:4531:C:H2'	2:A2:4532:U:C6	2.53	0.44
3:A3:125:HIS:CD2	3:A3:131:VAL:HG11	2.53	0.44
7:Bv:64:A:H4'	13:D1:27:PRO:HA	1.99	0.44
10:C1:93:ARG:HG2	10:C1:182:SER:HB3	2.00	0.44
13:D1:170:LYS:HD3	13:D1:175:LYS:HA	1.99	0.44
17:E2:284:ILE:HG23	17:E2:331:ILE:HG23	2.00	0.44
19:F1:47:ALA:HB3	19:F1:48:PRO:HD3	2.00	0.44
19:F1:75:GLY:HA2	19:F1:97:SER:OG	2.18	0.44
29:I3:67:SER:HB2	29:I3:109:LEU:HD12	2.00	0.44
35:L3:38:ARG:HA	51:T3:31:ARG:HB2	1.99	0.44
38:N2:87:LYS:HE3	38:N2:87:LYS:HB3	1.88	0.44
39:N3:87:ASP:CG	69:m2:926:G:H21	2.26	0.44
41:O3:134:PRO:HB3	69:m2:946:A:H5''	1.99	0.44
43:P3:101:PHE:HA	43:P3:113:HIS:CE1	2.52	0.44
54:W2:38:ILE:HD11	54:W2:46:VAL:HG21	2.00	0.44
55:X2:60:PRO:HD2	55:X2:100:ASN:HD21	1.83	0.44
58:a2:64:LEU:HA	58:a2:67:LEU:HD12	1.99	0.44
58:a2:69:LYS:HG2	58:a2:73:HIS:CD2	2.51	0.44
69:m2:42:A:H4'	69:m2:98:C:OP1	2.18	0.44
69:m2:1311:C:H2'	69:m2:1312:U:C6	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:v2:50:GLN:HG2	78:v2:50:GLN:O	2.16	0.44
80:x2:124:LYS:HB2	80:x2:124:LYS:HE3	1.71	0.44
2:A2:35:U:H4'	2:A2:1338:A:C2	2.53	0.43
2:A2:40:G:N2	2:A2:4032:A:H62	2.16	0.43
2:A2:64:A:H1'	2:A2:76:A:H1'	1.99	0.43
2:A2:74:G:O5'	19:F1:59:VAL:HG13	2.17	0.43
2:A2:1252:C:C2'	2:A2:1253:U:H5'	2.48	0.43
2:A2:1271:C:H5''	32:K2:69:LYS:HD2	2.00	0.43
2:A2:1361:G:O2'	2:A2:2567:A:H8	1.98	0.43
2:A2:1660:A:H2'	2:A2:1661:C:C6	2.52	0.43
2:A2:2360:G:O2'	2:A2:2361:G:H5'	2.17	0.43
2:A2:2389:C:H2'	2:A2:2390:U:H6	1.82	0.43
2:A2:2494:C:H5''	67:j2:69:TRP:CH2	2.53	0.43
20:F2:140:LYS:HE2	20:F2:245:HIS:HB2	2.00	0.43
35:L3:124:HIS:HA	51:T3:35:ARG:CZ	2.47	0.43
68:k2:39:ARG:HG3	68:k2:105:ASP:OD2	2.18	0.43
69:m2:300:G:H2'	69:m2:301:A:O4'	2.19	0.43
69:m2:961:G:H2'	69:m2:962:U:C6	2.52	0.43
69:m2:1391:C:O2'	73:q2:163:PRO:HD3	2.18	0.43
72:p2:168:MET:HG2	72:p2:197:ILE:HG21	1.98	0.43
74:r2:198:ARG:HA	74:r2:208:VAL:HG12	2.00	0.43
76:t2:37:LYS:C	76:t2:39:GLN:H	2.26	0.43
78:v2:64:TRP:O	78:v2:65:ARG:HD3	2.18	0.43
80:x2:25:LEU:HA	80:x2:28:MET:HE2	1.99	0.43
80:x2:83:MET:HE3	80:x2:84:ILE:O	2.18	0.43
1:A1:141:ASN:ND2	1:A1:234:LYS:HD3	2.33	0.43
2:A2:10:A:H2'	2:A2:11:G:C8	2.52	0.43
2:A2:939:C:H2'	2:A2:940:C:H6	1.83	0.43
2:A2:3560:G:H5''	2:A2:3561:A:OP2	2.17	0.43
4:B1:150:LYS:HE2	4:B1:177:MET:O	2.18	0.43
5:B2:112:U:H2'	5:B2:113:G:H8	1.83	0.43
14:D2:28:ARG:HB2	14:D2:123:ARG:CB	2.46	0.43
15:D3:1:MET:HE1	31:J3:255:LEU:HB2	2.00	0.43
19:F1:130:LYS:HE3	19:F1:132:SER:HB2	2.00	0.43
23:G2:271:MET:HB3	23:G2:276:LYS:NZ	2.33	0.43
29:I3:149:GLU:H	29:I3:171:ASP:HB3	1.83	0.43
29:I3:209:SER:O	29:I3:216:ALA:HA	2.19	0.43
31:J3:212:LYS:O	31:J3:216:MET:HG3	2.18	0.43
33:K3:137:ARG:HH21	33:K3:178:ARG:HE	1.64	0.43
35:L3:79:ARG:HH12	35:L3:83:ARG:HH11	1.66	0.43
35:L3:111:GLN:NE2	35:L3:127:ARG:HD2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:S2:17:ARG:O	48:S2:21:ALA:HB2	2.18	0.43
57:Z2:30:ILE:HB	57:Z2:33:VAL:HG12	2.00	0.43
69:m2:316:U:H2'	69:m2:317:C:H6	1.82	0.43
74:r2:173:ILE:HB	74:r2:235:TRP:CH2	2.53	0.43
75:s2:174:ALA:O	75:s2:178:ILE:HG12	2.17	0.43
2:A2:2194:G:H5'	2:A2:2533:G:OP2	2.18	0.43
3:A3:19:ASN:HD21	3:A3:32:ALA:C	2.26	0.43
6:B3:71:GLY:HA2	6:B3:121:ARG:HD3	2.00	0.43
13:D1:90:ARG:NH1	13:D1:134:VAL:HG21	2.33	0.43
20:F2:195:LYS:HB2	20:F2:195:LYS:HZ3	1.82	0.43
28:I2:119:VAL:O	28:I2:121:PRO:HD3	2.19	0.43
29:I3:126:ASP:O	29:I3:128:THR:HG23	2.17	0.43
33:K3:133:LEU:HD22	69:m2:150:A:H61	1.84	0.43
35:L3:78:LEU:HD11	35:L3:94:LEU:HG	1.99	0.43
46:R2:82:THR:HG21	59:b2:37:THR:HG22	2.00	0.43
55:X2:26:THR:HB	55:X2:85:ARG:HH11	1.81	0.43
55:X2:32:ARG:HB3	55:X2:48:GLU:HG3	2.00	0.43
61:d2:34:CYS:HB3	61:d2:38:GLY:H	1.83	0.43
62:e2:11:PHE:HA	62:e2:14:THR:HG22	1.99	0.43
69:m2:644:U:H1'	69:m2:646:OMG:HM21	1.99	0.43
69:m2:847:G:H2'	69:m2:848:G:O4'	2.18	0.43
85:m2:1935:B8N:C4	70:n2:33:C:H5'	2.48	0.43
73:q2:21:LEU:O	73:q2:25:LEU:HD23	2.17	0.43
76:t2:27:LEU:HD13	76:t2:45:ILE:HD11	1.99	0.43
76:t2:51:ILE:HB	76:t2:179:LYS:HE2	1.99	0.43
2:A2:158:A:H5''	2:A2:159:C:H2'	2.00	0.43
2:A2:271:C:H2'	2:A2:272:U:H6	1.81	0.43
2:A2:928:G:H1	2:A2:1064:G:N2	2.16	0.43
2:A2:1029:C:H2'	2:A2:1030:G:H8	1.84	0.43
2:A2:1327:U:H2'	2:A2:1328:A:C8	2.54	0.43
2:A2:1482:A:H4'	2:A2:1498:G:H22	1.81	0.43
2:A2:1680:G:H2'	2:A2:1681:C:C6	2.54	0.43
3:A3:62:ASP:O	3:A3:65:GLU:HG3	2.18	0.43
4:B1:190:LEU:HD23	4:B1:193:LEU:HD12	2.00	0.43
17:E2:92:TYR:HB2	17:E2:159:VAL:HB	1.99	0.43
31:J3:242:ASP:O	31:J3:246:LYS:HG3	2.18	0.43
37:M3:53:ALA:HB1	37:M3:80:ASP:H	1.82	0.43
47:R3:80:ARG:NH1	69:m2:1600:G:H5''	2.33	0.43
48:S2:47:MET:HE3	48:S2:119:LEU:HD12	2.00	0.43
60:c2:73:ILE:O	60:c2:77:VAL:HG22	2.18	0.43
69:m2:150:A:H3'	69:m2:151:C:H6	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:m2:1115:A:H4'	72:p2:202:GLN:NE2	2.33	0.43
69:m2:1231:G:H2'	69:m2:1232:C:C6	2.53	0.43
69:m2:1459:U:H2'	69:m2:1460:G:C8	2.51	0.43
69:m2:1595:C:C2	69:m2:1596:A:C8	3.06	0.43
2:A2:37:U:H2'	2:A2:38:A:O4'	2.18	0.43
2:A2:120:A:H2'	2:A2:149:A:H61	1.82	0.43
2:A2:1015:C:H2'	2:A2:1016:A:C8	2.53	0.43
2:A2:1115:C:H2'	2:A2:1117:A:C4	2.53	0.43
2:A2:3590:G:H2'	2:A2:3591:C:C6	2.54	0.43
2:A2:4244:C:H2'	2:A2:4245:C:C6	2.52	0.43
2:A2:4327:U:H4'	17:E2:281:ASN:O	2.18	0.43
4:B1:89:ARG:O	4:B1:93:THR:HG23	2.18	0.43
4:B1:103:ARG:HE	4:B1:193:LEU:HA	1.84	0.43
12:C3:51:LYS:HB3	12:C3:90:ASP:H	1.84	0.43
21:F3:90:GLU:HG2	21:F3:91:ALA:N	2.32	0.43
29:I3:18:VAL:HG21	29:I3:307:VAL:HG23	1.99	0.43
30:J2:4:TYR:CD2	30:J2:149:ILE:HD11	2.53	0.43
33:K3:28:TYR:HE1	33:K3:104:ALA:HB2	1.84	0.43
34:L2:60:ARG:HG3	34:L2:63:CYS:SG	2.58	0.43
35:L3:118:GLY:O	35:L3:119:LEU:HG	2.17	0.43
35:L3:131:ARG:HD2	35:L3:131:ARG:HA	1.78	0.43
38:N2:84:ILE:HD12	53:V2:23:LYS:HD3	1.99	0.43
41:O3:97:LEU:HD23	41:O3:97:LEU:HA	1.87	0.43
56:Y2:129:LEU:HD23	56:Y2:129:LEU:H	1.83	0.43
63:f2:28:ARG:HA	63:f2:33:ASN:ND2	2.31	0.43
69:m2:28:U:O2'	69:m2:29:G:H5'	2.19	0.43
69:m2:1145:A:H2'	69:m2:1146:A:C8	2.54	0.43
69:m2:1618:U:H2'	69:m2:1619:G:O4'	2.18	0.43
74:r2:59:ASP:HA	74:r2:62:LYS:HE2	2.00	0.43
76:t2:19:PHE:CZ	76:t2:49:LYS:HA	2.54	0.43
2:A2:153:G:H2'	2:A2:154:G:H8	1.83	0.43
2:A2:286:U:H2'	2:A2:287:U:C6	2.54	0.43
2:A2:287:U:H2'	2:A2:288:G:C8	2.52	0.43
2:A2:1509:C:H2'	2:A2:1510:G:N9	2.34	0.43
2:A2:1668:G:C8	13:D1:4:ARG:NH1	2.87	0.43
2:A2:1895:G:P	2:A2:2011:C:H42	2.41	0.43
2:A2:2129:A:H2'	2:A2:2130:A:H8	1.83	0.43
2:A2:2135:G:N2	2:A2:2179:OMG:H5''	2.33	0.43
2:A2:3366:G:N3	2:A2:3367:A:H1'	2.33	0.43
2:A2:3552:C:H1'	17:E2:268:ARG:HH22	1.84	0.43
4:B1:229:ARG:NH1	4:B1:233:ILE:HD11	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Bv:62:C:H2'	7:Bv:63:G:C8	2.53	0.43
11:C2:94:G:C5	61:d2:84:PRO:HG3	2.53	0.43
24:G3:49:PRO:HB3	75:s2:60:ARG:HH21	1.83	0.43
28:I2:51:LYS:HA	28:I2:141:LEU:HD11	2.00	0.43
29:I3:292:SER:HB2	29:I3:297:THR:HB	2.00	0.43
41:O3:98:ARG:HG2	41:O3:99:ALA:O	2.19	0.43
43:P3:50:PHE:CB	43:P3:63:VAL:HG12	2.48	0.43
61:d2:4:GLY:O	61:d2:8:PHE:HD1	2.00	0.43
69:m2:211:A:H1'	69:m2:212:U:H5	1.84	0.43
69:m2:215:G:H2'	69:m2:216:U:O4'	2.19	0.43
69:m2:1215:C:H2'	69:m2:1216:A:H8	1.83	0.43
69:m2:1239:C:O2'	80:x2:128:HIS:HD2	2.02	0.43
69:m2:1283:G:H2'	69:m2:1284:A:C8	2.53	0.43
72:p2:34:LYS:HB2	72:p2:97:LEU:HD23	2.00	0.43
72:p2:132:GLY:C	72:p2:221:PRO:HG3	2.44	0.43
74:r2:141:THR:HB	74:r2:145:ARG:H	1.84	0.43
2:A2:21:G:H1'	11:C2:103:A:N3	2.34	0.43
2:A2:283:G:H1'	60:c2:82:ARG:HH12	1.84	0.43
2:A2:389:A:H1'	48:S2:90:ALA:O	2.19	0.43
2:A2:705:G:H2'	2:A2:706:C:C6	2.54	0.43
2:A2:1061:U:H2'	2:A2:1062:C:C6	2.54	0.43
2:A2:1743:A:H2	2:A2:4085:G:HO2'	1.67	0.43
2:A2:3346:U:H2'	2:A2:3347:G:O4'	2.18	0.43
2:A2:4330:G:N2	2:A2:4365:G:H1'	2.33	0.43
11:C2:38:U:C6	59:b2:81:LEU:HD23	2.54	0.43
17:E2:224:LYS:HG2	17:E2:340:THR:HG22	2.01	0.43
21:F3:21:ILE:HD12	21:F3:72:HIS:ND1	2.33	0.43
23:G2:21:ARG:HG2	23:G2:21:ARG:HH11	1.83	0.43
23:G2:211:LEU:HD23	23:G2:211:LEU:HA	1.87	0.43
25:H1:49:ARG:NH1	25:H1:49:ARG:HB2	2.33	0.43
25:H1:139:HIS:O	25:H1:143:ARG:HG2	2.19	0.43
27:H3:36:LEU:HD23	27:H3:36:LEU:H	1.84	0.43
31:J3:207:ALA:HB2	69:m2:4:C:H4'	1.99	0.43
33:K3:23:LYS:HZ1	33:K3:41:LEU:HD12	1.84	0.43
33:K3:46:LYS:HA	33:K3:46:LYS:HD3	1.89	0.43
45:Q3:114:MET:HA	45:Q3:122:LYS:HG3	1.99	0.43
58:a2:40:LYS:HE3	58:a2:52:ARG:CZ	2.49	0.43
59:b2:52:LYS:HA	59:b2:52:LYS:HD3	1.84	0.43
69:m2:604:G:H1	69:m2:622:G:H21	1.65	0.43
76:t2:51:ILE:HD12	76:t2:51:ILE:HA	1.94	0.43
77:u2:113:TYR:CE2	77:u2:121:LEU:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:w2:59:LYS:HB3	79:w2:134:LEU:HD13	2.00	0.43
82:z2:58:MET:HE3	82:z2:58:MET:HB3	1.69	0.43
1:A1:243:LYS:HD2	1:A1:243:LYS:HA	1.81	0.43
2:A2:1322:C:H2'	2:A2:1323:G:H8	1.84	0.43
2:A2:1467:G:C6	2:A2:3570:U:H5''	2.54	0.43
2:A2:1613:G:H2'	2:A2:1614:C:H6	1.83	0.43
2:A2:1675:A:H5'	53:V2:7:HIS:O	2.19	0.43
2:A2:2113:G:H2'	2:A2:2114:U:O4'	2.18	0.43
2:A2:2498:A:H1'	14:D2:21:LYS:NZ	2.34	0.43
2:A2:3279:C:H2'	2:A2:3280:A:O4'	2.19	0.43
2:A2:3712:A:C4	2:A2:3713:U:C5	3.07	0.43
4:B1:34:LYS:HG3	4:B1:36:PRO:HD3	2.01	0.43
19:F1:26:PHE:CE2	20:F2:107:THR:HG22	2.54	0.43
24:G3:12:ALA:HB1	24:G3:32:VAL:HB	2.01	0.43
24:G3:44:ARG:NH1	24:G3:63:ARG:HB2	2.33	0.43
28:I2:83:THR:O	28:I2:87:MET:HG3	2.18	0.43
35:L3:38:ARG:HD3	69:m2:525:A:OP2	2.19	0.43
35:L3:160:SER:C	35:L3:161:LEU:HD23	2.44	0.43
45:Q3:87:PRO:HG2	45:Q3:90:ARG:HB2	2.01	0.43
47:R3:41:ARG:HH21	47:R3:78:LYS:NZ	2.17	0.43
57:Z2:76:ARG:HG2	57:Z2:85:ARG:HG2	2.01	0.43
68:k2:28:GLU:H	68:k2:28:GLU:HG2	1.70	0.43
69:m2:69:C:H2'	69:m2:70:G:O4'	2.18	0.43
69:m2:344:C:H2'	69:m2:345:A:O4'	2.18	0.43
69:m2:1745:G:H21	69:m2:1793:A:H62	1.67	0.43
75:s2:49:LEU:HB2	81:y2:50:LYS:HZ3	1.83	0.43
1:A1:93:MET:O	1:A1:96:MET:HG2	2.19	0.43
2:A2:222:C:H2'	2:A2:223:G:O4'	2.19	0.43
2:A2:1022:C:C4	2:A2:1023:C:C4	3.07	0.43
2:A2:1071:G:N2	2:A2:1078:G:H1	2.17	0.43
2:A2:1390:G:O2'	2:A2:1425:G:H4'	2.17	0.43
2:A2:2371:C:C2	2:A2:2477:G:N2	2.87	0.43
2:A2:3263:U:H2'	2:A2:3264:A:H8	1.84	0.43
2:A2:3317:G:O2'	14:D2:156:LYS:HD2	2.18	0.43
2:A2:3731:G:H2'	2:A2:3732:G:C8	2.54	0.43
3:A3:24:ARG:O	3:A3:55:ARG:HD3	2.19	0.43
13:D1:48:LEU:O	13:D1:139:ARG:HA	2.18	0.43
21:F3:46:GLU:OE2	21:F3:48:ALA:HB3	2.19	0.43
21:F3:59:PHE:HB3	21:F3:62:TYR:HD2	1.84	0.43
22:G1:11:ARG:HB3	22:G1:27:ILE:HD12	2.00	0.43
25:H1:36:LEU:HD21	25:H1:109:HIS:CB	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:H1:152:THR:OG1	59:b2:95:LEU:HD11	2.18	0.43
27:H3:32:ARG:NH2	27:H3:38:MET:HB2	2.30	0.43
31:J3:195:LEU:HB3	31:J3:222:CYS:SG	2.59	0.43
31:J3:206:SER:OG	31:J3:210:PRO:HB2	2.19	0.43
33:K3:135:PRO:HG2	33:K3:141:ILE:HG12	2.00	0.43
36:M2:16:CYS:SG	36:M2:54:MET:HE2	2.59	0.43
55:X2:19:GLU:O	55:X2:90:ARG:HD2	2.19	0.43
69:m2:479:G:C2	69:m2:480:G:C8	3.07	0.43
69:m2:514:A2M:H2'	69:m2:515:G:C8	2.41	0.43
69:m2:637:G:C6	69:m2:638:C:C4	3.07	0.43
69:m2:835:C:H2'	69:m2:836:C:C6	2.54	0.43
69:m2:942:U:H2'	69:m2:943:C:C6	2.54	0.43
2:A2:2:G:H2'	2:A2:3:C:C6	2.54	0.43
2:A2:940:C:H2'	2:A2:941:C:C6	2.54	0.43
2:A2:1196:G:H2'	2:A2:1197:G:H8	1.84	0.43
2:A2:1366:A:P	67:j2:4:ARG:HD3	2.59	0.43
2:A2:1836:G:H2'	2:A2:1837:C:C6	2.54	0.43
2:A2:2216:G:H2'	2:A2:2217:U:C6	2.54	0.43
2:A2:3996:U:H2'	2:A2:3997:C:C6	2.54	0.43
2:A2:4506:G:H2'	2:A2:4507:G:H8	1.83	0.43
2:A2:4542:G:H2'	2:A2:4543:G:H8	1.83	0.43
2:A2:4574:C:H5''	22:G1:114:LYS:HE2	2.01	0.43
2:A2:4601:A:H2'	2:A2:4602:A:C8	2.54	0.43
2:A2:4655:G:H2'	2:A2:4656:U:C6	2.54	0.43
18:E3:100:VAL:HG13	18:E3:122:VAL:HG13	2.00	0.43
24:G3:62:GLU:HB2	41:O3:75:MET:HE1	2.01	0.43
29:I3:59:LEU:HD13	29:I3:90:TRP:CD2	2.54	0.43
32:K2:65:ARG:O	32:K2:69:LYS:HG2	2.19	0.43
38:N2:89:ILE:HG13	38:N2:91:VAL:HG23	2.01	0.43
41:O3:150:ARG:NH1	69:m2:1065:C:H4'	2.34	0.43
54:W2:18:LEU:O	54:W2:22:MET:HG2	2.18	0.43
69:m2:318:G:H2'	69:m2:319:C:H6	1.82	0.43
69:m2:638:C:C4	69:m2:639:U:C4	3.07	0.43
69:m2:1090:U:H4'	69:m2:1091:G:OP2	2.19	0.43
69:m2:1619:G:N2	69:m2:1621:A:H3'	2.34	0.43
69:m2:1645:U:H2'	69:m2:1646:C:C6	2.54	0.43
69:m2:1669:U:H2'	69:m2:1670:U:C6	2.54	0.43
73:q2:146:ARG:HA	73:q2:146:ARG:HD2	1.84	0.43
75:s2:85:LYS:HB3	75:s2:88:MET:HE3	2.00	0.43
2:A2:278:G:O4'	25:H1:50:ARG:HD2	2.19	0.42
2:A2:3543:OMC:HM22	2:A2:3544:G:H5'	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A2:3894:U:N3	2:A2:3933:A:H2	2.08	0.42
2:A2:4104:U:H2'	2:A2:4174:G:O6	2.20	0.42
2:A2:4133:U:H2'	2:A2:4134:U:H6	1.84	0.42
2:A2:4550:C:H2'	2:A2:4551:C:C6	2.54	0.42
5:B2:75:G:H5''	36:M2:49:SER:O	2.19	0.42
5:B2:111:C:H2'	5:B2:112:U:O4'	2.19	0.42
7:Bv:33:U:H2'	7:Bv:34:G:H3'	2.01	0.42
12:C3:49:LYS:HB2	12:C3:92:HIS:HB3	2.01	0.42
12:C3:55:ARG:HG2	12:C3:87:ARG:CD	2.46	0.42
19:F1:31:ARG:HD3	19:F1:35:ARG:NH2	2.34	0.42
22:G1:26:ALA:HB2	22:G1:77:TRP:HZ3	1.84	0.42
23:G2:66:TYR:HE2	23:G2:68:ARG:HD3	1.83	0.42
33:K3:41:LEU:HD23	33:K3:41:LEU:H	1.83	0.42
39:N3:70:LYS:HE2	69:m2:1021:C:OP2	2.19	0.42
42:P2:21:PRO:HA	42:P2:54:ALA:HA	2.00	0.42
42:P2:32:THR:HG21	42:P2:105:ILE:HD12	2.01	0.42
45:Q3:36:PRO:HB2	45:Q3:39:GLU:OE1	2.18	0.42
45:Q3:122:LYS:NZ	69:m2:84:A:H5''	2.34	0.42
69:m2:1136:G:H2'	69:m2:1137:C:H6	1.84	0.42
69:m2:1364:U:H5''	69:m2:1365:C:C5	2.54	0.42
69:m2:1446:U:H2'	69:m2:1447:U:O4'	2.19	0.42
69:m2:1660:G:H2'	69:m2:1661:U:O4'	2.19	0.42
71:o2:195:TRP:HE1	71:o2:197:VAL:HB	1.83	0.42
75:s2:60:ARG:HG3	75:s2:61:PHE:CD2	2.54	0.42
78:v2:3:MET:HE3	78:v2:8:ARG:HB2	2.00	0.42
2:A2:752:G:H2'	2:A2:753:A:C8	2.54	0.42
2:A2:1332:C:H2'	2:A2:1333:C:C6	2.54	0.42
2:A2:1444:A:C8	14:D2:199:VAL:HG21	2.54	0.42
2:A2:2376:A:H2'	2:A2:2377:G:C8	2.53	0.42
2:A2:2499:A:H2'	2:A2:2500:A:C8	2.54	0.42
2:A2:3260:A:H2'	2:A2:3261:C:C6	2.54	0.42
2:A2:3266:A:H2'	2:A2:3267:A:C8	2.54	0.42
2:A2:3529:G:H2'	2:A2:3530:G:C8	2.53	0.42
2:A2:4152:PSU:H2'	2:A2:4153:U:C6	2.55	0.42
2:A2:4601:A:H2'	2:A2:4602:A:O4'	2.19	0.42
7:Bv:62:C:H2'	7:Bv:63:G:H8	1.84	0.42
10:C1:6:SER:OG	10:C1:59:LYS:HB3	2.19	0.42
12:C3:26:SER:HB3	12:C3:32:LEU:HB2	2.01	0.42
12:C3:64:THR:HG22	12:C3:77:TRP:CE3	2.55	0.42
12:C3:91:LEU:HD12	12:C3:91:LEU:HA	1.92	0.42
19:F1:182:LEU:HD21	52:U2:128:PHE:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:O3:46:ASP:OD2	41:O3:51:GLU:HB2	2.19	0.42
45:Q3:16:ARG:HA	45:Q3:19:GLN:HA	2.00	0.42
46:R2:123:LYS:HD3	46:R2:125:ASN:OD1	2.19	0.42
46:R2:126:THR:CG2	46:R2:134:LYS:HE2	2.49	0.42
57:Z2:106:TYR:HB2	57:Z2:107:PRO:HD3	2.02	0.42
58:a2:59:VAL:HB	58:a2:63:VAL:CG1	2.50	0.42
58:a2:61:PRO:O	58:a2:64:LEU:HB2	2.19	0.42
68:k2:85:ASN:OD1	68:k2:88:ALA:HB3	2.20	0.42
69:m2:99:A2M:HM'3	69:m2:99:A2M:H1'	1.84	0.42
69:m2:165:G:H2'	69:m2:166:A:H8	1.84	0.42
69:m2:1800:C:H2'	69:m2:1801:G:O4'	2.19	0.42
73:q2:59:LEU:HA	73:q2:66:ILE:HG23	2.00	0.42
74:r2:127:ARG:NH2	74:r2:142:HIS:HB2	2.35	0.42
2:A2:1228:G:H2'	2:A2:1229:C:C6	2.54	0.42
2:A2:1437:G:H2'	2:A2:1456:A:H62	1.84	0.42
2:A2:1597:A:H2'	2:A2:1598:U:O4'	2.19	0.42
2:A2:3593:C:H2'	2:A2:3594:G:C8	2.54	0.42
2:A2:4386:A:H2'	2:A2:4387:G:C8	2.53	0.42
3:A3:124:ARG:NH1	3:A3:129:LEU:HB3	2.26	0.42
11:C2:142:U:H4'	25:H1:139:HIS:HE2	1.83	0.42
20:F2:281:MET:HE2	32:K2:110:ARG:NH1	2.34	0.42
21:F3:12:LYS:HB2	21:F3:33:ASP:OD2	2.19	0.42
29:I3:106:LYS:HB2	29:I3:126:ASP:HB3	2.00	0.42
31:J3:172:ASN:O	31:J3:174:ILE:HG12	2.19	0.42
41:O3:42:VAL:HG23	41:O3:43:HIS:N	2.34	0.42
43:P3:102:ILE:O	43:P3:102:ILE:HG13	2.18	0.42
44:Q2:51:TRP:CD1	44:Q2:51:TRP:H	2.37	0.42
69:m2:1232:C:H2'	69:m2:1233:C:H6	1.84	0.42
69:m2:1440:A:H2'	69:m2:1441:A:C8	2.55	0.42
69:m2:1622:A:H1'	69:m2:1626:U:OP2	2.19	0.42
69:m2:1644:U:O2'	69:m2:1645:U:H5'	2.19	0.42
71:o2:123:VAL:HG22	71:o2:145:ILE:HB	2.01	0.42
75:s2:113:VAL:O	75:s2:117:ILE:HG12	2.19	0.42
2:A2:68:U:H2'	2:A2:69:A:O4'	2.20	0.42
2:A2:231:U:H4'	48:S2:100:HIS:CD2	2.55	0.42
2:A2:1053:G:H8	2:A2:1053:G:OP2	2.03	0.42
2:A2:1231:C:H2'	2:A2:1232:G:O4'	2.20	0.42
2:A2:1271:C:C2	2:A2:1272:A:C8	3.07	0.42
2:A2:2118:A2M:H2'	2:A2:2119:OMG:O4'	2.19	0.42
2:A2:2591:A:H1'	17:E2:228:TYR:CD2	2.55	0.42
2:A2:3366:G:N2	2:A2:3368:A:C6	2.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A2:4413:G:H2'	2:A2:4414:A:H8	1.84	0.42
4:B1:79:ALA:O	4:B1:82:GLN:HG2	2.19	0.42
4:B1:259:LYS:HA	4:B1:259:LYS:HD3	1.90	0.42
11:C2:19:C:H2'	11:C2:20:A:C8	2.54	0.42
13:D1:145:LYS:NZ	13:D1:167:ILE:HG13	2.34	0.42
19:F1:110:LEU:O	19:F1:114:VAL:HG23	2.19	0.42
29:I3:149:GLU:CB	29:I3:171:ASP:HB3	2.49	0.42
32:K2:81:VAL:O	32:K2:138:LEU:HD12	2.20	0.42
46:R2:71:LEU:HD12	46:R2:71:LEU:HA	1.89	0.42
46:R2:104:ALA:HA	46:R2:108:GLN:NE2	2.35	0.42
63:f2:14:ALA:O	63:f2:18:LYS:HG3	2.19	0.42
69:m2:431:C:H2'	69:m2:432:C:C6	2.54	0.42
69:m2:1103:U:H3	69:m2:1133:G:H1	1.67	0.42
69:m2:1421:C:H4'	69:m2:1422:G:H5'	2.00	0.42
69:m2:1531:C:H5'	69:m2:1668:C:OP1	2.19	0.42
69:m2:1683:U:H2'	69:m2:1684:C:C6	2.54	0.42
72:p2:127:VAL:O	72:p2:134:LEU:HD12	2.19	0.42
2:A2:7:C:H2'	2:A2:8:U:C6	2.54	0.42
2:A2:1006:G:C2	2:A2:1019:G:C2	3.08	0.42
2:A2:1168:A:H4'	2:A2:1169:G:O5'	2.19	0.42
2:A2:2591:A:H1'	17:E2:228:TYR:CE2	2.54	0.42
2:A2:3735:A:H61	4:B1:62:ARG:HH11	1.67	0.42
2:A2:4648:U:H2'	2:A2:4649:U:H6	1.84	0.42
2:A2:4655:G:H2'	2:A2:4656:U:H6	1.85	0.42
23:G2:264:LYS:HE3	23:G2:264:LYS:HB2	1.76	0.42
29:I3:259:TRP:CE3	29:I3:266:ILE:HG12	2.54	0.42
33:K3:67:VAL:HG11	33:K3:75:LEU:HD11	2.01	0.42
46:R2:104:ALA:HA	46:R2:108:GLN:HE21	1.83	0.42
67:j2:73:THR:HG22	67:j2:75:SER:H	1.84	0.42
69:m2:388:C:H2'	69:m2:389:C:C6	2.54	0.42
69:m2:466:A:H4'	69:m2:467:A:OP2	2.19	0.42
69:m2:915:A:OP1	76:t2:99:ARG:HD3	2.20	0.42
69:m2:1502:G:H2'	69:m2:1503:C:O4'	2.19	0.42
69:m2:1841:U:H2'	69:m2:1842:U:C6	2.55	0.42
69:m2:1860:G:H2'	69:m2:1861:A:C8	2.55	0.42
71:o2:90:PHE:CD1	71:o2:179:ALA:HB2	2.55	0.42
77:u2:67:TRP:CE3	77:u2:189:VAL:HG11	2.55	0.42
80:x2:52:LYS:HD3	80:x2:80:LEU:HD22	2.02	0.42
82:z2:106:LEU:HD23	82:z2:106:LEU:HA	1.90	0.42
2:A2:223:G:H2'	20:F2:164:THR:HG21	2.00	0.42
2:A2:2343:C:H41	58:a2:70:THR:HG21	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A2:2417:G:H2'	2:A2:2418:G:O4'	2.19	0.42
2:A2:3424:U:O2'	2:A2:3425:C:H5'	2.20	0.42
2:A2:4123:U:H2'	2:A2:4124:G:C8	2.54	0.42
2:A2:4263:A:H2'	2:A2:4264:C:H6	1.84	0.42
2:A2:4624:G:H2'	2:A2:4625:A:H5''	2.01	0.42
3:A3:40:TYR:CZ	3:A3:97:GLN:HG2	2.54	0.42
4:B1:70:LEU:HD23	4:B1:70:LEU:HA	1.92	0.42
6:B3:74:SER:O	6:B3:78:ILE:HG13	2.18	0.42
7:Bv:34:G:H2'	7:Bv:35:A:H8	1.83	0.42
10:C1:19:THR:OG1	10:C1:26:ILE:HB	2.19	0.42
16:E1:112:HIS:ND1	16:E1:117:ILE:HD11	2.34	0.42
17:E2:90:VAL:HG22	17:E2:104:THR:HG23	2.02	0.42
18:E3:26:GLN:HA	18:E3:29:LYS:HG2	2.02	0.42
22:G1:6:TYR:H	22:G1:11:ARG:NH2	2.17	0.42
26:H2:154:GLY:HA2	26:H2:210:ILE:HG13	2.01	0.42
26:H2:268:ILE:HG23	26:H2:274:LEU:HD23	2.01	0.42
32:K2:46:VAL:O	32:K2:50:ARG:HG3	2.19	0.42
33:K3:219:GLU:O	33:K3:222:GLU:HG3	2.19	0.42
42:P2:20:LEU:HD13	42:P2:26:ILE:HG21	2.00	0.42
46:R2:89:LYS:HB3	46:R2:95:THR:OG1	2.20	0.42
69:m2:129:C:N4	69:m2:181:A:H61	2.18	0.42
69:m2:297:C:H2'	69:m2:298:U:C6	2.55	0.42
69:m2:1151:A:O2'	69:m2:1152:A:H3'	2.20	0.42
69:m2:1337:G:H2'	69:m2:1338:C:O4'	2.20	0.42
82:z2:34:VAL:O	82:z2:38:ILE:HG12	2.19	0.42
2:A2:424:U:H2'	2:A2:425:U:C6	2.54	0.42
2:A2:802:A:C8	2:A2:803:C:H5	2.37	0.42
2:A2:1206:A:H2'	2:A2:1207:G:C8	2.53	0.42
2:A2:1454:G:N2	2:A2:3574:G:H21	2.18	0.42
2:A2:1874:C:H2'	2:A2:1875:C:H6	1.84	0.42
2:A2:2464:C:H2'	2:A2:2465:C:C6	2.54	0.42
2:A2:3325:G:H21	2:A2:3328:G:H21	1.62	0.42
2:A2:4677:G:H2'	2:A2:4678:C:H6	1.85	0.42
10:C1:77:VAL:O	10:C1:81:ILE:HG12	2.19	0.42
11:C2:137:A:H2'	11:C2:138:C:C6	2.55	0.42
13:D1:167:ILE:HD13	13:D1:167:ILE:HA	1.95	0.42
14:D2:54:ARG:HG2	14:D2:56:ALA:H	1.84	0.42
17:E2:17:LEU:HD21	17:E2:264:PHE:HD2	1.84	0.42
20:F2:32:ILE:O	32:K2:23:ILE:HD11	2.20	0.42
24:G3:47:LYS:HB2	75:s2:139:VAL:HG21	2.00	0.42
26:H2:102:THR:HA	26:H2:111:THR:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:I2:7:LEU:HD21	36:M2:167:PHE:CE1	2.54	0.42
28:I2:27:VAL:HG23	28:I2:98:ALA:HB1	2.02	0.42
32:K2:63:LEU:HD12	32:K2:66:MET:HE2	2.02	0.42
32:K2:177:ALA:O	32:K2:181:ARG:HB3	2.20	0.42
35:L3:32:ILE:CD1	35:L3:40:LYS:HG2	2.50	0.42
55:X2:75:LYS:HB2	55:X2:79:ASN:O	2.19	0.42
69:m2:182:C:H4'	69:m2:183:G:H5''	2.01	0.42
69:m2:187:G:C4	69:m2:188:C:C5	3.08	0.42
69:m2:1692:U:H2'	69:m2:1693:U:H6	1.84	0.42
71:o2:102:ARG:HG2	71:o2:104:THR:H	1.84	0.42
73:q2:159:HIS:C	73:q2:164:VAL:HG21	2.44	0.42
81:y2:48:GLN:O	81:y2:49:TYR:HB2	2.20	0.42
1:A1:136:LEU:HD21	1:A1:143:THR:HG22	2.02	0.42
2:A2:672:C:H2'	2:A2:673:G:C5	2.54	0.42
2:A2:949:G:H2'	2:A2:950:A:C8	2.54	0.42
2:A2:1702:C:H4'	56:Y2:60:TYR:CE1	2.54	0.42
2:A2:2389:C:C2	2:A2:2390:U:C5	3.07	0.42
2:A2:3910:C:H2'	2:A2:3911:C:C6	2.51	0.42
2:A2:4132:A:H2'	2:A2:4133:U:O4'	2.19	0.42
2:A2:4274:A:H4'	17:E2:13:SER:HB2	2.01	0.42
13:D1:54:SER:HB2	13:D1:135:ILE:HD11	2.02	0.42
16:E1:94:LEU:HD13	16:E1:166:PHE:CZ	2.55	0.42
17:E2:354:GLN:HB3	17:E2:359:ALA:HB1	2.01	0.42
20:F2:336:ARG:HA	20:F2:339:THR:HG22	2.02	0.42
21:F3:79:ILE:HD13	69:m2:1865:A:H1'	2.02	0.42
23:G2:21:ARG:HG2	23:G2:21:ARG:NH1	2.34	0.42
23:G2:222:GLN:HG3	23:G2:223:PHE:CD1	2.55	0.42
26:H2:64:TYR:HB2	26:H2:69:MET:HE2	2.02	0.42
26:H2:171:PHE:CE1	26:H2:180:LEU:HB3	2.54	0.42
27:H3:27:ARG:HD2	69:m2:1265:U:H4'	2.01	0.42
29:I3:253:GLY:O	29:I3:285:GLN:HA	2.19	0.42
33:K3:94:ARG:HD2	69:m2:457:A:OP1	2.20	0.42
38:N2:80:VAL:O	38:N2:80:VAL:HG13	2.19	0.42
41:O3:38:ASN:O	41:O3:39:ASP:HB2	2.19	0.42
43:P3:40:VAL:HG11	43:P3:103:VAL:HG22	2.02	0.42
46:R2:110:LYS:HG3	46:R2:121:VAL:HB	2.02	0.42
67:j2:28:LYS:HG3	67:j2:29:ILE:N	2.34	0.42
69:m2:600:G:H2'	69:m2:601:A:H8	1.84	0.42
69:m2:1203:U:H2'	69:m2:1204:U:C6	2.54	0.42
73:q2:68:GLU:OE2	78:v2:65:ARG:HD2	2.20	0.42
73:q2:119:CYS:O	73:q2:123:LEU:HD23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:x2:127:LYS:HD2	80:x2:127:LYS:HA	1.51	0.42
1:A1:118:ARG:HG3	1:A1:161:TYR:HA	2.01	0.42
1:A1:120:ILE:HD13	32:K2:3:VAL:HG13	2.00	0.42
2:A2:166:C:H2'	2:A2:167:C:H6	1.85	0.42
2:A2:270:U:H2'	2:A2:271:C:C6	2.55	0.42
2:A2:278:G:C1'	25:H1:50:ARG:HD2	2.49	0.42
2:A2:866:A:N6	2:A2:1894:G:H1'	2.34	0.42
2:A2:1348:C:H2'	2:A2:1349:U:O4'	2.20	0.42
2:A2:2063:A:H61	2:A2:2085:G:H1'	1.84	0.42
2:A2:2184:A:H2'	2:A2:2185:C:H6	1.84	0.42
2:A2:2639:G:H2'	2:A2:2640:A:H8	1.85	0.42
2:A2:3713:U:H2'	2:A2:3715:G:H8	1.85	0.42
2:A2:3885:A:C8	2:A2:3887:G:C8	3.08	0.42
2:A2:4412:G:H2'	2:A2:4413:G:O4'	2.20	0.42
7:Bv:8:U:H3	7:Bv:14:A:H2	1.66	0.42
11:C2:148:A:H2'	11:C2:149:G:C8	2.54	0.42
14:D2:65:ASP:HB3	14:D2:68:ARG:O	2.20	0.42
17:E2:105:VAL:HG11	17:E2:150:PHE:HE1	1.82	0.42
17:E2:160:ILE:HD12	17:E2:194:LEU:HD21	2.02	0.42
19:F1:92:ARG:NH1	19:F1:98:VAL:HB	2.35	0.42
20:F2:22:VAL:HG12	20:F2:23:THR:O	2.20	0.42
25:H1:140:LYS:NZ	25:H1:144:ARG:HH21	2.17	0.42
26:H2:102:THR:HG22	26:H2:111:THR:HB	2.01	0.42
31:J3:110:MET:HE3	31:J3:125:LYS:HD3	2.01	0.42
43:P3:6:VAL:HG22	43:P3:34:ILE:HD11	2.01	0.42
44:Q2:31:PHE:CB	44:Q2:37:GLU:HG2	2.49	0.42
45:Q3:89:HIS:HB3	69:m2:576:A:H4'	2.02	0.42
49:S3:32:PHE:CE1	49:S3:47:PHE:HD1	2.38	0.42
68:k2:51:VAL:HB	68:k2:113:ARG:HG2	2.01	0.42
69:m2:116:OMU:HM23	69:m2:116:OMU:H1'	1.92	0.42
69:m2:1220:C:H2'	69:m2:1221:C:H6	1.84	0.42
69:m2:1549:C:H2'	69:m2:1550:G:O4'	2.20	0.42
71:o2:189:ILE:HG13	71:o2:195:TRP:CH2	2.55	0.42
81:y2:90:LYS:HG3	81:y2:120:LEU:HD23	2.01	0.42
1:A1:88:ARG:HD2	1:A1:88:ARG:HA	1.75	0.42
1:A1:248:HIS:HB3	1:A1:251:GLU:HG2	2.02	0.42
2:A2:111:C:OP1	59:b2:106:LYS:HD3	2.20	0.42
2:A2:2407:G:C2	58:a2:50:PRO:HG3	2.55	0.42
2:A2:3778:A:C2	4:B1:34:LYS:HD2	2.55	0.42
5:B2:23:A:H2'	5:B2:24:C:C6	2.55	0.42
6:B3:100:ALA:O	6:B3:104:LEU:HG	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:E2:17:LEU:HB3	17:E2:18:PRO:HD3	2.02	0.42
17:E2:220:ILE:HB	17:E2:346:THR:HB	2.01	0.42
20:F2:32:ILE:HG22	20:F2:34:PRO:HD3	2.01	0.42
24:G3:35:MET:HE1	24:G3:55:VAL:HG22	2.02	0.42
29:I3:258:ILE:HG22	29:I3:267:VAL:HB	2.01	0.42
31:J3:84:PHE:CD2	31:J3:265:PRO:HD3	2.54	0.42
41:O3:52:THR:HG21	69:m2:954:G:N2	2.26	0.42
45:Q3:25:ILE:HD11	45:Q3:60:PHE:CE1	2.55	0.42
45:Q3:117:VAL:HG13	45:Q3:122:LYS:HA	2.01	0.42
57:Z2:50:VAL:HG22	57:Z2:69:VAL:HG23	2.01	0.42
69:m2:179:C:H5'	69:m2:180:G:OP2	2.20	0.42
69:m2:356:U:OP1	79:w2:107:LYS:HD3	2.20	0.42
69:m2:870:G:H3'	69:m2:871:A:H5''	2.02	0.42
69:m2:924:A:C2	69:m2:1024:U:H5	2.37	0.42
69:m2:1162:U:H2'	69:m2:1163:U:C6	2.54	0.42
69:m2:1720:G:H2'	69:m2:1721:A:H2	1.84	0.42
74:r2:47:PHE:HE2	74:r2:90:ILE:HG21	1.85	0.42
76:t2:40:LEU:HD21	76:t2:79:LEU:HD11	2.02	0.42
2:A2:1360:A:C2	2:A2:2568:A:H8	2.38	0.41
2:A2:1482:A:H62	2:A2:1683:OMC:H5	1.68	0.41
2:A2:1722:C:O2'	2:A2:1724:G:H5''	2.20	0.41
2:A2:3994:C:O3'	66:i2:37:GLY:HA3	2.19	0.41
2:A2:4127:G:OP2	2:A2:4128:C:H5''	2.20	0.41
2:A2:4546:G:H2'	2:A2:4547:C:C6	2.55	0.41
2:A2:4569:C:O2	2:A2:4570:U:H1'	2.20	0.41
13:D1:75:TYR:HD2	13:D1:151:ALA:HB2	1.84	0.41
17:E2:259:PRO:O	17:E2:261:ARG:N	2.53	0.41
20:F2:333:LYS:HE3	20:F2:337:ARG:NH2	2.36	0.41
25:H1:11:TRP:HZ3	25:H1:120:TRP:HZ3	1.67	0.41
38:N2:34:TYR:CE2	38:N2:93:ILE:HG23	2.54	0.41
52:U2:64:LYS:O	52:U2:67:GLN:HG2	2.20	0.41
55:X2:38:PHE:CD2	55:X2:78:ARG:HD3	2.55	0.41
57:Z2:28:LEU:HD22	57:Z2:101:ILE:HD12	2.01	0.41
69:m2:29:G:H2'	69:m2:30:C:H6	1.85	0.41
69:m2:215:G:C5	69:m2:216:U:C4	3.08	0.41
69:m2:423:G:H2'	69:m2:424:U:C6	2.55	0.41
69:m2:1203:U:H2'	69:m2:1204:U:H6	1.84	0.41
69:m2:1270:C:H1'	80:x2:99:GLY:O	2.20	0.41
69:m2:1274:C:H2'	69:m2:1275:C:C6	2.55	0.41
69:m2:1522:G:H5''	69:m2:1523:C:OP2	2.19	0.41
69:m2:1808:A:H2'	69:m2:1809:C:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:t2:158:LEU:HD21	76:t2:187:PHE:HD2	1.84	0.41
78:v2:53:LYS:HA	78:v2:65:ARG:O	2.20	0.41
79:w2:18:GLN:OE1	79:w2:34:PRO:HG3	2.19	0.41
79:w2:143:LEU:HA	79:w2:143:LEU:HD23	1.79	0.41
81:y2:52:LEU:HD23	81:y2:52:LEU:O	2.20	0.41
81:y2:86:GLN:HE22	81:y2:122:ALA:HA	1.85	0.41
1:A1:158:VAL:O	1:A1:162:ILE:HG12	2.20	0.41
1:A1:267:ARG:HA	1:A1:267:ARG:HD3	1.72	0.41
2:A2:18:C:H4'	25:H1:138:PHE:CD1	2.55	0.41
2:A2:1110:G:H2'	2:A2:1111:U:H6	1.85	0.41
2:A2:1230:C:H2'	2:A2:1231:C:C6	2.55	0.41
2:A2:1358:G:H2'	2:A2:1359:C:C6	2.55	0.41
2:A2:1455:A:H2	2:A2:3574:G:H4'	1.85	0.41
2:A2:1763:G:H2'	2:A2:1826:G:N2	2.35	0.41
2:A2:2430:G:O6	54:W2:30:GLY:HA3	2.20	0.41
2:A2:3840:U:H2'	2:A2:3841:U:H6	1.85	0.41
2:A2:3848:OMG:HM23	2:A2:3848:OMG:H1'	1.83	0.41
2:A2:3997:C:H2'	2:A2:3998:U:H6	1.86	0.41
3:A3:94:LYS:HD3	3:A3:94:LYS:HA	1.85	0.41
16:E1:87:LEU:HB3	16:E1:92:TYR:CD1	2.56	0.41
16:E1:124:GLY:H	16:E1:126:TYR:HE1	1.68	0.41
33:K3:164:LYS:HG2	69:m2:67:C:C2	2.55	0.41
35:L3:111:GLN:HE21	35:L3:145:PRO:CB	2.30	0.41
39:N3:20:ARG:HH12	43:P3:56:HIS:CE1	2.38	0.41
39:N3:76:LYS:HG2	39:N3:81:ALA:HB2	2.01	0.41
44:Q2:46:PRO:HG2	44:Q2:54:LEU:HD23	2.02	0.41
45:Q3:47:MET:HE3	69:m2:839:A:C8	2.55	0.41
45:Q3:107:ARG:O	45:Q3:111:LYS:HG3	2.20	0.41
55:X2:92:ARG:HA	55:X2:102:LEU:HD23	2.01	0.41
57:Z2:48:ALA:HB2	57:Z2:71:TRP:CZ3	2.55	0.41
58:a2:62:LYS:O	58:a2:65:MET:HG2	2.20	0.41
69:m2:519:OMC:H2'	69:m2:520:G:O4'	2.19	0.41
69:m2:565:G:C2	69:m2:566:A:C8	3.08	0.41
69:m2:872:A:C2	69:m2:917:G:C6	3.08	0.41
69:m2:1416:A:H5'	69:m2:1417:C:OP2	2.20	0.41
1:A1:201:LEU:HD21	1:A1:226:ALA:HA	2.03	0.41
2:A2:458:C:OP1	26:H2:121:ARG:HG2	2.20	0.41
2:A2:1281:C:C2	2:A2:1282:C:C5	3.08	0.41
2:A2:1649:C:H4'	32:K2:152:PHE:CZ	2.55	0.41
2:A2:3765:G:H8	2:A2:3765:G:OP2	2.03	0.41
2:A2:3942:U:OP1	66:i2:9:ARG:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:E1:9:GLU:C	16:E1:11:PRO:HD2	2.46	0.41
18:E3:76:LYS:HA	69:m2:484:G:OP1	2.20	0.41
23:G2:121:GLY:HA3	23:G2:168:ASP:O	2.20	0.41
26:H2:99:VAL:HG23	26:H2:114:VAL:HG23	2.02	0.41
26:H2:147:LEU:HD21	26:H2:151:ILE:HG22	2.01	0.41
31:J3:192:LEU:HB3	31:J3:227:ARG:HB3	2.01	0.41
31:J3:207:ALA:O	31:J3:210:PRO:HD2	2.20	0.41
39:N3:32:ASP:O	39:N3:35:GLU:HG3	2.20	0.41
50:T2:77:TYR:CD2	54:W2:39:ARG:HD2	2.54	0.41
66:i2:61:LYS:CE	66:i2:87:ARG:HH12	2.33	0.41
68:k2:26:SER:HB2	68:k2:31:ASN:ND2	2.35	0.41
68:k2:51:VAL:HG13	68:k2:60:VAL:HG13	2.03	0.41
69:m2:18:C:H2'	69:m2:19:A:O4'	2.20	0.41
69:m2:187:G:C6	69:m2:188:C:C4	3.08	0.41
69:m2:895:U:H2'	69:m2:896:G:O4'	2.21	0.41
69:m2:1392:U:H2'	69:m2:1393:C:H6	1.86	0.41
69:m2:1476:A:H2'	69:m2:1477:G:C8	2.55	0.41
69:m2:1714:A:H2'	69:m2:1715:C:H6	1.85	0.41
72:p2:25:PHE:HA	72:p2:28:LYS:HG3	2.02	0.41
72:p2:121:ILE:HD13	72:p2:164:ILE:HB	2.00	0.41
78:v2:8:ARG:HD2	78:v2:12:TYR:CZ	2.55	0.41
80:x2:29:SER:OG	80:x2:32:GLN:HG3	2.19	0.41
80:x2:37:TYR:OH	80:x2:86:LEU:HA	2.21	0.41
1:A1:176:ILE:HG22	1:A1:209:MET:HE1	2.03	0.41
2:A2:377:A:H2'	2:A2:378:A:O4'	2.21	0.41
2:A2:1330:2MG:H2'	2:A2:1331:A:N7	2.36	0.41
2:A2:2652:G:H2'	2:A2:2653:G:C8	2.55	0.41
2:A2:3314:C:H5''	14:D2:242:ARG:O	2.20	0.41
2:A2:4604:C:H2'	2:A2:4605:U:H6	1.85	0.41
3:A3:15:VAL:O	3:A3:19:ASN:HB3	2.20	0.41
15:D3:70:LEU:HD21	15:D3:74:LYS:HZ3	1.84	0.41
16:E1:33:LEU:HD11	16:E1:67:LYS:O	2.20	0.41
16:E1:163:MET:HE3	16:E1:174:ILE:HD13	2.03	0.41
20:F2:28:PHE:CD1	20:F2:132:ALA:HB2	2.55	0.41
20:F2:128:LEU:HD13	20:F2:260:LEU:HD21	2.01	0.41
32:K2:29:VAL:O	32:K2:33:ARG:HB2	2.19	0.41
54:W2:47:ILE:HA	54:W2:72:HIS:O	2.20	0.41
55:X2:25:TYR:CD1	55:X2:119:THR:HG23	2.54	0.41
55:X2:33:ILE:HD11	55:X2:45:ALA:HA	2.03	0.41
69:m2:217:G:H2'	69:m2:218:C:H6	1.85	0.41
70:n2:63:U:H2'	70:n2:64:C:H6	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:v2:71:LEU:HD23	78:v2:73:ASN:N	2.31	0.41
80:x2:100:LYS:O	80:x2:101:THR:C	2.63	0.41
82:z2:11:LYS:HE2	82:z2:11:LYS:HB3	1.78	0.41
1:A1:231:TRP:CD1	1:A1:232:PRO:HD2	2.55	0.41
1:A1:259:GLU:HG2	36:M2:38:VAL:HG22	2.02	0.41
2:A2:164:G:H2'	2:A2:165:A:H8	1.86	0.41
2:A2:263:G:H2'	2:A2:264:C:C6	2.56	0.41
2:A2:1613:G:H2'	2:A2:1614:C:C6	2.56	0.41
2:A2:3501:A:H2'	2:A2:3502:C:H6	1.83	0.41
2:A2:3891:A:H2'	2:A2:3892:G:C8	2.55	0.41
2:A2:3896:A:H2'	2:A2:3897:G:O4'	2.20	0.41
2:A2:3952:U:OP1	38:N2:87:LYS:HE3	2.21	0.41
2:A2:4591:G:H1'	26:H2:165:ARG:NH1	2.36	0.41
3:A3:12:ILE:HG23	3:A3:20:ILE:HG23	2.02	0.41
3:A3:136:THR:OG1	69:m2:1523:C:H2'	2.20	0.41
6:B3:44:GLU:OE1	6:B3:45:LEU:HD12	2.20	0.41
19:F1:28:GLN:HB3	19:F1:29:PRO:HD3	2.03	0.41
23:G2:164:LYS:HA	23:G2:167:VAL:HG22	2.02	0.41
28:I2:113:ASP:OD1	28:I2:114:LYS:HG3	2.20	0.41
33:K3:6:SER:OG	33:K3:112:VAL:HG22	2.20	0.41
33:K3:221:LYS:HD3	33:K3:221:LYS:HA	1.91	0.41
35:L3:130:ILE:HG21	35:L3:145:PRO:HA	2.03	0.41
41:O3:29:GLY:O	41:O3:93:LEU:HA	2.21	0.41
41:O3:51:GLU:HG3	72:p2:48:LEU:O	2.20	0.41
43:P3:24:GLN:HG2	43:P3:64:ASN:OD1	2.20	0.41
45:Q3:80:ASP:HA	45:Q3:83:LYS:NZ	2.35	0.41
58:a2:95:PHE:CD2	58:a2:96:LEU:HD22	2.55	0.41
61:d2:49:TRP:CE3	61:d2:50:SER:HB2	2.56	0.41
61:d2:67:LEU:HD23	61:d2:67:LEU:HA	1.93	0.41
65:h2:3:ALA:HB3	86:m2:1936:4AC:OP1	2.21	0.41
69:m2:217:G:H2'	69:m2:218:C:C6	2.55	0.41
69:m2:1515:C:H2'	69:m2:1516:G:H8	1.86	0.41
69:m2:1591:A:H2'	69:m2:1592:C:H6	1.86	0.41
73:q2:76:ARG:HG2	78:v2:61:GLN:HE21	1.86	0.41
74:r2:11:ARG:HH21	74:r2:24:THR:HB	1.86	0.41
74:r2:184:ILE:HD13	74:r2:226:PHE:CE1	2.54	0.41
78:v2:49:MET:HA	78:v2:55:ARG:HH12	1.85	0.41
2:A2:1332:C:H2'	2:A2:1333:C:H6	1.86	0.41
2:A2:1494:G:O5'	52:U2:29:PRO:HB2	2.20	0.41
2:A2:1523:G:H2'	2:A2:1524:C:H6	1.84	0.41
2:A2:3722:C:C2	2:A2:3723:A:C8	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A2:4326:C:H2'	2:A2:4327:U:C6	2.56	0.41
4:B1:94:GLN:HB3	4:B1:218:LEU:HD21	2.01	0.41
10:C1:45:LEU:HD22	10:C1:57:VAL:HG22	2.02	0.41
17:E2:85:VAL:CG2	17:E2:167:GLN:HE21	2.33	0.41
20:F2:33:ARG:HG3	20:F2:122:TYR:OH	2.19	0.41
25:H1:65:ARG:HD3	25:H1:127:TYR:CG	2.56	0.41
31:J3:200:ARG:O	35:L3:98:LEU:HB3	2.20	0.41
33:K3:186:GLN:HE22	69:m2:320:A:H61	1.67	0.41
39:N3:16:LEU:HB3	43:P3:57:ARG:NH2	2.36	0.41
41:O3:136:PRO:HB2	41:O3:139:SER:HB3	2.03	0.41
42:P2:96:LEU:HD13	44:Q2:20:ARG:HG2	2.02	0.41
46:R2:113:VAL:HG13	46:R2:117:TYR:HD2	1.85	0.41
48:S2:47:MET:HE3	48:S2:119:LEU:CD1	2.51	0.41
50:T2:103:ASP:HB3	50:T2:106:LEU:HD13	2.02	0.41
69:m2:293:G:H8	79:w2:41:GLY:HA3	1.85	0.41
71:o2:206:ASP:HA	71:o2:207:PRO:HD3	1.93	0.41
74:r2:114:ILE:HD13	74:r2:237:SER:OG	2.20	0.41
81:y2:131:LYS:N	81:y2:131:LYS:HD2	2.35	0.41
2:A2:38:A:H5''	52:U2:35:ALA:HB2	2.03	0.41
2:A2:166:C:H2'	2:A2:167:C:C6	2.56	0.41
2:A2:439:G:H2'	2:A2:440:U:O4'	2.21	0.41
2:A2:1724:G:OP1	36:M2:160:ARG:HD3	2.21	0.41
2:A2:2047:C:H2'	2:A2:2048:U:C6	2.56	0.41
2:A2:2164:U:H5	2:A2:2538:A:N1	2.19	0.41
2:A2:2393:G:N1	2:A2:2473:U:H2'	2.36	0.41
2:A2:2472:G:H2'	2:A2:2473:U:O4'	2.21	0.41
2:A2:4014:A:H4'	66:i2:39:ARG:HH12	1.85	0.41
2:A2:4382:C:H2'	2:A2:4383:G:O4'	2.21	0.41
13:D1:76:MET:HE2	13:D1:138:ILE:HG21	2.03	0.41
13:D1:103:LEU:HD23	13:D1:103:LEU:HA	1.93	0.41
17:E2:36:ASP:HB3	17:E2:39:LYS:NZ	2.36	0.41
17:E2:103:LYS:HE2	17:E2:103:LYS:HB2	1.92	0.41
19:F1:140:SER:HA	19:F1:143:GLU:HB3	2.01	0.41
20:F2:145:GLU:C	20:F2:147:VAL:H	2.27	0.41
25:H1:42:PRO:HG3	25:H1:53:TYR:CE1	2.56	0.41
30:J2:125:MET:HB2	30:J2:141:SER:OG	2.21	0.41
39:N3:114:ARG:HG2	69:m2:1011:A:O2'	2.20	0.41
54:W2:48:LEU:HD13	54:W2:71:VAL:HG13	2.01	0.41
55:X2:117:LEU:HD23	55:X2:117:LEU:HA	1.75	0.41
69:m2:90:G:H2'	69:m2:91:A:O4'	2.21	0.41
69:m2:347:U:H2'	69:m2:348:C:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:o2:33:GLN:OE1	71:o2:154:LEU:HB2	2.20	0.41
71:o2:195:TRP:CD1	71:o2:197:VAL:H	2.38	0.41
73:q2:99:ILE:HA	73:q2:99:ILE:HD12	1.79	0.41
76:t2:130:LEU:HG	76:t2:177:TYR:CE1	2.55	0.41
2:A2:130:G:H3'	2:A2:131:C:H5''	2.02	0.41
2:A2:712:G:H2'	2:A2:713:C:C6	2.55	0.41
2:A2:1376:A:H2'	2:A2:1377:A:O4'	2.21	0.41
2:A2:1532:U:H4'	38:N2:100:LYS:HB2	2.01	0.41
2:A2:2379:G:H2'	2:A2:2380:U:H6	1.85	0.41
2:A2:4065:C:H2'	2:A2:4066:A:O4'	2.19	0.41
2:A2:4156:C:H2'	2:A2:4157:C:C6	2.56	0.41
2:A2:4564:G:H2'	2:A2:4565:C:C6	2.55	0.41
5:B2:16:A:H2'	5:B2:17:C:C6	2.55	0.41
6:B3:71:GLY:N	6:B3:74:SER:HB3	2.33	0.41
7:Bv:53:G:H8	7:Bv:53:G:OP2	2.03	0.41
10:C1:88:PHE:CE1	10:C1:151:ILE:HD12	2.56	0.41
11:C2:115:G:H2'	11:C2:116:C:C6	2.55	0.41
13:D1:26:VAL:HG21	13:D1:96:VAL:HG21	2.02	0.41
16:E1:132:VAL:HG12	16:E1:134:LEU:HD12	2.02	0.41
20:F2:240:LEU:HD23	20:F2:240:LEU:HA	1.85	0.41
27:H3:33:LYS:C	27:H3:35:GLY:H	2.29	0.41
28:I2:88:LEU:HD23	28:I2:88:LEU:HA	1.90	0.41
29:I3:31:ILE:HB	29:I3:43:TRP:HB2	2.02	0.41
29:I3:59:LEU:HD13	29:I3:90:TRP:CG	2.55	0.41
29:I3:133:ASN:HB2	29:I3:138:CYS:SG	2.60	0.41
30:J2:91:LEU:HD23	30:J2:91:LEU:HA	1.94	0.41
31:J3:127:PHE:CD2	31:J3:141:VAL:HG22	2.55	0.41
42:P2:16:ILE:HD13	42:P2:57:VAL:HG23	2.03	0.41
67:j2:50:ARG:HB3	67:j2:54:ILE:HG22	2.03	0.41
69:m2:12:U:H2'	69:m2:13:C:H6	1.85	0.41
69:m2:113:G:C2	69:m2:295:C:C5	3.09	0.41
69:m2:187:G:H2'	69:m2:188:C:H6	1.85	0.41
69:m2:1558:A:H2'	69:m2:1558:A:N3	2.36	0.41
69:m2:1690:C:H2'	69:m2:1691:C:H6	1.86	0.41
69:m2:1694:U:H2'	69:m2:1695:G:C8	2.56	0.41
74:r2:168:LYS:HA	74:r2:168:LYS:HD2	1.75	0.41
77:u2:110:ARG:HH12	77:u2:121:LEU:C	2.28	0.41
81:y2:32:ILE:HD13	81:y2:39:LEU:HD22	2.03	0.41
81:y2:78:VAL:O	81:y2:82:TYR:HD1	2.03	0.41
1:A1:148:ASN:O	1:A1:152:ILE:HG12	2.20	0.41
1:A1:187:LYS:HE2	2:A2:2029:C:O2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:248:HIS:ND1	1:A1:250:VAL:HG22	2.35	0.41
2:A2:1059:C:H2'	2:A2:1060:G:O4'	2.20	0.41
2:A2:1489:C:H41	2:A2:4030:A:H5''	1.85	0.41
2:A2:1608:G:H2'	2:A2:1609:C:C6	2.56	0.41
2:A2:1695:C:C2	2:A2:1696:C:C5	3.09	0.41
2:A2:2160:G:N7	63:f2:2:SER:HB3	2.36	0.41
2:A2:2376:A:H2'	2:A2:2377:G:H8	1.86	0.41
2:A2:2451:A:H62	62:e2:35:LYS:HZ2	1.69	0.41
2:A2:3256:G:H2'	2:A2:3257:C:H6	1.85	0.41
2:A2:3954:U:H4'	38:N2:5:LYS:HE3	2.03	0.41
2:A2:4166:G:H2'	2:A2:4167:G:O4'	2.21	0.41
2:A2:4608:C:H2'	2:A2:4609:G:O4'	2.20	0.41
3:A3:68:ILE:HD13	3:A3:68:ILE:HA	1.94	0.41
5:B2:42:A:C5	5:B2:43:U:C5	3.09	0.41
5:B2:51:G:H21	16:E1:12:MET:CE	2.33	0.41
5:B2:52:C:H1'	16:E1:12:MET:HE3	2.03	0.41
6:B3:70:ALA:O	6:B3:121:ARG:HD3	2.21	0.41
14:D2:186:TYR:HB2	14:D2:196:TRP:CZ3	2.55	0.41
15:D3:14:PRO:HB2	15:D3:23:ILE:HG23	2.02	0.41
16:E1:87:LEU:HB3	16:E1:92:TYR:HD1	1.86	0.41
23:G2:10:LYS:HG2	23:G2:14:LYS:HE2	2.03	0.41
24:G3:33:GLU:HG2	24:G3:41:SER:HB2	2.02	0.41
26:H2:121:ARG:HG2	26:H2:121:ARG:H	1.70	0.41
28:I2:79:ILE:O	28:I2:83:THR:HG23	2.21	0.41
28:I2:116:LYS:HE3	36:M2:169:THR:HB	2.02	0.41
29:I3:45:LEU:HD23	29:I3:45:LEU:HA	1.89	0.41
29:I3:149:GLU:N	29:I3:171:ASP:HB3	2.36	0.41
29:I3:266:ILE:HA	29:I3:266:ILE:HD13	1.96	0.41
31:J3:166:ARG:HB2	31:J3:248:TYR:CD1	2.56	0.41
33:K3:3:LEU:HB3	33:K3:16:ILE:HB	2.02	0.41
33:K3:50:VAL:HG21	33:K3:111:LEU:HB3	2.01	0.41
35:L3:29:LEU:HD13	51:T3:41:ARG:HD2	2.02	0.41
37:M3:53:ALA:CB	37:M3:80:ASP:H	2.33	0.41
39:N3:3:ARG:HG2	39:N3:3:ARG:NH1	2.36	0.41
43:P3:32:LYS:HE3	43:P3:32:LYS:HB2	1.84	0.41
45:Q3:110:ARG:O	45:Q3:114:MET:HG3	2.21	0.41
46:R2:74:TYR:HB2	59:b2:25:LYS:HE3	2.02	0.41
49:S3:49:HIS:HA	49:S3:70:LYS:HA	2.02	0.41
66:i2:38:LYS:HA	66:i2:38:LYS:HD3	1.90	0.41
69:m2:158:A:H61	69:m2:465:C:H1'	1.86	0.41
69:m2:486:A2M:HM'3	69:m2:486:A2M:H1'	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:m2:603:OMG:H1'	69:m2:603:OMG:HM23	1.85	0.41
69:m2:982:A:H2'	69:m2:983:A:C8	2.56	0.41
69:m2:1131:G:H2'	69:m2:1132:G:C4	2.56	0.41
69:m2:1206:A:H2'	69:m2:1207:C:C6	2.55	0.41
69:m2:1522:G:N3	69:m2:1522:G:H2'	2.36	0.41
69:m2:1568:G:N2	69:m2:1571:A:H2	2.18	0.41
69:m2:1720:G:N2	69:m2:1816:G:H2'	2.36	0.41
71:o2:63:ARG:HG3	71:o2:185:MET:HE1	2.03	0.41
72:p2:49:VAL:HG21	72:p2:62:LEU:CD2	2.45	0.41
74:r2:48:LEU:HD11	74:r2:70:ILE:HG12	2.03	0.41
75:s2:20:PHE:HB3	75:s2:23:TRP:HD1	1.85	0.41
75:s2:32:ASP:OD2	75:s2:34:SER:HB3	2.21	0.41
76:t2:69:LEU:HD13	76:t2:96:ALA:HB2	2.02	0.41
76:t2:91:HIS:CE1	76:t2:169:LYS:HD2	2.56	0.41
77:u2:47:ARG:HG2	77:u2:47:ARG:NH1	2.34	0.41
77:u2:74:ARG:HG2	77:u2:108:PRO:HB3	2.03	0.41
77:u2:101:ILE:HD11	77:u2:198:TYR:CE2	2.56	0.41
82:z2:13:ALA:HA	82:z2:16:ILE:HG22	2.01	0.41
2:A2:176:G:H2'	2:A2:177:G:H8	1.86	0.41
2:A2:1079:A:OP1	53:V2:87:LYS:HD2	2.21	0.41
2:A2:1684:U:C4	2:A2:2034:A:C2	3.09	0.41
2:A2:1832:A:H2'	2:A2:1833:C:O4'	2.21	0.41
2:A2:2520:A:H2'	2:A2:2521:A:H8	1.86	0.41
2:A2:2600:A:N6	2:A2:3499:C:H42	2.12	0.41
2:A2:3958:OMU:H1'	2:A2:3958:OMU:HM23	1.82	0.41
6:B3:87:VAL:HG13	69:m2:1231:G:H21	1.85	0.41
10:C1:43:VAL:HG12	10:C1:59:LYS:HD3	2.02	0.41
12:C3:94:PRO:O	12:C3:98:VAL:HG23	2.21	0.41
15:D3:11:LEU:HD12	15:D3:12:TYR:CD1	2.55	0.41
16:E1:90:ARG:O	16:E1:91:GLU:HG3	2.21	0.41
19:F1:90:VAL:O	19:F1:94:ILE:HG12	2.20	0.41
20:F2:11:TYR:CZ	20:F2:148:PRO:HB2	2.56	0.41
20:F2:150:LEU:HB3	20:F2:151:PRO:HD3	2.01	0.41
31:J3:192:LEU:HB3	31:J3:227:ARG:CB	2.51	0.41
32:K2:42:THR:O	32:K2:46:VAL:HG23	2.21	0.41
33:K3:201:LYS:HE3	33:K3:201:LYS:HB3	1.92	0.41
35:L3:18:ARG:NH2	69:m2:4:C:H1'	2.35	0.41
35:L3:91:LYS:H	35:L3:91:LYS:HG3	1.69	0.41
40:O2:54:GLY:C	40:O2:56:LEU:H	2.27	0.41
45:Q3:86:GLU:OE1	45:Q3:87:PRO:HD2	2.21	0.41
49:S3:46:VAL:HG12	49:S3:54:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:W2:31:TYR:CZ	54:W2:35:LEU:HD11	2.56	0.41
68:k2:84:LYS:HE2	68:k2:84:LYS:HB3	1.66	0.41
69:m2:65:C:H5'	69:m2:78:C:H41	1.85	0.41
69:m2:314:G:O2'	69:m2:315:A:H5'	2.21	0.41
69:m2:385:G:C5	69:m2:386:U:C4	3.09	0.41
69:m2:1392:U:H2'	69:m2:1393:C:C6	2.56	0.41
69:m2:1416:A:H5'	69:m2:1417:C:P	2.61	0.41
70:n2:65:C:H2'	70:n2:66:U:C6	2.55	0.41
71:o2:53:ARG:HG3	71:o2:53:ARG:HH11	1.86	0.41
72:p2:36:PRO:HG2	72:p2:39:PHE:CE2	2.54	0.41
73:q2:139:SER:O	73:q2:182:LEU:HD12	2.21	0.41
73:q2:168:VAL:HG13	73:q2:187:LYS:HB2	2.03	0.41
1:A1:222:ARG:HA	1:A1:225:GLU:OE1	2.22	0.40
2:A2:62:A:H2'	2:A2:63:G:O4'	2.20	0.40
2:A2:300:A:H2'	2:A2:301:G:C8	2.51	0.40
2:A2:757:U:C2	2:A2:758:G:C8	3.09	0.40
2:A2:949:G:H2'	2:A2:950:A:H8	1.86	0.40
2:A2:1029:C:H2'	2:A2:1030:G:C8	2.56	0.40
2:A2:1233:A:N3	2:A2:1233:A:H2'	2.36	0.40
2:A2:1367:A:N6	2:A2:1386:G:H1'	2.35	0.40
2:A2:1475:C:H2'	2:A2:1476:C:C6	2.55	0.40
2:A2:2480:A:H1'	34:L2:93:VAL:HG21	2.03	0.40
2:A2:2514:G:C5	2:A2:2515:G:C6	3.09	0.40
2:A2:3308:A:H2'	2:A2:3309:A:C8	2.56	0.40
2:A2:3392:A:H2'	2:A2:3393:A:C8	2.55	0.40
2:A2:3600:G:H2'	2:A2:3601:A:H8	1.84	0.40
3:A3:44:VAL:HG11	3:A3:71:MET:HG3	2.03	0.40
6:B3:33:TRP:HH2	6:B3:99:VAL:HG22	1.85	0.40
10:C1:96:TYR:HB3	10:C1:101:ILE:CD1	2.51	0.40
15:D3:34:MET:HE2	15:D3:34:MET:HB3	1.88	0.40
16:E1:5:GLN:HA	16:E1:8:LYS:HE3	2.03	0.40
17:E2:379:PHE:CE2	17:E2:385:LYS:HG3	2.56	0.40
18:E3:60:LYS:HG2	18:E3:114:ASP:O	2.21	0.40
19:F1:200:LYS:HG2	19:F1:204:GLU:OE2	2.20	0.40
20:F2:342:ARG:HG2	20:F2:345:ARG:NH2	2.35	0.40
25:H1:75:VAL:HG11	25:H1:80:THR:HG22	2.04	0.40
33:K3:14:LYS:HE2	33:K3:121:ILE:HD13	2.03	0.40
36:M2:168:THR:OG1	36:M2:170:LYS:HG2	2.22	0.40
40:O2:25:CYS:C	40:O2:28:PRO:HD2	2.47	0.40
41:O3:42:VAL:HG21	41:O3:81:VAL:HG21	2.03	0.40
43:P3:25:VAL:HG12	43:P3:65:LEU:HD21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:P3:39:THR:O	43:P3:43:LYS:HG2	2.21	0.40
56:Y2:66:THR:HA	56:Y2:69:MET:SD	2.61	0.40
69:m2:346:U:H2'	69:m2:347:U:H6	1.86	0.40
69:m2:514:A2M:H4'	69:m2:578:A2M:H2	2.03	0.40
69:m2:637:G:H2'	69:m2:638:C:H6	1.85	0.40
69:m2:1489:A:H2'	69:m2:1490:C:C6	2.56	0.40
69:m2:1676:G:OP2	81:y2:78:VAL:HG21	2.21	0.40
69:m2:1838:G:H4'	69:m2:1839:G:C4	2.56	0.40
72:p2:103:MET:O	72:p2:214:LYS:HA	2.21	0.40
75:s2:201:LYS:HG3	75:s2:204:ARG:HH21	1.86	0.40
76:t2:98:ARG:CZ	76:t2:128:ALA:HB1	2.51	0.40
1:A1:250:VAL:HG12	36:M2:38:VAL:HG12	2.02	0.40
2:A2:23:C:H2'	2:A2:24:G:O4'	2.22	0.40
2:A2:654:G:H2'	2:A2:655:G:O4'	2.22	0.40
2:A2:1223:C:N4	2:A2:1224:G:C2	2.89	0.40
2:A2:2102:A:C2	56:Y2:31:ILE:HD11	2.56	0.40
2:A2:4108:OMC:HM23	2:A2:4108:OMC:H1'	1.88	0.40
6:B3:15:VAL:HG11	69:m2:1543:G:H4'	2.03	0.40
11:C2:116:C:H2'	11:C2:117:C:C6	2.57	0.40
13:D1:53:VAL:HG11	38:N2:158:PHE:HZ	1.85	0.40
13:D1:152:LEU:HD12	13:D1:165:ILE:HG23	2.03	0.40
17:E2:110:ILE:HG22	17:E2:115:LYS:HG3	2.03	0.40
20:F2:33:ARG:HG3	20:F2:122:TYR:CE2	2.55	0.40
29:I3:67:SER:HB3	29:I3:83:TRP:CD1	2.56	0.40
33:K3:50:VAL:CG2	33:K3:111:LEU:HB3	2.51	0.40
45:Q3:121:ALA:HA	45:Q3:124:ASN:HD21	1.86	0.40
59:b2:91:MET:HA	59:b2:94:ARG:HE	1.86	0.40
68:k2:37:SER:OG	68:k2:40:TYR:HD2	2.04	0.40
69:m2:356:U:P	79:w2:107:LYS:HD3	2.61	0.40
69:m2:641:C:N4	69:m2:642:A:H62	2.19	0.40
69:m2:869:OMG:HM23	69:m2:869:OMG:H1'	1.81	0.40
69:m2:946:A:H2'	69:m2:947:U:H6	1.86	0.40
69:m2:1067:G:H2'	69:m2:1068:U:C6	2.56	0.40
69:m2:1389:G:H2'	69:m2:1390:A:O4'	2.21	0.40
69:m2:1413:G:C6	69:m2:1433:G:C6	3.09	0.40
69:m2:1622:A:H3'	80:x2:40:ARG:HD3	2.03	0.40
72:p2:105:LEU:HD23	72:p2:105:LEU:HA	1.81	0.40
73:q2:35:SER:OG	73:q2:91:VAL:HG21	2.21	0.40
75:s2:19:LEU:HB3	75:s2:21:GLY:H	1.86	0.40
76:t2:134:VAL:HG12	76:t2:173:PHE:CD2	2.55	0.40
81:y2:55:VAL:CG2	81:y2:63:PHE:HB2	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A2:35:U:H4'	2:A2:1338:A:N1	2.37	0.40
2:A2:663:C:H2'	2:A2:664:C:C6	2.56	0.40
2:A2:879:C:H2'	2:A2:880:U:C6	2.56	0.40
2:A2:1115:C:H1'	2:A2:2070:G:OP1	2.20	0.40
2:A2:1579:C:H2'	2:A2:1580:C:C6	2.55	0.40
2:A2:2172:A:H2'	2:A2:2173:A:H8	1.86	0.40
2:A2:2325:U:H2'	2:A2:2326:C:C6	2.56	0.40
2:A2:3340:G:H2'	2:A2:3341:C:H6	1.85	0.40
2:A2:3442:U:O2	2:A2:3470:U:H4'	2.20	0.40
2:A2:3478:U:H2'	2:A2:3479:G:C8	2.56	0.40
2:A2:4406:G:C6	2:A2:4525:G:C2	3.10	0.40
2:A2:4632:G:H2'	2:A2:4633:C:H6	1.84	0.40
6:B3:23:LYS:HA	6:B3:54:TYR:CE1	2.56	0.40
11:C2:45:C:C2	11:C2:46:G:C8	3.10	0.40
16:E1:3:GLN:HG3	16:E1:6:GLY:H	1.86	0.40
20:F2:149:GLU:OE2	20:F2:151:PRO:HD2	2.22	0.40
27:H3:11:PRO:HG2	69:m2:1620:C:C5	2.56	0.40
35:L3:110:LEU:HB2	35:L3:147:PHE:HB3	2.04	0.40
42:P2:23:GLY:HA2	42:P2:38:TYR:CZ	2.56	0.40
42:P2:25:VAL:HA	42:P2:37:LEU:O	2.22	0.40
55:X2:29:ILE:HG21	55:X2:80:VAL:HG11	2.04	0.40
69:m2:115:U:H2'	69:m2:116:OMU:C6	2.51	0.40
69:m2:145:G:H2'	69:m2:146:G:C8	2.56	0.40
69:m2:423:G:OP1	79:w2:98:LYS:HA	2.21	0.40
69:m2:476:G:C2	69:m2:477:C:C5	3.09	0.40
69:m2:496:C:H2'	69:m2:497:U:H5'	2.03	0.40
69:m2:1218:C:N4	69:m2:1344:U:H5''	2.37	0.40
69:m2:1268:C:H2'	69:m2:1269:C:C6	2.56	0.40
69:m2:1831:G:H1'	69:m2:1852:A:H2	1.87	0.40
72:p2:28:LYS:NZ	72:p2:50:THR:HG22	2.36	0.40
77:u2:65:PHE:CD2	77:u2:104:ILE:HG13	2.55	0.40
82:z2:33:ARG:O	82:z2:36:GLU:HG2	2.22	0.40
2:A2:873:G:H2'	2:A2:874:C:C6	2.57	0.40
2:A2:928:G:H1	2:A2:1064:G:H1	1.70	0.40
2:A2:1254:C:H2'	2:A2:1255:C:C6	2.56	0.40
2:A2:1874:C:H2'	2:A2:1875:C:C6	2.56	0.40
2:A2:2168:U:H2'	2:A2:2169:G:C8	2.57	0.40
2:A2:3579:A:H2'	2:A2:3580:C:C6	2.56	0.40
2:A2:3839:G:H2'	2:A2:3840:U:O4'	2.22	0.40
2:A2:4368:C:OP2	17:E2:30:LYS:HD2	2.22	0.40
4:B1:87:LEU:HD23	4:B1:87:LEU:HA	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B1:231:ASP:HB3	4:B1:235:ARG:NH1	2.36	0.40
6:B3:56:ARG:HG3	6:B3:103:VAL:HG21	2.03	0.40
10:C1:6:SER:HB3	10:C1:67:LEU:HD11	2.04	0.40
11:C2:90:C:H2'	11:C2:91:A:C8	2.57	0.40
14:D2:6:ARG:HG2	14:D2:10:LYS:HZ1	1.86	0.40
23:G2:146:LEU:HD22	23:G2:163:LEU:HD12	2.02	0.40
23:G2:208:MET:HB2	23:G2:233:PRO:HG3	2.04	0.40
26:H2:125:THR:OG1	56:Y2:93:LYS:HG3	2.21	0.40
31:J3:204:ILE:HD11	31:J3:220:ASP:HA	2.03	0.40
34:L2:134:ASN:ND2	34:L2:135:LYS:N	2.69	0.40
36:M2:51:LEU:HA	36:M2:51:LEU:HD23	1.84	0.40
39:N3:49:GLN:O	39:N3:53:ILE:HG12	2.22	0.40
52:U2:15:VAL:HG23	52:U2:16:SER:N	2.37	0.40
55:X2:46:LEU:HD12	55:X2:64:ILE:HD13	2.02	0.40
69:m2:528:A:H61	69:m2:590:G:H1	1.67	0.40
69:m2:1642:A:OP2	69:m2:1642:A:H8	2.04	0.40
70:n2:30:G:C5	70:n2:31:C:C5	3.10	0.40
71:o2:119:PRO:HG2	71:o2:142:LEU:HD13	2.03	0.40
73:q2:126:ILE:HD13	73:q2:134:CYS:SG	2.62	0.40
77:u2:6:ASP:HB2	77:u2:8:TRP:CD1	2.56	0.40
77:u2:173:ALA:HB1	77:u2:188:TYR:O	2.21	0.40
1:A1:149:LYS:HB2	38:N2:133:ALA:HB3	2.04	0.40
2:A2:123:C:H2'	2:A2:124:C:C6	2.56	0.40
2:A2:145:G:H2'	2:A2:146:G:O4'	2.21	0.40
2:A2:955:U:H3	2:A2:1027:G:H1	1.69	0.40
2:A2:2256:C:H2'	2:A2:2257:G:H5'	2.02	0.40
2:A2:2283:G:H2'	2:A2:2284:A:O4'	2.22	0.40
2:A2:3388:A:H2'	2:A2:3389:A:C8	2.56	0.40
2:A2:4215:U:H2'	2:A2:4216:A:H8	1.87	0.40
2:A2:4302:G:H2'	2:A2:4303:A:O4'	2.20	0.40
3:A3:86:ARG:HD3	3:A3:98:VAL:CG1	2.52	0.40
4:B1:57:TRP:NE1	4:B1:65:ARG:HH12	2.20	0.40
5:B2:64:G:H2'	5:B2:65:G:H8	1.86	0.40
11:C2:81:C:H2'	11:C2:83:C:OP2	2.21	0.40
13:D1:36:LEU:HD12	13:D1:69:ARG:HD3	2.02	0.40
17:E2:18:PRO:O	17:E2:19:ARG:C	2.65	0.40
19:F1:170:THR:HG23	19:F1:173:GLU:H	1.86	0.40
34:L2:92:LYS:O	34:L2:96:MET:HG3	2.22	0.40
35:L3:37:LEU:HD11	35:L3:106:LEU:HD22	2.04	0.40
37:M3:26:LEU:HD13	37:M3:31:LEU:HD22	2.03	0.40
39:N3:16:LEU:CD1	39:N3:62:GLN:HG3	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:P3:89:TRP:HE3	43:P3:93:LEU:HD13	1.86	0.40
53:V2:90:LYS:O	53:V2:93:ARG:HG2	2.22	0.40
58:a2:86:CYS:O	58:a2:90:ARG:HG3	2.21	0.40
65:h2:14:LYS:HD2	69:m2:1174:U:H5''	2.03	0.40
69:m2:527:A:H61	69:m2:562:A:H61	1.68	0.40
69:m2:565:G:N3	69:m2:566:A:C8	2.90	0.40
69:m2:966:A:H1'	69:m2:1056:G:O2'	2.22	0.40
69:m2:1037:A:H2'	69:m2:1038:A:O4'	2.21	0.40
69:m2:1049:C:H2'	69:m2:1050:G:O4'	2.21	0.40
69:m2:1721:A:H2	69:m2:1816:G:H21	1.69	0.40
73:q2:123:LEU:HD21	73:q2:136:VAL:HB	2.04	0.40
74:r2:137:PRO:HD2	74:r2:149:TYR:CD1	2.57	0.40
76:t2:101:LEU:HD23	76:t2:116:ARG:HG3	2.02	0.40
78:v2:79:LEU:C	78:v2:81:ASP:H	2.29	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A1	220/270 (82%)	213 (97%)	7 (3%)	0	100	100
3	A3	137/152 (90%)	120 (88%)	16 (12%)	1 (1%)	18	49
4	B1	214/266 (80%)	207 (97%)	7 (3%)	0	100	100
6	B3	136/145 (94%)	127 (93%)	9 (7%)	0	100	100
10	C1	188/192 (98%)	182 (97%)	6 (3%)	0	100	100
12	C3	95/119 (80%)	91 (96%)	4 (4%)	0	100	100
13	D1	200/214 (94%)	194 (97%)	6 (3%)	0	100	100
14	D2	243/257 (95%)	229 (94%)	14 (6%)	0	100	100
15	D3	81/83 (98%)	75 (93%)	6 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	E1	172/178 (97%)	165 (96%)	7 (4%)	0	100	100
17	E2	400/403 (99%)	383 (96%)	17 (4%)	0	100	100
18	E3	137/142 (96%)	124 (90%)	13 (10%)	0	100	100
19	F1	201/211 (95%)	189 (94%)	12 (6%)	0	100	100
20	F2	350/419 (84%)	334 (95%)	16 (5%)	0	100	100
21	F3	95/114 (83%)	89 (94%)	6 (6%)	0	100	100
22	G1	137/217 (63%)	134 (98%)	3 (2%)	0	100	100
23	G2	291/297 (98%)	283 (97%)	8 (3%)	0	100	100
24	G3	52/69 (75%)	52 (100%)	0	0	100	100
25	H1	201/204 (98%)	195 (97%)	6 (3%)	0	100	100
26	H2	212/296 (72%)	207 (98%)	5 (2%)	0	100	100
27	H3	49/56 (88%)	44 (90%)	5 (10%)	0	100	100
28	I2	196/203 (97%)	190 (97%)	6 (3%)	0	100	100
29	I3	208/317 (66%)	183 (88%)	24 (12%)	1 (0%)	24	57
30	J2	151/184 (82%)	145 (96%)	6 (4%)	0	100	100
31	J3	215/293 (73%)	192 (89%)	22 (10%)	1 (0%)	24	57
32	K2	184/188 (98%)	172 (94%)	12 (6%)	0	100	100
33	K3	205/249 (82%)	200 (98%)	5 (2%)	0	100	100
34	L2	167/196 (85%)	164 (98%)	3 (2%)	0	100	100
35	L3	177/194 (91%)	158 (89%)	18 (10%)	1 (1%)	21	52
36	M2	173/176 (98%)	163 (94%)	10 (6%)	0	100	100
37	M3	74/132 (56%)	66 (89%)	8 (11%)	0	100	100
38	N2	157/160 (98%)	154 (98%)	3 (2%)	0	100	100
39	N3	147/151 (97%)	131 (89%)	16 (11%)	0	100	100
40	O2	99/128 (77%)	98 (99%)	1 (1%)	0	100	100
41	O3	133/151 (88%)	124 (93%)	9 (7%)	0	100	100
42	P2	127/140 (91%)	122 (96%)	5 (4%)	0	100	100
43	P3	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
44	Q2	60/157 (38%)	56 (93%)	4 (7%)	0	100	100
45	Q3	117/133 (88%)	108 (92%)	9 (8%)	0	100	100
46	R2	116/156 (74%)	113 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	R3	71/125 (57%)	67 (94%)	4 (6%)	0	100	100
48	S2	132/145 (91%)	128 (97%)	4 (3%)	0	100	100
49	S3	75/84 (89%)	70 (93%)	5 (7%)	0	100	100
50	T2	133/136 (98%)	131 (98%)	2 (2%)	0	100	100
51	T3	40/133 (30%)	39 (98%)	1 (2%)	0	100	100
52	U2	145/148 (98%)	137 (94%)	8 (6%)	0	100	100
53	V2	115/160 (72%)	112 (97%)	3 (3%)	0	100	100
54	W2	92/115 (80%)	89 (97%)	3 (3%)	0	100	100
55	X2	105/125 (84%)	100 (95%)	5 (5%)	0	100	100
56	Y2	126/135 (93%)	123 (98%)	3 (2%)	0	100	100
57	Z2	107/110 (97%)	105 (98%)	2 (2%)	0	100	100
58	a2	105/117 (90%)	102 (97%)	3 (3%)	0	100	100
59	b2	118/123 (96%)	117 (99%)	1 (1%)	0	100	100
60	c2	100/105 (95%)	97 (97%)	3 (3%)	0	100	100
61	d2	84/97 (87%)	80 (95%)	4 (5%)	0	100	100
62	e2	67/70 (96%)	67 (100%)	0	0	100	100
63	f2	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
64	g2	50/128 (39%)	49 (98%)	1 (2%)	0	100	100
65	h2	22/25 (88%)	22 (100%)	0	0	100	100
66	i2	101/105 (96%)	96 (95%)	5 (5%)	0	100	100
67	j2	87/92 (95%)	84 (97%)	3 (3%)	0	100	100
68	k2	123/137 (90%)	118 (96%)	5 (4%)	0	100	100
71	o2	213/295 (72%)	197 (92%)	16 (8%)	0	100	100
72	p2	210/264 (80%)	190 (90%)	20 (10%)	0	100	100
73	q2	211/242 (87%)	206 (98%)	5 (2%)	0	100	100
74	r2	255/257 (99%)	234 (92%)	21 (8%)	0	100	100
75	s2	181/204 (89%)	169 (93%)	12 (7%)	0	100	100
76	t2	166/194 (86%)	149 (90%)	17 (10%)	0	100	100
77	u2	175/208 (84%)	166 (95%)	9 (5%)	0	100	100
78	v2	81/165 (49%)	64 (79%)	16 (20%)	1 (1%)	10	37
79	w2	134/158 (85%)	124 (92%)	10 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
80	x2	118/145 (81%)	109 (92%)	9 (8%)	0	100	100
81	y2	137/146 (94%)	121 (88%)	16 (12%)	0	100	100
82	z2	123/135 (91%)	115 (94%)	8 (6%)	0	100	100
All	All	10694/12621 (85%)	10120 (95%)	569 (5%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A3	91	LYS
29	I3	52	TYR
31	J3	77	SER
78	v2	42	ASN
35	L3	122	SER

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A1	193/234 (82%)	193 (100%)	0	100	100
3	A3	121/132 (92%)	121 (100%)	0	100	100
4	B1	189/223 (85%)	187 (99%)	2 (1%)	65	78
6	B3	111/115 (96%)	111 (100%)	0	100	100
10	C1	169/171 (99%)	169 (100%)	0	100	100
12	C3	90/107 (84%)	90 (100%)	0	100	100
13	D1	174/181 (96%)	174 (100%)	0	100	100
14	D2	188/199 (94%)	188 (100%)	0	100	100
15	D3	53/67 (79%)	53 (100%)	0	100	100
16	E1	147/149 (99%)	147 (100%)	0	100	100
17	E2	347/348 (100%)	347 (100%)	0	100	100
18	E3	111/114 (97%)	111 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	F1	170/178 (96%)	170 (100%)	0	100	100
20	F2	298/348 (86%)	298 (100%)	0	100	100
21	F3	84/97 (87%)	84 (100%)	0	100	100
22	G1	118/157 (75%)	118 (100%)	0	100	100
23	G2	246/249 (99%)	246 (100%)	0	100	100
24	G3	49/62 (79%)	49 (100%)	0	100	100
25	H1	171/172 (99%)	171 (100%)	0	100	100
26	H2	196/256 (77%)	196 (100%)	0	100	100
27	H3	45/49 (92%)	45 (100%)	0	100	100
28	I2	170/173 (98%)	170 (100%)	0	100	100
29	I3	197/275 (72%)	197 (100%)	0	100	100
30	J2	134/163 (82%)	134 (100%)	0	100	100
31	J3	155/224 (69%)	155 (100%)	0	100	100
32	K2	164/165 (99%)	164 (100%)	0	100	100
33	K3	182/218 (84%)	182 (100%)	0	100	100
34	L2	149/175 (85%)	149 (100%)	0	100	100
35	L3	160/168 (95%)	160 (100%)	0	100	100
36	M2	155/156 (99%)	155 (100%)	0	100	100
37	M3	35/108 (32%)	35 (100%)	0	100	100
38	N2	139/140 (99%)	139 (100%)	0	100	100
39	N3	130/131 (99%)	130 (100%)	0	100	100
40	O2	91/114 (80%)	91 (100%)	0	100	100
41	O3	103/119 (87%)	103 (100%)	0	100	100
42	P2	100/107 (94%)	100 (100%)	0	100	100
43	P3	110/113 (97%)	110 (100%)	0	100	100
44	Q2	54/126 (43%)	54 (100%)	0	100	100
45	Q3	103/115 (90%)	103 (100%)	0	100	100
46	R2	106/133 (80%)	106 (100%)	0	100	100
47	R3	65/103 (63%)	65 (100%)	0	100	100
48	S2	124/135 (92%)	124 (100%)	0	100	100
49	S3	71/76 (93%)	71 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	T2	117/118 (99%)	117 (100%)	0	100	100
51	T3	35/105 (33%)	35 (100%)	0	100	100
52	U2	120/121 (99%)	120 (100%)	0	100	100
53	V2	98/124 (79%)	98 (100%)	0	100	100
54	W2	79/97 (81%)	79 (100%)	0	100	100
55	X2	98/110 (89%)	98 (100%)	0	100	100
56	Y2	114/121 (94%)	114 (100%)	0	100	100
57	Z2	88/89 (99%)	88 (100%)	0	100	100
58	a2	93/100 (93%)	93 (100%)	0	100	100
59	b2	108/110 (98%)	108 (100%)	0	100	100
60	c2	86/89 (97%)	86 (100%)	0	100	100
61	d2	73/80 (91%)	73 (100%)	0	100	100
62	e2	64/65 (98%)	64 (100%)	0	100	100
63	f2	47/48 (98%)	47 (100%)	0	100	100
64	g2	48/116 (41%)	48 (100%)	0	100	100
65	h2	23/24 (96%)	23 (100%)	0	100	100
66	i2	91/93 (98%)	91 (100%)	0	100	100
67	j2	73/75 (97%)	73 (100%)	0	100	100
68	k2	109/121 (90%)	109 (100%)	0	100	100
71	o2	180/242 (74%)	180 (100%)	0	100	100
72	p2	193/229 (84%)	193 (100%)	0	100	100
73	q2	176/201 (88%)	176 (100%)	0	100	100
74	r2	220/220 (100%)	220 (100%)	0	100	100
75	s2	157/170 (92%)	157 (100%)	0	100	100
76	t2	132/174 (76%)	132 (100%)	0	100	100
77	u2	137/180 (76%)	137 (100%)	0	100	100
78	v2	75/136 (55%)	75 (100%)	0	100	100
79	w2	125/142 (88%)	125 (100%)	0	100	100
80	x2	109/130 (84%)	105 (96%)	4 (4%)	30	61
81	y2	115/121 (95%)	115 (100%)	0	100	100
82	z2	113/121 (93%)	113 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9263/10717 (86%)	9257 (100%)	6 (0%)	87 90

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

Mol	Chain	Res	Type
4	B1	137[A]	ARG
4	B1	137[B]	ARG
80	x2	124	LYS
80	x2	125	PRO
80	x2	126	VAL
80	x2	127	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (107) such sidechains are listed below:

Mol	Chain	Res	Type
1	A1	80	HIS
1	A1	153	ASN
1	A1	228	ASN
3	A3	10	GLN
3	A3	19	ASN
3	A3	85	ASN
3	A3	97	GLN
4	B1	66	GLN
4	B1	100	HIS
4	B1	195	HIS
6	B3	63	HIS
10	C1	98	HIS
10	C1	108	ASN
10	C1	138	GLN
14	D2	22	HIS
14	D2	95	GLN
14	D2	97	ASN
14	D2	132	ASN
16	E1	110	GLN
17	E2	109	HIS
17	E2	167	GLN
17	E2	184	GLN
18	E3	16	HIS
19	F1	111	GLN
19	F1	175	ASN
20	F2	43	ASN

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Mol	Chain	Res	Type
20	F2	50	GLN
20	F2	198	ASN
20	F2	212	ASN
20	F2	282	HIS
20	F2	286	ASN
22	G1	20	HIS
22	G1	34	ASN
22	G1	66	HIS
23	G2	57	ASN
23	G2	63	GLN
23	G2	198	HIS
23	G2	291	GLN
25	H1	145	ASN
25	H1	196	ASN
27	H3	28	HIS
28	I2	180	GLN
28	I2	184	ASN
29	I3	64	HIS
29	I3	76	GLN
29	I3	285	GLN
30	J2	80	GLN
30	J2	97	ASN
32	K2	44	ASN
32	K2	57	ASN
33	K3	81	HIS
33	K3	155	GLN
33	K3	163	ASN
33	K3	186	GLN
34	L2	40	GLN
34	L2	86	ASN
34	L2	134	ASN
35	L3	134	HIS
35	L3	140	GLN
36	M2	50	GLN
36	M2	125	GLN
36	M2	173	ASN
39	N3	105	ASN
39	N3	123	HIS
44	Q2	17	HIS
45	Q3	94	HIS
46	R2	107	HIS
48	S2	14	ASN

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Mol	Chain	Res	Type
49	S3	9	HIS
50	T2	97	ASN
51	T3	39	ASN
53	V2	6	ASN
53	V2	27	GLN
53	V2	50	ASN
53	V2	60	ASN
54	W2	72	HIS
55	X2	93	ASN
58	a2	73	HIS
59	b2	62	ASN
59	b2	68	ASN
61	d2	76	HIS
63	f2	19	GLN
64	g2	90	ASN
66	i2	76	ASN
71	o2	141	ASN
71	o2	165	ASN
72	p2	53	GLN
72	p2	177	GLN
72	p2	179	ASN
72	p2	232	HIS
73	q2	101	GLN
74	r2	142	HIS
74	r2	157	ASN
74	r2	188	ASN
74	r2	216	ASN
75	s2	101	HIS
75	s2	203	ASN
76	t2	76	GLN
77	u2	84	ASN
77	u2	181	GLN
78	v2	61	GLN
79	w2	94	HIS
79	w2	106	HIS
80	x2	35	GLN
80	x2	128	HIS
81	y2	29	ASN
82	z2	74	GLN

### 5.3.3 RNA ⓘ



Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	C2	155/156 (99%)	28 (18%)	0
2	A2	3484/3615 (96%)	679 (19%)	13 (0%)
5	B2	118/121 (97%)	11 (9%)	0
69	m2	1612/1633 (98%)	391 (24%)	0
7	Bv	63/76 (82%)	28 (44%)	0
70	n2	70/73 (95%)	8 (11%)	0
8	Bx	9/10 (90%)	4 (44%)	0
All	All	5511/5684 (96%)	1149 (20%)	13 (0%)

All (1149) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	A2	2	G
2	A2	13	U
2	A2	17	A
2	A2	21	G
2	A2	25	A
2	A2	39	A
2	A2	42	A
2	A2	48	G
2	A2	57	G
2	A2	59	A
2	A2	63	G
2	A2	64	A
2	A2	65	A
2	A2	66	A
2	A2	71	C
2	A2	73	A
2	A2	74	G
2	A2	91	G
2	A2	104	G
2	A2	108	A
2	A2	109	G
2	A2	110	C
2	A2	119	G
2	A2	120	A
2	A2	131	C
2	A2	134	G
2	A2	144	G
2	A2	151	G
2	A2	159	C
2	A2	164	G
2	A2	172	C

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Mol	Chain	Res	Type
2	A2	183	C
2	A2	184	U
2	A2	185	C
2	A2	186	G
2	A2	188	G
2	A2	189	G
2	A2	197	A
2	A2	200	U
2	A2	201	C
2	A2	209	U
2	A2	216	C
2	A2	217	C
2	A2	218	A
2	A2	220	C
2	A2	233	U
2	A2	234	G
2	A2	237	G
2	A2	253	G
2	A2	254	G
2	A2	266	C
2	A2	267	G
2	A2	280	G
2	A2	297	U
2	A2	315	G
2	A2	316	U
2	A2	340	C
2	A2	341	G
2	A2	345	C
2	A2	362	A
2	A2	363	A
2	A2	379	G
2	A2	386	A
2	A2	387	G
2	A2	396	A
2	A2	401	G
2	A2	407	A
2	A2	410	A
2	A2	412	G
2	A2	413	G
2	A2	431	G
2	A2	432	U
2	A2	433	A

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Mol	Chain	Res	Type
2	A2	449	C
2	A2	450	G
2	A2	452	A
2	A2	453	G
2	A2	454	U
2	A2	467	U
2	A2	468	U
2	A2	469	C
2	A2	486	C
2	A2	498	G
2	A2	499	U
2	A2	500	G
2	A2	510	A
2	A2	511	U
2	A2	658	C
2	A2	659	C
2	A2	671	G
2	A2	673	G
2	A2	674	A
2	A2	675	C
2	A2	678	G
2	A2	681	G
2	A2	692	C
2	A2	693	A
2	A2	694	C
2	A2	699	A
2	A2	703	U
2	A2	704	G
2	A2	711	C
2	A2	715	G
2	A2	738	G
2	A2	747	G
2	A2	753	A
2	A2	767	G
2	A2	770	G
2	A2	805	C
2	A2	811	G
2	A2	812	U
2	A2	814	A
2	A2	816	A
2	A2	817	G
2	A2	820	C

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Mol	Chain	Res	Type
2	A2	824	G
2	A2	839	C
2	A2	841	A
2	A2	842	A
2	A2	843	U
2	A2	844	C
2	A2	857	A
2	A2	858	A
2	A2	869	C
2	A2	870	G
2	A2	876	G
2	A2	927	C
2	A2	929	G
2	A2	933	G
2	A2	934	C
2	A2	935	C
2	A2	936	C
2	A2	937	C
2	A2	938	U
2	A2	1000	G
2	A2	1002	G
2	A2	1004	C
2	A2	1005	G
2	A2	1006	G
2	A2	1010	G
2	A2	1011	U
2	A2	1012	C
2	A2	1013	C
2	A2	1014	C
2	A2	1015	C
2	A2	1019	G
2	A2	1021	G
2	A2	1022	C
2	A2	1024	C
2	A2	1031	U
2	A2	1032	C
2	A2	1036	G
2	A2	1038	G
2	A2	1043	C
2	A2	1044	G
2	A2	1048	C
2	A2	1049	C

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Mol	Chain	Res	Type
2	A2	1053	G
2	A2	1054	G
2	A2	1065	U
2	A2	1067	A
2	A2	1070	C
2	A2	1071	G
2	A2	1079	A
2	A2	1081	G
2	A2	1082	A
2	A2	1085	C
2	A2	1086	C
2	A2	1087	G
2	A2	1094	C
2	A2	1095	G
2	A2	1098	G
2	A2	1099	U
2	A2	1101	G
2	A2	1108	A
2	A2	1109	U
2	A2	1110	G
2	A2	1116	U
2	A2	1117	A
2	A2	1118	C
2	A2	1128	C
2	A2	1136	A
2	A2	1140	A2M
2	A2	1151	A
2	A2	1159	G
2	A2	1168	A
2	A2	1172	A
2	A2	1173	G
2	A2	1179	C
2	A2	1180	G
2	A2	1181	U
2	A2	1182	C
2	A2	1190	C
2	A2	1191	G
2	A2	1197	G
2	A2	1201	A
2	A2	1208	G
2	A2	1211	A
2	A2	1212	A

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Mol	Chain	Res	Type
2	A2	1224	G
2	A2	1233	A
2	A2	1237	G
2	A2	1251	U
2	A2	1253	U
2	A2	1259	C
2	A2	1278	G
2	A2	1294	C
2	A2	1295	G
2	A2	1296	C
2	A2	1302	G
2	A2	1310	A
2	A2	1311	G
2	A2	1315	G
2	A2	1317	G
2	A2	1331	A
2	A2	1338	A
2	A2	1347	A2M
2	A2	1348	C
2	A2	1360	A
2	A2	1379	C
2	A2	1391	U
2	A2	1399	G
2	A2	1404	U
2	A2	1409	U
2	A2	1410	G
2	A2	1425	G
2	A2	1426	A
2	A2	1437	G
2	A2	1438	OMG
2	A2	1444	A
2	A2	1446	G
2	A2	1447	A
2	A2	1454	G
2	A2	1467	G
2	A2	1474	C
2	A2	1489	C
2	A2	1490	PSU
2	A2	1491	C
2	A2	1504	G
2	A2	1511	C
2	A2	1512	U

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Mol	Chain	Res	Type
2	A2	1522	C
2	A2	1523	G
2	A2	1533	C
2	A2	1536	G
2	A2	1542	C
2	A2	1544	A
2	A2	1552	G
2	A2	1555	G
2	A2	1558	U
2	A2	1559	U
2	A2	1560	G
2	A2	1575	U
2	A2	1589	A
2	A2	1605	G
2	A2	1606	A
2	A2	1608	G
2	A2	1622	C
2	A2	1623	G
2	A2	1624	U
2	A2	1638	G
2	A2	1639	A
2	A2	1644	G
2	A2	1657	G
2	A2	1671	G
2	A2	1685	G
2	A2	1694	A
2	A2	1699	A
2	A2	1718	G
2	A2	1719	A
2	A2	1721	G
2	A2	1722	C
2	A2	1723	C
2	A2	1724	G
2	A2	1727	G
2	A2	1733	C
2	A2	1734	A
2	A2	1738	C
2	A2	1747	G
2	A2	1750	G
2	A2	1761	U
2	A2	1764	A
2	A2	1821	C

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Mol	Chain	Res	Type
2	A2	1822	U
2	A2	1823	G
2	A2	1825	C
2	A2	1827	A
2	A2	1828	A
2	A2	1834	U
2	A2	1848	G
2	A2	1850	U
2	A2	1854	G
2	A2	1857	G
2	A2	1858	G
2	A2	1871	A
2	A2	1886	C
2	A2	1887	G
2	A2	1893	C
2	A2	1895	G
2	A2	1897	A
2	A2	1899	G
2	A2	1900	G
2	A2	1904	G
2	A2	1905	G
2	A2	1909	G
2	A2	1910	G
2	A2	1912	A
2	A2	2006	C
2	A2	2008	G
2	A2	2009	G
2	A2	2012	C
2	A2	2014	G
2	A2	2015	C
2	A2	2021	C
2	A2	2023	A
2	A2	2024	C
2	A2	2025	G
2	A2	2044	C
2	A2	2049	G
2	A2	2052	G
2	A2	2055	A
2	A2	2056	G
2	A2	2061	G
2	A2	2068	A
2	A2	2069	G

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Mol	Chain	Res	Type
2	A2	2071	G
2	A2	2077	G
2	A2	2087	A
2	A2	2088	G
2	A2	2094	G
2	A2	2098	G
2	A2	2100	G
2	A2	2103	G
2	A2	2104	A
2	A2	2106	OMC
2	A2	2115	A
2	A2	2150	A
2	A2	2152	G
2	A2	2153	U
2	A2	2165	C
2	A2	2166	C
2	A2	2176	G
2	A2	2177	OMC
2	A2	2180	U
2	A2	2196	C
2	A2	2197	G
2	A2	2208	A
2	A2	2224	C
2	A2	2226	G
2	A2	2229	G
2	A2	2233	C
2	A2	2239	A
2	A2	2245	U
2	A2	2249	U
2	A2	2257	G
2	A2	2259	C
2	A2	2260	C
2	A2	2262	A
2	A2	2266	A
2	A2	2267	A
2	A2	2268	A
2	A2	2275	C
2	A2	2284	A
2	A2	2285	U
2	A2	2295	C
2	A2	2299	G
2	A2	2301	G

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Mol	Chain	Res	Type
2	A2	2302	G
2	A2	2308	A
2	A2	2328	A
2	A2	2341	G
2	A2	2342	A
2	A2	2344	C
2	A2	2356	A
2	A2	2357	G
2	A2	2361	G
2	A2	2382	C
2	A2	2383	U
2	A2	2408	C
2	A2	2413	G
2	A2	2417	G
2	A2	2424	C
2	A2	2425	C
2	A2	2430	G
2	A2	2431	A
2	A2	2442	U
2	A2	2449	G
2	A2	2450	A
2	A2	2451	A
2	A2	2458	G
2	A2	2463	U
2	A2	2464	C
2	A2	2466	G
2	A2	2476	G
2	A2	2479	G
2	A2	2481	G
2	A2	2491	G
2	A2	2493	C
2	A2	2494	C
2	A2	2498	A
2	A2	2509	G
2	A2	2513	G
2	A2	2514	G
2	A2	2515	G
2	A2	2517	G
2	A2	2518	U
2	A2	2519	A
2	A2	2524	U
2	A2	2525	C

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Mol	Chain	Res	Type
2	A2	2543	U
2	A2	2545	U
2	A2	2549	C
2	A2	2561	A
2	A2	2569	C
2	A2	2582	G
2	A2	2584	U
2	A2	2601	G
2	A2	2603	G
2	A2	2610	G
2	A2	2632	G
2	A2	2652	G
2	A2	3252	A
2	A2	3253	G
2	A2	3254	C
2	A2	3271	G
2	A2	3272	U
2	A2	3282	G
2	A2	3291	A
2	A2	3300	U
2	A2	3302	A
2	A2	3304	A
2	A2	3318	A
2	A2	3328	G
2	A2	3329	C
2	A2	3334	G
2	A2	3365	U
2	A2	3366	G
2	A2	3367	A
2	A2	3368	A
2	A2	3373	A
2	A2	3380	A2M
2	A2	3383	A
2	A2	3404	A
2	A2	3406	G
2	A2	3408	C
2	A2	3413	G
2	A2	3416	A
2	A2	3420	U
2	A2	3421	G
2	A2	3426	U
2	A2	3429	U

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Mol	Chain	Res	Type
2	A2	3430	A
2	A2	3431	A
2	A2	3433	G
2	A2	3439	A
2	A2	3440	A
2	A2	3441	A2M
2	A2	3442	U
2	A2	3455	A
2	A2	3458	U
2	A2	3466	C
2	A2	3467	G
2	A2	3470	U
2	A2	3473	A
2	A2	3475	G
2	A2	3494	U
2	A2	3495	G
2	A2	3496	U
2	A2	3515	G
2	A2	3523	A
2	A2	3532	A
2	A2	3533	A
2	A2	3534	C
2	A2	3535	G
2	A2	3548	U
2	A2	3553	G
2	A2	3557	A
2	A2	3562	A
2	A2	3563	G
2	A2	3564	A
2	A2	3571	U
2	A2	3585	G
2	A2	3586	U
2	A2	3595	G
2	A2	3598	A
2	A2	3604	C
2	A2	3606	U
2	A2	3607	G
2	A2	3611	G
2	A2	3612	G
2	A2	3614	G
2	A2	3615	U
2	A2	3706	A

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Mol	Chain	Res	Type
2	A2	3707	C
2	A2	3708	U
2	A2	3709	C
2	A2	3710	U
2	A2	3712	A
2	A2	3713	U
2	A2	3726	G
2	A2	3736	G
2	A2	3740	G
2	A2	3765	G
2	A2	3766	C
2	A2	3769	C
2	A2	3771	G
2	A2	3772	G
2	A2	3777	A
2	A2	3782	U
2	A2	3784	C
2	A2	3814	C
2	A2	3815	U
2	A2	3822	A
2	A2	3828	C
2	A2	3835	G
2	A2	3836	G
2	A2	3843	G
2	A2	3855	A
2	A2	3864	A
2	A2	3874	G
2	A2	3881	U
2	A2	3885	A
2	A2	3889	C
2	A2	3894	U
2	A2	3903	A
2	A2	3906	G
2	A2	3908	A
2	A2	3909	A
2	A2	3917	U
2	A2	3920	A
2	A2	3923	A
2	A2	3924	G
2	A2	3925	A
2	A2	3933	A
2	A2	3943	G

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Mol	Chain	Res	Type
2	A2	3949	G
2	A2	3956	A
2	A2	3957	G
2	A2	3966	C
2	A2	3978	G
2	A2	3981	G
2	A2	3982	G
2	A2	3984	C
2	A2	3991	A
2	A2	4002	C
2	A2	4004	U
2	A2	4006	U
2	A2	4023	G
2	A2	4025	G
2	A2	4029	G
2	A2	4030	A
2	A2	4031	A
2	A2	4032	A
2	A2	4033	A
2	A2	4039	C
2	A2	4043	G
2	A2	4046	A
2	A2	4050	C
2	A2	4067	1MA
2	A2	4068	G
2	A2	4073	C
2	A2	4074	A
2	A2	4082	G
2	A2	4085	G
2	A2	4090	U
2	A2	4100	G
2	A2	4101	A
2	A2	4104	U
2	A2	4105	C
2	A2	4116	A
2	A2	4118	C
2	A2	4127	G
2	A2	4151	OMG
2	A2	4152	PSU
2	A2	4162	A
2	A2	4164	U
2	A2	4165	A

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Mol	Chain	Res	Type
2	A2	4171	C
2	A2	4176	G
2	A2	4177	C
2	A2	4184	U
2	A2	4200	A
2	A2	4201	G
2	A2	4212	C
2	A2	4219	G
2	A2	4225	G
2	A2	4227	G
2	A2	4242	A
2	A2	4246	U
2	A2	4252	G
2	A2	4272	OMU
2	A2	4276	A
2	A2	4278	A
2	A2	4287	A
2	A2	4288	PSU
2	A2	4289	OMG
2	A2	4304	G
2	A2	4308	A
2	A2	4309	U
2	A2	4322	C
2	A2	4324	A
2	A2	4331	G
2	A2	4346	G
2	A2	4352	A
2	A2	4360	A
2	A2	4361	U
2	A2	4382	C
2	A2	4385	C
2	A2	4386	A
2	A2	4393	A
2	A2	4394	G
2	A2	4402	G
2	A2	4403	G
2	A2	4406	G
2	A2	4409	C
2	A2	4411	C
2	A2	4413	G
2	A2	4417	G
2	A2	4422	G

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Mol	Chain	Res	Type
2	A2	4428	C
2	A2	4429	G
2	A2	4434	U
2	A2	4497	U
2	A2	4498	C
2	A2	4499	G
2	A2	4504	C
2	A2	4508	G
2	A2	4513	G
2	A2	4515	G
2	A2	4516	C
2	A2	4520	G
2	A2	4521	A
2	A2	4522	G
2	A2	4523	C
2	A2	4525	G
2	A2	4527	U
2	A2	4528	C
2	A2	4540	C
2	A2	4541	G
2	A2	4545	U
2	A2	4546	G
2	A2	4548	G
2	A2	4552	G
2	A2	4553	G
2	A2	4555	A
2	A2	4557	G
2	A2	4560	G
2	A2	4565	C
2	A2	4569	C
2	A2	4570	U
2	A2	4571	C
2	A2	4582	U
2	A2	4583	U
2	A2	4587	G
2	A2	4588	C
2	A2	4589	A
2	A2	4591	G
2	A2	4597	G
2	A2	4609	G
2	A2	4610	C
2	A2	4621	G

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Mol	Chain	Res	Type
2	A2	4622	U
2	A2	4625	A
2	A2	4634	U
2	A2	4636	C
2	A2	4637	U
2	A2	4641	U
2	A2	4659	C
2	A2	4663	G
2	A2	4668	U
2	A2	4680	A
2	A2	4687	G
2	A2	4693	C
2	A2	4696	C
2	A2	4700	C
2	A2	4701	G
2	A2	4702	A
2	A2	4707	A
2	A2	4715	U
5	B2	7	G
5	B2	33	U
5	B2	38	U
5	B2	41	G
5	B2	53	U
5	B2	54	A
5	B2	64	G
5	B2	97	G
5	B2	100	A
5	B2	110	G
5	B2	119	U
7	Bv	3	C
7	Bv	4	C
7	Bv	7	A
7	Bv	9	A
7	Bv	10	G
7	Bv	11	C
7	Bv	12	U
7	Bv	14	A
7	Bv	19	G
7	Bv	23	A
7	Bv	30	G
7	Bv	32	U
7	Bv	34	G

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Mol	Chain	Res	Type
7	Bv	35	A
7	Bv	36	A
7	Bv	44	G
7	Bv	45	U
7	Bv	46	G
7	Bv	47	C
7	Bv	48	C
7	Bv	51	U
7	Bv	52	G
7	Bv	53	G
7	Bv	54	U
7	Bv	59	U
7	Bv	62	C
7	Bv	63	G
7	Bv	64	A
8	Bx	46	U
8	Bx	49	U
8	Bx	50	U
8	Bx	52	U
11	C2	25	G
11	C2	34	U
11	C2	35	C
11	C2	51	U
11	C2	52	A
11	C2	59	A
11	C2	62	A
11	C2	63	U
11	C2	75	OMG
11	C2	82	A
11	C2	84	A
11	C2	85	U
11	C2	87	G
11	C2	94	G
11	C2	99	U
11	C2	103	A
11	C2	105	C
11	C2	106	G
11	C2	110	U
11	C2	111	U
11	C2	114	G
11	C2	123	U
11	C2	125	C

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Mol	Chain	Res	Type
11	C2	126	C
11	C2	147	G
11	C2	150	C
11	C2	151	G
11	C2	155	C
69	m2	14	C
69	m2	29	G
69	m2	33	G
69	m2	41	G
69	m2	42	A
69	m2	46	A
69	m2	49	C
69	m2	56	G
69	m2	59	U
69	m2	60	A
69	m2	61	A
69	m2	65	C
69	m2	66	G
69	m2	67	C
69	m2	68	A
69	m2	78	C
69	m2	79	A
69	m2	82	G
69	m2	99	A2M
69	m2	103	A
69	m2	113	G
69	m2	115	U
69	m2	118	C
69	m2	125	C
69	m2	126	G
69	m2	127	C
69	m2	130	G
69	m2	142	C
69	m2	143	U
69	m2	144	U
69	m2	145	G
69	m2	146	G
69	m2	149	A
69	m2	150	A
69	m2	156	G
69	m2	158	A
69	m2	159	A

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Mol	Chain	Res	Type
69	m2	160	U
69	m2	161	U
69	m2	162	C
69	m2	163	U
69	m2	170	A
69	m2	171	A
69	m2	172	OMU
69	m2	173	A
69	m2	179	C
69	m2	180	G
69	m2	181	A
69	m2	182	C
69	m2	189	U
69	m2	191	A
69	m2	193	C
69	m2	195	C
69	m2	198	U
69	m2	199	U
69	m2	200	C
69	m2	201	C
69	m2	202	C
69	m2	204	G
69	m2	207	G
69	m2	209	G
69	m2	212	U
69	m2	217	G
69	m2	293	G
69	m2	296	U
69	m2	297	C
69	m2	301	A
69	m2	306	C
69	m2	307	U
69	m2	308	C
69	m2	310	G
69	m2	311	G
69	m2	313	C
69	m2	314	G
69	m2	315	A
69	m2	316	U
69	m2	317	C
69	m2	321	C
69	m2	322	G

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Mol	Chain	Res	Type
69	m2	323	C
69	m2	324	C
69	m2	332	G
69	m2	337	G
69	m2	342	C
69	m2	345	A
69	m2	349	G
69	m2	353	G
69	m2	362	A
69	m2	364	C
69	m2	365	A
69	m2	366	A
69	m2	370	U
69	m2	372	G
69	m2	379	G
69	m2	383	C
69	m2	384	C
69	m2	385	G
69	m2	387	G
69	m2	388	C
69	m2	395	U
69	m2	396	G
69	m2	402	C
69	m2	411	C
69	m2	415	G
69	m2	440	G
69	m2	441	A
69	m2	442	G
69	m2	446	G
69	m2	450	A
69	m2	451	A
69	m2	452	C
69	m2	454	G
69	m2	466	A
69	m2	467	A
69	m2	468	G
69	m2	473	G
69	m2	474	C
69	m2	476	G
69	m2	482	G
69	m2	484	G
69	m2	487	A

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Mol	Chain	Res	Type
69	m2	489	U
69	m2	494	C
69	m2	497	U
69	m2	502	A
69	m2	504	C
69	m2	513	U
69	m2	518	A
69	m2	520	G
69	m2	525	A
69	m2	527	A
69	m2	530	A
69	m2	532	U
69	m2	534	C
69	m2	555	A
69	m2	557	A
69	m2	558	U
69	m2	559	U
69	m2	562	A
69	m2	565	G
69	m2	570	C
69	m2	575	U
69	m2	576	A
69	m2	578	A2M
69	m2	585	A
69	m2	591	G
69	m2	592	A
69	m2	593	U
69	m2	594	C
69	m2	602	G
69	m2	606	A
69	m2	607	A
69	m2	608	G
69	m2	609	U
69	m2	616	C
69	m2	617	C
69	m2	619	G
69	m2	625	G
69	m2	630	A
69	m2	631	A
69	m2	632	U
69	m2	633	U
69	m2	641	C

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Mol	Chain	Res	Type
69	m2	645	A
69	m2	646	OMG
69	m2	662	C
69	m2	670	A2M
69	m2	671	A
69	m2	673	A
69	m2	674	A
69	m2	675	G
69	m2	686	G
69	m2	803	U
69	m2	817	U
69	m2	821	G
69	m2	823	G
69	m2	824	PSU
69	m2	832	A
69	m2	837	C
69	m2	839	A
69	m2	840	G
69	m2	842	C
69	m2	843	G
69	m2	845	C
69	m2	847	G
69	m2	849	A
69	m2	870	G
69	m2	871	A
69	m2	872	A
69	m2	875	G
69	m2	880	G
69	m2	882	G
69	m2	888	A
69	m2	889	U
69	m2	890	U
69	m2	891	U
69	m2	892	U
69	m2	893	G
69	m2	894	U
69	m2	898	U
69	m2	900	U
69	m2	902	C
69	m2	906	A
69	m2	912	G
69	m2	913	C

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Mol	Chain	Res	Type
69	m2	915	A
69	m2	916	U
69	m2	918	A
69	m2	921	A
69	m2	922	A
69	m2	932	C
69	m2	935	G
69	m2	936	G
69	m2	945	U
69	m2	958	G
69	m2	965	A
69	m2	973	G
69	m2	980	G
69	m2	992	A
69	m2	994	A
69	m2	1001	G
69	m2	1003	A
69	m2	1019	U
69	m2	1025	A
69	m2	1029	A
69	m2	1030	A
69	m2	1047	U
69	m2	1063	U
69	m2	1064	A
69	m2	1082	A
69	m2	1085	A
69	m2	1087	C
69	m2	1091	G
69	m2	1111	C
69	m2	1115	A
69	m2	1117	U
69	m2	1118	C
69	m2	1123	G
69	m2	1132	G
69	m2	1135	A
69	m2	1140	C
69	m2	1150	A
69	m2	1151	A
69	m2	1155	C
69	m2	1156	U
69	m2	1172	A
69	m2	1184	A

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Mol	Chain	Res	Type
69	m2	1185	A
69	m2	1196	A
69	m2	1197	A
69	m2	1209	G
69	m2	1210	A
69	m2	1217	C
69	m2	1218	C
69	m2	1219	A
69	m2	1225	A
69	m2	1226	G
69	m2	1229	G
69	m2	1233	C
69	m2	1244	U
69	m2	1245	PSU
69	m2	1252	A
69	m2	1253	A
69	m2	1255	A
69	m2	1258	G
69	m2	1259	G
69	m2	1261	A
69	m2	1268	C
69	m2	1273	C
69	m2	1275	C
69	m2	1276	G
69	m2	1285	C
69	m2	1289	A
69	m2	1290	U
69	m2	1302	U
69	m2	1304	G
69	m2	1305	C
69	m2	1306	U
69	m2	1308	U
69	m2	1310	U
69	m2	1315	A
69	m2	1316	U
69	m2	1317	U
69	m2	1338	C
69	m2	1340	G
69	m2	1345	U
69	m2	1346	A
69	m2	1350	G
69	m2	1358	G

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Mol	Chain	Res	Type
69	m2	1360	U
69	m2	1366	U
69	m2	1373	U
69	m2	1374	U
69	m2	1380	A
69	m2	1383	G
69	m2	1384	A
69	m2	1399	U
69	m2	1400	G
69	m2	1403	A
69	m2	1412	C
69	m2	1416	A
69	m2	1417	C
69	m2	1419	C
69	m2	1420	C
69	m2	1421	C
69	m2	1423	A
69	m2	1425	C
69	m2	1448	A
69	m2	1454	A
69	m2	1456	A
69	m2	1465	U
69	m2	1466	C
69	m2	1468	G
69	m2	1470	C
69	m2	1482	A
69	m2	1491	A
69	m2	1492	G
69	m2	1497	G
69	m2	1499	G
69	m2	1500	A
69	m2	1511	U
69	m2	1512	G
69	m2	1514	C
69	m2	1515	C
69	m2	1522	G
69	m2	1523	C
69	m2	1524	A
69	m2	1530	G
69	m2	1532	U
69	m2	1533	A
69	m2	1535	A

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Mol	Chain	Res	Type
69	m2	1546	C
69	m2	1547	A
69	m2	1559	C
69	m2	1572	G
69	m2	1577	G
69	m2	1581	A
69	m2	1582	A
69	m2	1590	A
69	m2	1603	A
69	m2	1606	G
69	m2	1608	G
69	m2	1623	U
69	m2	1625	A
69	m2	1627	U
69	m2	1628	C
69	m2	1634	G
69	m2	1635	A
69	m2	1636	A
69	m2	1641	G
69	m2	1642	A
69	m2	1645	U
69	m2	1648	C
69	m2	1649	A
69	m2	1650	G
69	m2	1656	G
69	m2	1664	U
69	m2	1665	A
69	m2	1666	A
69	m2	1667	G
69	m2	1688	G
69	m2	1697	A
69	m2	1698	C
69	m2	1700	C
69	m2	1703	C
69	m2	1707	C
69	m2	1717	A
69	m2	1723	G
69	m2	1724	G
69	m2	1726	A
69	m2	1729	G
69	m2	1746	G
69	m2	1788	U

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Mol	Chain	Res	Type
69	m2	1813	C
69	m2	1815	A
69	m2	1817	A
69	m2	1824	A
69	m2	1826	A
69	m2	1827	A
69	m2	1828	G
69	m2	1831	G
69	m2	1837	A
69	m2	1840	U
69	m2	1851	G
69	m2	1853	A
69	m2	1854	C
69	m2	1863	G
69	m2	1864	G
69	m2	1865	A
69	m2	1866	U
69	m2	1867	C
70	n2	8	U
70	n2	17	G
70	n2	18	G
70	n2	45	G
70	n2	55	C
70	n2	56	G
70	n2	69	G
70	n2	75	A

All (13) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	A2	236	G
2	A2	406	C
2	A2	1446	G
2	A2	1721	G
2	A2	2382	C
2	A2	2430	G
2	A2	2463	U
2	A2	3253	G
2	A2	3532	A
2	A2	3614	G
2	A2	4277	C
2	A2	4351	U

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Mol	Chain	Res	Type
2	A2	4582	U

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	5MC	A2	4099	2	18,22,23	0.47	0	26,32,35	0.61	0
2	OMC	A2	2559	2	19,22,23	0.42	0	26,31,34	0.38	0
69	A2M	m2	578	69	22,25,26	0.10	0	31,36,39	0.27	0
2	PSU	A2	3371	2	18,21,22	0.61	0	22,30,33	0.57	0
2	OMC	A2	2106	2	19,22,23	0.36	0	26,31,34	0.40	0
2	1MA	A2	4067	2	21,25,26	0.41	0	31,37,40	0.45	0
2	OMC	A2	3525	2	19,22,23	0.38	0	26,31,34	0.41	0
69	PSU	m2	824	69	18,21,22	0.58	0	22,30,33	0.64	1 (4%)
2	PSU	A2	3945	2	18,21,22	0.61	0	22,30,33	0.60	0
69	OMU	m2	172	69	19,22,23	0.29	0	26,31,34	0.58	1 (3%)
2	OMU	A2	4272	2	19,22,23	0.48	0	26,31,34	0.68	0
2	PSU	A2	4094	2	18,21,22	0.67	1 (5%)	22,30,33	0.58	0
69	A2M	m2	1680	69	22,25,26	0.16	0	31,36,39	0.23	0
2	A2M	A2	398	2	22,25,26	0.14	0	31,36,39	0.36	0
2	OMG	A2	3400	2	23,26,27	0.40	0	33,38,41	0.37	0
69	OMG	m2	646	69	23,26,27	0.49	0	33,38,41	0.39	0
2	OMG	A2	1438	2	23,26,27	0.34	0	33,38,41	0.39	0
69	OMG	m2	603	69	23,26,27	0.43	0	33,38,41	0.32	0
69	PSU	m2	614	69	18,21,22	0.60	1 (5%)	22,30,33	0.63	1 (4%)
69	B8T	m2	1339	69	19,22,23	0.48	0	26,31,34	0.42	0
69	PSU	m2	825	69	18,21,22	0.57	0	22,30,33	0.61	1 (4%)
2	OMC	A2	2579	2	19,22,23	0.39	0	26,31,34	0.42	0
2	OMC	A2	3543	2	19,22,23	0.38	0	26,31,34	0.46	0
2	PSU	A2	1395	2	18,21,22	0.73	1 (5%)	22,30,33	0.53	0
2	OMG	A2	3555	2,83	23,26,27	0.49	0	33,38,41	0.51	0
2	A2M	A2	3481	2	22,25,26	0.15	0	31,36,39	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	A2M	A2	1337	2	22,25,26	0.21	0	31,36,39	0.52	0
2	PSU	A2	1490	2	18,21,22	0.75	1 (5%)	22,30,33	0.42	0
69	OMG	m2	685	69	23,26,27	0.49	0	33,38,41	0.44	0
69	OMG	m2	511	69,83	23,26,27	0.35	0	33,38,41	0.43	0
2	A2M	A2	1347	2,83	22,25,26	0.13	0	31,36,39	0.53	0
2	OMC	A2	3357	2	19,22,23	0.34	0	26,31,34	0.49	0
2	OMC	A2	3464	2	19,22,23	0.37	0	26,31,34	0.40	0
2	A2M	A2	3374	2	22,25,26	0.15	0	31,36,39	0.37	0
2	OMU	A2	4150	2	19,22,23	0.34	0	26,31,34	0.50	0
2	OMG	A2	4044	2	23,26,27	0.45	0	33,38,41	0.35	0
69	OMU	m2	116	69	19,22,23	0.33	0	26,31,34	0.43	0
2	OMG	A2	2119	2	23,26,27	0.47	0	33,38,41	0.44	0
2	OMU	A2	3581	2	19,22,23	0.41	0	26,31,34	0.62	0
2	PSU	A2	4152	2	18,21,22	0.58	0	22,30,33	0.63	0
2	OMU	A2	2592	2	19,22,23	0.39	0	26,31,34	0.63	0
2	PSU	A2	2263	2	18,21,22	0.66	0	22,30,33	0.56	0
2	OMG	A2	1130	2	23,26,27	0.52	0	33,38,41	0.60	1 (3%)
2	OMC	A2	2120	2	19,22,23	0.40	0	26,31,34	0.48	0
69	OMC	m2	355	69	19,22,23	0.37	0	26,31,34	0.41	0
2	A2M	A2	4223	2	22,25,26	0.14	0	31,36,39	0.18	0
69	A2M	m2	27	69	22,25,26	0.20	0	31,36,39	0.30	0
69	A2M	m2	486	69	22,25,26	0.12	0	31,36,39	0.28	0
2	A2M	A2	1140	2	22,25,26	0.15	0	31,36,39	0.25	0
2	A2M	A2	3441	2	22,25,26	0.16	0	31,36,39	0.35	0
2	OMU	A2	3474	2	19,22,23	0.38	0	26,31,34	0.38	0
2	PSU	A2	4280	2	18,21,22	0.63	1 (5%)	22,30,33	0.57	0
2	PSU	A2	3385	2	18,21,22	0.63	0	22,30,33	0.56	0
69	OMC	m2	519	69	19,22,23	0.35	0	26,31,34	0.49	0
2	A2M	A2	2542	2	22,25,26	0.19	0	31,36,39	0.30	0
69	OMU	m2	121	69	19,22,23	0.37	0	26,31,34	0.48	0
2	OMG	A2	4275	2	23,26,27	0.46	0	33,38,41	0.52	0
2	PSU	A2	4183	2	18,21,22	0.63	0	22,30,33	0.42	0
2	5MC	A2	3438	2,83	18,22,23	0.39	0	26,32,35	0.45	0
2	OMG	A2	4289	2	23,26,27	0.47	0	33,38,41	0.40	0
2	OMC	A2	4188	2	19,22,23	0.42	0	26,31,34	0.53	0
2	OMC	A2	1683	2,83	19,22,23	0.42	0	26,31,34	0.63	0
2	OMC	A2	3497	2	19,22,23	0.40	0	26,31,34	0.36	0
69	OMU	m2	430	69	19,22,23	0.32	0	26,31,34	0.47	0
2	OMG	A2	3283	2	23,26,27	0.43	0	33,38,41	0.53	0
2	PSU	A2	4288	2	18,21,22	0.61	0	22,30,33	0.60	0
2	A2M	A2	4175	2,83	22,25,26	0.19	0	31,36,39	0.44	0
69	PSU	m2	1083	69	18,21,22	0.65	1 (5%)	22,30,33	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	A2M	A2	2156	2	22,25,26	0.18	0	31,36,39	0.21	0
2	OMC	A2	1154	2	19,22,23	0.40	0	26,31,34	0.57	0
2	A2M	A2	1137	2	22,25,26	0.13	0	31,36,39	0.26	0
69	A2M	m2	1033	69	22,25,26	0.18	0	31,36,39	0.29	0
69	OMG	m2	438	69	23,26,27	0.43	0	33,38,41	0.39	0
69	OMC	m2	1705	69	19,22,23	0.34	0	26,31,34	0.47	0
2	OMG	A2	3880	2	23,26,27	0.38	0	33,38,41	0.49	0
69	A2M	m2	670	69,83	22,25,26	0.21	0	31,36,39	0.29	0
2	A2M	A2	2118	2,83	22,25,26	0.16	0	31,36,39	0.24	0
2	PSU	A2	4055	2	18,21,22	0.69	1 (5%)	22,30,33	0.59	1 (4%)
2	OMG	A2	2179	2	23,26,27	0.42	0	33,38,41	0.40	0
2	A2M	A2	3380	2	22,25,26	0.13	0	31,36,39	0.31	0
2	OMG	A2	4022	2	23,26,27	0.46	0	33,38,41	0.39	0
2	OMG	A2	1335	2	23,26,27	0.45	0	33,38,41	0.40	0
2	A2M	A2	3486	2	22,25,26	0.17	0	31,36,39	0.44	0
2	OMC	A2	4108	2	19,22,23	0.40	0	26,31,34	0.39	0
2	OMC	A2	2177	2,83	19,22,23	0.39	0	26,31,34	0.38	0
2	OMG	A2	4151	2	23,26,27	0.40	0	33,38,41	0.46	0
69	PSU	m2	1245	69	18,21,22	0.65	0	22,30,33	0.58	0
2	A2M	A2	2570	2	22,25,26	0.19	0	31,36,39	0.26	0
2	OMC	A2	2616	2	19,22,23	0.35	0	26,31,34	0.42	0
2	OMU	A2	3958	2	19,22,23	0.40	0	26,31,34	0.53	0
2	PSU	A2	4102	2,83	18,21,22	0.68	1 (5%)	22,30,33	0.38	0
69	OMG	m2	869	69	23,26,27	0.35	0	33,38,41	0.34	0
2	OMG	A2	3448	2	23,26,27	0.42	0	33,38,41	0.32	0
69	A2M	m2	99	69,83	22,25,26	0.15	0	31,36,39	0.40	0
2	OMG	A2	4146	2	23,26,27	0.44	0	33,38,41	0.40	0
69	OMC	m2	174	69	19,22,23	0.38	0	26,31,34	0.52	0
69	UR3	m2	1832	69,83	19,22,23	0.41	0	26,32,35	0.37	0
2	A2M	A2	4270	2	22,25,26	0.20	0	31,36,39	0.50	1 (3%)
11	OMG	C2	75	11	23,26,27	0.44	0	33,38,41	0.37	0
2	A2M	A2	1673	2	22,25,26	0.18	0	31,36,39	0.41	0
2	OMG	A2	3848	2	23,26,27	0.43	0	33,38,41	0.43	0
69	OMG	m2	1330	69	23,26,27	0.39	0	33,38,41	0.39	0
69	A2M	m2	514	69	22,25,26	0.16	0	31,36,39	0.26	0
2	2MG	A2	1330	2	23,26,27	0.46	0	32,38,41	0.41	0
2	PSU	A2	1496	2	18,21,22	0.66	0	22,30,33	0.67	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5MC	A2	4099	2	-	3/7/25/26	0/2/2/2
2	OMC	A2	2559	2	-	0/9/27/28	0/2/2/2
69	A2M	m2	578	69	-	2/9/27/28	0/3/3/3
2	PSU	A2	3371	2	-	0/7/25/26	0/2/2/2
2	OMC	A2	2106	2	-	2/9/27/28	0/2/2/2
2	1MA	A2	4067	2	-	2/7/25/26	0/3/3/3
2	OMC	A2	3525	2	-	0/9/27/28	0/2/2/2
69	PSU	m2	824	69	-	0/7/25/26	0/2/2/2
2	PSU	A2	3945	2	-	0/7/25/26	0/2/2/2
69	OMU	m2	172	69	-	3/9/27/28	0/2/2/2
2	OMU	A2	4272	2	-	3/9/27/28	0/2/2/2
2	PSU	A2	4094	2	-	0/7/25/26	0/2/2/2
69	A2M	m2	1680	69	-	1/9/27/28	0/3/3/3
2	A2M	A2	398	2	-	2/9/27/28	0/3/3/3
2	OMG	A2	3400	2	-	0/9/27/28	0/3/3/3
69	OMG	m2	646	69	-	3/9/27/28	0/3/3/3
2	OMG	A2	1438	2	-	1/9/27/28	0/3/3/3
69	OMG	m2	603	69	-	0/9/27/28	0/3/3/3
69	PSU	m2	614	69	-	0/7/25/26	0/2/2/2
69	B8T	m2	1339	69	-	2/7/27/28	0/2/2/2
69	PSU	m2	825	69	-	0/7/25/26	0/2/2/2
2	OMC	A2	2579	2	-	1/9/27/28	0/2/2/2
2	OMC	A2	3543	2	-	1/9/27/28	0/2/2/2
2	PSU	A2	1395	2	-	0/7/25/26	0/2/2/2
2	OMG	A2	3555	2,83	-	0/9/27/28	0/3/3/3
2	A2M	A2	3481	2	-	0/9/27/28	0/3/3/3
2	A2M	A2	1337	2	-	1/9/27/28	0/3/3/3
2	PSU	A2	1490	2	-	4/7/25/26	0/2/2/2
69	OMG	m2	685	69	-	0/9/27/28	0/3/3/3
69	OMG	m2	511	69,83	-	0/9/27/28	0/3/3/3
2	A2M	A2	1347	2,83	-	3/9/27/28	0/3/3/3
2	OMC	A2	3357	2	-	4/9/27/28	0/2/2/2
2	OMC	A2	3464	2	-	0/9/27/28	0/2/2/2
2	A2M	A2	3374	2	-	0/9/27/28	0/3/3/3
2	OMU	A2	4150	2	-	0/9/27/28	0/2/2/2
2	OMG	A2	4044	2	-	0/9/27/28	0/3/3/3
69	OMU	m2	116	69	-	0/9/27/28	0/2/2/2
2	OMG	A2	2119	2	-	2/9/27/28	0/3/3/3
2	OMU	A2	3581	2	-	0/9/27/28	0/2/2/2
2	PSU	A2	4152	2	-	1/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMU	A2	2592	2	-	0/9/27/28	0/2/2/2
2	PSU	A2	2263	2	-	0/7/25/26	0/2/2/2
2	OMG	A2	1130	2	-	0/9/27/28	0/3/3/3
2	OMC	A2	2120	2	-	1/9/27/28	0/2/2/2
69	OMC	m2	355	69	-	1/9/27/28	0/2/2/2
2	A2M	A2	4223	2	-	0/9/27/28	0/3/3/3
69	A2M	m2	27	69	-	3/9/27/28	0/3/3/3
69	A2M	m2	486	69	-	0/9/27/28	0/3/3/3
2	A2M	A2	1140	2	-	3/9/27/28	0/3/3/3
2	A2M	A2	3441	2	-	5/9/27/28	0/3/3/3
2	OMU	A2	3474	2	-	2/9/27/28	0/2/2/2
2	PSU	A2	4280	2	-	2/7/25/26	0/2/2/2
2	PSU	A2	3385	2	-	0/7/25/26	0/2/2/2
69	OMC	m2	519	69	-	2/9/27/28	0/2/2/2
2	A2M	A2	2542	2	-	3/9/27/28	0/3/3/3
69	OMU	m2	121	69	-	0/9/27/28	0/2/2/2
2	OMG	A2	4275	2	-	0/9/27/28	0/3/3/3
2	PSU	A2	4183	2	-	2/7/25/26	0/2/2/2
2	5MC	A2	3438	2,83	-	0/7/25/26	0/2/2/2
2	OMG	A2	4289	2	-	3/9/27/28	0/3/3/3
2	OMC	A2	4188	2	-	0/9/27/28	0/2/2/2
2	OMC	A2	1683	2,83	-	0/9/27/28	0/2/2/2
2	OMC	A2	3497	2	-	1/9/27/28	0/2/2/2
69	OMU	m2	430	69	-	4/9/27/28	0/2/2/2
2	OMG	A2	3283	2	-	0/9/27/28	0/3/3/3
2	PSU	A2	4288	2	-	5/7/25/26	0/2/2/2
2	A2M	A2	4175	2,83	-	1/9/27/28	0/3/3/3
69	PSU	m2	1083	69	-	1/7/25/26	0/2/2/2
2	A2M	A2	2156	2	-	0/9/27/28	0/3/3/3
2	OMC	A2	1154	2	-	0/9/27/28	0/2/2/2
2	A2M	A2	1137	2	-	2/9/27/28	0/3/3/3
69	A2M	m2	1033	69	-	0/9/27/28	0/3/3/3
69	OMG	m2	438	69	-	0/9/27/28	0/3/3/3
69	OMC	m2	1705	69	-	0/9/27/28	0/2/2/2
2	OMG	A2	3880	2	-	1/9/27/28	0/3/3/3
69	A2M	m2	670	69,83	-	1/9/27/28	0/3/3/3
2	A2M	A2	2118	2,83	-	0/9/27/28	0/3/3/3
2	PSU	A2	4055	2	-	0/7/25/26	0/2/2/2
2	OMG	A2	2179	2	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A2M	A2	3380	2	-	2/9/27/28	0/3/3/3
2	OMG	A2	4022	2	-	0/9/27/28	0/3/3/3
2	OMG	A2	1335	2	-	0/9/27/28	0/3/3/3
2	A2M	A2	3486	2	-	0/9/27/28	0/3/3/3
2	OMC	A2	4108	2	-	0/9/27/28	0/2/2/2
2	OMC	A2	2177	2,83	-	2/9/27/28	0/2/2/2
2	OMG	A2	4151	2	-	0/9/27/28	0/3/3/3
69	PSU	m2	1245	69	-	2/7/25/26	0/2/2/2
2	A2M	A2	2570	2	-	0/9/27/28	0/3/3/3
2	OMC	A2	2616	2	-	0/9/27/28	0/2/2/2
2	OMU	A2	3958	2	-	1/9/27/28	0/2/2/2
2	PSU	A2	4102	2,83	-	1/7/25/26	0/2/2/2
69	OMG	m2	869	69	-	0/9/27/28	0/3/3/3
2	OMG	A2	3448	2	-	0/9/27/28	0/3/3/3
69	A2M	m2	99	69,83	-	3/9/27/28	0/3/3/3
2	OMG	A2	4146	2	-	0/9/27/28	0/3/3/3
69	OMC	m2	174	69	-	2/9/27/28	0/2/2/2
69	UR3	m2	1832	69,83	-	0/7/25/26	0/2/2/2
2	A2M	A2	4270	2	-	0/9/27/28	0/3/3/3
11	OMG	C2	75	11	-	2/9/27/28	0/3/3/3
2	A2M	A2	1673	2	-	0/9/27/28	0/3/3/3
2	OMG	A2	3848	2	-	0/9/27/28	0/3/3/3
69	OMG	m2	1330	69	-	0/9/27/28	0/3/3/3
69	A2M	m2	514	69	-	0/9/27/28	0/3/3/3
2	2MG	A2	1330	2	-	0/9/27/28	0/3/3/3
2	PSU	A2	1496	2	-	0/7/25/26	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A2	1490	PSU	O4'-C1'	-2.27	1.40	1.43
69	m2	1083	PSU	O4'-C1'	-2.27	1.40	1.43
2	A2	1395	PSU	O4'-C1'	-2.15	1.40	1.43
2	A2	4094	PSU	O4'-C1'	-2.15	1.40	1.43
2	A2	4102	PSU	O4'-C1'	-2.13	1.40	1.43
69	m2	614	PSU	O4'-C1'	-2.11	1.40	1.43
2	A2	4055	PSU	O4'-C1'	-2.10	1.40	1.43
2	A2	4280	PSU	O4'-C1'	-2.05	1.41	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
69	m2	614	PSU	O4'-C1'-C2'	2.21	108.26	105.14
69	m2	172	OMU	O2'-C2'-C1'	2.18	113.33	109.08
2	A2	4270	A2M	C2'-C3'-C4'	-2.17	97.28	101.99
69	m2	824	PSU	O4'-C1'-C2'	2.09	108.10	105.14
69	m2	825	PSU	O4'-C1'-C2'	2.05	108.04	105.14
2	A2	4055	PSU	O4'-C1'-C2'	2.01	107.98	105.14
2	A2	1130	OMG	C2'-C1'-N9	-2.00	110.33	114.22

There are no chirality outliers.

All (100) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	C2	75	OMG	O4'-C4'-C5'-O5'
11	C2	75	OMG	C3'-C4'-C5'-O5'
2	A2	398	A2M	C1'-C2'-O2'-CM'
2	A2	1140	A2M	O4'-C4'-C5'-O5'
2	A2	1140	A2M	C3'-C4'-C5'-O5'
2	A2	1347	A2M	C4'-C5'-O5'-P
2	A2	1347	A2M	O4'-C4'-C5'-O5'
2	A2	1347	A2M	C3'-C4'-C5'-O5'
2	A2	1490	PSU	C2'-C1'-C5-C4
2	A2	2106	OMC	C1'-C2'-O2'-CM2
2	A2	2177	OMC	C1'-C2'-O2'-CM2
2	A2	2179	OMG	C1'-C2'-O2'-CM2
2	A2	2579	OMC	C1'-C2'-O2'-CM2
2	A2	3357	OMC	C2'-C1'-N1-C2
2	A2	3357	OMC	C2'-C1'-N1-C6
2	A2	3380	A2M	O4'-C4'-C5'-O5'
2	A2	3380	A2M	C3'-C4'-C5'-O5'
2	A2	3497	OMC	C1'-C2'-O2'-CM2
2	A2	4175	A2M	C1'-C2'-O2'-CM'
2	A2	4183	PSU	O4'-C1'-C5-C4
2	A2	4183	PSU	O4'-C1'-C5-C6
2	A2	4272	OMU	C1'-C2'-O2'-CM2
2	A2	4272	OMU	O4'-C4'-C5'-O5'
2	A2	4288	PSU	C2'-C1'-C5-C4
2	A2	4288	PSU	C2'-C1'-C5-C6
2	A2	4288	PSU	C3'-C4'-C5'-O5'
2	A2	4289	OMG	O4'-C4'-C5'-O5'
2	A2	4289	OMG	C1'-C2'-O2'-CM2
69	m2	172	OMU	C1'-C2'-O2'-CM2
69	m2	174	OMC	O4'-C1'-N1-C2
69	m2	174	OMC	O4'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
69	m2	355	OMC	C1'-C2'-O2'-CM2
69	m2	430	OMU	C2'-C1'-N1-C2
69	m2	430	OMU	C2'-C1'-N1-C6
69	m2	646	OMG	C3'-C4'-C5'-O5'
2	A2	3441	A2M	O4'-C4'-C5'-O5'
2	A2	4272	OMU	C3'-C4'-C5'-O5'
2	A2	4289	OMG	C3'-C4'-C5'-O5'
2	A2	4067	1MA	O4'-C4'-C5'-O5'
2	A2	4067	1MA	C3'-C4'-C5'-O5'
2	A2	4288	PSU	O4'-C4'-C5'-O5'
69	m2	1245	PSU	O4'-C4'-C5'-O5'
2	A2	3880	OMG	C3'-C2'-O2'-CM2
69	m2	27	A2M	C3'-C4'-C5'-O5'
2	A2	4152	PSU	C4'-C5'-O5'-P
2	A2	1137	A2M	O4'-C4'-C5'-O5'
2	A2	1490	PSU	O4'-C4'-C5'-O5'
69	m2	519	OMC	O4'-C4'-C5'-O5'
69	m2	646	OMG	O4'-C4'-C5'-O5'
69	m2	1245	PSU	C3'-C4'-C5'-O5'
69	m2	519	OMC	C3'-C4'-C5'-O5'
69	m2	578	A2M	C4'-C5'-O5'-P
69	m2	27	A2M	O4'-C4'-C5'-O5'
2	A2	2119	OMG	O4'-C4'-C5'-O5'
69	m2	172	OMU	C4'-C5'-O5'-P
69	m2	646	OMG	C4'-C5'-O5'-P
2	A2	1490	PSU	C3'-C4'-C5'-O5'
2	A2	3441	A2M	C3'-C4'-C5'-O5'
2	A2	2542	A2M	C2'-C1'-N9-C8
2	A2	3441	A2M	C2'-C1'-N9-C8
69	m2	1339	B8T	C3'-C4'-C5'-O5'
2	A2	3474	OMU	C4'-C5'-O5'-P
2	A2	3543	OMC	C4'-C5'-O5'-P
2	A2	3357	OMC	O4'-C1'-N1-C6
69	m2	430	OMU	O4'-C1'-N1-C6
2	A2	1140	A2M	C4'-C5'-O5'-P
2	A2	1137	A2M	C3'-C4'-C5'-O5'
69	m2	670	A2M	O4'-C4'-C5'-O5'
2	A2	1490	PSU	O4'-C1'-C5-C4
2	A2	4102	PSU	O4'-C1'-C5-C4
2	A2	4280	PSU	O4'-C1'-C5-C4
2	A2	1438	OMG	C3'-C2'-O2'-CM2
2	A2	3441	A2M	C3'-C2'-O2'-CM'

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Mol	Chain	Res	Type	Atoms
2	A2	4099	5MC	O4'-C1'-N1-C6
2	A2	2177	OMC	O4'-C4'-C5'-O5'
2	A2	3357	OMC	O4'-C1'-N1-C2
2	A2	4099	5MC	C2'-C1'-N1-C6
2	A2	398	A2M	O4'-C4'-C5'-O5'
69	m2	99	A2M	O4'-C4'-C5'-O5'
2	A2	4099	5MC	O4'-C1'-N1-C2
2	A2	3958	OMU	C1'-C2'-O2'-CM2
69	m2	99	A2M	C1'-C2'-O2'-CM'
69	m2	1680	A2M	C1'-C2'-O2'-CM'
69	m2	27	A2M	C3'-C2'-O2'-CM'
2	A2	1337	A2M	O4'-C1'-N9-C8
2	A2	3441	A2M	O4'-C1'-N9-C8
2	A2	4280	PSU	O4'-C1'-C5-C6
2	A2	4288	PSU	O4'-C1'-C5-C6
69	m2	430	OMU	O4'-C1'-N1-C2
69	m2	1083	PSU	C4'-C5'-O5'-P
2	A2	2542	A2M	O4'-C1'-N9-C8
2	A2	2106	OMC	O4'-C4'-C5'-O5'
2	A2	2119	OMG	C3'-C4'-C5'-O5'
69	m2	172	OMU	O4'-C4'-C5'-O5'
2	A2	2120	OMC	C3'-C2'-O2'-CM2
2	A2	3474	OMU	C3'-C2'-O2'-CM2
69	m2	1339	B8T	O4'-C4'-C5'-O5'
69	m2	99	A2M	C4'-C5'-O5'-P
69	m2	578	A2M	C3'-C4'-C5'-O5'
2	A2	2542	A2M	C2'-C1'-N9-C4

There are no ring outliers.

46 monomers are involved in 64 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A2	4099	5MC	2	0
69	m2	578	A2M	2	0
2	A2	2106	OMC	1	0
2	A2	4067	1MA	1	0
69	m2	824	PSU	1	0
69	m2	172	OMU	1	0
2	A2	398	A2M	2	0
69	m2	646	OMG	1	0
69	m2	603	OMG	3	0
69	m2	825	PSU	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A2	2579	OMC	1	0
2	A2	3543	OMC	1	0
2	A2	1490	PSU	1	0
69	m2	511	OMG	3	0
2	A2	3374	A2M	1	0
2	A2	4044	OMG	2	0
69	m2	116	OMU	3	0
2	A2	2119	OMG	1	0
2	A2	4152	PSU	1	0
69	m2	355	OMC	1	0
69	m2	486	A2M	2	0
2	A2	1140	A2M	1	0
2	A2	3441	A2M	1	0
69	m2	519	OMC	1	0
69	m2	121	OMU	3	0
2	A2	4275	OMG	1	0
2	A2	1683	OMC	1	0
2	A2	4288	PSU	1	0
2	A2	1154	OMC	2	0
69	m2	1033	A2M	1	0
69	m2	1705	OMC	2	0
2	A2	2118	A2M	1	0
2	A2	2179	OMG	2	0
2	A2	3380	A2M	1	0
2	A2	4108	OMC	1	0
2	A2	2177	OMC	1	0
2	A2	2570	A2M	2	0
2	A2	3958	OMU	1	0
69	m2	869	OMG	2	0
69	m2	99	A2M	1	0
2	A2	4146	OMG	1	0
69	m2	174	OMC	1	0
2	A2	1673	A2M	2	0
2	A2	3848	OMG	1	0
69	m2	514	A2M	3	0
2	A2	1330	2MG	1	0

## 5.5 Carbohydrates

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 131 ligands modelled in this entry, 129 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
85	B8N	m2	1935	69	24,29,30	0.69	1 (4%)	29,42,45	0.66	1 (3%)
86	4AC	m2	1936	69	21,24,25	0.39	0	29,34,37	0.36	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	B8N	m2	1935	69	-	4/16/34/35	0/2/2/2
86	4AC	m2	1936	69	-	0/11/29/30	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	m2	1935	B8N	O4'-C1'	-2.09	1.40	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	m2	1935	B8N	O4'-C1'-C2'	2.03	108.01	105.14

There are no chirality outliers.

All (4) torsion outliers are listed below:

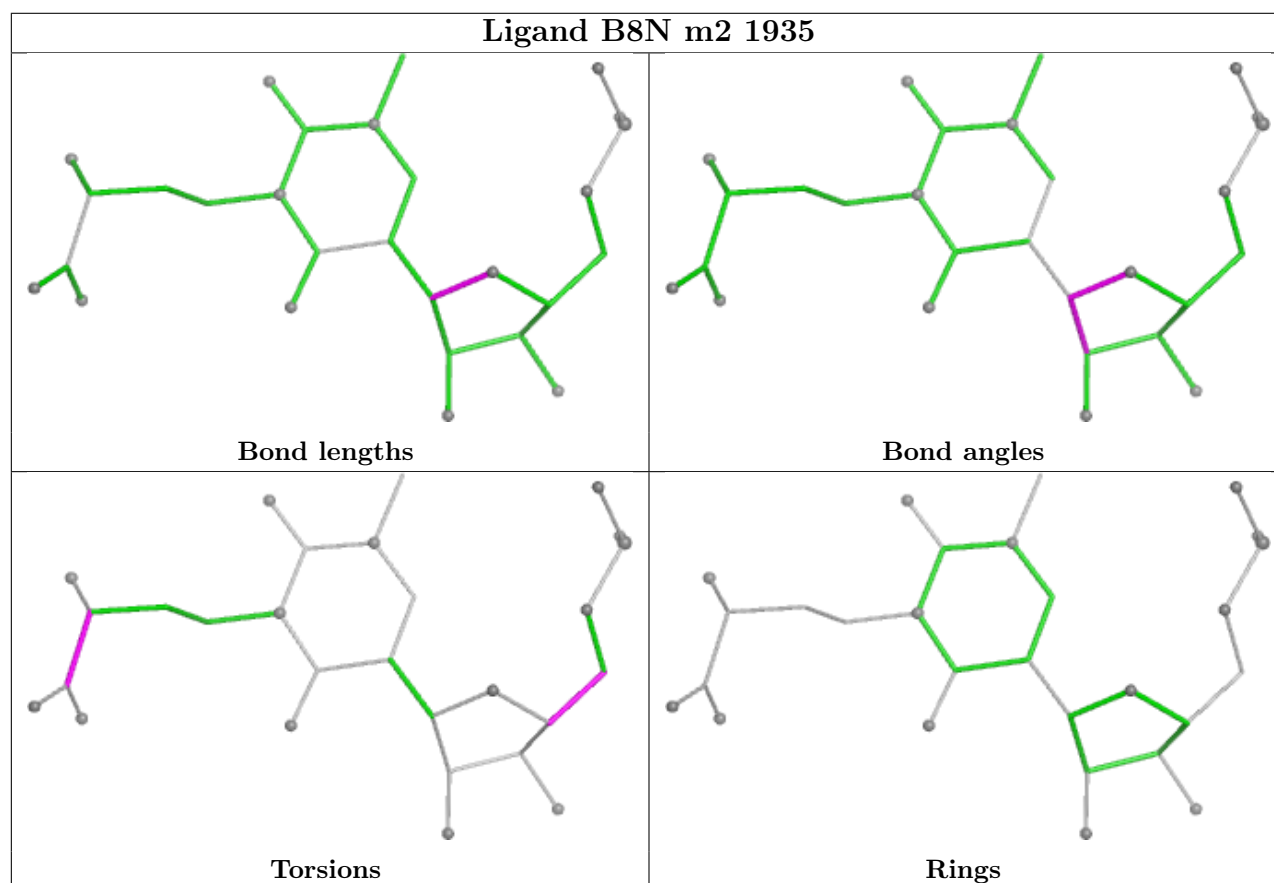
Mol	Chain	Res	Type	Atoms
85	m2	1935	B8N	O4'-C4'-C5'-O5'
85	m2	1935	B8N	C3'-C4'-C5'-O5'
85	m2	1935	B8N	N34-C33-C34-O36
85	m2	1935	B8N	N34-C33-C34-O35

There are no ring outliers.

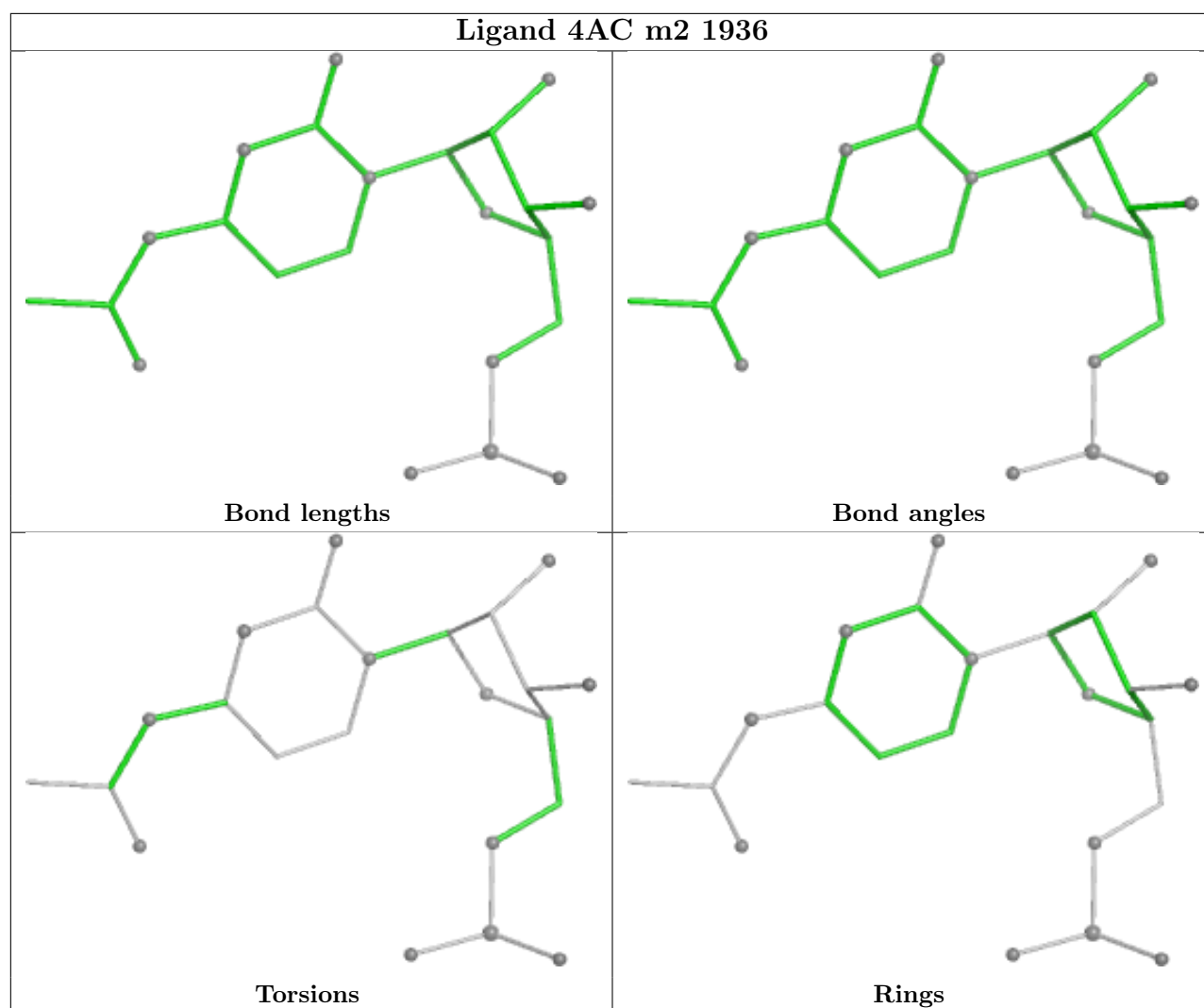
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
85	m2	1935	B8N	1	0
86	m2	1936	4AC	2	0

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







## 5.7 Other polymers [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
2	A2	15
69	m2	8
70	n2	2
51	T3	1
32	K2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	m2	130:G	O3'	141:A	P	26.12
1	A2	1512:U	O3'	1521:A	P	25.45
1	m2	690:U	O3'	801:U	P	17.62
1	A2	4437:C	O3'	4493:G	P	17.51
1	m2	536:G	O3'	554:U	P	16.80
1	A2	770:G	O3'	799:C	P	16.52
1	A2	859:G	O3'	866:A	P	16.11
1	A2	1564:C	O3'	1572:A	P	15.12
1	m2	324:C	O3'	331:G	P	14.73
1	m2	1753:C	O3'	1786:G	P	14.69
1	A2	1772:A	O3'	1820:C	P	14.03
1	T3	43:VAL	C	55:PRO	N	13.92
1	A2	1914:C	O3'	2004:G	P	13.66
1	A2	4668:U	O3'	4674:G	P	12.84
1	A2	481:G	O3'	485:U	P	11.75
1	A2	1055:G	O3'	1059:C	P	11.26
1	A2	866:A	O3'	868:C	P	9.59
1	A2	1072:U	O3'	1078:G	P	8.35
1	m2	227:G	O3'	289:U	P	8.04
1	n2	18:G	O3'	20:A	P	7.90
1	A2	956:C	O3'	999:C	P	7.48
1	m2	1843:C	O3'	1845:G	P	6.74
1	n2	45:G	O3'	47:C	P	6.51
1	m2	1249:C	O3'	1251:C	P	6.49
1	A2	4422:G	O3'	4424:U	P	4.82
1	A2	501:G	O3'	506:G	P	4.53
1	K2	157:GLY	C	158:THR	N	1.20

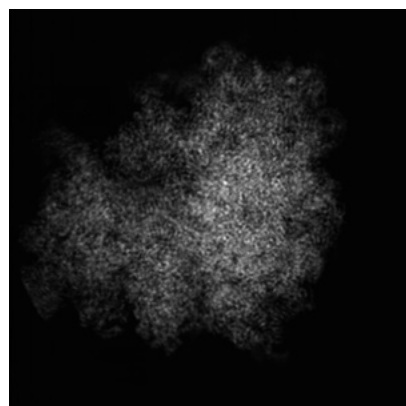
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53427. These allow visual inspection of the internal detail of the map and identification of artifacts.

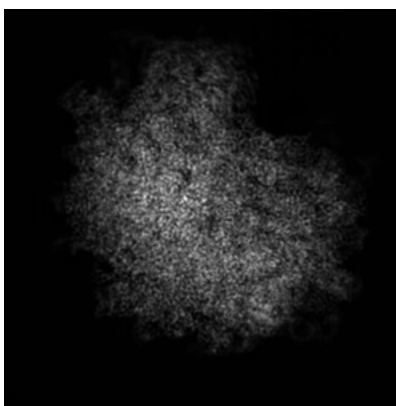
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

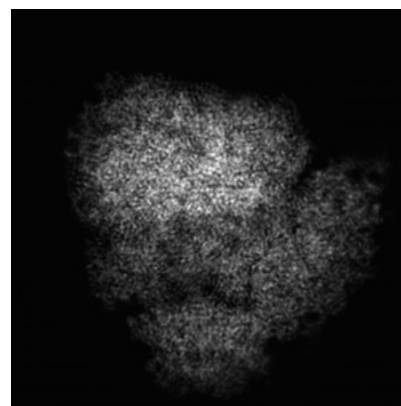
#### 6.1.1 Primary map



X

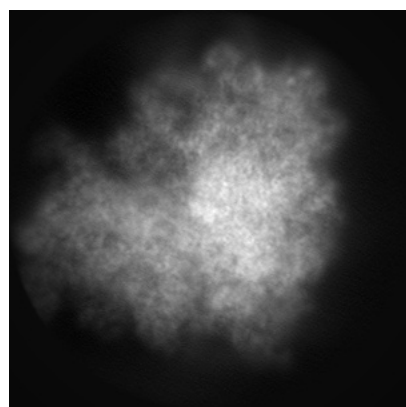


Y

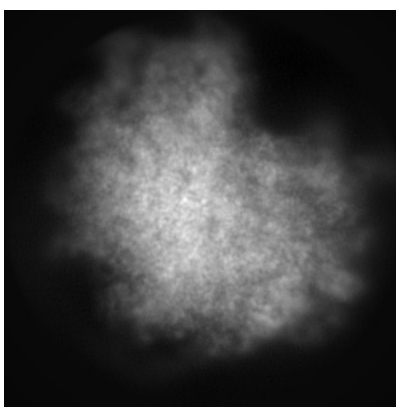


Z

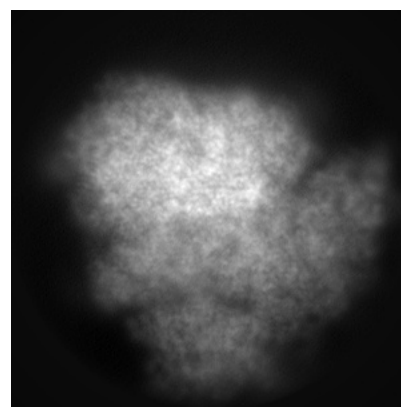
#### 6.1.2 Raw map



X



Y



Z

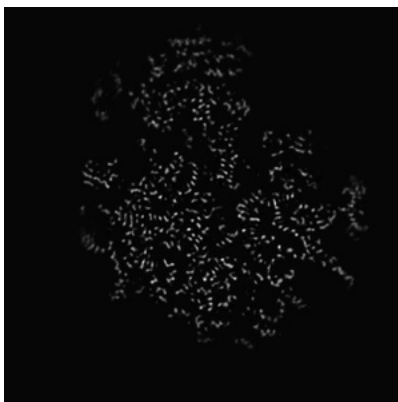
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

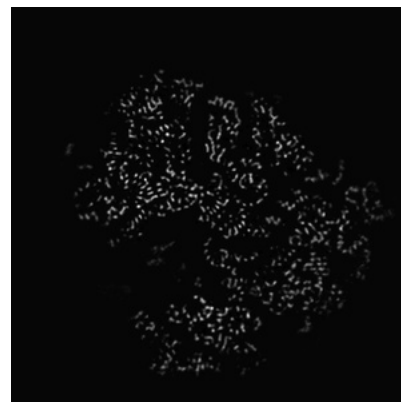
### 6.2.1 Primary map



X Index: 156

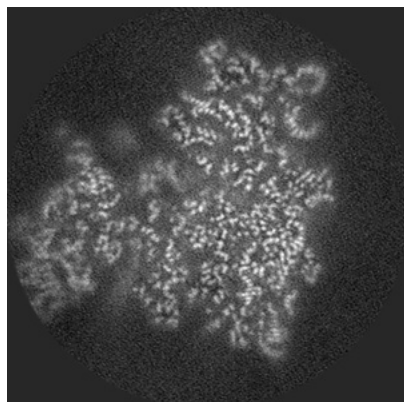


Y Index: 156

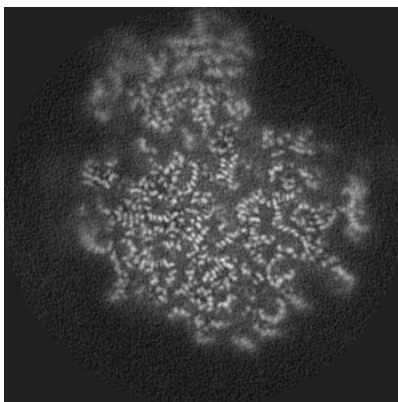


Z Index: 156

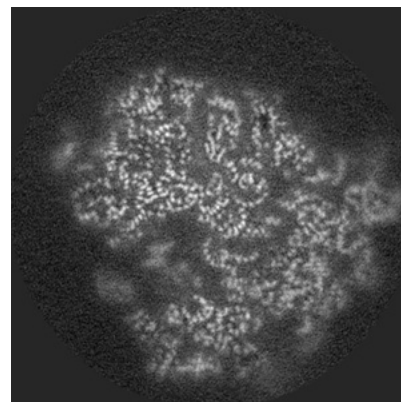
### 6.2.2 Raw map



X Index: 156



Y Index: 156

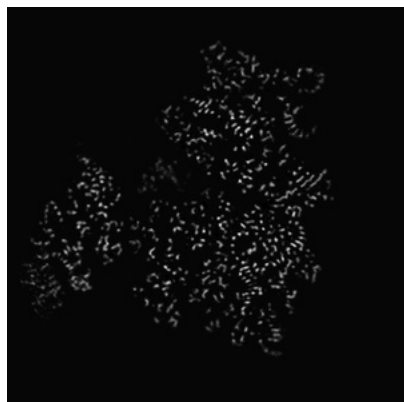


Z Index: 156

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

## 6.3 Largest variance slices [i](#)

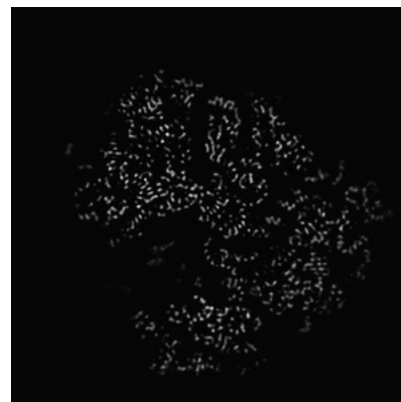
### 6.3.1 Primary map



X Index: 155

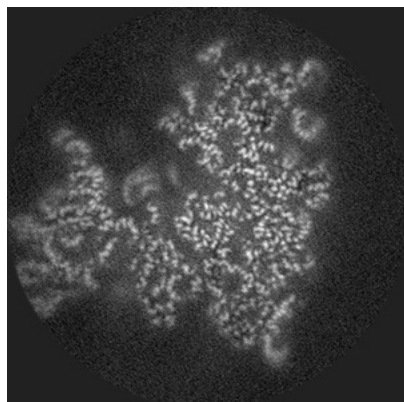


Y Index: 170

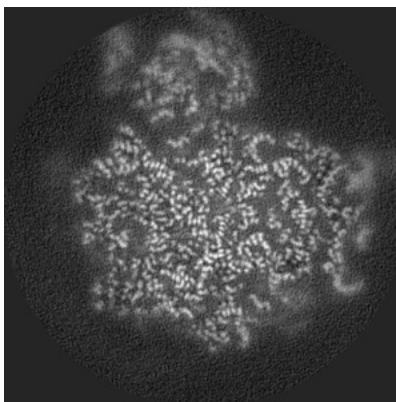


Z Index: 156

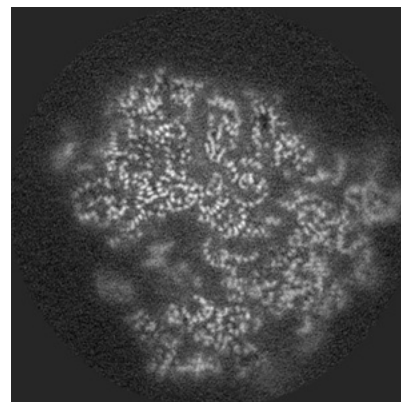
### 6.3.2 Raw map



X Index: 161



Y Index: 170



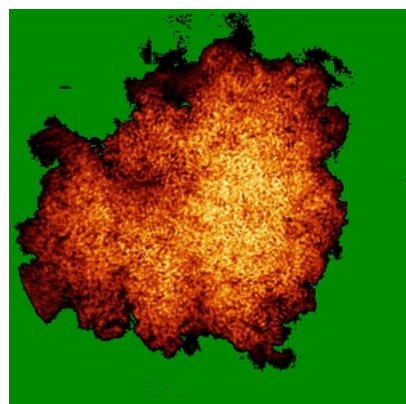
Z Index: 156

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

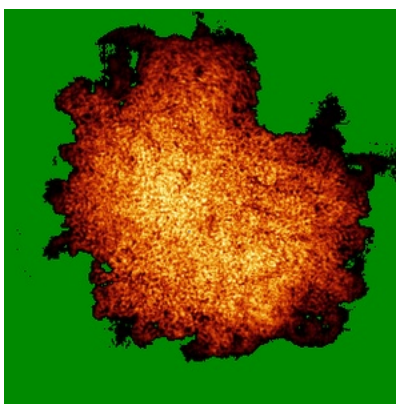


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

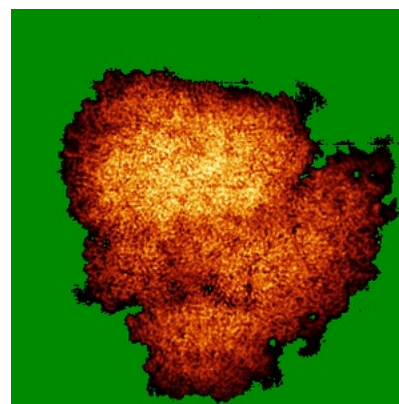
### 6.4.1 Primary map



X

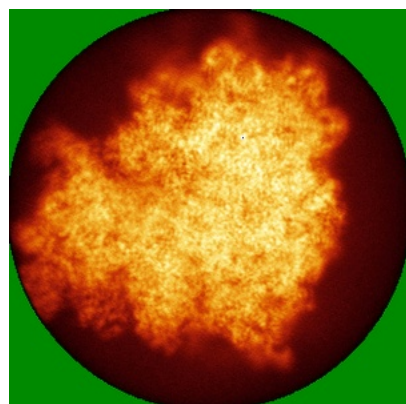


Y

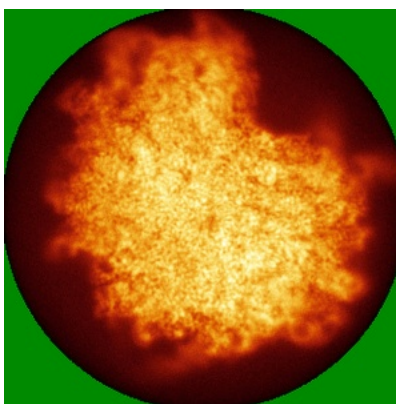


Z

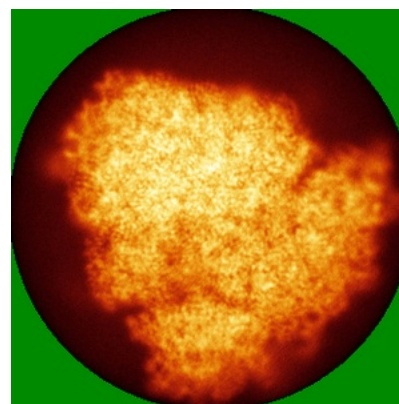
### 6.4.2 Raw map



X



Y

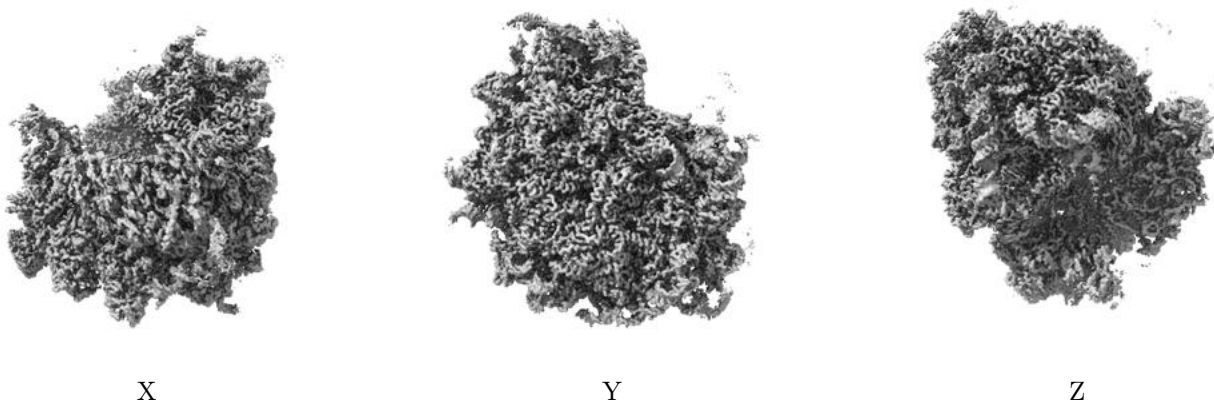


Z

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

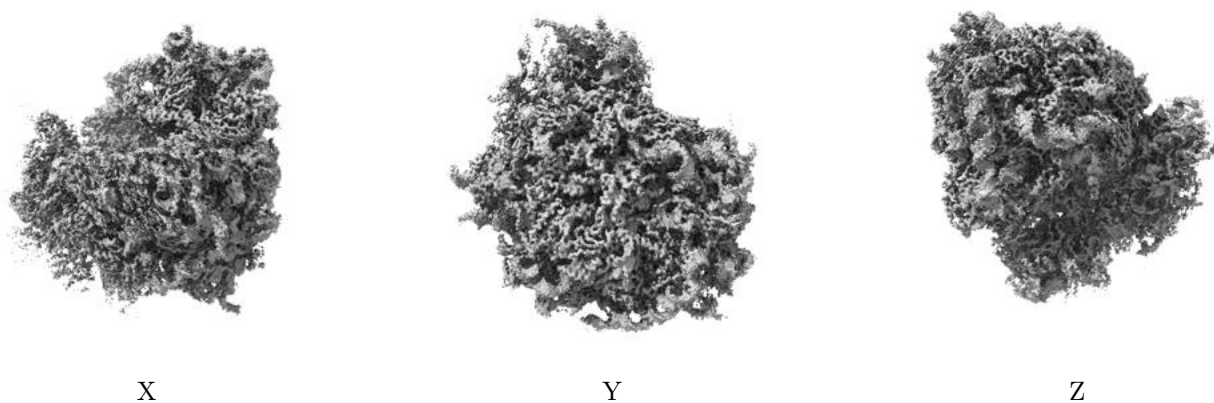
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0823. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

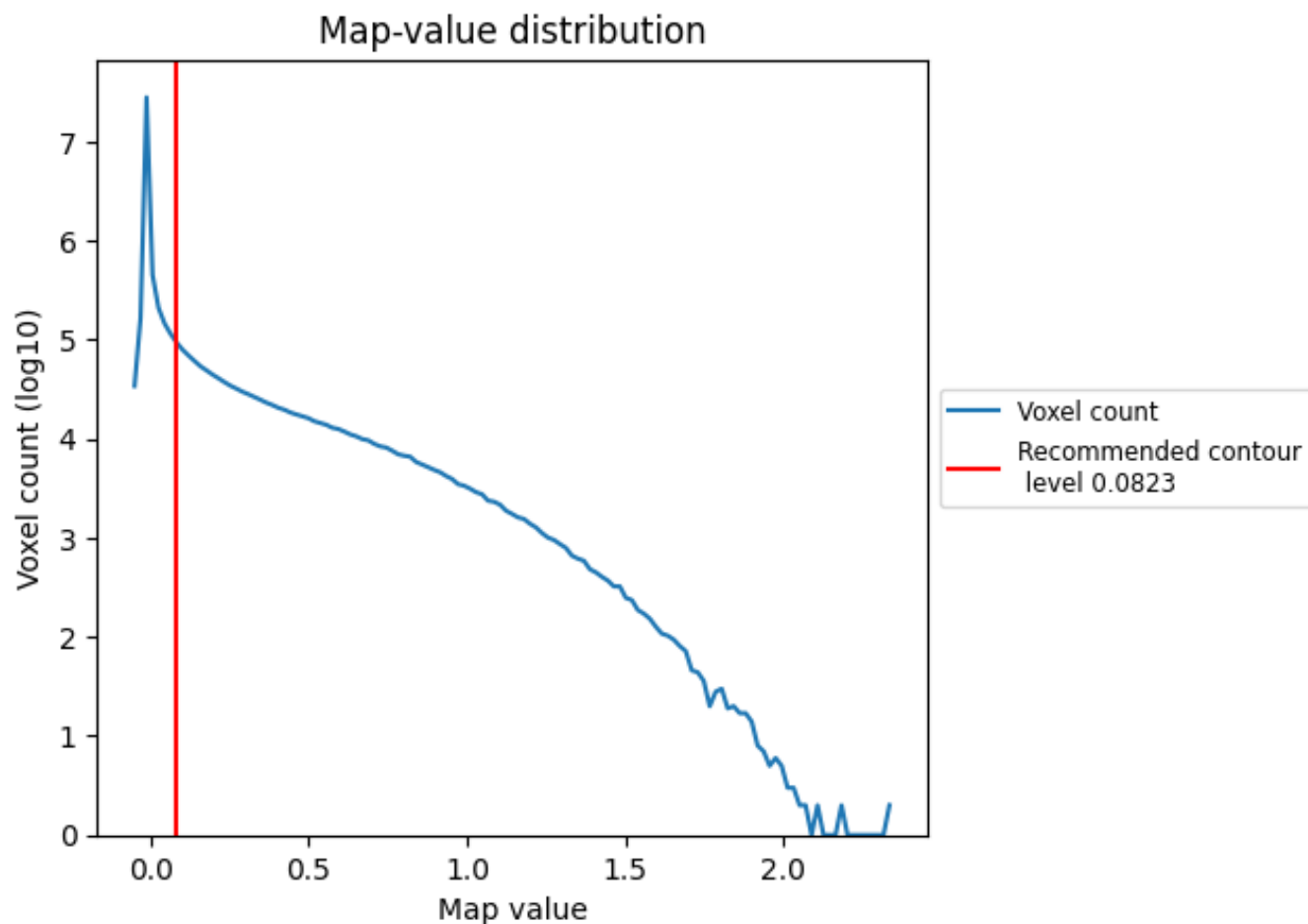
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

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

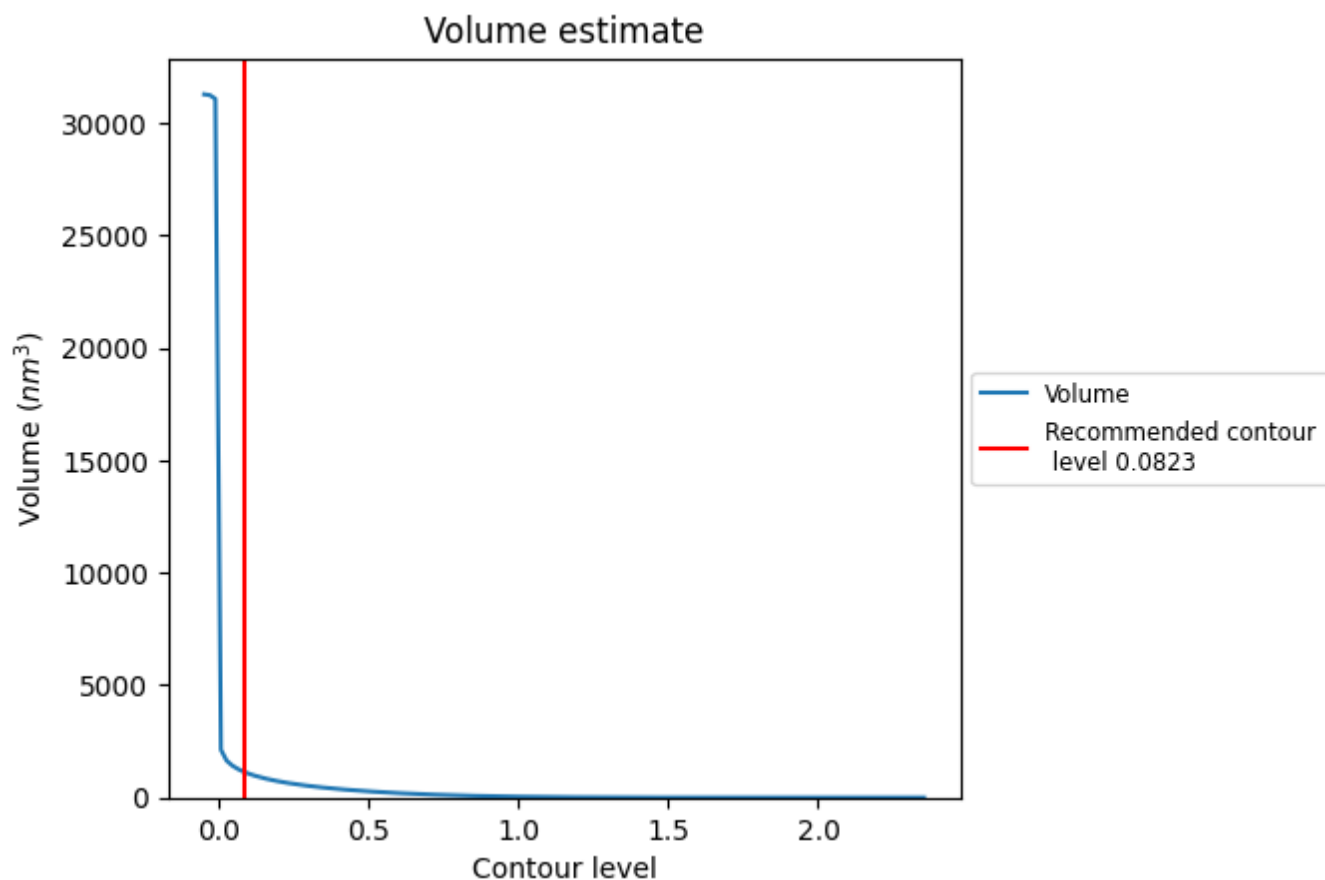
### 7.1 Map-value distribution [i](#)



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



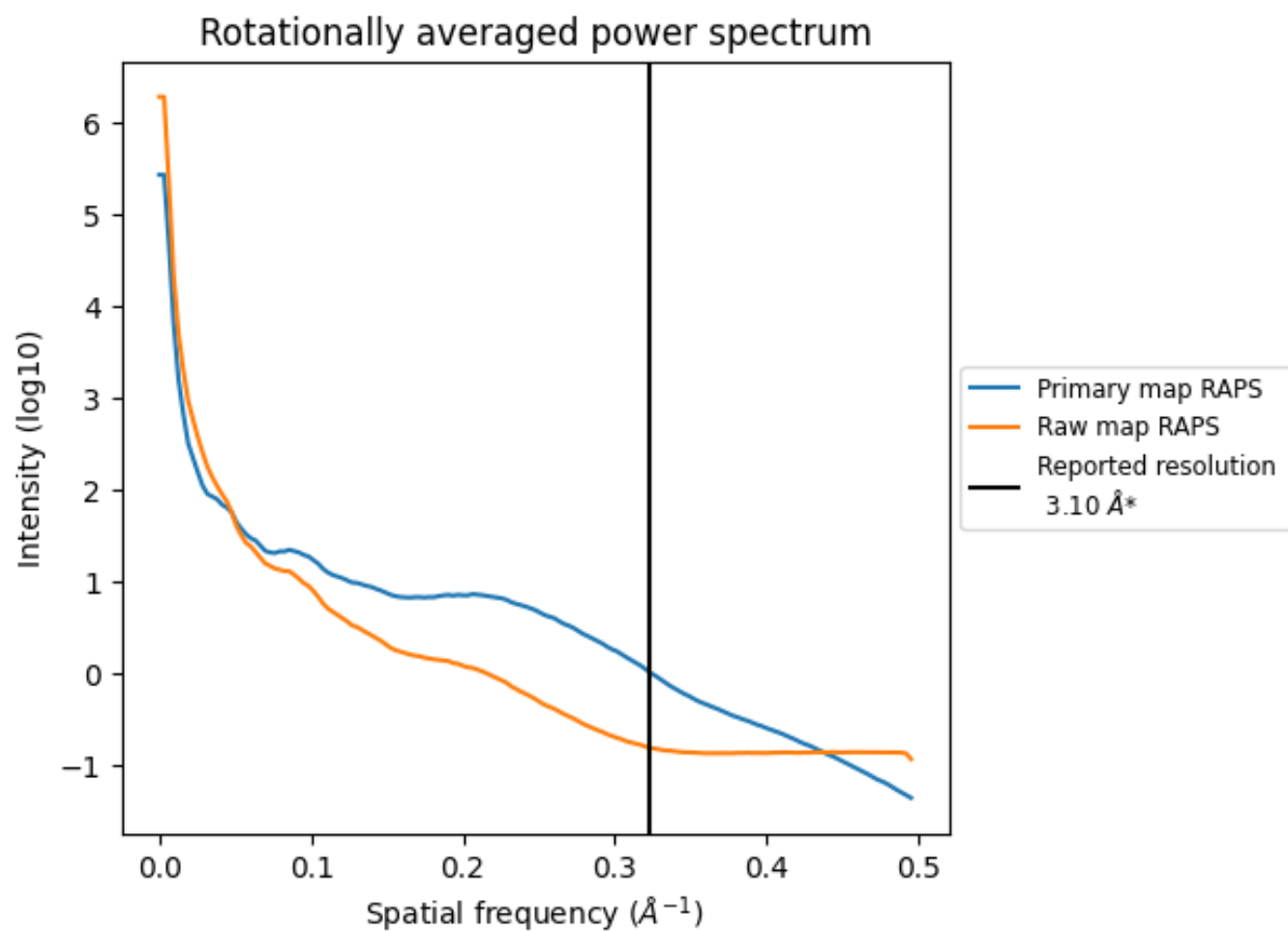
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1154 nm<sup>3</sup>; this corresponds to an approximate mass of 1043 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 ⓘ

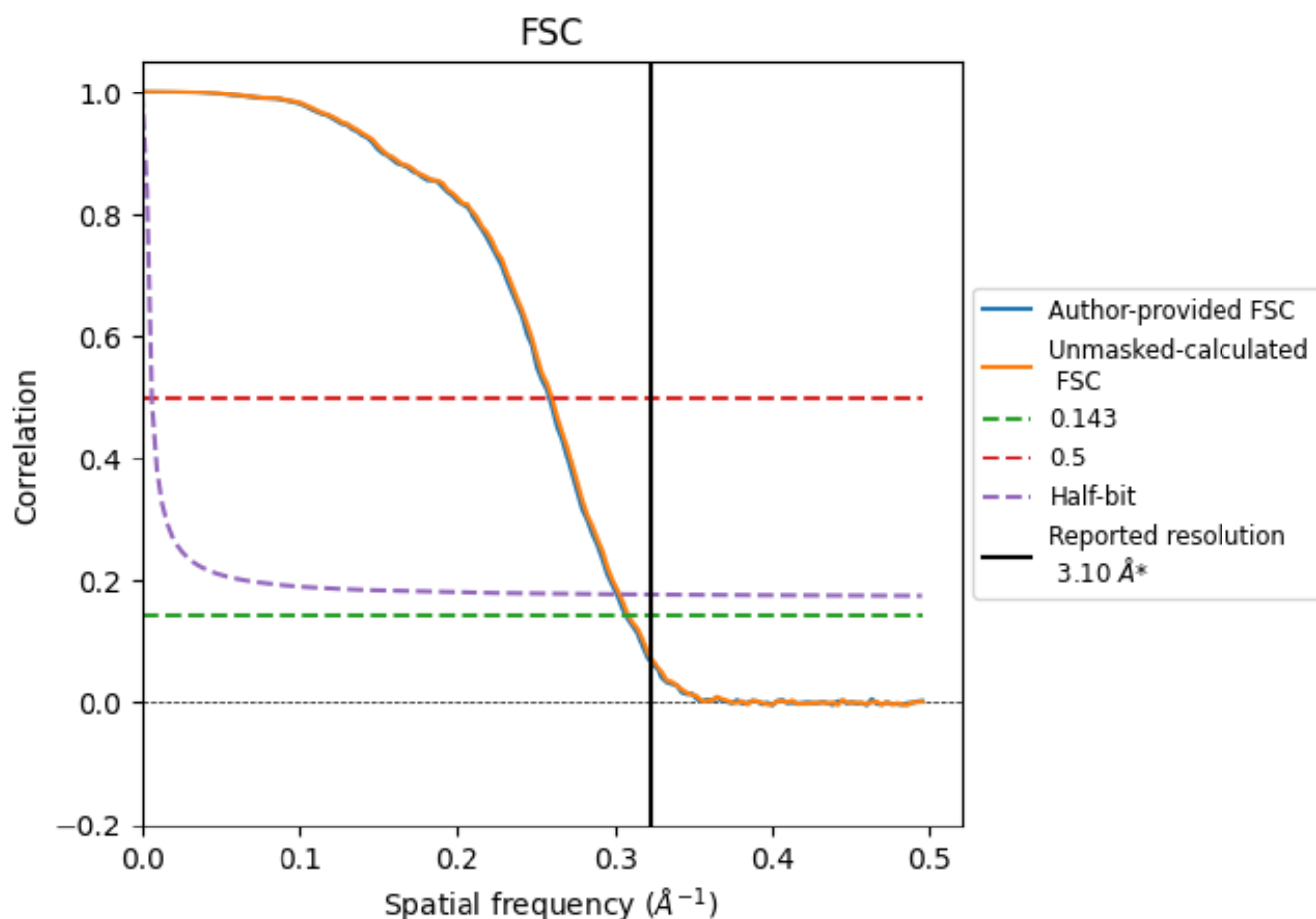


\*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

## 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 0.323  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

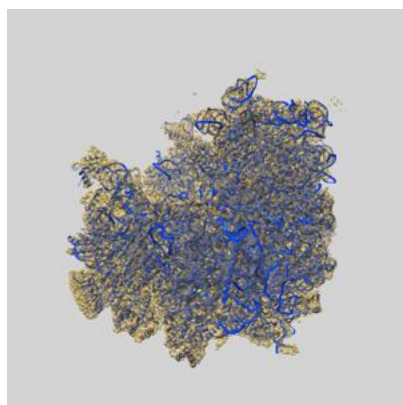
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.26	3.87	3.32
Unmasked-calculated*	3.24	3.85	3.30

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

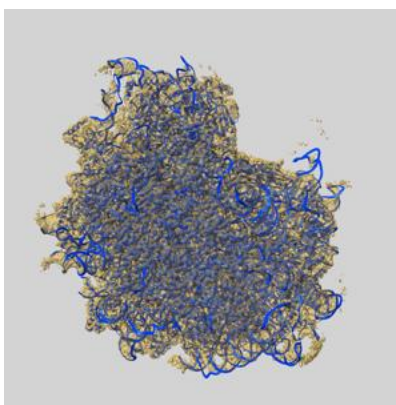
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-53427 and PDB model 9QWT. Per-residue inclusion information can be found in section [3](#) on page [23](#).

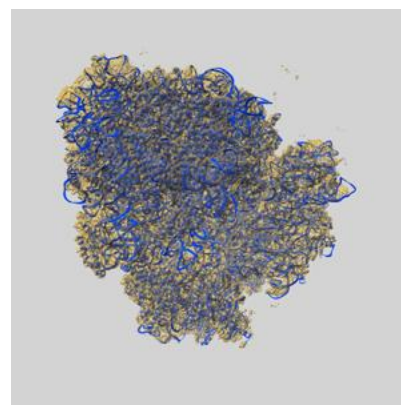
### 9.1 Map-model overlay [i](#)



X



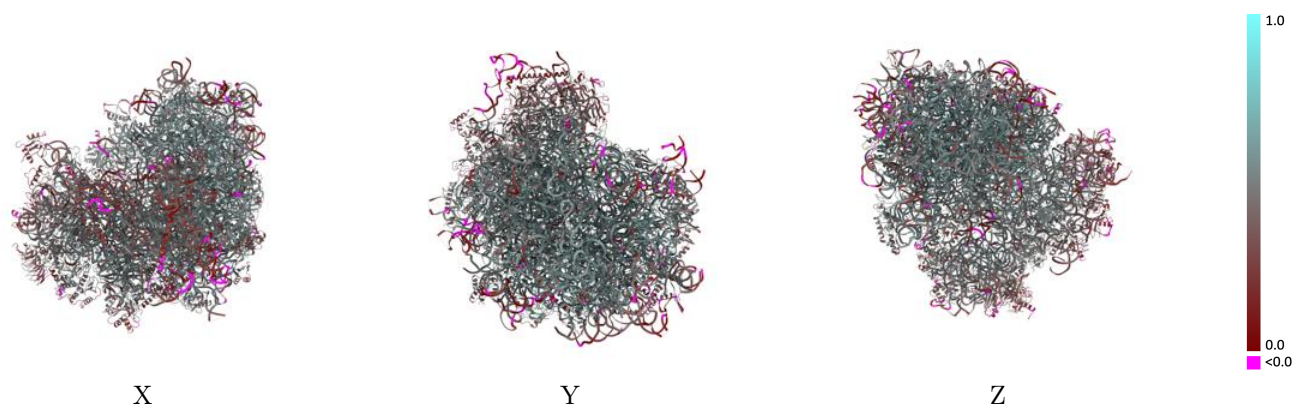
Y



Z

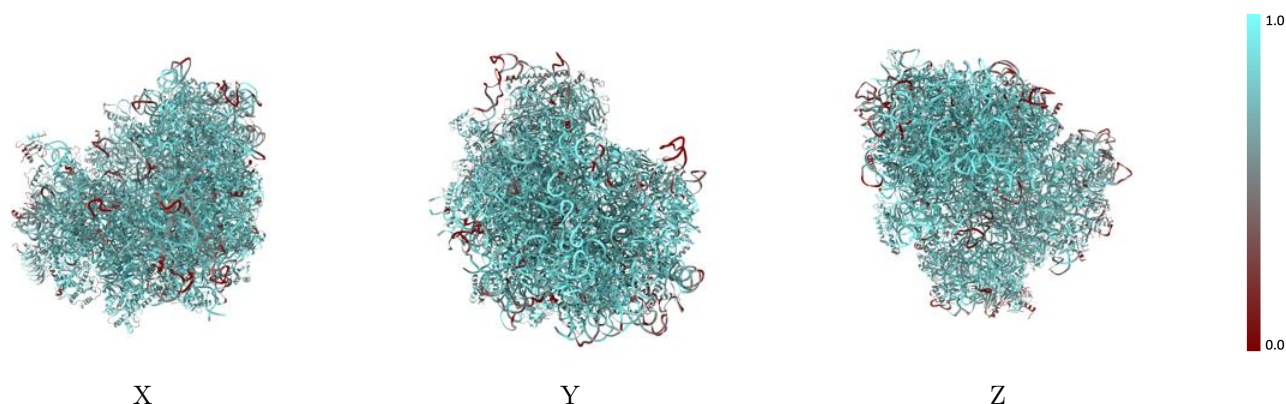
The images above show the 3D surface view of the map at the recommended contour level 0.0823 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



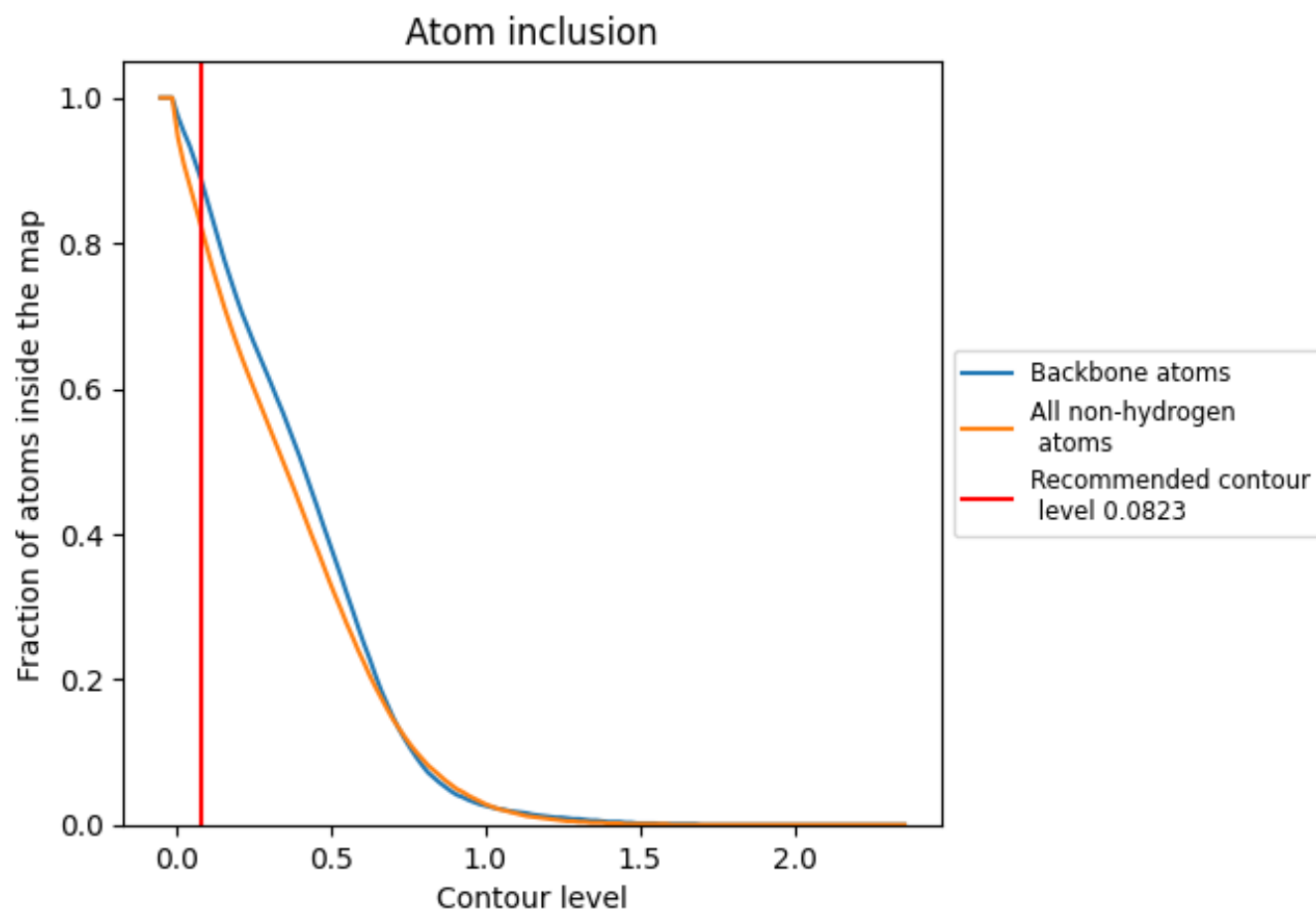
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0823).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 82% 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 (0.0823) and Q-score for the entire model and for each chain.





















































































Chain	Atom inclusion	Q-score
All	 0.8210	 0.4740
A1	 0.8390	 0.5160
A2	 0.8610	 0.4970
A3	 0.7650	 0.4220
B1	 0.7990	 0.4630
B2	 0.9370	 0.5460
B3	 0.6940	 0.3830
Bv	 0.5950	 0.3020
Bx	 0.8450	 0.4850
By	 0.0000	 0.0310
C1	 0.8080	 0.5000
C2	 0.8580	 0.5040
C3	 0.5720	 0.3270
D1	 0.8290	 0.5070
D2	 0.9090	 0.5630
D3	 0.8130	 0.4670
E1	 0.7540	 0.4390
E2	 0.8310	 0.5170
E3	 0.7700	 0.4400
F1	 0.8250	 0.4950
F2	 0.8710	 0.5350
F3	 0.8310	 0.4950
G1	 0.8500	 0.5040
G2	 0.7850	 0.4740
G3	 0.7150	 0.4290
H1	 0.9130	 0.5720
H2	 0.7770	 0.4820
H3	 0.8150	 0.4350
I2	 0.8760	 0.5370
I3	 0.6500	 0.3200
J2	 0.8670	 0.5380
J3	 0.8300	 0.4860
K2	 0.8880	 0.5460
K3	 0.5880	 0.2800
L2	 0.8110	 0.4850



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Chain	Atom inclusion	Q-score
L3	 0.6050	 0.3090
M2	 0.9020	 0.5490
M3	 0.3770	 0.1880
N2	 0.8240	 0.5040
N3	 0.7960	 0.4510
O2	 0.6980	 0.3980
O3	 0.7660	 0.4530
P2	 0.8750	 0.5430
P3	 0.8350	 0.4930
Q2	 0.8620	 0.5320
Q3	 0.4840	 0.2230
R2	 0.8170	 0.4990
R3	 0.6490	 0.3610
S2	 0.7800	 0.4950
S3	 0.7480	 0.4060
T2	 0.8220	 0.4860
T3	 0.6150	 0.3460
U2	 0.8870	 0.5540
V2	 0.6460	 0.3990
W2	 0.8320	 0.4850
X2	 0.7860	 0.4930
Y2	 0.8630	 0.5440
Z2	 0.9010	 0.5630
a2	 0.8540	 0.5190
b2	 0.8000	 0.4800
c2	 0.7670	 0.4610
d2	 0.8800	 0.5560
e2	 0.7190	 0.4100
f2	 0.8460	 0.5240
g2	 0.8150	 0.5190
h2	 0.8180	 0.4840
i2	 0.8190	 0.5090
j2	 0.8620	 0.5270
k2	 0.8640	 0.5300
m2	 0.8570	 0.4620
n2	 0.7190	 0.3850
o2	 0.7560	 0.4120
p2	 0.7970	 0.4600
q2	 0.6680	 0.3820
r2	 0.6620	 0.3470
s2	 0.7380	 0.4180
t2	 0.7390	 0.3830

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Chain	Atom inclusion	Q-score
u2	 0.7420	 0.3980
v2	 0.6300	 0.3030
w2	 0.7520	 0.4120
x2	 0.7190	 0.4120
y2	 0.7290	 0.4010
z2	 0.6660	 0.3350