



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 06:43 AM UTC

PDB ID : 9GYT / pdb_00009gyt
EMDB ID : EMD-51718
Title : High resolution structure of B. oleracea mitoribosome
Authors : Waltz, F.; Skaltsogiannis, V.; Giege, P.
Deposited on : 2024-10-02
Resolution : 2.11 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

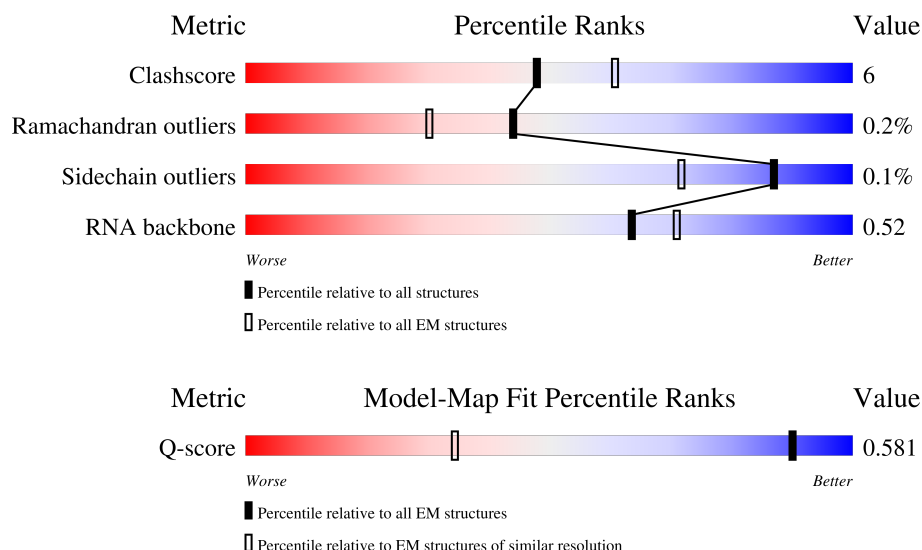
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.11 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.



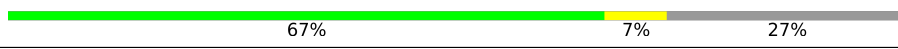
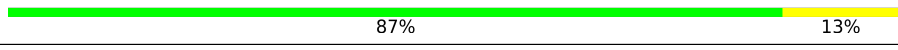
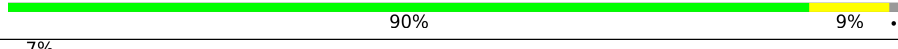
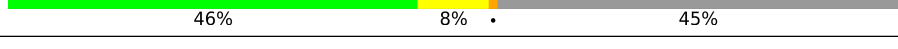
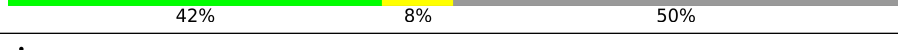
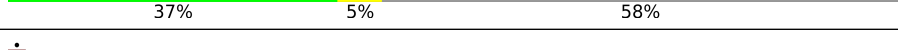
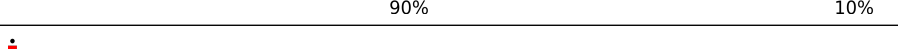
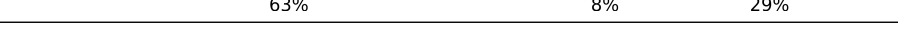
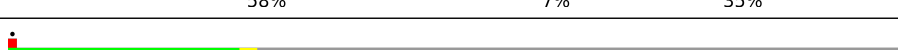
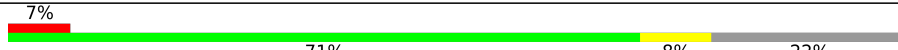
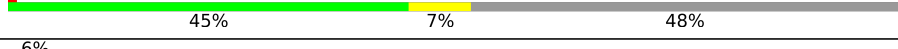
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	2361 (1.64 - 2.61)

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

Mol	Chain	Length	Quality of chain
1	3	118	
2	A	212	
3	B	554	

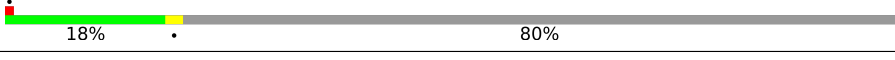
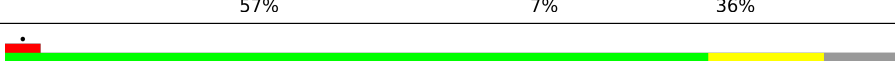
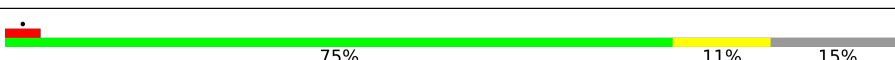
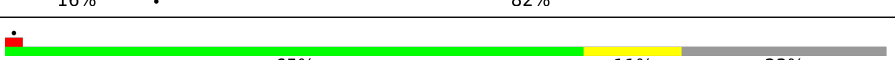
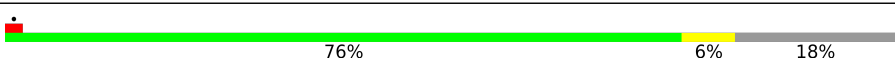
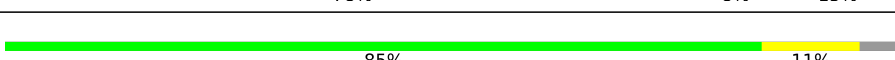
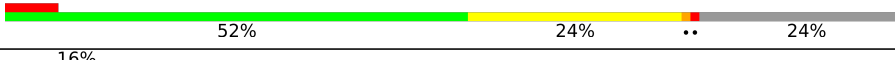
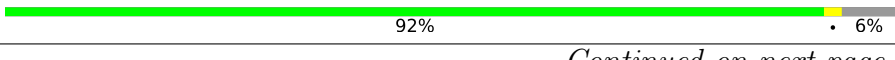
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Mol	Chain	Length	Quality of chain
4	C	362	
5	D	501	
6	E	138	
7	F	157	
8	G	129	
9	H	383	
10	I	228	
11	J	304	
12	K	125	
13	L	154	
14	M	155	
15	N	414	
16	O	136	
17	P	110	
18	Q	237	
19	R	212	
20	S	100	
21	T	94	
22	U	192	
23	V	193	
24	W	483	
25	X	496	
26	Y	102	
27	Z	153	
28	a	424	

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Mol	Chain	Length	Quality of chain
29	b	80	
30	c	128	
31	d	110	
32	e	383	
33	f	410	
34	g	668	
35	h	384	
36	i	725	
37	j	408	
38	k	153	
39	l	576	
40	1B	217	
41	1C	286	
42	1D	319	
43	1E	296	
44	1F	185	
45	1G	102	
46	1H	220	
47	1I	170	
48	1J	156	
49	1K	204	
50	1L	176	
51	1M	281	
52	1N	179	
53	1O	160	

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Mol	Chain	Length	Quality of chain
54	1P	114	
55	1Q	233	
56	1R	126	
57	1S	270	
58	1T	264	
59	1U	180	
60	1V	159	
61	1W	248	
62	1X	271	
63	1Y	156	
64	1Z	215	
65	1a	144	
66	1b	109	
67	1c	135	
68	1d	139	
69	1e	106	
70	1f	146	
71	1g	162	
72	1h	103	
73	1i	247	
74	1j	90	
75	1k	119	
76	1l	239	
77	1m	128	
78	1o	125	

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Mol	Chain	Length	Quality of chain
79	1p	130	
80	1q	78	
81	1r	167	
82	1s	181	
83	1t	491	
84	1u	752	
85	1v	514	
86	1	2922	
87	2	1766	

2 Entry composition

There are 92 unique types of molecules in this entry. The entry contains 233430 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	3	118	Total	C	N	O	P	0	0
			2513	1124	453	819	117		

- Molecule 2 is a protein called Ribosomal protein S2.

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

- Molecule 3 is a protein called Small ribosomal subunit protein uS3m.

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

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	22	TRP	ARG	conflict	UNP A0A068BCX1
B	62	ILE	LEU	conflict	UNP A0A068BCX1
B	172	LEU	SER	conflict	UNP A0A068BCX1
B	202	LYS	ARG	conflict	UNP A0A068BCX1
B	296	LEU	SER	conflict	UNP A0A068BCX1
B	512	CYS	ARG	conflict	UNP A0A068BCX1
B	524	VAL	ALA	conflict	UNP A0A068BCX1
B	533	LEU	SER	conflict	UNP A0A068BCX1

- Molecule 4 is a protein called uS4m.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	333	Total	C	N	O	S	0	0
			2806	1793	540	462	11		

- Molecule 5 is a protein called S5 DRBM domain-containing protein.

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

- Molecule 6 is a protein called bS6m.

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

- Molecule 7 is a protein called uS7m, Small ribosomal subunit protein uS7m.

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

- Molecule 8 is a protein called uS8m.

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

- Molecule 9 is a protein called uS9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	212	Total	C	N	O	S	0	0
			1671	1048	308	310	5		

- Molecule 10 is a protein called Small ribosomal subunit protein uS10 domain-containing protein.

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

- Molecule 11 is a protein called uS11m.

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

- Molecule 12 is a protein called uS12m.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	124	Total	C	N	O	S	0	0
			993	614	209	166	4		

- Molecule 13 is a protein called uS13m.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	110	Total	C	N	O	S	0	0
			873	529	185	154	5		

- Molecule 14 is a protein called uS14m.

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

- Molecule 15 is a protein called Small ribosomal subunit protein uS15c.

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

- Molecule 16 is a protein called 30S ribosomal protein S16.

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

- Molecule 17 is a protein called uS17m.

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

- Molecule 18 is a protein called bS18m.

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

- Molecule 19 is a protein called Small ribosomal subunit protein uS19m.

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

- Molecule 20 is a protein called Ribosomal protein S21.

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

- Molecule 21 is a protein called 30S ribosomal protein S31, mitochondrial.

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

- Molecule 22 is a protein called mS23.

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

- Molecule 23 is a protein called mS26.

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

- Molecule 24 is a protein called Small ribosomal subunit protein mS29.

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

- Molecule 25 is a protein called mS31/mS46.

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

- Molecule 26 is a protein called mS33.

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

- Molecule 27 is a protein called mS34.

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

- Molecule 28 is a protein called mS35.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	a	315	Total	C	N	O	S	0	0
			2486	1546	448	482	10		

- Molecule 29 is a protein called mS37.

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

- Molecule 30 is a protein called mS38.

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

- Molecule 31 is a protein called mS41.

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

- Molecule 32 is a protein called mS45.

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

- Molecule 33 is a protein called mS47.

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

- Molecule 34 is a protein called Small ribosomal subunit protein mS81 (rPPR8).

Mol	Chain	Residues	Atoms					AltConf	Trace
34	g	571	Total	C	N	O	S	0	0
			4527	2860	767	869	31		

- Molecule 35 is a protein called mS83 (rPPR10).

Mol	Chain	Residues	Atoms					AltConf	Trace
35	h	310	Total	C	N	O	S	0	0
			2463	1557	438	455	13		

- Molecule 36 is a protein called PROP1-like PPR domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	i	597	Total	C	N	O	S	0	0
			4766	3010	805	919	32		

- Molecule 37 is a protein called mS76 (rPPR1).

Mol	Chain	Residues	Atoms					AltConf	Trace
37	j	381	Total	C	N	O	S	0	0
			2980	1881	510	567	22		

- Molecule 38 is a protein called mS86.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	k	28	Total	C	N	O	S	0	0
			220	139	42	35	4		

- Molecule 39 is a protein called Small ribosomal subunit protein mS80 (rPPR6).

Mol	Chain	Residues	Atoms					AltConf	Trace
39	l	442	Total	C	N	O	S	0	0
			3468	2209	573	663	23		

- Molecule 40 is a protein called Large ribosomal subunit protein uL2 C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	1B	177	Total	C	N	O	S	0	0
			1326	819	259	234	14		

- Molecule 41 is a protein called uL2m N-ter mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	1C	215	Total	C	N	O	S	0	0
			1699	1083	314	296	6		

- Molecule 42 is a protein called uL3m.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	1D	264	Total	C	N	O	S	0	0
			2045	1309	367	358	11		

- Molecule 43 is a protein called uL4m.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	1E	221	Total	C	N	O	S	0	0
			1754	1104	334	309	7		

- Molecule 44 is a protein called uL5m.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	1F	158	Total	C	N	O	S	0	0
			1283	825	212	237	9		

- Molecule 45 is a protein called Large ribosomal subunit protein uL6 alpha-beta domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	1G	98	Total	C	N	O	S	0	0
			779	508	136	130	5		

- Molecule 46 is a protein called bL9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	1H	66	Total	C	N	O	S	0	0
			539	345	98	94	2		

- Molecule 47 is a protein called uL10m.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	1I	130	Total	C	N	O	S	0	0
			1036	669	178	184	5		

- Molecule 48 is a protein called uL11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	1J	147	Total	C	N	O	S	0	0
			1133	726	193	205	9		

- Molecule 49 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	1K	189	Total	C	N	O	S	0	0
			1526	955	299	265	7		

- Molecule 50 is a protein called uL14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	1L	127	Total	C	N	O	S	0	0
			966	609	184	168	5		

- Molecule 51 is a protein called uL15m.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	1M	210	Total	C	N	O	S	0	0
			1649	1052	321	273	3		

- Molecule 52 is a protein called Large ribosomal subunit protein uL16m.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	1N	148	Total	C	N	O	S	0	0
			1160	731	230	192	7		

- Molecule 53 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	1O	151	Total	C	N	O	S	0	0
			1231	767	244	214	6		

- Molecule 54 is a protein called Ribosomal protein L18e/L15P domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	1P	113	Total	C	N	O	S	0	0
			878	564	160	149	5		

- Molecule 55 is a protein called bL19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	1Q	122	Total	C	N	O	S	0	0
			1008	641	198	166	3		

- Molecule 56 is a protein called bL20m.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	1R	110	Total	C	N	O	S	0	0
			915	572	184	154	5		

- Molecule 57 is a protein called bL21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	1S	145	Total	C	N	O	S	0	0
			1164	748	204	210	2		

- Molecule 58 is a protein called Large ribosomal subunit protein uL22m.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	1T	155	Total	C	N	O	S	0	0
			1241	782	249	205	5		

- Molecule 59 is a protein called uL23m.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	1U	130	Total	C	N	O	S	0	0
			1048	675	190	181	2		

- Molecule 60 is a protein called uL24m.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	1V	158	Total	C	N	O	S	0	0
			1223	770	229	220	4		

- Molecule 61 is a protein called bL25-2m.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	1W	205	Total	C	N	O	S	0	0
			1591	1006	286	294	5		

- Molecule 62 is a protein called bL25m.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	1X	216	Total	C	N	O	S	0	0
			1670	1069	298	302	1		

- Molecule 63 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	1Y	103	Total	C	N	O	S	0	0
			800	502	157	140	1		

- Molecule 64 is a protein called bL28m.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	1Z	177	Total	C	N	O	S	0	0
			1439	908	269	253	9		

- Molecule 65 is a protein called uL29m.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	1a	110	Total	C	N	O	S	0	0
			928	588	172	158	10		

- Molecule 66 is a protein called uL30m.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	1b	100	Total	C	N	O	S	0	0
			801	501	159	136	5		

- Molecule 67 is a protein called bL31m.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	1c	59	Total	C	N	O	S	0	0
			489	313	98	73	5		

- Molecule 68 is a protein called bL32m.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	1d	49	Total	C	N	O	S	0	0
			379	240	80	55	4		

- Molecule 69 is a protein called bL33m.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	1e	54	Total	C	N	O	S	0	0
			459	300	85	72	2		

- Molecule 70 is a protein called Large ribosomal subunit protein bL34m.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	1f	44	Total	C	N	O	S	0	0
			364	224	88	52			

- Molecule 71 is a protein called bL35m.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	1g	91	Total	C	N	O	S	0	0
			773	496	155	119	3		

- Molecule 72 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	1h	38	Total	C	N	O	S	0	0
			309	190	65	49	5		

- Molecule 73 is a protein called mL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	1i	178	Total	C	N	O	S	0	0
			1378	856	245	267	10		

- Molecule 74 is a protein called mL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	1j	71	Total	C	N	O	S	0	0
			570	369	102	97	2		

- Molecule 75 is a protein called Large ribosomal subunit protein mL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	1k	118	Total	C	N	O	S	0	0
			952	599	184	165	4		

- Molecule 76 is a protein called mL46.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	1l	211	Total	C	N	O	S	0	0
			1739	1128	286	318	7		

- Molecule 77 is a protein called mL53.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	1m	122	Total	C	N	O	S	0	0
			970	610	170	184	6		

- Molecule 78 is a protein called mL54.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	1o	76	Total	C	N	O		0	0
			617	392	111	114			

- Molecule 79 is a protein called mL59/mL64.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	1p	117	Total	C	N	O	S	0	0
			992	626	189	169	8		

- Molecule 80 is a protein called mL60.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	1q	50	Total	C	N	O	S	0	0
			389	242	79	67	1		

- Molecule 81 is a protein called mL80.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	1r	92	Total	C	N	O	S	0	0
			735	469	139	122	5		

- Molecule 82 is a protein called mL87.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	1s	118	Total	C	N	O	S	0	0
			985	617	203	163	2		

- Molecule 83 is a protein called mL101 (rPPR4).

Mol	Chain	Residues	Atoms					AltConf	Trace
83	1t	484	Total	C	N	O	S	0	0
			3856	2433	665	733	25		

- Molecule 84 is a protein called mL102 (rPPR5).

Mol	Chain	Residues	Atoms					AltConf	Trace
84	1u	665	Total	C	N	O	S	0	0
			5269	3318	915	992	44		

- Molecule 85 is a protein called mL104 (rPPR9).

Mol	Chain	Residues	Atoms					AltConf	Trace
85	1v	433	Total	C	N	O	S	0	0
			3440	2169	613	634	24		

- Molecule 86 is a RNA chain called 26S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	1	2922	Total	C	N	O	P	5	0
			62518	27942	11365	20289	2922		

- Molecule 87 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	2	1766	Total	C	N	O	P	0	0
			37784	16899	6869	12250	1766		

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

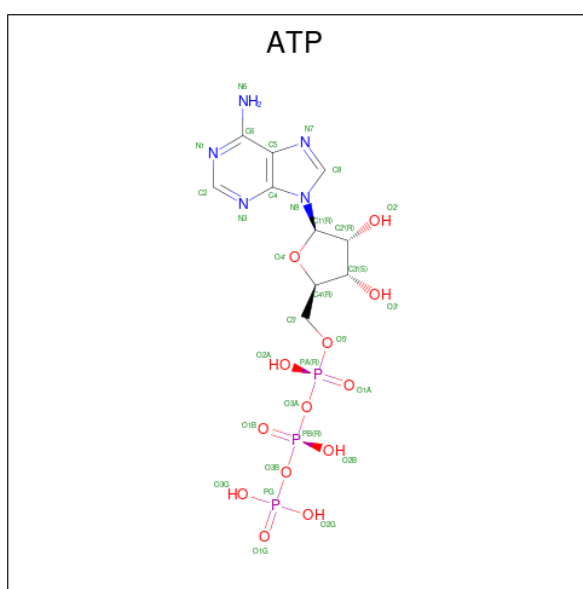
Mol	Chain	Residues	Atoms		AltConf
88	3	3	Total	Mg	0
			3	3	
88	T	1	Total	Mg	0
			1	1	
88	W	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
88	1D	2	Total	Mg	0
			2	2	
88	1q	2	Total	Mg	0
			2	2	
88	1	243	Total	Mg	0
			243	243	
88	2	97	Total	Mg	0
			97	97	

- Molecule 89 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 90 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
90	1B	2	Total	K	0
			2	2	
90	1E	1	Total	K	0
			1	1	
90	1	62	Total	K	0
			62	62	
90	2	19	Total	K	0
			19	19	

- Molecule 91 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
91	1d	1	Total 1	Zn 1	0
91	1h	1	Total 1	Zn 1	0

- Molecule 92 is water.

Mol	Chain	Residues	Atoms		AltConf
92	3	79	Total 79	O 79	0
92	A	37	Total 37	O 37	0
92	B	37	Total 37	O 37	0
92	C	63	Total 63	O 63	0
92	D	91	Total 91	O 91	0
92	E	18	Total 18	O 18	0
92	F	8	Total 8	O 8	0
92	G	37	Total 37	O 37	0
92	H	36	Total 36	O 36	0
92	I	28	Total 28	O 28	0
92	J	23	Total 23	O 23	0
92	K	25	Total 25	O 25	0
92	L	16	Total 16	O 16	0
92	M	23	Total 23	O 23	0
92	N	42	Total 42	O 42	0
92	O	39	Total 39	O 39	0
92	P	21	Total 21	O 21	0

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Mol	Chain	Residues	Atoms		AltConf
92	Q	25	Total 25	O 25	0
92	R	15	Total 15	O 15	0
92	S	16	Total 16	O 16	0
92	T	19	Total 19	O 19	0
92	U	15	Total 15	O 15	0
92	V	26	Total 26	O 26	0
92	W	49	Total 49	O 49	0
92	X	17	Total 17	O 17	0
92	Y	19	Total 19	O 19	0
92	Z	11	Total 11	O 11	0
92	a	33	Total 33	O 33	0
92	b	2	Total 2	O 2	0
92	c	6	Total 6	O 6	0
92	d	10	Total 10	O 10	0
92	e	87	Total 87	O 87	0
92	f	35	Total 35	O 35	0
92	h	17	Total 17	O 17	0
92	i	15	Total 15	O 15	0
92	k	2	Total 2	O 2	0
92	1B	44	Total 44	O 44	0
92	1C	33	Total 33	O 33	0

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Mol	Chain	Residues	Atoms		AltConf
92	1D	55	Total 55	O 55	0
92	1E	59	Total 59	O 59	0
92	1F	31	Total 31	O 31	0
92	1G	5	Total 5	O 5	0
92	1H	7	Total 7	O 7	0
92	1K	57	Total 57	O 57	0
92	1L	25	Total 25	O 25	0
92	1M	50	Total 50	O 50	0
92	1N	17	Total 17	O 17	0
92	1O	32	Total 32	O 32	0
92	1P	44	Total 44	O 44	0
92	1Q	24	Total 24	O 24	0
92	1R	34	Total 34	O 34	0
92	1S	29	Total 29	O 29	0
92	1T	40	Total 40	O 40	0
92	1U	22	Total 22	O 22	0
92	1V	36	Total 36	O 36	0
92	1W	5	Total 5	O 5	0
92	1X	26	Total 26	O 26	0
92	1Y	27	Total 27	O 27	0
92	1Z	34	Total 34	O 34	0

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Mol	Chain	Residues	Atoms		AltConf
92	1a	15	Total 15	O 15	0
92	1b	24	Total 24	O 24	0
92	1c	8	Total 8	O 8	0
92	1d	9	Total 9	O 9	0
92	1e	6	Total 6	O 6	0
92	1f	21	Total 21	O 21	0
92	1g	35	Total 35	O 35	0
92	1h	5	Total 5	O 5	0
92	1i	55	Total 55	O 55	0
92	1j	34	Total 34	O 34	0
92	1k	24	Total 24	O 24	0
92	1l	56	Total 56	O 56	0
92	1m	3	Total 3	O 3	0
92	1p	33	Total 33	O 33	0
92	1q	17	Total 17	O 17	0
92	1r	9	Total 9	O 9	0
92	1s	22	Total 22	O 22	0
92	1t	88	Total 88	O 88	0
92	1u	15	Total 15	O 15	0
92	1v	16	Total 16	O 16	0
92	1	5283	Total 5283	O 5283	0

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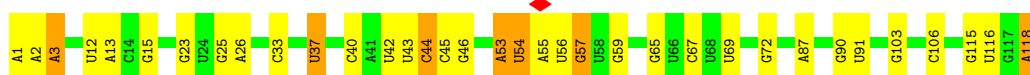
Mol	Chain	Residues	Atoms		AltConf
92	2	2491	Total	O	0
			2491	2491	

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 5S rRNA

Chain 3: 



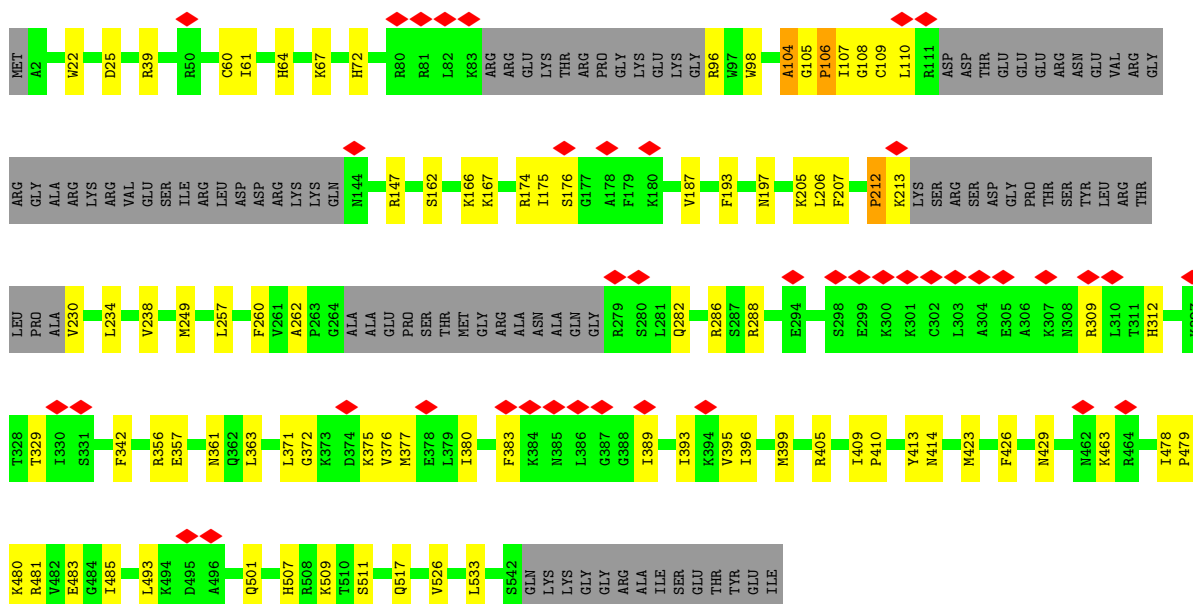
- Molecule 2: Ribosomal protein S2

Chain A: 

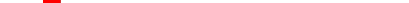


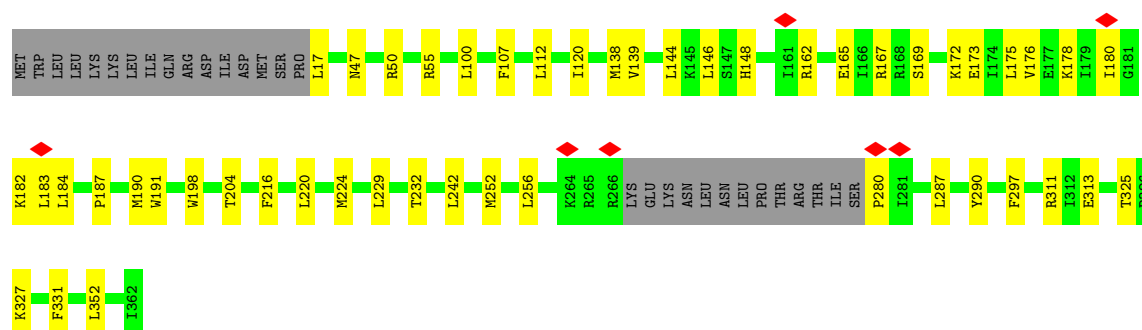
- Molecule 3: Small ribosomal subunit protein uS3m

Chain B: 



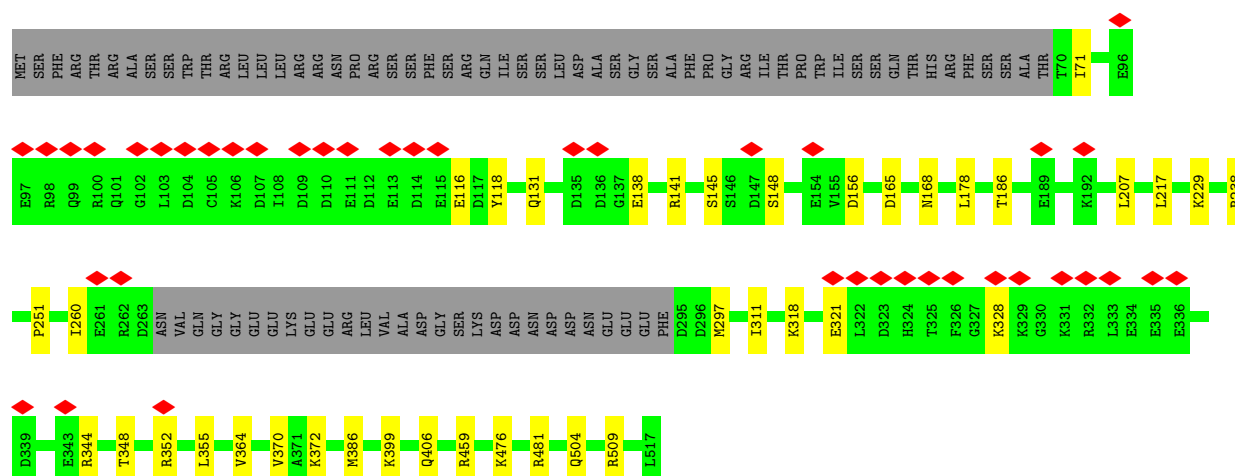
- Molecule 4: uS4m

Chain C:  78% 14% 8%



- Molecule 5: S5 DRBM domain-containing protein

Chain D: 8% 75% 8% 17%

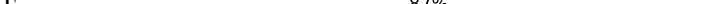


- Molecule 6: bS6m

Chain E:  67% 7% 27%



- Molecule 7: uS7m, Small ribosomal subunit protein uS7m

Chain F:  87% 13%



- Molecule 8: uS8m

Chain G: 90% 9%

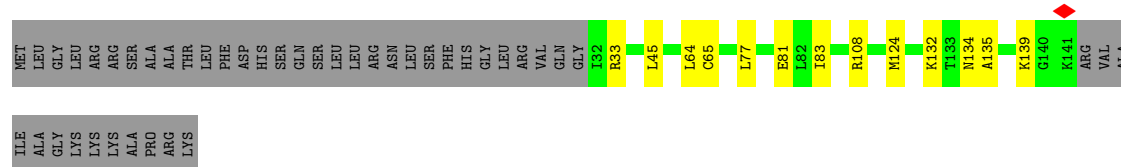
- Molecule 12: uS12m

Chain K:  90% 10%



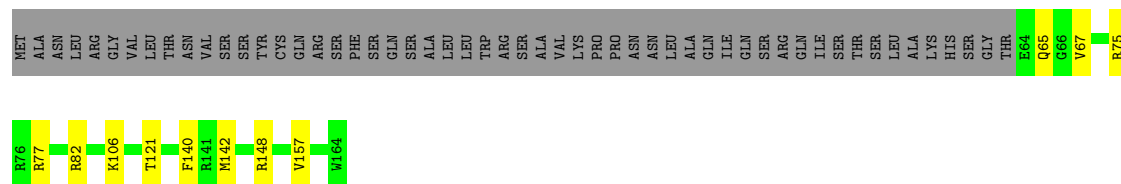
- Molecule 13: uS13m

Chain L:  63% 8% 29%



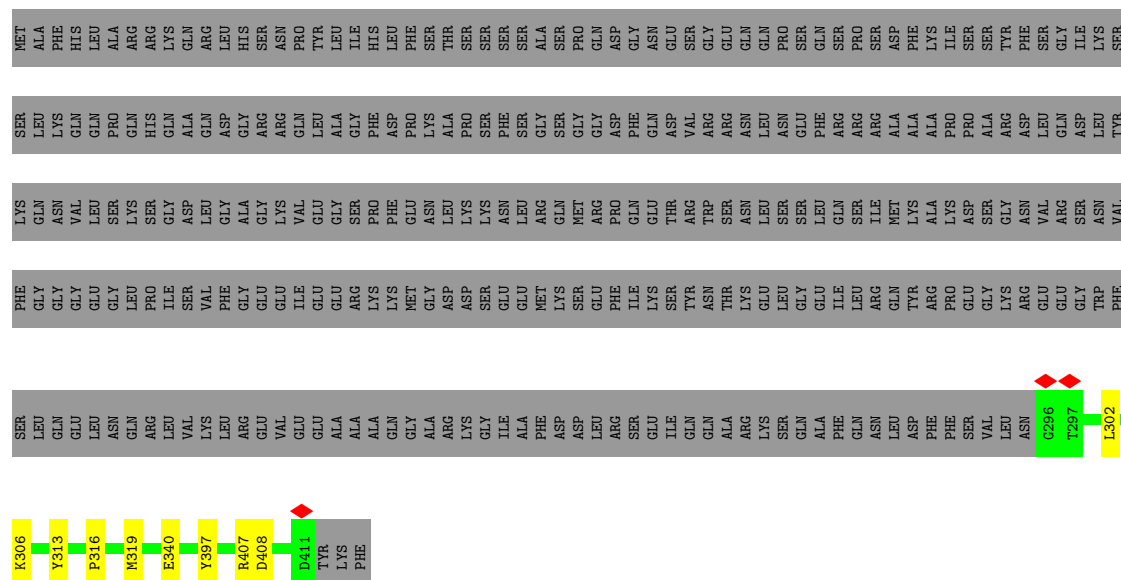
- Molecule 14: uS14m

Chain M:  58% 7% 35%



- Molecule 15: Small ribosomal subunit protein uS15c

Chain N:  26% 72%



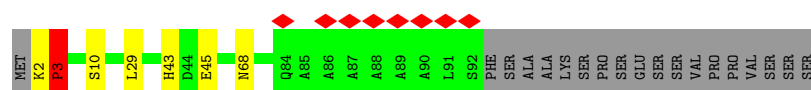
- Molecule 16: 30S ribosomal protein S16

Chain O:  73% 8% 19%



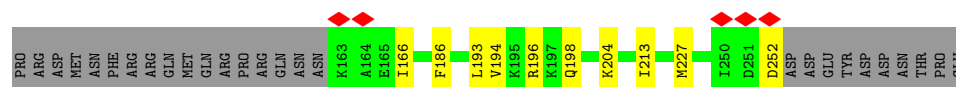
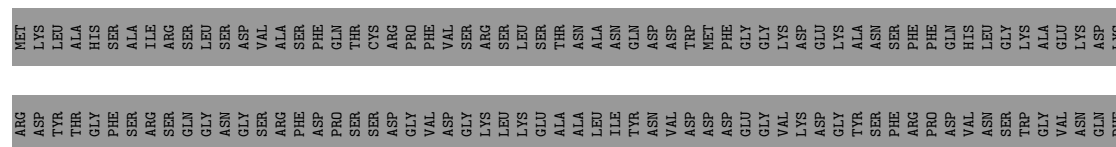
• Molecule 17: uS17m

Chain P:  7% 76% 5% 17%



• Molecule 18: bS18m

Chain Q:  34% 62%



• Molecule 19: Small ribosomal subunit protein uS19m

Chain R:  7% 71% 8% 22%



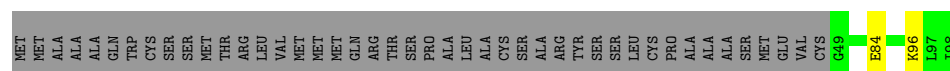
• Molecule 20: Ribosomal protein S21

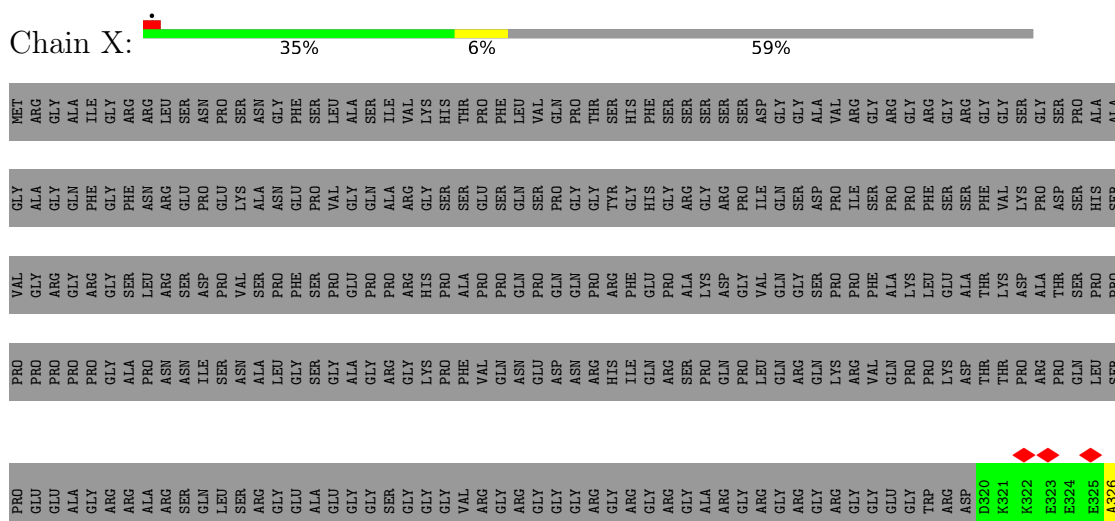
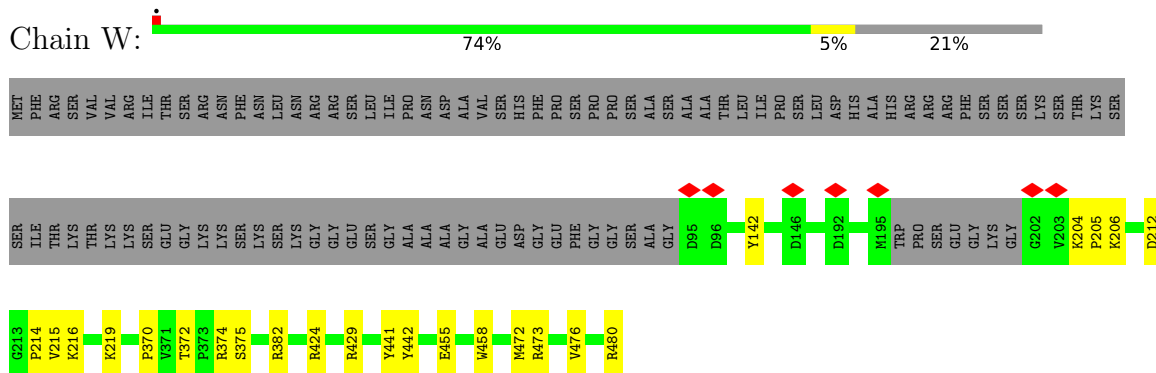
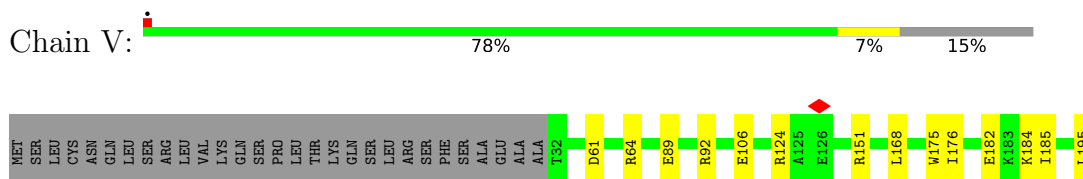
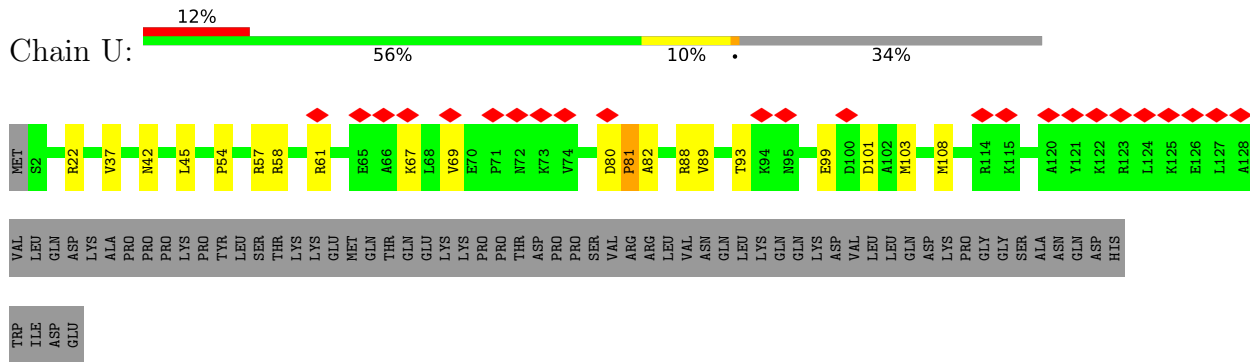
Chain S:  66% 9% 25%

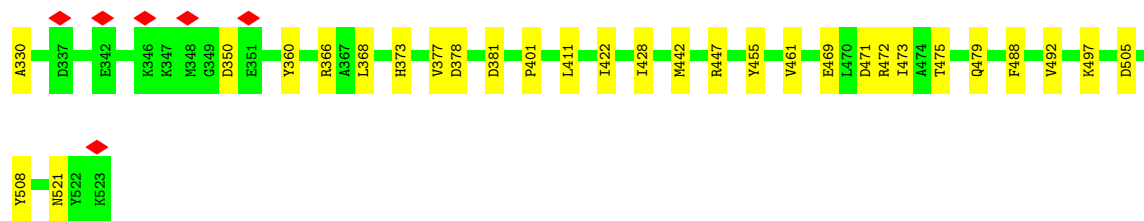


• Molecule 21: 30S ribosomal protein S31, mitochondrial

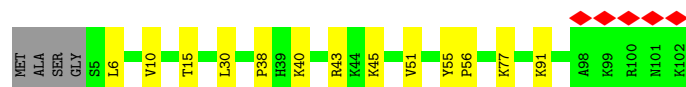
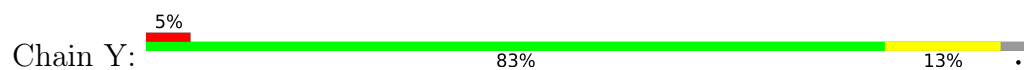
Chain T:  51% 47%



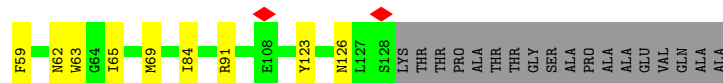
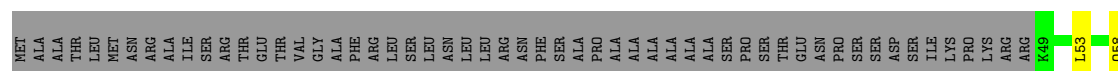




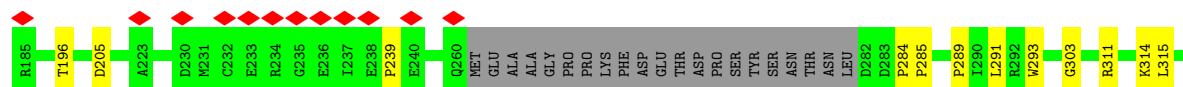
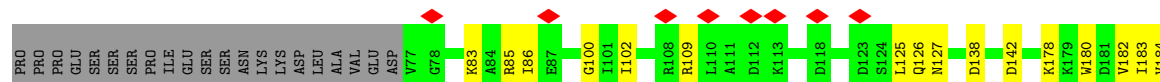
• Molecule 26: mS33



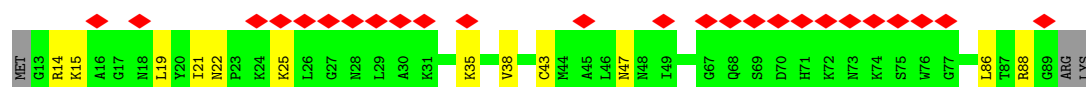
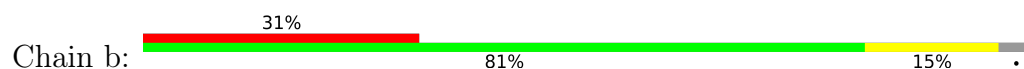
• Molecule 27: mS34

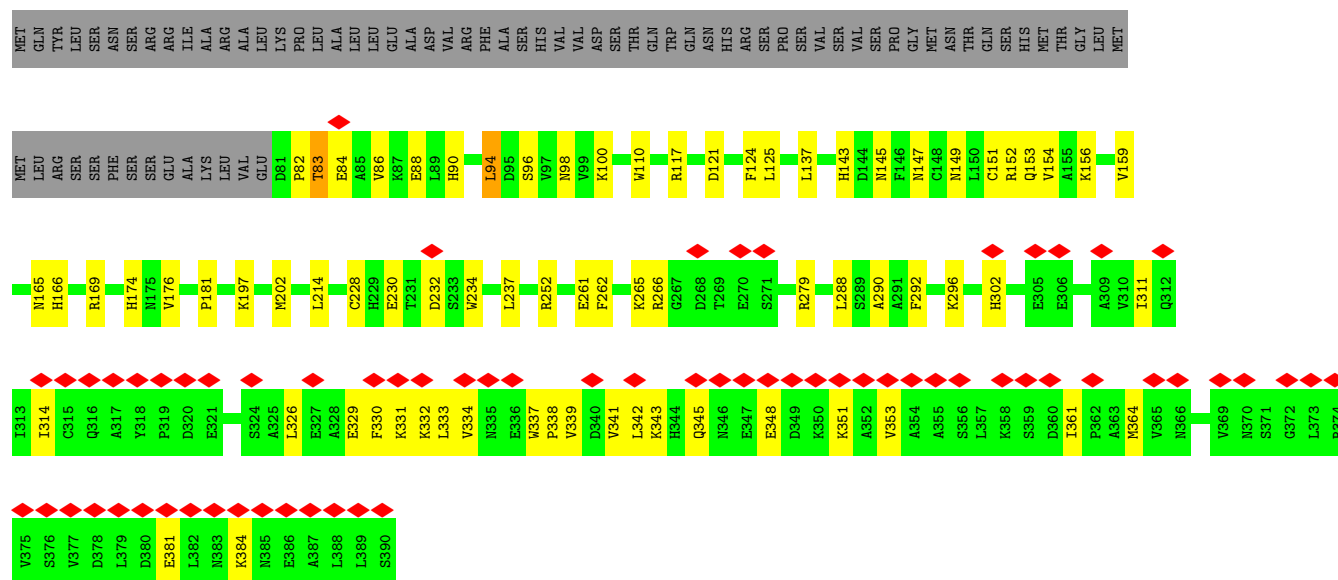
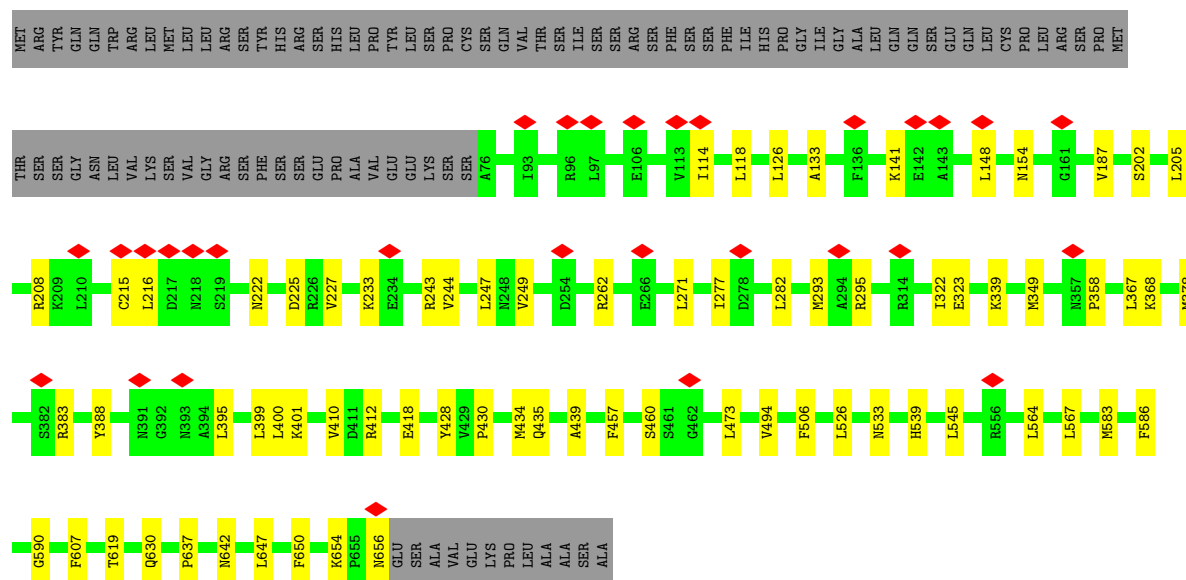


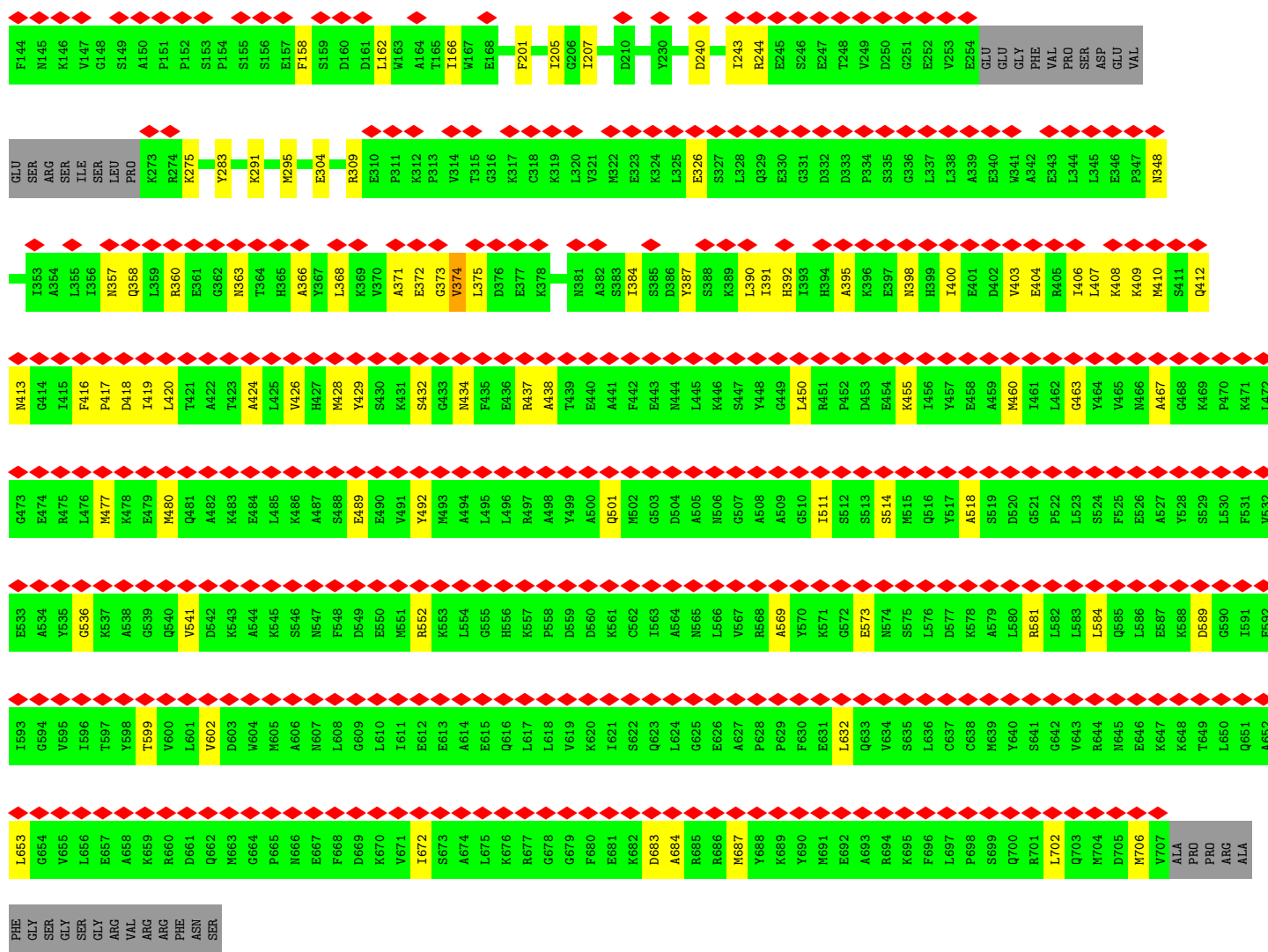
• Molecule 28: mS35



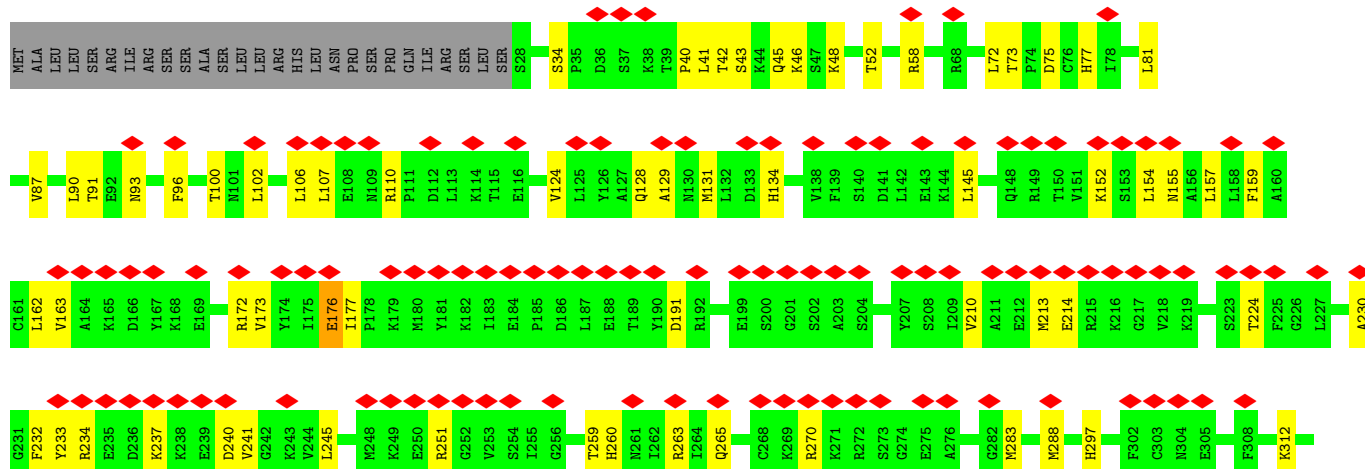
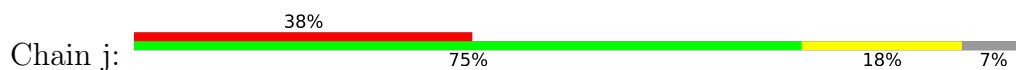
• Molecule 29: mS37

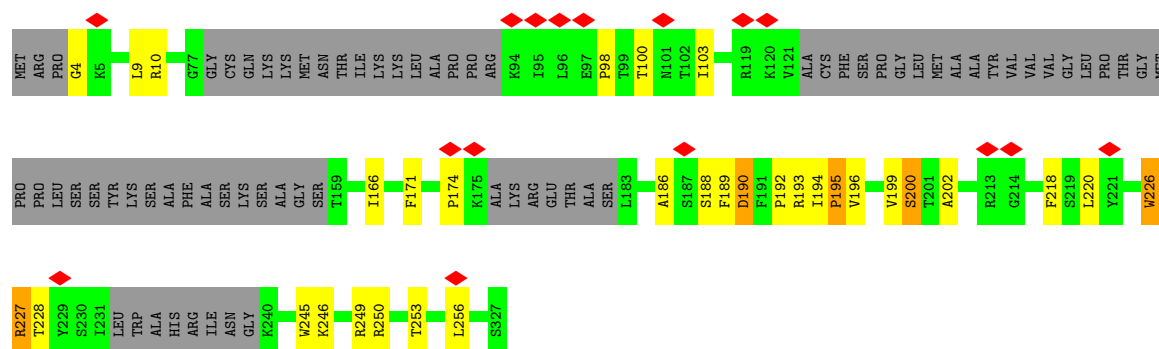




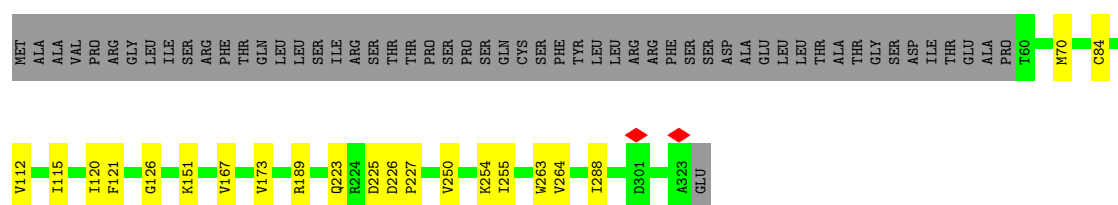
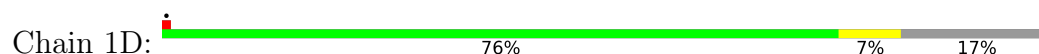


• Molecule 37: mS76 (rPPR1)

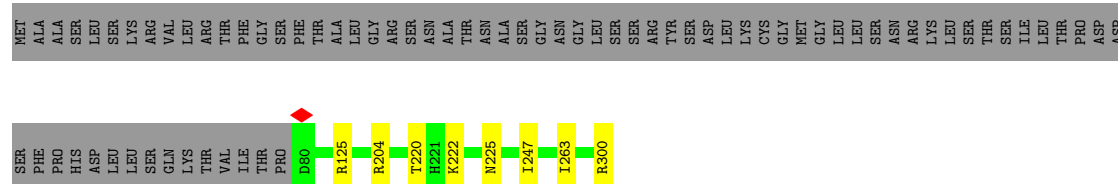




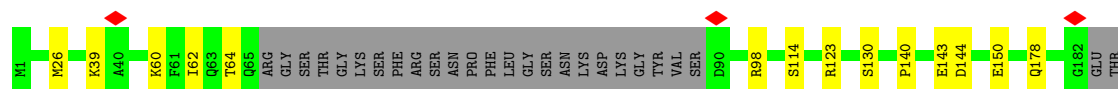
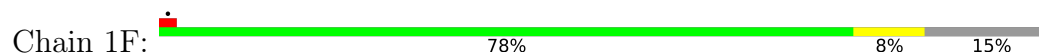
• Molecule 42: uL3m



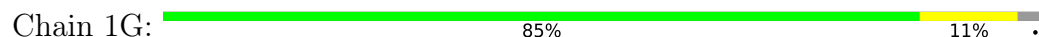
• Molecule 43: uL4m



• Molecule 44: uL5m

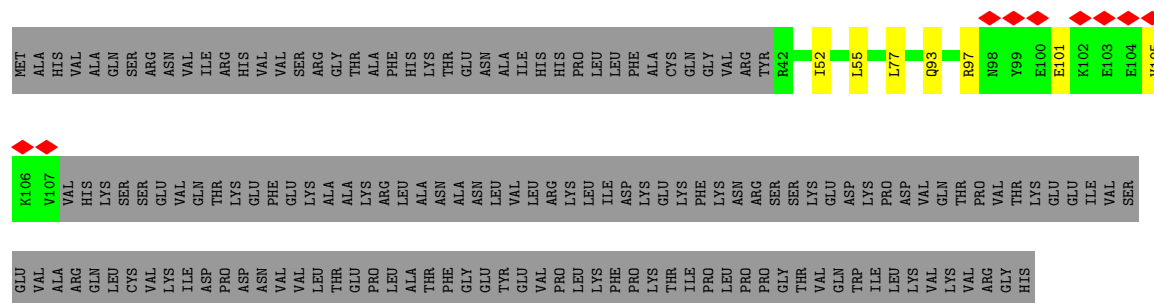


• Molecule 45: Large ribosomal subunit protein uL6 alpha-beta domain-containing protein

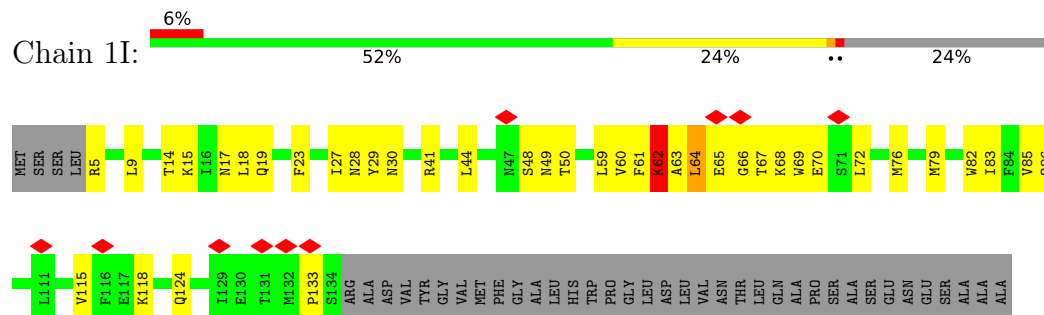


• Molecule 46: bL9m

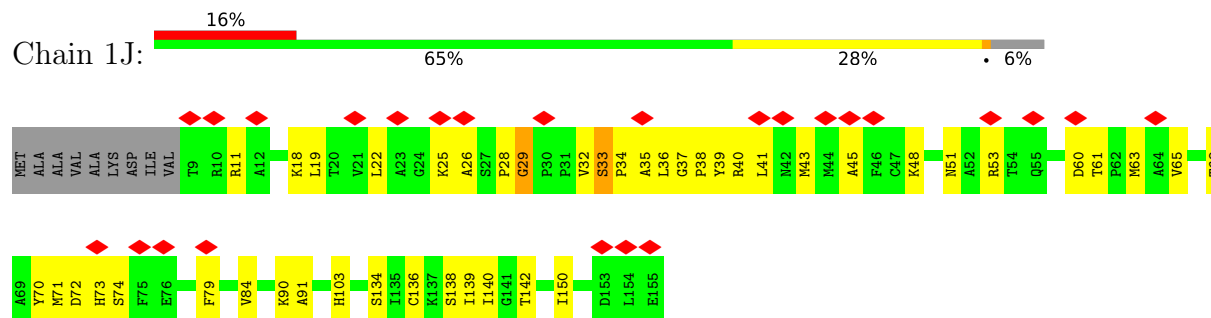




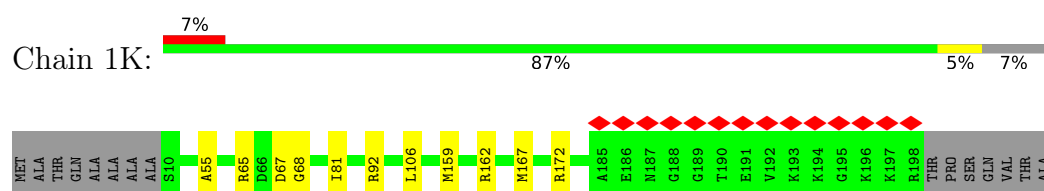
• Molecule 47: uL10m



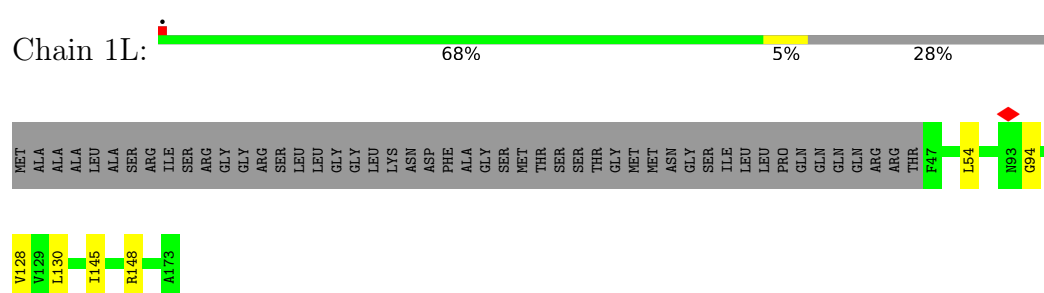
• Molecule 48: uL11m



• Molecule 49: 50S ribosomal protein L13

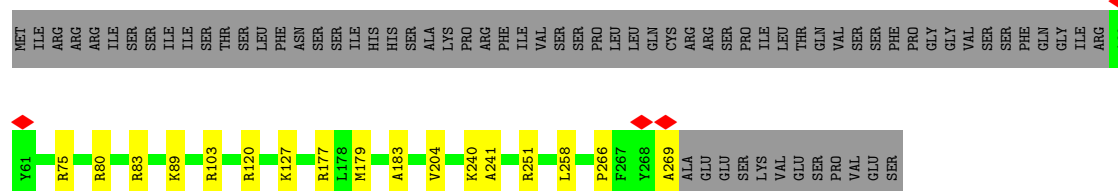


• Molecule 50: uL14m



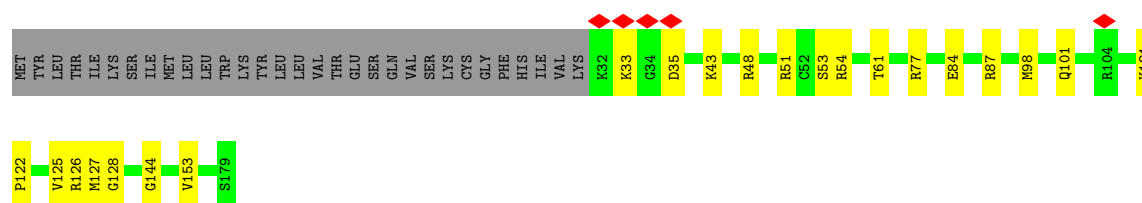
- Molecule 51: uL15m

Chain 1M:



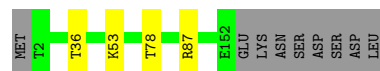
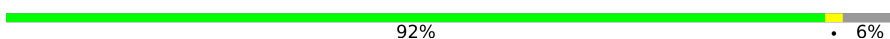
- Molecule 52: Large ribosomal subunit protein uL16m

Chain 1N:



- Molecule 53: 50S ribosomal protein L17

Chain 10:



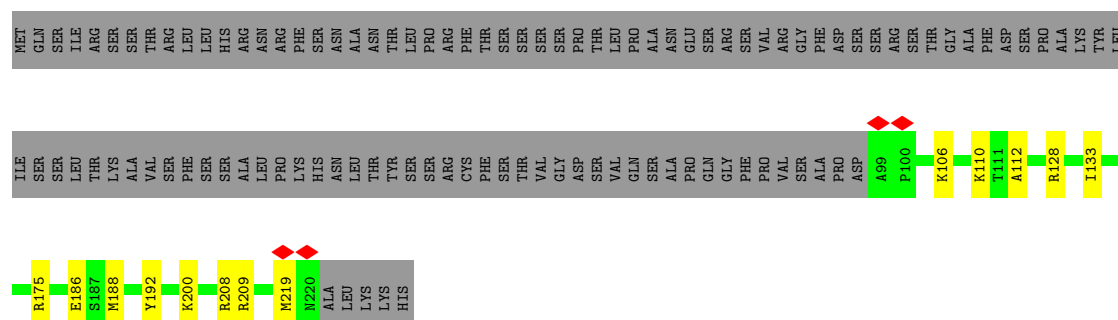
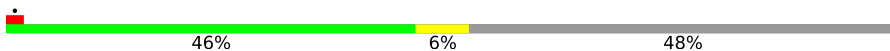
- Molecule 54: Ribosomal protein L18e/L15P domain-containing protein

Chain 1P:



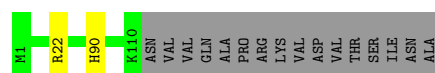
- Molecule 55: bL19m

Chain 1Q:



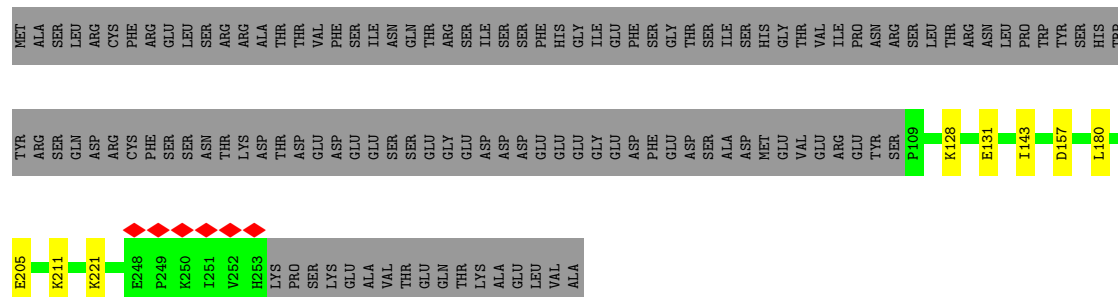
- Molecule 56: bL20m

Chain 1R:  86% 13%



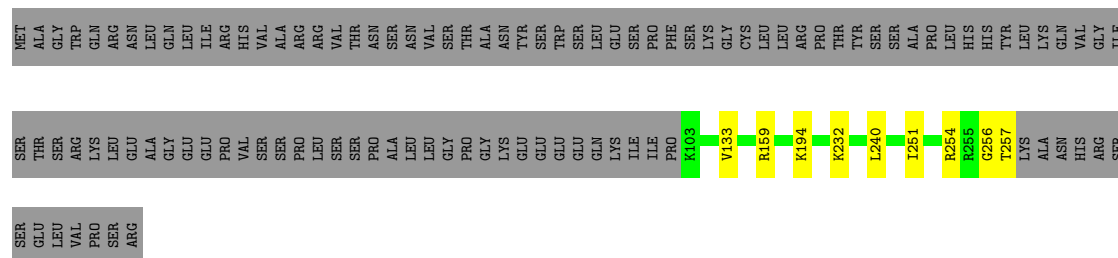
• Molecule 57: bL21m

Chain 1S:  51% 46%



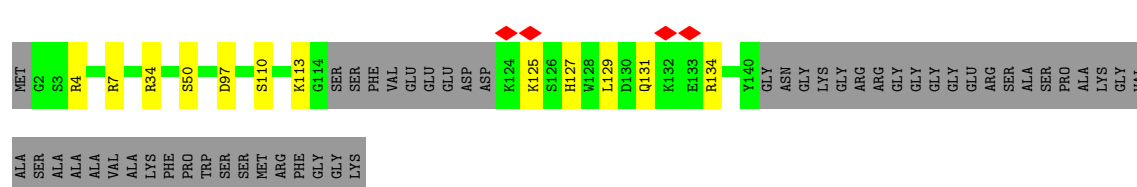
• Molecule 58: Large ribosomal subunit protein uL22m

Chain 1T:  55% 41%



• Molecule 59: uL23m

Chain 1U:  66% 7% 28%



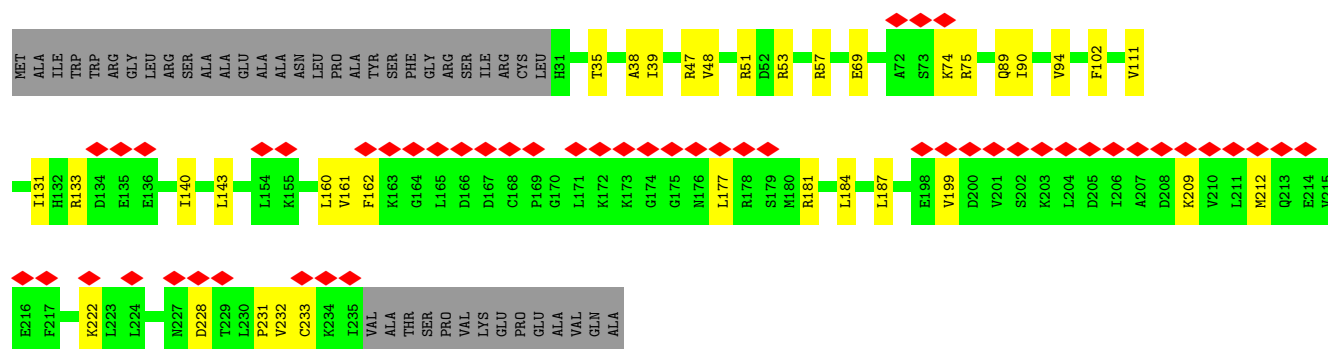
• Molecule 60: uL24m

Chain 1V:  87% 13%

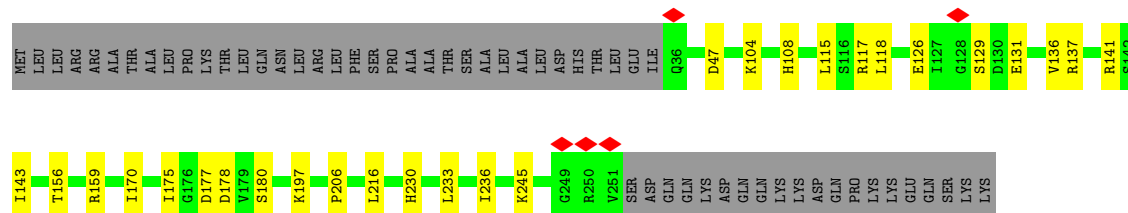


• Molecule 61: bL25-2m

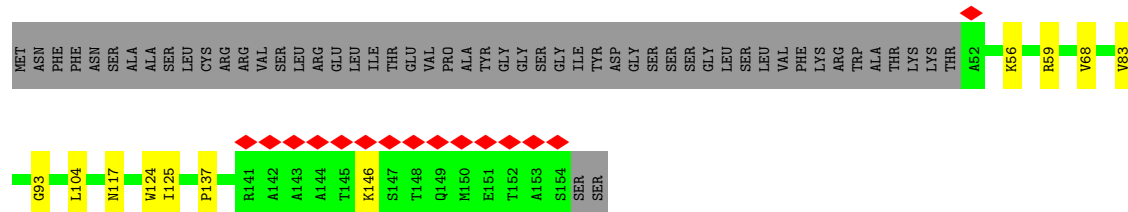
Chain 1W:  21% 69% 14% 17%



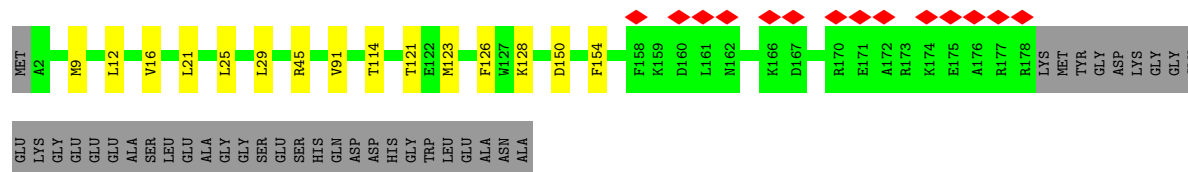
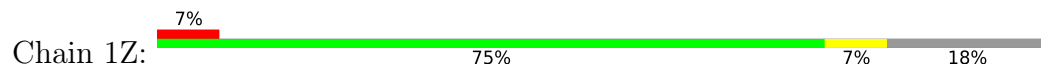
• Molecule 62: bL25m



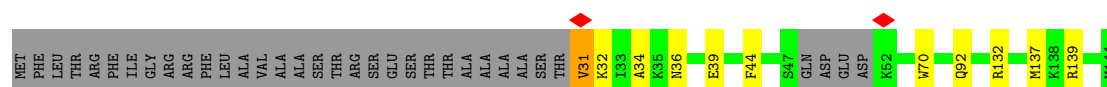
• Molecule 63: 50S ribosomal protein L27



• Molecule 64: bL28m

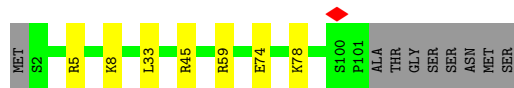


• Molecule 65: uL29m



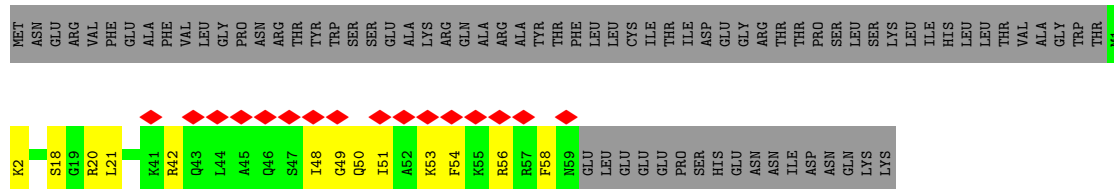
- Molecule 66: uL30m

Chain 1b:  85% 6% 8%



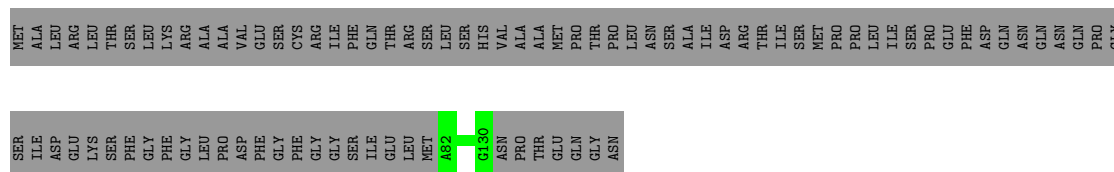
- Molecule 67: bL31m

Chain 1c:  12% 34% 10% 56%



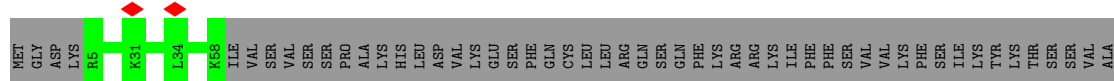
- Molecule 68: bL32m

Chain 1d:  35% 65%



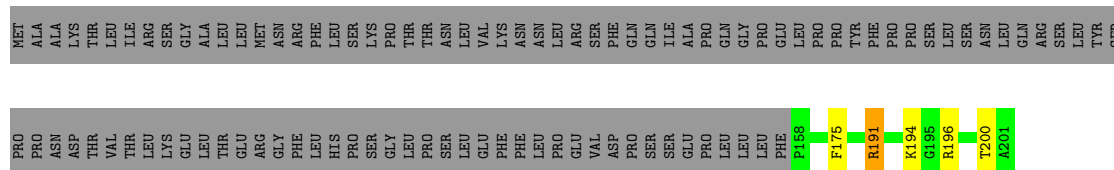
- Molecule 69: bL33m

Chain 1e:  51% 49%



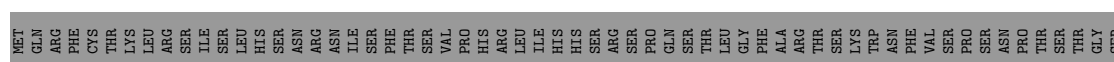
- Molecule 70: Large ribosomal subunit protein bL34m

Chain 1f:  27% 70%



- Molecule 71: bL35m

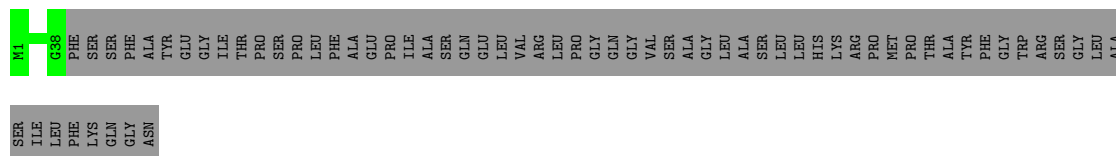
Chain 1g:  51% 6% 44%





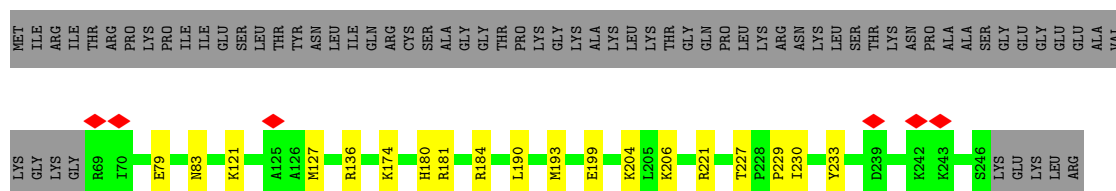
- Molecule 72: Ribosomal protein

Chain 1h: 37% 63%



- Molecule 73: mL40

Chain 1i: 64% 8% 28%



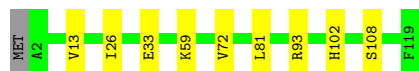
- Molecule 74: mL41

Chain 1j: 72% 7% 21%



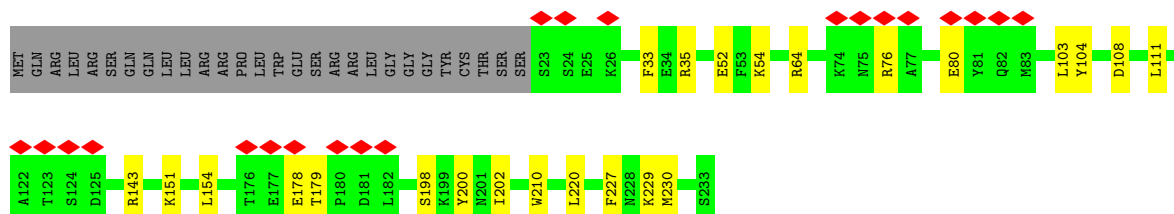
- Molecule 75: Large ribosomal subunit protein mL43

Chain 1k: 92% 8%



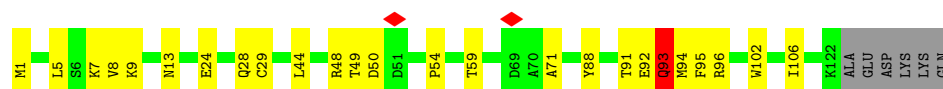
- Molecule 76: mL46

Chain 1l: 9% 78% 10% 12%

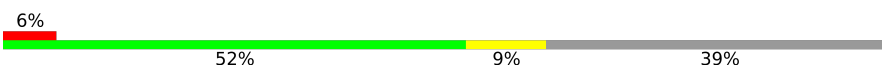


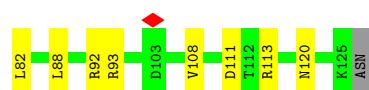
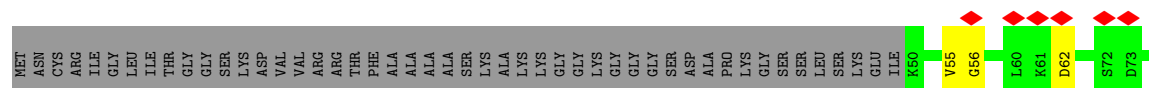
- Molecule 77: mL53

Chain 1m:  76% 19% 5%



• Molecule 78: mL54

Chain 1o:  52% 9% 39%



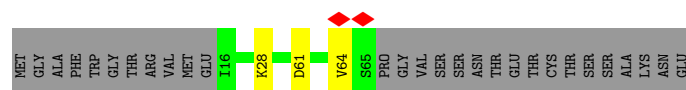
• Molecule 79: mL59/mL64

Chain 1p:  86% 10% 6%

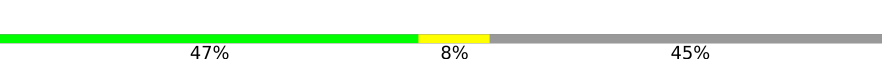


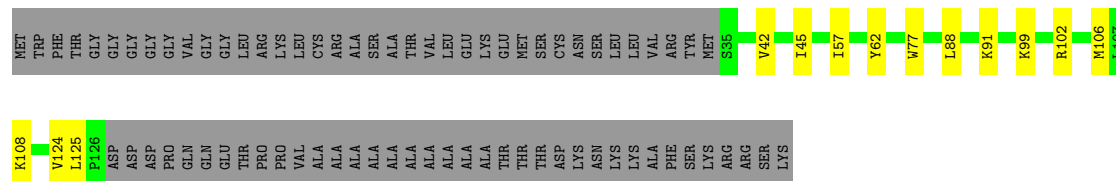
• Molecule 80: mL60

Chain 1q:  60% 36% 6%



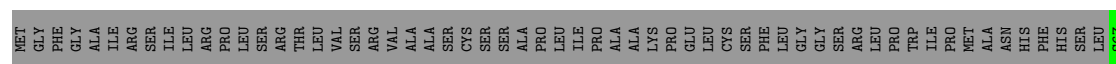
• Molecule 81: mL80

Chain 1r:  47% 45% 8%



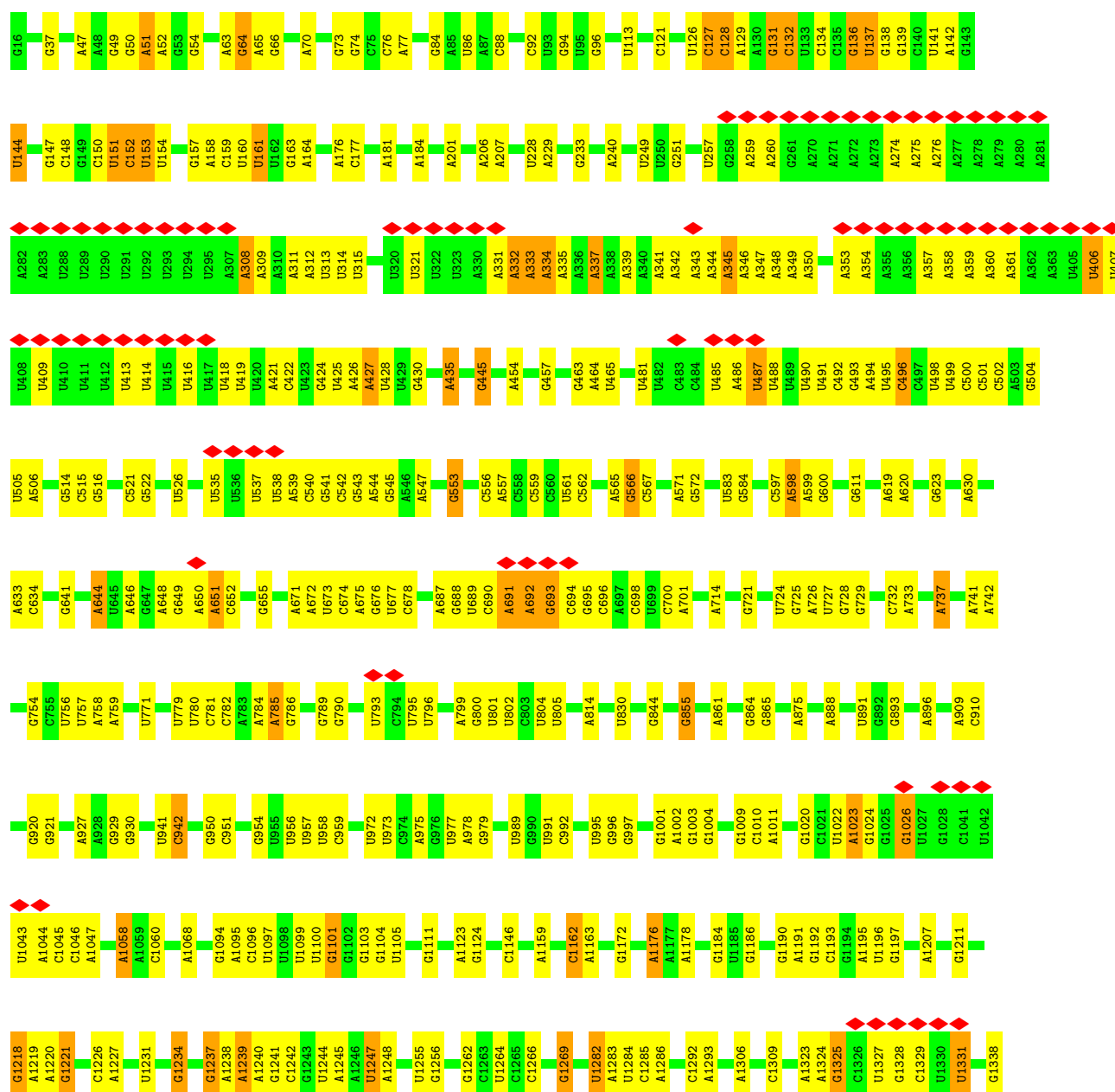
• Molecule 82: mL87

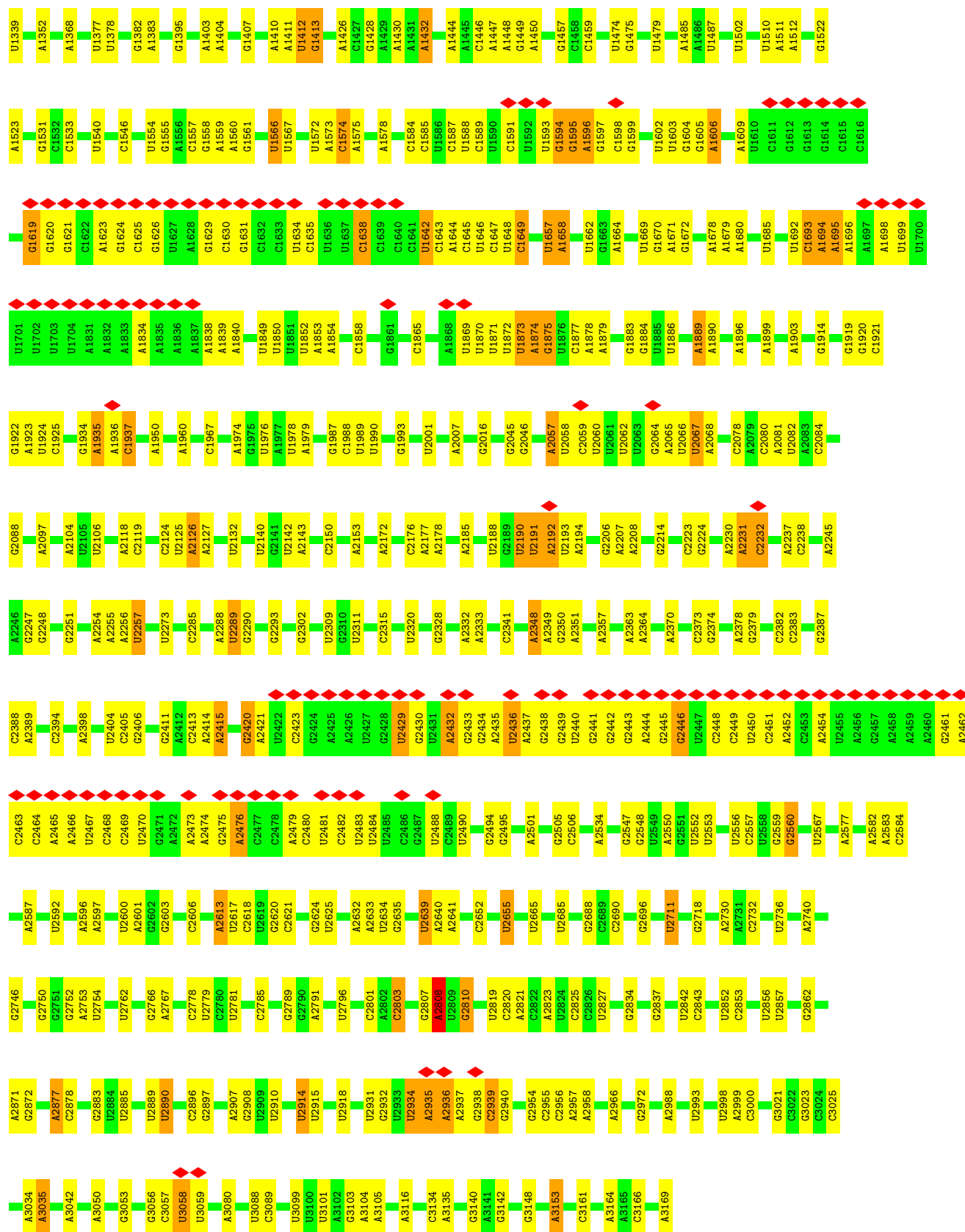
Chain 1s:  59% 35% 7%



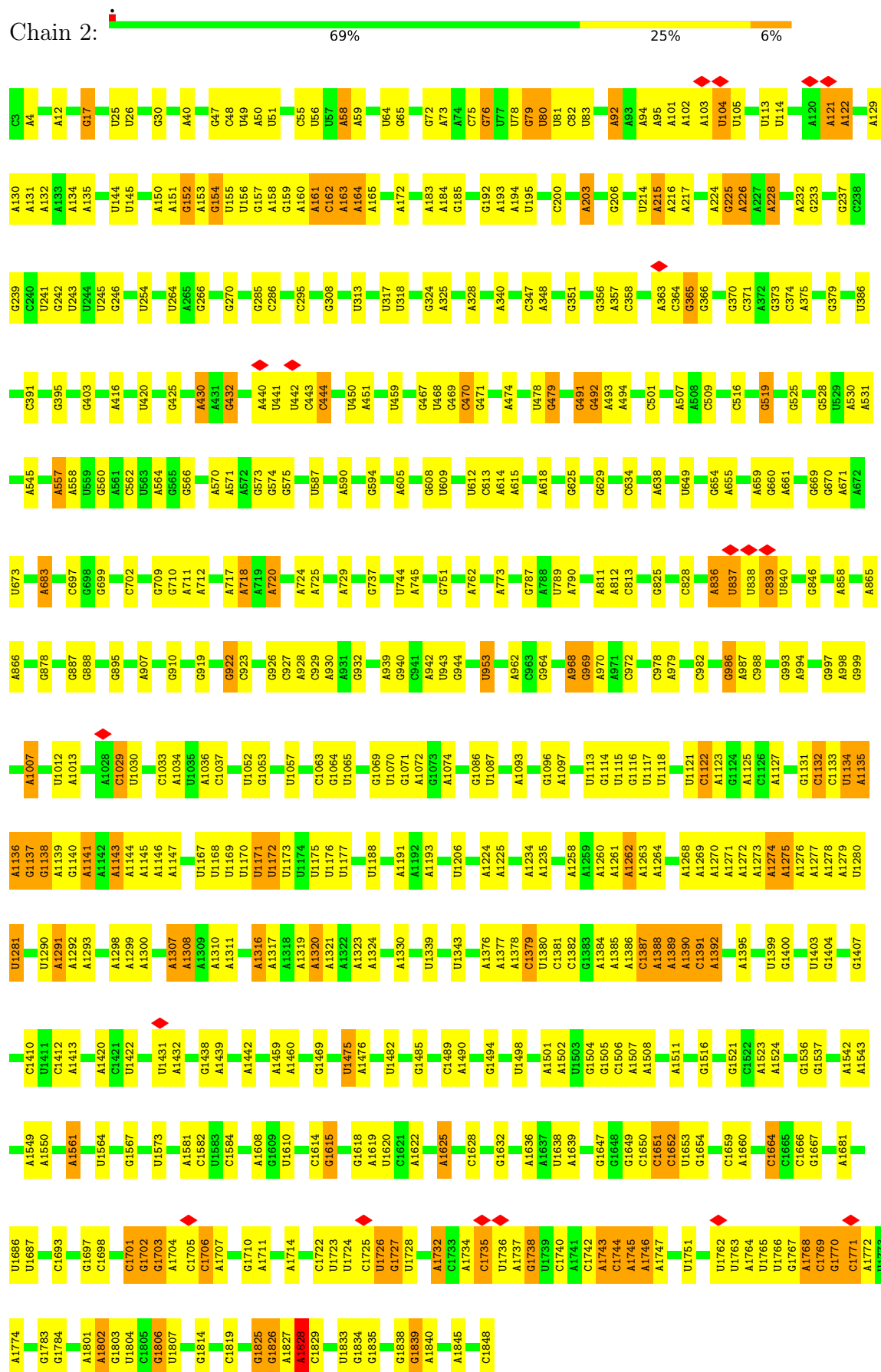


- Molecule 86: 26S rRNA





• Molecule 87: 18S rRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	219403	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	41.66	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	165000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	1.628	Depositor
Minimum map value	0.000	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.0854	Depositor
Map size (Å)	551.12396, 551.12396, 551.12396	wwPDB
Map dimensions	588, 588, 588	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93728566, 0.93728566, 0.93728566	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	3	0.21	0/2810	0.39	0/4378
2	A	0.28	0/1647	0.44	0/2227
3	B	0.26	0/3969	0.47	2/5320 (0.0%)
4	C	0.29	0/2859	0.54	1/3828 (0.0%)
5	D	0.30	0/3474	0.48	0/4647
6	E	0.31	0/838	0.41	0/1121
7	F	0.16	0/1225	0.48	0/1641
8	G	0.36	0/1054	0.50	0/1418
9	H	0.19	0/1696	0.48	2/2273 (0.1%)
10	I	0.17	0/964	0.42	0/1293
11	J	0.40	0/1000	0.53	0/1340
12	K	0.32	0/1010	0.44	0/1345
13	L	0.14	0/883	0.37	0/1176
14	M	0.14	0/856	0.30	0/1134
15	N	0.30	0/958	0.44	0/1280
16	O	0.35	0/890	0.49	0/1196
17	P	0.30	0/730	0.51	1/984 (0.1%)
18	Q	0.27	0/733	0.44	0/978
19	R	0.14	0/1323	0.35	0/1772
20	S	0.24	0/614	0.36	0/809
21	T	0.14	0/416	0.31	0/547
22	U	0.28	0/1036	0.57	1/1395 (0.1%)
23	V	0.26	0/1423	0.43	0/1895
24	W	0.14	0/3139	0.33	0/4250
25	X	0.36	0/1644	0.55	1/2216 (0.0%)
26	Y	0.48	1/807 (0.1%)	0.44	0/1077
27	Z	0.20	0/669	0.39	0/900
28	a	0.18	0/2523	0.50	3/3386 (0.1%)
29	b	0.20	0/618	0.59	0/822
30	c	0.31	0/233	0.44	0/296
31	d	0.29	0/628	0.42	0/840
32	e	0.32	0/2118	0.54	0/2828

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	f	0.26	0/2981	0.49	0/4033
34	g	0.16	0/4599	0.43	0/6181
35	h	0.38	0/2511	0.59	1/3391 (0.0%)
36	i	0.20	0/4847	0.47	2/6505 (0.0%)
37	j	0.21	0/3028	0.58	2/4067 (0.0%)
38	k	0.18	0/224	0.37	0/297
39	l	0.25	3/3523 (0.1%)	0.41	2/4739 (0.0%)
40	1B	0.22	0/1348	0.47	0/1797
41	1C	0.29	0/1730	0.52	1/2314 (0.0%)
42	1D	0.21	0/2099	0.44	0/2836
43	1E	0.19	0/1787	0.38	0/2412
44	1F	0.15	0/1310	0.39	0/1768
45	1G	0.16	0/796	0.38	0/1067
46	1H	0.19	0/547	0.44	0/731
47	1I	0.50	0/1054	0.74	5/1417 (0.4%)
48	1J	0.32	0/1160	0.64	0/1569
49	1K	0.20	0/1553	0.37	0/2080
50	1L	0.18	0/976	0.40	0/1304
51	1M	0.22	0/1682	0.46	0/2248
52	1N	0.19	0/1184	0.39	0/1580
53	1O	0.22	0/1255	0.45	0/1687
54	1P	0.18	0/895	0.36	0/1206
55	1Q	0.20	0/1022	0.38	0/1368
56	1R	0.25	0/930	0.43	0/1234
57	1S	0.22	0/1186	0.41	0/1596
58	1T	0.20	0/1259	0.39	0/1687
59	1U	0.19	0/1065	0.38	0/1421
60	1V	0.23	0/1247	0.38	0/1681
61	1W	0.23	0/1614	0.41	0/2175
62	1X	0.17	0/1703	0.40	0/2307
63	1Y	0.19	0/817	0.37	0/1095
64	1Z	0.24	0/1463	0.41	0/1946
65	1a	0.30	0/946	0.43	0/1262
66	1b	0.21	0/816	0.48	0/1096
67	1c	0.13	0/501	0.32	0/666
68	1d	0.21	0/387	0.47	0/514
69	1e	0.16	0/468	0.35	0/618
70	1f	0.37	0/370	0.60	1/486 (0.2%)
71	1g	0.35	0/792	0.56	1/1051 (0.1%)
72	1h	0.19	0/312	0.37	0/409
73	1i	0.14	0/1394	0.33	0/1868
74	1j	0.22	0/586	0.43	0/789
75	1k	0.20	0/970	0.37	0/1309

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	1l	0.14	0/1789	0.36	0/2421
77	1m	0.37	1/987 (0.1%)	0.77	1/1331 (0.1%)
78	1o	0.23	0/628	0.41	0/848
79	1p	0.19	0/1014	0.33	0/1349
80	1q	0.19	0/393	0.33	0/525
81	1r	0.22	0/750	0.46	0/1005
82	1s	0.20	0/1001	0.40	0/1327
83	1t	0.16	0/3919	0.41	0/5272
84	1u	0.18	0/5350	0.47	0/7190
85	1v	0.20	0/3497	0.45	0/4685
86	1	0.27	2/69709 (0.0%)	0.42	10/108649 (0.0%)
87	2	0.34	1/42141 (0.0%)	0.42	3/65658 (0.0%)
All	All	0.27	8/236902 (0.0%)	0.44	40/342679 (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
42	1D	0	1
52	1N	0	1
77	1m	0	1
83	1t	0	1
All	All	0	4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	1	1574	C	O3'-P	-19.72	1.31	1.61
87	2	922	G	O3'-P	-14.68	1.39	1.61
86	1	1264	U	O3'-P	14.61	1.83	1.61
77	1m	93	GLN	C-N	-9.46	1.20	1.33
39	l	485	ARG	N-CA	-7.08	1.37	1.46
39	l	484	ILE	C-N	-5.74	1.26	1.33
26	Y	45	LYS	CA-C	-5.64	1.45	1.52
39	l	485	ARG	CA-CB	-5.13	1.45	1.53

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
77	1m	93	GLN	O-C-N	-22.73	92.37	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	1	1657	U	O3'-P-O5'	22.11	137.16	104.00
86	1	1657	U	P-O3'-C3'	-21.86	87.42	120.20
86	1	1574	C	P-O3'-C3'	14.35	141.72	120.20
87	2	922	G	P-O3'-C3'	-11.37	103.15	120.20
86	1	1657	U	OP1-P-O3'	-11.07	74.80	108.00
28	a	239	PRO	N-CA-CB	10.65	109.82	102.79
86	1	1574	C	O3'-P-O5'	9.29	117.94	104.00
22	U	81	PRO	CA-N-CD	-9.04	99.34	112.00
47	1I	62	LYS	N-CA-C	-8.94	91.77	110.80
17	P	3	PRO	CA-N-CD	-8.69	99.83	112.00
3	B	212	PRO	CA-N-CD	-8.66	99.88	112.00
71	1g	119	LYS	N-CA-C	8.44	121.54	111.33
87	2	922	G	O3'-P-O5'	8.28	116.42	104.00
28	a	284	PRO	N-CA-CB	7.62	110.47	103.08
47	1I	63	ALA	N-CA-C	-7.55	102.59	112.41
41	1C	200	SER	N-CA-C	7.32	119.89	111.11
86	1	1264	U	O3'-P-O5'	7.17	114.75	104.00
4	C	280	PRO	N-CA-CB	6.89	110.58	103.00
47	1I	89	ASP	CA-C-N	6.88	124.58	120.24
47	1I	89	ASP	C-N-CA	6.88	124.58	120.24
87	2	922	G	OP1-P-O3'	-6.68	87.97	108.00
47	1I	64	LEU	N-CA-C	-6.38	103.11	113.19
35	h	94	LEU	N-CA-C	-6.26	105.60	113.18
70	1f	191	ARG	CG-CD-NE	6.08	125.39	112.00
28	a	285	PRO	N-CA-CB	6.03	110.28	102.86
3	B	104	ALA	N-CA-C	-5.94	98.59	108.32
86	1	1566	U	P-O3'-C3'	5.78	128.87	120.20
25	X	479	GLN	N-CA-C	5.34	117.86	111.71
86	1	655	G	O4'-C1'-N9	5.20	115.99	108.20
9	H	224	VAL	CA-C-N	5.15	131.25	121.97
9	H	224	VAL	C-N-CA	5.15	131.25	121.97
37	j	176	GLU	CA-C-N	5.08	124.39	120.33
37	j	176	GLU	C-N-CA	5.08	124.39	120.33
36	i	416	PHE	N-CA-C	5.07	114.13	108.25
86	1	2057	A	P-O3'-C3'	5.06	127.79	120.20
39	l	484	ILE	CA-C-N	-5.04	113.13	120.29
39	l	484	ILE	C-N-CA	-5.04	113.13	120.29
86	1	1574	C	OP2-P-O3'	-5.04	92.89	108.00
36	i	501	GLN	N-CA-CB	5.01	118.02	110.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
42	1D	225	ASP	Peptide
52	1N	126	ARG	Peptide
77	1m	93	GLN	Mainchain
83	1t	462	HIS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	3	2513	0	1275	22	0
2	A	1611	0	1633	23	0
3	B	3877	0	4008	103	0
4	C	2806	0	2971	33	0
5	D	3425	0	3453	33	0
6	E	823	0	879	19	0
7	F	1254	0	1268	20	0
8	G	1037	0	1058	8	0
9	H	1671	0	1713	23	0
10	I	941	0	970	14	0
11	J	988	0	1020	20	0
12	K	993	0	1051	7	0
13	L	873	0	904	11	0
14	M	843	0	884	20	0
15	N	941	0	978	11	0
16	O	869	0	898	8	0
17	P	717	0	755	17	0
18	Q	724	0	744	9	0
19	R	1299	0	1307	33	0
20	S	611	0	687	18	0
21	T	408	0	444	2	0
22	U	1014	0	1061	44	0
23	V	1399	0	1427	10	0
24	W	3062	0	3029	16	0
25	X	1613	0	1559	39	0
26	Y	793	0	834	12	0
27	Z	649	0	661	45	0
28	a	2486	0	2376	70	0
29	b	610	0	626	51	0
30	c	232	0	278	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	d	616	0	674	10	0
32	e	2074	0	2074	24	0
33	f	2922	0	2870	69	0
34	g	4527	0	4564	44	0
35	h	2463	0	2488	82	0
36	i	4766	0	4759	97	0
37	j	2980	0	3031	60	0
38	k	220	0	223	3	0
39	l	3468	0	3522	125	0
40	1B	1326	0	1397	23	0
41	1C	1699	0	1754	44	0
42	1D	2045	0	2080	18	0
43	1E	1754	0	1815	7	0
44	1F	1283	0	1272	18	0
45	1G	779	0	810	6	0
46	1H	539	0	574	6	0
47	1I	1036	0	1084	41	0
48	1J	1133	0	1166	77	0
49	1K	1526	0	1586	10	0
50	1L	966	0	1048	8	0
51	1M	1649	0	1765	15	0
52	1N	1160	0	1206	17	0
53	1O	1231	0	1262	3	0
54	1P	878	0	939	24	0
55	1Q	1008	0	1101	14	0
56	1R	915	0	946	2	0
57	1S	1164	0	1223	7	0
58	1T	1241	0	1346	8	0
59	1U	1048	0	1123	20	0
60	1V	1223	0	1278	16	0
61	1W	1591	0	1675	38	0
62	1X	1670	0	1751	20	0
63	1Y	800	0	820	15	0
64	1Z	1439	0	1483	27	0
65	1a	928	0	959	8	0
66	1b	801	0	837	8	0
67	1c	489	0	511	41	0
68	1d	379	0	416	0	0
69	1e	459	0	491	0	0
70	1f	364	0	398	3	0
71	1g	773	0	843	9	0
72	1h	309	0	337	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
73	1i	1378	0	1426	19	0
74	1j	570	0	592	9	0
75	1k	952	0	987	6	0
76	1l	1739	0	1705	30	0
77	1m	970	0	979	31	0
78	1o	617	0	641	14	0
79	1p	992	0	1027	5	0
80	1q	389	0	416	2	0
81	1r	735	0	781	19	0
82	1s	985	0	1072	8	0
83	1t	3856	0	3912	39	0
84	1u	5269	0	5341	116	0
85	1v	3440	0	3497	57	0
86	1	62518	0	31501	367	0
87	2	37784	0	19036	433	0
88	1	243	0	0	0	0
88	1D	2	0	0	0	0
88	1q	2	0	0	0	0
88	2	97	0	0	0	0
88	3	3	0	0	0	0
88	T	1	0	0	0	0
88	W	1	0	0	0	0
89	W	31	0	12	1	0
90	1	62	0	0	0	0
90	1B	2	0	0	0	0
90	1E	1	0	0	0	0
90	2	19	0	0	0	0
91	1d	1	0	0	0	0
91	1h	1	0	0	0	0
92	1	5283	0	0	6	0
92	1B	44	0	0	0	0
92	1C	33	0	0	0	0
92	1D	55	0	0	0	0
92	1E	59	0	0	0	0
92	1F	31	0	0	0	0
92	1G	5	0	0	0	0
92	1H	7	0	0	0	0
92	1K	57	0	0	0	0
92	1L	25	0	0	2	0
92	1M	50	0	0	2	0
92	1N	17	0	0	1	0
92	1O	32	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
92	1P	44	0	0	0	0
92	1Q	24	0	0	1	0
92	1R	34	0	0	0	0
92	1S	29	0	0	1	0
92	1T	40	0	0	1	0
92	1U	22	0	0	2	0
92	1V	36	0	0	1	0
92	1W	5	0	0	0	0
92	1X	26	0	0	0	0
92	1Y	27	0	0	0	0
92	1Z	34	0	0	0	0
92	1a	15	0	0	0	0
92	1b	24	0	0	1	0
92	1c	8	0	0	0	0
92	1d	9	0	0	0	0
92	1e	6	0	0	0	0
92	1f	21	0	0	0	0
92	1g	35	0	0	1	0
92	1h	5	0	0	0	0
92	1i	55	0	0	1	0
92	1j	34	0	0	0	0
92	1k	24	0	0	0	0
92	1l	56	0	0	1	0
92	1m	3	0	0	0	0
92	1p	33	0	0	0	0
92	1q	17	0	0	0	0
92	1r	9	0	0	1	0
92	1s	22	0	0	0	0
92	1t	88	0	0	7	0
92	1u	15	0	0	0	0
92	1v	16	0	0	0	0
92	2	2491	0	0	5	0
92	3	79	0	0	1	0
92	A	37	0	0	1	0
92	B	37	0	0	0	0
92	C	63	0	0	0	0
92	D	91	0	0	3	0
92	E	18	0	0	0	0
92	F	8	0	0	1	0
92	G	37	0	0	1	0
92	H	36	0	0	0	0
92	I	28	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
92	J	23	0	0	1	0
92	K	25	0	0	0	0
92	L	16	0	0	1	0
92	M	23	0	0	3	0
92	N	42	0	0	0	0
92	O	39	0	0	2	0
92	P	21	0	0	0	0
92	Q	25	0	0	1	0
92	R	15	0	0	0	0
92	S	16	0	0	1	0
92	T	19	0	0	0	0
92	U	15	0	0	0	0
92	V	26	0	0	0	0
92	W	49	0	0	0	0
92	X	17	0	0	0	0
92	Y	19	0	0	0	0
92	Z	11	0	0	0	0
92	a	33	0	0	0	0
92	b	2	0	0	2	0
92	c	6	0	0	0	0
92	d	10	0	0	0	0
92	e	87	0	0	0	0
92	f	35	0	0	0	0
92	h	17	0	0	0	0
92	i	15	0	0	0	0
92	k	2	0	0	0	0
All	All	233430	0	175177	2315	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (2315) 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)
86:1:2257:5MU:C5	86:1:2257:5MU:C4	1.82	1.65
27:Z:91:ARG:NH2	87:2:152:G:C5	1.67	1.61
41:1C:100:THR:CG2	64:1Z:154:PHE:HZ	1.06	1.59
29:b:21:ILE:HA	87:2:1845:A:C2	1.37	1.59
41:1C:100:THR:CG2	64:1Z:154:PHE:CZ	1.81	1.57
39:l:279:ARG:NH1	39:l:281:PHE:CZ	1.69	1.54
39:l:545:HIS:HB3	87:2:1392:A:C2	1.40	1.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:1J:32:VAL:HG12	48:1J:43:MET:CE	1.28	1.53
48:1J:32:VAL:CG1	48:1J:43:MET:HE1	1.36	1.53
36:i:400:ILE:HD11	36:i:429:TYR:CE1	1.45	1.51
6:E:81:TYR:HE2	40:1B:52:HIS:CE1	1.30	1.50
33:f:290:VAL:CG1	33:f:299:LYS:HE2	1.39	1.49
39:l:545:HIS:CB	87:2:1392:A:C2	1.97	1.47
33:f:336:TYR:CE2	33:f:340:LEU:HD11	1.48	1.47
29:b:21:ILE:HB	87:2:1845:A:N1	1.30	1.46
36:i:400:ILE:CD1	36:i:429:TYR:HE1	1.25	1.46
6:E:81:TYR:CE2	40:1B:52:HIS:ND1	1.82	1.46
6:E:81:TYR:HE2	40:1B:52:HIS:ND1	1.07	1.45
76:1l:104:TYR:CZ	76:1l:198:SER:OG	1.67	1.45
29:b:21:ILE:CB	87:2:1845:A:N1	1.82	1.42
6:E:84:LYS:HE2	40:1B:56:ASN:ND2	1.18	1.41
76:1l:104:TYR:CE2	76:1l:198:SER:OG	1.72	1.41
29:b:21:ILE:HB	87:2:1845:A:C6	1.56	1.39
39:l:547:ASN:HB2	87:2:1391:C:N3	1.33	1.39
41:1C:100:THR:HG21	64:1Z:154:PHE:CZ	1.45	1.39
77:1m:92:GLU:HG3	77:1m:102:TRP:CD1	1.58	1.39
47:1I:49:ASN:HB2	47:1I:87:THR:CG2	1.54	1.35
48:1J:22:LEU:CD2	48:1J:60:ASP:OD1	1.75	1.35
6:E:78:GLU:O	40:1B:52:HIS:NE2	1.58	1.32
6:E:81:TYR:CE2	40:1B:52:HIS:CE1	2.15	1.32
39:l:474:LYS:HG2	87:2:1141:A:C2	1.64	1.30
6:E:78:GLU:O	40:1B:52:HIS:CE1	1.85	1.29
39:l:485:ARG:NH1	39:l:488:CYS:CB	1.97	1.28
50:1L:148:ARG:NH2	87:2:358:C:OP1	1.67	1.27
39:l:279:ARG:NH1	39:l:281:PHE:CE2	2.04	1.25
48:1J:34:PRO:O	48:1J:38:PRO:CD	1.84	1.25
37:j:107:LEU:HD21	37:j:145:LEU:CD1	1.66	1.25
39:l:545:HIS:CG	87:2:1392:A:C2	2.22	1.25
85:1v:179:ASP:OD1	85:1v:216:LEU:HD11	1.15	1.24
22:U:61:ARG:CD	87:2:837:U:O2'	1.86	1.24
22:U:61:ARG:CG	87:2:837:U:O2'	1.86	1.23
22:U:67:LYS:CG	22:U:69:VAL:HG23	1.67	1.23
36:i:400:ILE:CD1	36:i:429:TYR:CE1	2.10	1.23
19:R:167:PRO:HG3	67:1c:54:PHE:CD2	1.72	1.22
27:Z:59:PHE:CD1	35:h:176:VAL:HG13	1.74	1.22
48:1J:29:GLY:O	48:1J:33:SER:HB2	1.35	1.21
15:N:407:ARG:HH22	86:1:861:A:P	1.64	1.21
22:U:61:ARG:HD2	87:2:837:U:O2'	1.41	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:b:21:ILE:CA	87:2:1845:A:N1	2.02	1.21
33:f:336:TYR:CZ	33:f:340:LEU:HD11	1.73	1.20
29:b:21:ILE:CA	87:2:1845:A:C2	2.24	1.19
33:f:336:TYR:CE2	33:f:340:LEU:CD1	2.24	1.19
39:l:545:HIS:CB	87:2:1392:A:N1	2.03	1.19
84:1u:363:TYR:HE1	84:1u:382:VAL:CG1	1.55	1.19
44:1F:123:ARG:NE	86:1:2613:A:OP1	1.74	1.18
6:E:84:LYS:CE	40:1B:56:ASN:ND2	2.07	1.17
39:l:547:ASN:HB2	87:2:1391:C:C4	1.80	1.17
41:1C:100:THR:HG23	64:1Z:154:PHE:CZ	1.73	1.16
27:Z:91:ARG:NH2	87:2:152:G:C4	2.14	1.16
27:Z:59:PHE:CE1	35:h:176:VAL:HG13	1.82	1.15
47:1I:49:ASN:HB2	47:1I:87:THR:HG21	1.17	1.14
19:R:167:PRO:CD	67:1c:54:PHE:CE2	2.30	1.14
37:j:107:LEU:HD21	37:j:145:LEU:HD13	1.17	1.13
6:E:84:LYS:CE	40:1B:56:ASN:HD22	1.62	1.13
36:i:395:ALA:HB2	36:i:428:MET:HG3	1.20	1.13
85:1v:267:PHE:CE2	85:1v:271:MET:SD	2.41	1.13
39:l:485:ARG:NH1	39:l:488:CYS:HB2	1.62	1.13
27:Z:59:PHE:CE1	35:h:176:VAL:CG1	2.30	1.13
34:g:630:GLN:NE2	39:l:437:GLY:O	1.79	1.13
81:1r:62:TYR:CE1	81:1r:124:VAL:HG13	1.83	1.13
37:j:191:ASP:OD1	37:j:224:THR:HG22	1.48	1.12
84:1u:323:PRO:O	84:1u:354:PHE:CD1	2.02	1.12
48:1J:33:SER:HB3	48:1J:34:PRO:CD	1.79	1.11
54:1P:91:LYS:CB	86:1:2639:U:O4	1.98	1.11
22:U:80:ASP:HB2	22:U:81:PRO:HD3	1.14	1.11
48:1J:34:PRO:O	48:1J:38:PRO:HD3	0.93	1.11
15:N:407:ARG:HH12	86:1:861:A:P	1.73	1.10
39:l:545:HIS:HB3	87:2:1392:A:N1	1.64	1.10
39:l:547:ASN:ND2	87:2:1391:C:H42	1.49	1.10
47:1I:49:ASN:CB	47:1I:87:THR:CG2	2.29	1.10
33:f:290:VAL:CG1	33:f:299:LYS:CE	2.29	1.10
22:U:81:PRO:HD2	22:U:82:ALA:H	1.13	1.10
2:A:115:LYS:HD2	87:2:1097:A:OP1	1.50	1.09
77:1m:92:GLU:CG	77:1m:102:TRP:CD1	2.34	1.09
36:i:395:ALA:HB2	36:i:428:MET:CG	1.82	1.09
39:l:485:ARG:HH12	39:l:488:CYS:CB	1.61	1.09
48:1J:22:LEU:HD21	48:1J:60:ASP:OD1	1.42	1.09
85:1v:179:ASP:OD1	85:1v:216:LEU:CD1	1.98	1.09
54:1P:81:ASP:OD2	63:1Y:146:LYS:HD3	1.50	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Z:91:ARG:NH2	87:2:152:G:C6	2.20	1.09
39:l:545:HIS:CB	87:2:1392:A:H2	1.50	1.09
48:1J:22:LEU:HD23	48:1J:60:ASP:OD1	1.44	1.09
76:1l:104:TYR:OH	76:1l:198:SER:CB	2.00	1.09
33:f:290:VAL:HG13	33:f:299:LYS:HE2	1.31	1.08
29:b:14:ARG:HH11	87:2:922:G:H4'	1.16	1.07
14:M:140:PHE:HB3	14:M:142:MET:HE3	1.14	1.07
29:b:21:ILE:CB	87:2:1845:A:C6	2.33	1.06
33:f:290:VAL:HG11	33:f:299:LYS:HE2	1.09	1.06
77:1m:92:GLU:HG3	77:1m:102:TRP:CG	1.90	1.06
3:B:107:ILE:O	3:B:110:LEU:CD2	2.02	1.06
22:U:67:LYS:HG3	22:U:69:VAL:HG23	1.14	1.06
27:Z:59:PHE:CD1	35:h:176:VAL:CG1	2.38	1.06
19:R:167:PRO:CG	67:1c:54:PHE:CD2	2.40	1.05
48:1J:33:SER:CB	48:1J:34:PRO:HD3	1.86	1.05
28:a:391:LYS:HE3	39:l:560:MET:HG2	1.34	1.04
64:1Z:150:ASP:O	64:1Z:154:PHE:CD2	2.11	1.04
62:1X:175:ILE:HG21	78:1o:93:ARG:HH12	0.90	1.04
11:J:272:ARG:HG3	20:S:40:LEU:HD23	1.39	1.03
62:1X:175:ILE:HG21	78:1o:93:ARG:NH1	1.71	1.03
33:f:290:VAL:HG11	33:f:299:LYS:CE	1.89	1.03
47:1I:49:ASN:HB2	47:1I:87:THR:HG23	1.40	1.03
86:1:2046:G:OP1	92:1:3601:HOH:O	1.75	1.03
39:l:547:ASN:HD22	87:2:1391:C:N4	1.56	1.02
48:1J:33:SER:CB	48:1J:34:PRO:CD	2.36	1.02
61:1W:69:GLU:OE1	61:1W:74:LYS:HB3	1.57	1.02
29:b:21:ILE:HA	87:2:1845:A:N1	1.69	1.02
33:f:389:THR:CG2	33:f:397:GLU:OE1	2.08	1.02
33:f:266:LYS:HB3	33:f:269:MET:HE3	1.41	1.01
34:g:642:ASN:HB3	39:l:372:ILE:HG21	1.37	1.01
49:1K:92:ARG:HH11	86:1:1282:U:H4'	1.25	1.01
54:1P:81:ASP:CG	63:1Y:146:LYS:HD3	1.84	1.01
62:1X:175:ILE:CG2	78:1o:93:ARG:HH12	1.71	1.01
85:1v:256:CYS:SG	85:1v:285:VAL:HG12	2.01	1.01
1:3:45:C:O2	44:1F:98:ARG:NH1	1.92	1.01
20:S:93:ILE:HG12	92:b:102:HOH:O	1.58	1.01
54:1P:91:LYS:CG	86:1:2639:U:O4	2.08	1.01
19:R:167:PRO:HD2	67:1c:54:PHE:CE2	1.94	1.01
39:l:545:HIS:HB2	87:2:1392:A:N1	1.72	1.01
54:1P:91:LYS:HB3	86:1:2639:U:O4	1.57	1.01
17:P:2:LYS:HB3	17:P:3:PRO:HD3	1.42	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:167:PRO:CG	67:1c:54:PHE:CE2	2.44	1.00
84:1u:112:ILE:HD12	84:1u:119:LEU:HD21	1.39	1.00
28:a:390:VAL:CG1	39:l:553:LEU:HD23	1.92	1.00
76:1l:104:TYR:OH	76:1l:198:SER:HB3	1.60	1.00
39:l:547:ASN:CB	87:2:1391:C:N3	2.24	1.00
22:U:61:ARG:HG2	87:2:837:U:O2'	1.61	0.99
77:1m:92:GLU:HG3	77:1m:102:TRP:NE1	1.77	0.99
87:2:1726:U:H3	87:2:1744:C:N4	1.58	0.99
61:1W:47:ARG:NH2	86:1:1596:A:OP2	1.94	0.99
25:X:366:ARG:HH12	28:a:126:GLN:NE2	1.61	0.98
15:N:407:ARG:NH2	86:1:861:A:P	2.36	0.98
39:l:502:GLU:HG2	39:l:506:PHE:HE2	1.27	0.98
39:l:485:ARG:HH12	39:l:488:CYS:HB3	1.26	0.98
19:R:167:PRO:CD	67:1c:54:PHE:CD2	2.46	0.98
29:b:21:ILE:HB	87:2:1845:A:N6	1.79	0.98
39:l:545:HIS:CG	87:2:1392:A:H2	1.72	0.97
22:U:80:ASP:HB2	22:U:81:PRO:CD	1.95	0.97
27:Z:59:PHE:HZ	87:2:153:A:C2	1.82	0.97
54:1P:91:LYS:HG2	86:1:2639:U:O4	1.64	0.97
39:l:279:ARG:HD3	39:l:281:PHE:HE2	1.29	0.97
3:B:383:PHE:HD1	3:B:389:ILE:HG12	1.31	0.96
64:1Z:150:ASP:O	64:1Z:154:PHE:HD2	1.43	0.96
84:1u:323:PRO:O	84:1u:354:PHE:CE1	2.17	0.96
84:1u:363:TYR:CE1	84:1u:382:VAL:CG1	2.47	0.96
36:i:395:ALA:CB	36:i:428:MET:CG	2.44	0.96
39:l:547:ASN:CB	87:2:1391:C:C4	2.47	0.96
77:1m:91:THR:HG22	77:1m:95:PHE:CE2	2.00	0.96
19:R:167:PRO:HG3	67:1c:54:PHE:HD2	1.25	0.96
28:a:391:LYS:HE3	39:l:560:MET:CG	1.96	0.96
36:i:404:GLU:CD	36:i:437:ARG:CZ	2.38	0.96
86:1:2231:A:H2	87:2:1802:A:O2'	1.48	0.95
17:P:2:LYS:HB3	17:P:3:PRO:CD	1.97	0.95
84:1u:290:VAL:HG11	84:1u:324:SER:HB2	1.46	0.95
86:1:2415:A:H61	86:1:2495:G:H1	1.14	0.95
37:j:191:ASP:OD1	37:j:224:THR:CG2	2.15	0.94
39:l:502:GLU:HG2	39:l:506:PHE:CE2	2.02	0.94
85:1v:311:LEU:O	85:1v:315:THR:HG23	1.66	0.94
3:B:249:MET:HE1	28:a:358:GLU:OE1	1.66	0.94
3:B:371:LEU:CD2	3:B:375:LYS:NZ	2.30	0.94
11:J:250:VAL:HG13	11:J:255:LEU:HD12	1.49	0.94
84:1u:99:GLU:HG3	84:1u:101:THR:HG23	1.48	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:1l:104:TYR:CZ	76:1l:198:SER:CB	2.50	0.94
33:f:389:THR:HG23	33:f:397:GLU:OE1	1.66	0.94
27:Z:58:GLN:HE22	87:2:153:A:N6	1.66	0.93
84:1u:112:ILE:CD1	84:1u:119:LEU:CD2	2.46	0.93
39:l:485:ARG:NH1	39:l:488:CYS:SG	2.42	0.93
59:1U:131:GLN:OE1	59:1U:134:ARG:CD	2.16	0.93
76:1l:154:LEU:HD23	76:1l:202:ILE:HD13	1.50	0.93
27:Z:59:PHE:CE1	35:h:176:VAL:HG11	2.03	0.93
84:1u:112:ILE:HD11	84:1u:119:LEU:CD2	1.97	0.93
20:S:86:PHE:CE1	29:b:19:LEU:HD23	2.04	0.93
3:B:371:LEU:HD23	3:B:375:LYS:HZ1	1.34	0.93
35:h:341:VAL:HG23	35:h:342:LEU:HD12	1.51	0.93
15:N:407:ARG:NH1	86:1:861:A:P	2.42	0.92
29:b:14:ARG:NH1	87:2:922:G:H4'	1.82	0.92
33:f:260:ASN:OD1	33:f:261:THR:HG23	1.68	0.92
48:1J:33:SER:OG	48:1J:34:PRO:HD3	1.69	0.92
48:1J:34:PRO:C	48:1J:38:PRO:HD3	1.93	0.92
27:Z:59:PHE:HE1	35:h:176:VAL:CG1	1.76	0.92
87:2:1381:C:H2'	87:2:1382:C:C6	2.05	0.92
27:Z:59:PHE:HE1	35:h:176:VAL:HG11	1.35	0.91
39:l:474:LYS:HG2	87:2:1141:A:H2	1.33	0.91
48:1J:53:ARG:HH11	48:1J:79:PHE:HE2	1.16	0.91
86:1:2420:G:H1	86:1:2490:U:H3	1.11	0.91
22:U:80:ASP:CB	22:U:81:PRO:HD3	2.01	0.91
33:f:266:LYS:HB3	33:f:269:MET:CE	2.01	0.91
29:b:14:ARG:CD	87:2:922:G:O2'	2.19	0.90
29:b:21:ILE:HA	87:2:1845:A:H2	1.08	0.90
27:Z:91:ARG:NH2	87:2:152:G:N7	2.18	0.90
87:2:858:A:H5'	87:2:1070:U:O4	1.70	0.90
84:1u:296:MET:O	84:1u:300:TYR:HD2	1.54	0.90
39:l:513:ASP:OD1	87:2:1138:G:H1'	1.72	0.90
29:b:14:ARG:HD2	87:2:922:G:O2'	1.72	0.90
48:1J:53:ARG:NH1	48:1J:79:PHE:HE2	1.69	0.90
41:1C:100:THR:CG2	64:1Z:154:PHE:CE2	2.54	0.89
19:R:190:GLY:HA2	67:1c:50:GLN:OE1	1.72	0.89
33:f:323:GLY:CA	33:f:334:ARG:NH2	2.36	0.89
36:i:395:ALA:CB	36:i:428:MET:HG2	2.01	0.89
3:B:383:PHE:CD1	3:B:389:ILE:HG12	2.08	0.89
84:1u:336:VAL:O	84:1u:336:VAL:HG12	1.70	0.89
3:B:371:LEU:CD2	3:B:375:LYS:HZ1	1.84	0.89
48:1J:72:ASP:O	48:1J:73:HIS:ND1	2.06	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:1V:140:MET:HE3	74:1j:82:ILE:HD11	1.54	0.89
41:1C:100:THR:HG21	64:1Z:154:PHE:CE2	2.07	0.89
59:1U:34:ARG:NH2	92:1U:201:HOH:O	2.05	0.89
1:3:40:C:OP2	92:3:301:HOH:O	1.90	0.89
48:1J:29:GLY:O	48:1J:33:SER:CB	2.19	0.89
48:1J:33:SER:HB3	48:1J:34:PRO:HD2	1.54	0.88
3:B:205:LYS:HB2	28:a:183:ILE:HG12	1.55	0.88
35:h:149:ASN:HD22	35:h:152:ARG:HH21	0.92	0.88
37:j:107:LEU:CD2	37:j:145:LEU:HD13	2.02	0.88
37:j:173:VAL:HB	37:j:177:ILE:HD12	1.52	0.88
32:e:299:LEU:HD22	32:e:384:LEU:HD21	1.53	0.88
84:1u:112:ILE:CD1	84:1u:119:LEU:HD21	2.02	0.88
3:B:175:ILE:HD11	25:X:447:ARG:NH2	1.88	0.88
3:B:107:ILE:O	3:B:110:LEU:HD21	1.73	0.88
35:h:149:ASN:ND2	35:h:152:ARG:HH21	1.70	0.88
48:1J:22:LEU:HD23	48:1J:60:ASP:HA	1.53	0.87
84:1u:158:GLU:HG2	84:1u:190:ILE:HD13	1.56	0.87
85:1v:267:PHE:CZ	85:1v:271:MET:SD	2.67	0.87
3:B:176:SER:HG	3:B:230:VAL:N	1.71	0.87
48:1J:103:HIS:CE1	52:1N:101:GLN:HE22	1.92	0.87
41:1C:100:THR:HG21	64:1Z:154:PHE:HZ	0.75	0.87
59:1U:127:HIS:CD2	83:1t:118:GLU:OE1	2.28	0.87
3:B:509:LYS:HZ2	3:B:517:GLN:HE22	1.20	0.87
19:R:140:PRO:HD3	67:1c:58:PHE:CG	2.09	0.87
37:j:107:LEU:CD2	37:j:145:LEU:CD1	2.50	0.87
85:1v:421:LYS:HD2	85:1v:458:ARG:HH22	1.38	0.87
20:S:86:PHE:CE1	29:b:19:LEU:CD2	2.58	0.86
20:S:86:PHE:HE1	29:b:19:LEU:CG	1.87	0.86
27:Z:59:PHE:HD1	35:h:176:VAL:HG13	1.38	0.86
87:2:1071:G:O2'	92:2:2101:HOH:O	1.85	0.86
36:i:392:HIS:CE1	36:i:424:ALA:HB2	2.11	0.86
49:1K:92:ARG:NH1	86:1:1282:U:H4'	1.91	0.86
47:1I:49:ASN:CB	47:1I:87:THR:HG21	1.99	0.86
39:l:485:ARG:HH11	39:l:488:CYS:CB	1.87	0.86
22:U:81:PRO:HD2	22:U:82:ALA:N	1.89	0.86
87:2:163:A:H4'	87:2:164:A:H5'	1.56	0.86
31:d:57:VAL:HG12	37:j:40:PRO:HG2	1.58	0.86
3:B:509:LYS:NZ	3:B:517:GLN:HE22	1.74	0.86
3:B:371:LEU:HD23	3:B:375:LYS:NZ	1.91	0.85
22:U:67:LYS:HG2	22:U:69:VAL:HG23	1.57	0.85
29:b:21:ILE:CG2	87:2:1845:A:C6	2.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
87:2:79:G:H22	87:2:161:A:H2	1.23	0.85
54:1P:81:ASP:CG	63:1Y:146:LYS:CD	2.48	0.85
27:Z:123:TYR:CE1	87:2:155:U:C2	2.65	0.85
3:B:363:LEU:HB3	25:X:360:TYR:OH	1.77	0.85
14:M:140:PHE:HB3	14:M:142:MET:CE	2.03	0.85
17:P:68:ASN:ND2	87:2:254:U:H5''	1.92	0.85
39:l:502:GLU:CG	39:l:506:PHE:HE2	1.89	0.84
71:lg:123:ARG:HH22	86:1:782:C:N4	1.74	0.84
36:i:404:GLU:OE2	36:i:437:ARG:CZ	2.25	0.84
37:j:77:HIS:NE2	37:j:81:LEU:HD11	1.92	0.84
50:1L:148:ARG:NH2	87:2:358:C:P	2.50	0.84
85:1v:174:GLY:O	85:1v:175:ALA:CB	2.25	0.84
39:l:279:ARG:NH1	39:l:281:PHE:HZ	1.33	0.84
1:3:57:G:H21	44:1F:26:MET:HE1	1.41	0.83
37:j:230:ALA:O	37:j:234:ARG:HG2	1.78	0.83
37:j:107:LEU:HD21	37:j:145:LEU:HD11	1.59	0.83
20:S:86:PHE:CE1	29:b:19:LEU:HG	2.14	0.83
19:R:167:PRO:HG3	67:1c:54:PHE:CE2	2.10	0.83
19:R:167:PRO:HD3	67:1c:54:PHE:CD2	2.11	0.83
84:1u:189:LYS:HD2	84:1u:225:THR:CG2	2.08	0.83
39:l:485:ARG:HH11	39:l:488:CYS:HB2	1.36	0.83
77:1m:92:GLU:CG	77:1m:102:TRP:NE1	2.39	0.83
27:Z:59:PHE:CZ	87:2:153:A:C2	2.66	0.83
85:1v:71:ASP:N	85:1v:72:PRO:HD2	1.92	0.83
86:1:1594:G:O6	86:1:1658:A:C6	2.31	0.83
33:f:323:GLY:HA2	33:f:334:ARG:HH22	1.44	0.83
39:l:474:LYS:HE3	87:2:1141:A:N1	1.93	0.83
36:i:404:GLU:CD	36:i:437:ARG:NH2	2.37	0.83
28:a:390:VAL:HG11	39:l:553:LEU:HD23	1.61	0.82
41:1C:100:THR:HG22	64:1Z:154:PHE:CZ	2.07	0.82
36:i:403:VAL:HG11	36:i:428:MET:HE2	1.58	0.82
39:l:513:ASP:OD2	87:2:1139:A:O4'	1.97	0.82
14:M:157:VAL:HG22	92:M:219:HOH:O	1.77	0.82
27:Z:123:TYR:CD1	87:2:155:U:C2	2.68	0.82
87:2:1144:A:H2'	87:2:1145:A:H8	1.44	0.82
48:1J:32:VAL:O	48:1J:43:MET:CE	2.27	0.81
19:R:189:GLU:HG2	67:1c:51:ILE:CD1	2.10	0.81
59:1U:131:GLN:OE1	59:1U:134:ARG:HD2	1.81	0.81
74:1j:82:ILE:O	74:1j:83:GLU:HG3	1.80	0.81
28:a:393:ARG:HH21	87:2:1388:A:P	2.04	0.81
29:b:14:ARG:HD2	87:2:922:G:HO2'	1.41	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:1C:192:PRO:O	41:1C:195:PRO:HD2	1.80	0.81
71:1g:123:ARG:NH2	86:1:782:C:N4	2.28	0.81
27:Z:59:PHE:HD1	35:h:176:VAL:CG1	1.92	0.81
76:1l:154:LEU:HD23	76:1l:202:ILE:CD1	2.10	0.81
47:1I:49:ASN:CB	47:1I:87:THR:HG23	2.04	0.81
77:1m:92:GLU:HG3	77:1m:102:TRP:CE2	2.16	0.81
84:1u:363:TYR:HE1	84:1u:382:VAL:HG13	1.44	0.81
33:f:389:THR:HG22	33:f:397:GLU:HB2	1.64	0.80
33:f:323:GLY:HA2	33:f:334:ARG:NH2	1.95	0.80
86:1:2237:A:N1	87:2:1804:U:O2'	2.15	0.80
35:h:149:ASN:HD22	35:h:152:ARG:NH2	1.75	0.80
39:l:474:LYS:CG	87:2:1141:A:C2	2.57	0.80
48:1J:36:LEU:C	48:1J:38:PRO:HD2	2.06	0.80
17:P:68:ASN:ND2	87:2:254:U:C5'	2.45	0.80
77:1m:92:GLU:CD	77:1m:102:TRP:CD1	2.59	0.80
84:1u:189:LYS:HD2	84:1u:225:THR:HG21	1.61	0.80
87:2:1702:G:H2'	87:2:1703:G:C8	2.16	0.80
86:1:1871:U:H2'	86:1:1872:U:C6	2.16	0.80
48:1J:36:LEU:HD12	48:1J:43:MET:SD	2.21	0.80
81:1r:62:TYR:HE1	81:1r:124:VAL:HG13	1.47	0.80
3:B:371:LEU:HD22	3:B:375:LYS:HZ2	1.46	0.80
61:1W:102:PHE:CE2	61:1W:131:ILE:CG2	2.65	0.80
86:1:1594:G:C6	86:1:1658:A:C6	2.70	0.80
48:1J:33:SER:HB3	48:1J:34:PRO:HD3	1.49	0.79
48:1J:11:ARG:HD2	48:1J:70:TYR:CD1	2.16	0.79
59:1U:127:HIS:HD2	83:1t:118:GLU:OE1	1.64	0.79
54:1P:81:ASP:HB3	63:1Y:146:LYS:HD2	1.63	0.79
76:1l:178:GLU:CD	76:1l:179:THR:HG23	2.07	0.79
85:1v:256:CYS:CB	85:1v:285:VAL:HG12	2.12	0.79
10:I:232:SER:O	28:a:376:ALA:HB1	1.82	0.79
39:l:549:ILE:HD12	87:2:1389:A:O2'	1.82	0.79
1:3:115:G:OP2	54:1P:51:LYS:CE	2.30	0.79
3:B:205:LYS:CB	28:a:183:ILE:HG12	2.11	0.79
35:h:82:PRO:HG3	35:h:124:PHE:CZ	2.18	0.79
22:U:61:ARG:HG2	87:2:837:U:HO2'	1.47	0.79
27:Z:63:TRP:CG	35:h:137:LEU:HD22	2.18	0.79
86:1:1695:A:H2'	86:1:1696:A:C8	2.17	0.78
39:l:549:ILE:CD1	87:2:1389:A:O2'	2.30	0.78
61:1W:102:PHE:CD2	61:1W:131:ILE:HG21	2.18	0.78
36:i:410:MET:HE1	36:i:417:PRO:HG3	1.63	0.78
2:A:28:LYS:HD3	22:U:45:LEU:HD13	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:86:PHE:HE1	29:b:19:LEU:CD2	1.96	0.78
86:1:2415:A:N6	86:1:2495:G:H1	1.81	0.78
6:E:25:ARG:NE	40:1B:51:LEU:O	2.16	0.78
41:1C:100:THR:HG23	64:1Z:154:PHE:HZ	1.13	0.78
36:i:403:VAL:HG11	36:i:428:MET:CE	2.13	0.78
41:1C:189:PHE:O	41:1C:190:ASP:HB2	1.85	0.77
14:M:140:PHE:CB	14:M:142:MET:HE3	2.06	0.77
20:S:93:ILE:CG2	29:b:86:LEU:HD13	2.15	0.77
27:Z:59:PHE:HZ	87:2:153:A:N3	1.80	0.77
27:Z:65:ILE:HD11	35:h:143:HIS:ND1	2.00	0.77
41:1C:194:ILE:CG2	41:1C:195:PRO:HD3	2.14	0.77
3:B:371:LEU:HD22	3:B:375:LYS:NZ	1.99	0.77
27:Z:58:GLN:NE2	87:2:153:A:N6	2.32	0.77
28:a:291:LEU:HB3	28:a:315:LEU:HD11	1.67	0.77
36:i:395:ALA:HB1	36:i:428:MET:HG2	1.65	0.77
59:1U:34:ARG:CZ	92:1U:201:HOH:O	2.33	0.77
14:M:121:THR:HG23	87:2:1622:A:N7	1.99	0.77
27:Z:91:ARG:CZ	87:2:152:G:C6	2.68	0.77
7:F:140:ARG:NE	11:J:237:TYR:OH	2.18	0.77
36:i:398:ASN:OD1	36:i:432:SER:HB3	1.85	0.77
28:a:390:VAL:HG13	39:l:553:LEU:HD23	1.67	0.77
83:1t:18:LYS:HD3	92:1t:501:HOH:O	1.83	0.77
19:R:140:PRO:HD3	67:1c:58:PHE:CD1	2.19	0.77
81:1r:62:TYR:CZ	81:1r:124:VAL:CG1	2.68	0.77
1:3:57:G:N2	44:1F:26:MET:HE1	1.99	0.76
47:1I:65:GLU:O	47:1I:67:THR:HG23	1.84	0.76
39:l:517:LYS:HZ2	87:2:1385:A:C1'	1.98	0.76
86:1:2231:A:C2	87:2:1802:A:C8	2.73	0.76
22:U:67:LYS:CG	22:U:69:VAL:CG2	2.57	0.76
87:2:1381:C:H2'	87:2:1382:C:H6	1.44	0.76
77:1m:91:THR:CG2	77:1m:95:PHE:CE2	2.69	0.76
84:1u:296:MET:O	84:1u:300:TYR:CD2	2.38	0.76
77:1m:91:THR:HG22	77:1m:95:PHE:HE2	1.50	0.76
84:1u:363:TYR:HE1	84:1u:382:VAL:HG12	1.49	0.76
50:1L:148:ARG:HD2	92:1L:205:HOH:O	1.84	0.76
81:1r:62:TYR:CZ	81:1r:124:VAL:HG13	2.20	0.76
85:1v:71:ASP:N	85:1v:72:PRO:CD	2.49	0.76
36:i:438:ALA:HB1	36:i:460:MET:HE1	1.67	0.75
86:1:1325:G:H1	86:1:1331:U:H3	1.31	0.75
20:S:86:PHE:CE1	29:b:19:LEU:CG	2.69	0.75
35:h:342:LEU:HD11	35:h:353:VAL:CG1	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:162:SER:OG	3:B:429:ASN:ND2	2.19	0.75
35:h:86:VAL:HG21	35:h:121:ASP:HB2	1.66	0.75
3:B:478:ILE:HG22	3:B:479:PRO:O	1.87	0.75
60:1V:109:THR:HB	86:1:435:A:H5''	1.68	0.75
76:1l:154:LEU:CD2	76:1l:202:ILE:CD1	2.63	0.75
18:Q:193:LEU:HD21	18:Q:213:ILE:HG21	1.68	0.75
59:1U:131:GLN:OE1	59:1U:134:ARG:NE	2.18	0.75
22:U:61:ARG:HD2	87:2:837:U:C2'	2.17	0.75
84:1u:224:ASP:OD1	84:1u:257:THR:OG1	2.04	0.75
61:1W:69:GLU:OE1	61:1W:74:LYS:CB	2.33	0.75
85:1v:256:CYS:HB2	85:1v:285:VAL:CG1	2.16	0.75
9:H:240:GLY:H	36:i:295:MET:HE1	1.52	0.75
33:f:249:LEU:O	33:f:253:SER:OG	2.05	0.75
39:l:513:ASP:OD1	87:2:1138:G:O2'	2.03	0.75
87:2:1769:C:H2'	87:2:1770:G:C8	2.23	0.74
77:1m:92:GLU:HG3	77:1m:102:TRP:CD2	2.22	0.74
22:U:81:PRO:CD	22:U:82:ALA:H	1.97	0.74
35:h:342:LEU:HD11	35:h:353:VAL:HG11	1.69	0.74
28:a:390:VAL:HG11	39:l:553:LEU:HA	1.69	0.74
33:f:105:LEU:N	33:f:106:PRO:HD2	2.01	0.74
42:1D:115:ILE:HG12	42:1D:121:PHE:CE2	2.23	0.74
87:2:1726:U:H3	87:2:1744:C:H42	0.77	0.74
17:P:43:HIS:HE2	17:P:45:GLU:HG2	1.51	0.74
33:f:221:PHE:CE2	33:f:256:VAL:HG11	2.23	0.74
36:i:392:HIS:CE1	36:i:424:ALA:CB	2.71	0.74
39:l:547:ASN:CB	87:2:1391:C:N4	2.51	0.74
28:a:178:LYS:O	28:a:182:VAL:HG23	1.88	0.73
61:1W:102:PHE:CE2	61:1W:131:ILE:HG21	2.23	0.73
67:1c:56:ARG:HH22	87:2:1573:U:H5''	1.53	0.73
28:a:393:ARG:NH2	87:2:1388:A:O5'	2.20	0.73
85:1v:256:CYS:CB	85:1v:285:VAL:CG1	2.65	0.73
3:B:147:ARG:HH21	25:X:472:ARG:HH22	1.33	0.73
20:S:86:PHE:HE1	29:b:19:LEU:HG	1.49	0.73
36:i:400:ILE:HD13	36:i:429:TYR:CE1	2.19	0.73
46:1H:101:GLU:O	46:1H:105:VAL:HG23	1.87	0.73
29:b:21:ILE:CG2	87:2:1845:A:N1	2.51	0.73
35:h:341:VAL:HG23	35:h:342:LEU:CD1	2.17	0.73
3:B:96:ARG:NH1	25:X:326:ALA:CB	2.51	0.73
5:D:138:GLU:HB2	5:D:141:ARG:HB2	1.71	0.73
47:1I:64:LEU:HD22	47:1I:69:TRP:HB2	1.71	0.73
61:1W:184:LEU:HD22	61:1W:212:MET:HE1	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:1m:92:GLU:CD	77:1m:102:TRP:NE1	2.47	0.73
87:2:26:U:H3	87:2:910:G:H1	1.34	0.73
1:3:33:C:O2'	73:1i:180:HIS:HE1	1.70	0.73
87:2:1144:A:H2'	87:2:1145:A:C8	2.23	0.73
42:1D:189:ARG:HH12	86:1:3101:U:H4'	1.54	0.73
1:3:115:G:OP2	54:1P:51:LYS:HE3	1.89	0.72
29:b:14:ARG:HD3	87:2:922:G:O2'	1.89	0.72
44:1F:123:ARG:CZ	86:1:2613:A:OP1	2.37	0.72
84:1u:112:ILE:HD13	84:1u:115:TRP:CE2	2.24	0.72
27:Z:63:TRP:CD1	35:h:137:LEU:HD22	2.23	0.72
84:1u:323:PRO:O	84:1u:354:PHE:HD1	1.70	0.72
85:1v:174:GLY:O	85:1v:175:ALA:HB3	1.87	0.72
2:A:28:LYS:HB3	22:U:45:LEU:HD11	1.72	0.72
39:l:547:ASN:HB2	87:2:1391:C:C2	2.23	0.72
15:N:407:ARG:CZ	86:1:861:A:P	2.77	0.72
19:R:167:PRO:HD2	67:1c:54:PHE:CZ	2.22	0.72
84:1u:279:ASP:O	84:1u:282:ILE:HG22	1.90	0.72
87:2:1145:A:N1	87:2:1378:A:H2	1.87	0.72
33:f:266:LYS:HD2	33:f:269:MET:HE1	1.72	0.72
61:1W:184:LEU:CD2	61:1W:212:MET:HE1	2.19	0.72
81:1r:62:TYR:CE1	81:1r:124:VAL:CG1	2.69	0.72
87:2:1704:A:H2	87:2:1706:C:H41	1.37	0.72
25:X:366:ARG:HH12	28:a:126:GLN:HE22	1.37	0.72
3:B:509:LYS:HZ2	3:B:517:GLN:NE2	1.88	0.72
34:g:647:LEU:HD13	39:l:404:ALA:O	1.90	0.72
35:h:288:LEU:HD11	35:h:326:LEU:CD2	2.20	0.72
7:F:140:ARG:CZ	11:J:237:TYR:OH	2.38	0.72
20:S:86:PHE:HE1	29:b:19:LEU:HD23	1.54	0.71
22:U:37:VAL:HG11	33:f:236:LYS:HD2	1.71	0.71
86:1:1695:A:H2'	86:1:1696:A:H8	1.54	0.71
4:C:139:VAL:HG11	4:C:144:LEU:HD22	1.72	0.71
42:1D:115:ILE:CG1	42:1D:121:PHE:CE2	2.73	0.71
85:1v:211:ARG:NH1	85:1v:242:PHE:O	2.22	0.71
47:1I:27:ILE:CD1	47:1I:83:ILE:HD11	2.20	0.71
64:1Z:150:ASP:HB3	64:1Z:154:PHE:HE2	1.55	0.71
84:1u:154:MET:SD	84:1u:190:ILE:HD12	2.31	0.71
86:1:1693:C:H3'	86:1:1694:A:H8	1.54	0.71
22:U:80:ASP:CB	22:U:81:PRO:CD	2.65	0.71
22:U:89:VAL:O	22:U:93:THR:HG23	1.90	0.71
25:X:366:ARG:NH1	28:a:126:GLN:NE2	2.38	0.71
13:L:83:ILE:HD11	76:1l:80:GLU:OE2	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:1I:61:PHE:HB2	47:1I:76:MET:SD	2.31	0.71
48:1J:37:GLY:N	48:1J:38:PRO:HD2	2.06	0.71
36:i:400:ILE:HD11	36:i:429:TYR:HE1	0.54	0.71
48:1J:28:PRO:HB3	48:1J:43:MET:HE3	1.72	0.71
22:U:99:GLU:HG3	22:U:103:MET:HE1	1.73	0.70
81:1r:62:TYR:OH	81:1r:124:VAL:CG1	2.39	0.70
86:1:1692:U:H2'	86:1:1693:C:C6	2.26	0.70
37:j:77:HIS:ND1	87:2:92:A:OP1	2.23	0.70
61:1W:184:LEU:HD13	61:1W:212:MET:HE1	1.74	0.70
1:3:57:G:H21	44:1F:26:MET:CE	2.04	0.70
84:1u:112:ILE:HD11	84:1u:119:LEU:HD22	1.71	0.70
37:j:107:LEU:CD2	37:j:145:LEU:HD11	2.18	0.70
66:1b:74:GLU:HG2	66:1b:78:LYS:HE3	1.71	0.70
22:U:67:LYS:HG2	22:U:69:VAL:CG2	2.20	0.70
48:1J:37:GLY:N	48:1J:38:PRO:CD	2.55	0.70
87:2:660:G:H22	87:2:737:G:H1	1.38	0.70
3:B:249:MET:SD	28:a:358:GLU:HG2	2.32	0.70
33:f:323:GLY:CA	33:f:334:ARG:HH22	1.98	0.70
3:B:376:VAL:HG12	3:B:380:ILE:HG23	1.73	0.70
4:C:178:LYS:HZ1	4:C:311:ARG:HG2	1.55	0.70
28:a:180:TRP:O	28:a:184:VAL:HG23	1.92	0.70
35:h:121:ASP:HA	35:h:124:PHE:HD2	1.56	0.70
36:i:404:GLU:OE2	36:i:429:TYR:OH	2.10	0.70
23:V:176:ILE:HG12	23:V:184:LYS:HD2	1.73	0.69
39:l:474:LYS:HG2	87:2:1141:A:N1	2.05	0.69
87:2:1681:A:H5'	92:2:4433:HOH:O	1.90	0.69
4:C:175:LEU:HD11	4:C:198:TRP:HB3	1.74	0.69
42:1D:115:ILE:HG12	42:1D:121:PHE:CZ	2.27	0.69
59:1U:131:GLN:HB2	59:1U:134:ARG:HD2	1.74	0.69
84:1u:99:GLU:HG3	84:1u:101:THR:CG2	2.21	0.69
1:3:3:A:H61	1:3:116:U:H3	1.38	0.69
33:f:389:THR:HG21	33:f:397:GLU:OE1	1.93	0.69
87:2:1703:G:H1	87:2:1768:A:N6	1.90	0.69
3:B:107:ILE:O	3:B:110:LEU:HD23	1.93	0.69
35:h:166:HIS:CE1	35:h:169:ARG:HH11	2.11	0.69
61:1W:184:LEU:CD1	61:1W:212:MET:HE1	2.22	0.69
85:1v:142:ASP:OD1	85:1v:143:ASP:N	2.26	0.69
39:l:279:ARG:CD	39:l:281:PHE:HE2	2.05	0.69
39:l:517:LYS:NZ	87:2:1385:A:O4'	2.23	0.69
83:1t:448:PHE:HA	83:1t:451:LEU:HB2	1.75	0.69
86:1:2238:C:OP1	87:2:1826:G:H1'	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:1J:103:HIS:HE1	52:1N:101:GLN:HE22	1.39	0.68
36:i:400:ILE:HG12	36:i:434:ASN:ND2	2.08	0.68
77:1m:91:THR:O	77:1m:95:PHE:CD2	2.47	0.68
3:B:96:ARG:NH1	25:X:326:ALA:HB1	2.08	0.68
55:1Q:154:ARG:NH2	87:2:365:G:OP2	2.27	0.68
22:U:108:MET:HE1	36:i:450:LEU:HD22	1.75	0.68
47:1I:9:LEU:HD11	78:1o:108:VAL:HG21	1.75	0.68
48:1J:72:ASP:O	48:1J:73:HIS:CG	2.45	0.68
87:2:673:U:H3	87:2:709:G:H22	1.39	0.68
76:1l:33:PHE:CE2	76:1l:154:LEU:HD11	2.29	0.68
87:2:200:C:H5	87:2:246:G:H1	1.42	0.68
39:l:279:ARG:O	39:l:279:ARG:HG2	1.94	0.68
12:K:114:ARG:HB2	12:K:119:ALA:HB3	1.74	0.68
61:1W:131:ILE:HG22	61:1W:143:LEU:HD23	1.76	0.68
2:A:28:LYS:CG	22:U:45:LEU:HD11	2.22	0.67
2:A:28:LYS:CD	22:U:45:LEU:HD13	2.24	0.67
37:j:152:LYS:HA	37:j:155:ASN:HB2	1.76	0.67
51:1M:80:ARG:NH2	86:1:1407:G:N7	2.42	0.67
87:2:1388:A:H2'	87:2:1388:A:N3	2.09	0.67
48:1J:32:VAL:O	48:1J:43:MET:HE2	1.94	0.67
84:1u:336:VAL:O	84:1u:336:VAL:CG1	2.42	0.67
28:a:387:THR:OG1	39:l:555:ARG:HB2	1.94	0.67
35:h:82:PRO:HG3	35:h:124:PHE:CE2	2.29	0.67
29:b:15:LYS:HG3	87:2:1652:C:C5'	2.24	0.67
1:3:115:G:OP2	54:1P:51:LYS:HE2	1.95	0.67
48:1J:22:LEU:HD23	48:1J:60:ASP:CG	2.19	0.67
3:B:206:LEU:HB2	28:a:183:ILE:HG23	1.76	0.67
5:D:217:LEU:HD11	36:i:207:ILE:HD11	1.76	0.67
77:1m:88:TYR:CZ	77:1m:102:TRP:HZ2	2.13	0.67
84:1u:189:LYS:CD	84:1u:225:THR:HG21	2.25	0.67
87:2:1275:A:N6	87:2:1281:U:O4	2.28	0.67
54:1P:81:ASP:OD1	63:1Y:146:LYS:NZ	2.26	0.67
39:l:439:LYS:CE	39:l:471:LYS:O	2.42	0.67
47:1I:27:ILE:HD12	47:1I:83:ILE:HD11	1.77	0.67
84:1u:112:ILE:HD13	84:1u:115:TRP:CD2	2.30	0.67
84:1u:279:ASP:HA	84:1u:282:ILE:HG22	1.74	0.67
84:1u:406:GLN:NE2	84:1u:411:ASP:O	2.28	0.67
2:A:28:LYS:HD3	22:U:45:LEU:CD1	2.24	0.66
4:C:187:PRO:HD2	4:C:190:MET:HE2	1.77	0.66
13:L:108:ARG:HD2	67:1c:50:GLN:NE2	2.10	0.66
61:1W:47:ARG:HE	86:1:1595:G:H3'	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:140:ARG:CZ	11:J:237:TYR:HH	2.07	0.66
2:A:28:LYS:CB	22:U:45:LEU:HD11	2.25	0.66
48:1J:25:LYS:O	48:1J:25:LYS:HG2	1.95	0.66
29:b:15:LYS:CG	87:2:1652:C:H5'	2.26	0.66
86:1:2232:C:N4	92:1:3609:HOH:O	2.29	0.66
29:b:21:ILE:CB	87:2:1845:A:C2	2.66	0.66
39:l:206:ARG:HA	87:2:1330:A:O2'	1.96	0.66
47:1I:30:ASN:ND2	47:1I:79:MET:SD	2.69	0.66
11:J:205:THR:HG21	11:J:239:ALA:HA	1.78	0.66
84:1u:351:MET:HE2	84:1u:357:GLU:HA	1.77	0.66
47:1I:68:LYS:HA	47:1I:118:LYS:HE2	1.78	0.66
87:2:1377:A:H2'	87:2:1378:A:C8	2.31	0.66
86:1:2238:C:OP1	87:2:1826:G:C1'	2.44	0.66
87:2:79:G:N2	87:2:161:A:H2	1.94	0.66
27:Z:84:ILE:H	35:h:143:HIS:HE1	1.44	0.66
59:1U:129:LEU:HD11	83:1t:110:GLU:OE1	1.95	0.66
86:1:1978:U:O2'	86:1:2084:C:O2'	2.14	0.65
33:f:83:ASN:O	33:f:138:LYS:NZ	2.28	0.65
87:2:858:A:H5'	87:2:1070:U:C4	2.30	0.65
61:1W:102:PHE:CD2	61:1W:131:ILE:CG2	2.79	0.65
13:L:83:ILE:HD11	76:1l:80:GLU:CD	2.22	0.65
31:d:57:VAL:HG12	37:j:40:PRO:CG	2.27	0.65
37:j:173:VAL:HB	37:j:177:ILE:CD1	2.25	0.65
33:f:336:TYR:CE2	33:f:340:LEU:HD12	2.27	0.65
14:M:157:VAL:HG23	92:M:206:HOH:O	1.95	0.65
29:b:21:ILE:HG22	87:2:1845:A:C2	2.32	0.65
86:1:2231:A:H2	87:2:1802:A:HO2'	0.70	0.65
87:2:1136:A:H2'	87:2:1390:A:N1	2.10	0.65
32:e:312:LEU:HD21	32:e:370:MET:HE1	1.79	0.65
39:l:517:LYS:NZ	87:2:1385:A:C1'	2.58	0.65
3:B:376:VAL:HG12	3:B:376:VAL:O	1.97	0.65
19:R:190:GLY:HA2	67:1c:50:GLN:CD	2.22	0.65
36:i:390:LEU:HB3	36:i:406:ILE:HD13	1.79	0.65
84:1u:403:LEU:HD22	84:1u:437:LEU:HD11	1.78	0.64
85:1v:283:TYR:HB3	85:1v:313:MET:HE2	1.79	0.64
87:2:1524:A:H2	87:2:1537:G:H21	1.44	0.64
1:3:44:C:C6	44:1F:62:ILE:HB	2.32	0.64
86:1:64:G:O2'	86:1:66:G:N7	2.28	0.64
3:B:110:LEU:HG	28:a:83:LYS:HB2	1.80	0.64
3:B:249:MET:HE1	28:a:358:GLU:CD	2.22	0.64
22:U:81:PRO:CD	22:U:82:ALA:N	2.58	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:488:PHE:O	25:X:492:VAL:HG23	1.97	0.64
36:i:426:VAL:HG13	36:i:460:MET:HE3	1.80	0.64
84:1u:363:TYR:CE1	84:1u:382:VAL:HG12	2.25	0.64
26:Y:43:ARG:NH1	87:2:1537:G:N7	2.44	0.64
39:l:545:HIS:HB3	87:2:1392:A:H2	0.96	0.64
86:1:1871:U:H2'	86:1:1872:U:H6	1.61	0.64
87:2:1825:2MG:N2	87:2:1828:MA6:OP2	2.29	0.64
3:B:509:LYS:NZ	3:B:517:GLN:NE2	2.44	0.64
37:j:128:GLN:HG3	37:j:163:VAL:HG11	1.79	0.64
86:1:2934:U:O2'	86:1:2936:A:N6	2.30	0.64
61:1W:184:LEU:HD22	61:1W:212:MET:CE	2.28	0.64
3:B:175:ILE:HD11	25:X:447:ARG:HH22	1.61	0.64
11:J:246:ILE:O	11:J:250:VAL:HG23	1.98	0.64
49:1K:159:MET:HE2	86:1:1162:C:H42	1.62	0.64
86:1:1873:U:H2'	86:1:1874:A:O4'	1.98	0.64
55:1Q:209:ARG:HH22	86:1:2078:C:H5	1.46	0.64
13:L:33:ARG:NH1	44:1F:150:GLU:OE2	2.31	0.64
84:1u:154:MET:SD	84:1u:190:ILE:CD1	2.86	0.64
86:1:690:C:O2'	86:1:691:A:N7	2.29	0.64
86:1:3000:C:H5'	86:1:3153:A:H5'	1.80	0.64
87:2:969:G:H22	87:2:1625:A:H5'	1.63	0.64
59:1U:7:ARG:NH1	86:1:152:C:OP1	2.30	0.63
3:B:371:LEU:CD2	3:B:375:LYS:HZ2	2.03	0.63
61:1W:177:LEU:HD11	61:1W:233:CYS:HB2	1.79	0.63
35:h:147:ASN:ND2	87:2:1745:A:OP2	2.31	0.63
77:1m:54:PRO:HD2	77:1m:71:ALA:HB2	1.80	0.63
84:1u:158:GLU:CG	84:1u:190:ILE:HD13	2.28	0.63
6:E:81:TYR:CD2	40:1B:52:HIS:CE1	2.82	0.63
22:U:88:ARG:NH1	36:i:420:LEU:HD21	2.13	0.63
85:1v:120:PRO:O	85:1v:156:ARG:NH1	2.32	0.63
87:2:609:U:H3	87:2:625:G:H22	1.47	0.63
67:1c:48:ILE:HG12	67:1c:53:LYS:HG3	1.79	0.63
76:1l:154:LEU:CD2	76:1l:202:ILE:HD13	2.22	0.63
17:P:68:ASN:HD22	87:2:254:U:H5''	1.63	0.63
83:1t:18:LYS:NZ	92:1t:501:HOH:O	2.14	0.63
35:h:202:MET:HE1	35:h:228:CYS:HB3	1.81	0.63
39:l:547:ASN:HB3	87:2:1391:C:N4	2.14	0.63
41:1C:194:ILE:HG23	41:1C:195:PRO:HD3	1.79	0.63
87:2:1145:A:H2'	87:2:1146:A:C8	2.34	0.63
22:U:67:LYS:HG3	22:U:69:VAL:CG2	2.08	0.63
35:h:288:LEU:HD11	35:h:326:LEU:HD21	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:1J:32:VAL:CG1	48:1J:43:MET:CE	2.23	0.63
9:H:298:ARG:HH21	9:H:300:VAL:HG21	1.63	0.63
34:g:339:LYS:HE2	34:g:383:ARG:HH12	1.64	0.62
77:1m:92:GLU:OE2	77:1m:96:ARG:CZ	2.46	0.62
44:1F:123:ARG:CD	86:1:2613:A:OP1	2.47	0.62
86:1:1432:A:OP2	86:1:1988:C:N4	2.31	0.62
87:2:65:G:H1	87:2:374:C:H5	1.47	0.62
1:3:54:U:O2'	73:1i:181:ARG:NH1	2.32	0.62
3:B:167:LYS:NZ	28:a:127:ASN:OD1	2.31	0.62
37:j:48:LYS:O	37:j:52:THR:HG23	1.99	0.62
83:1t:462:HIS:CE1	85:1v:242:PHE:H	2.17	0.62
48:1J:28:PRO:CB	48:1J:43:MET:HE3	2.28	0.62
57:1S:205:GLU:OE2	75:1k:93:ARG:NH1	2.32	0.62
12:K:6:GLN:HG2	12:K:9:ARG:HH21	1.63	0.62
81:1r:57:ILE:HG21	81:1r:88:LEU:HD21	1.81	0.62
16:O:79:ARG:HG2	32:e:334:ILE:HD12	1.82	0.62
32:e:299:LEU:HD22	32:e:384:LEU:CD2	2.26	0.62
85:1v:421:LYS:HD2	85:1v:458:ARG:NH2	2.11	0.62
17:P:3:PRO:HD2	17:P:3:PRO:O	1.97	0.62
86:1:2889:U:H2'	86:1:2890:U:H2'	1.82	0.62
39:l:485:ARG:HH22	39:l:521:SER:HG	1.47	0.62
84:1u:363:TYR:CE1	84:1u:382:VAL:HG13	2.25	0.62
86:1:1191:A:H2'	86:1:1192:G:C8	2.34	0.62
87:2:1650:C:O2'	87:2:1651:C:H5'	1.99	0.62
48:1J:72:ASP:C	48:1J:73:HIS:ND1	2.57	0.62
60:1V:140:MET:HE3	74:1j:82:ILE:CD1	2.28	0.62
87:2:1701:C:H3'	87:2:1702:G:H8	1.64	0.62
7:F:143:ALA:O	7:F:144:HIS:ND1	2.32	0.62
87:2:81:U:H3	87:2:159:G:H22	1.45	0.62
22:U:54:PRO:O	22:U:58:ARG:HG3	2.00	0.61
86:1:1594:G:C5	86:1:1658:A:C2	2.87	0.61
4:C:325:THR:HG21	4:C:327:LYS:HE2	1.83	0.61
33:f:57:ASP:OD1	33:f:94:SER:OG	2.17	0.61
33:f:105:LEU:N	33:f:106:PRO:CD	2.64	0.61
48:1J:32:VAL:O	48:1J:43:MET:HE1	2.00	0.61
86:1:2150:C:O2'	86:1:2289:U:OP2	2.18	0.61
39:l:178:LEU:HD23	39:l:216:LEU:HD21	1.81	0.61
3:B:96:ARG:NH1	25:X:326:ALA:HB3	2.14	0.61
5:D:459:ARG:NH2	92:D:602:HOH:O	2.33	0.61
7:F:141:SER:HB3	11:J:237:TYR:CE2	2.35	0.61
35:h:90:HIS:NE2	35:h:94:LEU:HD22	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:j:77:HIS:CD2	37:j:81:LEU:HD11	2.35	0.61
86:l:228:U:H3	86:l:240:A:H2	1.47	0.61
81:l:r:62:TYR:CZ	81:l:r:124:VAL:HG11	2.35	0.61
7:F:17:ASN:OD1	7:F:25:ARG:NH1	2.34	0.61
25:X:373:HIS:O	25:X:377:VAL:HG23	1.99	0.61
36:i:404:GLU:OE2	36:i:437:ARG:NE	2.33	0.61
39:l:517:LYS:NZ	87:2:1385:A:H1'	2.16	0.61
39:l:549:ILE:CD1	87:2:1389:A:H1'	2.30	0.61
36:i:398:ASN:OD1	36:i:432:SER:CB	2.48	0.61
39:l:513:ASP:CG	87:2:1138:G:O2'	2.43	0.61
65:1a:31:VAL:O	65:1a:44:PHE:HB2	2.01	0.61
19:R:189:GLU:HG2	67:1c:51:ILE:HD11	1.82	0.61
29:b:21:ILE:HG22	87:2:1845:A:C6	2.34	0.61
5:D:352:ARG:NH2	87:2:1065:U:H4'	2.16	0.61
25:X:381:ASP:OD1	25:X:455:TYR:OH	2.19	0.61
35:h:252:ARG:NH1	87:2:1732:A:OP2	2.33	0.61
41:1C:192:PRO:C	41:1C:195:PRO:HD2	2.25	0.61
86:l:1874:A:H2'	86:l:1875:G:H5''	1.83	0.61
87:2:1703:G:H3'	87:2:1704:A:C8	2.36	0.61
10:I:131:CYS:HB2	10:I:217:GLN:HB2	1.82	0.60
36:i:407:LEU:HD12	36:i:410:MET:HE3	1.81	0.60
41:1C:245:TRP:HB2	64:1Z:91:VAL:HG22	1.83	0.60
86:l:1186:G:H1	86:l:1269:G:H22	1.49	0.60
87:2:836:A:O2'	87:2:839:C:N4	2.34	0.60
22:U:57:ARG:NH1	87:2:837:U:OP2	2.34	0.60
27:Z:63:TRP:CD2	35:h:137:LEU:HD22	2.37	0.60
27:Z:91:ARG:NH2	87:2:152:G:C8	2.69	0.60
36:i:541:VAL:HG21	36:i:573:GLU:HB2	1.83	0.60
87:2:1703:G:H1	87:2:1768:A:H62	1.47	0.60
3:B:207:PHE:HZ	3:B:213:LYS:HE3	1.65	0.60
85:1v:253:SER:HA	85:1v:285:VAL:HG11	1.81	0.60
14:M:77:ARG:NH1	26:Y:51:VAL:HG13	2.16	0.60
41:1C:194:ILE:HG22	41:1C:195:PRO:HD3	1.81	0.60
11:J:290:ASN:HD21	20:S:36:LEU:HB2	1.67	0.60
37:j:91:THR:HG21	37:j:129:ALA:HA	1.83	0.60
29:b:15:LYS:HG3	87:2:1652:C:H5'	1.82	0.60
41:1C:4:GLY:N	86:l:1558:G:N7	2.50	0.60
33:f:286:MET:O	33:f:290:VAL:HG23	2.02	0.60
42:1D:254:LYS:HB3	42:1D:263:TRP:HB2	1.84	0.60
52:1N:51:ARG:NH1	86:l:1104:G:OP2	2.35	0.60
10:I:224:LEU:HB3	28:a:289:PRO:HG2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:157:VAL:CG2	92:M:219:HOH:O	2.41	0.59
33:f:323:GLY:HA3	33:f:334:ARG:NH2	2.17	0.59
35:h:165:ASN:O	35:h:169:ARG:HG3	2.02	0.59
17:P:68:ASN:ND2	87:2:254:U:H5'	2.17	0.59
36:i:404:GLU:HG3	36:i:437:ARG:NH1	2.17	0.59
47:1I:5:ARG:NH2	78:1o:111:ASP:OD2	2.35	0.59
86:1:1218:G:N2	86:1:1245:A:O2'	2.35	0.59
87:2:1727:G:H1	87:2:1743:A:H2	1.44	0.59
2:A:70:VAL:HG11	2:A:145:VAL:HG21	1.84	0.59
5:D:344:ARG:NH1	5:D:348:THR:OG1	2.35	0.59
9:H:307:TYR:HH	87:2:1410:C:HO2'	1.48	0.59
33:f:290:VAL:HG13	33:f:299:LYS:CE	2.16	0.59
37:j:237:LYS:HB3	37:j:240:ASP:HB2	1.85	0.59
65:1a:132:ARG:NH2	86:1:132:C:O2	2.35	0.59
81:1r:124:VAL:HG12	81:1r:125:LEU:N	2.18	0.59
83:1t:130:LEU:HD23	83:1t:160:SER:HB3	1.84	0.59
84:1u:290:VAL:CG1	84:1u:324:SER:HB2	2.26	0.59
86:1:1694:A:O2'	86:1:1695:A:H5'	2.03	0.59
3:B:96:ARG:HH12	25:X:326:ALA:CB	2.14	0.59
3:B:238:VAL:HG22	25:X:411:LEU:HD21	1.84	0.59
9:H:412:GLU:OE2	9:H:415:LYS:NZ	2.36	0.59
84:1u:676:ARG:HG3	84:1u:678:LEU:HD23	1.84	0.59
5:D:186:THR:HG23	36:i:244:ARG:HH12	1.67	0.59
87:2:787:G:N2	87:2:1806:G:O3'	2.32	0.59
7:F:140:ARG:NH2	11:J:237:TYR:OH	2.36	0.59
35:h:82:PRO:CG	35:h:124:PHE:CZ	2.85	0.59
67:1c:49:GLY:O	67:1c:53:LYS:HG3	2.03	0.59
87:2:1144:A:H61	87:2:1379:C:N4	2.01	0.59
1:3:1:A:N7	1:3:118:A:O2'	2.35	0.59
36:i:489:GLU:HA	36:i:492:TYR:HD2	1.65	0.59
39:l:513:ASP:OD1	87:2:1138:G:C1'	2.49	0.59
45:1G:19:ARG:NH1	45:1G:21:GLU:OE1	2.36	0.59
86:1:1692:U:H2'	86:1:1693:C:C1'	2.33	0.59
87:2:1770:G:H3'	87:2:1771:C:H4'	1.84	0.59
19:R:140:PRO:HG3	67:1c:58:PHE:CD2	2.38	0.59
37:j:96:PHE:O	37:j:100:THR:HG23	2.02	0.59
39:l:549:ILE:HD11	87:2:1389:A:O2'	2.01	0.59
14:M:106:LYS:HD2	25:X:521:ASN:HD21	1.67	0.59
33:f:336:TYR:CD2	33:f:340:LEU:CD1	2.85	0.59
37:j:102:LEU:O	37:j:106:LEU:HG	2.02	0.59
27:Z:59:PHE:CZ	87:2:153:A:N3	2.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:1D:115:ILE:HG13	42:1D:121:PHE:CE2	2.38	0.58
86:1:888:A:O2'	86:1:2001:U:OP1	2.21	0.58
87:2:669:G:H2'	87:2:670:G:C8	2.38	0.58
4:C:167:ARG:NH1	5:D:118:TYR:O	2.36	0.58
7:F:31:ILE:HD13	7:F:107:LEU:HD23	1.85	0.58
33:f:347:VAL:HG11	33:f:380:MET:SD	2.44	0.58
36:i:400:ILE:CD1	36:i:429:TYR:CD1	2.82	0.58
37:j:154:LEU:HA	37:j:157:LEU:HB2	1.83	0.58
40:1B:87:LEU:O	86:1:2142:U:O2'	2.21	0.58
54:1P:81:ASP:CB	63:1Y:146:LYS:HD2	2.32	0.58
87:2:79:G:HO2'	87:2:80:U:H6	1.52	0.58
18:Q:204:LYS:HD2	87:2:659:A:H5''	1.84	0.58
24:W:372:THR:HG22	24:W:374:ARG:H	1.67	0.58
27:Z:59:PHE:HD2	87:2:155:U:H5''	1.68	0.58
33:f:90:LEU:HD23	33:f:141:ILE:HB	1.85	0.58
35:h:381:GLU:HA	35:h:384:LYS:HB2	1.84	0.58
47:1I:14:THR:HA	47:1I:17:ASN:HB2	1.84	0.58
66:1b:74:GLU:CG	66:1b:78:LYS:HE3	2.34	0.58
87:2:858:A:OP1	87:2:1070:U:C5	2.56	0.58
3:B:108:GLY:O	3:B:109:CYS:HB2	2.02	0.58
33:f:159:GLY:O	33:f:162:ARG:NH1	2.36	0.58
85:1v:179:ASP:CG	85:1v:216:LEU:HD11	2.16	0.58
86:1:445:G:H21	86:1:465:U:H3'	1.67	0.58
81:1r:62:TYR:OH	81:1r:124:VAL:HG11	2.04	0.58
86:1:2238:C:P	87:2:1826:G:H1'	2.43	0.58
87:2:131:A:H2'	87:2:132:A:H8	1.68	0.58
3:B:107:ILE:O	3:B:107:ILE:HG23	2.04	0.58
17:P:43:HIS:CD2	17:P:45:GLU:HG3	2.37	0.58
33:f:266:LYS:CB	33:f:269:MET:CE	2.79	0.58
50:1L:94:GLY:O	50:1L:97:LYS:NZ	2.37	0.58
35:h:348:GLU:HA	35:h:351:LYS:HD2	1.86	0.58
54:1P:11:ARG:HD2	63:1Y:93:GLY:O	2.03	0.58
84:1u:158:GLU:O	84:1u:162:GLN:HG3	2.04	0.58
86:1:136:G:O2'	86:1:137:U:O2	2.21	0.58
39:l:439:LYS:HE3	39:l:471:LYS:O	2.04	0.58
86:1:2238:C:OP1	87:2:1826:G:N9	2.37	0.58
87:2:79:G:H1'	87:2:80:U:OP1	2.03	0.58
28:a:391:LYS:HE3	39:l:560:MET:HG3	1.85	0.58
33:f:117:GLU:O	33:f:121:HIS:CD2	2.57	0.58
47:1I:61:PHE:O	47:1I:62:LYS:HB2	2.04	0.58
77:1m:9:LYS:HG3	77:1m:44:LEU:HD22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:1s:86:ARG:HA	82:1s:89:LEU:HD12	1.86	0.58
33:f:389:THR:HG21	33:f:397:GLU:CD	2.29	0.57
62:1X:175:ILE:HG22	78:1o:93:ARG:HH22	1.66	0.57
84:1u:189:LYS:HD2	84:1u:225:THR:HG23	1.84	0.57
87:2:939:A:H2'	87:2:940:G:C8	2.39	0.57
87:2:1378:A:H2'	87:2:1379:C:O2	2.04	0.57
36:i:138:GLU:OE1	36:i:141:ARG:NH2	2.37	0.57
33:f:347:VAL:CG1	33:f:380:MET:SD	2.93	0.57
58:1T:254:ARG:NH1	92:1T:301:HOH:O	2.37	0.57
86:1:1872:U:H2'	86:1:1873:U:C6	2.39	0.57
4:C:204:THR:HA	5:D:116:GLU:HG2	1.86	0.57
37:j:214:GLU:OE2	37:j:251:ARG:NH1	2.37	0.57
42:1D:115:ILE:HD13	42:1D:120:ILE:CA	2.34	0.57
85:1v:92:GLN:OE1	85:1v:97:ARG:NH2	2.35	0.57
1:3:33:C:O2'	73:1i:180:HIS:CE1	2.55	0.57
3:B:410:PRO:HB2	3:B:413:TYR:HB2	1.87	0.57
37:j:131:MET:HG2	37:j:134:HIS:HB2	1.87	0.57
37:j:389:LYS:HZ1	37:j:399:TRP:HD1	1.51	0.57
9:H:226:LYS:O	9:H:230:ARG:NH2	2.38	0.57
24:W:473:ARG:NH1	89:W:501:ATP:O3'	2.38	0.57
35:h:288:LEU:CD1	35:h:326:LEU:HD21	2.35	0.57
36:i:372:GLU:O	36:i:409:LYS:NZ	2.38	0.57
86:1:1693:C:H3'	86:1:1694:A:C8	2.38	0.57
3:B:262:ALA:H	28:a:196:THR:HG21	1.70	0.57
16:O:21:MET:HE1	16:O:36:VAL:HG22	1.87	0.57
36:i:400:ILE:HD13	36:i:429:TYR:CD1	2.39	0.57
48:1J:72:ASP:O	48:1J:73:HIS:CE1	2.58	0.57
39:l:547:ASN:HD22	87:2:1391:C:H42	0.71	0.57
39:l:547:ASN:HB3	87:2:1391:C:C4	2.40	0.57
84:1u:167:ASN:HB2	86:1:494:A:H5''	1.87	0.57
87:2:161:A:H2'	87:2:162:C:H4'	1.85	0.57
6:E:84:LYS:HE2	40:1B:56:ASN:HD22	0.76	0.57
84:1u:570:ILE:HG21	84:1u:603:ILE:HD11	1.87	0.57
85:1v:394:LYS:HE2	86:1:144:U:H5'	1.87	0.57
84:1u:279:ASP:C	84:1u:282:ILE:HG22	2.30	0.56
2:A:28:LYS:HG2	22:U:45:LEU:HD11	1.85	0.56
29:b:21:ILE:HB	87:2:1845:A:H61	1.67	0.56
36:i:368:LEU:O	36:i:372:GLU:HG2	2.05	0.56
55:1Q:175:ARG:NH1	55:1Q:186:GLU:OE2	2.38	0.56
28:a:387:THR:OG1	39:l:555:ARG:CB	2.53	0.56
35:h:121:ASP:HA	35:h:124:PHE:CD2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:j:233:TYR:O	37:j:270:ARG:NH1	2.38	0.56
41:1C:192:PRO:HG2	41:1C:195:PRO:HG2	1.88	0.56
48:1J:35:ALA:C	48:1J:38:PRO:HD2	2.31	0.56
48:1J:140:ILE:HD12	48:1J:150:ILE:HG12	1.88	0.56
55:1Q:219:MET:SD	87:2:1693:C:C5'	2.93	0.56
4:C:169:SER:O	4:C:173:GLU:HB2	2.06	0.56
31:d:57:VAL:CG1	37:j:40:PRO:HG2	2.33	0.56
34:g:215:CYS:SG	34:g:216:LEU:N	2.78	0.56
34:g:322:ILE:HD13	34:g:358:PRO:HA	1.87	0.56
54:1P:15:TYR:CE1	63:1Y:137:PRO:HD3	2.40	0.56
81:1r:106:MET:HG2	83:1t:6:LEU:HD11	1.85	0.56
4:C:47:ASN:OD1	4:C:50:ARG:NH2	2.33	0.56
84:1u:112:ILE:HG21	84:1u:115:TRP:CE2	2.40	0.56
86:1:1594:G:C5	86:1:1658:A:N1	2.74	0.56
87:2:1135:A:HO2'	87:2:1136:A:H8	1.52	0.56
7:F:38:ARG:HH12	7:F:109:LYS:HA	1.69	0.56
14:M:106:LYS:CD	25:X:521:ASN:HD21	2.18	0.56
35:h:232:ASP:OD1	35:h:266:ARG:NH1	2.37	0.56
61:1W:212:MET:SD	61:1W:232:VAL:CG1	2.94	0.56
65:1a:139:ARG:NH1	86:1:153:U:OP1	2.38	0.56
84:1u:548:LEU:HA	84:1u:551:LYS:HG2	1.87	0.56
87:2:968:A:H4'	87:2:969:G:H5''	1.87	0.56
25:X:366:ARG:NH1	28:a:126:GLN:HE22	2.00	0.56
28:a:293:TRP:CD2	28:a:315:LEU:HD13	2.41	0.56
41:1C:192:PRO:HG2	41:1C:195:PRO:CG	2.34	0.56
55:1Q:219:MET:SD	87:2:1693:C:H5''	2.46	0.56
61:1W:48:VAL:HG23	86:1:1596:A:OP1	2.05	0.56
87:2:1701:C:H3'	87:2:1702:G:C8	2.40	0.56
4:C:139:VAL:HG11	4:C:144:LEU:CD2	2.34	0.56
6:E:43:PHE:HB2	6:E:64:LEU:HB3	1.88	0.56
17:P:43:HIS:NE2	17:P:45:GLU:HG2	2.20	0.56
35:h:302:HIS:ND1	35:h:302:HIS:O	2.39	0.56
47:1I:28:ASN:ND2	47:1I:30:ASN:OD1	2.28	0.56
62:1X:197:LYS:HG2	62:1X:236:ILE:HD12	1.87	0.56
86:1:1872:U:H2'	86:1:1873:U:H6	1.71	0.56
86:1:2420:G:N2	86:1:2490:U:O2	2.31	0.56
5:D:145:SER:HB2	5:D:148:SER:HB2	1.88	0.56
28:a:407:LYS:HG2	39:l:527:LEU:HD12	1.88	0.56
79:1p:89:ILE:HG22	79:1p:93:LYS:HE2	1.88	0.56
84:1u:290:VAL:HG11	84:1u:324:SER:CB	2.30	0.56
85:1v:198:PHE:HA	85:1v:201:MET:HE3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:1:728:G:O2'	86:1:1411:A:OP1	2.24	0.56
19:R:66:LYS:N	87:2:1136:A:OP1	2.39	0.56
33:f:260:ASN:OD1	33:f:261:THR:N	2.39	0.56
84:1u:279:ASP:O	84:1u:282:ILE:CG2	2.53	0.56
86:1:1221:G:O2'	86:1:1239:A:OP2	2.24	0.56
7:F:25:ARG:NH2	87:2:1636:A:OP1	2.40	0.55
18:Q:227:MET:HE1	20:S:47:MET:HE1	1.87	0.55
76:1l:154:LEU:HD22	76:1l:200:TYR:HB3	1.88	0.55
4:C:256:LEU:HD11	4:C:287:LEU:HD23	1.88	0.55
25:X:471:ASP:O	25:X:475:THR:HG23	2.06	0.55
39:l:279:ARG:HD3	39:l:281:PHE:CE2	2.21	0.55
84:1u:112:ILE:HG21	84:1u:115:TRP:CZ2	2.41	0.55
87:2:1649:G:H2'	87:2:1650:C:C6	2.41	0.55
4:C:172:LYS:O	4:C:176:VAL:HB	2.05	0.55
86:1:1873:U:H4'	86:1:1874:A:OP1	2.05	0.55
5:D:406:GLN:NE2	92:D:606:HOH:O	2.38	0.55
23:V:106:GLU:OE2	87:2:634:C:O2'	2.21	0.55
33:f:145:ASP:OD2	33:f:224:HIS:CE1	2.58	0.55
34:g:114:ILE:HA	34:g:118:LEU:HD23	1.88	0.55
36:i:357:ASN:OD1	36:i:360:ARG:NH2	2.39	0.55
39:l:495:GLU:HA	39:l:498:LYS:HD2	1.87	0.55
48:1J:91:ALA:HA	78:1o:55:VAL:HB	1.88	0.55
64:1Z:114:THR:O	64:1Z:128:LYS:NZ	2.34	0.55
84:1u:541:ARG:NH2	84:1u:572:ASP:OD1	2.38	0.55
85:1v:267:PHE:CE2	85:1v:271:MET:CE	2.89	0.55
87:2:232:A:N6	92:2:2213:HOH:O	2.40	0.55
87:2:1137:G:C4'	87:2:1389:A:H61	2.18	0.55
87:2:1727:G:N1	87:2:1743:A:C2	2.67	0.55
87:2:1839:G:H2'	87:2:1840:A:C8	2.42	0.55
7:F:38:ARG:HH22	7:F:109:LYS:HG3	1.72	0.55
9:H:387:LEU:HD22	9:H:394:MET:HE1	1.89	0.55
36:i:404:GLU:HG3	36:i:437:ARG:HH12	1.70	0.55
41:1C:246:LYS:HE3	64:1Z:45:ARG:HD2	1.89	0.55
48:1J:34:PRO:O	48:1J:38:PRO:CG	2.51	0.55
52:1N:121:LYS:NZ	52:1N:127:MET:O	2.39	0.55
81:1r:106:MET:CG	83:1t:6:LEU:HD11	2.36	0.55
86:1:1693:C:O2'	86:1:1694:A:H5'	2.06	0.55
36:i:403:VAL:HG21	36:i:428:MET:HE2	1.87	0.55
43:1E:247:ILE:HG21	43:1E:263:ILE:HD12	1.88	0.55
48:1J:18:LYS:HE2	86:1:1211:G:H8	1.71	0.55
48:1J:28:PRO:CB	48:1J:43:MET:CE	2.84	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:1M:251:ARG:NH1	86:1:786:G:OP1	2.39	0.55
86:1:2190:U:O2'	86:1:2191:U:O4'	2.24	0.55
9:H:336:ASP:OD2	24:W:429:ARG:NH1	2.40	0.55
36:i:599:THR:HG22	36:i:632:LEU:HD22	1.89	0.55
44:1F:178:GLN:NE2	73:1i:221:ARG:O	2.35	0.55
73:1i:79:GLU:OE2	73:1i:83:ASN:ND2	2.40	0.55
86:1:855:G:H1	86:1:865:G:H22	1.53	0.55
6:E:46:VAL:HG12	23:V:195:LEU:HD23	1.89	0.55
35:h:153:GLN:HA	35:h:156:LYS:HG2	1.88	0.55
36:i:400:ILE:CG1	36:i:434:ASN:ND2	2.69	0.55
55:1Q:128:ARG:NH2	55:1Q:133:ILE:O	2.40	0.55
67:1c:18:SER:HB3	73:1i:229:PRO:HB3	1.88	0.55
86:1:1325:G:O6	86:1:1331:U:O4	2.25	0.55
76:1l:178:GLU:OE2	76:1l:179:THR:HG23	2.06	0.55
84:1u:230:ILE:HG13	84:1u:231:LEU:HD12	1.89	0.55
87:2:1746:A:H2'	87:2:1747:A:C8	2.42	0.55
30:c:137:LYS:HA	86:1:2251:G:H5''	1.88	0.55
70:1f:175:PHE:HA	70:1f:200:THR:HG21	1.88	0.55
86:1:855:G:H22	86:1:865:G:H22	1.55	0.55
3:B:405:ARG:CD	28:a:125:LEU:HD22	2.37	0.54
27:Z:65:ILE:CD1	35:h:143:HIS:ND1	2.69	0.54
34:g:141:LYS:HA	34:g:148:LEU:HD11	1.88	0.54
42:1D:250:VAL:HG12	42:1D:264:VAL:HG22	1.89	0.54
45:1G:88:TYR:HB2	45:1G:91:GLU:HB2	1.89	0.54
81:1r:57:ILE:CG2	81:1r:88:LEU:HD21	2.37	0.54
33:f:331:CYS:HA	33:f:334:ARG:NH1	2.22	0.54
34:g:439:ALA:HB1	34:g:473:LEU:HG	1.89	0.54
51:1M:240:LYS:NZ	92:1M:306:HOH:O	2.40	0.54
77:1m:88:TYR:CZ	77:1m:102:TRP:CZ2	2.95	0.54
81:1r:102:ARG:NH2	92:1r:201:HOH:O	2.39	0.54
86:1:1023:A:N6	86:1:1047:A:O2'	2.41	0.54
87:2:160:A:H2'	87:2:161:A:C8	2.43	0.54
3:B:405:ARG:CD	28:a:125:LEU:CD2	2.85	0.54
36:i:392:HIS:NE2	36:i:424:ALA:HB2	2.23	0.54
61:1W:47:ARG:CZ	86:1:1596:A:OP2	2.55	0.54
76:1l:220:LEU:HD13	76:1l:227:PHE:CE2	2.42	0.54
3:B:176:SER:OG	3:B:230:VAL:N	2.39	0.54
34:g:367:LEU:HD12	34:g:399:LEU:HD11	1.88	0.54
51:1M:183:ALA:HB1	51:1M:204:VAL:HG11	1.88	0.54
74:1j:37:LYS:O	86:1:121:C:O2'	2.20	0.54
84:1u:279:ASP:CA	84:1u:282:ILE:HG22	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:98:TRP:HB2	25:X:330:ALA:HB1	1.90	0.54
29:b:21:ILE:CG2	87:2:1845:A:C2	2.90	0.54
36:i:392:HIS:NE2	36:i:424:ALA:CB	2.71	0.54
60:1V:121:ILE:HD12	60:1V:124:ILE:HD12	1.90	0.54
87:2:1171:U:H2'	87:2:1172:U:C6	2.42	0.54
14:M:121:THR:HG22	87:2:972:C:H42	1.73	0.54
19:R:167:PRO:HD3	67:1c:54:PHE:CG	2.43	0.54
43:1E:125:ARG:NH2	86:1:804:U:O3'	2.41	0.54
86:1:2191:U:H2'	86:1:2192:A:H4'	1.89	0.54
86:1:2231:A:H2	87:2:1802:A:C2'	2.20	0.54
35:h:166:HIS:CE1	35:h:169:ARG:NH1	2.75	0.54
56:1R:22:ARG:HH12	86:1:1410:A:H5'	1.73	0.54
79:1p:16:VAL:O	79:1p:16:VAL:HG12	2.06	0.54
84:1u:550:ILE:HG22	84:1u:554:MET:HE2	1.90	0.54
85:1v:256:CYS:SG	85:1v:285:VAL:CG1	2.87	0.54
87:2:80:U:H2'	87:2:81:U:C6	2.42	0.54
4:C:182:LYS:HZ2	4:C:224:MET:HG3	1.72	0.54
14:M:121:THR:HG23	87:2:1622:A:C5	2.43	0.54
27:Z:63:TRP:CD2	35:h:137:LEU:CD2	2.91	0.54
27:Z:123:TYR:CE1	87:2:155:U:N1	2.76	0.54
34:g:227:VAL:HG22	34:g:247:LEU:HD13	1.90	0.54
37:j:260:HIS:CE1	37:j:283:MET:HE3	2.42	0.54
37:j:354:MET:HE3	37:j:391:LYS:HD2	1.88	0.54
41:1C:100:THR:HG22	64:1Z:154:PHE:CE2	2.35	0.54
82:1s:128:ARG:NH2	86:1:1967:C:OP1	2.35	0.54
84:1u:340:ARG:HB3	84:1u:343:ASP:HB2	1.90	0.54
9:H:224:VAL:HG12	9:H:225:ILE:H	1.73	0.54
13:L:124:MET:HE1	87:2:1489:C:H3'	1.90	0.54
33:f:198:GLU:OE2	33:f:324:ARG:NH2	2.41	0.54
36:i:400:ILE:HD13	36:i:434:ASN:HD22	1.73	0.54
60:1V:17:ARG:NH1	86:1:84:G:OP2	2.40	0.54
77:1m:93:GLN:C	77:1m:95:PHE:N	2.64	0.54
84:1u:472:MET:HE2	84:1u:477:TYR:HB3	1.88	0.54
84:1u:566:LEU:O	84:1u:570:ILE:HG12	2.07	0.54
86:1:1001:G:H2'	86:1:1002:A:C8	2.43	0.54
86:1:1594:G:C6	86:1:1658:A:C5	2.94	0.54
2:A:28:LYS:CG	22:U:45:LEU:CD1	2.85	0.54
3:B:39:ARG:NH1	3:B:60:CYS:O	2.39	0.54
3:B:206:LEU:CB	28:a:183:ILE:HG23	2.38	0.54
3:B:212:PRO:HD2	3:B:212:PRO:O	2.07	0.54
87:2:683:A:O2'	87:2:697:C:N4	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:207:PHE:CZ	3:B:213:LYS:HE3	2.42	0.53
61:1W:212:MET:SD	61:1W:232:VAL:HG13	2.48	0.53
87:2:1137:G:C2'	87:2:1138:G:H5'	2.38	0.53
87:2:1388:A:HO2'	87:2:1389:A:H8	1.55	0.53
87:2:1650:C:C2'	87:2:1651:C:H5'	2.38	0.53
36:i:404:GLU:OE1	36:i:437:ARG:NH2	2.41	0.53
39:l:485:ARG:NH2	39:l:521:SER:OG	2.32	0.53
52:1N:84:GLU:OE2	52:1N:87:ARG:NH2	2.40	0.53
67:1c:48:ILE:HG23	67:1c:53:LYS:CE	2.38	0.53
73:1i:230:ILE:HB	73:1i:233:TYR:HB2	1.90	0.53
87:2:79:G:O2'	87:2:80:U:H5''	2.07	0.53
87:2:929:C:H2'	87:2:930:A:H8	1.73	0.53
2:A:16:SER:HB2	2:A:178:ALA:HB1	1.90	0.53
82:1s:118:ARG:NH1	86:1:1889:A:OP1	2.42	0.53
84:1u:382:VAL:HA	84:1u:385:SER:OG	2.08	0.53
60:1V:2:GLY:N	92:1V:207:HOH:O	2.40	0.53
67:1c:21:LEU:H	73:1i:227:THR:HB	1.73	0.53
5:D:364:VAL:HA	5:D:386:MET:HG2	1.89	0.53
20:S:86:PHE:CD1	29:b:19:LEU:HG	2.42	0.53
52:1N:48:ARG:HG3	86:1:1058:A:C5	2.43	0.53
84:1u:189:LYS:HG3	84:1u:225:THR:OG1	2.09	0.53
85:1v:256:CYS:HG	85:1v:285:VAL:HG12	1.74	0.53
86:1:2600:U:H2'	86:1:2601:A:C8	2.44	0.53
87:2:670:G:H2'	87:2:671:A:C8	2.44	0.53
11:J:260:VAL:HG11	11:J:275:ILE:HG12	1.89	0.53
14:M:106:LYS:CD	25:X:521:ASN:ND2	2.72	0.53
34:g:154:ASN:HB3	34:g:187:VAL:HG21	1.91	0.53
39:l:502:GLU:CG	39:l:506:PHE:CE2	2.76	0.53
86:1:1870:U:H2'	86:1:1871:U:C6	2.43	0.53
86:1:1870:U:H2'	86:1:1871:U:H6	1.73	0.53
34:g:400:LEU:HD22	34:g:428:TYR:HE2	1.73	0.53
39:l:513:ASP:OD2	87:2:1138:G:O2'	2.27	0.53
42:1D:115:ILE:HD13	42:1D:120:ILE:C	2.33	0.53
84:1u:279:ASP:HA	84:1u:282:ILE:CG2	2.39	0.53
45:1G:31:LEU:HD13	45:1G:76:LYS:HB2	1.89	0.53
47:1I:41:ARG:NH2	86:1:1234:G:OP1	2.42	0.53
51:1M:103:ARG:NH1	86:1:951:C:OP2	2.41	0.53
87:2:1136:A:H3'	87:2:1390:A:H61	1.74	0.53
28:a:311:ARG:O	28:a:360:ASN:ND2	2.42	0.53
39:l:513:ASP:CG	87:2:1138:G:H1'	2.34	0.53
83:1t:22:ASP:OD1	83:1t:28:ARG:NH2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
87:2:1137:G:O2'	87:2:1389:A:N1	2.33	0.53
1:3:44:C:C5	44:1F:62:ILE:HG21	2.43	0.53
3:B:107:ILE:HG23	3:B:110:LEU:HD21	1.90	0.53
23:V:89:GLU:OE2	23:V:92:ARG:NH2	2.42	0.53
24:W:372:THR:HB	24:W:375:SER:HB3	1.91	0.53
29:b:21:ILE:HG22	87:2:1845:A:C5	2.44	0.53
57:1S:221:LYS:HD2	86:1:1123:A:H5''	1.91	0.53
61:1W:38:ALA:HB3	61:1W:111:VAL:HG22	1.90	0.53
61:1W:181:ARG:NH2	86:1:1638:C:OP1	2.42	0.53
71:1g:89:LYS:NZ	86:1:2718:G:OP1	2.42	0.53
87:2:1387:C:O2	87:2:1387:C:C2'	2.56	0.53
39:l:522:PHE:HD1	39:l:528:ASP:HB3	1.73	0.52
42:1D:223:GLN:HB2	42:1D:227:PRO:HD3	1.91	0.52
85:1v:107:PRO:O	85:1v:108:THR:HG23	2.09	0.52
86:1:1935:A:O2'	86:1:1937:C:OP1	2.26	0.52
4:C:162:ARG:NH2	4:C:165:GLU:OE1	2.42	0.52
15:N:340:GLU:OE2	23:V:151:ARG:NH2	2.42	0.52
62:1X:115:LEU:HD21	62:1X:143:ILE:HG22	1.91	0.52
77:1m:92:GLU:CG	77:1m:102:TRP:CE2	2.90	0.52
5:D:131:GLN:NE2	87:2:430:A:OP1	2.35	0.52
26:Y:91:LYS:NZ	87:2:1475:U:OP2	2.40	0.52
29:b:43:CYS:SG	29:b:47:ASN:ND2	2.83	0.52
37:j:172:ARG:NH2	37:j:176:GLU:OE1	2.41	0.52
39:l:411:ASN:OD1	39:l:444:THR:OG1	2.27	0.52
70:1f:194:LYS:HD3	70:1f:196:ARG:HD3	1.91	0.52
84:1u:325:VAL:HG23	84:1u:354:PHE:CZ	2.45	0.52
87:2:203:A:H62	87:2:243:U:H3	1.56	0.52
87:2:1224:A:H2'	87:2:1225:A:H8	1.74	0.52
3:B:375:LYS:HZ1	28:a:102:ILE:HG12	1.74	0.52
47:1I:72:LEU:HD13	47:1I:115:VAL:HG23	1.91	0.52
48:1J:28:PRO:HB2	48:1J:43:MET:CE	2.39	0.52
59:1U:129:LEU:HD13	83:1t:110:GLU:HB3	1.92	0.52
61:1W:35:THR:O	61:1W:89:GLN:NE2	2.42	0.52
66:1b:45:ARG:NH2	92:1b:202:HOH:O	2.42	0.52
67:1c:20:ARG:HE	73:1i:229:PRO:HG3	1.74	0.52
86:1:343:A:N6	86:1:490:U:OP2	2.36	0.52
3:B:511:SER:O	3:B:517:GLN:OE1	2.27	0.52
11:J:250:VAL:HG13	11:J:255:LEU:CD1	2.33	0.52
17:P:68:ASN:HD21	87:2:254:U:C5'	2.23	0.52
27:Z:123:TYR:CD1	87:2:155:U:O2	2.62	0.52
47:1I:59:LEU:O	47:1I:60:VAL:C	2.51	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:1t:462:HIS:CE1	85:1v:242:PHE:N	2.69	0.52
86:1:2446:G:N3	86:1:2476:A:O2'	2.37	0.52
1:3:43:U:O4	44:1F:64:THR:HA	2.09	0.52
13:L:45:LEU:HD22	13:L:64:LEU:HD21	1.92	0.52
24:W:215:VAL:HG22	24:W:216:LYS:HG2	1.91	0.52
34:g:630:GLN:HG2	34:g:650:PHE:CE1	2.44	0.52
37:j:366:LYS:HA	37:j:369:VAL:HG12	1.91	0.52
47:1I:15:LYS:O	47:1I:19:GLN:HG3	2.10	0.52
61:1W:39:ILE:HD12	61:1W:57:ARG:HH22	1.73	0.52
86:1:1606:A:N6	86:1:1646:U:O2'	2.39	0.52
86:1:3057:C:O2	86:1:3058:U:N3	2.40	0.52
87:2:1697:G:H2'	87:2:1698:C:C6	2.45	0.52
9:H:269:ASN:OD1	9:H:272:ARG:NH2	2.37	0.52
52:1N:128:GLY:O	86:1:2584:C:O2'	2.28	0.52
55:1Q:208:ARG:C	55:1Q:209:ARG:HD2	2.35	0.52
67:1c:56:ARG:NH2	87:2:1573:U:H5''	2.24	0.52
76:1I:220:LEU:HD13	76:1I:227:PHE:HE2	1.74	0.52
92:A:319:HOH:O	38:k:20:MET:HE2	2.10	0.52
3:B:104:ALA:HB2	3:B:405:ARG:O	2.10	0.52
85:1v:495:THR:O	85:1v:499:ARG:HG3	2.10	0.52
86:1:1693:C:C3'	86:1:1694:A:H8	2.23	0.52
87:2:922:G:C6	87:2:923:C:C4	2.98	0.52
87:2:1833:U:H2'	87:2:1834:G:C8	2.45	0.52
7:F:124:SER:HA	7:F:127:ARG:HD3	1.91	0.52
31:d:44:GLU:OE2	37:j:42:THR:HB	2.09	0.52
32:e:194:LYS:NZ	32:e:227:GLU:OE1	2.41	0.52
48:1J:36:LEU:HB3	48:1J:41:LEU:HB2	1.92	0.52
51:1M:127:LYS:NZ	86:1:229:A:H5'	2.25	0.52
54:1P:87:ILE:HD11	54:1P:113:LEU:HD22	1.92	0.52
3:B:193:PHE:O	3:B:197:ASN:HB2	2.10	0.52
4:C:17:LEU:HD13	87:2:451:A:H4'	1.92	0.52
29:b:25:LYS:HD3	87:2:1845:A:C6	2.45	0.52
32:e:384:LEU:C	32:e:384:LEU:HD12	2.35	0.52
35:h:288:LEU:HD11	35:h:326:LEU:HD23	1.92	0.52
48:1J:22:LEU:HD23	48:1J:60:ASP:CA	2.33	0.52
60:1V:38:VAL:HG22	60:1V:45:VAL:HG12	1.92	0.52
61:1W:160:LEU:HD23	61:1W:161:VAL:N	2.25	0.52
83:1t:123:GLU:OE1	83:1t:155:THR:OG1	2.28	0.52
84:1u:112:ILE:HG23	84:1u:112:ILE:O	2.09	0.52
84:1u:367:LEU:HD11	84:1u:383:LEU:HD21	1.92	0.52
85:1v:107:PRO:C	85:1v:108:THR:HG23	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:1:1875:G:H4'	86:1:1875:G:OP1	2.10	0.52
17:P:43:HIS:HD2	17:P:45:GLU:HG3	1.75	0.51
20:S:45:ARG:HH21	20:S:49:SER:HB3	1.75	0.51
35:h:96:SER:HA	35:h:100:LYS:HE2	1.92	0.51
5:D:238:ARG:NH2	32:e:285:ASP:OD1	2.41	0.51
8:G:15:ASN:OD1	8:G:18:ARG:NH2	2.43	0.51
20:S:38:LYS:NZ	92:S:201:HOH:O	2.43	0.51
23:V:182:GLU:HA	23:V:185:ILE:HD12	1.93	0.51
39:l:157:LEU:HG	39:l:187:ILE:HG23	1.92	0.51
48:1J:32:VAL:CB	48:1J:43:MET:HE1	2.29	0.51
64:1Z:12:LEU:HD21	64:1Z:29:LEU:HD22	1.91	0.51
52:1N:77:ARG:NH2	92:1N:202:HOH:O	2.43	0.51
85:1v:107:PRO:O	85:1v:108:THR:CG2	2.58	0.51
85:1v:174:GLY:O	85:1v:175:ALA:HB2	2.10	0.51
86:1:1412:U:H5''	86:1:1413:G:H5''	1.92	0.51
33:f:253:SER:HB3	36:i:283:TYR:OH	2.10	0.51
34:g:642:ASN:CB	39:l:372:ILE:HG21	2.25	0.51
83:1t:91:SER:HB3	86:1:1575:A:H5'	1.91	0.51
87:2:564:A:N6	92:2:2271:HOH:O	2.43	0.51
87:2:710:G:H2'	87:2:711:A:C8	2.46	0.51
87:2:969:G:OP2	87:2:1620:U:O2'	2.25	0.51
3:B:166:LYS:NZ	25:X:378:ASP:OD1	2.44	0.51
5:D:399:LYS:NZ	92:D:608:HOH:O	2.43	0.51
7:F:19:ARG:HG2	7:F:93:LEU:HD13	1.92	0.51
33:f:397:GLU:O	33:f:399:LYS:NZ	2.44	0.51
34:g:208:ARG:HH22	34:g:222:ASN:HA	1.75	0.51
52:1N:43:LYS:NZ	86:1:1060:C:OP1	2.40	0.51
85:1v:512:LYS:NZ	86:1:37:G:O6	2.44	0.51
2:A:28:LYS:CD	22:U:45:LEU:CD1	2.85	0.51
3:B:175:ILE:HD11	25:X:447:ARG:HH21	1.73	0.51
9:H:241:ILE:HB	36:i:295:MET:HE2	1.92	0.51
9:H:321:ILE:HG22	9:H:363:ILE:HG12	1.91	0.51
9:H:352:LEU:HD23	9:H:387:LEU:HD11	1.93	0.51
21:T:84:GLU:HG2	24:W:382:ARG:HE	1.76	0.51
28:a:333:ARG:NH2	87:2:1131:G:OP1	2.44	0.51
63:1Y:56:LYS:O	63:1Y:59:ARG:NH1	2.39	0.51
75:1k:33:GLU:HG2	75:1k:81:LEU:HD22	1.92	0.51
86:1:2433:G:O2'	86:1:2469:C:N3	2.43	0.51
87:2:1618:G:H2'	87:2:1619:A:C8	2.46	0.51
87:2:1703:G:H3'	87:2:1704:A:H8	1.75	0.51
19:R:189:GLU:HG2	67:1c:51:ILE:HG13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:d:39:LYS:HE2	37:j:43:SER:HB3	1.93	0.51
37:j:245:LEU:HD21	37:j:263:ARG:HH21	1.74	0.51
47:1I:23:PHE:HB3	47:1I:85:VAL:HB	1.93	0.51
86:1:2934:U:OP1	86:1:2935:A:N6	2.43	0.51
4:C:290:TYR:HD2	5:D:178:LEU:HD21	1.76	0.51
26:Y:6:LEU:O	26:Y:10:VAL:HG23	2.11	0.51
31:d:92:LEU:HD13	87:2:478:U:H5'	1.92	0.51
35:h:330:PHE:HA	35:h:333:LEU:HD13	1.93	0.51
35:h:342:LEU:HA	35:h:345:GLN:HG2	1.93	0.51
36:i:387:TYR:OH	36:i:413:ASN:ND2	2.44	0.51
41:1C:196:VAL:CG2	41:1C:226:TRP:HZ3	2.24	0.51
60:1V:159:LEU:HD11	65:1a:137:MET:HG3	1.93	0.51
61:1W:209:LYS:HD2	61:1W:231:PRO:HG3	1.91	0.51
83:1t:462:HIS:HE1	85:1v:242:PHE:H	1.59	0.51
84:1u:138:ARG:HH22	86:1:496:C:H5	1.59	0.51
4:C:182:LYS:HG3	4:C:220:LEU:HD22	1.92	0.51
14:M:77:ARG:HH11	26:Y:51:VAL:HG13	1.76	0.51
37:j:58:ARG:HD2	37:j:93:ASN:HD21	1.76	0.51
48:1J:32:VAL:HG12	48:1J:43:MET:HE3	1.68	0.51
84:1u:289:ASP:O	84:1u:293:TYR:HD2	1.94	0.51
87:2:474:A:H61	87:2:479:G:H5'	1.75	0.51
87:2:1273:A:N1	87:2:1274:A:N6	2.58	0.51
87:2:1653:U:H2'	87:2:1654:G:C8	2.46	0.51
13:L:135:ALA:HB3	13:L:139:LYS:HE3	1.92	0.51
30:c:112:ASP:N	87:2:570:A:OP2	2.44	0.51
54:1P:91:LYS:CA	86:1:2639:U:O4	2.59	0.51
62:1X:47:ASP:O	62:1X:117:ARG:NH2	2.40	0.51
74:1j:17:ARG:NH2	86:1:598:A:O2'	2.44	0.51
81:1r:77:TRP:CD1	81:1r:91:LYS:HE2	2.46	0.51
81:1r:124:VAL:CG1	81:1r:125:LEU:N	2.74	0.51
86:1:345:A:H2'	86:1:346:A:C8	2.45	0.51
31:d:46:LEU:HD11	31:d:60:LEU:HD12	1.92	0.50
39:l:548:ALA:HB3	87:2:1391:C:O2	2.11	0.50
43:1E:300:ARG:NH2	86:1:757:U:OP2	2.39	0.50
85:1v:252:ILE:CD1	85:1v:267:PHE:HD2	2.24	0.50
86:1:2808:2MA:O2'	86:1:2810:G:OP2	2.24	0.50
3:B:309:ARG:HA	3:B:312:HIS:HB2	1.94	0.50
7:F:145:PHE:HZ	11:J:232:ARG:NH1	2.09	0.50
35:h:84:GLU:O	35:h:88:GLU:HG3	2.11	0.50
47:1I:17:ASN:HA	47:1I:86:GLN:HE21	1.76	0.50
50:1L:122:ARG:NH2	86:1:2007:A:OP1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:1P:94:ARG:CZ	86:1:2603:G:H5'	2.42	0.50
85:1v:94:ILE:HB	85:1v:128:GLY:HA3	1.93	0.50
85:1v:252:ILE:HD11	85:1v:267:PHE:HD2	1.76	0.50
86:1:1585:C:N4	92:1:4021:HOH:O	2.44	0.50
3:B:405:ARG:HD3	28:a:125:LEU:HD22	1.93	0.50
25:X:469:GLU:O	25:X:473:ILE:HG13	2.11	0.50
39:l:547:ASN:ND2	87:2:1391:C:N4	2.33	0.50
49:1K:65:ARG:HG2	49:1K:67:ASP:HB2	1.92	0.50
67:1c:48:ILE:HG23	67:1c:53:LYS:HE2	1.93	0.50
84:1u:124:LEU:HB3	84:1u:159:MET:HE1	1.93	0.50
84:1u:315:GLU:O	84:1u:319:LYS:HG2	2.11	0.50
86:1:275:A:H2'	86:1:276:A:H8	1.75	0.50
4:C:55:ARG:NH2	5:D:406:GLN:OE1	2.44	0.50
37:j:312:LYS:NZ	37:j:342:ASP:OD2	2.43	0.50
48:1J:39:TYR:HH	86:1:1247:U:H3	1.57	0.50
61:1W:90:ILE:O	61:1W:94:VAL:HG23	2.12	0.50
66:1b:59:ARG:NH2	80:1q:61:ASP:OD1	2.43	0.50
86:1:151:U:H1'	86:1:152:C:H5'	1.93	0.50
87:2:1737:A:H3'	87:2:1738:G:H21	1.77	0.50
10:I:156:MET:HB2	10:I:185:LYS:HB3	1.92	0.50
27:Z:62:ASN:N	35:h:145:ASN:OD1	2.41	0.50
36:i:404:GLU:CG	36:i:437:ARG:NH1	2.75	0.50
41:1C:193:ARG:NH2	46:1H:77:LEU:HD23	2.27	0.50
84:1u:270:ARG:HB3	84:1u:273:THR:HB	1.92	0.50
86:1:1624:G:H21	86:1:1625:C:H41	1.59	0.50
86:1:2414:A:H2'	86:1:2415:A:C8	2.46	0.50
87:2:612:U:H2'	87:2:613:C:C6	2.46	0.50
34:g:654:LYS:HE3	34:g:656:ASN:HB2	1.93	0.50
41:1C:100:THR:HG23	64:1Z:154:PHE:CE1	2.37	0.50
62:1X:136:VAL:HG21	62:1X:159:ARG:HG2	1.94	0.50
73:1i:127:MET:O	76:1l:64:ARG:NH1	2.45	0.50
3:B:206:LEU:CA	28:a:183:ILE:HG23	2.41	0.50
18:Q:193:LEU:HD21	18:Q:213:ILE:CG2	2.39	0.50
19:R:189:GLU:HG2	67:1c:51:ILE:CG1	2.41	0.50
26:Y:77:LYS:NZ	87:2:1469:G:OP1	2.39	0.50
37:j:45:GLN:HA	37:j:48:LYS:HB3	1.94	0.50
39:l:502:GLU:O	39:l:506:PHE:HD2	1.94	0.50
41:1C:194:ILE:N	41:1C:195:PRO:CD	2.74	0.50
48:1J:134:SER:HB3	86:1:1231:U:H4'	1.92	0.50
86:1:958:U:H2'	86:1:959:C:C6	2.47	0.50
86:1:1594:G:O6	86:1:1658:A:N6	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:1:1594:G:C6	86:1:1658:A:N1	2.79	0.50
86:1:2856:U:H3	86:1:2862:G:H22	1.58	0.50
87:2:1137:G:H2'	87:2:1138:G:H5'	1.93	0.50
87:2:1137:G:N7	87:2:1384:A:C2	2.80	0.50
2:A:58:ALA:HB2	2:A:195:CYS:HB3	1.93	0.50
11:J:270:LYS:NZ	92:J:401:HOH:O	2.44	0.50
28:a:405:GLN:O	28:a:409:MET:HG2	2.11	0.50
29:b:21:ILE:HG22	87:2:1845:A:C4	2.47	0.50
32:e:299:LEU:CD2	32:e:384:LEU:CD2	2.89	0.50
36:i:371:ALA:C	36:i:373:GLY:H	2.18	0.50
73:1i:184:ARG:NH1	92:1i:303:HOH:O	2.45	0.50
74:1j:82:ILE:O	74:1j:83:GLU:CG	2.57	0.50
85:1v:143:ASP:OD2	85:1v:175:ALA:HB3	2.12	0.50
85:1v:326:ASN:OD1	85:1v:359:THR:OG1	2.28	0.50
3:B:376:VAL:O	3:B:376:VAL:CG1	2.59	0.50
27:Z:123:TYR:HE1	87:2:155:U:N1	2.09	0.50
36:i:326:GLU:OE2	36:i:358:GLN:NE2	2.44	0.50
39:l:143:SER:HB2	39:l:146:PHE:HB3	1.94	0.50
39:l:474:LYS:CE	87:2:1141:A:N1	2.70	0.50
47:1I:61:PHE:HB2	47:1I:76:MET:HE1	1.94	0.50
3:B:205:LYS:CB	28:a:183:ILE:CG1	2.87	0.49
33:f:266:LYS:CD	33:f:269:MET:HE1	2.41	0.49
37:j:259:THR:O	37:j:263:ARG:HG2	2.12	0.49
39:l:174:LEU:HB3	39:l:197:LEU:HD11	1.94	0.49
46:1H:52:ILE:HB	46:1H:55:LEU:HB2	1.93	0.49
51:1M:241:ALA:HB2	51:1M:258:LEU:HG	1.94	0.49
62:1X:141:ARG:HB3	62:1X:156:THR:HG22	1.95	0.49
71:1g:147:LYS:NZ	92:1g:201:HOH:O	2.45	0.49
76:1l:35:ARG:HG3	76:1l:103:LEU:HD22	1.92	0.49
86:1:2350:G:N2	86:1:2877:A:OP2	2.45	0.49
86:1:2363:A:H2'	86:1:2364:A:C8	2.47	0.49
86:1:2633:A:H2'	86:1:2634:U:C6	2.47	0.49
34:g:401:LYS:HA	34:g:434:MET:HE3	1.93	0.49
39:l:549:ILE:CD1	87:2:1389:A:C1'	2.89	0.49
63:1Y:117:ASN:HB2	63:1Y:124:TRP:HZ3	1.77	0.49
85:1v:233:MET:O	85:1v:237:THR:OG1	2.29	0.49
10:I:176:ARG:NH2	87:2:1628:C:O2'	2.39	0.49
34:g:247:LEU:HB3	34:g:249:VAL:HG23	1.94	0.49
39:l:235:ASN:ND2	39:l:268:THR:OG1	2.42	0.49
47:1I:124:GLN:OE1	77:1m:49:THR:OG1	2.26	0.49
61:1W:48:VAL:CG2	86:1:1596:A:H5'	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:1i:193:MET:HE1	76:1l:230:MET:HA	1.93	0.49
76:1l:108:ASP:OD1	76:1l:108:ASP:N	2.44	0.49
22:U:108:MET:CE	36:i:450:LEU:HD22	2.42	0.49
27:Z:58:GLN:HE22	87:2:153:A:H61	1.54	0.49
33:f:347:VAL:HG12	33:f:347:VAL:O	2.11	0.49
34:g:430:PRO:O	34:g:435:GLN:NE2	2.45	0.49
39:l:232:GLU:OE2	39:l:267:LYS:NZ	2.44	0.49
86:1:2238:C:OP1	87:2:1826:G:C8	2.65	0.49
87:2:1498:U:O2'	87:2:1567:G:OP1	2.29	0.49
3:B:405:ARG:HD3	28:a:125:LEU:CD2	2.42	0.49
33:f:104:VAL:C	33:f:106:PRO:HD2	2.37	0.49
33:f:266:LYS:HD2	33:f:269:MET:CE	2.42	0.49
34:g:583:MET:HB3	34:g:619:THR:HG21	1.93	0.49
35:h:125:LEU:HD21	35:h:154:VAL:HG23	1.94	0.49
37:j:389:LYS:HZ1	37:j:399:TRP:CD1	2.30	0.49
48:1J:18:LYS:CE	86:1:1211:G:C8	2.95	0.49
49:1K:167:MET:HE3	49:1K:172:ARG:HG3	1.95	0.49
62:1X:129:SER:OG	62:1X:131:GLU:OE1	2.30	0.49
84:1u:154:MET:O	84:1u:158:GLU:HG3	2.12	0.49
86:1:1426:A:N7	92:1:3745:HOH:O	2.35	0.49
86:1:1693:C:C2'	86:1:1694:A:H5'	2.42	0.49
87:2:709:G:H2'	87:2:710:G:C8	2.47	0.49
87:2:1388:A:O2'	87:2:1389:A:H8	1.94	0.49
3:B:67:LYS:HD3	28:a:303:GLY:HA2	1.92	0.49
35:h:181:PRO:HB2	35:h:214:LEU:HD11	1.94	0.49
60:1V:156:MET:HE3	60:1V:157:PRO:HD2	1.95	0.49
83:1t:63:LYS:NZ	92:1t:509:HOH:O	2.43	0.49
87:2:613:C:H2'	87:2:614:A:C8	2.47	0.49
87:2:1494:G:N2	92:2:2227:HOH:O	2.45	0.49
7:F:24:LYS:NZ	92:F:202:HOH:O	2.44	0.49
29:b:21:ILE:C	87:2:1845:A:N1	2.68	0.49
35:h:331:LYS:HA	35:h:334:VAL:HG22	1.93	0.49
36:i:304:GLU:OE2	36:i:348:ASN:ND2	2.44	0.49
60:1V:127:THR:HG23	86:1:92:C:H41	1.77	0.49
86:1:1589:C:N4	92:1:4038:HOH:O	2.45	0.49
86:1:1694:A:C2'	86:1:1695:A:H5'	2.42	0.49
86:1:2126:A:H2'	86:1:2127:A:C8	2.47	0.49
87:2:1298:A:H2'	87:2:1299:A:H8	1.77	0.49
24:W:204:LYS:HD3	24:W:205:PRO:HD2	1.95	0.49
48:1J:35:ALA:C	48:1J:38:PRO:CD	2.86	0.49
55:1Q:128:ARG:NH1	55:1Q:192:TYR:OH	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:1k:13:VAL:HB	75:1k:59:LYS:HB3	1.95	0.49
84:1u:141:GLU:OE1	84:1u:179:LYS:NZ	2.41	0.49
86:1:334:A:H2'	86:1:335:A:H8	1.77	0.49
86:1:2432:A:N7	86:1:2433:G:N2	2.45	0.49
87:2:1666:C:H2'	87:2:1667:G:C8	2.47	0.49
3:B:342:PHE:HZ	10:I:206:ARG:HG2	1.78	0.49
23:V:124:ARG:NH2	87:2:590:A:OP1	2.45	0.49
40:1B:40:LYS:HA	40:1B:43:VAL:HG22	1.95	0.49
57:1S:143:ILE:HD12	57:1S:180:LEU:HB3	1.94	0.49
59:1U:131:GLN:OE1	59:1U:134:ARG:CG	2.59	0.49
60:1V:95:LYS:HE3	60:1V:105:VAL:HG11	1.94	0.49
65:1a:34:ALA:HB1	65:1a:39:GLU:HB2	1.95	0.49
86:1:2827:U:O2'	86:1:2956:C:OP1	2.23	0.49
9:H:395:ARG:NH2	87:2:1442:A:OP2	2.46	0.49
11:J:289:GLN:NE2	18:Q:252:ASP:OD2	2.45	0.49
32:e:212:MET:HE3	32:e:257:ARG:HG2	1.94	0.49
41:1C:249:ARG:HG3	64:1Z:126:PHE:CE1	2.48	0.49
48:1J:68:THR:O	48:1J:70:TYR:CE2	2.66	0.49
83:1t:463:PRO:HG2	83:1t:467:GLN:HB2	1.95	0.49
87:2:718:A:H2	87:2:729:A:H61	1.61	0.49
3:B:372:GLY:HA2	3:B:376:VAL:CG2	2.43	0.48
5:D:297:MET:HE1	5:D:355:LEU:HD11	1.94	0.48
10:I:160:ARG:NH2	92:I:303:HOH:O	2.45	0.48
35:h:197:LYS:HE2	35:h:230:GLU:HB3	1.95	0.48
41:1C:250:ARG:HG3	41:1C:256:LEU:HD12	1.94	0.48
42:1D:112:VAL:HG23	42:1D:167:VAL:HG23	1.94	0.48
16:O:14:ASN:ND2	92:O:202:HOH:O	2.41	0.48
19:R:175:ARG:HB3	19:R:182:HIS:HB3	1.94	0.48
34:g:271:LEU:HA	34:g:293:MET:HE1	1.94	0.48
51:1M:75:ARG:NH1	86:1:1403:A:OP2	2.29	0.48
51:1M:266:PRO:HB2	51:1M:269:ALA:HB3	1.95	0.48
84:1u:522:GLY:O	84:1u:556:LYS:NZ	2.40	0.48
86:1:801:U:H2'	86:1:802:U:C6	2.47	0.48
86:1:1609:A:H61	86:1:1642:U:H3	1.61	0.48
87:2:1137:G:H3'	87:2:1138:G:N2	2.29	0.48
19:R:189:GLU:O	67:1c:50:GLN:HB2	2.14	0.48
39:l:549:ILE:HD12	87:2:1389:A:H1'	1.95	0.48
84:1u:417:GLU:HA	84:1u:420:LYS:HE3	1.94	0.48
86:1:160:U:O2'	86:1:161:U:O2	2.31	0.48
3:B:405:ARG:HD2	28:a:125:LEU:CD2	2.43	0.48
5:D:318:LYS:HA	5:D:321:GLU:HG2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:j:159:PHE:HA	37:j:162:LEU:HG	1.95	0.48
83:1t:291:ARG:NH1	83:1t:324:GLU:OE2	2.35	0.48
86:1:1002:A:H61	86:1:1068:A:H61	1.61	0.48
2:A:28:LYS:HG2	22:U:45:LEU:CD1	2.43	0.48
9:H:406:ARG:NH1	9:H:407:ASP:O	2.46	0.48
48:1J:90:LYS:HE3	78:1o:56:GLY:HA3	1.95	0.48
73:1i:136:ARG:NH1	76:1l:52:GLU:OE2	2.46	0.48
86:1:737:A:N1	86:1:954:G:O2'	2.38	0.48
86:1:1191:A:H2'	86:1:1192:G:H8	1.76	0.48
87:2:1263:A:H2'	87:2:1264:A:C8	2.49	0.48
10:I:170:HIS:CE1	10:I:171:VAL:HG22	2.48	0.48
18:Q:194:VAL:HG13	18:Q:198:GLN:OE1	2.14	0.48
22:U:101:ASP:OD1	36:i:455:LYS:HE3	2.14	0.48
34:g:225:ASP:OD1	34:g:262:ARG:NH1	2.46	0.48
54:1P:81:ASP:CB	63:1Y:146:LYS:CD	2.92	0.48
61:1W:160:LEU:HD22	61:1W:162:PHE:CE1	2.48	0.48
82:1s:101:THR:HB	82:1s:104:GLU:HB2	1.94	0.48
87:2:1734:A:H2'	87:2:1735:C:H4'	1.96	0.48
5:D:229:LYS:NZ	32:e:258:GLU:OE2	2.46	0.48
5:D:352:ARG:HH22	87:2:1065:U:H4'	1.79	0.48
8:G:38:ARG:NH2	92:G:204:HOH:O	2.46	0.48
39:l:337:ARG:NH1	87:2:1320:A:N3	2.61	0.48
39:l:513:ASP:OD2	87:2:1138:G:C2'	2.62	0.48
53:1O:53:LYS:NZ	53:1O:87:ARG:O	2.46	0.48
86:1:2237:A:O3'	87:2:1826:G:H1'	2.13	0.48
86:1:2559:G:O2'	86:1:2801:C:OP1	2.31	0.48
87:2:101:A:O2'	87:2:102:A:O4'	2.31	0.48
87:2:670:G:H2'	87:2:671:A:H8	1.77	0.48
34:g:233:LYS:HD3	34:g:243:ARG:HH22	1.78	0.48
41:1C:199:VAL:HG23	46:1H:93:GLN:HB3	1.96	0.48
82:1s:177:ARG:HA	82:1s:180:GLU:HB2	1.96	0.48
86:1:347:A:H2'	86:1:348:A:C8	2.48	0.48
86:1:544:A:H2'	86:1:545:G:C8	2.48	0.48
86:1:2820:C:H2'	86:1:2821:A:H8	1.78	0.48
87:2:1137:G:N7	87:2:1384:A:N1	2.61	0.48
36:i:514:SER:O	36:i:518:ALA:HB3	2.13	0.48
42:1D:173:VAL:HG22	42:1D:255:ILE:HD12	1.96	0.48
62:1X:104:LYS:O	62:1X:108:HIS:ND1	2.45	0.48
83:1t:104:ARG:NH2	92:1t:515:HOH:O	2.47	0.48
83:1t:462:HIS:HE1	85:1v:242:PHE:N	2.09	0.48
84:1u:332:ILE:O	84:1u:336:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:1:692:A:O2'	86:1:693:G:O4'	2.29	0.48
87:2:225:G:O2'	87:2:226:A:N7	2.39	0.48
87:2:997:G:H1	87:2:1029:C:H41	1.60	0.48
87:2:1063:C:H2'	87:2:1064:G:H8	1.78	0.48
39:l:176:ARG:HA	39:l:179:LYS:HD2	1.96	0.48
52:1N:53:SER:OG	86:1:1101:G:OP1	2.26	0.48
80:1q:28:LYS:NZ	86:1:1286:A:OP2	2.33	0.48
84:1u:436:VAL:O	84:1u:440:ASN:ND2	2.47	0.48
19:R:149:LYS:HE2	19:R:153:ALA:HB2	1.96	0.47
33:f:336:TYR:CD2	33:f:340:LEU:HD12	2.48	0.47
83:1t:411:ASP:OD1	83:1t:414:ARG:NH1	2.45	0.47
84:1u:363:TYR:HE1	84:1u:382:VAL:HG11	1.66	0.47
13:L:65:CYS:HB3	24:W:370:PRO:HD3	1.95	0.47
32:e:265:SER:O	32:e:265:SER:OG	2.31	0.47
37:j:210:VAL:HA	37:j:213:MET:HB3	1.96	0.47
39:l:485:ARG:HD2	39:l:485:ARG:HA	1.39	0.47
85:1v:433:ASP:OD1	85:1v:467:TYR:OH	2.28	0.47
86:1:1619:G:N1	86:1:1634:U:N3	2.61	0.47
87:2:1137:G:C1'	87:2:1389:A:H61	2.27	0.47
87:2:1167:U:H2'	87:2:1168:U:H6	1.79	0.47
4:C:287:LEU:HD22	5:D:178:LEU:HD23	1.95	0.47
4:C:331:PHE:HB2	32:e:214:GLN:HB3	1.97	0.47
14:M:106:LYS:HD2	25:X:521:ASN:ND2	2.29	0.47
36:i:410:MET:HE1	36:i:417:PRO:CG	2.39	0.47
41:1C:193:ARG:HG3	41:1C:226:TRP:CZ2	2.49	0.47
45:1G:60:ILE:HG23	77:1m:106:ILE:HD11	1.96	0.47
47:1I:49:ASN:HB3	47:1I:87:THR:CG2	2.37	0.47
86:1:977:U:H2'	86:1:978:A:C8	2.48	0.47
87:2:1299:A:H2'	87:2:1300:A:C8	2.49	0.47
22:U:101:ASP:OD1	36:i:455:LYS:HG2	2.14	0.47
33:f:301:THR:O	33:f:305:VAL:HG23	2.13	0.47
41:1C:227:ARG:HB2	41:1C:228:THR:H	1.53	0.47
52:1N:48:ARG:HG3	86:1:1058:A:N7	2.30	0.47
59:1U:4:ARG:NH2	86:1:134:C:N3	2.62	0.47
64:1Z:21:LEU:HD23	64:1Z:25:LEU:HD23	1.95	0.47
83:1t:376:MET:HB3	83:1t:391:CYS:HB2	1.96	0.47
86:1:630:A:N6	92:1:4115:HOH:O	2.47	0.47
87:2:858:A:H5'	87:2:1070:U:C5	2.49	0.47
3:B:205:LYS:HB3	28:a:183:ILE:HG12	1.95	0.47
5:D:165:ASP:HA	5:D:168:ASN:HB2	1.97	0.47
41:1C:174:PRO:HD3	41:1C:253:THR:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:1J:36:LEU:CA	48:1J:38:PRO:HD2	2.44	0.47
49:1K:81:ILE:HD13	49:1K:106:LEU:HD21	1.95	0.47
86:1:127:C:H1'	86:1:128:C:H5'	1.96	0.47
86:1:1026:G:N2	86:1:1043:U:O2	2.44	0.47
7:F:45:ASP:OD2	24:W:480:ARG:NH2	2.48	0.47
29:b:22:ASN:N	87:2:1845:A:N1	2.61	0.47
34:g:368:LYS:NZ	87:2:1293:A:OP1	2.47	0.47
35:h:342:LEU:HD11	35:h:353:VAL:HG12	1.93	0.47
57:1S:211:LYS:NZ	92:1S:303:HOH:O	2.45	0.47
87:2:1069:G:N2	87:2:1072:A:OP2	2.37	0.47
87:2:1147:A:H2	87:2:1376:A:N1	2.12	0.47
32:e:344:LYS:HA	32:e:350:GLY:HA2	1.97	0.47
33:f:290:VAL:HG11	33:f:299:LYS:NZ	2.30	0.47
33:f:389:THR:CG2	33:f:397:GLU:CD	2.84	0.47
34:g:349:MET:HE2	34:g:388:TYR:HA	1.95	0.47
35:h:296:LYS:HD2	35:h:337:TRP:CE2	2.50	0.47
39:l:240:LEU:HA	39:l:243:LYS:HD2	1.96	0.47
40:1B:66:GLY:HA2	40:1B:101:PRO:HG3	1.97	0.47
43:1E:220:THR:OG1	43:1E:225:ASN:ND2	2.47	0.47
47:1I:65:GLU:HA	47:1I:70:GLU:OE1	2.14	0.47
47:1I:65:GLU:HG2	47:1I:66:GLY:N	2.30	0.47
53:1O:36:THR:HG21	86:1:1993:G:H5'	1.97	0.47
84:1u:656:VAL:HA	84:1u:659:GLU:HG2	1.95	0.47
85:1v:201:MET:O	85:1v:206:GLY:N	2.47	0.47
86:1:732:C:H2'	86:1:733:A:C8	2.50	0.47
86:1:1693:C:C2	86:1:1694:A:C8	3.03	0.47
86:1:2078:C:N3	86:1:3025:C:O2'	2.41	0.47
86:1:2177:A:H2'	86:1:2178:A:C8	2.50	0.47
87:2:1726:U:C4	87:2:1744:C:N4	2.79	0.47
3:B:363:LEU:HD23	25:X:360:TYR:OH	2.15	0.47
8:G:104:THR:HG22	87:2:638:A:N3	2.29	0.47
39:l:517:LYS:HD3	87:2:1384:A:O2'	2.15	0.47
41:1C:199:VAL:HG12	41:1C:202:ALA:CB	2.45	0.47
48:1J:40:ARG:NH2	48:1J:71:MET:O	2.48	0.47
51:1M:120:ARG:NH2	71:1g:135:GLU:OE1	2.41	0.47
74:1j:82:ILE:C	74:1j:83:GLU:HG3	2.38	0.47
76:1l:111:LEU:HD13	76:1l:210:TRP:HB3	1.97	0.47
79:1p:75:LYS:HB2	86:1:559:C:H5''	1.97	0.47
87:2:215:A:H2'	87:2:216:A:C8	2.50	0.47
26:Y:10:VAL:HA	28:a:385:ILE:HD11	1.95	0.47
34:g:378:MET:HE2	34:g:418:GLU:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:1:1694:A:H3'	86:1:1694:A:OP2	2.14	0.47
87:2:1143:A:N1	87:2:1381:C:O2'	2.48	0.47
10:I:133:ALA:HB3	10:I:215:GLU:HB3	1.97	0.47
18:Q:196:ARG:NH1	92:Q:303:HOH:O	2.42	0.47
34:g:494:VAL:HG11	34:g:533:ASN:HB3	1.97	0.47
44:1F:39:LYS:NZ	44:1F:130:SER:OG	2.44	0.47
56:1R:90:HIS:O	75:1k:108:SER:OG	2.27	0.47
58:1T:232:LYS:HG2	86:1:2940:G:H5''	1.97	0.47
61:1W:187:LEU:HD23	61:1W:222:LYS:HE3	1.97	0.47
77:1m:5:LEU:HD23	77:1m:8:VAL:HG22	1.97	0.47
83:1t:469:LEU:HD12	83:1t:473:LYS:HG2	1.97	0.47
86:1:641:G:H22	86:1:644:A:H5'	1.79	0.47
86:1:2207:A:H2'	86:1:2208:A:C8	2.50	0.47
87:2:1135:A:O2'	87:2:1136:A:H8	1.97	0.47
33:f:230:VAL:HG22	33:f:252:TYR:HB3	1.97	0.46
35:h:110:TRP:HE1	87:2:1745:A:H5'	1.80	0.46
36:i:384:ILE:HA	36:i:387:TYR:HD2	1.79	0.46
58:1T:194:LYS:HA	86:1:896:A:H5'	1.98	0.46
67:1c:48:ILE:O	67:1c:53:LYS:HE3	2.15	0.46
84:1u:243:PHE:HA	84:1u:246:MET:HB3	1.97	0.46
86:1:1446:C:H2'	86:1:1447:A:H8	1.80	0.46
87:2:1013:A:H2	87:2:1482:U:H1'	1.79	0.46
87:2:1651:C:HO2'	87:2:1652:C:H6	1.59	0.46
4:C:100:LEU:HD12	4:C:352:LEU:HD21	1.97	0.46
24:W:212:ASP:OD2	24:W:424:ARG:NH1	2.46	0.46
27:Z:63:TRP:CE2	35:h:137:LEU:CD2	2.98	0.46
34:g:295:ARG:NH1	34:g:323:GLU:OE1	2.48	0.46
35:h:174:HIS:HB2	87:2:154:G:H1'	1.96	0.46
87:2:1145:A:N1	87:2:1378:A:C2	2.76	0.46
3:B:414:ASN:OD1	28:a:142:ASP:HB3	2.16	0.46
11:J:208:THR:OG1	87:2:702:C:O2'	2.32	0.46
54:1P:94:ARG:CZ	86:1:2603:G:C5'	2.93	0.46
83:1t:106:ILE:HG12	83:1t:138:MET:HE1	1.97	0.46
86:1:346:A:H2'	86:1:347:A:C8	2.50	0.46
87:2:986:G:O2'	87:2:987:A:N7	2.48	0.46
2:A:161:ASP:N	2:A:161:ASP:OD1	2.49	0.46
62:1X:180:SER:OG	62:1X:216:LEU:O	2.34	0.46
85:1v:80:SER:OG	85:1v:119:SER:OG	2.31	0.46
86:1:2634:U:H2'	86:1:2635:G:C8	2.51	0.46
87:2:986:G:H2'	87:2:988:C:H41	1.79	0.46
87:2:1701:C:C3'	87:2:1702:G:H8	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Y:40:LYS:NZ	87:2:1536:G:N7	2.63	0.46
35:h:338:PRO:HA	35:h:341:VAL:HG22	1.98	0.46
36:i:653:LEU:HD11	36:i:687:MET:HE3	1.97	0.46
61:1W:102:PHE:HE2	61:1W:131:ILE:CG2	2.24	0.46
84:1u:189:LYS:CG	84:1u:225:THR:HG21	2.46	0.46
86:1:855:G:H1	86:1:865:G:H1	1.62	0.46
86:1:1987:G:H5''	86:1:1988:C:H5'	1.96	0.46
86:1:2382:C:H2'	86:1:2383:C:C6	2.51	0.46
86:1:2413:C:H2'	86:1:2414:A:H8	1.80	0.46
87:2:25:U:H2'	87:2:26:U:C6	2.51	0.46
87:2:1298:A:H2'	87:2:1299:A:C8	2.50	0.46
3:B:205:LYS:HB2	28:a:183:ILE:CG1	2.37	0.46
4:C:180:ILE:HG22	4:C:191:TRP:CZ2	2.51	0.46
10:I:153:TYR:O	87:2:1115:U:O2'	2.32	0.46
31:d:43:PRO:CG	37:j:42:THR:HA	2.46	0.46
35:h:234:TRP:HA	35:h:237:LEU:HD12	1.97	0.46
37:j:34:SER:HB3	37:j:41:LEU:HD11	1.97	0.46
48:1J:28:PRO:HB2	48:1J:43:MET:HE2	1.97	0.46
48:1J:39:TYR:OH	86:1:1247:U:N3	2.45	0.46
48:1J:45:ALA:HA	48:1J:48:LYS:HG2	1.97	0.46
84:1u:514:LEU:HB3	84:1u:530:ILE:HD13	1.97	0.46
86:1:1693:C:H2'	86:1:1694:A:C8	2.51	0.46
86:1:2624:G:OP2	86:1:2624:G:N2	2.41	0.46
86:1:2957:A:H2'	86:1:2958:A:C8	2.51	0.46
4:C:242:LEU:HD22	4:C:297:PHE:HB3	1.98	0.46
33:f:389:THR:CG2	33:f:397:GLU:HB2	2.39	0.46
34:g:395:LEU:HD12	34:g:428:TYR:HB2	1.98	0.46
43:1E:204:ARG:HD3	43:1E:204:ARG:HA	1.76	0.46
61:1W:51:ARG:NH1	83:1t:292:LEU:O	2.47	0.46
66:1b:74:GLU:O	66:1b:78:LYS:HG3	2.15	0.46
84:1u:189:LYS:HE2	84:1u:221:LYS:HB3	1.97	0.46
86:1:1839:A:H61	86:1:1865:C:H42	1.64	0.46
86:1:2837:G:O2'	86:1:2966:A:N1	2.47	0.46
87:2:1649:G:H2'	87:2:1650:C:H6	1.81	0.46
3:B:22:TRP:HB3	3:B:64:HIS:HB2	1.97	0.46
15:N:313:TYR:CE1	23:V:168:LEU:HD21	2.50	0.46
35:h:361:ILE:HD12	35:h:364:MET:HB3	1.97	0.46
36:i:514:SER:O	36:i:518:ALA:CB	2.64	0.46
39:l:529:TRP:HE1	39:l:557:VAL:HB	1.79	0.46
50:1L:130:LEU:HB3	50:1L:145:ILE:HD12	1.98	0.46
83:1t:465:MET:O	83:1t:465:MET:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
87:2:131:A:H2'	87:2:132:A:C8	2.49	0.46
87:2:1767:G:H3'	87:2:1768:A:H5''	1.98	0.46
35:h:149:ASN:HB2	35:h:152:ARG:NH2	2.30	0.46
36:i:429:TYR:CZ	36:i:437:ARG:HD3	2.50	0.46
39:l:217:VAL:HG11	39:l:237:LEU:HD11	1.97	0.46
39:l:485:ARG:NH2	39:l:521:SER:HG	2.09	0.46
41:1C:10:ARG:NH2	86:1:1555:G:N7	2.57	0.46
45:1G:7:ARG:HH21	45:1G:66:HIS:CD2	2.34	0.46
61:1W:69:GLU:O	61:1W:75:ARG:NH2	2.46	0.46
66:1b:33:LEU:HD12	86:1:995:U:H5''	1.98	0.46
77:1m:7:LYS:HB3	77:1m:59:THR:HG22	1.96	0.46
86:1:2118:A:H2'	86:1:2119:C:C6	2.51	0.46
86:1:2560:OMG:HM23	86:1:2560:OMG:H1'	1.74	0.46
87:2:654:G:H2'	87:2:655:A:C8	2.50	0.46
87:2:1138:G:N3	87:2:1138:G:H3'	2.31	0.46
87:2:1388:A:O2'	87:2:1389:A:OP2	2.34	0.46
11:J:200:LEU:HD22	11:J:270:LYS:HE2	1.97	0.46
35:h:311:ILE:HA	35:h:314:ILE:HG22	1.98	0.46
39:l:442:VAL:HG11	39:l:476:SER:H	1.81	0.46
47:1I:68:LYS:HG3	47:1I:118:LYS:HE3	1.98	0.46
48:1J:33:SER:HG	48:1J:34:PRO:HD3	1.73	0.46
60:1V:42:GLN:OE1	60:1V:44:ARG:NH1	2.46	0.46
71:1g:135:GLU:OE2	86:1:2665:U:O2'	2.28	0.46
86:1:346:A:H2'	86:1:347:A:H8	1.81	0.46
86:1:2363:A:H2'	86:1:2364:A:H8	1.81	0.46
87:2:1549:A:H2'	87:2:1550:A:C8	2.51	0.46
36:i:104:PHE:HZ	36:i:166:ILE:HG23	1.80	0.45
36:i:121:LYS:HA	36:i:124:ILE:HD12	1.98	0.45
39:l:204:ASP:OD2	39:l:206:ARG:NH2	2.44	0.45
84:1u:290:VAL:CG1	84:1u:324:SER:CB	2.92	0.45
86:1:486:A:H4'	86:1:487:U:H5'	1.98	0.45
86:1:2231:A:N1	87:2:1802:A:C8	2.84	0.45
87:2:72:G:H4'	87:2:73:A:H5''	1.98	0.45
36:i:374:VAL:HG22	36:i:374:VAL:O	2.16	0.45
48:1J:18:LYS:HD3	86:1:1211:G:C8	2.51	0.45
57:1S:128:LYS:HB2	57:1S:131:GLU:HG3	1.96	0.45
76:1l:178:GLU:OE1	76:1l:179:THR:HG23	2.15	0.45
86:1:1186:G:H22	86:1:1269:G:N2	2.14	0.45
86:1:1680:A:H61	86:1:1886:U:H3	1.63	0.45
87:2:48:C:H2'	87:2:49:U:C6	2.50	0.45
3:B:405:ARG:HD2	28:a:125:LEU:HD22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:372:LYS:NZ	87:2:1074:A:OP1	2.41	0.45
32:e:189:MET:HG2	32:e:205:LEU:HD22	1.98	0.45
33:f:180:HIS:CE1	33:f:182:ASP:HB3	2.51	0.45
34:g:607:PHE:HE2	34:g:637:PRO:HD2	1.81	0.45
37:j:378:VAL:HG12	37:j:382:LYS:HE2	1.97	0.45
40:1B:88:VAL:HG21	40:1B:95:ALA:HB2	1.98	0.45
84:1u:130:LEU:HD21	84:1u:160:LEU:HA	1.98	0.45
86:1:978:A:H2'	86:1:979:G:H8	1.80	0.45
86:1:2106:U:H1'	86:1:2914:U:H5''	1.99	0.45
87:2:993:G:H2'	87:2:994:A:H8	1.80	0.45
87:2:1502:A:H62	87:2:1561:A:H61	1.64	0.45
1:3:53:A:O3'	73:1i:174:LYS:HG2	2.16	0.45
25:X:497:LYS:HB2	25:X:497:LYS:HE3	1.70	0.45
32:e:256:ASP:OD1	32:e:256:ASP:N	2.49	0.45
71:1g:153:ARG:NH1	86:1:2655:U:OP2	2.50	0.45
77:1m:92:GLU:O	77:1m:95:PHE:HB2	2.17	0.45
83:1t:8:ARG:NH1	86:1:1662:U:OP2	2.46	0.45
87:2:216:A:H2'	87:2:217:A:C8	2.51	0.45
87:2:1269:A:H2'	87:2:1270:A:C8	2.52	0.45
9:H:422:ARG:HG3	87:2:1610:U:H4'	1.99	0.45
23:V:61:ASP:OD1	23:V:64:ARG:NH1	2.49	0.45
35:h:83:THR:O	35:h:86:VAL:HG22	2.17	0.45
39:l:256:LYS:HA	39:l:259:GLU:HB2	1.99	0.45
40:1B:94:ASN:HB3	40:1B:128:THR:HG22	1.98	0.45
61:1W:48:VAL:HG23	86:1:1596:A:H5'	1.99	0.45
64:1Z:121:THR:HG22	64:1Z:123:MET:H	1.81	0.45
86:1:1558:G:H2'	86:1:1559:A:C8	2.51	0.45
25:X:366:ARG:HH12	28:a:126:GLN:HE21	1.58	0.45
28:a:293:TRP:CE2	28:a:315:LEU:HD13	2.52	0.45
31:d:60:LEU:HD22	31:d:64:LEU:HD12	1.99	0.45
33:f:290:VAL:CG2	33:f:298:CYS:HB3	2.46	0.45
34:g:202:SER:HA	34:g:205:LEU:HD13	1.99	0.45
36:i:158:PHE:HB3	36:i:162:LEU:HD23	1.98	0.45
36:i:552:ARG:NH2	36:i:589:ASP:OD2	2.50	0.45
47:1I:50:THR:HG22	47:1I:85:VAL:HG13	1.99	0.45
86:1:553:G:OP2	86:1:2711:U:O2'	2.26	0.45
87:2:1387:C:O2	87:2:1387:C:H2'	2.17	0.45
9:H:219:LYS:O	9:H:222:THR:OG1	2.30	0.45
13:L:77:LEU:HD22	13:L:81:GLU:HB3	1.99	0.45
19:R:206:LYS:HE2	19:R:206:LYS:HB2	1.80	0.45
28:a:325:SER:OG	28:a:326:LYS:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:f:266:LYS:CG	33:f:269:MET:CE	2.94	0.45
49:1K:92:ARG:HH11	86:1:1282:U:C4'	2.12	0.45
59:1U:97:ASP:OD1	59:1U:97:ASP:N	2.49	0.45
61:1W:53:ARG:NH2	86:1:1649:C:O3'	2.50	0.45
76:1L:143:ARG:NH2	92:1L:307:HOH:O	2.40	0.45
84:1u:324:SER:O	84:1u:327:SER:OG	2.31	0.45
86:1:741:A:H2'	86:1:742:A:C8	2.52	0.45
4:C:229:LEU:O	4:C:232:THR:OG1	2.32	0.45
6:E:79:LEU:HA	40:1B:52:HIS:HE1	1.82	0.45
12:K:70:GLU:HG2	87:2:519:G:H4'	1.99	0.45
29:b:35:LYS:HA	29:b:38:VAL:HG22	1.99	0.45
43:1E:222:LYS:NZ	86:1:454:A:OP1	2.42	0.45
86:1:978:A:H2'	86:1:979:G:C8	2.52	0.45
86:1:1009:G:H2'	86:1:1010:C:C6	2.52	0.45
86:1:2231:A:C2	87:2:1802:A:N9	2.85	0.45
87:2:1704:A:N3	87:2:1706:C:H5	2.15	0.45
2:A:141:ARG:HG2	2:A:168:PHE:CE2	2.52	0.45
48:1J:28:PRO:HB3	48:1J:43:MET:CE	2.45	0.45
48:1J:84:VAL:HG21	48:1J:139:ILE:HG12	1.98	0.45
51:1M:83:ARG:HA	86:1:956:U:H2'	1.99	0.45
59:1U:131:GLN:OE1	59:1U:134:ARG:HG2	2.16	0.45
82:1s:100:TYR:CZ	82:1s:102:PRO:HA	2.52	0.45
83:1t:452:ILE:HG21	83:1t:484:LEU:HD13	1.99	0.45
86:1:556:C:H2'	86:1:557:A:C8	2.51	0.45
86:1:2766:G:H2'	86:1:2767:A:C8	2.52	0.45
87:2:164:A:H2'	87:2:165:A:C8	2.51	0.45
14:M:148:ARG:NH2	87:2:1052:U:OP1	2.40	0.45
17:P:43:HIS:CD2	17:P:45:GLU:CG	2.99	0.45
19:R:51:PHE:HB3	19:R:57:VAL:HG21	1.98	0.45
32:e:367:VAL:HA	32:e:370:MET:HE2	1.98	0.45
33:f:347:VAL:HG11	33:f:380:MET:CG	2.46	0.45
35:h:166:HIS:HA	35:h:169:ARG:HD3	1.99	0.45
39:l:474:LYS:HE3	87:2:1141:A:C6	2.52	0.45
42:1D:223:GLN:O	86:1:2370:A:O2'	2.35	0.45
84:1u:406:GLN:HE21	84:1u:411:ASP:HB3	1.81	0.45
85:1v:283:TYR:OH	85:1v:316:ARG:HG3	2.17	0.45
86:1:1192:G:H2'	86:1:1193:C:H6	1.80	0.45
17:P:3:PRO:CD	17:P:3:PRO:O	2.62	0.44
27:Z:59:PHE:CZ	87:2:153:A:C4	3.05	0.44
35:h:292:PHE:CE1	35:h:329:GLU:HB3	2.51	0.44
36:i:395:ALA:HB1	36:i:428:MET:CG	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:1N:35:ASP:OD1	52:1N:35:ASP:N	2.50	0.44
59:1U:50:SER:HB3	74:1j:65:ILE:HD12	1.99	0.44
63:1Y:104:LEU:HD12	63:1Y:125:ILE:HD12	1.99	0.44
86:1:176:A:H2'	86:1:177:C:C6	2.52	0.44
86:1:864:G:H2'	86:1:865:G:H8	1.82	0.44
86:1:1234:G:N3	86:1:1255:U:O2'	2.46	0.44
86:1:2441:G:H2'	86:1:2442:G:H8	1.82	0.44
86:1:2494:G:H2'	86:1:2495:G:C8	2.52	0.44
87:2:432:G:O2'	87:2:444:C:N3	2.43	0.44
3:B:105:GLY:O	3:B:106:PRO:C	2.60	0.44
3:B:399:MET:HE3	28:a:102:ILE:HD12	2.00	0.44
19:R:167:PRO:CD	67:1c:54:PHE:CZ	2.90	0.44
33:f:260:ASN:OD1	33:f:261:THR:CG2	2.54	0.44
34:g:277:ILE:HG13	34:g:282:LEU:HB2	1.99	0.44
36:i:371:ALA:C	36:i:373:GLY:N	2.75	0.44
37:j:72:LEU:O	37:j:110:ARG:NH1	2.50	0.44
61:1W:51:ARG:NE	86:1:1595:G:OP1	2.39	0.44
86:1:2556:U:H2'	86:1:2557:C:H6	1.82	0.44
87:2:711:A:H2'	87:2:712:A:C8	2.53	0.44
87:2:1744:C:H2'	87:2:1746:A:N7	2.32	0.44
3:B:107:ILE:HD13	28:a:86:ILE:HG21	1.99	0.44
35:h:83:THR:HG21	35:h:117:ARG:HB2	2.00	0.44
62:1X:126:GLU:HG3	62:1X:129:SER:HB2	1.99	0.44
65:1a:31:VAL:HG12	65:1a:32:LYS:H	1.80	0.44
71:1g:137:LYS:HD3	71:1g:137:LYS:HA	1.84	0.44
81:1r:42:VAL:HA	81:1r:45:ILE:HD12	1.99	0.44
84:1u:614:ASN:HB3	84:1u:617:LEU:HD12	2.00	0.44
86:1:359:A:H2'	86:1:360:A:C8	2.53	0.44
87:2:812:A:OP1	87:2:1835:G:O2'	2.26	0.44
87:2:1701:C:H2'	87:2:1702:G:O4'	2.17	0.44
5:D:481:ARG:NH2	87:2:557:A:OP1	2.50	0.44
17:P:10:SER:OG	87:2:295:C:OP1	2.27	0.44
19:R:140:PRO:CD	67:1c:58:PHE:CG	2.93	0.44
33:f:329:ASP:N	33:f:329:ASP:OD1	2.49	0.44
34:g:202:SER:O	34:g:205:LEU:HB3	2.17	0.44
34:g:410:VAL:HG23	34:g:412:ARG:HB2	1.99	0.44
34:g:457:PHE:O	34:g:460:SER:OG	2.33	0.44
36:i:240:ASP:HA	36:i:243:ILE:HG22	1.99	0.44
41:1C:98:PRO:HD2	41:1C:220:LEU:HG	2.00	0.44
54:1P:15:TYR:CD1	63:1Y:137:PRO:HD3	2.52	0.44
61:1W:69:GLU:OE1	61:1W:74:LYS:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:1:1594:G:H1	86:1:1657:U:H3	1.64	0.44
87:2:50:A:H2'	87:2:51:U:C6	2.53	0.44
87:2:724:A:H2'	87:2:725:A:C8	2.53	0.44
2:A:36:ASN:O	38:k:16:GLN:NE2	2.51	0.44
6:E:29:HIS:CE1	40:1B:52:HIS:CD2	3.05	0.44
16:O:9:ARG:NH1	92:O:203:HOH:O	2.43	0.44
34:g:647:LEU:CD1	39:l:404:ALA:O	2.64	0.44
36:i:581:ARG:HA	36:i:584:LEU:HG	2.00	0.44
3:B:509:LYS:NZ	3:B:511:SER:OG	2.50	0.44
27:Z:59:PHE:HE2	87:2:153:A:H2'	1.83	0.44
44:1F:144:ASP:OD1	76:1l:76:ARG:NH2	2.50	0.44
47:1I:61:PHE:N	47:1I:76:MET:HE1	2.33	0.44
48:1J:136:CYS:O	48:1J:140:ILE:HG12	2.17	0.44
49:1K:162:ARG:HD3	86:1:1162:C:C2	2.53	0.44
54:1P:4:PRO:HA	54:1P:5:PRO:HD3	1.93	0.44
60:1V:97:LEU:HD23	60:1V:97:LEU:HA	1.89	0.44
79:1p:21:ARG:HE	79:1p:21:ARG:HB3	1.69	0.44
84:1u:292:THR:HG22	84:1u:296:MET:HE1	2.00	0.44
86:1:413:U:H2'	86:1:414:U:C6	2.52	0.44
86:1:583:U:H2'	86:1:584:G:C8	2.53	0.44
86:1:1026:G:H1	86:1:1043:U:H3	1.66	0.44
86:1:2600:U:OP1	86:1:2685:U:O2'	2.36	0.44
86:1:2632:A:H2'	86:1:2633:A:C8	2.53	0.44
87:2:1113:U:H2'	87:2:1114:G:C8	2.52	0.44
87:2:1686:U:H2'	87:2:1687:U:C6	2.53	0.44
2:A:10:LYS:HD2	9:H:246:LEU:HG	1.99	0.44
2:A:118:SER:OG	2:A:119:ARG:N	2.51	0.44
5:D:156:ASP:OD1	5:D:156:ASP:N	2.48	0.44
6:E:81:TYR:CE2	40:1B:52:HIS:HE1	2.14	0.44
8:G:30:SER:HB3	87:2:587:U:H5''	1.99	0.44
35:h:156:LYS:HA	35:h:159:VAL:HG12	1.99	0.44
44:1F:114:SER:O	67:1c:42:ARG:NH1	2.51	0.44
84:1u:210:LYS:HG2	84:1u:213:GLU:OE1	2.17	0.44
84:1u:276:ARG:NH1	86:1:335:A:OP1	2.50	0.44
86:1:347:A:H2'	86:1:348:A:H8	1.83	0.44
86:1:2413:C:H2'	86:1:2414:A:C8	2.52	0.44
86:1:2429:U:H1'	86:1:2436:U:H4'	2.00	0.44
87:2:241:U:H2'	87:2:242:G:H8	1.83	0.44
87:2:978:C:H2'	87:2:979:A:H8	1.82	0.44
2:A:22:ALA:O	2:A:163:ASN:ND2	2.51	0.44
28:a:387:THR:CB	39:l:555:ARG:HB2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:g:126:LEU:HB3	34:g:133:ALA:HB2	2.00	0.44
41:1C:186:ALA:O	41:1C:188:SER:N	2.51	0.44
86:1:1323:A:H2'	86:1:1324:A:H8	1.82	0.44
86:1:3034:A:H1'	86:1:3035:A:H2'	1.99	0.44
87:2:356:G:H2'	87:2:357:A:C8	2.53	0.44
87:2:887:G:H2'	87:2:888:G:C8	2.53	0.44
87:2:1033:C:H2'	87:2:1034:A:H8	1.81	0.44
87:2:1147:A:C2	87:2:1376:A:N1	2.86	0.44
87:2:1388:A:O2'	87:2:1389:A:P	2.76	0.44
87:2:1504:G:H2'	87:2:1505:G:C8	2.53	0.44
3:B:463:LYS:HA	3:B:463:LYS:HD3	1.81	0.44
14:M:82:ARG:NH1	87:2:1007:A:OP2	2.44	0.44
25:X:469:GLU:OE2	25:X:472:ARG:NH2	2.50	0.44
29:b:88:ARG:NH1	92:b:101:HOH:O	2.51	0.44
35:h:332:LYS:HD3	35:h:332:LYS:HA	1.82	0.44
39:l:279:ARG:O	39:l:279:ARG:CG	2.63	0.44
41:1C:249:ARG:HG3	64:1Z:126:PHE:CZ	2.53	0.44
48:1J:11:ARG:H	48:1J:11:ARG:HG2	1.57	0.44
73:li:204:LYS:HB3	73:li:204:LYS:HE3	1.90	0.44
84:1u:157:ILE:HG23	84:1u:169:ALA:HB1	2.00	0.44
84:1u:449:ARG:HA	84:1u:452:LYS:HD3	1.99	0.44
84:1u:454:LEU:HD12	84:1u:457:LEU:HD23	2.00	0.44
84:1u:626:LEU:HD13	84:1u:657:LEU:HD11	1.99	0.44
86:1:1176:A:OP1	86:1:1284:U:O2'	2.27	0.44
86:1:1178:A:N3	86:1:2791:A:O2'	2.45	0.44
87:2:467:G:H2'	87:2:468:U:C6	2.52	0.44
8:G:24:VAL:HG22	8:G:62:VAL:HB	2.00	0.43
12:K:39:THR:HG22	12:K:51:LYS:HD3	1.99	0.43
24:W:442:TYR:HD2	24:W:476:VAL:HG21	1.83	0.43
37:j:330:TYR:O	37:j:334:VAL:HG23	2.18	0.43
50:1L:54:LEU:HD22	50:1L:128:VAL:HG13	1.98	0.43
86:1:728:G:H2'	86:1:729:G:C8	2.52	0.43
86:1:3103:G:O2'	86:1:3105:A:OP2	2.31	0.43
4:C:184:LEU:HD11	4:C:216:PHE:HZ	1.83	0.43
7:F:99:ARG:NH2	7:F:117:ASP:OD2	2.51	0.43
19:R:167:PRO:CG	67:1c:54:PHE:HE2	2.22	0.43
25:X:505:ASP:HA	25:X:508:TYR:CE2	2.53	0.43
63:1Y:68:VAL:HG22	63:1Y:83:VAL:HG22	2.00	0.43
76:1l:151:LYS:HB2	76:1l:151:LYS:HE2	1.75	0.43
86:1:565:A:H5''	86:1:566:G:H5''	2.01	0.43
86:1:1692:U:H2'	86:1:1693:C:O4'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
87:2:104:U:H2'	87:2:105:U:C6	2.53	0.43
87:2:158:A:H2'	87:2:159:G:H8	1.83	0.43
87:2:557:A:H4'	87:2:558:A:H3'	1.99	0.43
87:2:939:A:H2'	87:2:940:G:H8	1.82	0.43
87:2:1323:A:H2'	87:2:1324:A:H8	1.83	0.43
87:2:1506:C:H2'	87:2:1507:A:H8	1.83	0.43
3:B:234:LEU:HD21	25:X:422:ILE:HG21	2.01	0.43
6:E:78:GLU:C	40:1B:52:HIS:NE2	2.61	0.43
13:L:134:ASN:ND2	87:2:942:A:N7	2.67	0.43
16:O:6:ARG:HB2	87:2:395:G:H5''	1.99	0.43
41:1C:199:VAL:HG12	41:1C:202:ALA:HB2	2.00	0.43
48:1J:18:LYS:CE	86:1:1211:G:H8	2.29	0.43
60:1V:118:ARG:NH2	86:1:94:G:O6	2.50	0.43
78:1o:62:ASP:OD1	78:1o:62:ASP:N	2.49	0.43
86:1:427:A:H2'	86:1:430:G:C8	2.54	0.43
86:1:505:U:H2'	86:1:506:A:H8	1.83	0.43
86:1:1191:A:O2'	86:1:1192:G:H5'	2.18	0.43
87:2:1268:A:H2'	87:2:1269:A:H8	1.83	0.43
87:2:1270:A:H2'	87:2:1271:A:C8	2.52	0.43
87:2:1438:G:H2'	87:2:1439:A:H8	1.83	0.43
7:F:145:PHE:HZ	11:J:232:ARG:CZ	2.31	0.43
19:R:189:GLU:CG	67:1c:51:ILE:CD1	2.90	0.43
24:W:206:LYS:HE3	24:W:206:LYS:HB2	1.80	0.43
27:Z:63:TRP:CE2	35:h:137:LEU:HD22	2.53	0.43
34:g:244:VAL:HA	34:g:247:LEU:HD12	2.01	0.43
34:g:526:LEU:HD13	34:g:545:LEU:HD22	2.00	0.43
36:i:463:GLY:O	36:i:467:ALA:N	2.51	0.43
39:l:502:GLU:HG2	39:l:506:PHE:CD2	2.51	0.43
42:1D:84:CYS:HA	55:1Q:112:ALA:HB1	1.99	0.43
48:1J:72:ASP:C	48:1J:73:HIS:CG	2.96	0.43
55:1Q:209:ARG:NH2	92:1Q:306:HOH:O	2.51	0.43
77:1m:13:ASN:ND2	77:1m:48:ARG:O	2.44	0.43
83:1t:18:LYS:CD	92:1t:501:HOH:O	2.56	0.43
83:1t:420:PHE:HD1	83:1t:425:ASP:HB3	1.82	0.43
84:1u:616:ASP:OD1	84:1u:616:ASP:N	2.51	0.43
84:1u:721:ASP:HA	84:1u:724:ILE:HG22	2.01	0.43
86:1:1377:U:H2'	86:1:1378:U:C6	2.53	0.43
10:I:132:ILE:HB	10:I:188:LEU:HB2	2.01	0.43
36:i:404:GLU:CG	36:i:437:ARG:CZ	2.96	0.43
37:j:87:VAL:O	37:j:91:THR:HG23	2.18	0.43
83:1t:256:GLU:OE2	83:1t:274:TYR:OH	2.28	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
84:1u:88:GLU:HG2	84:1u:122:ASN:HB2	1.99	0.43
86:1:996:G:H2'	86:1:997:G:H8	1.84	0.43
86:1:1186:G:H1	86:1:1269:G:N2	2.14	0.43
86:1:1449:G:H2'	86:1:1450:A:C8	2.53	0.43
87:2:58:A:O2'	87:2:379:G:N2	2.51	0.43
87:2:1307:A:N1	87:2:1308:A:N6	2.67	0.43
87:2:1744:C:H2'	87:2:1746:A:C8	2.54	0.43
3:B:257:LEU:HA	3:B:260:PHE:HD2	1.83	0.43
4:C:112:LEU:HD22	4:C:120:ILE:HG12	2.01	0.43
9:H:204:GLU:HA	9:H:207:GLU:HG3	2.01	0.43
18:Q:166:ILE:HD13	18:Q:186:PHE:CZ	2.53	0.43
22:U:61:ARG:HG3	87:2:837:U:O2'	1.99	0.43
22:U:88:ARG:NH1	36:i:420:LEU:CD2	2.80	0.43
33:f:226:ARG:HH11	38:k:3:TYR:HE2	1.67	0.43
37:j:283:MET:HG3	37:j:288:MET:HG3	2.00	0.43
47:1I:64:LEU:O	47:1I:67:THR:OG1	2.36	0.43
48:1J:150:ILE:HG23	78:1o:82:LEU:HD11	2.00	0.43
58:1T:254:ARG:O	58:1T:256:GLY:N	2.52	0.43
77:1m:93:GLN:C	77:1m:95:PHE:H	2.25	0.43
86:1:2935:A:H2	86:1:2939:C:H3'	1.84	0.43
4:C:138:MET:HE3	4:C:138:MET:HB3	1.94	0.43
15:N:302:LEU:HD23	15:N:302:LEU:HA	1.90	0.43
29:b:22:ASN:HB2	29:b:25:LYS:HB2	2.00	0.43
33:f:103:ASP:O	33:f:106:PRO:HD2	2.18	0.43
35:h:94:LEU:O	35:h:98:ASN:HB2	2.19	0.43
35:h:166:HIS:ND1	35:h:169:ARG:NH1	2.64	0.43
39:l:145:GLU:OE1	39:l:176:ARG:NH2	2.51	0.43
40:1B:52:HIS:CG	40:1B:52:HIS:O	2.71	0.43
44:1F:140:PRO:HA	44:1F:143:GLU:HG2	2.01	0.43
84:1u:511:LEU:HD22	84:1u:530:ILE:HG23	1.99	0.43
86:1:51:A:H2'	86:1:52:A:C8	2.53	0.43
87:2:113:U:H2'	87:2:114:U:C6	2.54	0.43
87:2:113:U:H2'	87:2:114:U:H6	1.84	0.43
87:2:121:A:H2'	87:2:122:A:C8	2.54	0.43
87:2:953:U:O2	87:2:1485:G:O2'	2.25	0.43
87:2:1504:G:H2'	87:2:1505:G:H8	1.83	0.43
5:D:251:PRO:HB2	22:U:22:ARG:HB3	2.01	0.43
12:K:116:LYS:NZ	87:2:501:C:OP1	2.40	0.43
20:S:27:ILE:HD12	20:S:47:MET:HE2	2.00	0.43
33:f:107:LEU:HB3	33:f:119:CYS:SG	2.58	0.43
47:1I:44:LEU:O	47:1I:48:SER:OG	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:1I:61:PHE:HB2	47:1I:76:MET:CE	2.48	0.43
73:1i:190:LEU:HA	73:1i:193:MET:HE2	2.01	0.43
74:1j:80:CYS:O	74:1j:82:ILE:HG13	2.19	0.43
86:1:727:U:H2'	86:1:728:G:C8	2.53	0.43
86:1:1474:U:H2'	86:1:1475:G:C8	2.54	0.43
87:2:718:A:O2'	87:2:720:A:OP2	2.25	0.43
87:2:1234:A:H2'	87:2:1235:A:H8	1.83	0.43
4:C:242:LEU:HD23	5:D:207:LEU:HD13	2.00	0.43
9:H:311:ARG:H	9:H:381:LEU:HD23	1.83	0.43
16:O:46:GLN:HE21	87:2:615:A:H5''	1.84	0.43
28:a:390:VAL:HG13	39:l:553:LEU:CD2	2.43	0.43
33:f:221:PHE:CE2	33:f:256:VAL:CG1	2.98	0.43
34:g:586:PHE:HD1	34:g:590:GLY:HA3	1.84	0.43
35:h:339:VAL:O	35:h:343:LYS:HG2	2.17	0.43
37:j:77:HIS:CE1	87:2:92:A:OP1	2.71	0.43
37:j:265:GLN:HB2	37:j:297:HIS:CE1	2.54	0.43
39:l:137:LEU:HB3	39:l:169:ILE:HG23	2.00	0.43
66:1b:45:ARG:HD3	86:1:1309:C:H5''	2.01	0.43
84:1u:208:PHE:O	84:1u:218:ARG:NH1	2.44	0.43
87:2:943:U:H2'	87:2:944:G:C8	2.54	0.43
87:2:1134:U:O2'	87:2:1135:A:H5'	2.19	0.43
87:2:1701:C:H4'	87:2:1702:G:OP1	2.18	0.43
3:B:205:LYS:HB3	28:a:183:ILE:CG1	2.48	0.43
9:H:318:ARG:HH21	9:H:366:THR:HG21	1.83	0.43
19:R:64:THR:HG22	19:R:71:SER:HA	1.99	0.43
48:1J:19:LEU:N	48:1J:65:VAL:O	2.52	0.43
48:1J:84:VAL:HG11	48:1J:142:THR:HG21	2.01	0.43
62:1X:245:LYS:HD3	86:1:1020:G:H5''	2.00	0.43
64:1Z:9:MET:HE1	64:1Z:29:LEU:HB3	2.00	0.43
84:1u:176:MET:HE2	84:1u:176:MET:HB3	1.85	0.43
84:1u:362:THR:HG22	84:1u:366:LEU:HD23	2.00	0.43
84:1u:601:MET:O	84:1u:605:ILE:HG12	2.18	0.43
85:1v:428:GLY:N	86:1:144:U:O4	2.48	0.43
86:1:153:U:H2'	86:1:154:U:H6	1.82	0.43
86:1:864:G:H2'	86:1:865:G:C8	2.53	0.43
36:i:684:ALA:HB1	36:i:706:MET:HE1	2.01	0.42
41:1C:199:VAL:HG12	41:1C:199:VAL:O	2.19	0.42
47:1I:18:LEU:HD21	47:1I:64:LEU:HD21	2.01	0.42
47:1I:60:VAL:HG21	47:1I:82:TRP:CD1	2.54	0.42
48:1J:33:SER:OG	48:1J:34:PRO:CD	2.52	0.42
77:1m:92:GLU:OE2	77:1m:96:ARG:NH2	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:1:1186:G:H22	86:1:1269:G:H22	1.66	0.42
86:1:2405:C:H2'	86:1:2406:G:H8	1.83	0.42
87:2:1121:U:H5''	87:2:1122:C:H5'	2.01	0.42
4:C:107:PHE:HD1	4:C:146:LEU:HD11	1.84	0.42
25:X:350:ASP:OD1	25:X:350:ASP:O	2.37	0.42
28:a:330:ARG:NH1	87:2:1132:C:OP1	2.53	0.42
30:c:121:LYS:NZ	87:2:1819:C:OP2	2.48	0.42
36:i:201:PHE:O	36:i:205:ILE:HG12	2.19	0.42
36:i:408:LYS:O	36:i:412:GLN:HG2	2.20	0.42
41:1C:9:LEU:HD12	82:1s:108:SER:HA	2.01	0.42
47:1I:49:ASN:CG	47:1I:87:THR:HG21	2.44	0.42
52:1N:98:MET:HE1	52:1N:153:VAL:HA	2.00	0.42
62:1X:177:ASP:N	62:1X:177:ASP:OD1	2.50	0.42
66:1b:5:ARG:HA	66:1b:8:LYS:HD2	2.01	0.42
83:1t:216:ILE:HD12	83:1t:219:MET:HE3	2.01	0.42
85:1v:281:LEU:O	85:1v:285:VAL:HG23	2.18	0.42
86:1:153:U:H2'	86:1:154:U:C6	2.54	0.42
86:1:721:G:H2'	86:1:2348:A:N7	2.35	0.42
86:1:1558:G:H2'	86:1:1559:A:H8	1.84	0.42
86:1:2582:A:H2'	86:1:2583:A:C8	2.54	0.42
87:2:228:A:N1	87:2:239:G:O2'	2.45	0.42
87:2:1268:A:H2'	87:2:1269:A:C8	2.54	0.42
5:D:328:LYS:HA	5:D:328:LYS:HD3	1.89	0.42
5:D:504:GLN:HG3	5:D:509:ARG:O	2.19	0.42
24:W:142:TYR:CE2	24:W:441:TYR:HB2	2.54	0.42
26:Y:30:LEU:HD23	26:Y:30:LEU:HA	1.89	0.42
36:i:392:HIS:CE1	36:i:424:ALA:HB1	2.51	0.42
48:1J:26:ALA:HB3	48:1J:51:ASN:HD21	1.84	0.42
81:1r:99:LYS:NZ	86:1:3140:G:OP1	2.45	0.42
85:1v:150:VAL:HG21	85:1v:177:THR:HG23	2.01	0.42
87:2:129:A:H2'	87:2:130:A:H8	1.84	0.42
87:2:144:U:H2'	87:2:145:U:H6	1.84	0.42
87:2:313:U:OP1	87:2:608:G:O2'	2.27	0.42
87:2:1138:G:H2'	87:2:1139:A:O4'	2.19	0.42
3:B:485:ILE:HG22	3:B:507:HIS:HB3	2.00	0.42
36:i:400:ILE:HG12	36:i:434:ASN:HD21	1.83	0.42
39:l:513:ASP:OD1	87:2:1138:G:C2'	2.67	0.42
41:1C:103:ILE:HD11	41:1C:218:PHE:HE2	1.84	0.42
52:1N:33:LYS:HB2	52:1N:33:LYS:HE2	1.85	0.42
59:1U:129:LEU:CD1	83:1t:110:GLU:HB3	2.49	0.42
73:1i:199:GLU:HA	73:1i:206:LYS:HE2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
84:1u:231:LEU:HD23	84:1u:264:GLY:HA3	2.02	0.42
84:1u:659:GLU:HG3	84:1u:660:LYS:HD2	2.00	0.42
86:1:360:A:H2'	86:1:361:A:C8	2.54	0.42
86:1:804:U:H2'	86:1:805:U:C6	2.55	0.42
86:1:1096:C:H2'	86:1:1097:U:H6	1.85	0.42
86:1:1560:A:H2'	86:1:1561:G:C8	2.55	0.42
87:2:1485:G:OP2	87:2:1584:C:N4	2.38	0.42
4:C:313:GLU:HG2	32:e:253:VAL:HB	2.02	0.42
35:h:149:ASN:HA	35:h:152:ARG:CZ	2.49	0.42
39:l:414:VAL:HG11	39:l:444:THR:HG23	2.02	0.42
84:1u:261:MET:HE2	84:1u:261:MET:HB3	1.80	0.42
84:1u:325:VAL:CG2	84:1u:354:PHE:CE2	3.02	0.42
86:1:648:A:H8	86:1:651:A:H2	1.68	0.42
86:1:941:U:H2'	86:1:942:C:C6	2.53	0.42
86:1:2067:U:H2'	86:1:2068:A:C8	2.55	0.42
87:2:1271:A:H2'	87:2:1272:A:C8	2.55	0.42
87:2:1710:G:H2'	87:2:1711:A:H8	1.84	0.42
19:R:24:GLY:HA2	19:R:27:ARG:HE	1.83	0.42
29:b:15:LYS:HA	87:2:1652:C:H4'	2.01	0.42
33:f:107:LEU:HD22	33:f:119:CYS:HA	2.02	0.42
39:l:441:ASP:N	39:l:441:ASP:OD1	2.51	0.42
39:l:446:THR:HG1	39:l:479:THR:HG1	1.67	0.42
39:l:553:LEU:O	39:l:557:VAL:HG22	2.20	0.42
43:1E:300:ARG:HD3	86:1:756:U:C5	2.54	0.42
55:1Q:188:MET:HE2	86:1:2993:U:H4'	2.01	0.42
57:1S:157:ASP:OD2	75:1k:102:HIS:NE2	2.41	0.42
76:1l:229:LYS:HB2	76:1l:229:LYS:HE3	1.86	0.42
79:1p:16:VAL:O	79:1p:16:VAL:CG1	2.66	0.42
84:1u:154:MET:HE1	84:1u:190:ILE:HD12	2.01	0.42
86:1:1594:G:O6	86:1:1658:A:C5	2.70	0.42
86:1:1874:A:H3'	86:1:1875:G:H5''	1.99	0.42
87:2:1269:A:H2'	87:2:1270:A:H8	1.84	0.42
1:3:44:C:C6	44:1F:62:ILE:CG2	3.03	0.42
3:B:147:ARG:HB3	25:X:508:TYR:CZ	2.55	0.42
5:D:476:LYS:NZ	87:2:17:G:OP2	2.45	0.42
17:P:68:ASN:HD21	87:2:254:U:H5''	1.76	0.42
25:X:488:PHE:HE1	26:Y:38:PRO:HG3	1.85	0.42
32:e:299:LEU:CD2	32:e:384:LEU:HD21	2.35	0.42
35:h:149:ASN:ND2	35:h:152:ARG:NH2	2.50	0.42
35:h:261:GLU:O	35:h:265:LYS:HG2	2.20	0.42
36:i:418:ASP:O	36:i:419:ILE:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:i:602:VAL:HB	36:i:632:LEU:HD11	2.01	0.42
49:1K:159:MET:HE2	86:1:1162:C:N4	2.33	0.42
78:1o:88:LEU:HD21	78:1o:92:ARG:HH22	1.85	0.42
85:1v:219:LYS:O	85:1v:223:GLU:HG2	2.19	0.42
86:1:333:A:O2'	86:1:334:A:H8	2.02	0.42
86:1:571:A:H2'	86:1:572:G:C8	2.55	0.42
87:2:1710:G:H2'	87:2:1711:A:C8	2.54	0.42
1:3:44:C:O2'	44:1F:60:LYS:O	2.28	0.42
3:B:405:ARG:CD	28:a:125:LEU:HD23	2.50	0.42
29:b:25:LYS:O	29:b:25:LYS:HG2	2.18	0.42
30:c:137:LYS:HG2	86:1:2251:G:OP1	2.18	0.42
37:j:41:LEU:HB2	37:j:46:LYS:HG3	2.02	0.42
47:1I:49:ASN:HB3	47:1I:87:THR:HG23	1.94	0.42
60:1V:120:GLU:OE1	60:1V:123:LYS:NZ	2.46	0.42
86:1:1878:A:H2'	86:1:1879:A:C8	2.55	0.42
86:1:2842:U:H2'	86:1:2843:C:C6	2.55	0.42
86:1:2939:C:H2'	86:1:2940:G:C8	2.54	0.42
14:M:65:GLN:NE2	14:M:67:VAL:O	2.44	0.42
15:N:397:TYR:OH	15:N:408:ASP:OD1	2.28	0.42
39:l:279:ARG:CD	39:l:281:PHE:CE2	2.95	0.42
51:1M:89:LYS:NZ	92:1M:311:HOH:O	2.53	0.42
51:1M:177:ARG:HG2	51:1M:179:MET:SD	2.60	0.42
60:1V:157:PRO:HD3	65:1a:70:TRP:CD1	2.54	0.42
61:1W:160:LEU:HD11	61:1W:199:VAL:HG11	2.02	0.42
62:1X:118:LEU:HB3	62:1X:137:ARG:HE	1.85	0.42
84:1u:154:MET:CE	84:1u:190:ILE:HD12	2.50	0.42
84:1u:681:GLU:HG3	84:1u:683:SER:H	1.85	0.42
86:1:131:G:O2'	86:1:132:C:O5'	2.34	0.42
86:1:1446:C:H2'	86:1:1447:A:C8	2.55	0.42
86:1:2178:A:N6	86:1:2206:G:H1'	2.35	0.42
87:2:72:G:O6	87:2:163:A:N6	2.53	0.42
87:2:1290:U:H4'	87:2:1291:A:H5'	2.01	0.42
3:B:249:MET:SD	28:a:358:GLU:CG	3.06	0.42
5:D:370:VAL:HG11	87:2:1072:A:H5''	2.02	0.42
27:Z:126:ASN:OD1	87:2:113:U:OP1	2.38	0.42
28:a:85:ARG:NH1	28:a:100:GLY:O	2.47	0.42
28:a:393:ARG:NH2	87:2:1388:A:OP1	2.51	0.42
36:i:291:LYS:O	36:i:295:MET:HG2	2.19	0.42
42:1D:126:GLY:HA3	42:1D:151:LYS:HG3	2.02	0.42
47:1I:61:PHE:CB	47:1I:76:MET:HE1	2.50	0.42
59:1U:34:ARG:HD2	65:1a:92:GLN:OE1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:1U:125:LYS:HE2	59:1U:125:LYS:HB3	1.88	0.42
73:1i:136:ARG:HA	73:1i:136:ARG:HD3	1.91	0.42
84:1u:244:ASN:O	84:1u:248:SER:OG	2.31	0.42
84:1u:308:GLU:HG3	84:1u:311:LYS:HE3	2.02	0.42
87:2:134:A:H2'	87:2:135:A:C8	2.55	0.42
87:2:192:G:H2'	87:2:193:A:C8	2.55	0.42
87:2:1653:U:H2'	87:2:1654:G:H8	1.84	0.42
87:2:1727:G:N1	87:2:1743:A:H2	2.14	0.42
8:G:79:ASP:OD1	8:G:123:GLN:NE2	2.52	0.41
16:O:85:PRO:HA	16:O:86:PRO:HD3	1.95	0.41
25:X:411:LEU:HG	25:X:442:MET:HE1	2.02	0.41
32:e:169:LYS:HE2	32:e:169:LYS:HB3	1.90	0.41
36:i:672:ILE:HG22	36:i:702:LEU:HD11	2.00	0.41
39:l:439:LYS:HE2	39:l:471:LYS:O	2.18	0.41
62:1X:175:ILE:CG2	78:1o:93:ARG:NH1	2.54	0.41
67:1c:48:ILE:HG23	67:1c:53:LYS:HE3	2.00	0.41
77:1m:24:GLU:O	77:1m:28:GLN:HG2	2.20	0.41
84:1u:88:GLU:HG3	84:1u:119:LEU:HD12	2.02	0.41
85:1v:256:CYS:HB2	85:1v:285:VAL:HG11	1.96	0.41
86:1:732:C:H2'	86:1:733:A:H8	1.84	0.41
86:1:1873:U:H2'	86:1:1874:A:C8	2.55	0.41
2:A:157:VAL:HG22	2:A:174:TYR:HB2	2.03	0.41
3:B:423:MET:HA	3:B:426:PHE:CE2	2.55	0.41
3:B:480:LYS:HE2	3:B:480:LYS:HB2	1.92	0.41
3:B:493:LEU:HD12	3:B:501:GLN:HG2	2.01	0.41
14:M:121:THR:HG22	87:2:972:C:N4	2.33	0.41
15:N:306:LYS:NZ	23:V:175:TRP:O	2.52	0.41
25:X:505:ASP:OD1	25:X:505:ASP:N	2.53	0.41
33:f:347:VAL:HG11	33:f:380:MET:HG2	2.02	0.41
36:i:387:TYR:CG	36:i:410:MET:HG3	2.55	0.41
61:1W:133:ARG:HG2	61:1W:140:ILE:HD13	2.01	0.41
62:1X:230:HIS:HB3	62:1X:233:LEU:HD13	2.02	0.41
78:1o:120:ASN:HB3	86:1:1240:A:H5'	2.02	0.41
86:1:677:U:H2'	86:1:678:C:C6	2.55	0.41
86:1:1226:C:H2'	86:1:1227:A:H8	1.85	0.41
86:1:2067:U:H2'	86:1:2068:A:H8	1.84	0.41
86:1:2231:A:C2	87:2:1802:A:O2'	2.39	0.41
86:1:2819:U:H2'	86:1:2820:C:C6	2.54	0.41
86:1:3134:C:H2'	86:1:3135:A:H8	1.85	0.41
1:3:37:U:OP1	76:1l:54:LYS:HE3	2.21	0.41
8:G:10:LEU:HB3	8:G:71:CYS:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:170:HIS:ND1	10:I:171:VAL:HG22	2.34	0.41
28:a:403:LYS:C	39:l:527:LEU:HD11	2.45	0.41
28:a:405:GLN:HA	28:a:408:ILE:HG12	2.03	0.41
33:f:120:LYS:HG2	33:f:340:LEU:HD22	2.03	0.41
41:1C:166:ILE:HG23	64:1Z:16:VAL:HG21	2.02	0.41
42:1D:70:MET:HB3	42:1D:288:ILE:HG23	2.01	0.41
59:1U:110:SER:HA	59:1U:113:LYS:HE2	2.01	0.41
86:1:521:C:H2'	86:1:522:G:C8	2.56	0.41
86:1:2852:U:H2'	86:1:2853:C:C6	2.54	0.41
87:2:94:A:H2'	87:2:95:A:C8	2.56	0.41
39:l:198:LEU:HD12	39:l:213:LEU:HD21	2.02	0.41
48:1J:53:ARG:NH1	48:1J:79:PHE:CE2	2.59	0.41
49:1K:55:ALA:HB2	49:1K:68:GLY:HA2	2.01	0.41
71:1g:159:PRO:HA	71:1g:160:PRO:HD3	1.95	0.41
84:1u:339:GLU:O	84:1u:341:VAL:N	2.52	0.41
86:1:977:U:H2'	86:1:978:A:H8	1.85	0.41
86:1:2552:U:H2'	86:1:2553:U:C6	2.56	0.41
87:2:78:U:HO2'	87:2:79:G:H8	1.68	0.41
3:B:61:ILE:HB	3:B:72:HIS:HB2	2.03	0.41
3:B:174:ARG:CZ	25:X:366:ARG:HD3	2.50	0.41
34:g:539:HIS:ND1	87:2:1172:U:O2'	2.40	0.41
35:h:149:ASN:CB	35:h:152:ARG:NH2	2.83	0.41
36:i:391:ILE:HG12	36:i:403:VAL:HG13	2.02	0.41
39:l:549:ILE:HD11	87:2:1389:A:H4'	2.01	0.41
41:1C:199:VAL:HG22	46:1H:97:ARG:HB2	2.03	0.41
55:1Q:200:LYS:HE2	55:1Q:200:LYS:HB2	1.90	0.41
58:1T:133:VAL:HG11	58:1T:159:ARG:HD3	2.02	0.41
62:1X:178:ASP:OD1	62:1X:178:ASP:N	2.51	0.41
64:1Z:150:ASP:HB3	64:1Z:154:PHE:CE2	2.44	0.41
81:1r:108:LYS:HB2	81:1r:125:LEU:HD21	2.02	0.41
83:1t:130:LEU:HB2	83:1t:145:LEU:HD22	2.02	0.41
86:1:561:U:H2'	86:1:562:C:C6	2.55	0.41
86:1:691:A:H1'	86:1:692:A:H5'	2.03	0.41
86:1:784:A:H2'	86:1:785:A:C8	2.56	0.41
86:1:1978:U:H2'	86:1:1979:A:C8	2.56	0.41
87:2:161:A:C2	87:2:162:C:H1'	2.55	0.41
87:2:241:U:H2'	87:2:242:G:C8	2.56	0.41
87:2:491:G:H2'	87:2:492:G:C8	2.55	0.41
2:A:186:TYR:CG	9:H:264:LEU:HD13	2.56	0.41
4:C:148:HIS:CE1	32:e:384:LEU:HD11	2.55	0.41
7:F:34:GLN:HB2	7:F:108:GLU:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:22:ALA:HB3	22:U:42:ASN:HB2	2.02	0.41
9:H:307:TYR:OH	87:2:1410:C:O2'	2.24	0.41
26:Y:15:THR:HB	28:a:334:GLU:HG2	2.03	0.41
29:b:21:ILE:CB	87:2:1845:A:N6	2.65	0.41
29:b:25:LYS:HD3	87:2:1845:A:C5	2.55	0.41
35:h:151:CYS:HA	35:h:154:VAL:HG12	2.03	0.41
36:i:477:MET:HA	36:i:480:MET:HE2	2.03	0.41
36:i:477:MET:HE2	36:i:511:ILE:HD13	2.01	0.41
36:i:683:ASP:O	36:i:687:MET:HG2	2.20	0.41
37:j:73:THR:HG22	37:j:75:ASP:H	1.85	0.41
37:j:77:HIS:CE1	87:2:92:A:P	3.14	0.41
37:j:232:PHE:HE2	37:j:240:ASP:HB3	1.85	0.41
55:1Q:219:MET:SD	87:2:1693:C:H5'	2.60	0.41
83:1t:10:ARG:NH2	92:1t:518:HOH:O	2.54	0.41
86:1:1594:G:C6	86:1:1658:A:C2	3.09	0.41
86:1:1874:A:H2'	86:1:1875:G:O4'	2.21	0.41
86:1:2567:U:O2'	86:1:2732:C:OP2	2.35	0.41
87:2:1316:A:H2'	87:2:1317:A:C8	2.55	0.41
87:2:1403:U:H2'	87:2:1404:G:H8	1.85	0.41
3:B:187:VAL:HG11	3:B:329:THR:H	1.86	0.41
3:B:212:PRO:O	3:B:212:PRO:CD	2.68	0.41
6:E:78:GLU:HB3	40:1B:52:HIS:NE2	2.36	0.41
41:1C:171:PHE:HB3	64:1Z:126:PHE:CD1	2.56	0.41
57:1S:221:LYS:HA	57:1S:221:LYS:HD3	1.83	0.41
84:1u:477:TYR:HA	84:1u:480:ILE:HG22	2.03	0.41
86:1:349:A:H2'	86:1:350:A:C8	2.56	0.41
86:1:543:G:H2'	86:1:544:A:C8	2.55	0.41
86:1:2931:U:H2'	86:1:2932:G:C8	2.55	0.41
87:2:1506:C:H2'	87:2:1507:A:C8	2.56	0.41
3:B:282:GLN:O	3:B:286:ARG:HG3	2.20	0.41
4:C:252:MET:HE2	32:e:150:SER:HB3	2.03	0.41
13:L:132:LYS:NZ	92:L:201:HOH:O	2.54	0.41
21:T:96:LYS:HB2	87:2:1400:G:H4'	2.02	0.41
36:i:275:LYS:HD3	36:i:275:LYS:HA	1.91	0.41
37:j:124:VAL:HG12	37:j:128:GLN:HE22	1.84	0.41
41:1C:193:ARG:CZ	46:1H:77:LEU:HD23	2.51	0.41
50:1L:148:ARG:CD	92:1L:205:HOH:O	2.55	0.41
58:1T:257:THR:HA	86:1:3166[A]:C:N3	2.36	0.41
64:1Z:45:ARG:NH2	86:1:1522:G:N7	2.68	0.41
85:1v:298:ASP:OD2	85:1v:301:ARG:HG3	2.21	0.41
86:1:1511:A:H2'	86:1:1512:A:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
87:2:1507:A:H2'	87:2:1508:A:C8	2.55	0.41
87:2:1814:G:H8	87:2:1814:G:H2'	1.70	0.41
1:3:42:U:C6	67:1c:2:LYS:HE3	2.55	0.41
10:I:197:LEU:HD23	10:I:197:LEU:HA	1.93	0.41
11:J:272:ARG:O	11:J:276:VAL:HG23	2.21	0.41
16:O:101:ARG:HA	16:O:102:PRO:HD3	1.95	0.41
17:P:29:LEU:HD11	87:2:562:C:C4	2.56	0.41
20:S:36:LEU:HG	20:S:40:LEU:HD13	2.03	0.41
27:Z:91:ARG:NH1	87:2:152:G:N1	2.68	0.41
28:a:138:ASP:O	28:a:142:ASP:HB2	2.21	0.41
34:g:564:LEU:HD12	34:g:567:LEU:HD12	2.03	0.41
36:i:375:LEU:HD21	36:i:409:LYS:NZ	2.35	0.41
36:i:403:VAL:CG1	36:i:428:MET:HE2	2.41	0.41
39:l:485:ARG:NH1	39:l:488:CYS:HB3	1.95	0.41
39:l:517:LYS:CD	87:2:1384:A:O2'	2.68	0.41
47:1I:29:TYR:OH	86:1:1256:G:O2'	2.30	0.41
48:1J:61:THR:O	48:1J:63:MET:N	2.54	0.41
48:1J:70:TYR:HD2	48:1J:74:SER:O	2.03	0.41
70:1f:191:ARG:HD3	70:1f:191:ARG:HA	1.78	0.41
78:1o:113:ARG:HG2	86:1:1237:G:H5'	2.03	0.41
83:1t:7:SER:HB2	86:1:1664:A:N1	2.36	0.41
83:1t:18:LYS:CE	92:1t:501:HOH:O	2.65	0.41
83:1t:321:LEU:HD23	83:1t:321:LEU:HA	1.93	0.41
84:1u:87:LEU:HD11	84:1u:111:LEU:HG	2.02	0.41
86:1:314:U:H2'	86:1:315:U:H6	1.86	0.41
86:1:758:A:H2'	86:1:759:A:C8	2.55	0.41
86:1:844:G:O2'	86:1:1974:A:N3	2.48	0.41
86:1:2388:C:H2'	86:1:2389:A:C8	2.56	0.41
86:1:2404:U:H2'	86:1:2405:C:C6	2.56	0.41
87:2:64:U:H2'	87:2:65:G:C8	2.56	0.41
87:2:75:C:H2'	87:2:76:G:C8	2.56	0.41
87:2:1381:C:C2	87:2:1382:C:C5	3.09	0.41
87:2:1412:C:H2'	87:2:1413:A:C8	2.56	0.41
87:2:1614:C:H2'	87:2:1615:G:C8	2.56	0.41
87:2:1743:A:H2'	87:2:1744:C:H4'	2.02	0.41
1:3:37:U:OP1	76:1l:54:LYS:HG3	2.21	0.41
7:F:140:ARG:NH2	11:J:237:TYR:HH	2.16	0.41
14:M:75:ARG:NH2	87:2:987:A:O2'	2.52	0.41
27:Z:53:LEU:HG	27:Z:69:MET:HE2	2.03	0.41
27:Z:91:ARG:NH1	87:2:152:G:C6	2.89	0.41
31:d:74:ARG:HD3	87:2:470:C:H5'	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:1m:50:ASP:N	77:1m:50:ASP:OD1	2.53	0.41
86:1:274:A:H2'	86:1:275:A:C8	2.56	0.41
86:1:1095:A:H2'	86:1:1096:C:C6	2.56	0.41
87:2:328:A:O2'	87:2:605:A:N1	2.47	0.41
87:2:1703:G:C2'	87:2:1704:A:H5'	2.51	0.41
2:A:150:ALA:HB2	2:A:171:LYS:HB3	2.04	0.40
3:B:393:ILE:HA	3:B:396:ILE:HG22	2.02	0.40
4:C:183:LEU:HB3	5:D:71:ILE:HD12	2.02	0.40
15:N:316:PRO:HA	15:N:319:MET:HE2	2.02	0.40
24:W:455:GLU:HA	24:W:458:TRP:CD1	2.56	0.40
29:b:15:LYS:HD2	87:2:1652:C:OP1	2.21	0.40
34:g:506:PHE:HZ	34:g:526:LEU:HA	1.86	0.40
37:j:214:GLU:OE1	37:j:251:ARG:NH2	2.49	0.40
51:1M:258:LEU:HD23	51:1M:258:LEU:HA	1.88	0.40
54:1P:91:LYS:HG2	86:1:2639:U:C4	2.51	0.40
67:1c:48:ILE:HG12	67:1c:53:LYS:CG	2.48	0.40
86:1:76:C:H2'	86:1:77:A:H8	1.85	0.40
86:1:1447:A:H2'	86:1:1448:A:C8	2.55	0.40
87:2:1052:U:H2'	87:2:1053:G:H8	1.86	0.40
3:B:25:ASP:OD2	10:I:135:ARG:NH1	2.54	0.40
3:B:288:ARG:NE	28:a:205:ASP:OD1	2.46	0.40
3:B:312:HIS:O	3:B:312:HIS:ND1	2.52	0.40
5:D:311:ILE:HG21	5:D:344:ARG:HB2	2.02	0.40
9:H:305:ARG:NH2	87:2:1122:C:O2	2.37	0.40
19:R:140:PRO:HD3	67:1c:58:PHE:CD2	2.52	0.40
24:W:214:PRO:O	24:W:219:LYS:NZ	2.54	0.40
25:X:401:PRO:HD2	28:a:365:LEU:HD22	2.03	0.40
32:e:186:LYS:HA	32:e:189:MET:HE3	2.02	0.40
33:f:144:MET:HE1	33:f:157:ILE:HD13	2.04	0.40
36:i:309:ARG:HA	36:i:309:ARG:HD3	1.81	0.40
42:1D:115:ILE:CD1	42:1D:120:ILE:CA	2.99	0.40
52:1N:122:PRO:HG2	52:1N:125:VAL:HG21	2.02	0.40
54:1P:81:ASP:CG	63:1Y:146:LYS:HZ3	2.22	0.40
73:1i:121:LYS:HB3	73:1i:121:LYS:HE3	1.77	0.40
77:1m:1:MET:HE2	77:1m:29:CYS:HB3	2.03	0.40
85:1v:141:HIS:NE2	85:1v:146:VAL:HB	2.36	0.40
86:1:332:A:O2'	86:1:333:A:H5''	2.21	0.40
86:1:996:G:H2'	86:1:997:G:C8	2.56	0.40
86:1:1382:G:H2'	86:1:1383:A:C8	2.56	0.40
86:1:3088:U:H2'	86:1:3089:C:H6	1.86	0.40
3:B:357:GLU:O	3:B:361:ASN:ND2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:377:MET:HA	3:B:380:ILE:HG12	2.04	0.40
35:h:237:LEU:HD11	35:h:262:PHE:CD2	2.55	0.40
35:h:279:ARG:HH22	35:h:290:ALA:HB1	1.86	0.40
36:i:363:ASN:HB3	36:i:366:ALA:HB3	2.01	0.40
42:1D:115:ILE:HD13	42:1D:120:ILE:N	2.35	0.40
45:1G:9:LEU:HB2	45:1G:55:VAL:HB	2.03	0.40
48:1J:138:SER:O	48:1J:142:THR:HG23	2.22	0.40
55:1Q:106:LYS:HG2	55:1Q:110:LYS:HD2	2.03	0.40
62:1X:170:ILE:HG12	62:1X:206:PRO:HG2	2.02	0.40
75:1k:26:ILE:HD12	75:1k:72:VAL:HG21	2.03	0.40
84:1u:308:GLU:HA	84:1u:311:LYS:HG2	2.03	0.40
84:1u:722:GLU:O	84:1u:726:SER:OG	2.32	0.40
85:1v:211:ARG:CZ	85:1v:242:PHE:O	2.70	0.40
86:1:358:A:H2'	86:1:359:A:H8	1.86	0.40
86:1:543:G:H2'	86:1:544:A:H8	1.86	0.40
86:1:1698:A:H61	86:1:1838:A:H61	1.68	0.40
86:1:2332:A:H2'	86:1:2333:A:C8	2.55	0.40
87:2:161:A:H3'	87:2:162:C:H5''	2.03	0.40
87:2:1262:A:O2'	87:2:1263:A:O4'	2.34	0.40
3:B:356:ARG:NH1	25:X:368:LEU:O	2.53	0.40
3:B:395:VAL:HG22	28:a:109:ARG:HG3	2.03	0.40
12:K:46:ASN:ND2	12:K:89:ASP:OD1	2.35	0.40
18:Q:193:LEU:CD2	18:Q:213:ILE:HG21	2.47	0.40
27:Z:63:TRP:CE2	35:h:137:LEU:HD23	2.57	0.40
32:e:383:ILE:O	32:e:384:LEU:HG	2.22	0.40
36:i:536:GLY:HA2	36:i:569:ALA:HB2	2.03	0.40
37:j:233:TYR:CE1	37:j:241:VAL:HG21	2.55	0.40
52:1N:54:ARG:HD3	86:1:1101:G:C5	2.56	0.40
52:1N:61:THR:HG21	52:1N:144:GLY:O	2.21	0.40
84:1u:241:ARG:HH11	86:1:337:A:H3'	1.86	0.40
85:1v:271:MET:HE3	85:1v:271:MET:HB2	1.92	0.40
86:1:406:U:H2'	86:1:407:U:C6	2.56	0.40
86:1:600:G:O2'	86:1:611:G:O6	2.39	0.40
86:1:1192:G:H2'	86:1:1193:C:C6	2.56	0.40
87:2:1275:A:H2'	87:2:1276:A:C8	2.57	0.40
3:B:526:VAL:HB	3:B:533:LEU:HB3	2.02	0.40
12:K:83:ARG:HB3	12:K:98:ILE:HD11	2.03	0.40
24:W:472:MET:O	24:W:476:VAL:HG23	2.22	0.40
26:Y:55:TYR:HA	26:Y:56:PRO:HD3	1.92	0.40
28:a:314:LYS:HB3	28:a:314:LYS:HE3	1.98	0.40
29:b:15:LYS:HG3	87:2:1652:C:H5''	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:e:304:LEU:O	32:e:308:GLU:HG2	2.22	0.40
37:j:90:LEU:HD23	37:j:90:LEU:HA	1.89	0.40
39:l:548:ALA:N	87:2:1391:C:O2	2.55	0.40
51:1M:127:LYS:HZ3	86:1:229:A:H5'	1.86	0.40
53:1O:78:THR:HB	82:1s:168:TRP:CE2	2.56	0.40
58:1T:240:LEU:HD23	58:1T:240:LEU:HA	1.94	0.40
58:1T:251:ILE:HD12	58:1T:254:ARG:HH21	1.86	0.40
84:1u:263:TRP:CD1	86:1:308:A:H4'	2.57	0.40
84:1u:368:PRO:HD3	84:1u:398:ILE:HD11	2.04	0.40
85:1v:335:ILE:HG13	85:1v:337:ARG:HG3	2.04	0.40
86:1:2896:C:H2'	86:1:2897:G:C8	2.57	0.40
87:2:1638:U:H2'	87:2:1639:A:C8	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	202/212 (95%)	192 (95%)	10 (5%)	0	100	100
3	B	457/554 (82%)	426 (93%)	29 (6%)	2 (0%)	30	28
4	C	329/362 (91%)	322 (98%)	7 (2%)	0	100	100
5	D	413/501 (82%)	394 (95%)	18 (4%)	1 (0%)	43	44
6	E	99/138 (72%)	97 (98%)	2 (2%)	0	100	100
7	F	146/157 (93%)	141 (97%)	5 (3%)	0	100	100
8	G	126/129 (98%)	122 (97%)	4 (3%)	0	100	100
9	H	208/383 (54%)	196 (94%)	11 (5%)	1 (0%)	24	22
10	I	111/228 (49%)	107 (96%)	4 (4%)	0	100	100
11	J	125/304 (41%)	120 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	K	122/125 (98%)	119 (98%)	3 (2%)	0	100	100
13	L	108/154 (70%)	105 (97%)	3 (3%)	0	100	100
14	M	99/155 (64%)	97 (98%)	2 (2%)	0	100	100
15	N	114/414 (28%)	113 (99%)	1 (1%)	0	100	100
16	O	108/136 (79%)	107 (99%)	1 (1%)	0	100	100
17	P	89/110 (81%)	87 (98%)	1 (1%)	1 (1%)	11	7
18	Q	88/237 (37%)	87 (99%)	1 (1%)	0	100	100
19	R	162/212 (76%)	159 (98%)	3 (2%)	0	100	100
20	S	73/100 (73%)	73 (100%)	0	0	100	100
21	T	48/94 (51%)	46 (96%)	2 (4%)	0	100	100
22	U	125/192 (65%)	119 (95%)	6 (5%)	0	100	100
23	V	162/193 (84%)	160 (99%)	2 (1%)	0	100	100
24	W	376/483 (78%)	372 (99%)	4 (1%)	0	100	100
25	X	202/496 (41%)	193 (96%)	7 (4%)	2 (1%)	12	8
26	Y	96/102 (94%)	96 (100%)	0	0	100	100
27	Z	78/153 (51%)	75 (96%)	3 (4%)	0	100	100
28	a	311/424 (73%)	303 (97%)	8 (3%)	0	100	100
29	b	75/80 (94%)	66 (88%)	9 (12%)	0	100	100
30	c	24/128 (19%)	24 (100%)	0	0	100	100
31	d	76/110 (69%)	74 (97%)	2 (3%)	0	100	100
32	e	244/383 (64%)	230 (94%)	13 (5%)	1 (0%)	30	28
33	f	375/410 (92%)	361 (96%)	14 (4%)	0	100	100
34	g	569/668 (85%)	556 (98%)	13 (2%)	0	100	100
35	h	308/384 (80%)	301 (98%)	7 (2%)	0	100	100
36	i	593/725 (82%)	576 (97%)	16 (3%)	1 (0%)	43	44
37	j	379/408 (93%)	366 (97%)	13 (3%)	0	100	100
38	k	26/153 (17%)	23 (88%)	3 (12%)	0	100	100
39	l	440/576 (76%)	438 (100%)	2 (0%)	0	100	100
40	1B	175/217 (81%)	171 (98%)	4 (2%)	0	100	100
41	1C	203/286 (71%)	187 (92%)	14 (7%)	2 (1%)	12	8
42	1D	262/319 (82%)	258 (98%)	3 (1%)	1 (0%)	30	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	1E	219/296 (74%)	217 (99%)	2 (1%)	0	100	100
44	1F	154/185 (83%)	148 (96%)	6 (4%)	0	100	100
45	1G	96/102 (94%)	94 (98%)	2 (2%)	0	100	100
46	1H	64/220 (29%)	63 (98%)	1 (2%)	0	100	100
47	1I	128/170 (75%)	114 (89%)	12 (9%)	2 (2%)	7	3
48	1J	145/156 (93%)	131 (90%)	12 (8%)	2 (1%)	9	5
49	1K	187/204 (92%)	184 (98%)	3 (2%)	0	100	100
50	1L	125/176 (71%)	120 (96%)	5 (4%)	0	100	100
51	1M	208/281 (74%)	199 (96%)	9 (4%)	0	100	100
52	1N	146/179 (82%)	143 (98%)	3 (2%)	0	100	100
53	1O	149/160 (93%)	142 (95%)	7 (5%)	0	100	100
54	1P	111/114 (97%)	108 (97%)	3 (3%)	0	100	100
55	1Q	120/233 (52%)	118 (98%)	2 (2%)	0	100	100
56	1R	108/126 (86%)	107 (99%)	1 (1%)	0	100	100
57	1S	143/270 (53%)	140 (98%)	3 (2%)	0	100	100
58	1T	153/264 (58%)	151 (99%)	2 (1%)	0	100	100
59	1U	126/180 (70%)	124 (98%)	2 (2%)	0	100	100
60	1V	156/159 (98%)	153 (98%)	3 (2%)	0	100	100
61	1W	203/248 (82%)	197 (97%)	5 (2%)	1 (0%)	24	22
62	1X	214/271 (79%)	209 (98%)	5 (2%)	0	100	100
63	1Y	101/156 (65%)	100 (99%)	1 (1%)	0	100	100
64	1Z	175/215 (81%)	174 (99%)	1 (1%)	0	100	100
65	1a	106/144 (74%)	106 (100%)	0	0	100	100
66	1b	98/109 (90%)	93 (95%)	5 (5%)	0	100	100
67	1c	57/135 (42%)	55 (96%)	2 (4%)	0	100	100
68	1d	47/139 (34%)	46 (98%)	1 (2%)	0	100	100
69	1e	52/106 (49%)	51 (98%)	1 (2%)	0	100	100
70	1f	42/146 (29%)	42 (100%)	0	0	100	100
71	1g	89/162 (55%)	89 (100%)	0	0	100	100
72	1h	36/103 (35%)	35 (97%)	1 (3%)	0	100	100
73	1i	176/247 (71%)	175 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
74	1j	69/90 (77%)	69 (100%)	0	0	100	100
75	1k	116/119 (98%)	114 (98%)	2 (2%)	0	100	100
76	1l	209/239 (87%)	198 (95%)	11 (5%)	0	100	100
77	1m	120/128 (94%)	113 (94%)	5 (4%)	2 (2%)	7	3
78	1o	74/125 (59%)	71 (96%)	3 (4%)	0	100	100
79	1p	115/130 (88%)	115 (100%)	0	0	100	100
80	1q	48/78 (62%)	47 (98%)	0	1 (2%)	5	2
81	1r	90/167 (54%)	85 (94%)	5 (6%)	0	100	100
82	1s	116/181 (64%)	114 (98%)	2 (2%)	0	100	100
83	1t	482/491 (98%)	473 (98%)	7 (2%)	2 (0%)	30	28
84	1u	663/752 (88%)	631 (95%)	32 (5%)	0	100	100
85	1v	429/514 (84%)	418 (97%)	10 (2%)	1 (0%)	43	44
All	All	14791/20265 (73%)	14335 (97%)	433 (3%)	23 (0%)	44	44

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	H	225	ILE
41	1C	227	ARG
47	1I	62	LYS
47	1I	133	PRO
48	1J	33	SER
77	1m	94	MET
85	1v	175	ALA
3	B	106	PRO
36	i	374	VAL
61	1W	228	ASP
77	1m	93	GLN
83	1t	445	ALA
32	e	180	TYR
41	1C	190	ASP
25	X	461	VAL
48	1J	29	GLY
83	1t	473	LYS
25	X	428	ILE
3	B	409	ILE
5	D	260	ILE
80	1q	64	VAL

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Mol	Chain	Res	Type
17	P	3	PRO
42	1D	226	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	177/182 (97%)	177 (100%)	0	100	100
3	B	421/492 (86%)	419 (100%)	2 (0%)	81	87
4	C	312/343 (91%)	312 (100%)	0	100	100
5	D	370/444 (83%)	370 (100%)	0	100	100
6	E	90/126 (71%)	90 (100%)	0	100	100
7	F	124/124 (100%)	124 (100%)	0	100	100
8	G	112/113 (99%)	112 (100%)	0	100	100
9	H	175/320 (55%)	175 (100%)	0	100	100
10	I	104/197 (53%)	104 (100%)	0	100	100
11	J	108/256 (42%)	108 (100%)	0	100	100
12	K	106/107 (99%)	106 (100%)	0	100	100
13	L	93/128 (73%)	93 (100%)	0	100	100
14	M	90/137 (66%)	90 (100%)	0	100	100
15	N	107/362 (30%)	107 (100%)	0	100	100
16	O	93/117 (80%)	93 (100%)	0	100	100
17	P	78/95 (82%)	78 (100%)	0	100	100
18	Q	75/203 (37%)	75 (100%)	0	100	100
19	R	141/180 (78%)	141 (100%)	0	100	100
20	S	68/90 (76%)	68 (100%)	0	100	100
21	T	44/79 (56%)	44 (100%)	0	100	100
22	U	109/170 (64%)	109 (100%)	0	100	100
23	V	147/173 (85%)	147 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	W	328/410 (80%)	328 (100%)	0	100	100
25	X	174/395 (44%)	174 (100%)	0	100	100
26	Y	84/86 (98%)	84 (100%)	0	100	100
27	Z	65/119 (55%)	65 (100%)	0	100	100
28	a	252/375 (67%)	252 (100%)	0	100	100
29	b	68/71 (96%)	68 (100%)	0	100	100
30	c	25/116 (22%)	25 (100%)	0	100	100
31	d	65/93 (70%)	65 (100%)	0	100	100
32	e	226/339 (67%)	226 (100%)	0	100	100
33	f	321/351 (92%)	321 (100%)	0	100	100
34	g	510/597 (85%)	510 (100%)	0	100	100
35	h	271/337 (80%)	270 (100%)	1 (0%)	84	89
36	i	511/629 (81%)	511 (100%)	0	100	100
37	j	329/355 (93%)	329 (100%)	0	100	100
38	k	21/109 (19%)	21 (100%)	0	100	100
39	l	378/492 (77%)	377 (100%)	1 (0%)	86	91
40	1B	141/173 (82%)	141 (100%)	0	100	100
41	1C	184/239 (77%)	181 (98%)	3 (2%)	55	63
42	1D	216/264 (82%)	216 (100%)	0	100	100
43	1E	192/256 (75%)	192 (100%)	0	100	100
44	1F	145/168 (86%)	145 (100%)	0	100	100
45	1G	82/86 (95%)	82 (100%)	0	100	100
46	1H	58/196 (30%)	58 (100%)	0	100	100
47	1I	113/143 (79%)	113 (100%)	0	100	100
48	1J	125/131 (95%)	125 (100%)	0	100	100
49	1K	161/170 (95%)	161 (100%)	0	100	100
50	1L	103/140 (74%)	103 (100%)	0	100	100
51	1M	169/235 (72%)	169 (100%)	0	100	100
52	1N	116/146 (80%)	116 (100%)	0	100	100
53	1O	129/139 (93%)	129 (100%)	0	100	100
54	1P	94/95 (99%)	94 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	1Q	110/208 (53%)	110 (100%)	0	100	100
56	1R	96/110 (87%)	96 (100%)	0	100	100
57	1S	130/244 (53%)	130 (100%)	0	100	100
58	1T	133/229 (58%)	133 (100%)	0	100	100
59	1U	114/147 (78%)	114 (100%)	0	100	100
60	1V	132/133 (99%)	132 (100%)	0	100	100
61	1W	181/213 (85%)	181 (100%)	0	100	100
62	1X	186/235 (79%)	186 (100%)	0	100	100
63	1Y	83/127 (65%)	83 (100%)	0	100	100
64	1Z	148/175 (85%)	148 (100%)	0	100	100
65	1a	102/128 (80%)	100 (98%)	2 (2%)	48	55
66	1b	88/95 (93%)	88 (100%)	0	100	100
67	1c	51/119 (43%)	51 (100%)	0	100	100
68	1d	42/119 (35%)	42 (100%)	0	100	100
69	1e	49/98 (50%)	49 (100%)	0	100	100
70	1f	35/129 (27%)	35 (100%)	0	100	100
71	1g	84/152 (55%)	84 (100%)	0	100	100
72	1h	36/87 (41%)	36 (100%)	0	100	100
73	1i	147/203 (72%)	147 (100%)	0	100	100
74	1j	64/79 (81%)	64 (100%)	0	100	100
75	1k	105/106 (99%)	105 (100%)	0	100	100
76	1l	189/214 (88%)	189 (100%)	0	100	100
77	1m	107/112 (96%)	107 (100%)	0	100	100
78	1o	69/105 (66%)	69 (100%)	0	100	100
79	1p	101/108 (94%)	101 (100%)	0	100	100
80	1q	41/65 (63%)	41 (100%)	0	100	100
81	1r	83/138 (60%)	83 (100%)	0	100	100
82	1s	103/155 (66%)	103 (100%)	0	100	100
83	1t	417/423 (99%)	417 (100%)	0	100	100
84	1u	577/660 (87%)	577 (100%)	0	100	100
85	1v	366/446 (82%)	366 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	12969/17455 (74%)	12960 (100%)	9 (0%)	87 93

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	481	ARG
3	B	483	GLU
35	h	83	THR
39	l	485	ARG
41	1C	195	PRO
41	1C	200	SER
41	1C	226	TRP
65	1a	31	VAL
65	1a	36	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (106) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	4	HIS
2	A	99	ASN
3	B	64	HIS
3	B	240	GLN
3	B	358	GLN
3	B	361	ASN
3	B	516	ASN
3	B	517	GLN
4	C	158	ASN
4	C	185	HIS
4	C	186	GLN
4	C	284	ASN
4	C	349	ASN
5	D	234	GLN
5	D	309	ASN
5	D	482	ASN
6	E	63	GLN
7	F	34	GLN
8	G	65	GLN
9	H	299	GLN
10	I	139	ASN
10	I	213	GLN
13	L	92	HIS

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Mol	Chain	Res	Type
14	M	74	HIS
15	N	370	HIS
15	N	380	HIS
17	P	68	ASN
20	S	48	GLN
20	S	63	HIS
24	W	186	ASN
24	W	307	GLN
24	W	425	GLN
24	W	426	ASN
25	X	467	ASN
25	X	521	ASN
26	Y	93	HIS
27	Z	58	GLN
28	a	126	GLN
28	a	158	ASN
29	b	68	GLN
33	f	121	HIS
34	g	518	GLN
34	g	534	GLN
34	g	573	HIS
34	g	638	ASN
35	h	106	ASN
35	h	149	ASN
35	h	316	GLN
36	i	413	ASN
36	i	434	ASN
36	i	565	ASN
37	j	93	ASN
37	j	260	HIS
37	j	265	GLN
38	k	16	GLN
39	l	173	ASN
39	l	235	ASN
39	l	387	ASN
39	l	481	HIS
39	l	547	ASN
40	1B	56	ASN
41	1C	32	HIS
41	1C	64	ASN
41	1C	68	GLN
41	1C	101	ASN

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Mol	Chain	Res	Type
43	1E	225	ASN
46	1H	72	HIS
47	1I	80	ASN
48	1J	51	ASN
48	1J	103	HIS
49	1K	14	ASN
50	1L	69	GLN
51	1M	97	HIS
52	1N	93	HIS
52	1N	160	GLN
53	1O	74	HIS
54	1P	33	GLN
55	1Q	143	GLN
56	1R	61	HIS
57	1S	253	HIS
58	1T	116	GLN
59	1U	11	HIS
59	1U	127	HIS
61	1W	115	GLN
62	1X	98	GLN
64	1Z	140	GLN
65	1a	36	ASN
65	1a	142	ASN
67	1c	50	GLN
73	1i	101	GLN
73	1i	180	HIS
74	1j	56	GLN
74	1j	79	GLN
76	1l	60	GLN
76	1l	97	ASN
77	1m	93	GLN
79	1p	96	ASN
79	1p	106	GLN
83	1t	281	ASN
83	1t	307	GLN
84	1u	406	GLN
85	1v	99	HIS
85	1v	226	HIS
85	1v	303	GLN
85	1v	330	ASN
85	1v	442	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	3	117/118 (99%)	26 (22%)	1 (0%)
86	1	2910/2922 (99%)	548 (18%)	30 (1%)
87	2	1752/1766 (99%)	300 (17%)	25 (1%)
All	All	4779/4806 (99%)	874 (18%)	56 (1%)

All (874) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	3	2	A
1	3	3	A
1	3	13	A
1	3	15	G
1	3	23	G
1	3	25	G
1	3	26	A
1	3	37	U
1	3	44	C
1	3	46	G
1	3	53	A
1	3	54	U
1	3	55	A
1	3	56	U
1	3	57	G
1	3	59	G
1	3	65	G
1	3	67	C
1	3	69	U
1	3	72	G
1	3	87	A
1	3	90	G
1	3	91	U
1	3	103	G
1	3	106	C
1	3	118	A
86	1	47	A
86	1	49	G
86	1	50	G
86	1	51	A
86	1	54	G
86	1	63	A
86	1	64	G

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Mol	Chain	Res	Type
86	1	65	A
86	1	70	A
86	1	73	G
86	1	74	G
86	1	86	U
86	1	88	C
86	1	96	G
86	1	113	U
86	1	126	U
86	1	127	C
86	1	128	C
86	1	129	A
86	1	131	G
86	1	132	C
86	1	136	G
86	1	137	U
86	1	138	G
86	1	139	G
86	1	141	U
86	1	142	A
86	1	144	U
86	1	147	G
86	1	148	C
86	1	150	C
86	1	151	U
86	1	152	C
86	1	153	U
86	1	157	G
86	1	158	A
86	1	159	C
86	1	161	U
86	1	163	G
86	1	164	A
86	1	181	A
86	1	184	A
86	1	201	A
86	1	206	A
86	1	207	A
86	1	233	G
86	1	249	U
86	1	251	G
86	1	257	U

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Mol	Chain	Res	Type
86	1	259	A
86	1	260	A
86	1	308	A
86	1	309	A
86	1	311	A
86	1	313	U
86	1	321	U
86	1	331	A
86	1	332	A
86	1	333	A
86	1	334	A
86	1	337	A
86	1	339	A
86	1	341	A
86	1	342	A
86	1	344	A
86	1	345	A
86	1	353	A
86	1	354	A
86	1	357	A
86	1	406	U
86	1	409	U
86	1	416	U
86	1	418	U
86	1	419	U
86	1	421	A
86	1	422	C
86	1	424	G
86	1	425	U
86	1	426	A
86	1	427	A
86	1	428	U
86	1	435	A
86	1	445	G
86	1	457	G
86	1	463	G
86	1	464	A
86	1	481	U
86	1	485	U
86	1	487	U
86	1	488	U
86	1	491	U

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Mol	Chain	Res	Type
86	1	493	G
86	1	495	U
86	1	496	C
86	1	498	U
86	1	499	U
86	1	500	C
86	1	501	C
86	1	502	C
86	1	504	G
86	1	514	G
86	1	515	C
86	1	516	G
86	1	526	U
86	1	535	U
86	1	537	U
86	1	538	U
86	1	539	A
86	1	540	C
86	1	541	G
86	1	542	C
86	1	547	A
86	1	553	G
86	1	567	C
86	1	597	C
86	1	598	A
86	1	599	A
86	1	620	A
86	1	623	G
86	1	633	A
86	1	634	C
86	1	644	A
86	1	646	A
86	1	649	G
86	1	650	A
86	1	651	A
86	1	652	C
86	1	671	A
86	1	672	A
86	1	673	U
86	1	674	C
86	1	675	A
86	1	676	G

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Mol	Chain	Res	Type
86	1	687	A
86	1	689	U
86	1	691	A
86	1	692	A
86	1	693	G
86	1	694	C
86	1	695	G
86	1	696	C
86	1	698	C
86	1	700	C
86	1	701	A
86	1	714	A
86	1	724	U
86	1	725	G
86	1	726	A
86	1	737	A
86	1	754	G
86	1	771	U
86	1	779	U
86	1	780	U
86	1	781	C
86	1	785	A
86	1	789	G
86	1	790	G
86	1	793	U
86	1	795	U
86	1	796	U
86	1	799	A
86	1	800	G
86	1	814	A
86	1	830	U
86	1	855	G
86	1	875	A
86	1	893	G
86	1	909	A
86	1	910	C
86	1	920	G
86	1	921	G
86	1	927	A
86	1	929	G
86	1	930	G
86	1	942	C

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Mol	Chain	Res	Type
86	1	950	G
86	1	957	U
86	1	972	U
86	1	973	U
86	1	975	A
86	1	989	U
86	1	992	C
86	1	1003	G
86	1	1004	G
86	1	1011	A
86	1	1022	U
86	1	1023	A
86	1	1024	G
86	1	1026	G
86	1	1044	A
86	1	1045	C
86	1	1046	C
86	1	1058	A
86	1	1094	G
86	1	1099	U
86	1	1101	G
86	1	1103	G
86	1	1111	G
86	1	1124	G
86	1	1146	C
86	1	1159	A
86	1	1162	C
86	1	1163	A
86	1	1172	G
86	1	1176	A
86	1	1184	G
86	1	1190	G
86	1	1195	A
86	1	1196	U
86	1	1197	G
86	1	1207	A
86	1	1218	G
86	1	1219	A
86	1	1220	A
86	1	1221	G
86	1	1234	G
86	1	1237	G

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Mol	Chain	Res	Type
86	1	1238	A
86	1	1239	A
86	1	1241	G
86	1	1242	C
86	1	1244	U
86	1	1247	U
86	1	1248	A
86	1	1262	G
86	1	1266	C
86	1	1269	G
86	1	1282	U
86	1	1283	A
86	1	1285	C
86	1	1292	C
86	1	1293	A
86	1	1306	A
86	1	1325	G
86	1	1327	U
86	1	1328	G
86	1	1329	C
86	1	1331	U
86	1	1338	G
86	1	1339	U
86	1	1352	A
86	1	1368	A
86	1	1395	G
86	1	1404	A
86	1	1412	U
86	1	1413	G
86	1	1428	G
86	1	1430	A
86	1	1432	A
86	1	1444	A
86	1	1457	G
86	1	1459	C
86	1	1479	U
86	1	1485	A
86	1	1487	U
86	1	1502	U
86	1	1510	U
86	1	1523	A
86	1	1531	G

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Mol	Chain	Res	Type
86	1	1533	C
86	1	1540	U
86	1	1546	C
86	1	1554	U
86	1	1557	C
86	1	1566	U
86	1	1567	U
86	1	1572	U
86	1	1573	A
86	1	1574	C
86	1	1578	A
86	1	1584	C
86	1	1587	C
86	1	1588	U
86	1	1591	C
86	1	1593	U
86	1	1594	G
86	1	1595	G
86	1	1596	A
86	1	1597	G
86	1	1598	C
86	1	1599	G
86	1	1602	U
86	1	1603	U
86	1	1604	G
86	1	1605	G
86	1	1606	A
86	1	1619	G
86	1	1620	G
86	1	1621	G
86	1	1623	A
86	1	1626	G
86	1	1629	G
86	1	1630	C
86	1	1631	G
86	1	1635	C
86	1	1638	C
86	1	1643	C
86	1	1644	A
86	1	1645	C
86	1	1647	C
86	1	1648	U

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Mol	Chain	Res	Type
86	1	1649	C
86	1	1658	A
86	1	1669	U
86	1	1670	G
86	1	1671	A
86	1	1672	G
86	1	1678	A
86	1	1679	A
86	1	1685	U
86	1	1693	C
86	1	1694	A
86	1	1695	A
86	1	1699	U
86	1	1834	A
86	1	1840	A
86	1	1849	U
86	1	1850	U
86	1	1852	U
86	1	1853	A
86	1	1854	A
86	1	1858	C
86	1	1869	U
86	1	1874	A
86	1	1875	G
86	1	1877	C
86	1	1883	G
86	1	1884	G
86	1	1889	A
86	1	1890	A
86	1	1896	A
86	1	1899	A
86	1	1903	A
86	1	1914	G
86	1	1919	G
86	1	1920	G
86	1	1921	C
86	1	1922	G
86	1	1923	A
86	1	1924	U
86	1	1925	C
86	1	1934	G
86	1	1935	A

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Mol	Chain	Res	Type
86	1	1936	A
86	1	1937	C
86	1	1950	A
86	1	1960	A
86	1	1976	U
86	1	1989	U
86	1	1990	U
86	1	2016	G
86	1	2045	G
86	1	2058	U
86	1	2060	U
86	1	2062	U
86	1	2064	G
86	1	2065	A
86	1	2066	U
86	1	2067	U
86	1	2080	C
86	1	2081	A
86	1	2082	U
86	1	2088	G
86	1	2097	A
86	1	2104	A
86	1	2124	C
86	1	2125	U
86	1	2126	A
86	1	2132	U
86	1	2140	U
86	1	2143	A
86	1	2153	A
86	1	2172	A
86	1	2176	C
86	1	2185	A
86	1	2190	U
86	1	2191	U
86	1	2192	A
86	1	2193	U
86	1	2194	A
86	1	2214	G
86	1	2223	C
86	1	2224	G
86	1	2230	A
86	1	2231	A

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Mol	Chain	Res	Type
86	1	2232	C
86	1	2245	A
86	1	2247	G
86	1	2248	G
86	1	2254	A
86	1	2255	A
86	1	2256	A
86	1	2273	U
86	1	2285	C
86	1	2288	A
86	1	2289	U
86	1	2290	G
86	1	2293	G
86	1	2302	G
86	1	2309	U
86	1	2311	U
86	1	2315	C
86	1	2320	U
86	1	2328	G
86	1	2341	C
86	1	2348	A
86	1	2349	A
86	1	2351	A
86	1	2357	A
86	1	2373	C
86	1	2374	G
86	1	2378	A
86	1	2379	G
86	1	2387	G
86	1	2394	C
86	1	2398	A
86	1	2411	G
86	1	2415	A
86	1	2420	G
86	1	2421	A
86	1	2423	C
86	1	2429	U
86	1	2430	G
86	1	2432	A
86	1	2434	G
86	1	2435	A
86	1	2436	U

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Mol	Chain	Res	Type
86	1	2437	A
86	1	2438	G
86	1	2439	G
86	1	2440	U
86	1	2443	G
86	1	2444	A
86	1	2445	G
86	1	2446	G
86	1	2448	C
86	1	2449	C
86	1	2450	U
86	1	2451	C
86	1	2452	A
86	1	2454	A
86	1	2461	G
86	1	2462	A
86	1	2463	C
86	1	2464	C
86	1	2465	A
86	1	2466	A
86	1	2467	U
86	1	2468	C
86	1	2470	U
86	1	2473	A
86	1	2474	A
86	1	2475	G
86	1	2476	A
86	1	2479	A
86	1	2480	C
86	1	2481	U
86	1	2482	C
86	1	2483	U
86	1	2484	U
86	1	2488	U
86	1	2501	A
86	1	2506	C
86	1	2534	A
86	1	2547	G
86	1	2548	G
86	1	2550	A
86	1	2577	A
86	1	2587	A

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Mol	Chain	Res	Type
86	1	2592	U
86	1	2596	A
86	1	2597	A
86	1	2606	C
86	1	2613	A
86	1	2618	C
86	1	2620	G
86	1	2621	C
86	1	2625	U
86	1	2639	U
86	1	2640	A
86	1	2641	A
86	1	2652	C
86	1	2655	U
86	1	2688	G
86	1	2690	C
86	1	2696	G
86	1	2711	U
86	1	2730	A
86	1	2736	U
86	1	2740	A
86	1	2746	G
86	1	2750	G
86	1	2752	G
86	1	2753	A
86	1	2779	U
86	1	2781	U
86	1	2785	C
86	1	2789	G
86	1	2796	U
86	1	2803	OMC
86	1	2807	G
86	1	2808	2MA
86	1	2810	G
86	1	2823	A
86	1	2825	C
86	1	2834	G
86	1	2871	A
86	1	2872	G
86	1	2877	A
86	1	2878	C
86	1	2883	G

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Mol	Chain	Res	Type
86	1	2890	U
86	1	2907	A
86	1	2908	G
86	1	2914	U
86	1	2915	U
86	1	2918	U
86	1	2934	U
86	1	2935	A
86	1	2936	A
86	1	2937	A
86	1	2938	G
86	1	2939	C
86	1	2954	G
86	1	2955	C
86	1	2972	G
86	1	2988	A
86	1	2998	U
86	1	2999	A
86	1	3021	G
86	1	3023	G
86	1	3035	A
86	1	3042	A
86	1	3050	A
86	1	3053	G
86	1	3056	G
86	1	3058	U
86	1	3059	U
86	1	3080	A
86	1	3099	U
86	1	3104	A
86	1	3116	A
86	1	3142	G
86	1	3148	G
86	1	3153	A
86	1	3161	C
86	1	3164	A
86	1	3169	A
87	2	4	A
87	2	12	A
87	2	17	G
87	2	30	G
87	2	40	A

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Mol	Chain	Res	Type
87	2	47	G
87	2	55	C
87	2	56	U
87	2	58	A
87	2	59	A
87	2	76	G
87	2	79	G
87	2	80	U
87	2	82	C
87	2	83	U
87	2	92	A
87	2	104	U
87	2	121	A
87	2	122	A
87	2	150	A
87	2	151	A
87	2	152	G
87	2	154	G
87	2	156	U
87	2	157	G
87	2	161	A
87	2	162	C
87	2	163	A
87	2	164	A
87	2	172	A
87	2	183	A
87	2	184	A
87	2	185	G
87	2	194	A
87	2	195	U
87	2	203	A
87	2	206	G
87	2	214	U
87	2	215	A
87	2	224	A
87	2	225	G
87	2	226	A
87	2	228	A
87	2	233	G
87	2	237	G
87	2	245	U
87	2	264	U

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Mol	Chain	Res	Type
87	2	266	G
87	2	270	G
87	2	285	G
87	2	286	C
87	2	308	G
87	2	317	U
87	2	318	U
87	2	325	A
87	2	340	A
87	2	347	C
87	2	348	A
87	2	351	G
87	2	363	A
87	2	364	C
87	2	365	G
87	2	366	G
87	2	370	G
87	2	371	C
87	2	373	G
87	2	375	A
87	2	386	U
87	2	391	C
87	2	403	G
87	2	416	A
87	2	420	U
87	2	425	G
87	2	430	A
87	2	432	G
87	2	440	A
87	2	441	U
87	2	442	U
87	2	443	C
87	2	444	C
87	2	450	U
87	2	459	U
87	2	469	G
87	2	470	C
87	2	471	G
87	2	479	G
87	2	492	G
87	2	494	A
87	2	507	A

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Mol	Chain	Res	Type
87	2	509	C
87	2	516	C
87	2	519	G
87	2	528	G
87	2	530	A
87	2	531	A
87	2	545	A
87	2	557	A
87	2	560	G
87	2	566	G
87	2	571	A
87	2	573	G
87	2	574	G
87	2	575	G
87	2	594	G
87	2	618	A
87	2	629	G
87	2	649	U
87	2	661	A
87	2	683	A
87	2	699	G
87	2	717	A
87	2	718	A
87	2	720	A
87	2	744	U
87	2	745	A
87	2	751	G
87	2	762	A
87	2	773	A
87	2	789	U
87	2	790	A
87	2	811	A
87	2	813	C
87	2	825	G
87	2	828	C
87	2	836	A
87	2	837	U
87	2	838	U
87	2	839	C
87	2	840	U
87	2	846	G
87	2	865	A

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Mol	Chain	Res	Type
87	2	866	A
87	2	878	G
87	2	895	G
87	2	907	A
87	2	919	G
87	2	926	G
87	2	927	C
87	2	928	A
87	2	932	G
87	2	953	U
87	2	962	A
87	2	964	G
87	2	968	A
87	2	969	G
87	2	970	A
87	2	982	C
87	2	986	G
87	2	998	A
87	2	999	G
87	2	1007	A
87	2	1012	U
87	2	1029	C
87	2	1030	U
87	2	1036	A
87	2	1037	C
87	2	1057	U
87	2	1086	G
87	2	1087	U
87	2	1093	A
87	2	1096	G
87	2	1116	G
87	2	1117	U
87	2	1118	U
87	2	1122	C
87	2	1123	A
87	2	1125	A
87	2	1127	A
87	2	1132	C
87	2	1133	C
87	2	1134	U
87	2	1135	A
87	2	1136	A

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Mol	Chain	Res	Type
87	2	1137	G
87	2	1138	G
87	2	1140	G
87	2	1141	A
87	2	1143	A
87	2	1169	U
87	2	1170	U
87	2	1171	U
87	2	1172	U
87	2	1173	U
87	2	1175	U
87	2	1176	U
87	2	1177	U
87	2	1188	U
87	2	1191	A
87	2	1193	A
87	2	1206	U
87	2	1258	A
87	2	1260	A
87	2	1261	A
87	2	1262	A
87	2	1274	A
87	2	1275	A
87	2	1277	A
87	2	1278	A
87	2	1279	A
87	2	1280	U
87	2	1281	U
87	2	1291	A
87	2	1292	A
87	2	1307	A
87	2	1308	A
87	2	1310	A
87	2	1311	A
87	2	1316	A
87	2	1319	A
87	2	1320	A
87	2	1321	A
87	2	1339	U
87	2	1343	U
87	2	1379	C
87	2	1380	U

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Mol	Chain	Res	Type
87	2	1386	A
87	2	1387	C
87	2	1388	A
87	2	1389	A
87	2	1390	A
87	2	1391	C
87	2	1392	A
87	2	1395	A
87	2	1399	U
87	2	1407	G
87	2	1420	A
87	2	1422	U
87	2	1431	U
87	2	1432	A
87	2	1459	A
87	2	1460	A
87	2	1475	U
87	2	1476	A
87	2	1490	A
87	2	1501	A
87	2	1511	A
87	2	1516	G
87	2	1521	G
87	2	1523	A
87	2	1542	A
87	2	1543	A
87	2	1561	A
87	2	1564	U
87	2	1581	A
87	2	1582	C
87	2	1608	A
87	2	1615	G
87	2	1625	A
87	2	1632	G
87	2	1647	G
87	2	1651	C
87	2	1652	C
87	2	1659	C
87	2	1660	A
87	2	1664	4OC
87	2	1702	G
87	2	1703	G

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Mol	Chain	Res	Type
87	2	1706	C
87	2	1707	A
87	2	1714	A
87	2	1722	C
87	2	1723	U
87	2	1724	U
87	2	1725	C
87	2	1727	G
87	2	1728	U
87	2	1732	A
87	2	1735	C
87	2	1736	U
87	2	1738	G
87	2	1740	C
87	2	1742	C
87	2	1743	A
87	2	1744	C
87	2	1745	A
87	2	1746	A
87	2	1751	U
87	2	1762	U
87	2	1763	U
87	2	1764	A
87	2	1765	U
87	2	1766	U
87	2	1768	A
87	2	1769	C
87	2	1770	G
87	2	1771	C
87	2	1772	A
87	2	1774	A
87	2	1783	G
87	2	1784	G
87	2	1801	A
87	2	1802	A
87	2	1803	G
87	2	1806	G
87	2	1826	G
87	2	1828	MA6
87	2	1829	C
87	2	1838	G
87	2	1839	G

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Mol	Chain	Res	Type
87	2	1848	C

All (56) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	3	12	U
86	1	131	G
86	1	163	G
86	1	308	A
86	1	312	A
86	1	421	A
86	1	427	A
86	1	487	U
86	1	492	C
86	1	515	C
86	1	540	C
86	1	566	G
86	1	619	A
86	1	688	G
86	1	929	G
86	1	991	U
86	1	1100	U
86	1	1566	U
86	1	1598	C
86	1	1642	U
86	1	1693	C
86	1	1873	U
86	1	1923	A
86	1	2057	A
86	1	2059	C
86	1	2445	G
86	1	2461	G
86	1	2505	G
86	1	2617	U
86	1	2778	C
86	1	2998	U
87	2	79	G
87	2	82	C
87	2	103	A
87	2	162	C
87	2	225	G
87	2	317	U

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Mol	Chain	Res	Type
87	2	324	G
87	2	491	G
87	2	493	A
87	2	573	G
87	2	998	A
87	2	1117	U
87	2	1171	U
87	2	1277	A
87	2	1278	A
87	2	1280	U
87	2	1319	A
87	2	1386	A
87	2	1390	A
87	2	1701	C
87	2	1705	C
87	2	1706	C
87	2	1726	U
87	2	1769	C
87	2	1802	A

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

18 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$
86	PSU	1	2885	86,90	18,21,22	4.34	9 (50%)	21,30,33	2.06	6 (28%)
86	H2U	1	2754	86	18,21,22	0.49	0	19,30,33	0.98	1 (5%)
86	PSU	1	2910	86	18,21,22	4.40	7 (38%)	21,30,33	2.00	4 (19%)
86	PSU	1	891	86,88	18,21,22	4.38	8 (44%)	21,30,33	2.06	5 (23%)
87	MA6	2	1828	87	23,26,27	1.80	6 (26%)	33,38,41	3.44	12 (36%)
86	PSU	1	2188	86	18,21,22	4.35	7 (38%)	21,30,33	2.14	5 (23%)
87	UR3	2	1807	87	19,22,23	2.70	7 (36%)	26,32,35	1.72	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	5MU	1	2257	86,90	19,22,23	7.76	9 (47%)	27,32,35	3.40	10 (37%)
87	2MG	2	1825	87	23,26,27	2.70	8 (34%)	33,38,41	3.27	15 (45%)
87	MA6	2	1827	87	23,26,27	1.87	6 (26%)	33,38,41	3.28	12 (36%)
86	OMU	1	2857	86,88	19,22,23	3.11	8 (42%)	25,31,34	1.78	4 (16%)
87	G7M	2	525	87	23,26,27	2.15	8 (34%)	34,39,42	3.01	10 (29%)
87	4OC	2	1664	87	20,23,24	3.12	8 (40%)	25,32,35	1.00	3 (12%)
86	PSU	1	1105	86	18,21,22	4.26	7 (38%)	21,30,33	2.11	5 (23%)
86	PSU	1	2762	86	18,21,22	4.32	7 (38%)	21,30,33	2.08	6 (28%)
86	OMC	1	2803	86	19,22,23	2.90	8 (42%)	25,31,34	0.88	1 (4%)
86	OMG	1	2560	86,90	23,26,27	2.42	7 (30%)	32,38,41	2.29	10 (31%)
86	2MA	1	2808	86,90,88	22,25,26	4.11	7 (31%)	32,37,40	2.53	9 (28%)

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
86	PSU	1	2885	86,90	-	1/7/25/26	0/2/2/2
86	H2U	1	2754	86	-	0/7/38/39	0/2/2/2
86	PSU	1	2910	86	-	0/7/25/26	0/2/2/2
86	PSU	1	891	86,88	-	1/7/25/26	0/2/2/2
87	MA6	2	1828	87	-	1/11/29/30	0/3/3/3
86	PSU	1	2188	86	-	0/7/25/26	0/2/2/2
87	UR3	2	1807	87	-	0/7/25/26	0/2/2/2
86	5MU	1	2257	86,90	-	0/7/25/26	0/2/2/2
87	2MG	2	1825	87	-	0/9/27/28	0/3/3/3
87	MA6	2	1827	87	-	0/11/29/30	0/3/3/3
86	OMU	1	2857	86,88	-	0/9/27/28	0/2/2/2
87	G7M	2	525	87	-	3/7/25/26	0/3/3/3
87	4OC	2	1664	87	-	2/9/29/30	0/2/2/2
86	PSU	1	1105	86	-	0/7/25/26	0/2/2/2
86	PSU	1	2762	86	-	0/7/25/26	0/2/2/2
86	OMC	1	2803	86	-	0/9/27/28	0/2/2/2
86	OMG	1	2560	86,90	-	1/9/27/28	0/3/3/3
86	2MA	1	2808	86,90,88	-	2/7/25/26	0/3/3/3

All (127) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	1	2257	5MU	C4-C5	23.19	1.82	1.44
86	1	2257	5MU	C6-N1	15.60	1.64	1.38
86	1	2808	2MA	C4-N3	13.16	1.51	1.34
86	1	2257	5MU	C4-N3	-12.39	1.15	1.38
86	1	2257	5MU	C6-C5	-11.79	1.15	1.34
86	1	2910	PSU	C6-C5	11.61	1.48	1.35
86	1	2885	PSU	C6-C5	11.51	1.48	1.35
86	1	891	PSU	C6-C5	11.48	1.48	1.35
86	1	2188	PSU	C6-C5	11.43	1.47	1.35
86	1	2762	PSU	C6-C5	11.32	1.47	1.35
86	1	1105	PSU	C6-C5	11.12	1.47	1.35
86	1	2910	PSU	C2-N1	10.01	1.49	1.36
86	1	891	PSU	C2-N1	9.78	1.49	1.36
86	1	1105	PSU	C2-N1	9.68	1.49	1.36
86	1	2762	PSU	C2-N1	9.66	1.49	1.36
86	1	2188	PSU	C2-N1	9.63	1.49	1.36
86	1	2885	PSU	C2-N1	9.30	1.48	1.36
86	1	2808	2MA	C2-N3	8.10	1.47	1.34
86	1	2885	PSU	C2-N3	7.45	1.49	1.37
86	1	891	PSU	C2-N3	7.40	1.49	1.37
86	1	2188	PSU	C2-N3	7.40	1.49	1.37
86	1	2762	PSU	C2-N3	7.38	1.49	1.37
86	1	2857	OMU	C2-N1	7.38	1.50	1.38
87	2	1825	2MG	C2-N2	7.28	1.48	1.33
86	1	2910	PSU	C2-N3	7.17	1.49	1.37
86	1	1105	PSU	C2-N3	7.09	1.49	1.37
86	1	2808	2MA	C6-N1	6.86	1.44	1.35
87	2	1664	4OC	C4-N3	6.86	1.44	1.32
87	2	1807	UR3	C2-N1	6.80	1.47	1.38
86	1	2857	OMU	C2-N3	6.70	1.49	1.38
87	2	1825	2MG	C2-N3	6.66	1.44	1.32
86	1	2560	OMG	C4-N3	6.49	1.49	1.34
87	2	1664	4OC	C6-C5	6.21	1.49	1.35
86	1	2803	OMC	C2-N3	6.14	1.48	1.36
87	2	525	G7M	C4-N3	6.01	1.48	1.34
87	2	1807	UR3	C6-C5	6.01	1.49	1.35
87	2	1664	4OC	C2-N3	5.88	1.48	1.36
86	1	2803	OMC	C6-C5	5.78	1.48	1.35
86	1	2808	2MA	C2-N1	5.58	1.43	1.34
86	1	2857	OMU	C6-C5	5.48	1.47	1.35
86	1	2560	OMG	C2-N3	5.48	1.46	1.33
86	1	2257	5MU	C2-N3	5.33	1.47	1.38
87	2	1825	2MG	C4-N3	5.30	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	1	2910	PSU	C6-N1	5.23	1.44	1.36
87	2	1664	4OC	C4-N4	5.17	1.46	1.36
86	1	891	PSU	C6-N1	5.15	1.44	1.36
86	1	2808	2MA	C5-C6	5.07	1.55	1.41
86	1	2188	PSU	C6-N1	4.98	1.44	1.36
87	2	1828	MA6	C6-N6	4.94	1.50	1.36
87	2	1827	MA6	C6-N6	4.92	1.50	1.36
86	1	2762	PSU	C6-N1	4.89	1.44	1.36
86	1	1105	PSU	C6-N1	4.87	1.44	1.36
86	1	2803	OMC	C4-N3	4.78	1.44	1.34
86	1	2885	PSU	C6-N1	4.77	1.44	1.36
86	1	2560	OMG	C2-N2	4.66	1.45	1.34
87	2	1807	UR3	C2-N3	4.65	1.48	1.39
86	1	2803	OMC	C2-N1	4.63	1.49	1.40
86	1	2803	OMC	C4-N4	4.49	1.44	1.33
87	2	525	G7M	C5-N7	-4.48	1.34	1.39
86	1	2857	OMU	C4-N3	4.17	1.45	1.38
87	2	1825	2MG	C2-N1	3.99	1.43	1.36
86	1	2257	5MU	C2-N1	3.92	1.44	1.38
87	2	525	G7M	C2-N2	3.82	1.43	1.34
87	2	1664	4OC	C2-N1	3.74	1.47	1.40
87	2	1827	MA6	C5-C4	-3.68	1.32	1.39
86	1	2885	PSU	C4-N3	3.54	1.45	1.38
86	1	2762	PSU	C4-N3	3.52	1.45	1.38
86	1	891	PSU	C4-N3	3.50	1.45	1.38
86	1	2188	PSU	C4-N3	3.48	1.45	1.38
87	2	1828	MA6	C5-N7	-3.44	1.32	1.39
87	2	1664	4OC	C5-C4	3.43	1.48	1.41
86	1	2808	2MA	C6-N6	-3.41	1.25	1.34
86	1	1105	PSU	C4-N3	3.39	1.45	1.38
86	1	2257	5MU	O4-C4	-3.38	1.17	1.23
86	1	2910	PSU	C4-N3	3.34	1.45	1.38
87	2	1827	MA6	C5-N7	-3.32	1.33	1.39
86	1	2857	OMU	C6-N1	3.31	1.46	1.38
86	1	2560	OMG	C5-N7	-3.26	1.32	1.39
87	2	1664	4OC	O2-C2	-3.24	1.17	1.23
87	2	525	G7M	C2-N3	3.23	1.41	1.33
86	1	2857	OMU	O4-C4	-3.20	1.18	1.24
87	2	1828	MA6	C5-C4	-3.17	1.33	1.39
87	2	1664	4OC	C6-N1	3.07	1.45	1.38
86	1	2257	5MU	O2-C2	-3.03	1.17	1.23
87	2	1807	UR3	O2-C2	-3.01	1.16	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	1	2857	OMU	O2-C2	-3.00	1.17	1.23
86	1	2803	OMC	C6-N1	3.00	1.45	1.38
87	2	1827	MA6	C8-N9	-2.98	1.32	1.37
86	1	2803	OMC	O2-C2	-2.95	1.18	1.23
86	1	2885	PSU	O4-C4	-2.94	1.18	1.23
86	1	1105	PSU	O4-C4	-2.91	1.18	1.23
86	1	2910	PSU	O4-C4	-2.85	1.18	1.23
87	2	1828	MA6	C8-N9	-2.83	1.32	1.37
86	1	2560	OMG	O6-C6	-2.82	1.18	1.23
87	2	1807	UR3	C6-N1	2.78	1.44	1.38
86	1	2762	PSU	O4-C4	-2.78	1.18	1.23
86	1	891	PSU	O4-C4	-2.76	1.18	1.23
86	1	2188	PSU	O4-C4	-2.69	1.18	1.23
86	1	2808	2MA	C5-N7	-2.65	1.34	1.39
87	2	1807	UR3	O4-C4	-2.64	1.18	1.23
87	2	1828	MA6	C10-N6	2.59	1.51	1.45
86	1	2560	OMG	C2-N1	2.53	1.43	1.37
86	1	2885	PSU	O2-C2	-2.53	1.18	1.23
86	1	1105	PSU	O2-C2	-2.52	1.18	1.23
87	2	1825	2MG	C5-C6	2.48	1.53	1.44
86	1	2188	PSU	O2-C2	-2.46	1.18	1.23
87	2	525	G7M	C5-C6	2.42	1.49	1.43
86	1	2560	OMG	C5-C6	2.41	1.53	1.44
86	1	2910	PSU	O2-C2	-2.41	1.18	1.23
86	1	891	PSU	O2-C2	-2.39	1.18	1.23
86	1	2857	OMU	C5-C4	2.38	1.48	1.43
87	2	1827	MA6	C4-N9	-2.37	1.32	1.37
86	1	2762	PSU	O2-C2	-2.37	1.18	1.23
86	1	2885	PSU	O4'-C1'	-2.34	1.40	1.43
87	2	1827	MA6	C10-N6	2.32	1.50	1.45
87	2	525	G7M	C4-N9	-2.30	1.32	1.38
86	1	2803	OMC	C5-C4	2.29	1.48	1.42
87	2	1825	2MG	C4-N9	-2.24	1.32	1.38
86	1	891	PSU	O4'-C1'	-2.24	1.40	1.43
87	2	1807	UR3	C5-C4	2.16	1.49	1.43
86	1	2885	PSU	C1'-C5	2.14	1.55	1.50
87	2	525	G7M	C2-N1	2.14	1.42	1.37
87	2	525	G7M	C6-N1	2.13	1.42	1.38
87	2	1825	2MG	C5-N7	-2.13	1.34	1.39
86	1	2257	5MU	C5M-C5	2.12	1.55	1.50
87	2	1828	MA6	C4-N9	-2.11	1.33	1.37
87	2	1825	2MG	C6-N1	2.03	1.42	1.38

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	2	1828	MA6	N1-C6-N6	-12.50	101.62	116.86
87	2	1827	MA6	N1-C6-N6	-11.04	103.40	116.86
86	1	2257	5MU	C5-C4-N3	9.98	124.00	115.32
87	2	525	G7M	CN7-N7-C5	9.14	138.19	126.80
86	1	2808	2MA	C5-C4-N3	-8.74	117.98	127.18
87	2	1825	2MG	N1-C2-N2	8.62	125.36	116.56
87	2	1828	MA6	C5-C6-N6	8.45	138.71	125.33
86	1	2257	5MU	C5-C6-N1	-8.06	114.56	123.31
87	2	1827	MA6	C5-C6-N6	7.63	137.40	125.33
87	2	525	G7M	CN7-N7-C8	-7.15	113.96	124.79
86	1	2257	5MU	C4-N3-C2	-7.11	118.01	127.34
87	2	1825	2MG	C1'-N9-C8	-6.64	107.88	126.73
87	2	1825	2MG	C1'-N9-C4	6.43	145.49	126.49
87	2	1807	UR3	C4-N3-C2	-6.36	119.46	124.58
86	1	2808	2MA	N3-C4-N9	6.35	135.05	126.99
87	2	525	G7M	C1'-N9-C4	6.35	145.24	126.49
87	2	1825	2MG	C2-N3-C4	6.27	119.85	112.00
87	2	1827	MA6	N1-C2-N3	-6.10	119.35	128.58
87	2	1828	MA6	N1-C2-N3	-6.05	119.42	128.58
86	1	2560	OMG	C5-C4-N3	-6.00	118.84	128.39
87	2	525	G7M	C1'-N9-C8	-5.68	107.56	126.74
86	1	2857	OMU	C4-N3-C2	-5.38	119.93	126.61
87	2	1825	2MG	N2-C2-N3	-5.30	113.76	120.51
87	2	1827	MA6	N9-C8-N7	-5.30	106.42	113.94
86	1	2188	PSU	C4-N3-C2	-5.19	119.22	126.37
86	1	1105	PSU	C4-N3-C2	-5.15	119.28	126.37
86	1	891	PSU	C4-N3-C2	-5.11	119.33	126.37
86	1	2257	5MU	N3-C2-N1	5.05	121.46	114.89
87	2	1825	2MG	C2-N1-C6	-5.01	118.49	124.55
86	1	2910	PSU	C4-N3-C2	-5.01	119.47	126.37
86	1	2188	PSU	N1-C2-N3	4.95	120.39	115.17
86	1	1105	PSU	N1-C2-N3	4.88	120.32	115.17
86	1	2762	PSU	C4-N3-C2	-4.86	119.68	126.37
87	2	1828	MA6	C5-C4-N3	-4.80	120.11	126.72
86	1	2560	OMG	C2-N3-C4	4.77	120.52	112.30
86	1	891	PSU	N1-C2-N3	4.76	120.19	115.17
86	1	2560	OMG	C1'-N9-C4	-4.70	112.60	126.49
86	1	2762	PSU	N1-C2-N3	4.61	120.03	115.17
86	1	2910	PSU	N1-C2-N3	4.60	120.02	115.17
86	1	2885	PSU	N1-C2-N3	4.57	119.99	115.17
86	1	2885	PSU	C4-N3-C2	-4.57	120.08	126.37
87	2	1828	MA6	N9-C8-N7	-4.56	107.47	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	2	1825	2MG	CM2-N2-C2	-4.52	113.94	123.65
86	1	2560	OMG	C1'-N9-C8	4.44	139.35	126.73
87	2	525	G7M	C2-N3-C4	4.40	119.87	112.30
87	2	1825	2MG	C5-C4-N3	-4.28	121.58	128.39
87	2	525	G7M	C5-C6-N1	4.20	120.53	111.84
86	1	2257	5MU	C5M-C5-C6	-4.17	117.20	122.85
86	1	2560	OMG	N9-C4-N3	4.00	133.94	125.95
87	2	1827	MA6	C4-N9-C8	3.98	109.91	105.74
87	2	1827	MA6	C5-C4-N3	-3.90	121.35	126.72
86	1	2257	5MU	O4-C4-C5	-3.85	120.51	124.92
86	1	2857	OMU	N3-C2-N1	3.84	119.89	114.89
87	2	1827	MA6	C2-N1-C6	3.83	121.17	111.83
87	2	525	G7M	C5-C4-N3	-3.80	120.98	128.15
86	1	2857	OMU	C5-C4-N3	3.78	120.09	114.80
86	1	2808	2MA	N9-C8-N7	-3.73	108.64	113.94
87	2	1828	MA6	C2-N1-C6	3.73	120.94	111.83
86	1	2762	PSU	C6-C5-C4	3.70	120.67	118.17
87	2	525	G7M	O6-C6-C5	-3.60	119.97	128.01
86	1	2257	5MU	C6-C5-C4	3.57	120.96	118.02
87	2	1807	UR3	C5-C4-N3	3.55	119.71	115.04
87	2	1828	MA6	C4-C5-C6	3.54	119.57	115.91
86	1	2885	PSU	C6-N1-C2	-3.53	119.42	122.69
87	2	1827	MA6	C4-C5-C6	3.53	119.56	115.91
87	2	525	G7M	C2-N1-C6	-3.51	118.75	125.11
87	2	1828	MA6	C2-N3-C4	3.48	120.33	111.83
86	1	891	PSU	C6-C5-C4	3.44	120.50	118.17
86	1	2808	2MA	N3-C2-N1	-3.43	119.72	125.77
86	1	1105	PSU	C6-C5-C4	3.42	120.48	118.17
86	1	2188	PSU	C6-C5-C4	3.34	120.43	118.17
87	2	1828	MA6	N3-C4-N9	3.31	132.81	127.17
86	1	2560	OMG	C2-N1-C6	-3.30	119.12	125.11
87	2	1827	MA6	C5-N7-C8	3.28	108.61	103.45
86	1	891	PSU	C6-N1-C2	-3.27	119.66	122.69
86	1	2762	PSU	C6-N1-C2	-3.24	119.68	122.69
86	1	2188	PSU	C6-N1-C2	-3.22	119.71	122.69
86	1	1105	PSU	C6-N1-C2	-3.14	119.78	122.69
87	2	1828	MA6	C5-N7-C8	3.12	108.35	103.45
87	2	1827	MA6	C2-N3-C4	3.09	119.38	111.83
86	1	2885	PSU	O2-C2-N1	-3.09	119.61	122.79
86	1	2808	2MA	C4-N9-C1'	-3.08	119.44	126.63
87	2	1825	2MG	N9-C8-N7	-3.07	107.71	113.40
87	2	1825	2MG	C5-C4-N9	3.05	111.12	105.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	2	1828	MA6	C4-N9-C8	2.98	108.86	105.74
86	1	2188	PSU	O2-C2-N1	-2.97	119.72	122.79
86	1	2910	PSU	C6-C5-C4	2.97	120.18	118.17
86	1	2754	H2U	C5-C4-N3	-2.96	113.54	116.69
86	1	2257	5MU	O2-C2-N1	-2.95	118.96	122.80
86	1	2910	PSU	C6-N1-C2	-2.94	119.96	122.69
87	2	1827	MA6	C4-N9-C1'	-2.93	119.78	126.63
87	2	1825	2MG	C5-C6-N1	2.91	120.67	113.25
86	1	2857	OMU	O4-C4-C5	-2.90	120.16	125.16
86	1	2808	2MA	C5-N7-C8	2.89	107.99	103.45
86	1	2257	5MU	C5M-C5-C4	2.86	121.83	118.78
87	2	1827	MA6	N3-C4-N9	2.80	131.93	127.17
87	2	1825	2MG	C4-C5-N7	-2.76	106.30	110.67
86	1	2808	2MA	C6-C5-C4	2.73	120.90	117.18
86	1	2885	PSU	C6-C5-C4	2.69	119.99	118.17
86	1	2560	OMG	C5-C6-N1	2.68	120.09	113.25
87	2	1825	2MG	C6-C5-N7	2.68	135.16	130.29
86	1	2560	OMG	N9-C8-N7	-2.66	108.46	113.40
86	1	2762	PSU	O2-C2-N1	-2.66	120.04	122.79
86	1	2885	PSU	O4'-C1'-C2'	2.60	108.75	105.15
86	1	2808	2MA	C1'-N9-C8	2.59	132.83	127.09
86	1	891	PSU	O2-C2-N1	-2.56	120.15	122.79
86	1	2560	OMG	O6-C6-C5	-2.53	119.85	126.53
86	1	2257	5MU	O4-C4-N3	-2.46	115.49	120.11
86	1	1105	PSU	O2-C2-N1	-2.44	120.27	122.79
87	2	1807	UR3	C6-N1-C2	-2.42	119.82	121.80
87	2	1825	2MG	C8-N7-C5	2.33	108.42	104.26
87	2	1825	2MG	O6-C6-C5	-2.27	120.55	126.53
86	1	2808	2MA	CM2-C2-N3	2.25	120.49	117.13
87	2	525	G7M	N2-C2-N1	2.21	121.42	116.76
86	1	2803	OMC	O2-C2-N3	-2.17	118.90	122.33
86	1	2762	PSU	O4'-C1'-C2'	2.17	108.16	105.15
86	1	2560	OMG	C8-N7-C5	2.13	108.06	104.26
87	2	1664	4OC	O2-C2-N3	-2.12	118.98	122.33
87	2	1828	MA6	C4-C5-N7	-2.05	108.24	110.58
87	2	1664	4OC	CM4-N4-C4	-2.03	118.48	122.45
87	2	1664	4OC	C6-C5-C4	2.03	119.45	117.00
87	2	1807	UR3	C3U-N3-C2	2.02	120.85	117.33

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
86	1	2560	OMG	C1'-C2'-O2'-CM2
86	1	2808	2MA	O4'-C4'-C5'-O5'
87	2	1664	4OC	O4'-C4'-C5'-O5'
86	1	2808	2MA	C3'-C4'-C5'-O5'
87	2	1664	4OC	C3'-C4'-C5'-O5'
87	2	525	G7M	C3'-C4'-C5'-O5'
87	2	525	G7M	O4'-C4'-C5'-O5'
86	1	2885	PSU	O4'-C4'-C5'-O5'
87	2	525	G7M	C4'-C5'-O5'-P
87	2	1828	MA6	C4'-C5'-O5'-P
86	1	891	PSU	O4'-C1'-C5-C6

There are no ring outliers.

5 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	2	1828	MA6	1	0
86	1	2257	5MU	1	0
87	2	1825	2MG	1	0
86	1	2560	OMG	1	0
86	1	2808	2MA	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 436 ligands modelled in this entry, 435 are monoatomic - leaving 1 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	$\# Z > 2$
89	ATP	W	501	88	32,33,33	0.32	0	48,52,52	0.27	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
89	ATP	W	501	88	-	4/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

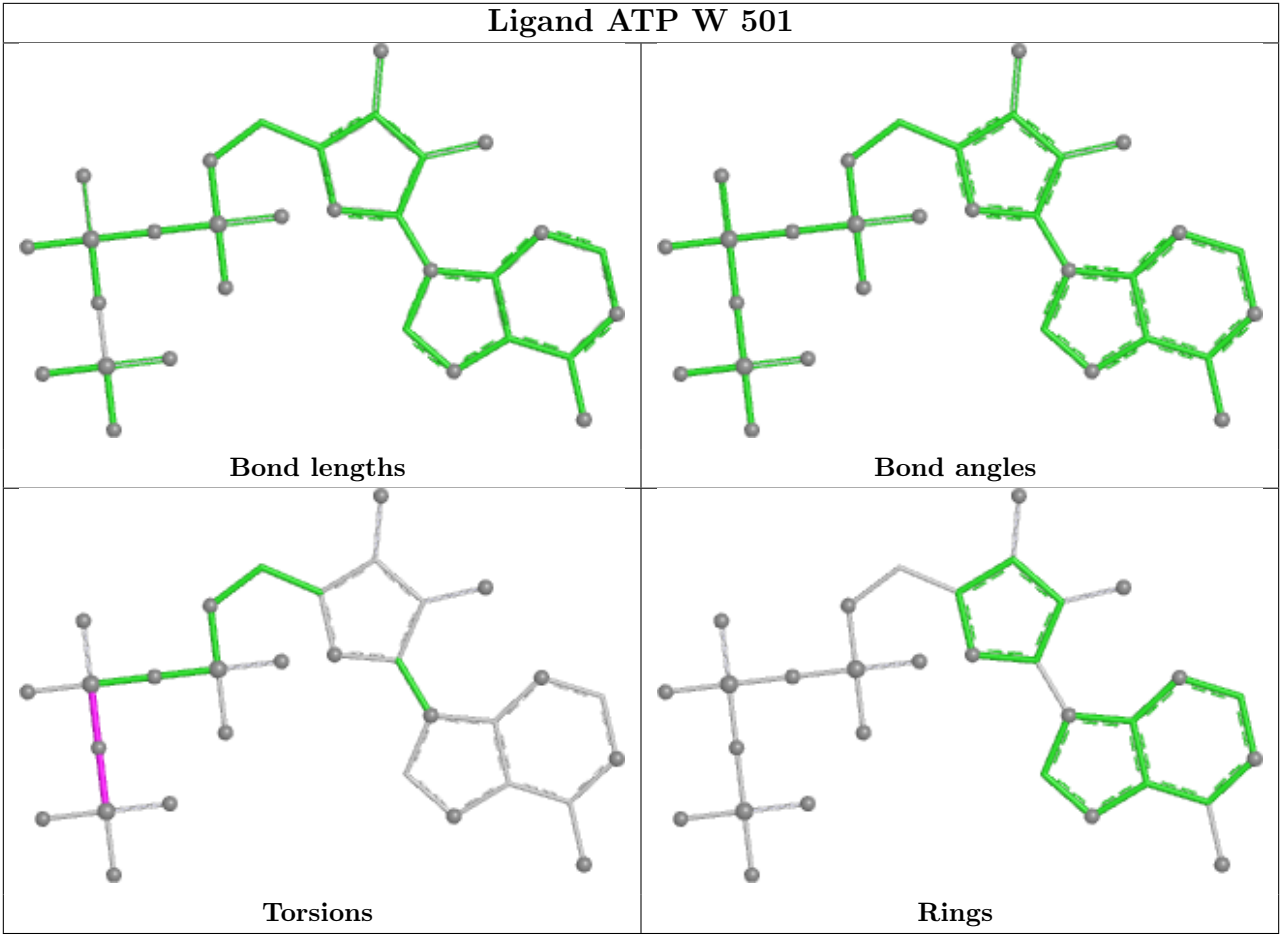
Mol	Chain	Res	Type	Atoms
89	W	501	ATP	PG-O3B-PB-O1B
89	W	501	ATP	PB-O3B-PG-O1G
89	W	501	ATP	PB-O3B-PG-O2G
89	W	501	ATP	PB-O3B-PG-O3G

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
89	W	501	ATP	1	0

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
87	2	18
86	1	16
41	1C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1C	256:LEU	C	298:ALA	N	39.42
1	1	261:G	O3'	270:A	P	27.88
1	1	295:U	O3'	307:A	P	27.72

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	1193:A	O3'	1197:U	P	23.87
1	2	95:A	O3'	101:A	P	23.32
1	2	1147:A	O3'	1164:U	P	22.59
1	2	1330:A	O3'	1335:U	P	18.04
1	1	363:A	O3'	405:U	P	17.68
1	1	283:A	O3'	288:U	P	17.02
1	1	1704:U	O3'	1831:A	P	16.95
1	1	1028:G	O3'	1041:C	P	16.82
1	2	124:A	O3'	129:A	P	15.54
1	1	323:U	O3'	330:A	P	15.13
1	1	2613:A	O3'	2617:U	P	14.54
1	2	1247:A	O3'	1250:U	P	14.54
1	2	137:A	O3'	142:U	P	14.49
1	2	1345:U	O3'	1376:A	P	13.61
1	1	1664:A	O3'	1667:C	P	12.66
1	2	116:U	O3'	120:A	P	12.62
1	1	2509:C	O3'	2528:G	P	10.63
1	2	1216:A	O3'	1221:A	P	9.18
1	2	84:A	O3'	86:A	P	7.96
1	2	1842:U	O3'	1845:A	P	7.74
1	2	1254:U	O3'	1257:A	P	6.90
1	1	859:U	O3'	861:A	P	4.06
1	2	1826:G	O3'	1827:MA6	P	3.25
1	2	1824:G	O3'	1825:2MG	P	3.17
1	1	2802:A	O3'	2803:OMC	P	3.11
1	1	2158:U	O3'	2159:G	P	3.09
1	1	2347:G	O3'	2348:A	P	3.08
1	2	1663:G	O3'	1664:4OC	P	3.06
1	2	1806:G	O3'	1807:UR3	P	3.05
1	1	1264:U	O3'	1265:C	P	1.83
1	2	922:G	O3'	923:C	P	1.39
1	1	1574:C	O3'	1575:A	P	1.31

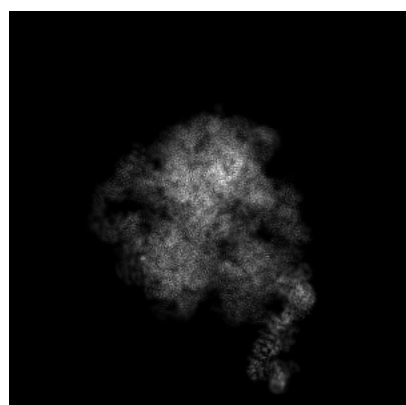
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51718. These allow visual inspection of the internal detail of the map and identification of artifacts.

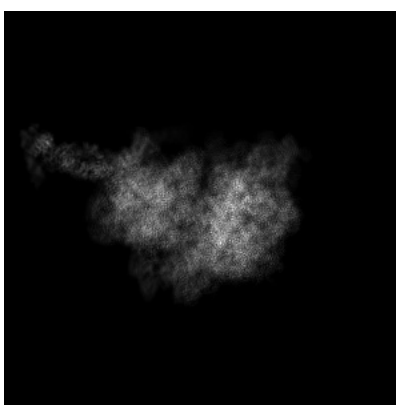
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

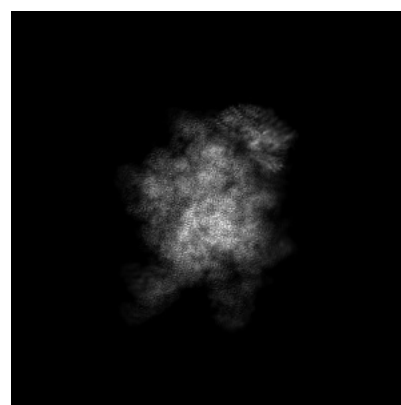
6.1.1 Primary map



X



Y

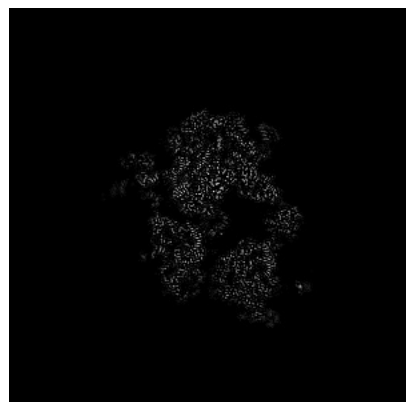


Z

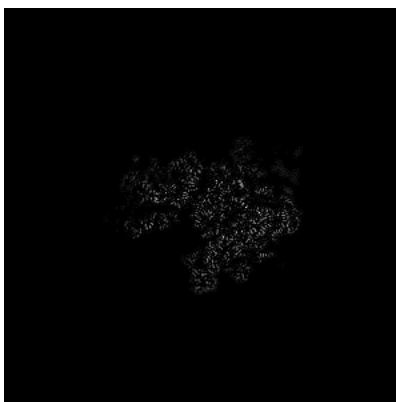
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 294



Y Index: 294

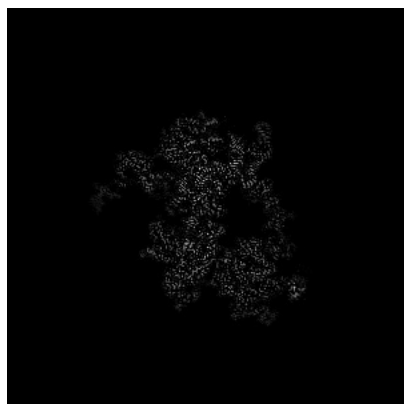


Z Index: 294

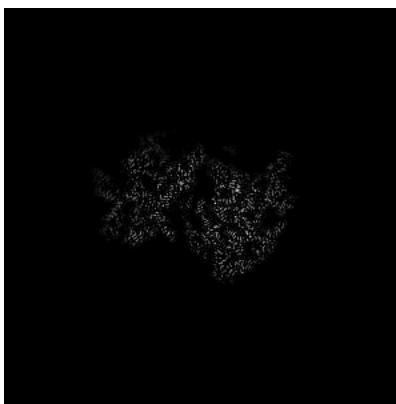
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

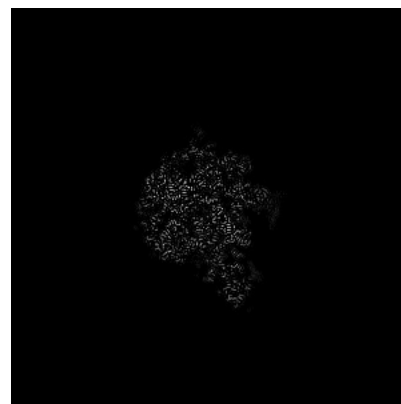
6.3.1 Primary map



X Index: 306



Y Index: 261

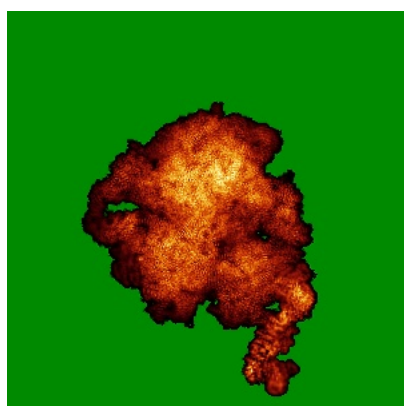


Z Index: 341

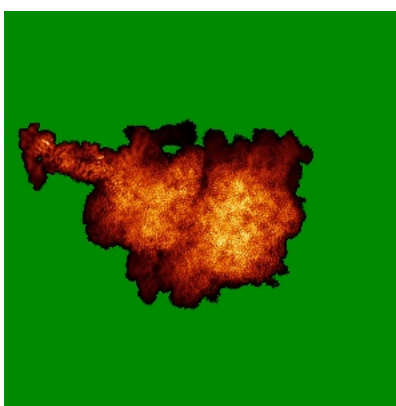
The images above show the largest variance slices of the map in three orthogonal directions.

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

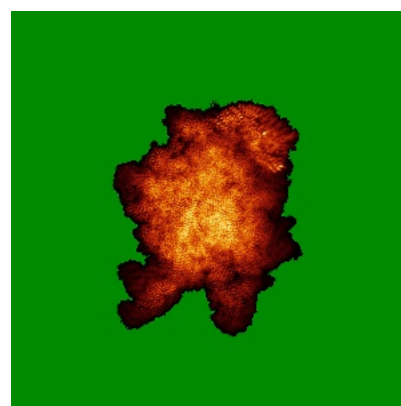
6.4.1 Primary map



X



Y

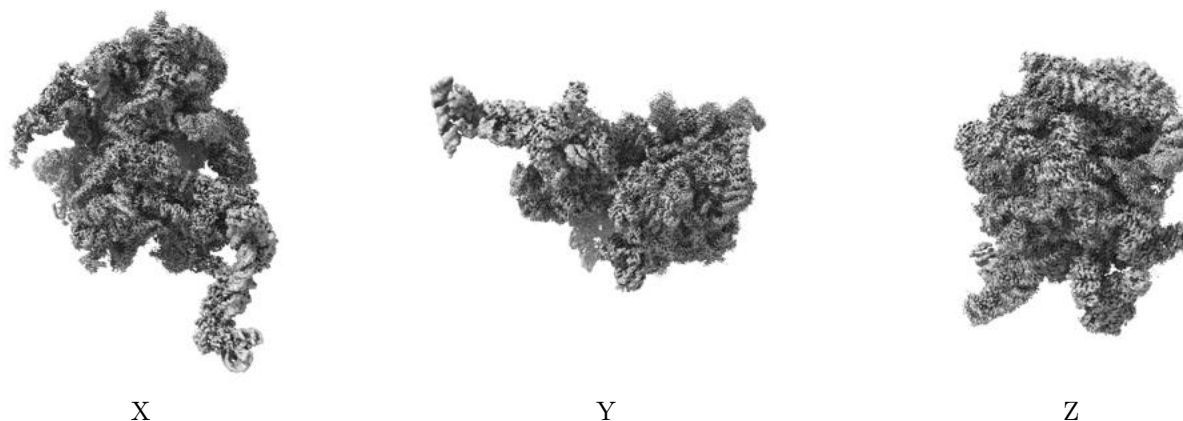


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0854. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

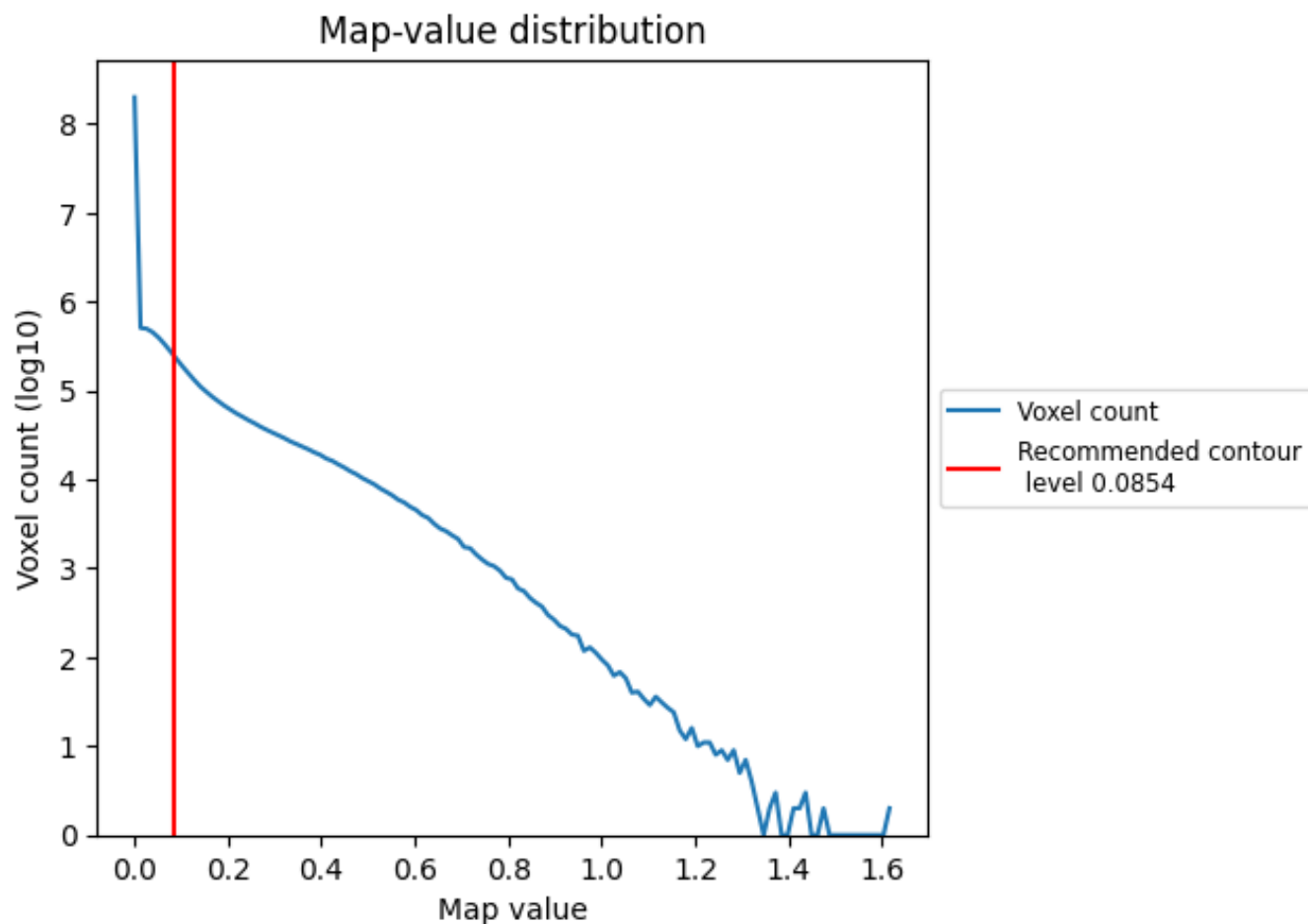
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

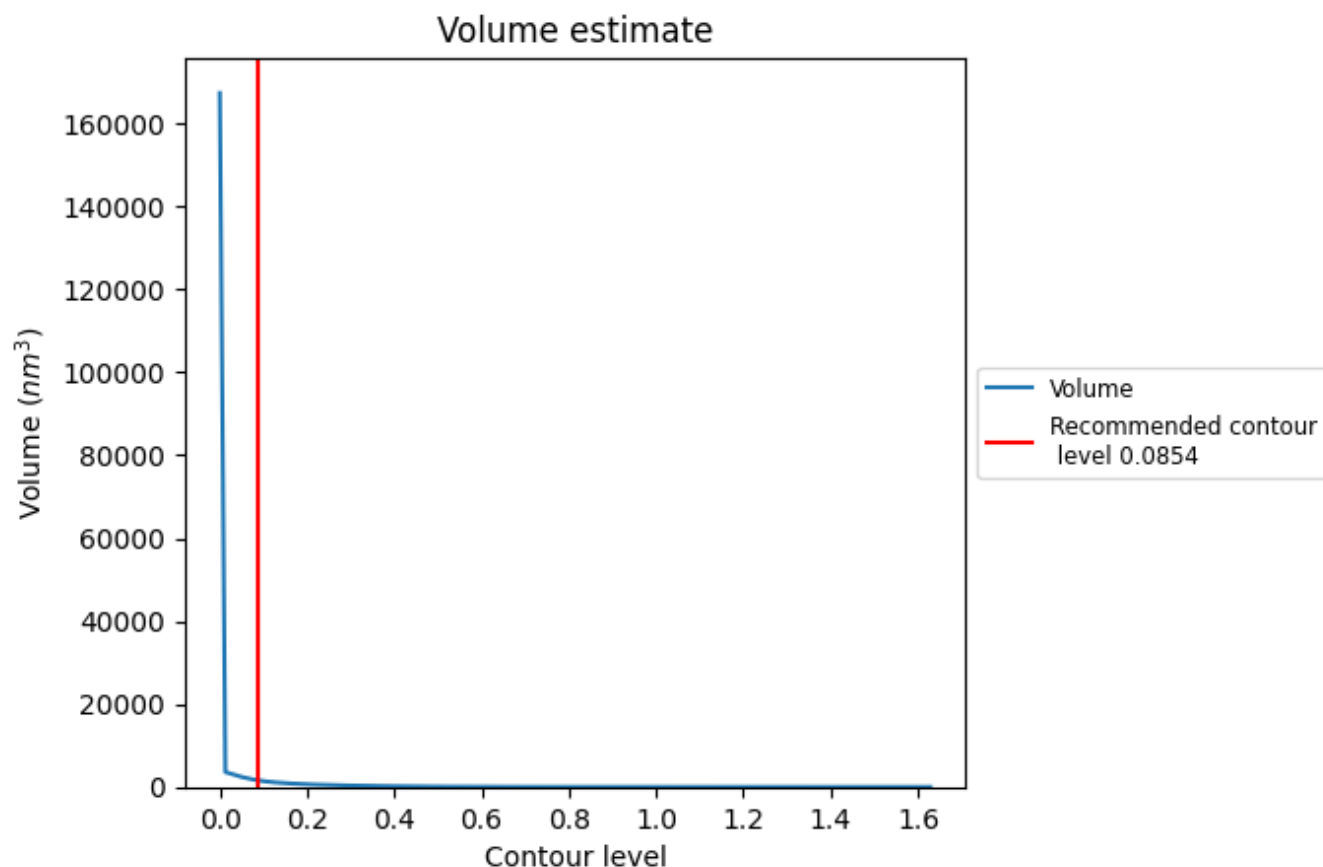
This section contains the results of statistical analysis of the map.

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.

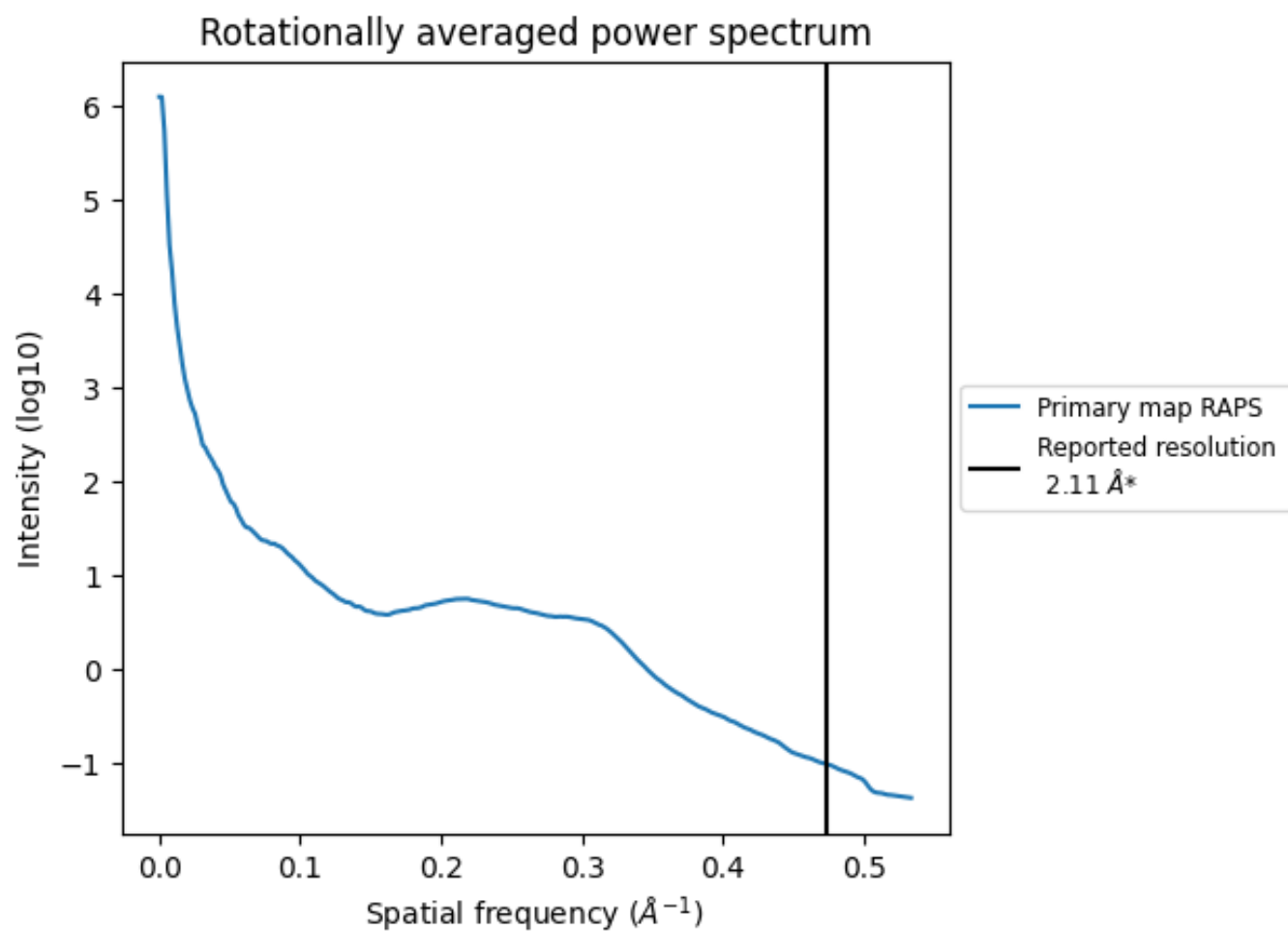
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1634 nm^3 ; this corresponds to an approximate mass of 1476 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 0.474 Å⁻¹

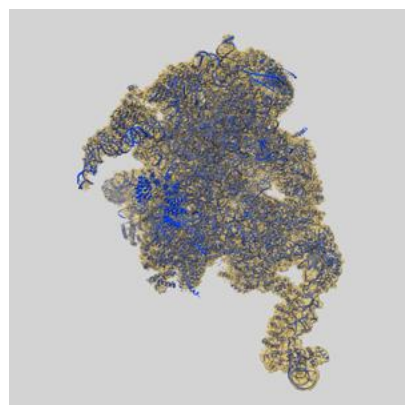
8 Fourier-Shell correlation

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

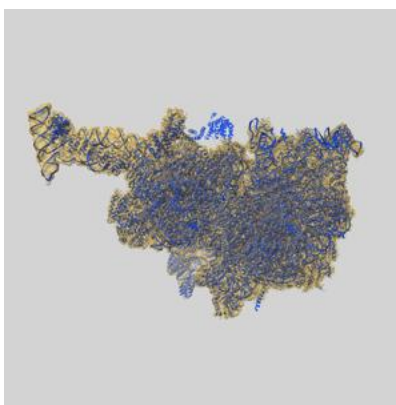
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51718 and PDB model 9GYT. Per-residue inclusion information can be found in section [3](#) on page [26](#).

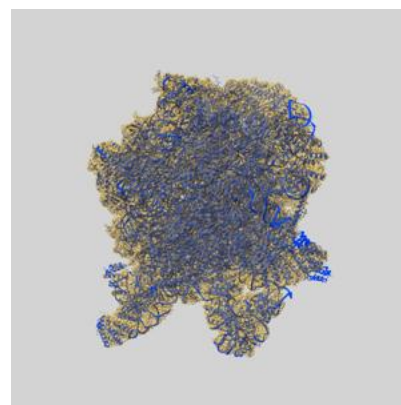
9.1 Map-model overlay [i](#)



X



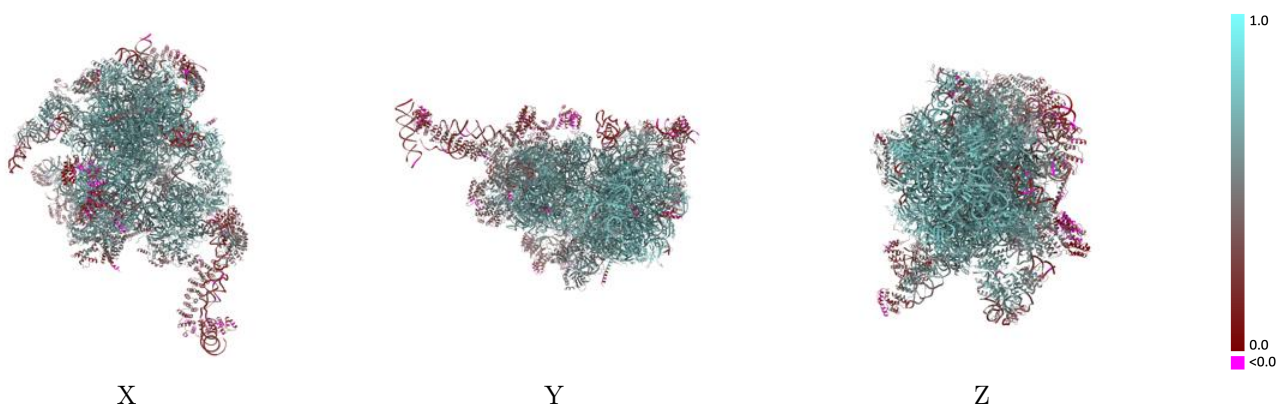
Y



Z

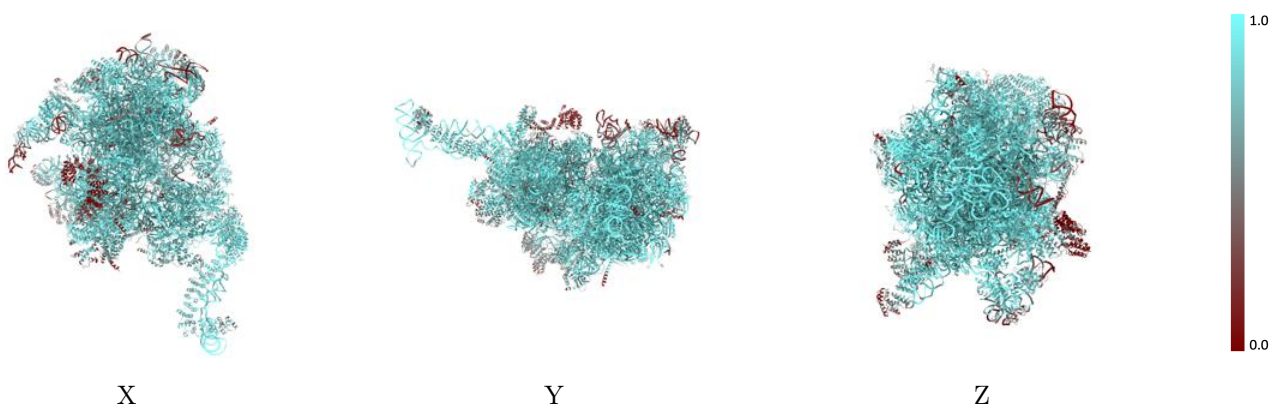
The images above show the 3D surface view of the map at the recommended contour level 0.0854 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



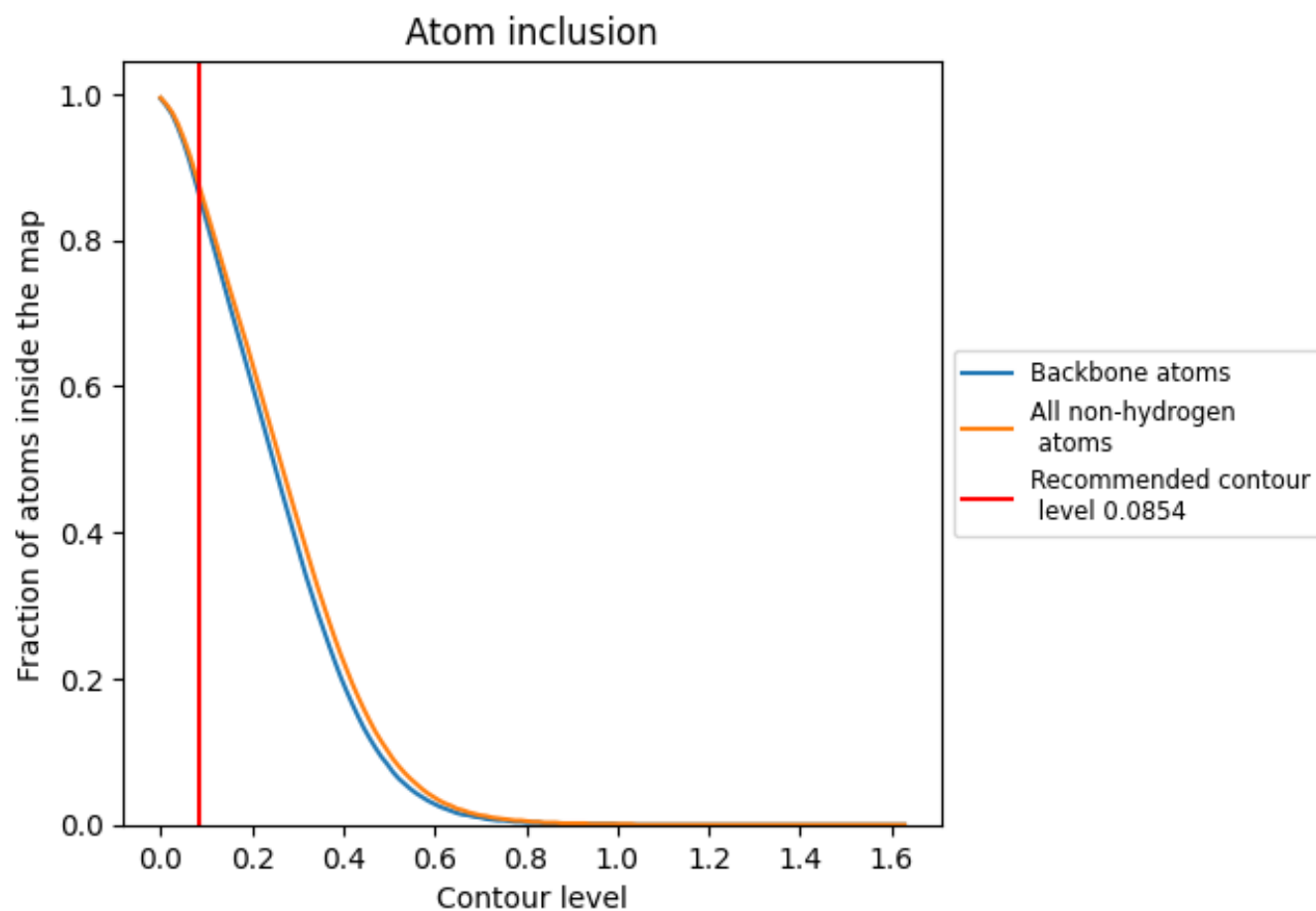
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0854).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 87% 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 (0.0854) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8730	 0.5810
1	 0.9140	 0.6380
1B	 0.9310	 0.6780
1C	 0.8420	 0.5920
1D	 0.9590	 0.7210
1E	 0.9700	 0.7220
1F	 0.9040	 0.6440
1G	 0.9160	 0.5480
1H	 0.8000	 0.5810
1I	 0.7430	 0.4950
1J	 0.6340	 0.4180
1K	 0.9110	 0.6820
1L	 0.9480	 0.7120
1M	 0.9510	 0.6950
1N	 0.9180	 0.6650
1O	 0.9740	 0.7340
1P	 0.9630	 0.6850
1Q	 0.9270	 0.6930
1R	 0.9920	 0.7440
1S	 0.9270	 0.7020
1T	 0.9730	 0.7250
1U	 0.9160	 0.6810
1V	 0.9540	 0.6840
1W	 0.6620	 0.4450
1X	 0.8900	 0.5470
1Y	 0.8530	 0.6500
1Z	 0.8660	 0.6270
1a	 0.9500	 0.7110
1b	 0.9630	 0.7110
1c	 0.7440	 0.5150
1d	 0.9780	 0.7300
1e	 0.9150	 0.6870
1f	 0.9970	 0.7550
1g	 0.9680	 0.7190
1h	 0.9770	 0.6650



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Chain	Atom inclusion	Q-score
1i	 0.8650	 0.6140
1j	 0.9600	 0.7060
1k	 0.9750	 0.7230
1l	 0.8370	 0.5930
1m	 0.7710	 0.4910
1o	 0.7110	 0.4740
1p	 0.8940	 0.6540
1q	 0.9500	 0.7200
1r	 0.9380	 0.6260
1s	 0.8990	 0.6380
1t	 0.8670	 0.5770
1u	 0.7150	 0.3900
1v	 0.7710	 0.5120
2	 0.9610	 0.5970
3	 0.9600	 0.6550
A	 0.9440	 0.6520
B	 0.8170	 0.5150
C	 0.8900	 0.5870
D	 0.8020	 0.5460
E	 0.9420	 0.6630
F	 0.8840	 0.5870
G	 0.9610	 0.6960
H	 0.8030	 0.5390
I	 0.9550	 0.6640
J	 0.8910	 0.5930
K	 0.9470	 0.6780
L	 0.9160	 0.6490
M	 0.9640	 0.6740
N	 0.9250	 0.6530
O	 0.9820	 0.6970
P	 0.9090	 0.6510
Q	 0.8910	 0.6360
R	 0.7870	 0.4500
S	 0.8530	 0.5930
T	 0.9800	 0.6850
U	 0.7060	 0.4060
V	 0.8600	 0.5930
W	 0.8980	 0.6200
X	 0.8350	 0.5370
Y	 0.8580	 0.6060
Z	 0.9150	 0.5670
a	 0.8090	 0.4920

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Chain	Atom inclusion	Q-score
b	 0.5470	 0.3570
c	 0.9150	 0.6460
d	 0.9270	 0.6350
e	 0.8990	 0.6140
f	 0.8660	 0.5550
g	 0.7740	 0.2500
h	 0.6800	 0.3890
i	 0.2500	 0.1700
j	 0.4440	 0.2560
k	 0.7440	 0.5090
l	 0.8270	 0.3330