



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 07:59 AM UTC

PDB ID : 7B7D / pdb_00007b7d
EMDB ID : EMD-12081
Title : Yeast 80S ribosome bound to eEF3 and A/A- and P/P-tRNAs
Authors : Ranjan, N.; Pochopien, A.A.; Wu, C.C.; Beckert, B.; Blanchet, S.; Green, R.;
Rodnina, M.V.; Wilson, D.N.
Deposited on : 2020-12-10
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

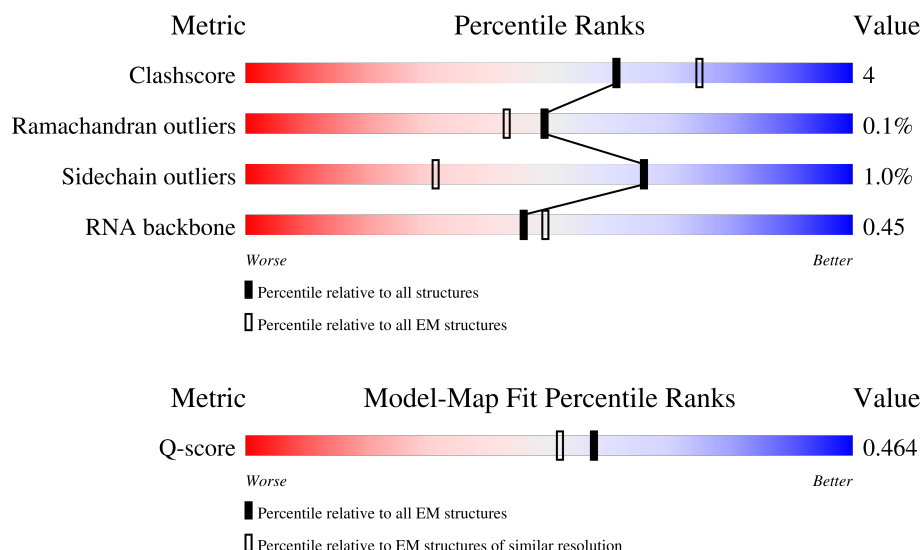
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.30 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	15087 (2.80 - 3.80)

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	2	1771	14% 56% 36% 7%
2	1	7	86% 14%
3	P	206	18% 80% 20%

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Mol	Chain	Length	Quality of chain
4	Q	232	
5	E	117	
6	R	216	
7	A	222	
8	S	258	
9	B	206	
10	T	228	
11	U	184	
12	V	198	
13	W	184	
14	C	92	
15	X	142	
16	D	121	
17	Y	150	
18	Z	127	
19	F	141	
20	G	125	
21	H	145	
22	I	143	
23	J	100	
24	a	87	
25	b	129	
26	c	144	
27	d	134	
28	K	82	

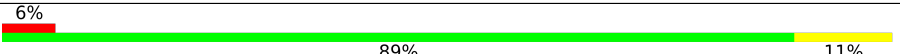
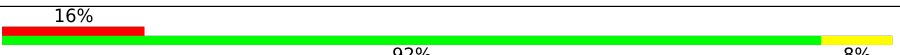
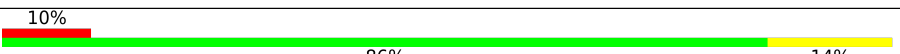
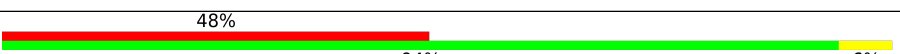
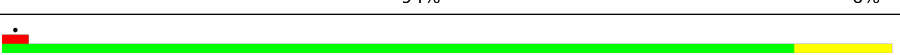
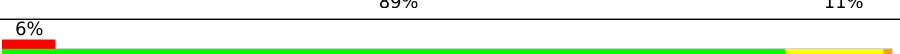
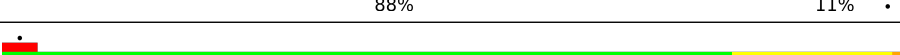
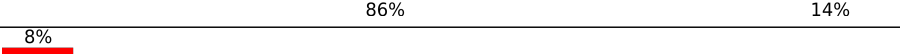
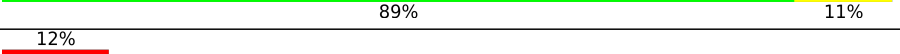
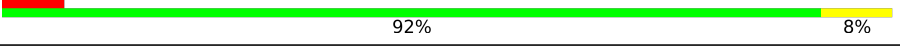
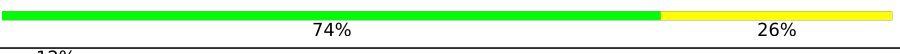
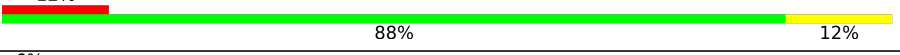
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Mol	Chain	Length	Quality of chain
29	e	97	
30	f	81	
31	M	53	
32	g	60	
33	N	73	
34	O	312	
35	L	63	
36	LA	3223	
37	LB	121	
38	LC	158	
39	LD	251	
40	LE	386	
41	LF	361	
42	LG	294	
43	LH	175	
44	LI	222	
45	LJ	233	
46	LK	191	
47	LL	218	
48	LM	169	
49	LN	193	
50	LO	136	
51	LP	203	
52	LQ	197	
53	LR	183	

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Mol	Chain	Length	Quality of chain
54	Lm	185	
55	Ln	188	
56	Lo	171	
57	Lp	159	
58	Lq	100	
59	Lr	136	
60	LS	126	
61	LT	121	
62	LU	125	
63	LV	135	
64	LW	148	
65	LX	58	
66	LY	96	
67	LZ	109	
68	La	127	
69	Lb	106	
70	Lc	112	
71	Ld	119	
72	Le	99	
73	Lf	81	
74	Lg	77	
75	Lh	50	
76	Li	52	
77	Lj	25	
78	Lk	103	

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Mol	Chain	Length	Quality of chain
79	Ll	91	5% 88% 12%
80	Sm	75	59% 63% 36%
80	Sn	75	16% 60% 35% 5%
81	EF	1044	30% 76% 17% 6%

2 Entry composition

There are 82 unique types of molecules in this entry. The entry contains 211144 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1771	Total	C	N	O	P	0	0
			37739	16872	6683	12413	1771		

- Molecule 2 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	7	Total	C	N	O	P	0	0
			149	67	26	49	7		

- Molecule 3 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	P	206	Total	C	N	O	S	0	0
			1603	1030	284	287	2		

- Molecule 4 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Q	226	Total	C	N	O	S	0	0
			1798	1139	330	325	4		

- Molecule 5 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	117	Total	C	N	O	S	0	0
			916	583	171	155	7		

- Molecule 6 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	R	216	Total	C	N	O	S	0	0
			1626	1042	287	295	2		

- Molecule 7 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	222	Total	C	N	O	S	0	0
			1729	1098	312	313	6		

- Molecule 8 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	S	258	Total	C	N	O	S	0	0
			2056	1308	387	358	3		

- Molecule 9 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	206	Total	C	N	O	S	0	0
			1605	1005	299	298	3		

- Molecule 10 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	T	228	Total	C	N	O	S	0	0
			1815	1138	351	323	3		

- Molecule 11 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	U	184	Total	C	N	O	S	0	0
			1473	946	263	264			

- Molecule 12 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	V	187	Total	C	N	O	S	0	0
			1476	916	295	263	2		

- Molecule 13 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	W	184	Total	C	N	O	S	0	0
			1479	935	285	258	1		

- Molecule 14 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	C	92	Total	C	N	O	S	0	0
			752	487	122	141	2		

- Molecule 15 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	X	142	Total	C	N	O	S	0	0
			1142	733	217	189	3		

- Molecule 16 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	D	121	Total	C	N	O	S	0	0
			875	551	153	169	2		

- Molecule 17 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Y	150	Total	C	N	O	S	0	0
			1192	759	224	207	2		

- Molecule 18 is a protein called 40S ribosomal protein S14-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Z	127	Total	C	N	O	S	0	0
			923	568	185	167	3		

- Molecule 19 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	F	141	Total	C	N	O	0	0
			1105	708	203	194		

- Molecule 20 is a protein called 40S ribosomal protein S17-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	G	121	Total	C	N	O	S	0	0
			948	596	179	171	2		

- Molecule 21 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	H	145	Total	C	N	O	S	0	0
			1188	741	237	208	2		

- Molecule 22 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	I	143	Total	C	N	O	S	0	0
			1112	694	208	208	2		

- Molecule 23 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	J	100	Total	C	N	O	S	0	0
			797	506	144	146	1		

- Molecule 24 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	87	Total	C	N	O	S	0	0
			673	415	125	131	2		

- Molecule 25 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	129	Total	C	N	O	S	0	0
			1021	650	188	180	3		

- Molecule 26 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	144	Total	C	N	O	S	0	0
			1121	708	220	191	2		

- Molecule 27 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	d	134	Total	C	N	O	0	0
			1073	676	208	189		

- Molecule 28 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	K	82	Total	C	N	O	0	0
			651	416	123	112		

- Molecule 29 is a protein called 40S ribosomal protein S26-B.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	e	97	Total	C	N	O	S	0
			765	473	160	127	5	0

- Molecule 30 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	f	81	Total	C	N	O	S	0
			610	382	110	113	5	0

- Molecule 31 is a protein called 40S ribosomal protein S29-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	M	53	Total	C	N	O	S	0
			442	274	92	72	4	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
32	g	60	Total	C	N	O	S	0
			472	298	97	76	1	0

- Molecule 33 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	N	73	Total	C	N	O	S	0
			556	352	105	95	4	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	97	ALA	LYS	conflict	UNP P05759

- Molecule 34 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	O	312	Total	C	N	O	S	0	0
			2383	1514	409	452	8		

- Molecule 35 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	L	63	Total	C	N	O	S	0	0
			491	303	96	91	1		

- Molecule 36 is a RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	LA	3223	Total	C	N	O	P	0	0
			68931	30790	12416	22502	3223		

- Molecule 37 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	LB	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 38 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	LC	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 39 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	LD	251	Total	C	N	O	S	0	0
			1899	1182	385	331	1		

- Molecule 40 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	LE	386	Total	C	N	O	S	0	0
			3075	1950	584	533	8		

- Molecule 41 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	LF	361	Total	C	N	O	S	0	0
			2748	1729	522	494	3		

- Molecule 42 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	LG	294	Total	C	N	O	S	0	0
			2351	1484	410	455	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
43	LH	167	Total	C	N	O	0	0
			1307	843	234	230		

- Molecule 44 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	LI	222	Total	C	N	O	S	0	0
			1784	1151	324	308	1		

- Molecule 45 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	LJ	233	Total	C	N	O	S	0	0
			1804	1151	323	327	3		

- Molecule 46 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	LK	191	Total	C	N	O	S	0	0
			1508	957	274	273	4		

- Molecule 47 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	LL	218	Total	C	N	O	S	0	0
			1764	1117	334	306	7		

- Molecule 48 is a protein called 60S ribosomal protein L11-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	LM	169	Total	C	N	O	S	0	0
			1346	843	252	247	4		

- Molecule 49 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	LN	193	Total	C	N	O		0	0
			1543	962	315	266			

- Molecule 50 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	LO	136	Total	C	N	O	S	0	0
			1053	675	199	177	2		

- Molecule 51 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	LP	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 52 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	LQ	197	Total	C	N	O	S	197	0
			1555	1003	289	262	1		

- Molecule 53 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	LR	183	Total	C	N	O		0	0
			1416	879	284	253			

- Molecule 54 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Lm	185	Total	C	N	O	S	0	0
			1441	908	290	241	2		

- Molecule 55 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	Ln	188	Total	C	N	O		
			1515	932	323	260	0	0

- Molecule 56 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	Lo	171	Total	C	N	O	S		
			1437	925	266	243	3	0	0

- Molecule 57 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Lp	159	Total	C	N	O	S		
			1272	802	245	221	4	0	0

- Molecule 58 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
58	Lq	100	Total	C	N	O		
			796	516	131	149	0	0

- Molecule 59 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Lr	136	Total	C	N	O	S		
			1003	628	189	179	7	0	0

- Molecule 60 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	LS	126	Total	C	N	O	S		
			836	525	165	145	1	0	0

- Molecule 61 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	LT	121	Total	C	N	O	S		
			964	620	169	173	2	0	0

- Molecule 62 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
62	LU	125	Total	C	N	O	0	0
			984	620	191	173		

- Molecule 63 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
63	LV	135	Total	C	N	O	0	0
			1080	701	199	180		

- Molecule 64 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	LW	148	Total	C	N	O	S	0	0
			1169	747	231	188	3		

- Molecule 65 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
65	LX	58	Total	C	N	O	0	0
			462	289	100	73		

- Molecule 66 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	LY	96	Total	C	N	O	S	0	0
			737	476	123	137	1		

- Molecule 67 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	LZ	109	Total	C	N	O	S	0	0
			876	556	167	152	1		

- Molecule 68 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	La	127	Total	C	N	O	S	0	0
			1013	642	205	165	1		

- Molecule 69 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Lb	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 70 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Lc	112	Total	C	N	O	S	0	0
			880	545	179	152	4		

- Molecule 71 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Ld	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 72 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Le	99	Total	C	N	O	S	0	0
			766	478	154	132	2		

- Molecule 73 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Lf	81	Total	C	N	O	S	0	0
			645	393	141	106	5		

- Molecule 74 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
74	Lg	77	Total	C	N	O	0	0
			612	391	115	106		

- Molecule 75 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Lh	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 76 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Li	52	Total	C	N	O	S	0	0
			410	254	86	65	5		

- Molecule 77 is a protein called 60S ribosomal protein L41-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Lj	25	Total	C	N	O	S	0	0
			229	139	62	27	1		

- Molecule 78 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Lk	103	Total	C	N	O	S	0	0
			824	517	167	135	5		

- Molecule 79 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Ll	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 80 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Sn	75	Total	C	N	O	P	0	0
			1606	716	297	518	75		
80	Sm	75	Total	C	N	O	P	0	0
			1605	716	297	517	75		

- Molecule 81 is a protein called Elongation factor 3A.

Mol	Chain	Residues	Atoms						AltConf	Trace
81	EF	977	Total	C	N	O	S	Se	0	0
			7479	4729	1294	1419	32	5		

There are 5 discrepancies between the modelled and reference sequences:

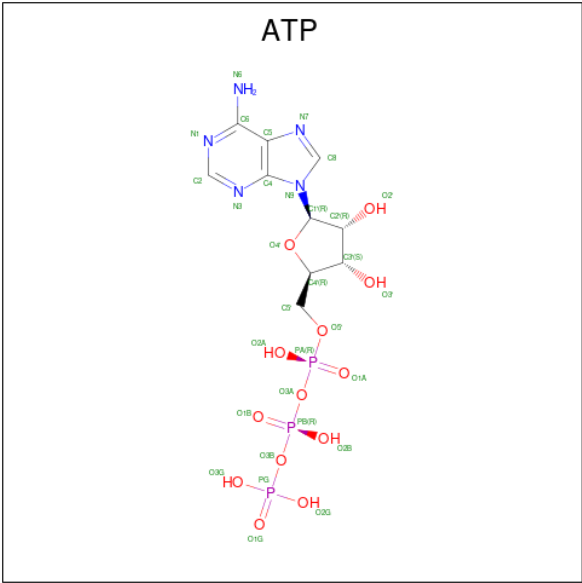
Chain	Residue	Modelled	Actual	Comment	Reference
EF	24	ASP	ASN	conflict	UNP P16521
EF	152	PHE	ILE	conflict	UNP P16521
EF	331	LEU	VAL	conflict	UNP P16521
EF	541	GLY	SER	conflict	UNP P16521

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Chain	Residue	Modelled	Actual	Comment	Reference
EF	542	SER	ALA	conflict	UNP P16521

- Molecule 82 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



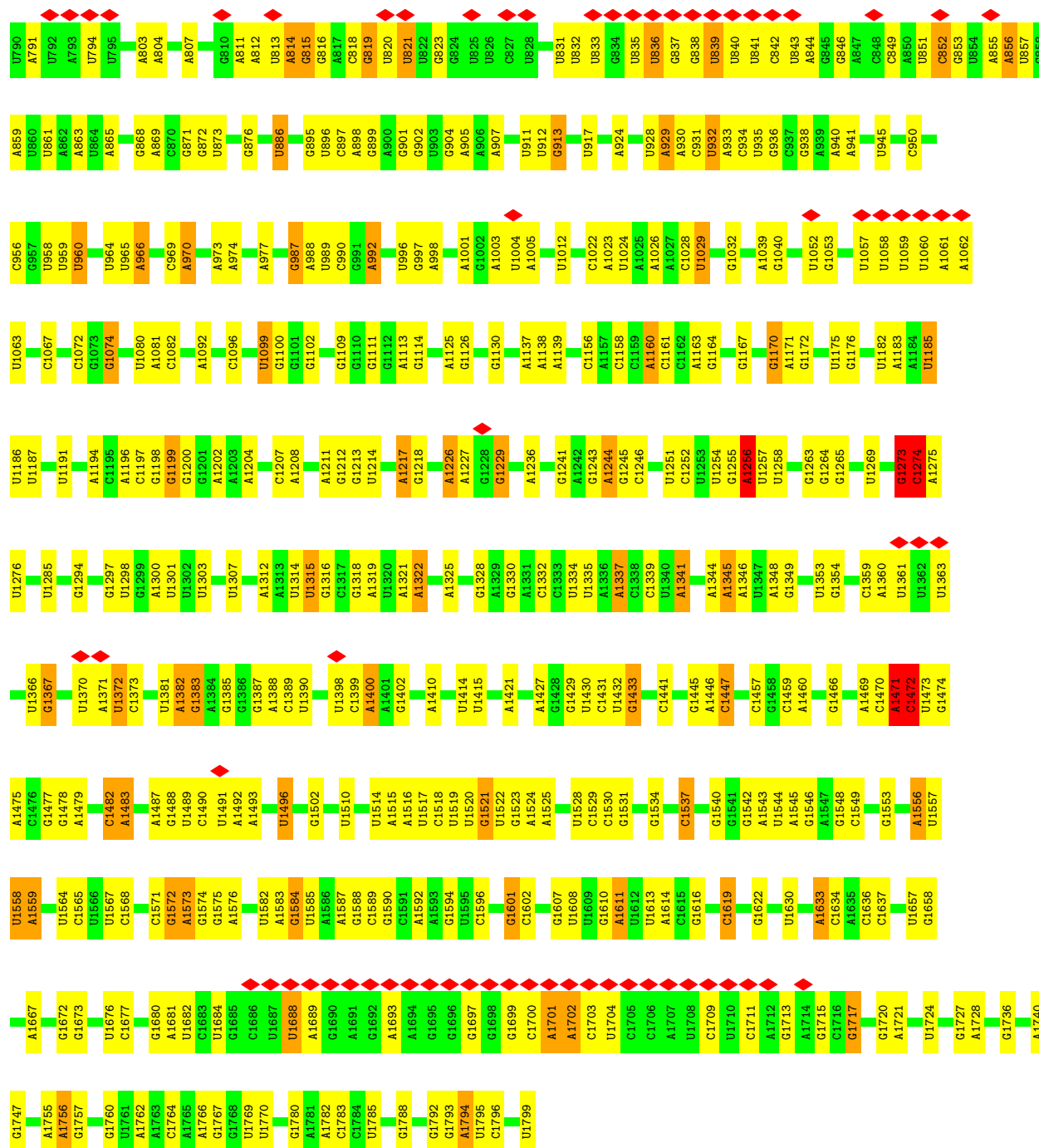
Mol	Chain	Residues	Atoms					AltConf
82	EF	1	Total	C	N	O	P	0
			31	10	5	13	3	
82	EF	1	Total	C	N	O	P	0
			31	10	5	13	3	

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.

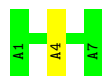
• Molecule 1: 18S rRNA





• Molecule 2: mRNA

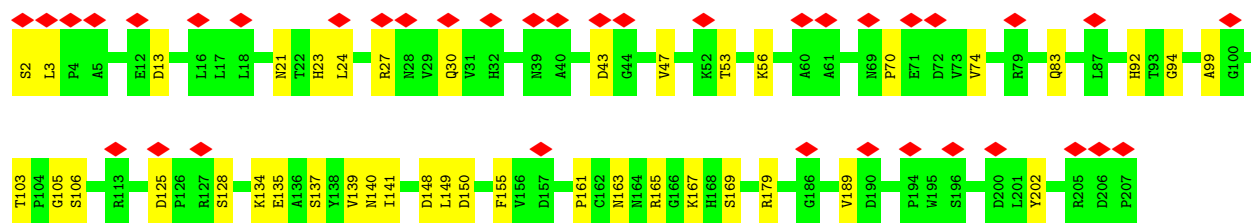
Chain 1:



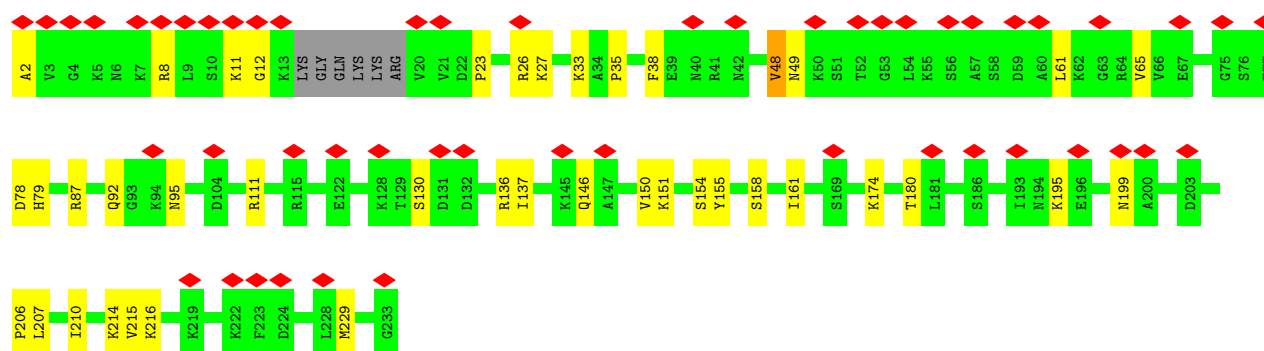
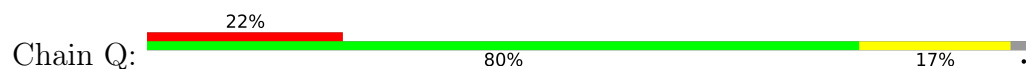
• Molecule 3: 40S ribosomal protein S0-A

Chain P:

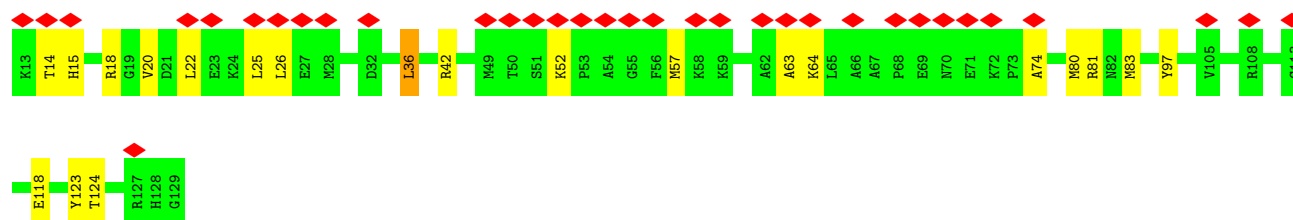
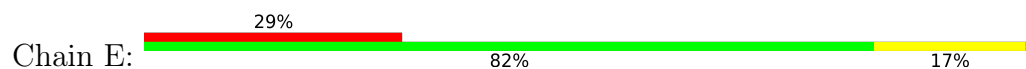




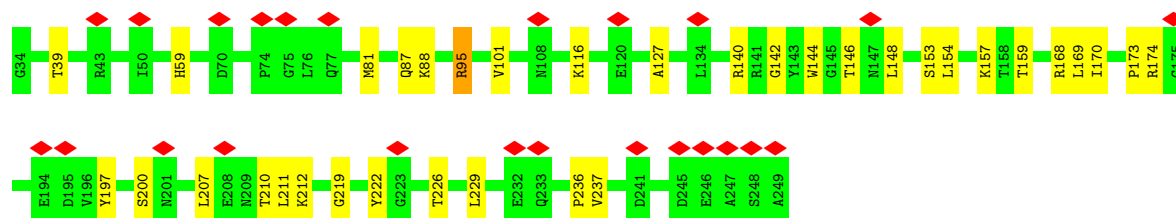
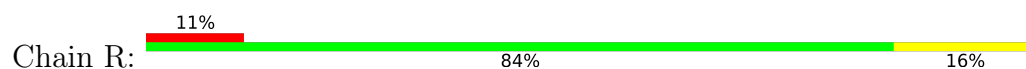
• Molecule 4: 40S ribosomal protein S1-A



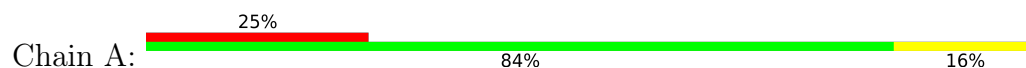
• Molecule 5: 40S ribosomal protein S15

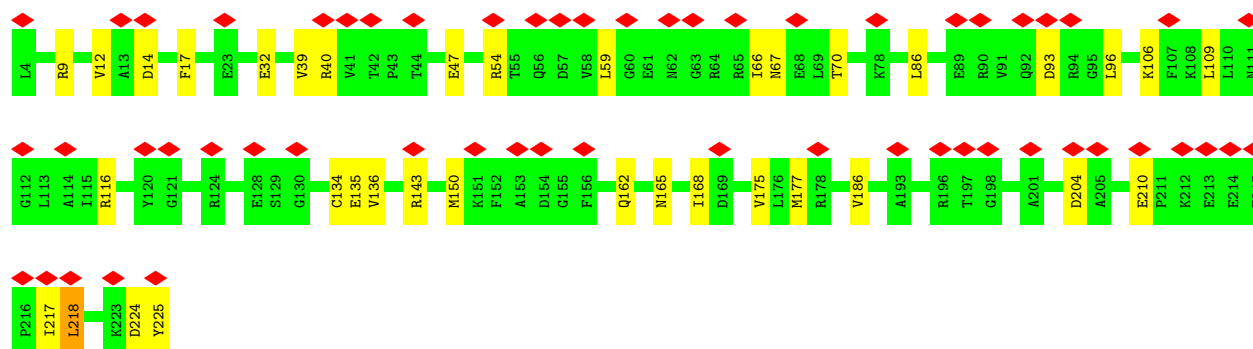


• Molecule 6: 40S ribosomal protein S2

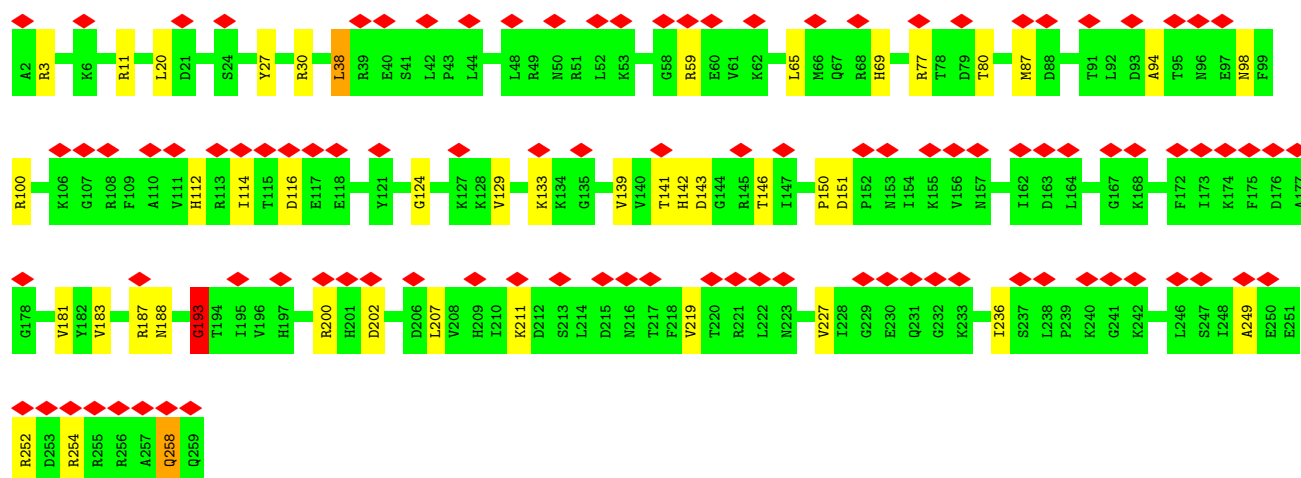
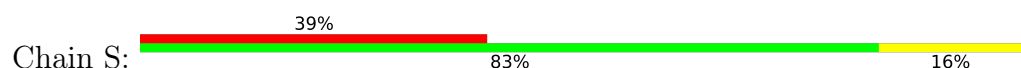


• Molecule 7: 40S ribosomal protein S3

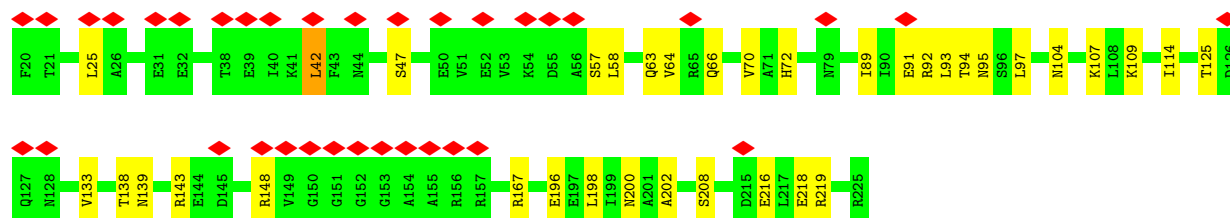
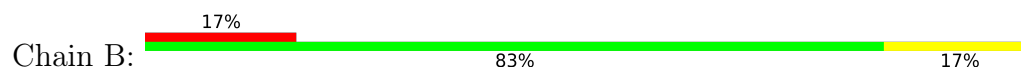




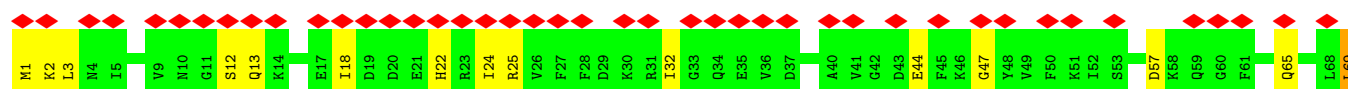
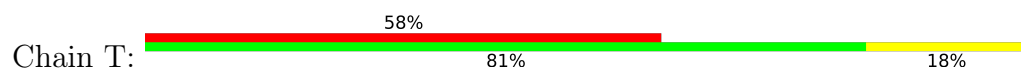
• Molecule 8: 40S ribosomal protein S4-A

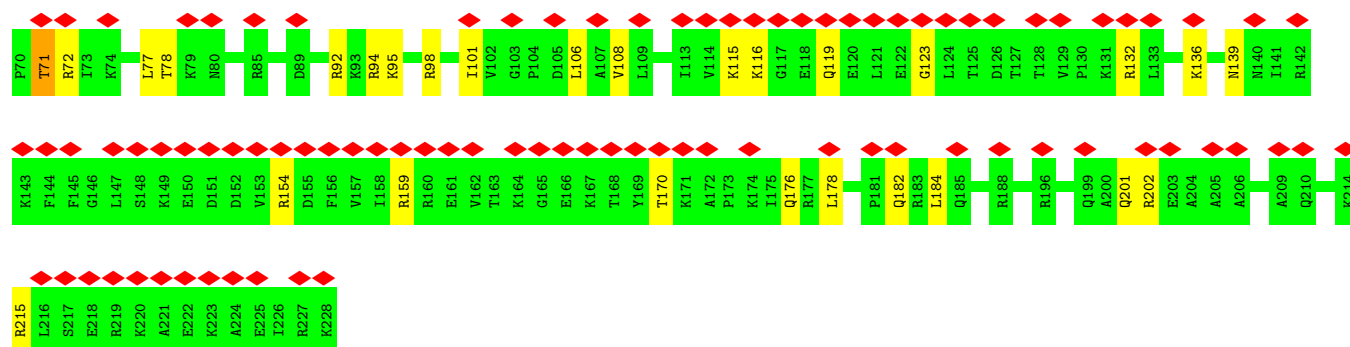


• Molecule 9: 40S ribosomal protein S5

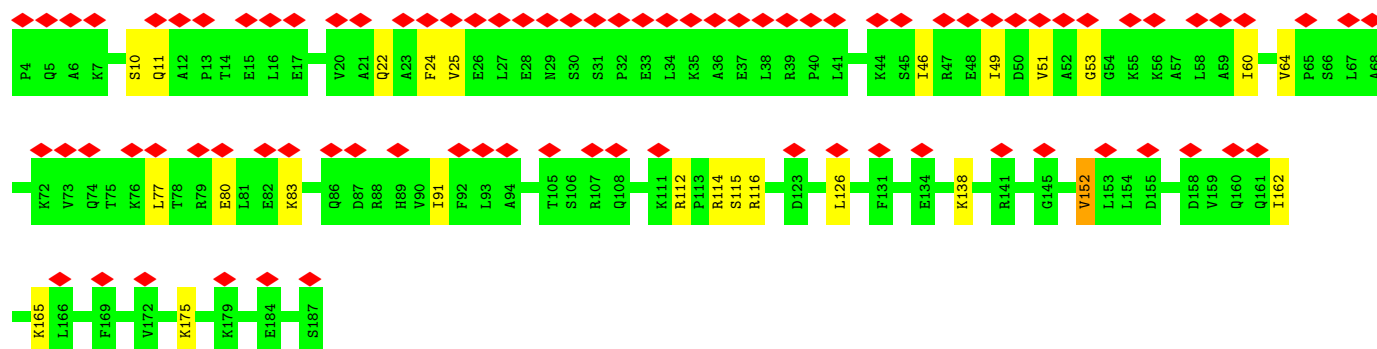
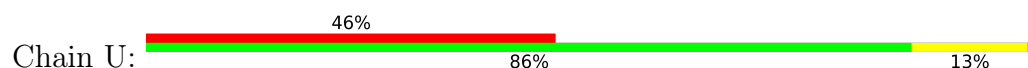


• Molecule 10: 40S ribosomal protein S6-A

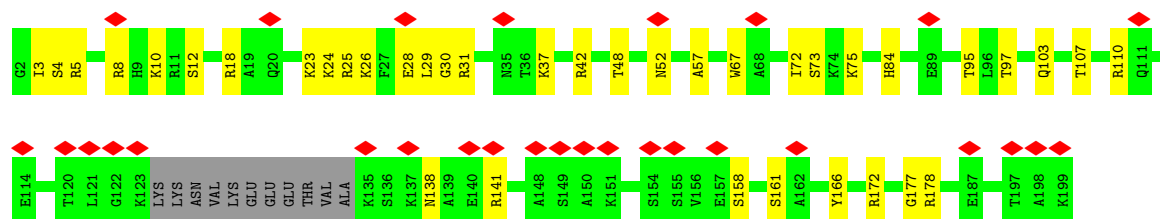
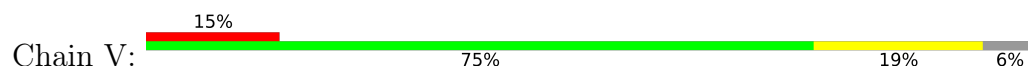




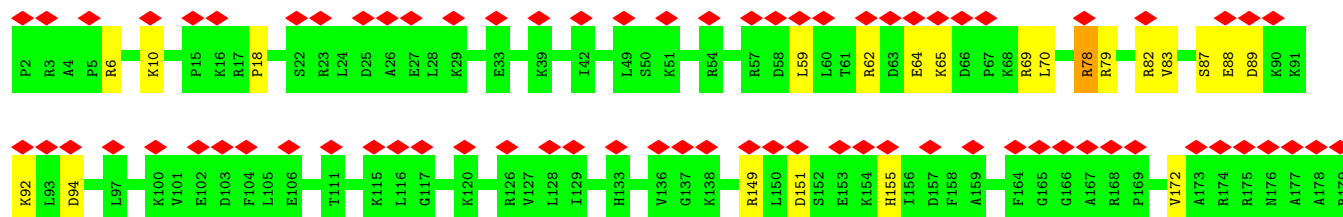
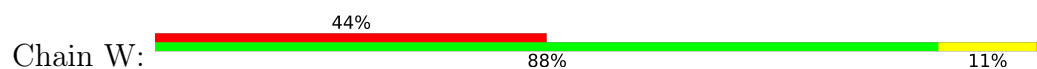
• Molecule 11: 40S ribosomal protein S7-A

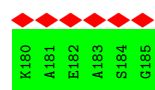


• Molecule 12: 40S ribosomal protein S8-A

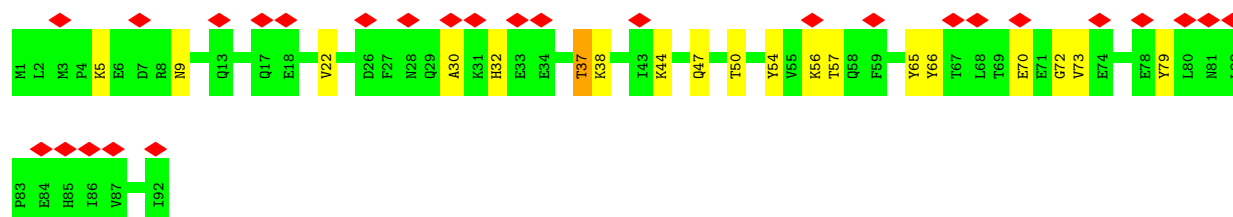
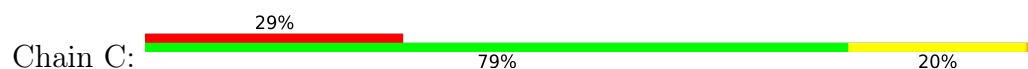


• Molecule 13: 40S ribosomal protein S9-A

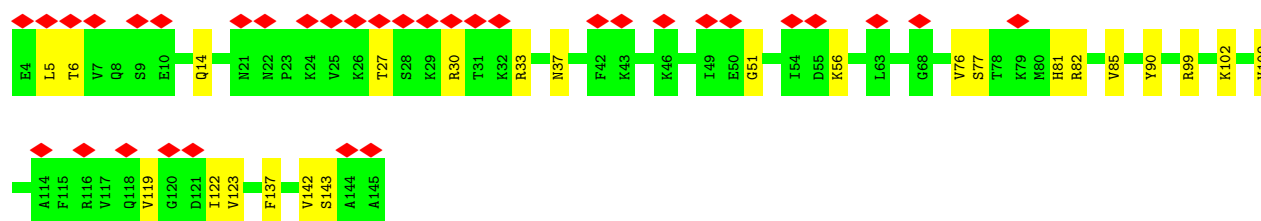
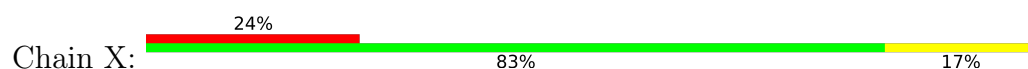




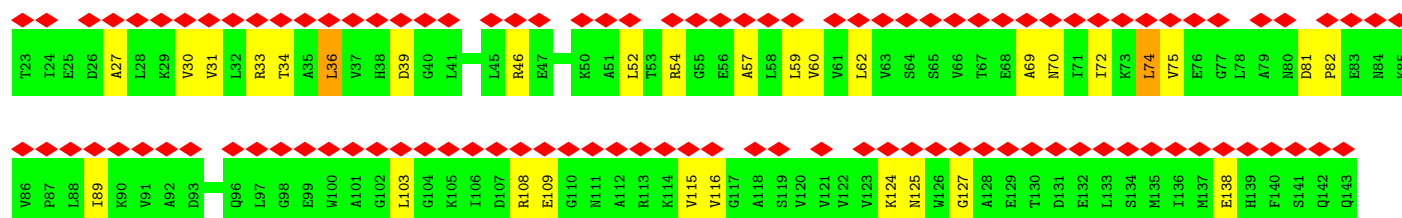
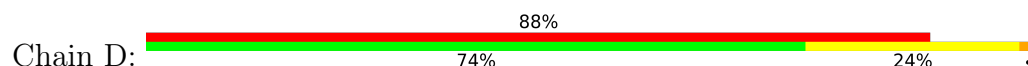
• Molecule 14: 40S ribosomal protein S10-A



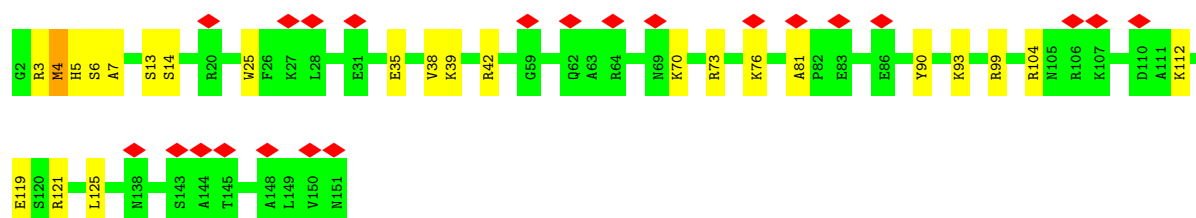
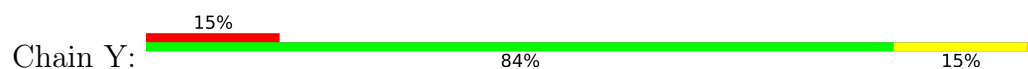
• Molecule 15: 40S ribosomal protein S11-A



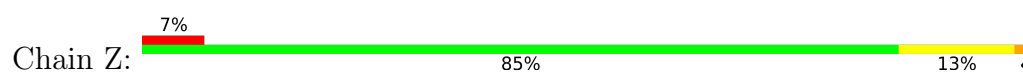
• Molecule 16: 40S ribosomal protein S12



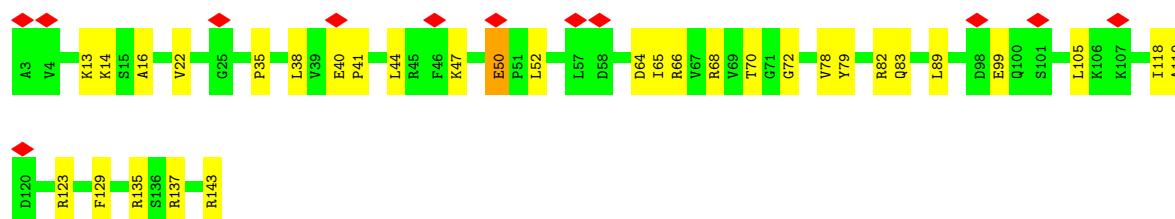
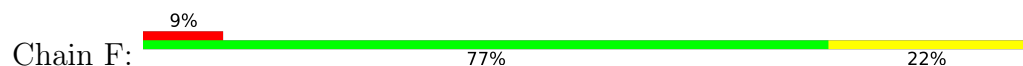
• Molecule 17: 40S ribosomal protein S13



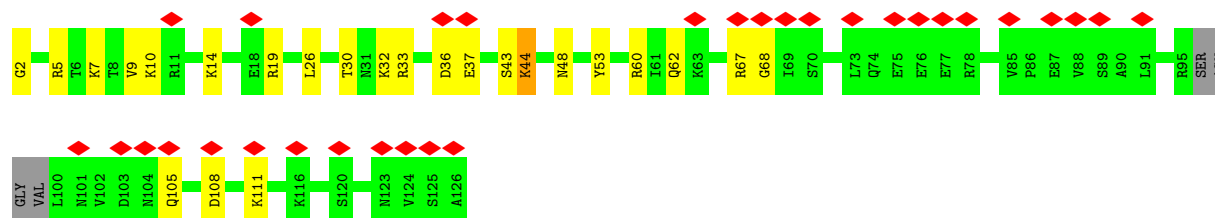
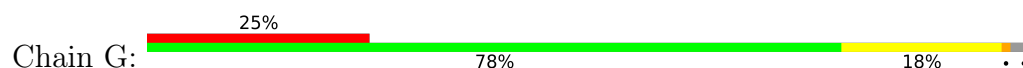
• Molecule 18: 40S ribosomal protein S14-B



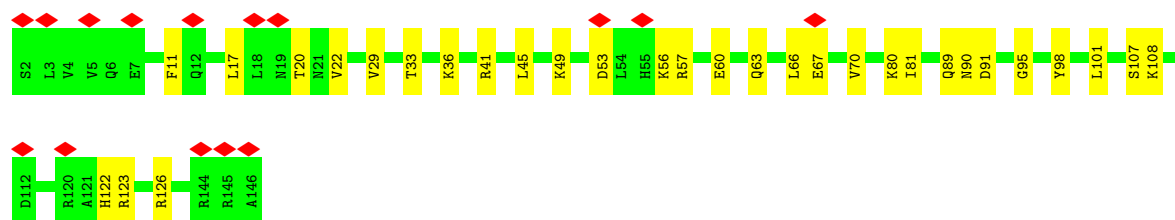
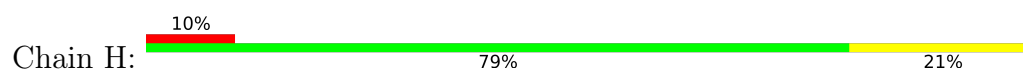
- Molecule 19: 40S ribosomal protein S16-A



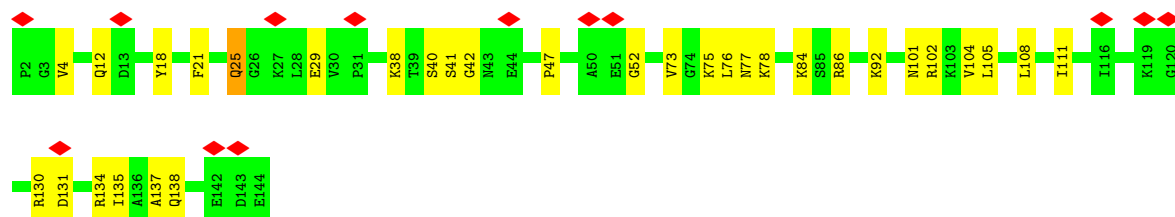
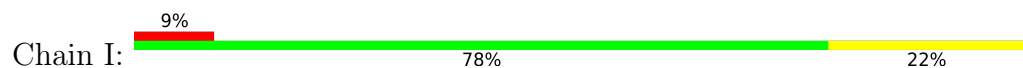
- Molecule 20: 40S ribosomal protein S17-B



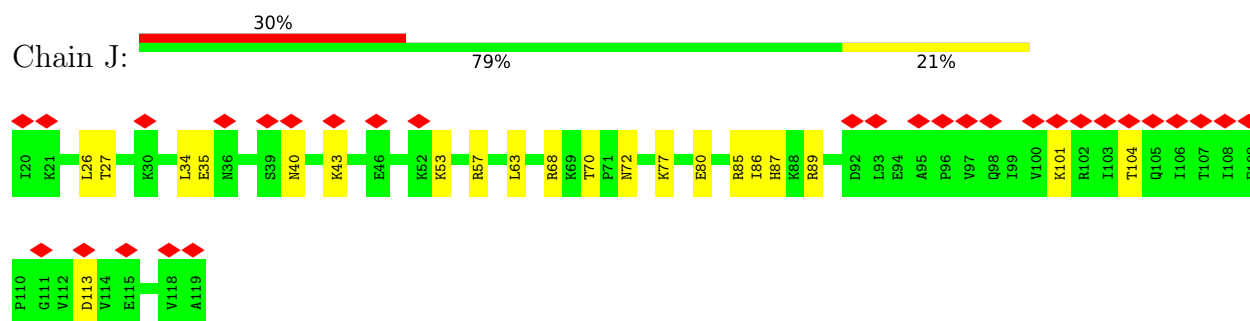
- Molecule 21: 40S ribosomal protein S18-A



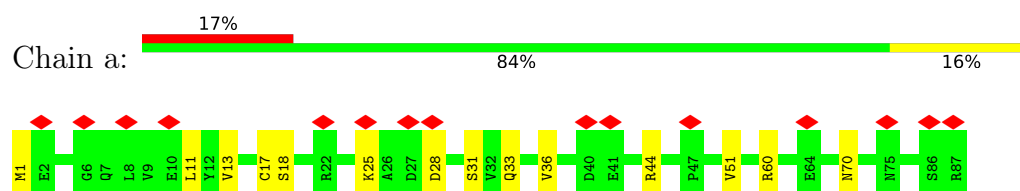
- Molecule 22: 40S ribosomal protein S19-A



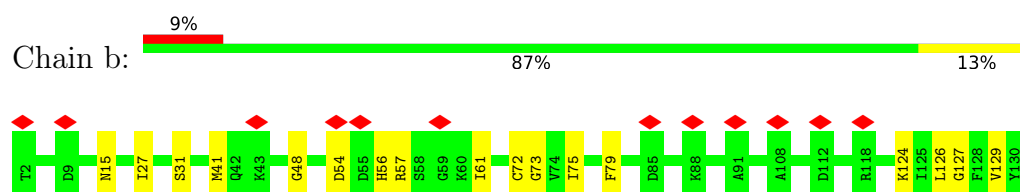
- Molecule 23: 40S ribosomal protein S20



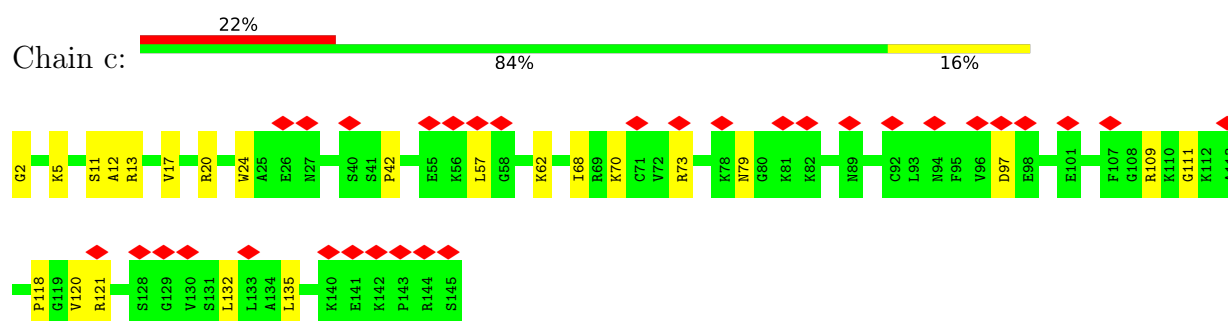
- Molecule 24: 40S ribosomal protein S21-A



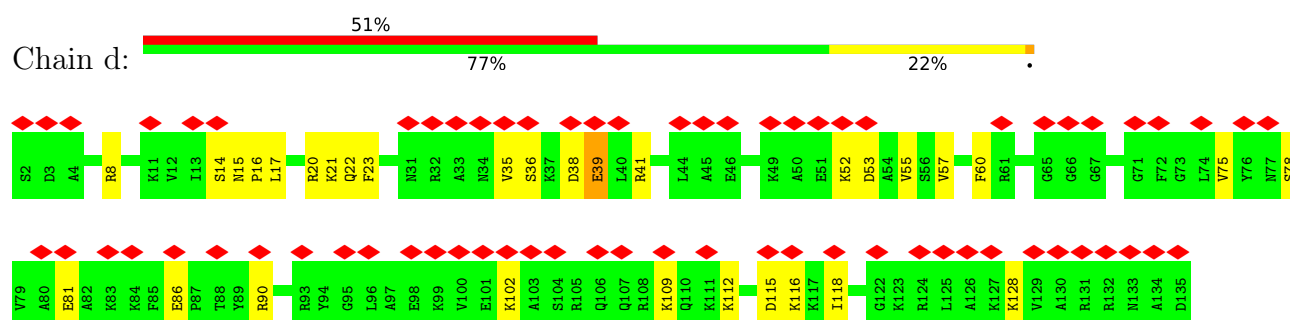
- Molecule 25: 40S ribosomal protein S22-A



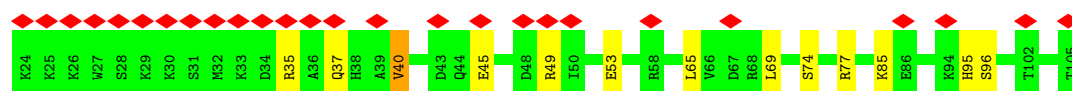
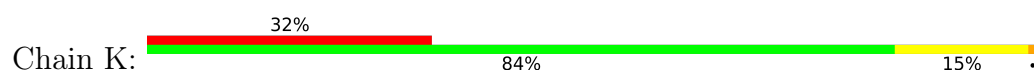
- Molecule 26: 40S ribosomal protein S23-A



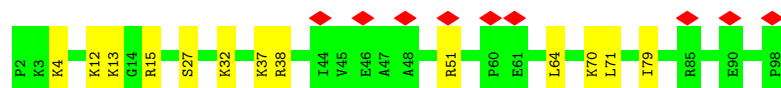
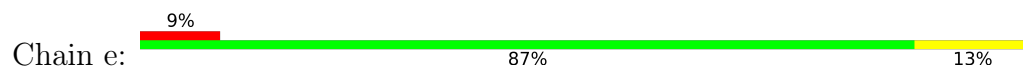
- Molecule 27: 40S ribosomal protein S24-A



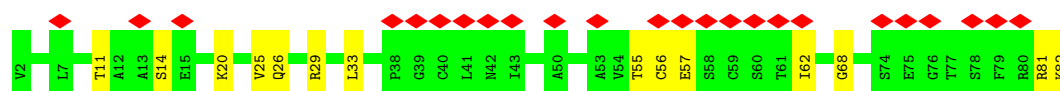
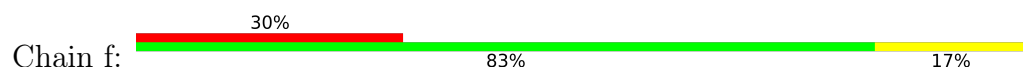
- Molecule 28: 40S ribosomal protein S25-A



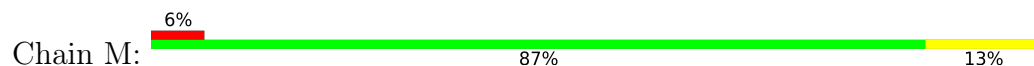
- Molecule 29: 40S ribosomal protein S26-B



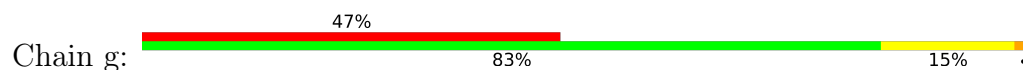
- Molecule 30: 40S ribosomal protein S27-A



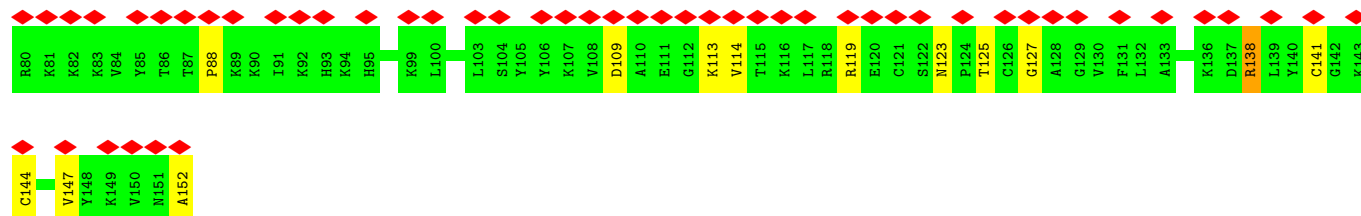
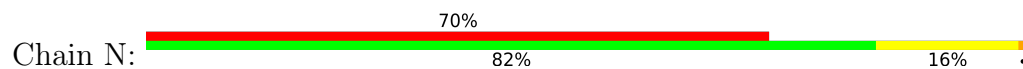
- Molecule 31: 40S ribosomal protein S29-A



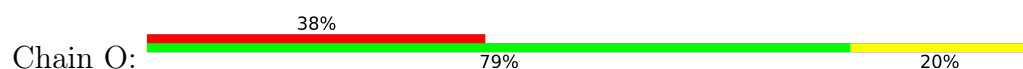
- Molecule 32: 40S ribosomal protein S30-A

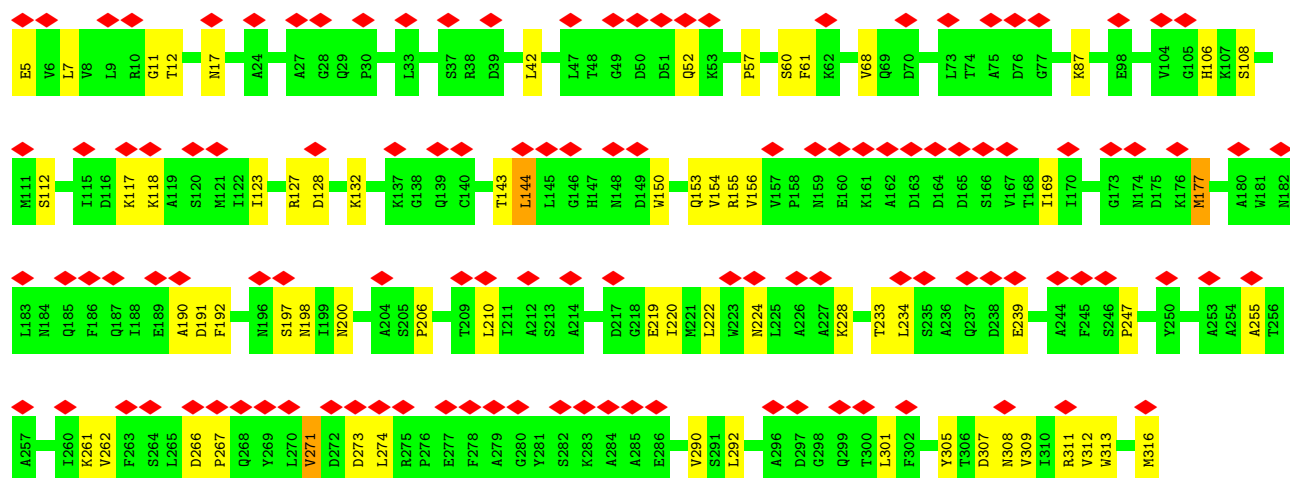


- Molecule 33: Ubiquitin-40S ribosomal protein S31

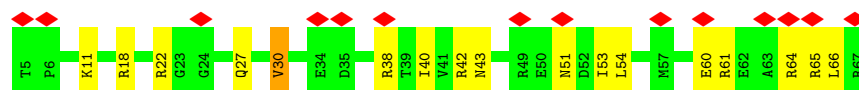
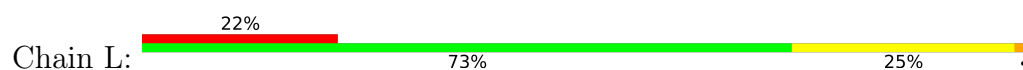


- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

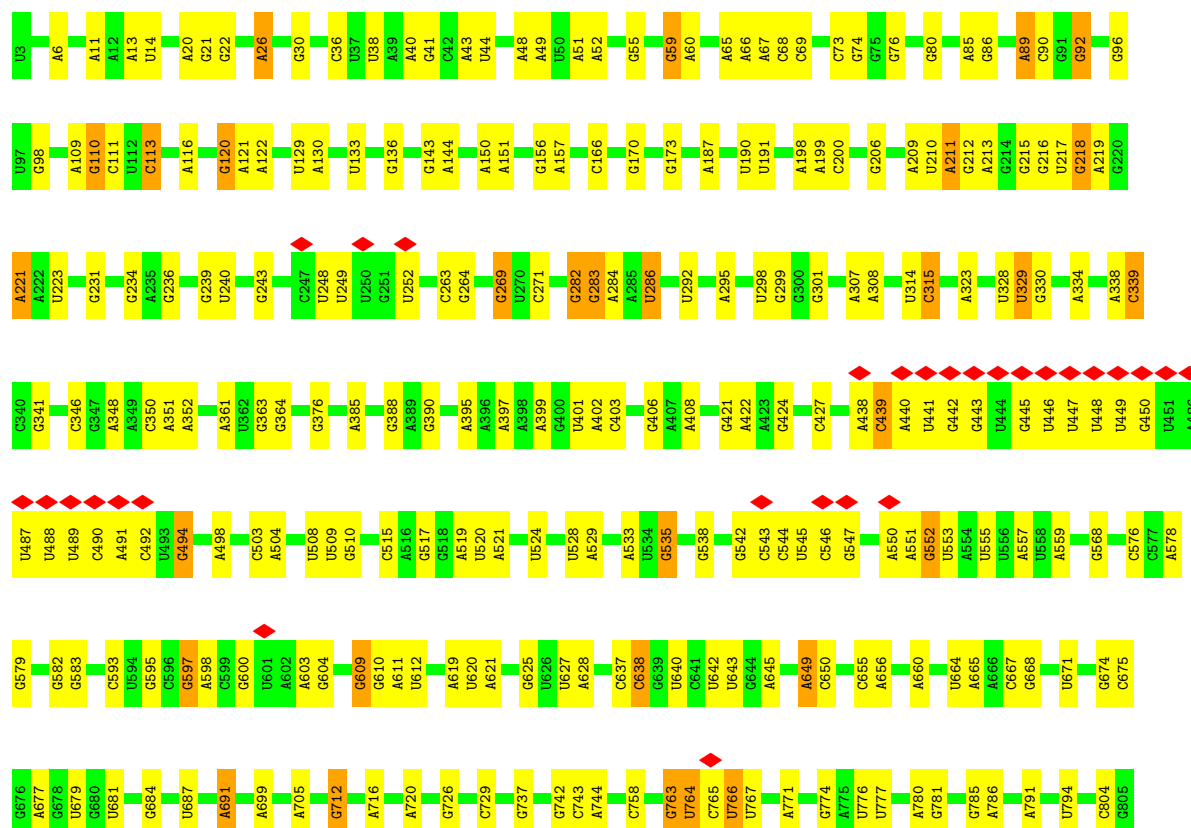


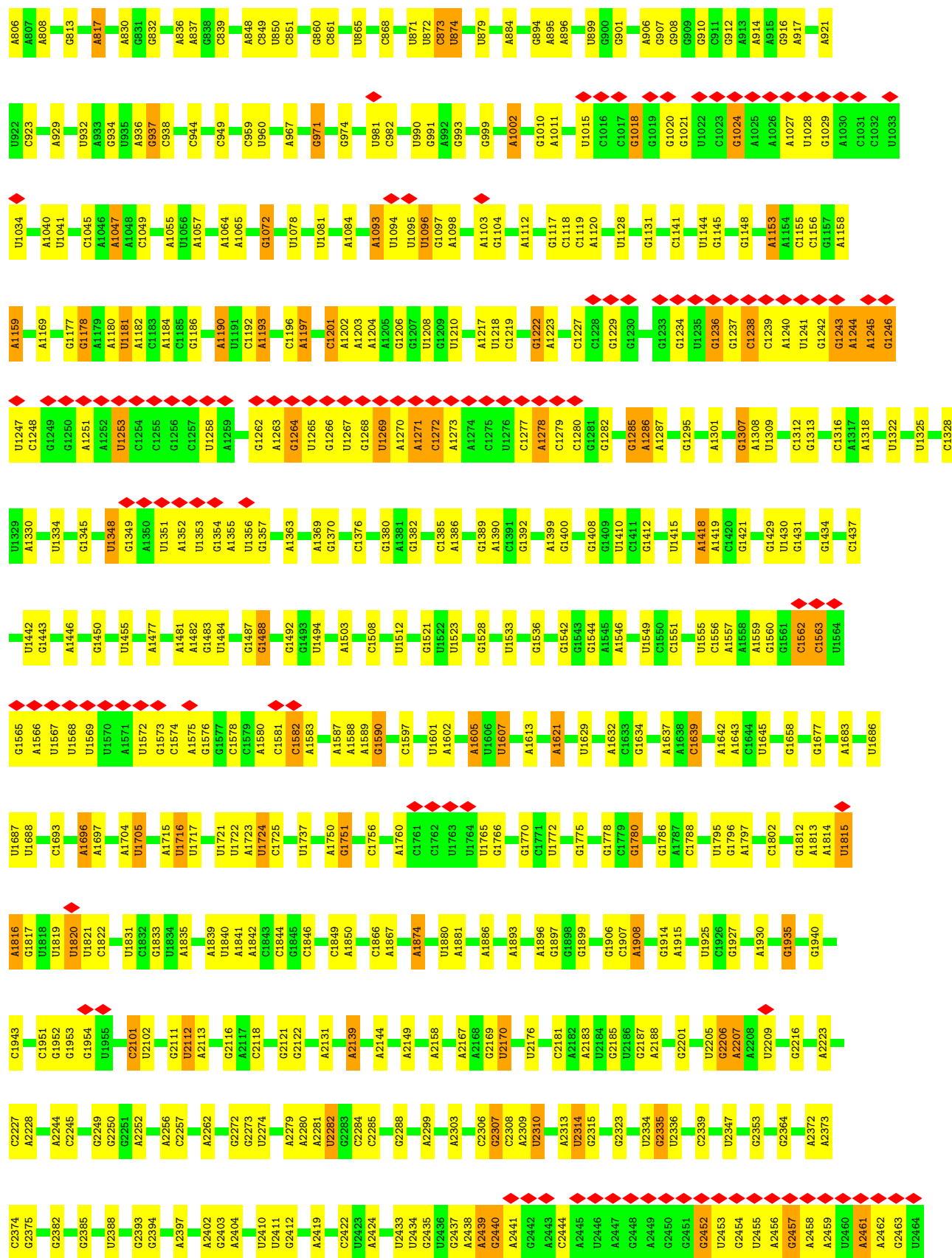


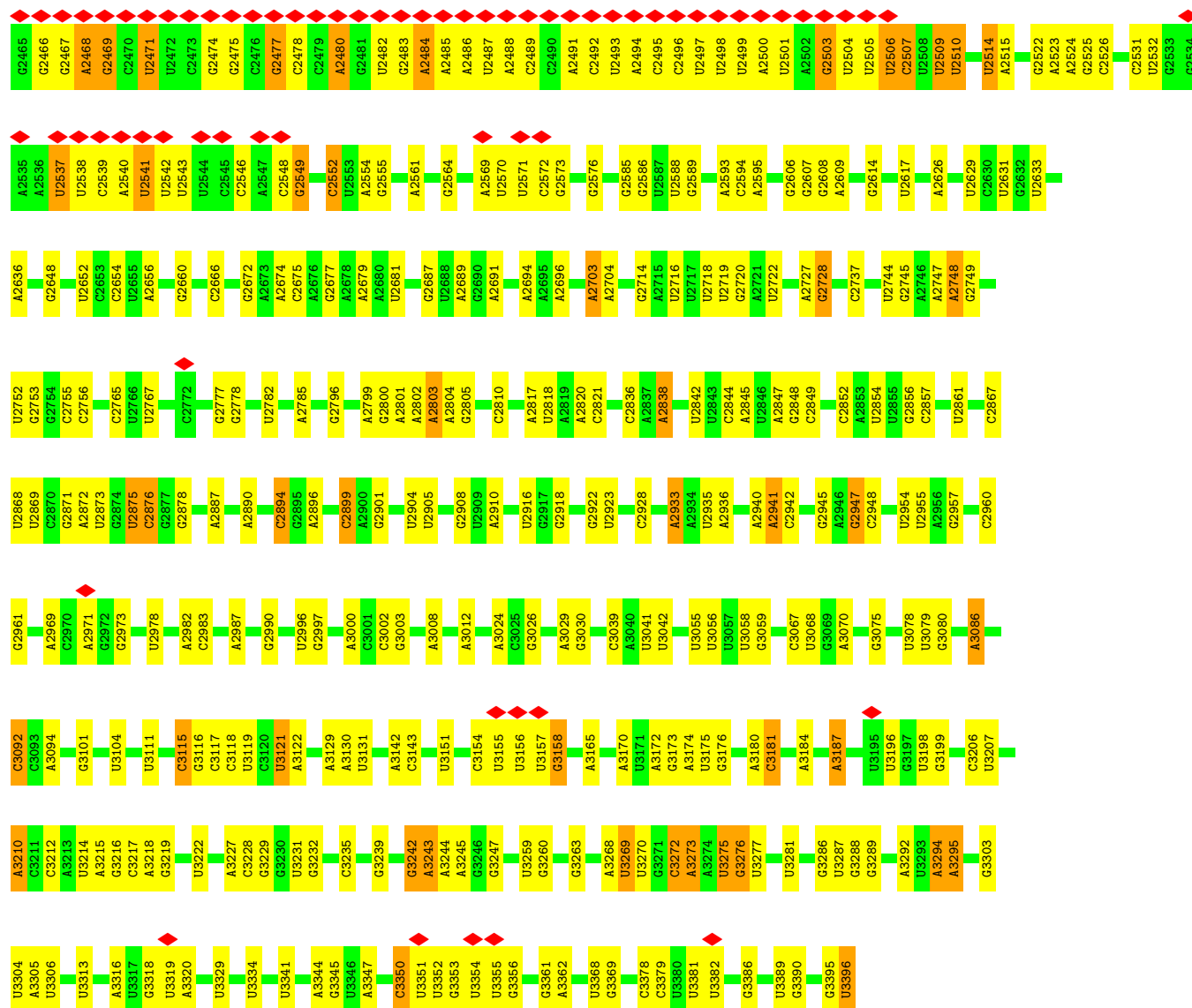
• Molecule 35: 40S ribosomal protein S28-A



• Molecule 36: 25S rRNA



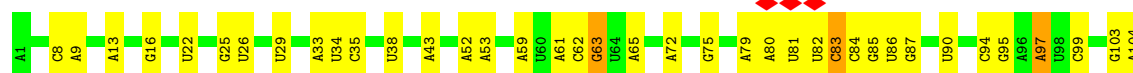




• Molecule 37: 5S rRNA

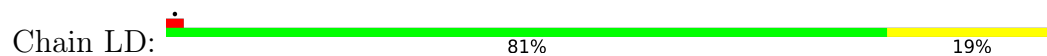


• Molecule 38: 5.8S rRNA

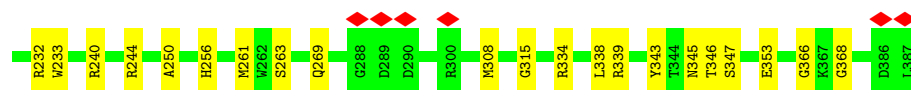
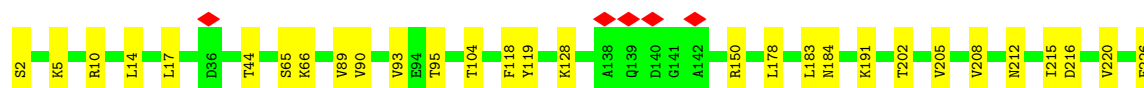
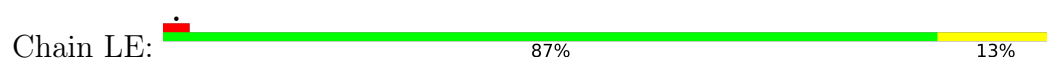




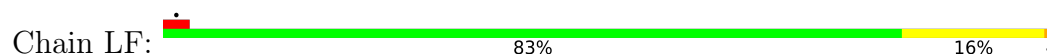
- Molecule 39: 60S ribosomal protein L2-A



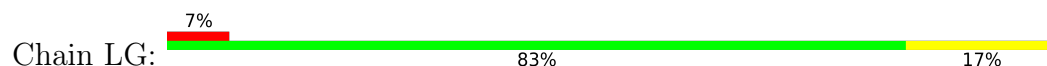
- Molecule 40: 60S ribosomal protein L3

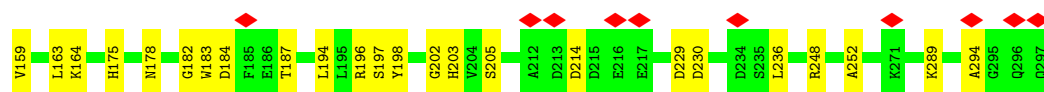


- Molecule 41: 60S ribosomal protein L4-A

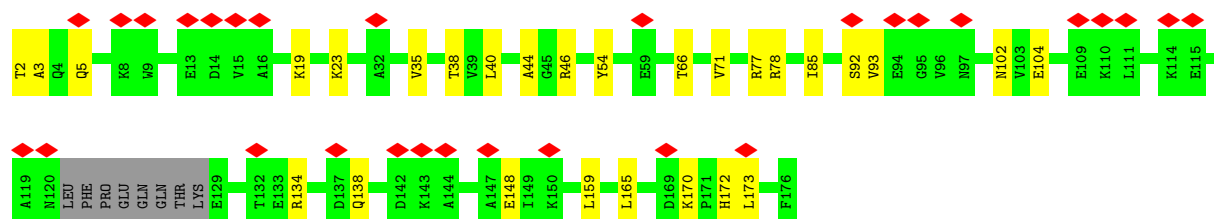
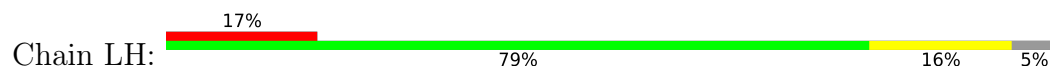


- Molecule 42: 60S ribosomal protein L5

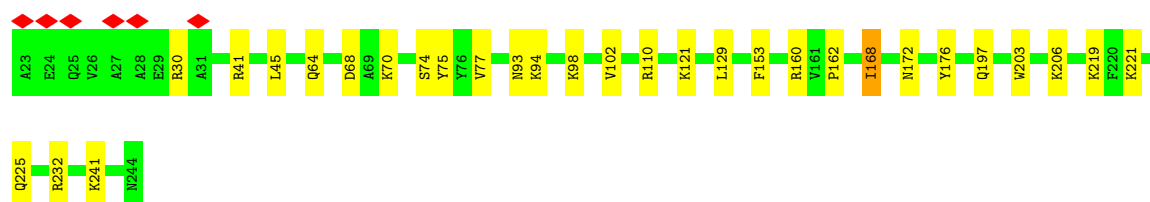
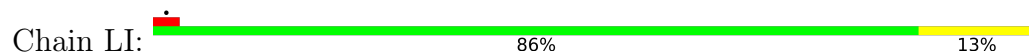




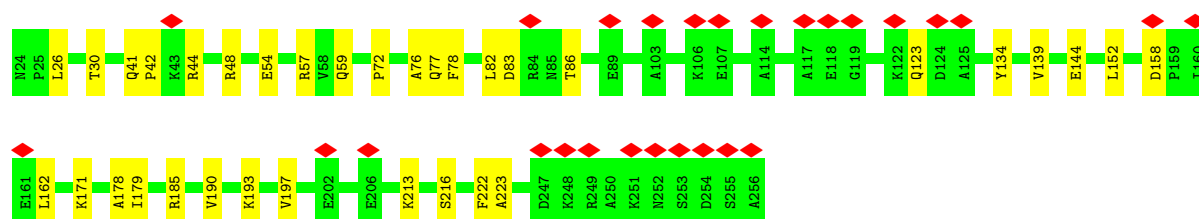
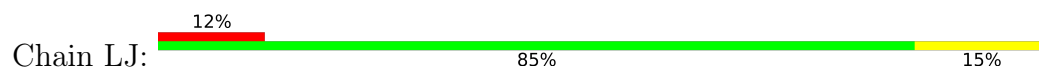
- Molecule 43: 60S ribosomal protein L6-B



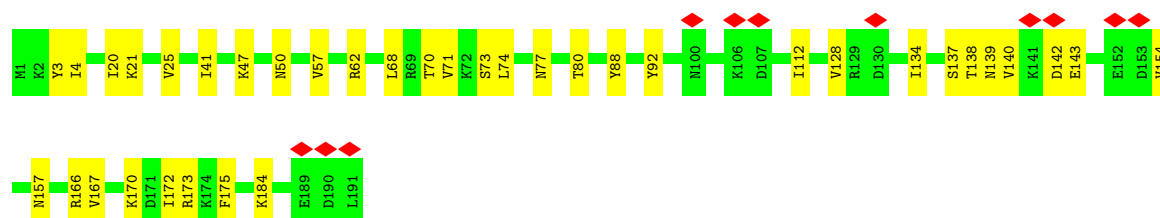
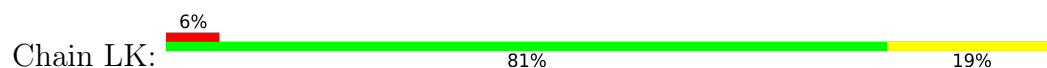
- Molecule 44: 60S ribosomal protein L7-A



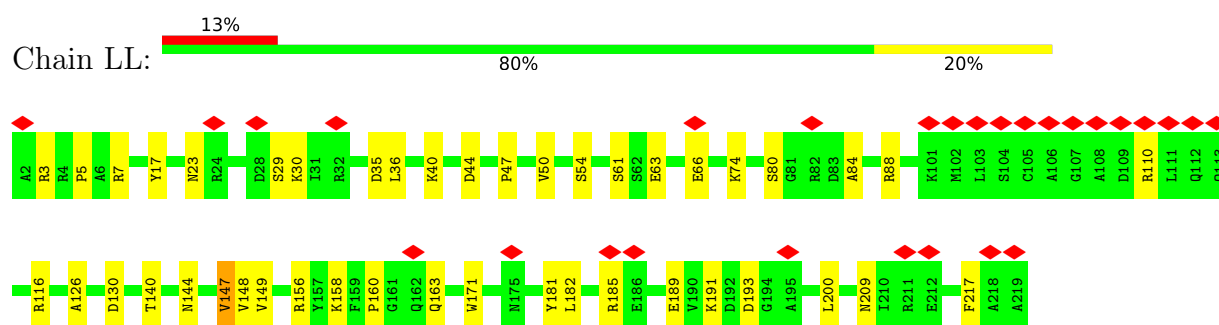
- Molecule 45: 60S ribosomal protein L8-A



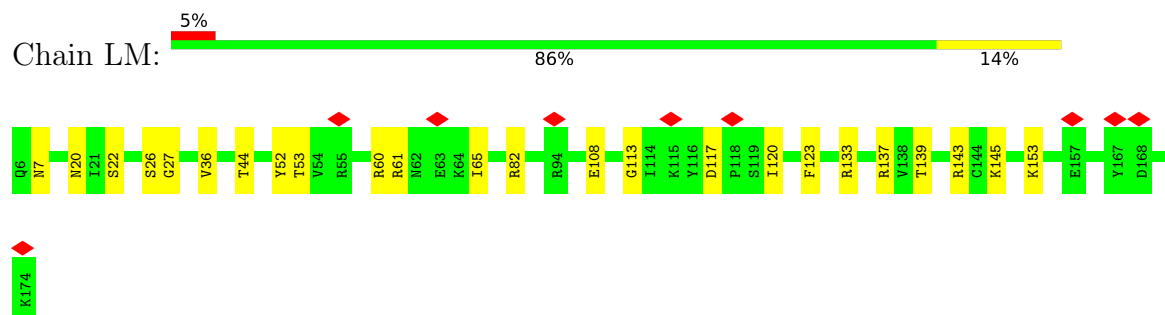
- Molecule 46: 60S ribosomal protein L9-A



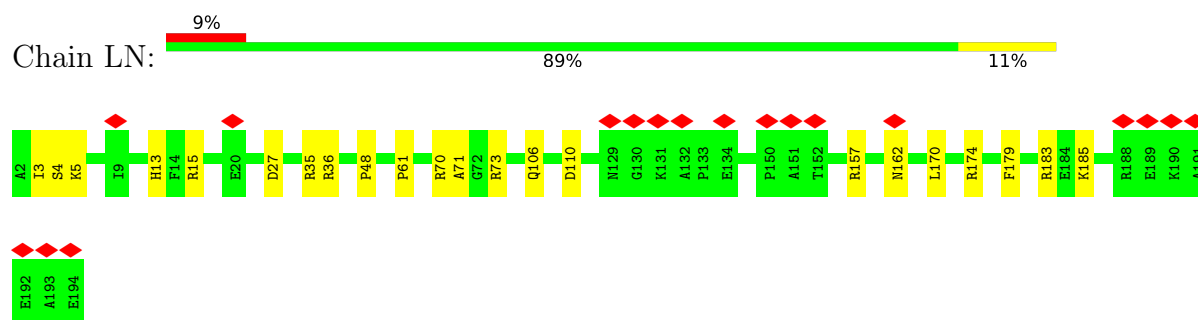
- Molecule 47: 60S ribosomal protein L10



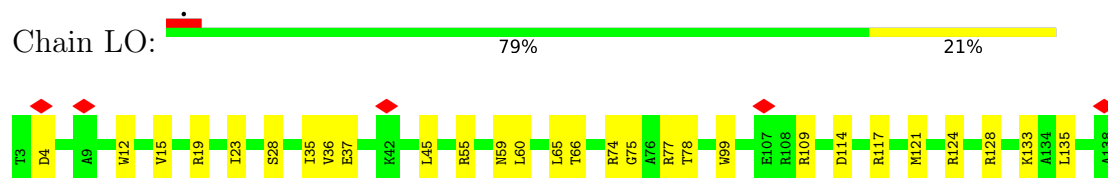
- Molecule 48: 60S ribosomal protein L11-B



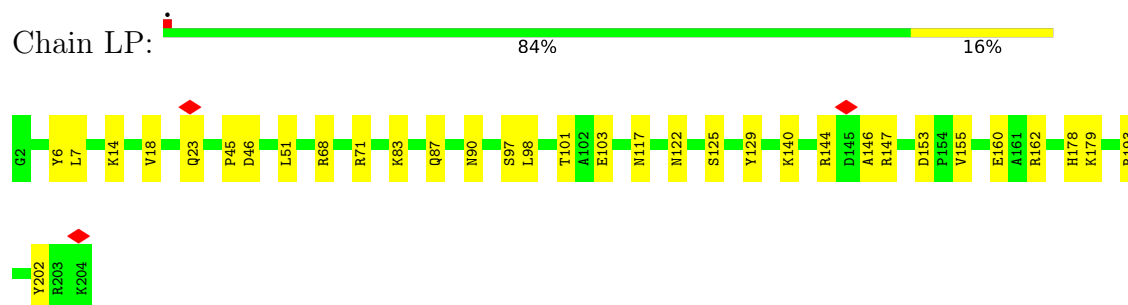
- Molecule 49: 60S ribosomal protein L13-A



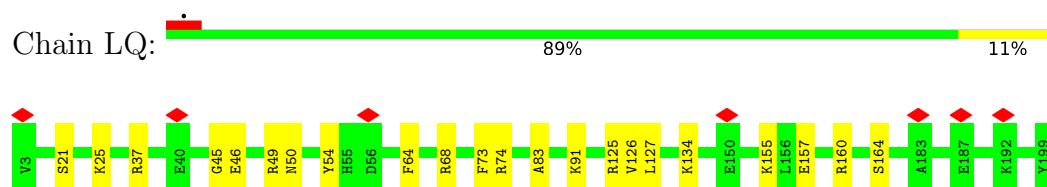
- Molecule 50: 60S ribosomal protein L14-A



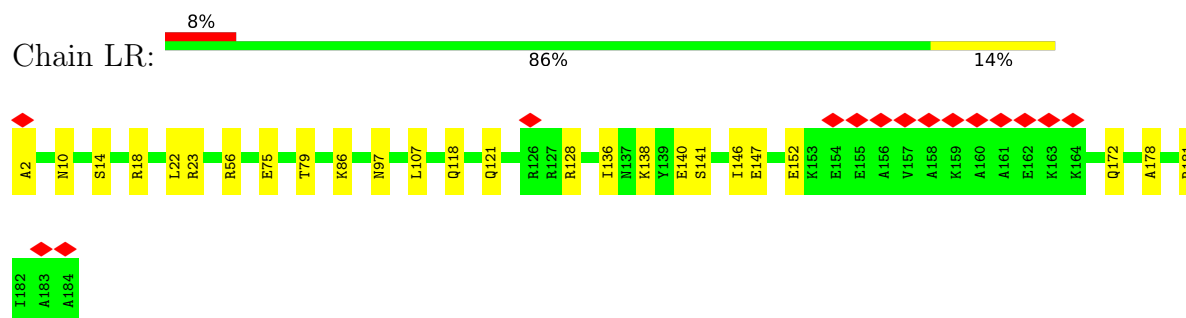
- Molecule 51: 60S ribosomal protein L15-A



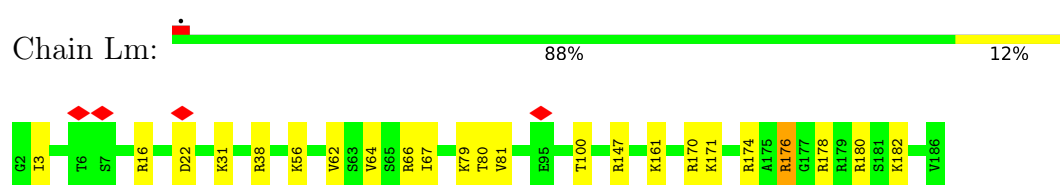
- Molecule 52: 60S ribosomal protein L16-A



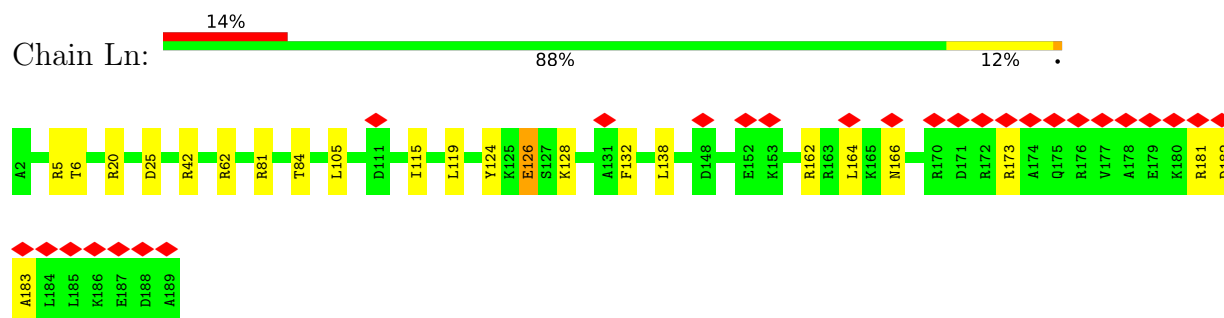
- Molecule 53: 60S ribosomal protein L17-A



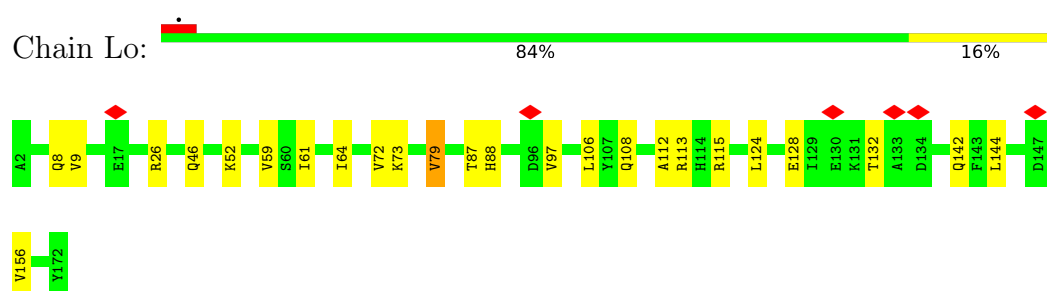
- Molecule 54: 60S ribosomal protein L18-A



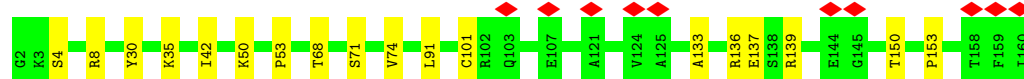
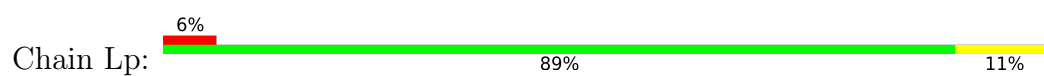
- Molecule 55: 60S ribosomal protein L19-A



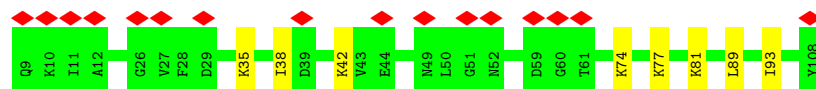
- Molecule 56: 60S ribosomal protein L20-A



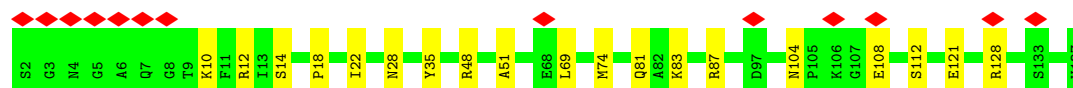
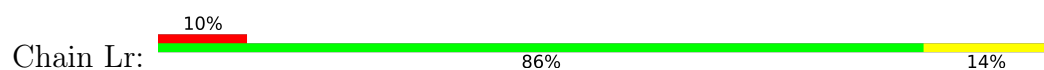
- Molecule 57: 60S ribosomal protein L21-A



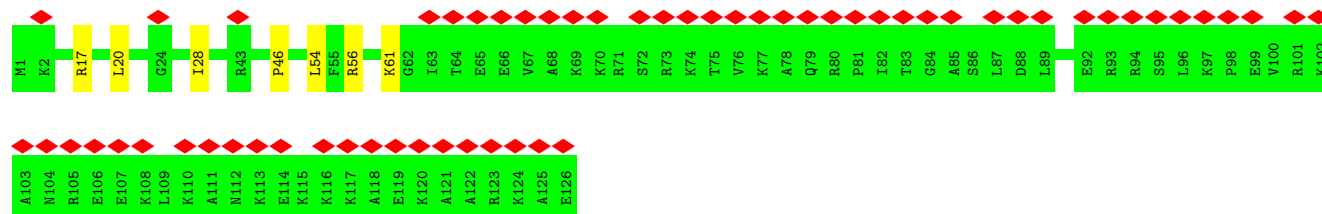
- Molecule 58: 60S ribosomal protein L22-A



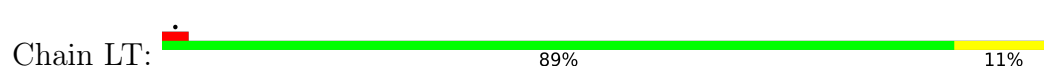
- Molecule 59: 60S ribosomal protein L23-A



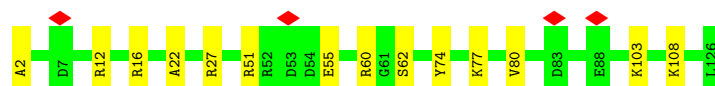
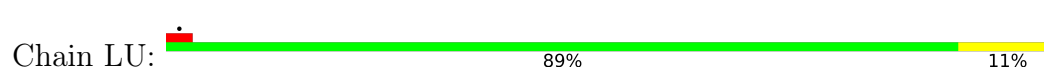
- Molecule 60: 60S ribosomal protein L24-A



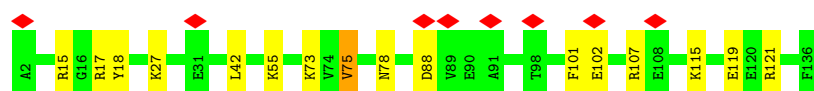
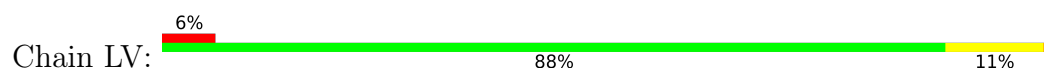
- Molecule 61: 60S ribosomal protein L25



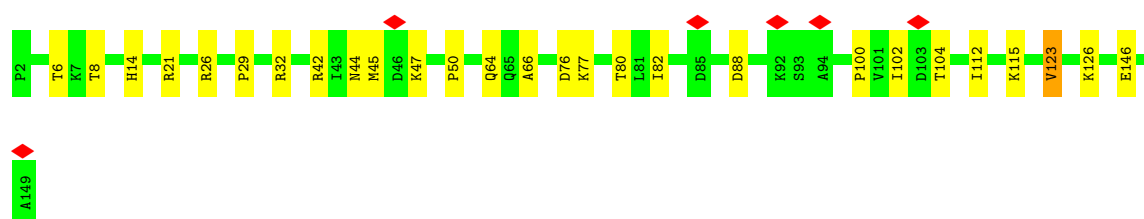
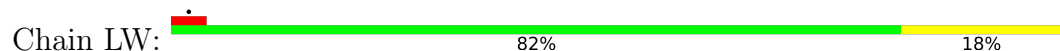
- Molecule 62: 60S ribosomal protein L26-A



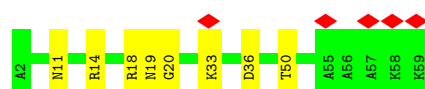
- Molecule 63: 60S ribosomal protein L27-A



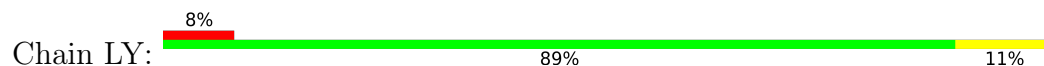
- Molecule 64: 60S ribosomal protein L28



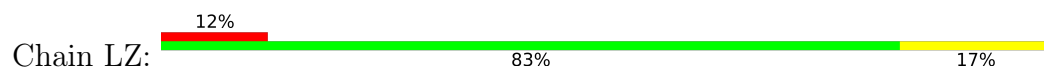
- Molecule 65: 60S ribosomal protein L29



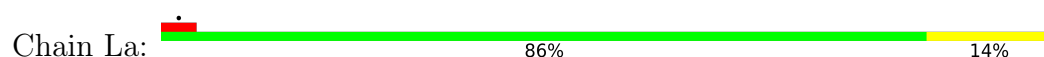
- Molecule 66: 60S ribosomal protein L30



- Molecule 67: 60S ribosomal protein L31-A

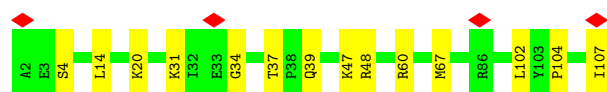


- Molecule 68: 60S ribosomal protein L32

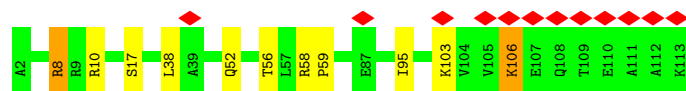


- Molecule 69: 60S ribosomal protein L33-A

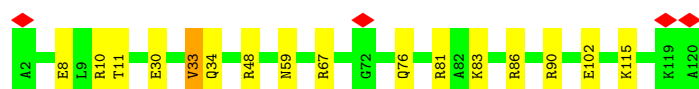




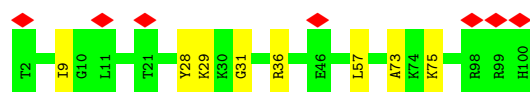
- Molecule 70: 60S ribosomal protein L34-A



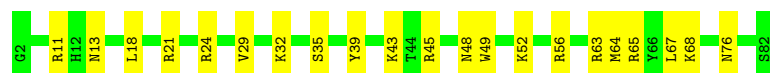
- Molecule 71: 60S ribosomal protein L35-A



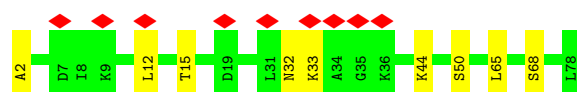
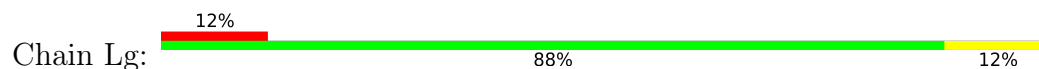
- Molecule 72: 60S ribosomal protein L36-A



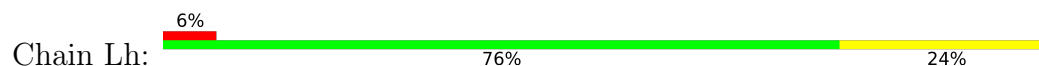
- Molecule 73: 60S ribosomal protein L37-A



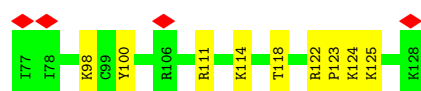
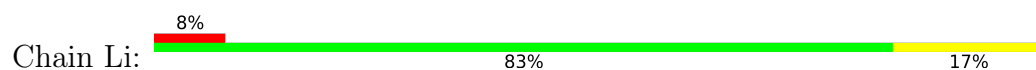
- Molecule 74: 60S ribosomal protein L38



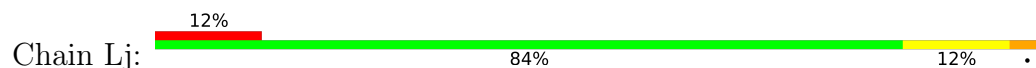
- Molecule 75: 60S ribosomal protein L39



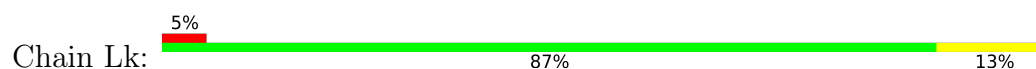
- Molecule 76: Ubiquitin-60S ribosomal protein L40



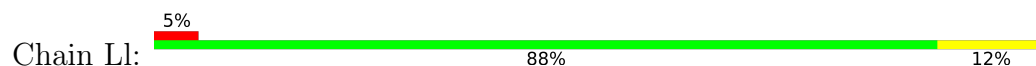
- Molecule 77: 60S ribosomal protein L41-B



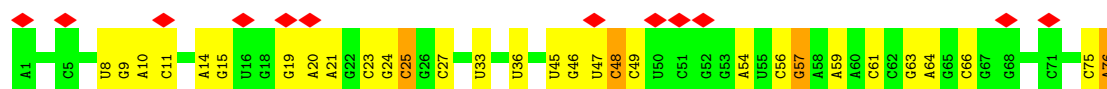
- Molecule 78: 60S ribosomal protein L42-A



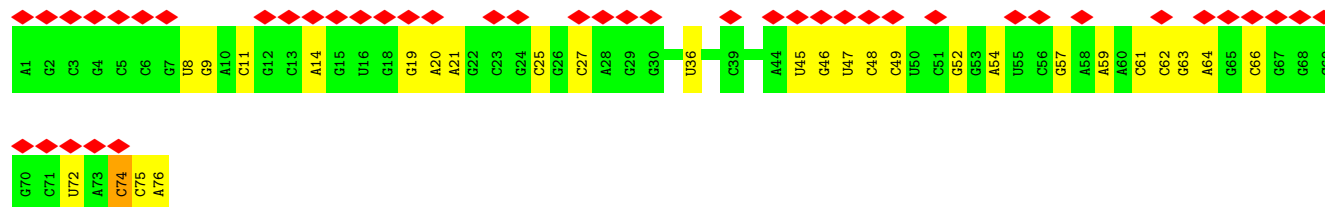
- Molecule 79: 60S ribosomal protein L43-A



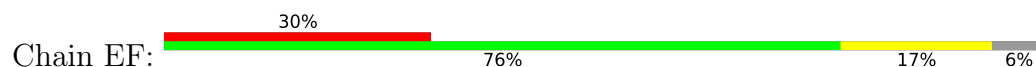
- Molecule 80: tRNA



- Molecule 80: tRNA



- Molecule 81: Elongation factor 3A



GLU	G898	G899	G900	K901	V902	V905	L906	G909	V918	E921	P922	Y925	L926	D927	R928	D929	V945	I946	F947	I948	E953	F954	T955	L958	T959	E960	D967	G968	R969	S973	G974	H975	N976	W977	VAL	SER	GLY	GLN	GLY	ALA	GLY	PRO	ARG	ILE	GLU	LYS	LYS	GLU	ASP	GLU	PHE					
	E781	A782	M783	N784	K785	K788	I789	E790	G791	T792	F793	R794	R802	F805	T808	Y809	E810	Y811	L817	G818	E819	N820	I821	C822	M823	K824	S825	E826	R827	W828	V829	D835	R841	E846	K850	A862	L869	I874	C882	L883	D884	P885	E886	G895	L896	S897										
	V668	E672	S679	Q682	T683	T684	Q689	C690	S691	L692	S693	S694	R695	N702	N711	L717	L718	F719	T720	V724	E728	N729	I735	F740	T750	E753	Q756	W757	R758	F759	Q760	T761	G762	E763	D764	S765	E766	D769	Q774	I775	N776	D779	A780													
	Y584	L585	G589	I590	T591	S592	T593	I594	T595	S596	H597	D598	F601	E607	T608	I609	I610	Y612	E613	G614	L615	K616	L617	K621	G622	N623	F624	T625	E626	F627	V628	K629	K630	C631	P632	A633	A634	K635	A636	V637	E638	L640	S641	N642	T643	D644	L645	E646	L655	K663	A664					
	E424	D425	E426	G427	E428	D429	L430	C431	A438	K442	L445	T448	L452	A455	R456	R457	Y458	G459	I460	G461	G462	P463	N464	G465	G466	G467	K468	R473	A474	D481	G482	F483	Q486	E487	R490	T491	V492	E495	H496	D497	I498	T501	H502	S503	D504	V507	L508									
	K358	E362	T363	I364	A365	A366	A369	D370	L371	I372	R375	I376	I377	D378	Q379	Q380	A381	W382	F383	T384	H385	Y389	M390	T391	I392	F393	L394	H395	E396	K397	K398	A399	K400	D401	I402	L403	D404	E405	F406	R407	K408	R409	A410	V411	D412	N413	I414	P415	V416	G417	P418	N419	F420	D421	D422	E423
	G260	I261	K262	K264	I268	I269	D270	L275	V281	I282	A283	L286	G287	K288	A301	E307	L310	K314	E324	D325	D326	A327	I328	F329	E330	L331	S332	H333	A334	G335	D336	V337	S338	Q342	V343	V344	N345	E346	T239	P240	L243	S244	R252	R257	E258	T259	P355	R356	F357							
	N65	A66	M67	Q68	A69	V70	A71	H72	N75	Q77	S77	N78	L79	S80	P81	S82	V83	E84	V88	Q89	L90	P92	C95	T96	N97	N100	K101	D102	K103	S110	I116	V117	N118	G230	A231	A236	V123	A124	I125	K126	A127	L128	N134	N140	Q143	A151	F152	S153	A154							
	D157	A158	D161	E169	L174	S175	E176	W179	D180	T181	K182	M193	T194	K195	A196	V200	D201	N202	K203	D204	I205	E206	R207	P210	S211	L212	A217	V222	V226	H227	L228	L229	G230	A236	E237	V238	T239	P240	L243	S244	R252	R257	E258	T259	P355	R356	F357									
	MET	S1	D2	S3	Q4	Q5	S6	I7	K8	V9	L10	E11	F14	Q15	K16	L17	S18	V19	A20	T21	A22	D23	D24	R25	H26	E27	I28	A29	S30	E31	V32	A33	S34	F35	G38	N39	I40	I41	E42	H43	D44	W45	P46	E47	H48	F49	F50	G51	E52	K55	G56	I57	K58	D59	K60	A64

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.391	Depositor
Minimum map value	-0.234	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.04	Depositor
Map size ($\text{\AA}$)	455.28, 455.28, 455.28	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.084, 1.084, 1.084	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ATP

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	2	0.43	0/42211	0.70	25/65773 (0.0%)
2	1	0.35	0/166	0.42	0/256
3	P	0.42	0/1644	0.88	1/2249 (0.0%)
4	Q	0.44	0/1823	0.98	0/2447
5	E	0.51	0/936	1.04	2/1259 (0.2%)
6	R	0.46	0/1656	0.94	0/2251
7	A	0.45	0/1754	0.99	5/2361 (0.2%)
8	S	0.40	0/2097	0.95	2/2823 (0.1%)
9	B	0.45	0/1625	0.99	3/2197 (0.1%)
10	T	0.39	0/1839	0.96	0/2460
11	U	0.42	0/1498	0.95	0/2019
12	V	0.42	0/1501	0.89	0/2006
13	W	0.39	0/1504	0.94	0/2016
14	C	0.47	0/769	1.00	0/1039
15	X	0.41	0/1168	0.85	0/1575
16	D	0.47	0/883	1.16	3/1199 (0.3%)
17	Y	0.43	0/1215	0.92	2/1638 (0.1%)
18	Z	0.50	0/934	1.04	1/1257 (0.1%)
19	F	0.49	0/1125	1.00	1/1510 (0.1%)
20	G	0.43	0/957	0.90	0/1283
21	H	0.47	0/1207	1.00	0/1623
22	I	0.51	0/1130	1.02	2/1517 (0.1%)
23	J	0.49	0/807	0.98	0/1091
24	a	0.41	0/682	0.89	0/921
25	b	0.47	0/1038	0.95	1/1395 (0.1%)
26	c	0.47	0/1139	0.95	0/1518
27	d	0.38	0/1087	0.98	2/1449 (0.1%)
28	K	0.43	0/661	1.06	1/888 (0.1%)
29	e	0.46	0/778	0.98	0/1042
30	f	0.37	0/620	0.93	0/838
31	M	0.43	0/452	0.94	0/600
32	g	0.42	0/480	0.99	0/639

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	N	0.37	0/567	1.04	0/764
34	O	0.38	0/2436	0.93	3/3318 (0.1%)
35	L	0.50	0/493	1.18	2/663 (0.3%)
36	LA	0.52	0/77157	0.64	15/120295 (0.0%)
37	LB	0.48	0/2883	0.60	0/4491
38	LC	0.51	0/3746	0.61	0/5832
39	LD	0.61	0/1933	0.90	0/2598
40	LE	0.53	0/3146	0.85	0/4228
41	LF	0.52	0/2800	0.91	2/3790 (0.1%)
42	LG	0.51	0/2400	0.91	5/3239 (0.2%)
43	LH	0.44	0/1329	0.94	1/1794 (0.1%)
44	LI	0.52	0/1821	0.91	0/2451
45	LJ	0.50	0/1836	0.90	0/2481
46	LK	0.48	0/1529	0.95	2/2060 (0.1%)
47	LL	0.48	0/1801	0.93	0/2416
48	LM	0.51	0/1367	0.95	1/1834 (0.1%)
49	LN	0.52	0/1568	0.87	0/2106
50	LO	0.45	0/1068	0.87	0/1438
51	LP	0.59	0/1757	0.88	0/2354
52	LQ	0.51	0/1585	0.85	0/2128
53	LR	0.54	0/1439	0.84	0/1938
54	Lm	0.54	0/1465	0.93	0/1965
55	Ln	0.50	0/1532	0.92	2/2043 (0.1%)
56	Lo	0.51	0/1473	0.81	0/1980
57	Lp	0.54	0/1296	0.88	1/1739 (0.1%)
58	Lq	0.45	0/812	0.89	0/1099
59	Lr	0.52	0/1018	0.88	1/1369 (0.1%)
60	LS	0.41	0/850	0.82	0/1152
61	LT	0.52	0/979	0.86	0/1321
62	LU	0.45	0/995	0.84	0/1329
63	LV	0.47	0/1106	0.86	0/1485
64	LW	0.58	0/1200	0.88	0/1607
65	LX	0.46	0/473	0.84	0/629
66	LY	0.45	0/745	0.82	0/1001
67	LZ	0.52	0/890	0.85	0/1196
68	La	0.48	0/1034	0.78	0/1385
69	Lb	0.56	0/868	0.87	1/1168 (0.1%)
70	Lc	0.60	0/890	0.96	2/1189 (0.2%)
71	Ld	0.44	0/978	0.79	0/1301
72	Le	0.44	0/772	0.88	0/1026
73	Lf	0.67	0/660	1.04	1/875 (0.1%)
74	Lg	0.48	0/618	0.94	0/826
75	Lh	0.59	0/443	0.98	0/588

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
76	Li	0.51	0/416	0.93	0/553
77	Lj	0.49	0/230	0.95	0/296
78	Lk	0.52	0/836	0.87	0/1104
79	Ll	0.56	0/701	0.83	0/934
80	Sm	0.34	0/1795	0.73	2/2797 (0.1%)
80	Sn	0.39	0/1796	0.72	0/2799
81	EF	0.33	0/7610	0.71	6/10311 (0.1%)
All	All	0.48	0/226528	0.77	98/332424 (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
8	S	0	1
9	B	0	2
11	U	0	1
16	D	0	1
19	F	0	1
25	b	0	1
33	N	0	1
36	LA	0	1
41	LF	0	3
44	LI	0	1
45	LJ	0	3
54	Lm	0	1
64	LW	0	2
65	LX	0	2
66	LY	0	1
67	LZ	0	1
71	Ld	0	1
81	EF	0	6
All	All	0	30

There are no bond length outliers.

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	d	39	GLU	CA-CB-CG	8.91	131.92	114.10
81	EF	415	PRO	N-CA-CB	7.58	110.39	103.34
80	Sm	74	C	O3'-P-O5'	7.39	115.08	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	EF	418	PRO	N-CA-CB	7.38	111.00	103.25
7	A	218	LEU	CA-CB-CG	7.22	141.58	116.30
1	2	400	A	C2'-C3'-O3'	7.21	120.32	109.50
19	F	50	GLU	CA-CB-CG	7.21	128.52	114.10
35	L	54	LEU	CA-CB-CG	7.06	141.01	116.30
35	L	66	LEU	CA-CB-CG	6.95	140.62	116.30
8	S	193	GLY	N-CA-C	6.68	129.00	113.18
36	LA	2112	U	P-O3'-C3'	6.58	130.06	120.20
36	LA	2541	U	P-O3'-C3'	6.48	129.92	120.20
36	LA	2537	U	P-O3'-C3'	6.31	129.67	120.20
18	Z	52	ARG	CB-CA-C	-6.26	99.24	110.70
1	2	322	G	P-O3'-C3'	6.26	129.59	120.20
1	2	1471	A	C5'-C4'-C3'	-6.24	106.65	116.00
17	Y	3	ARG	CB-CG-CD	6.24	125.64	111.30
42	LG	229	ASP	CA-C-N	6.22	131.59	122.63
42	LG	229	ASP	C-N-CA	6.22	131.59	122.63
36	LA	1716	U	P-O3'-C3'	6.08	129.32	120.20
27	d	39	GLU	N-CA-CB	6.02	118.75	110.01
17	Y	4	MET	N-CA-C	6.02	121.30	111.37
36	LA	2101	C	P-O3'-C3'	5.98	129.17	120.20
36	LA	3275	U	OP1-P-O3'	5.97	125.92	108.00
70	Lc	106	LYS	CA-CB-CG	5.93	125.97	114.10
9	B	148	ARG	CA-CB-CG	5.91	125.93	114.10
41	LF	4	PRO	CA-C-N	5.91	135.79	122.19
41	LF	4	PRO	C-N-CA	5.91	135.79	122.19
48	LM	108	GLU	CA-CB-CG	5.85	125.80	114.10
22	I	52	GLY	CA-C-N	5.84	132.70	121.54
22	I	52	GLY	C-N-CA	5.84	132.70	121.54
59	Lr	83	LYS	CB-CG-CD	5.82	124.69	111.30
1	2	639	U	P-O3'-C3'	5.79	128.89	120.20
1	2	1256	A	P-O3'-C3'	5.69	128.73	120.20
1	2	322	G	C2'-C3'-O3'	5.68	118.03	109.50
46	LK	112	ILE	N-CA-C	-5.68	100.40	109.20
36	LA	1815	U	P-O3'-C3'	5.67	128.70	120.20
36	LA	2495	C	O3'-P-O5'	5.67	112.50	104.00
1	2	400	A	P-O3'-C3'	5.64	128.66	120.20
80	Sm	72	U	C5'-C4'-C3'	5.63	124.44	116.00
55	Ln	181	ARG	CA-CB-CG	5.60	125.30	114.10
28	K	53	GLU	CA-CB-CG	5.58	125.26	114.10
1	2	1472	C	O5'-C5'-C4'	5.58	120.06	111.70
1	2	1382	A	P-O3'-C3'	5.57	128.55	120.20
1	2	1633	A	P-O3'-C3'	5.57	128.55	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	LA	1307	G	C2'-C3'-O3'	5.57	117.85	109.50
1	2	819	G	P-O3'-C3'	5.55	128.53	120.20
1	2	215	A	P-O3'-C3'	5.55	128.52	120.20
34	O	177	MET	CA-CB-CG	5.54	125.17	114.10
25	b	48	GLY	N-CA-C	5.53	116.96	111.21
1	2	1273	G	P-O3'-C3'	5.50	128.45	120.20
5	E	36	LEU	CA-CB-CG	5.50	135.55	116.30
36	LA	2452	G	P-O5'-C5'	5.48	129.12	120.90
1	2	555	A	P-O3'-C3'	5.43	128.34	120.20
1	2	738	G	P-O3'-C3'	5.43	128.34	120.20
42	LG	120	LYS	CB-CG-CD	5.42	123.76	111.30
42	LG	41	LYS	CA-CB-CG	5.40	124.91	114.10
1	2	77	U	P-O3'-C3'	5.40	128.30	120.20
57	Lp	137	GLU	CB-CA-C	5.39	119.78	110.45
1	2	738	G	O3'-P-O5'	5.36	112.03	104.00
1	2	224	C	P-O3'-C3'	5.35	128.22	120.20
1	2	278	U	P-O3'-C3'	5.31	128.16	120.20
34	O	307	ASP	CA-C-N	5.29	131.63	121.54
34	O	307	ASP	C-N-CA	5.29	131.63	121.54
3	P	74	VAL	CA-CB-CG1	5.28	119.38	110.40
16	D	36	LEU	CA-CB-CG	5.28	134.78	116.30
9	B	64	VAL	CA-C-N	5.25	131.30	123.05
9	B	64	VAL	C-N-CA	5.25	131.30	123.05
46	LK	140	VAL	CA-CB-CG2	5.25	119.32	110.40
5	E	57	MET	CB-CG-SD	5.24	128.43	112.70
1	2	1756	A	P-O5'-C5'	5.23	128.74	120.90
36	LA	1582	C	P-O3'-C3'	5.22	128.02	120.20
43	LH	77	ARG	N-CA-CB	5.20	120.30	111.57
55	Ln	126	GLU	CA-CB-CG	5.19	124.48	114.10
81	EF	101	LYS	CA-C-N	5.18	131.44	121.54
81	EF	101	LYS	C-N-CA	5.18	131.44	121.54
36	LA	3350	C	P-O3'-C3'	5.17	127.95	120.20
36	LA	763	G	P-O3'-C3'	5.14	127.91	120.20
73	Lf	24	ARG	CA-CB-CG	5.13	124.36	114.10
8	S	38	LEU	CA-CB-CG	5.12	134.23	116.30
81	EF	684	THR	CA-C-N	5.11	131.30	121.54
81	EF	684	THR	C-N-CA	5.11	131.30	121.54
70	Lc	8	ARG	N-CA-CB	-5.11	102.63	110.44
1	2	139	C	P-O3'-C3'	5.09	127.84	120.20
1	2	740	A	P-O5'-C5'	5.09	128.53	120.90
7	A	217	ILE	CA-C-N	5.08	131.23	121.54
7	A	217	ILE	C-N-CA	5.08	131.23	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	LA	3276	G	O5'-C5'-C4'	5.06	119.30	111.70
7	A	93	ASP	CA-CB-CG	5.06	117.66	112.60
16	D	125	ASN	CA-C-N	5.04	130.47	122.61
16	D	125	ASN	C-N-CA	5.04	130.47	122.61
69	Lb	67	MET	N-CA-CB	5.03	118.67	110.77
1	2	1274	C	P-O3'-C3'	5.03	127.75	120.20
1	2	640	U	P-O3'-C3'	5.03	127.74	120.20
36	LA	1716	U	C4'-C3'-O3'	5.02	116.94	109.40
7	A	143	ARG	CA-CB-CG	5.01	124.11	114.10
42	LG	230	ASP	CA-CB-CG	5.01	117.61	112.60
1	2	1573	A	P-O3'-C3'	5.00	127.70	120.20

There are no chirality outliers.

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	B	125	THR	Peptide
9	B	42	LEU	Peptide
16	D	108	ARG	Peptide
81	EF	465	GLY	Peptide
81	EF	663	LYS	Peptide
81	EF	760	GLN	Peptide
81	EF	78	ASN	Peptide
81	EF	80	SER	Peptide
81	EF	955	THR	Peptide
19	F	40	GLU	Peptide
36	LA	1273	A	Sidechain
41	LF	13	GLY	Peptide
41	LF	3	ARG	Peptide
41	LF	318	LEU	Peptide
44	LI	232	ARG	Peptide
45	LJ	30	THR	Peptide
45	LJ	76	ALA	Peptide
45	LJ	77	GLN	Peptide
64	LW	115	LYS	Peptide
64	LW	14	HIS	Peptide
65	LX	19	ASN	Peptide
65	LX	20	GLY	Peptide
66	LY	47	ASN	Peptide
67	LZ	7	VAL	Peptide
71	Ld	83	LYS	Peptide
54	Lm	161	LYS	Peptide

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Mol	Chain	Res	Type	Group
33	N	147	VAL	Peptide
8	S	193	GLY	Peptide
11	U	64	VAL	Peptide
25	b	54	ASP	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	2	37739	0	18987	297	0
2	1	149	0	75	0	0
3	P	1603	0	1610	24	0
4	Q	1798	0	1890	28	0
5	E	916	0	941	15	0
6	R	1626	0	1715	23	0
7	A	1729	0	1812	18	0
8	S	2056	0	2140	30	0
9	B	1605	0	1669	21	0
10	T	1815	0	1894	32	0
11	U	1473	0	1555	14	0
12	V	1476	0	1501	27	0
13	W	1479	0	1556	19	0
14	C	752	0	719	11	0
15	X	1142	0	1209	15	0
16	D	875	0	878	19	0
17	Y	1192	0	1255	16	0
18	Z	923	0	948	13	0
19	F	1105	0	1166	24	0
20	G	948	0	990	19	0
21	H	1188	0	1218	21	0
22	I	1112	0	1124	24	0
23	J	797	0	863	18	0
24	a	673	0	662	11	0
25	b	1021	0	1060	10	0
26	c	1121	0	1196	16	0
27	d	1073	0	1132	19	0
28	K	651	0	682	7	0
29	e	765	0	814	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	f	610	0	633	10	0
31	M	442	0	432	7	0
32	g	472	0	521	10	0
33	N	556	0	552	10	0
34	O	2383	0	2332	37	0
35	L	491	0	524	10	0
36	LA	68931	0	34637	373	0
37	LB	2579	0	1304	22	0
38	LC	3353	0	1695	25	0
39	LD	1899	0	1957	34	0
40	LE	3075	0	3142	33	0
41	LF	2748	0	2859	44	0
42	LG	2351	0	2294	34	0
43	LH	1307	0	1377	19	0
44	LI	1784	0	1862	25	0
45	LJ	1804	0	1877	22	0
46	LK	1508	0	1572	22	0
47	LL	1764	0	1804	28	0
48	LM	1346	0	1370	19	0
49	LN	1543	0	1608	19	0
50	LO	1053	0	1149	20	0
51	LP	1720	0	1779	26	0
52	LQ	1555	0	1659	16	0
53	LR	1416	0	1433	14	0
54	Lm	1441	0	1543	19	0
55	Ln	1515	0	1606	21	0
56	Lo	1437	0	1475	22	0
57	Lp	1272	0	1312	13	0
58	Lq	796	0	812	4	0
59	Lr	1003	0	1048	12	0
60	LS	836	0	706	4	0
61	LT	964	0	1025	7	0
62	LU	984	0	1075	11	0
63	LV	1080	0	1122	11	0
64	LW	1169	0	1211	23	0
65	LX	462	0	491	5	0
66	LY	737	0	792	6	0
67	LZ	876	0	912	8	0
68	La	1013	0	1077	13	0
69	Lb	850	0	880	8	0
70	Lc	880	0	945	9	0
71	Ld	969	0	1078	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
72	Le	766	0	844	8	0
73	Lf	645	0	649	18	0
74	Lg	612	0	682	6	0
75	Lh	436	0	475	11	0
76	Li	410	0	446	7	0
77	Lj	229	0	273	3	0
78	Lk	824	0	892	12	0
79	Ll	694	0	738	9	0
80	Sm	1605	0	816	3	0
80	Sn	1606	0	816	10	0
81	EF	7479	0	7407	102	0
82	EF	62	0	24	5	0
All	All	211144	0	156805	1568	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 4.

All (1568) 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)
36:LA:1896:A:H61	36:LA:2339:C:N4	1.57	1.01
36:LA:2471:U:H3	36:LA:2475:G:H1	1.01	0.97
1:2:1697:G:H1	1:2:1704:U:H3	1.05	0.96
36:LA:1896:A:N6	36:LA:2339:C:H42	1.63	0.94
1:2:821:U:H3	1:2:852:C:N4	1.64	0.94
36:LA:1018:G:H1	36:LA:1034:U:H3	1.16	0.86
1:2:1229:G:H21	1:2:1256:A:H62	1.18	0.85
1:2:1588:G:H1	1:2:1608:U:H3	1.19	0.85
1:2:1229:G:N2	1:2:1256:A:H62	1.77	0.83
1:2:821:U:H3	1:2:852:C:H42	1.24	0.83
1:2:174:U:H3	1:2:266:A:H62	1.26	0.83
36:LA:1896:A:H61	36:LA:2339:C:H42	0.86	0.82
1:2:1229:G:H21	1:2:1256:A:N6	1.77	0.82
1:2:1502:G:N7	22:I:102:ARG:NH2	2.31	0.79
81:EF:464:ASN:HD21	81:EF:899:GLY:HA3	1.48	0.78
19:F:50:GLU:OE2	19:F:82:ARG:NH2	2.20	0.74
28:K:65:LEU:O	28:K:69:LEU:HB2	1.88	0.74
1:2:1012:U:H4'	39:LD:247:ARG:HB3	1.70	0.73
36:LA:2206:G:N3	36:LA:2207:A:N6	2.36	0.73
36:LA:2987:A:H5''	52:LQ:68[A]:ARG:HH12	1.53	0.72
22:I:4:VAL:HG21	22:I:137:ALA:HB2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:EF:729:ASN:HD21	81:EF:802:ARG:HH22	1.38	0.72
39:LD:32:LEU:HD13	39:LD:163:ARG:HD2	1.70	0.71
36:LA:1634:G:N7	63:LV:17:ARG:NH1	2.39	0.71
35:L:64:ARG:HG3	35:L:65:ARG:HG2	1.72	0.70
1:2:1584:G:N2	1:2:1611:A:OP2	2.25	0.70
36:LA:1613:A:OP1	74:Lg:2:ALA:N	2.25	0.69
12:V:37:LYS:HE2	12:V:95:THR:HG22	1.75	0.69
10:T:2:LYS:HB3	10:T:108:VAL:HG22	1.75	0.69
36:LA:640:U:OP1	64:LW:21:ARG:NH2	2.25	0.69
1:2:323:A:OP2	12:V:10:LYS:NZ	2.23	0.68
11:U:49:ILE:HD12	11:U:175:LYS:HG2	1.75	0.68
48:LM:117:ASP:HB3	48:LM:120:ILE:HG12	1.74	0.68
36:LA:1907:C:O2	40:LE:240:ARG:NH2	2.24	0.68
3:P:70:PRO:HB2	3:P:94:GLY:HA3	1.75	0.68
10:T:78:THR:HG22	10:T:92:ARG:HG2	1.76	0.68
36:LA:2908:G:O2'	76:Li:114:LYS:NZ	2.27	0.68
16:D:103:LEU:HB2	16:D:115:VAL:HG12	1.76	0.67
36:LA:1562:C:H42	36:LA:1578:C:H42	1.40	0.67
12:V:5:ARG:NH1	12:V:29:LEU:O	2.28	0.67
1:2:259:U:OP1	12:V:75:LYS:NZ	2.28	0.67
1:2:853:G:OP1	55:Ln:173:ARG:NH1	2.28	0.67
43:LH:66:THR:OG1	43:LH:138:GLN:NE2	2.27	0.67
36:LA:1236:G:N2	36:LA:1272:C:OP1	2.27	0.67
47:LL:110:ARG:NH1	80:Sn:75:C:OP2	2.28	0.67
39:LD:80:GLU:HG3	79:Ll:66:GLY:HA2	1.76	0.66
42:LG:50:ARG:NH1	42:LG:147:ASP:OD2	2.28	0.66
36:LA:1389:G:OP1	68:La:104:ASN:ND2	2.27	0.66
36:LA:1363:A:OP1	44:LI:160:ARG:NH1	2.28	0.66
1:2:1330:G:H22	7:A:204:ASP:HB3	1.61	0.66
34:O:17:ASN:HA	34:O:308:ASN:HD22	1.61	0.66
36:LA:2799:A:O2'	64:LW:42:ARG:NH1	2.28	0.66
36:LA:3272:C:OP2	43:LH:78:ARG:NH1	2.29	0.66
47:LL:140:THR:HG21	47:LL:148:VAL:HG11	1.76	0.66
8:S:94:ALA:HB1	27:d:16:PRO:HB2	1.78	0.65
8:S:151:ASP:OD1	10:T:215:ARG:NH2	2.29	0.65
38:LC:75:G:OP2	62:LU:74:TYR:OH	2.12	0.65
1:2:821:U:O2	1:2:852:C:N3	2.28	0.65
7:A:106:LYS:HG3	7:A:175:VAL:HG22	1.79	0.65
36:LA:3158:G:O6	36:LA:3292:A:N1	2.29	0.65
46:LK:20:ILE:HG12	46:LK:25:VAL:HG22	1.78	0.65
67:LZ:47:ASP:OD1	67:LZ:87:ASN:ND2	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:868:G:OP1	17:Y:121:ARG:NH1	2.29	0.65
1:2:127:G:O6	10:T:202:ARG:NH2	2.30	0.65
36:LA:684:G:H5'	49:LN:35:ARG:HH12	1.61	0.65
1:2:913:G:H5'	36:LA:2207:A:H1'	1.79	0.65
11:U:46:ILE:HG12	11:U:60:ILE:HG12	1.78	0.65
1:2:105:A:O2'	12:V:8:ARG:NH1	2.30	0.65
1:2:992:A:H2	1:2:1012:U:H3	1.43	0.65
36:LA:813:G:O2'	73:Lf:45:ARG:NH2	2.29	0.65
1:2:821:U:N3	1:2:852:C:N4	2.39	0.64
1:2:907:A:N3	1:2:997:G:O2'	2.30	0.64
1:2:1520:U:OP2	22:I:75:LYS:NZ	2.30	0.64
17:Y:99:ARG:NH2	17:Y:119:GLU:OE2	2.29	0.64
1:2:1445:G:N2	33:N:88:PRO:O	2.30	0.64
9:B:42:LEU:HD22	9:B:47:SER:HA	1.80	0.64
1:2:1256:A:H5'	14:C:5:LYS:HD2	1.80	0.64
1:2:1482:C:O2'	19:F:72:GLY:O	2.13	0.64
38:LC:97:A:OP1	71:Ld:67:ARG:NH2	2.31	0.64
1:2:330:G:OP2	12:V:172:ARG:NH1	2.30	0.64
1:2:895:G:H1	1:2:917:U:H3	1.45	0.64
1:2:1335:U:H5'	23:J:85:ARG:HH22	1.63	0.64
36:LA:2185:G:O2'	36:LA:2314:U:OP2	2.16	0.64
22:I:25:GLN:HG2	81:EF:179:TRP:HB3	1.78	0.64
36:LA:576:C:OP1	44:LI:241:LYS:NZ	2.31	0.64
36:LA:3158:G:H1	36:LA:3292:A:H2	1.42	0.64
38:LC:53:A:O2'	75:Lh:40:LYS:NZ	2.31	0.64
9:B:63:GLN:NE2	9:B:66:GLN:OE1	2.30	0.64
36:LA:1055:A:N3	37:LB:81:U:O2'	2.30	0.64
36:LA:1210:U:OP1	46:LK:62:ARG:NH1	2.31	0.64
1:2:1601:G:OP1	22:I:86:ARG:NH1	2.31	0.64
1:2:1429:G:N3	23:J:72:ASN:ND2	2.45	0.63
1:2:1534:G:OP2	28:K:74:SER:OG	2.17	0.63
36:LA:2176:U:OP1	39:LD:54:ARG:NH2	2.31	0.63
34:O:11:GLY:HA2	34:O:52:GLN:HA	1.80	0.63
36:LA:1385:C:O2	43:LH:2:THR:N	2.32	0.63
37:LB:6:C:O2'	42:LG:50:ARG:NH2	2.31	0.63
42:LG:294:ALA:HB1	47:LL:217:PHE:HB3	1.79	0.63
49:LN:4:SER:O	64:LW:44:ASN:ND2	2.30	0.63
1:2:68:A:N6	10:T:132:ARG:O	2.32	0.63
1:2:1587:A:O2'	9:B:104:ASN:ND2	2.32	0.63
15:X:102:LYS:O	26:c:13:ARG:NH2	2.32	0.63
29:e:37:LYS:O	29:e:38:ARG:NH1	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:Lh:27:ILE:O	75:Lh:33:ASN:ND2	2.32	0.63
1:2:1339:C:O2'	1:2:1341:A:N7	2.31	0.63
1:2:268:C:OP1	10:T:176:GLN:NE2	2.32	0.63
8:S:69:HIS:HB3	27:d:17:LEU:HD22	1.81	0.63
41:LF:112:LYS:HG3	51:LP:202:TYR:HB3	1.79	0.63
8:S:100:ARG:HB3	8:S:112:HIS:HB3	1.81	0.63
36:LA:55:G:OP1	73:Lf:43:LYS:NZ	2.29	0.63
1:2:154:G:OP1	10:T:2:LYS:NZ	2.32	0.63
51:LP:155:VAL:O	51:LP:162:ARG:NH2	2.28	0.63
36:LA:1390:A:N6	36:LA:1418:A:O2'	2.32	0.62
1:2:1594:G:OP2	1:2:1596:C:N4	2.32	0.62
15:X:27:THR:O	15:X:30:ARG:NH1	2.32	0.62
29:e:32:LYS:O	29:e:37:LYS:NZ	2.31	0.62
36:LA:67:A:N6	36:LA:271:C:O2'	2.31	0.62
18:Z:71:CYS:HB2	18:Z:76:ILE:HD12	1.80	0.62
18:Z:31:THR:HG22	18:Z:38:THR:HA	1.81	0.62
1:2:578:U:H4'	1:2:579:A:H5'	1.81	0.62
41:LF:285:ASP:HB3	41:LF:288:ARG:HE	1.65	0.62
81:EF:174:LEU:HD22	81:EF:193:MET:HG3	1.82	0.62
81:EF:805:PHE:HB2	81:EF:810:GLU:HG3	1.82	0.62
10:T:44:GLU:O	10:T:119:GLN:NE2	2.31	0.62
36:LA:791:A:OP1	41:LF:108:LYS:NZ	2.31	0.62
1:2:647:G:H22	1:2:687:G:H1	1.48	0.62
1:2:815:G:O2'	55:Ln:162:ARG:NH2	2.32	0.62
1:2:765:G:H1	13:W:149:ARG:HD3	1.64	0.62
16:D:39:ASP:O	16:D:124:LYS:NZ	2.31	0.62
24:a:17:CYS:SG	24:a:18:SER:N	2.73	0.62
1:2:447:U:O2'	8:S:27:TYR:O	2.18	0.61
1:2:950:C:O2'	17:Y:104:ARG:NH1	2.33	0.61
1:2:1496:U:HO2'	1:2:1519:U:HO2'	1.47	0.61
36:LA:283:G:OP1	78:Lk:45:ARG:NH1	2.33	0.61
36:LA:364:G:OP2	73:Lf:52:LYS:NZ	2.33	0.61
36:LA:2838:A:H4'	47:LL:74:LYS:HG2	1.82	0.61
56:Lo:26:ARG:NH1	57:Lp:150:THR:OG1	2.33	0.61
1:2:1747:G:HO2'	36:LA:2303:A:HO2'	1.48	0.61
26:c:42:PRO:O	26:c:79:ASN:ND2	2.32	0.61
1:2:1213:G:O2'	1:2:1244:A:N7	2.33	0.61
36:LA:1169:A:H4'	44:LI:219:LYS:HE2	1.82	0.61
1:2:140:A:H1'	10:T:184:LEU:HD11	1.82	0.61
44:LI:121:LYS:HB2	57:Lp:133:ALA:HB3	1.82	0.61
48:LM:139:THR:O	48:LM:145:LYS:NZ	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:EF:466:CYS:HA	82:EF:1102:ATP:H4'	1.82	0.61
1:2:1102:G:N7	26:c:2:GLY:N	2.49	0.61
36:LA:2852:C:N3	47:LL:158:LYS:NZ	2.49	0.61
3:P:21:ASN:HB3	3:P:24:LEU:HD12	1.83	0.61
3:P:148:ASP:OD2	3:P:165:ARG:NH1	2.34	0.61
20:G:26:LEU:HD11	20:G:62:GLN:HG3	1.81	0.61
33:N:123:ASN:ND2	33:N:125:THR:OG1	2.33	0.61
36:LA:901:G:OP1	73:Lf:13:ASN:ND2	2.34	0.61
80:Sn:15:G:H22	80:Sn:48:C:H42	1.46	0.61
36:LA:804:C:OP1	41:LF:98:ARG:NH1	2.34	0.61
36:LA:1915:A:H5''	55:Ln:84:THR:HG22	1.83	0.61
7:A:40:ARG:NH2	7:A:47:GLU:OE2	2.34	0.61
36:LA:593:C:OP2	43:LH:19:LYS:NZ	2.34	0.61
1:2:393:C:N4	1:2:401:A:OP2	2.34	0.61
3:P:13:ASP:OD1	3:P:179:ARG:NH2	2.32	0.61
1:2:886:U:OP1	4:Q:214:LYS:NZ	2.34	0.60
34:O:206:PRO:HG2	34:O:247:PRO:HA	1.82	0.60
81:EF:263:ARG:NH2	81:EF:886:GLU:OE1	2.34	0.60
1:2:1544:U:H3	1:2:1567:U:H3	1.49	0.60
6:R:222:TYR:OH	24:a:11:LEU:O	2.19	0.60
38:LC:52:A:OP1	75:Lh:21:ARG:NH1	2.34	0.60
81:EF:460:ILE:HG22	81:EF:468:LYS:HZ2	1.65	0.60
27:d:55:VAL:HG23	27:d:75:VAL:HG12	1.82	0.60
36:LA:2681:U:H5'	48:LM:65:ILE:HD11	1.82	0.60
81:EF:464:ASN:ND2	82:EF:1102:ATP:O3G	2.34	0.60
9:B:94:THR:HA	9:B:97:LEU:HD12	1.83	0.60
36:LA:2424:A:OP1	51:LP:90:ASN:ND2	2.33	0.60
36:LA:2666:C:OP2	36:LA:2687:G:N1	2.32	0.60
39:LD:95:SER:O	39:LD:100:ASN:ND2	2.32	0.60
50:LO:15:VAL:HG23	50:LO:35:ILE:HD13	1.83	0.60
27:d:115:ASP:HA	27:d:118:ILE:HG12	1.84	0.60
49:LN:157:ARG:NH2	64:LW:146:GLU:OE2	2.34	0.60
19:F:143:ARG:NH1	80:Sn:33:U:OP2	2.35	0.60
34:O:262:VAL:HG13	34:O:271:VAL:HG23	1.83	0.60
1:2:639:U:OP1	11:U:112:ARG:NH2	2.32	0.60
36:LA:388:G:H1'	53:LR:97:ASN:HD21	1.66	0.60
81:EF:869:LEU:HB2	81:EF:874:ILE:HD11	1.83	0.60
36:LA:524:U:OP1	50:LO:77:ARG:NH2	2.35	0.60
36:LA:912:G:OP2	39:LD:9:ARG:NH1	2.35	0.60
36:LA:999:G:N3	36:LA:1002:A:N6	2.49	0.60
7:A:59:LEU:HD23	7:A:66:ILE:HG13	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:LA:2969:A:N7	39:LD:215:ASN:ND2	2.49	0.59
39:LD:27:ALA:O	39:LD:128:ARG:NH2	2.35	0.59
61:LT:90:ALA:O	61:LT:120:LYS:NZ	2.34	0.59
19:F:83:GLN:HE22	19:F:119:ALA:HB2	1.66	0.59
36:LA:2307:G:O2'	36:LA:2310:U:OP2	2.19	0.59
36:LA:2382:G:N7	52:LQ:91[A]:LYS:NZ	2.45	0.59
36:LA:1010:G:N2	47:LL:193:ASP:OD2	2.36	0.59
42:LG:122:VAL:O	42:LG:248:ARG:NH2	2.35	0.59
45:LJ:171:LYS:NZ	45:LJ:223:ALA:O	2.33	0.59
19:F:129:PHE:O	19:F:137:ARG:NH1	2.35	0.59
36:LA:1778:G:O2'	36:LA:1780:G:OP2	2.20	0.59
36:LA:1874:A:N7	55:Ln:20:ARG:NH1	2.50	0.59
36:LA:68:C:OP2	36:LA:301:G:N2	2.32	0.59
49:LN:70:ARG:NH1	49:LN:71:ALA:O	2.35	0.59
53:LR:107:LEU:HD23	53:LR:152:GLU:HG3	1.85	0.59
22:I:21:PHE:O	22:I:25:GLN:HB2	2.03	0.59
36:LA:2181:C:OP1	39:LD:193:ARG:NH2	2.32	0.59
38:LC:94:C:OP1	73:Lf:76:ASN:ND2	2.29	0.59
9:B:139:ASN:ND2	9:B:202:ALA:O	2.35	0.59
1:2:273:G:H1	1:2:283:U:H3	1.51	0.59
1:2:897:C:O2	18:Z:41:ARG:NH2	2.36	0.59
21:H:49:LYS:NZ	21:H:80:LYS:O	2.35	0.59
30:f:55:THR:HB	30:f:62:ILE:HD13	1.84	0.59
42:LG:126:GLU:HA	42:LG:196:ARG:HD2	1.85	0.59
81:EF:897:SER:HA	81:EF:901:LYS:HE2	1.85	0.59
1:2:446:A:OP1	8:S:59:ARG:NH1	2.36	0.59
9:B:94:THR:HG22	9:B:114:ILE:HG13	1.84	0.59
13:W:62:ARG:O	13:W:69:ARG:NH1	2.36	0.59
36:LA:743:C:O3'	54:Lm:66:ARG:NH2	2.36	0.59
47:LL:44:ASP:HA	47:LL:171:TRP:HE1	1.68	0.59
48:LM:133:ARG:NH1	48:LM:153:LYS:O	2.36	0.59
22:I:134:ARG:HD3	81:EF:182:LYS:HB2	1.85	0.59
47:LL:182:LEU:HD23	47:LL:185:ARG:HD3	1.84	0.59
54:Lm:176:ARG:HH12	64:LW:42:ARG:HH21	1.51	0.59
1:2:393:C:O2'	10:T:92:ARG:NH1	2.35	0.58
12:V:138:ASN:OD1	12:V:141:ARG:NH2	2.31	0.58
36:LA:836:A:O2'	79:LL:9:GLY:O	2.21	0.58
76:Li:122:ARG:NH1	76:Li:123:PRO:O	2.36	0.58
1:2:1565:C:OP1	21:H:41:ARG:NH1	2.32	0.58
6:R:236:PRO:O	24:a:33:GLN:NE2	2.36	0.58
28:K:35:ARG:O	28:K:37:GLN:NE2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:LA:2444:C:O2	36:LA:2503:G:N1	2.36	0.58
27:d:86:GLU:OE1	27:d:90:ARG:NH1	2.36	0.58
56:Lo:73:LYS:NZ	56:Lo:97:VAL:O	2.37	0.58
62:LU:55:GLU:HB3	62:LU:108:LYS:HB2	1.86	0.58
1:2:153:G:O6	27:d:128:LYS:NZ	2.36	0.58
1:2:623:A:N6	1:2:970:A:OP1	2.36	0.58
37:LB:77:G:N2	37:LB:102:A:OP2	2.35	0.58
1:2:572:C:OP1	26:c:109:ARG:NH1	2.35	0.58
45:LJ:162:LEU:HD23	51:LP:7:LEU:HD21	1.86	0.58
74:Lg:2:ALA:N	74:Lg:50:SER:HG	2.01	0.58
1:2:1673:G:O6	1:2:1728:A:N1	2.36	0.58
29:e:13:LYS:O	29:e:15:ARG:NH1	2.36	0.58
36:LA:408:A:N3	36:LA:655:C:O2'	2.33	0.58
37:LB:13:A:OP2	37:LB:67:G:N2	2.35	0.58
1:2:486:G:N2	1:2:501:U:O2'	2.37	0.58
4:Q:158:SER:HA	4:Q:161:ILE:HD12	1.84	0.58
36:LA:691:A:OP1	41:LF:46:LYS:NZ	2.32	0.58
36:LA:1551:C:HO2'	36:LA:2170:U:HO2'	1.51	0.58
46:LK:3:TYR:HA	56:Lo:142:GLN:HE22	1.67	0.58
64:LW:76:ASP:OD1	64:LW:76:ASP:N	2.36	0.58
1:2:458:G:OP1	27:d:109:LYS:NZ	2.36	0.58
36:LA:1369:A:OP1	64:LW:21:ARG:NH1	2.36	0.58
46:LK:137:SER:OG	46:LK:143:GLU:OE1	2.22	0.58
81:EF:775:ILE:HG23	81:EF:850:LYS:HZ1	1.69	0.58
25:b:15:ASN:ND2	25:b:72:CYS:O	2.36	0.58
37:LB:34:C:HO2'	42:LG:198:TYR:HH	1.49	0.58
81:EF:577:ASN:HD22	81:EF:702:ASN:HD22	1.52	0.58
29:e:37:LYS:HG2	29:e:70:LYS:HE2	1.86	0.58
36:LA:1899:G:O2'	36:LA:2334:U:O4	2.19	0.58
1:2:1388:A:OP2	20:G:32:LYS:NZ	2.36	0.57
13:W:59:LEU:HD22	13:W:69:ARG:HA	1.85	0.57
36:LA:1078:U:H4'	42:LG:46:THR:HG21	1.86	0.57
36:LA:1546:A:N7	51:LP:71:ARG:NH2	2.48	0.57
36:LA:2441:A:H2	36:LA:2506:U:H3	1.52	0.57
36:LA:3115:C:O2	36:LA:3117:C:N4	2.37	0.57
1:2:58:U:O2'	1:2:451:A:N3	2.35	0.57
1:2:636:A:H5''	25:b:31:SER:HB3	1.86	0.57
1:2:1114:G:O2'	1:2:1130:G:O6	2.22	0.57
23:J:35:GLU:OE2	23:J:89:ARG:NH1	2.37	0.57
36:LA:687:U:OP2	49:LN:36:ARG:NH2	2.36	0.57
81:EF:442:LYS:NZ	82:EF:1102:ATP:N3	2.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:127:G:N2	1:2:178:U:O2	2.38	0.57
1:2:936:G:OP1	1:2:1074:G:N2	2.34	0.57
36:LA:1723:A:OP1	55:Ln:128:LYS:NZ	2.37	0.57
12:V:57:ALA:HB2	12:V:177:GLY:HA2	1.86	0.57
21:H:63:GLN:HA	21:H:66:LEU:HG	1.87	0.57
36:LA:1737:U:O2	70:Lc:52:GLN:NE2	2.34	0.57
36:LA:2940:A:OP2	40:LE:2:SER:N	2.37	0.57
36:LA:3344:A:N6	36:LA:3361:G:O2'	2.38	0.57
39:LD:150:LEU:HD11	39:LD:156:LYS:HE2	1.86	0.57
81:EF:758:ARG:HE	81:EF:766:GLU:HG3	1.69	0.57
36:LA:212:G:OP2	62:LU:2:ALA:N	2.38	0.57
36:LA:860:G:OP1	79:Ll:17:ARG:NH2	2.38	0.57
36:LA:2948:C:OP1	40:LE:244:ARG:NH2	2.37	0.57
41:LF:329:PRO:HB2	44:LI:45:LEU:HD13	1.87	0.57
73:Lf:63:ARG:O	73:Lf:68:LYS:NZ	2.37	0.57
6:R:140:ARG:HH21	6:R:229:LEU:HD11	1.69	0.57
7:A:136:VAL:HG23	7:A:186:VAL:HG22	1.85	0.57
36:LA:729:C:O2'	54:Lm:79:LYS:NZ	2.36	0.57
36:LA:3041:U:OP1	59:Lr:12:ARG:NH1	2.37	0.57
36:LA:89:A:N7	54:Lm:171:LYS:NZ	2.52	0.57
7:A:134:CYS:SG	7:A:135:GLU:N	2.78	0.57
40:LE:368:GLY:O	60:LS:17:ARG:NH1	2.38	0.57
42:LG:214:ASP:HA	81:EF:689:GLN:HE22	1.70	0.57
1:2:905:A:H5''	18:Z:52:ARG:HG2	1.86	0.57
23:J:34:LEU:HD21	23:J:89:ARG:HD3	1.87	0.57
36:LA:1914:G:N2	55:Ln:81:ARG:O	2.35	0.57
41:LF:237:GLN:O	41:LF:246:ARG:NH1	2.38	0.57
81:EF:16:LYS:O	81:EF:65:ASN:ND2	2.38	0.57
1:2:217:A:N1	1:2:844:A:O2'	2.36	0.57
4:Q:23:PRO:HB2	4:Q:27:LYS:HE2	1.85	0.57
34:O:42:LEU:HB2	34:O:61:PHE:HB2	1.86	0.57
1:2:1126:G:OP1	77:Lj:15:ARG:NH1	2.38	0.56
1:2:1332:C:OP1	20:G:43:SER:OG	2.22	0.56
39:LD:47:GLN:HE21	39:LD:60:LYS:HD2	1.70	0.56
59:Lr:108:GLU:HG3	59:Lr:128:ARG:HG2	1.87	0.56
1:2:1433:G:N1	31:M:45:GLU:OE2	2.37	0.56
1:2:151:G:N3	10:T:13:GLN:NE2	2.54	0.56
1:2:477:A:OP2	32:g:28:LYS:NZ	2.39	0.56
1:2:1022:C:O2'	1:2:1125:A:N1	2.39	0.56
16:D:52:LEU:HA	16:D:57:ALA:HB2	1.86	0.56
36:LA:38:U:H4'	64:LW:32:ARG:HD2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:LA:1412:G:OP1	68:La:105:ARG:NH2	2.39	0.56
41:LF:188:ARG:NE	41:LF:197:ARG:O	2.32	0.56
45:LJ:152:LEU:HD23	45:LJ:178:ALA:HB3	1.88	0.56
81:EF:750:THR:HG23	81:EF:753:GLU:H	1.69	0.56
80:Sn:15:G:H22	80:Sn:48:C:N4	2.03	0.56
81:EF:544:SER:OG	81:EF:545:GLY:N	2.38	0.56
81:EF:668:VAL:HG12	81:EF:724:VAL:HA	1.88	0.56
16:D:54:ARG:NH2	33:N:127:GLY:O	2.38	0.56
36:LA:1018:G:N2	36:LA:1034:U:O2	2.34	0.56
36:LA:1057:A:OP1	44:LI:98:LYS:NZ	2.38	0.56
40:LE:14:LEU:HA	40:LE:17:LEU:HD13	1.88	0.56
45:LJ:162:LEU:HD21	51:LP:45:PRO:HG2	1.85	0.56
63:LV:27:LYS:HB3	63:LV:42:LEU:HB2	1.87	0.56
1:2:699:U:O2	1:2:739:G:O6	2.24	0.56
7:A:210:GLU:OE2	20:G:19:ARG:NH1	2.38	0.56
27:d:38:ASP:O	27:d:52:LYS:NZ	2.39	0.56
36:LA:533:A:O2'	36:LA:535:G:OP2	2.23	0.56
36:LA:1597:C:OP2	70:Lc:8:ARG:NH2	2.38	0.56
1:2:334:G:O6	12:V:5:ARG:NH2	2.35	0.56
1:2:539:G:N3	1:2:540:G:N2	2.53	0.56
12:V:107:THR:HA	12:V:110:ARG:HG2	1.88	0.56
36:LA:2183:A:H5''	39:LD:7:ASN:HB3	1.87	0.56
1:2:234:G:N2	1:2:235:G:N3	2.53	0.56
9:B:216:GLU:OE1	9:B:219:ARG:NH1	2.39	0.56
30:f:56:CYS:SG	30:f:57:GLU:N	2.78	0.56
36:LA:2471:U:O4	36:LA:2475:G:O6	2.24	0.56
41:LF:45:ASN:O	41:LF:110:ASN:ND2	2.39	0.56
27:d:57:VAL:HB	27:d:60:PHE:HE2	1.71	0.56
35:L:42:ARG:HH21	35:L:61:ARG:HH11	1.52	0.56
81:EF:574:ASP:O	81:EF:578:VAL:N	2.38	0.56
11:U:162:ILE:HA	11:U:165:LYS:HE2	1.87	0.56
28:K:95:HIS:ND1	28:K:96:SER:O	2.39	0.56
1:2:567:A:OP1	26:c:70:LYS:NZ	2.39	0.55
6:R:88:LYS:HD2	6:R:95:ARG:HD2	1.88	0.55
41:LF:57:GLY:HA3	41:LF:98:ARG:HB3	1.88	0.55
1:2:477:A:O2'	32:g:33:ARG:NH2	2.31	0.55
22:I:73:VAL:O	22:I:77:ASN:ND2	2.39	0.55
70:Lc:103:LYS:HD2	70:Lc:106:LYS:HE3	1.89	0.55
1:2:17:C:O2'	1:2:1137:A:N1	2.35	0.55
36:LA:504:A:O2'	41:LF:315:LYS:NZ	2.40	0.55
39:LD:242:ARG:NH1	39:LD:243:THR:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:Lm:62:VAL:HG13	54:Lm:66:ARG:HD3	1.88	0.55
9:B:133:VAL:HG12	9:B:198:LEU:HD13	1.88	0.55
39:LD:101:VAL:HG22	39:LD:165:VAL:HG22	1.88	0.55
1:2:4:C:OP2	6:R:200:SER:OG	2.20	0.55
36:LA:1494:U:OP1	75:Lh:42:ARG:NH1	2.33	0.55
1:2:61:A:O2'	1:2:62:A:O4'	2.25	0.55
40:LE:212:ASN:ND2	40:LE:353:GLU:OE1	2.40	0.55
1:2:868:G:H1	1:2:960:U:H3	1.54	0.55
1:2:1525:A:N3	1:2:1589:C:O2'	2.40	0.55
9:B:89:ILE:HD12	9:B:92:ARG:HD3	1.87	0.55
10:T:154:ARG:HG2	10:T:178:LEU:HD21	1.89	0.55
12:V:3:ILE:O	12:V:30:GLY:N	2.40	0.55
35:L:27:GLN:OE1	35:L:43:ASN:ND2	2.40	0.55
38:LC:126:A:O2'	38:LC:129:C:N4	2.39	0.55
36:LA:20:A:OP2	71:Ld:86:ARG:NH2	2.39	0.55
36:LA:2679:A:HO2'	48:LM:52:TYR:HH	1.54	0.55
36:LA:3092:C:O2'	36:LA:3094:A:OP2	2.22	0.55
39:LD:62:VAL:HG22	39:LD:73:GLU:HG3	1.88	0.55
66:LY:40:LYS:HB3	66:LY:101:LEU:HD21	1.89	0.55
81:EF:117:VAL:HG22	81:EF:128:LEU:HD11	1.89	0.55
81:EF:575:THR:HA	81:EF:578:VAL:HB	1.89	0.55
1:2:400:A:H5''	12:V:25:ARG:HA	1.89	0.55
3:P:56:LYS:NZ	24:a:70:ASN:OD1	2.30	0.55
36:LA:3303:G:O2'	36:LA:3305:A:N6	2.40	0.55
81:EF:672:GLU:O	81:EF:720:THR:OG1	2.24	0.55
1:2:299:A:OP1	8:S:30:ARG:NH1	2.33	0.55
3:P:140:ASN:ND2	24:a:31:SER:O	2.38	0.55
36:LA:329:U:N3	41:LF:54:GLU:OE2	2.37	0.55
37:LB:64:A:OP2	42:LG:289:LYS:NZ	2.33	0.55
41:LF:329:PRO:HG3	44:LI:41:ARG:HD2	1.88	0.55
1:2:1298:U:O3'	6:R:212:LYS:NZ	2.38	0.54
4:Q:2:ALA:N	18:Z:48:VAL:O	2.40	0.54
10:T:69:LEU:HD12	10:T:71:THR:H	1.72	0.54
36:LA:1011:A:OP1	47:LL:40:LYS:NZ	2.39	0.54
36:LA:1222:G:N2	36:LA:1285:G:O2'	2.40	0.54
81:EF:331:LEU:HD23	81:EF:333:HIS:H	1.72	0.54
4:Q:195:LYS:O	4:Q:199:ASN:ND2	2.41	0.54
22:I:138:GLN:NE2	81:EF:181:THR:O	2.40	0.54
1:2:849:C:OP1	55:Ln:162:ARG:NH2	2.40	0.54
1:2:930:A:N3	4:Q:111:ARG:NH2	2.53	0.54
1:2:1383:G:OP1	23:J:89:ARG:NH2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:O:42:LEU:HD11	34:O:68:VAL:HG21	1.90	0.54
36:LA:643:U:O2'	36:LA:1153:A:N1	2.38	0.54
36:LA:1181:U:O4	52:LQ:21[A]:SER:OG	2.24	0.54
36:LA:1886:A:O2'	40:LE:226:PHE:O	2.25	0.54
63:LV:88:ASP:O	63:LV:121:ARG:NH1	2.35	0.54
1:2:391:A:OP2	12:V:23:LYS:NZ	2.38	0.54
1:2:405:C:O2'	10:T:92:ARG:O	2.25	0.54
36:LA:638:C:OP1	68:La:21:HIS:NE2	2.32	0.54
36:LA:1721:U:OP2	55:Ln:124:TYR:OH	2.24	0.54
36:LA:2782:U:OP1	49:LN:185:LYS:NZ	2.40	0.54
44:LI:102:VAL:HG21	44:LI:129:LEU:HD12	1.90	0.54
73:Lf:29:VAL:O	73:Lf:32:LYS:NZ	2.35	0.54
1:2:1530:C:H1'	22:I:12:GLN:HE22	1.72	0.54
3:P:23:HIS:HD2	3:P:47:VAL:HG13	1.73	0.54
36:LA:1238:C:N4	36:LA:1245:A:OP1	2.40	0.54
42:LG:128:GLU:O	42:LG:164:LYS:NZ	2.39	0.54
1:2:1182:U:H4'	5:E:124:THR:HB	1.88	0.54
36:LA:2608:G:OP1	39:LD:2:GLY:N	2.41	0.54
71:Ld:76:GLN:O	71:Ld:81:ARG:NH2	2.41	0.54
54:Lm:178:ARG:HH11	64:LW:50:PRO:HG2	1.73	0.54
67:LZ:13:THR:OG1	67:LZ:72:ARG:NH1	2.35	0.54
1:2:590:C:OP1	32:g:42:ARG:NH2	2.35	0.54
44:LI:168:ILE:O	44:LI:172:ASN:ND2	2.41	0.54
81:EF:200:VAL:HG11	81:EF:205:ILE:HD11	1.88	0.54
1:2:57:G:OP2	27:d:116:LYS:NZ	2.41	0.54
36:LA:2631:U:OP2	57:Lp:4:SER:OG	2.26	0.54
1:2:1204:A:N3	31:M:10:HIS:NE2	2.50	0.54
1:2:1548:G:O2'	21:H:89:GLN:NE2	2.39	0.54
36:LA:1639:C:HO2'	36:LA:1737:U:HO2'	1.56	0.54
81:EF:918:VAL:HG13	81:EF:946:ILE:HB	1.89	0.54
1:2:395:U:H3	1:2:399:A:H62	1.55	0.53
1:2:1297:G:N2	1:2:1300:A:OP2	2.27	0.53
3:P:134:LYS:O	3:P:137:SER:OG	2.24	0.53
37:LB:45:A:OP1	42:LG:151:GLN:NE2	2.34	0.53
37:LB:72:A:O2'	37:LB:74:C:OP1	2.25	0.53
53:LR:172:GLN:NE2	69:Lb:60:ARG:O	2.38	0.53
1:2:869:A:H61	1:2:958:U:H3	1.55	0.53
1:2:1303:U:O2'	1:2:1322:A:OP2	2.25	0.53
6:R:170:ILE:HB	6:R:197:TYR:HB2	1.89	0.53
9:B:91:GLU:O	9:B:95:ASN:ND2	2.42	0.53
36:LA:86:G:O2'	36:LA:98:G:O6	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:LA:2896:A:OP1	76:Li:124:LYS:NZ	2.39	0.53
37:LB:28:C:OP1	48:LM:137:ARG:NH1	2.38	0.53
81:EF:153:SER:O	81:EF:195:LYS:NZ	2.41	0.53
36:LA:2679:A:O2'	48:LM:52:TYR:OH	2.24	0.53
36:LA:2848:G:OP1	76:Li:100:TYR:OH	2.24	0.53
44:LI:153:PHE:HD1	44:LI:162:PRO:HA	1.73	0.53
46:LK:92:TYR:HB2	46:LK:142:ASP:HB3	1.90	0.53
81:EF:811:TYR:OH	81:EF:841:ARG:NH1	2.41	0.53
34:O:132:LYS:HA	34:O:143:THR:HA	1.91	0.53
36:LA:3067:C:H3'	55:Ln:62:ARG:HH12	1.73	0.53
49:LN:4:SER:OG	49:LN:5:LYS:NZ	2.42	0.53
14:C:70:GLU:HA	14:C:73:VAL:HG12	1.90	0.53
36:LA:361:A:O2'	73:Lf:45:ARG:NH2	2.41	0.53
36:LA:2478:C:OP2	36:LA:2480:A:N6	2.42	0.53
36:LA:2716:U:H5'	78:Lk:8:ARG:HH22	1.74	0.53
47:LL:50:VAL:HG11	47:LL:149:VAL:HG22	1.90	0.53
36:LA:671:U:H5''	54:Lm:16:ARG:HH22	1.74	0.53
36:LA:1312:C:O2'	52:LQ:83[A]:ALA:O	2.26	0.53
36:LA:1492:G:N7	75:Lh:2:ALA:N	2.57	0.53
38:LC:65:A:O2'	71:Ld:10:ARG:NH2	2.42	0.53
81:EF:97:ASN:OD1	81:EF:100:ASN:ND2	2.42	0.53
36:LA:216:G:OP1	62:LU:16:ARG:NH1	2.42	0.53
59:Lr:87:ARG:NE	59:Lr:121:GLU:OE2	2.38	0.53
67:LZ:44:MET:O	67:LZ:77:ARG:NH1	2.42	0.53
41:LF:33:ASP:OD1	41:LF:33:ASP:N	2.40	0.53
19:F:35:PRO:HD2	19:F:38:LEU:HD12	1.91	0.53
23:J:40:ASN:HA	23:J:43:LYS:HG2	1.90	0.53
36:LA:1348:U:OP2	54:Lm:38:ARG:NH2	2.42	0.53
36:LA:2681:U:O2	48:LM:20:ASN:ND2	2.42	0.53
41:LF:152:VAL:HG21	41:LF:156:LEU:HD13	1.91	0.53
46:LK:167:VAL:HB	46:LK:172:ILE:HG22	1.91	0.53
1:2:396:G:N1	1:2:399:A:OP2	2.41	0.53
1:2:929:A:OP1	1:2:931:C:N4	2.42	0.53
6:R:153:SER:OG	6:R:154:LEU:N	2.42	0.53
36:LA:1621:A:N7	36:LA:1820:U:O4	2.42	0.53
36:LA:2552:C:H2'	66:LY:50:VAL:HG11	1.91	0.53
46:LK:173:ARG:NH1	76:Li:125:LYS:O	2.41	0.53
1:2:59:C:O2'	1:2:60:U:O4'	2.27	0.52
1:2:629:U:OP2	1:2:969:C:N4	2.41	0.52
25:b:79:PHE:O	25:b:124:LYS:HA	2.09	0.52
38:LC:150:G:O2'	45:LJ:59:GLN:NE2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:LI:74:SER:OG	44:LI:75:TYR:N	2.43	0.52
81:EF:612:TYR:HB3	81:EF:617:LEU:HD23	1.91	0.52
1:2:207:U:O2	12:V:178:ARG:NH2	2.41	0.52
1:2:220:A:OP2	1:2:831:U:O2'	2.26	0.52
1:2:930:A:H1'	4:Q:111:ARG:HH12	1.74	0.52
7:A:70:THR:HG22	7:A:86:LEU:HD13	1.91	0.52
34:O:153:GLN:OE1	34:O:155:ARG:NH1	2.41	0.52
36:LA:1833:G:O2'	75:Lh:3:ALA:O	2.26	0.52
41:LF:291:ASN:HA	41:LF:296:GLN:HE21	1.74	0.52
54:Lm:22:ASP:OD1	54:Lm:22:ASP:N	2.42	0.52
80:Sm:52:G:H1	80:Sm:62:C:H42	1.57	0.52
1:2:1611:A:O2'	9:B:95:ASN:O	2.27	0.52
34:O:12:THR:HG22	34:O:311:ARG:HG2	1.90	0.52
35:L:11:LYS:HE3	35:L:51:ASN:HA	1.91	0.52
36:LA:2461:A:O2'	36:LA:2485:A:N1	2.42	0.52
36:LA:2469:G:N1	36:LA:2477:G:O6	2.43	0.52
8:S:87:MET:HE1	8:S:236:ILE:HG21	1.91	0.52
15:X:122:ILE:HG13	15:X:143:SER:HB2	1.91	0.52
17:Y:76:LYS:HA	17:Y:81:ALA:HB2	1.91	0.52
36:LA:110:G:OP2	49:LN:73:ARG:NH1	2.38	0.52
36:LA:170:G:N2	36:LA:248:U:O2	2.43	0.52
36:LA:1488:G:O2'	70:Lc:10:ARG:O	2.27	0.52
37:LB:101:G:N7	56:Lo:52:LYS:NZ	2.57	0.52
53:LR:56:ARG:NH1	53:LR:75:GLU:OE2	2.38	0.52
80:Sn:15:G:N2	80:Sn:48:C:H42	2.07	0.52
81:EF:711:ASN:HB3	81:EF:717:LEU:HD13	1.92	0.52
10:T:3:LEU:HD13	10:T:18:ILE:HG13	1.92	0.52
16:D:82:PRO:HD3	33:N:113:LYS:HD2	1.92	0.52
21:H:57:ARG:HE	28:K:40:VAL:HG22	1.75	0.52
27:d:14:SER:HA	27:d:21:LYS:HG3	1.92	0.52
1:2:65:A:H2	1:2:84:A:H62	1.56	0.52
1:2:1568:C:OP1	21:H:36:LYS:NZ	2.43	0.52
22:I:18:TYR:HD1	22:I:135:ILE:HG21	1.75	0.52
45:LJ:134:TYR:HB3	45:LJ:190:VAL:HG11	1.91	0.52
51:LP:103:GLU:HG3	51:LP:160:GLU:HB2	1.92	0.52
1:2:1582:U:OP1	19:F:135:ARG:NH1	2.42	0.52
12:V:84:HIS:NE2	12:V:97:THR:OG1	2.36	0.52
36:LA:2675:C:N4	48:LM:22:SER:OG	2.43	0.52
14:C:57:THR:HA	14:C:65:TYR:O	2.09	0.52
34:O:200:ASN:ND2	34:O:239:GLU:OE2	2.42	0.52
36:LA:668:G:H1	36:LA:794:U:H3	1.56	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:LA:1024:G:H21	36:LA:1027:A:H62	1.58	0.52
36:LA:1597:C:H5'	36:LA:1696:A:H1'	1.92	0.52
36:LA:1605:A:O2'	36:LA:1607:U:OP2	2.26	0.52
36:LA:2353:G:H5''	53:LR:86:LYS:HB2	1.90	0.52
36:LA:3295:A:H5'	40:LE:119:TYR:HE1	1.75	0.52
49:LN:48:PRO:HG2	71:Ld:115:LYS:HD3	1.92	0.52
55:Ln:126:GLU:HG3	55:Ln:132:PHE:HE2	1.74	0.52
21:H:17:LEU:O	21:H:20:THR:OG1	2.26	0.52
23:J:80:GLU:OE1	31:M:44:ARG:NH1	2.42	0.52
36:LA:649:A:OP2	36:LA:2868:U:O2'	2.26	0.52
45:LJ:82:LEU:HD13	45:LJ:222:PHE:HE2	1.75	0.52
47:LL:156:ARG:HG3	47:LL:163:GLN:HB2	1.92	0.52
1:2:327:U:O2'	15:X:14:GLN:NE2	2.43	0.52
3:P:27:ARG:NH1	3:P:43:ASP:O	2.43	0.52
12:V:12:SER:HB3	12:V:18:ARG:HE	1.75	0.52
26:c:97:ASP:OD1	26:c:97:ASP:N	2.41	0.52
36:LA:1844:C:O2'	73:Lf:11:ARG:NH2	2.43	0.52
39:LD:30:ARG:O	39:LD:163:ARG:NH2	2.34	0.52
63:LV:102:GLU:H	63:LV:107:ARG:HH21	1.58	0.52
27:d:36:SER:N	27:d:39:GLU:OE2	2.39	0.51
36:LA:406:G:OP1	36:LA:1415:U:O2'	2.27	0.51
36:LA:1222:G:HO2'	36:LA:1285:G:H1	1.55	0.51
36:LA:1264:G:N2	36:LA:1265:U:O4	2.37	0.51
36:LA:3227:A:O3'	50:LO:133:LYS:NZ	2.43	0.51
36:LA:3379:C:H4'	40:LE:315:GLY:HA2	1.91	0.51
1:2:343:C:H2'	1:2:344:A:H8	1.74	0.51
1:2:511:A:H5''	13:W:172:VAL:HG13	1.92	0.51
1:2:856:A:N6	11:U:115:SER:O	2.31	0.51
1:2:1433:G:N2	31:M:42:CYS:SG	2.78	0.51
26:c:17:VAL:HG12	26:c:20:ARG:HH12	1.73	0.51
36:LA:89:A:OP2	54:Lm:170:ARG:NH2	2.43	0.51
1:2:123:G:OP1	8:S:77:ARG:NH2	2.44	0.51
1:2:1171:A:H2'	1:2:1172:G:C8	2.45	0.51
8:S:254:ARG:HG2	8:S:258:GLN:HE22	1.75	0.51
27:d:78:SER:OG	27:d:81:GLU:OE1	2.27	0.51
33:N:109:ASP:H	33:N:114:VAL:HG12	1.75	0.51
36:LA:1112:A:N3	36:LA:1370:G:O2'	2.42	0.51
1:2:451:A:N6	1:2:453:U:O2	2.43	0.51
1:2:814:A:O2'	55:Ln:166:ASN:ND2	2.44	0.51
1:2:1254:U:OP2	16:D:46:ARG:NH2	2.43	0.51
36:LA:218:G:O6	62:LU:62:SER:OG	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:LA:597:G:N2	41:LF:322:GLN:OE1	2.38	0.51
1:2:1487:A:OP1	31:M:34:TYR:OH	2.25	0.51
3:P:83:GLN:HG2	3:P:99:ALA:HB1	1.93	0.51
20:G:14:LYS:NZ	20:G:68:GLY:O	2.43	0.51
36:LA:508:U:H3	36:LA:583:G:H1	1.57	0.51
36:LA:3039:C:O2'	59:Lr:10:LYS:O	2.27	0.51
45:LJ:78:PHE:HD1	45:LJ:179:ILE:HD13	1.76	0.51
51:LP:23:GLN:NE2	51:LP:122:ASN:OD1	2.42	0.51
56:Lo:9:VAL:HG22	56:Lo:61:ILE:HG13	1.91	0.51
59:Lr:104:ASN:OD1	59:Lr:108:GLU:N	2.43	0.51
1:2:1688:U:H3	1:2:1713:G:H1	1.58	0.51
36:LA:542:G:O6	36:LA:550:A:N6	2.44	0.51
36:LA:2564:G:OP2	63:LV:55:LYS:NZ	2.43	0.51
37:LB:34:C:O2'	42:LG:198:TYR:OH	2.20	0.51
53:LR:22:LEU:HD12	53:LR:146:ILE:HD12	1.91	0.51
54:Lm:67:ILE:HG12	54:Lm:81:VAL:HG11	1.92	0.51
55:Ln:105:LEU:HD23	55:Ln:138:LEU:HD23	1.92	0.51
1:2:1236:A:N3	33:N:138:ARG:NH2	2.59	0.51
36:LA:2144:A:OP1	36:LA:2323:G:N2	2.37	0.51
39:LD:137:ILE:HD11	39:LD:149:ARG:HB2	1.93	0.51
44:LI:64:GLN:NE2	44:LI:68:ASP:OD1	2.43	0.51
61:LT:105:VAL:HG21	61:LT:135:ILE:HD13	1.91	0.51
36:LA:363:G:N2	41:LF:82:THR:OG1	2.44	0.51
9:B:200:ASN:HB3	9:B:208:SER:HB2	1.93	0.51
29:e:37:LYS:HA	29:e:71:LEU:O	2.11	0.51
36:LA:3395:G:N2	36:LA:3396:U:O4	2.40	0.51
1:2:896:U:OP1	4:Q:26:ARG:NH2	2.43	0.51
45:LJ:41:GLN:OE1	45:LJ:44:ARG:NH1	2.31	0.51
81:EF:355:PRO:O	81:EF:358:LYS:NZ	2.44	0.51
81:EF:921:GLU:H	81:EF:948:ILE:HG22	1.76	0.51
1:2:1337:A:OP1	19:F:123:ARG:NH2	2.40	0.50
4:Q:65:VAL:HG22	4:Q:87:ARG:HG3	1.93	0.50
42:LG:117:GLU:HG2	42:LG:118:THR:H	1.75	0.50
56:Lo:112:ALA:O	56:Lo:115:ARG:NH1	2.44	0.50
59:Lr:28:ASN:OD1	59:Lr:112:SER:N	2.39	0.50
70:Lc:38:LEU:O	70:Lc:58:ARG:NH1	2.44	0.50
81:EF:632:PRO:O	81:EF:635:LYS:NZ	2.38	0.50
5:E:14:THR:OG1	5:E:15:HIS:N	2.44	0.50
19:F:89:LEU:HG	19:F:105:LEU:HD21	1.93	0.50
36:LA:3070:A:OP1	55:Ln:62:ARG:NH2	2.37	0.50
36:LA:3210:A:OP1	50:LO:109:ARG:NH1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:LB:44:C:OP2	48:LM:137:ARG:NH2	2.39	0.50
47:LL:84:ALA:O	47:LL:144:ASN:ND2	2.45	0.50
49:LN:3:ILE:HG21	64:LW:45:MET:HE3	1.93	0.50
1:2:329:G:H2'	1:2:330:G:H8	1.75	0.50
1:2:634:G:N2	1:2:965:U:OP2	2.41	0.50
34:O:255:ALA:HB2	34:O:292:LEU:HD23	1.93	0.50
42:LG:75:LEU:O	42:LG:112:LYS:NZ	2.45	0.50
62:LU:74:TYR:HD2	62:LU:77:LYS:HB2	1.75	0.50
81:EF:401:ASP:O	81:EF:405:GLU:N	2.42	0.50
1:2:1558:U:OP2	1:2:1559:A:O2'	2.22	0.50
3:P:92:HIS:ND1	3:P:202:TYR:OH	2.36	0.50
42:LG:205:SER:HB3	42:LG:236:LEU:HD11	1.94	0.50
43:LH:71:VAL:HG11	43:LH:159:LEU:HB2	1.92	0.50
68:La:23:ASP:OD1	68:La:23:ASP:N	2.44	0.50
1:2:143:G:OP2	10:T:139:ASN:ND2	2.42	0.50
30:f:55:THR:OG1	30:f:56:CYS:N	2.45	0.50
36:LA:937:G:H5''	64:LW:29:PRO:HA	1.94	0.50
50:LO:23:ILE:HG21	50:LO:28:SER:HB2	1.94	0.50
53:LR:128:ARG:HD3	53:LR:136:ILE:HD12	1.93	0.50
81:EF:534:GLU:HG2	81:EF:535:MET:HG2	1.94	0.50
1:2:174:U:H3	1:2:266:A:N6	2.04	0.50
1:2:472:U:O2'	1:2:769:A:N3	2.40	0.50
1:2:478:A:N1	1:2:510:G:O6	2.45	0.50
1:2:1677:C:OP1	12:V:42:ARG:NH1	2.45	0.50
21:H:49:LYS:HD2	81:EF:301:ALA:HB2	1.94	0.50
36:LA:3306:U:OP1	40:LE:269:GLN:NE2	2.42	0.50
73:Lf:35:SER:O	73:Lf:45:ARG:NH1	2.44	0.50
1:2:1198:G:OP1	1:2:1199:G:O2'	2.26	0.50
36:LA:1705:U:O2	36:LA:1786:G:O2'	2.30	0.50
45:LJ:144:GLU:OE2	51:LP:6:TYR:OH	2.25	0.50
81:EF:817:LEU:N	81:EF:829:VAL:O	2.39	0.50
1:2:125:U:OP1	10:T:201:GLN:NE2	2.45	0.50
1:2:1470:C:H5''	1:2:1471:A:H5''	1.94	0.50
1:2:1474:G:OP1	9:B:109:LYS:NZ	2.45	0.50
3:P:30:GLN:HE22	3:P:149:LEU:HB3	1.76	0.50
3:P:103:THR:O	3:P:106:SER:OG	2.28	0.50
11:U:126:LEU:HD21	11:U:152:VAL:HG11	1.93	0.50
36:LA:424:G:O2'	68:La:23:ASP:OD2	2.27	0.50
36:LA:929:A:O2'	73:Lf:49:TRP:O	2.30	0.50
68:La:59:SER:HB2	68:La:64:LYS:HE2	1.94	0.50
36:LA:519:A:O5'	44:LI:70:LYS:NZ	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:LA:938:C:OP2	64:LW:26:ARG:NH1	2.45	0.50
38:LC:83:C:O2	62:LU:51:ARG:NH2	2.45	0.50
56:Lo:132:THR:HB	56:Lo:144:LEU:HD13	1.92	0.50
60:LS:46:PRO:HB2	60:LS:54:LEU:HD23	1.94	0.50
81:EF:222:VAL:HG21	81:EF:252:ARG:HG2	1.92	0.50
8:S:11:ARG:HH22	8:S:20:LEU:HB3	1.76	0.49
34:O:108:SER:OG	34:O:128:ASP:N	2.45	0.49
37:LB:44:C:H4'	42:LG:152:ARG:HG3	1.94	0.49
1:2:1211:A:N3	5:E:97:TYR:OH	2.43	0.49
34:O:156:VAL:HG12	34:O:169:ILE:HG22	1.93	0.49
36:LA:1802:C:O2'	70:Lc:59:PRO:O	2.28	0.49
38:LC:43:A:H62	73:Lf:65:ARG:HH12	1.59	0.49
41:LF:35:VAL:HG21	41:LF:244:LEU:HD21	1.93	0.49
81:EF:460:ILE:HG12	81:EF:610:ILE:HB	1.94	0.49
1:2:1466:G:O2'	1:2:1602:C:OP1	2.29	0.49
1:2:1483:A:H4'	19:F:72:GLY:H	1.77	0.49
8:S:249:ALA:HA	8:S:252:ARG:HG2	1.94	0.49
25:b:73:GLY:O	25:b:127:GLY:HA3	2.12	0.49
36:LA:144:A:OP1	45:LJ:193:LYS:NZ	2.43	0.49
36:LA:1382:G:OP2	41:LF:188:ARG:NH1	2.38	0.49
36:LA:3242:G:O6	40:LE:150:ARG:NH2	2.45	0.49
41:LF:39:PHE:HA	41:LF:42:VAL:HG12	1.94	0.49
48:LM:82:ARG:HH21	48:LM:113:GLY:HA3	1.76	0.49
49:LN:170:LEU:HB3	72:Le:9:ILE:HD11	1.94	0.49
74:Lg:32:ASN:OD1	74:Lg:33:LYS:N	2.46	0.49
81:EF:228:LEU:HA	81:EF:231:ALA:HB3	1.95	0.49
1:2:1067:C:H5''	4:Q:150:VAL:HG22	1.93	0.49
1:2:1359:C:OP1	22:I:130:ARG:NH2	2.45	0.49
1:2:1794:A:OP2	29:e:4:LYS:NZ	2.38	0.49
11:U:51:VAL:HG23	11:U:53:GLY:H	1.77	0.49
18:Z:92:LYS:HE3	18:Z:122:PRO:HD2	1.94	0.49
34:O:177:MET:HE3	34:O:191:ASP:HB3	1.94	0.49
36:LA:2439:A:H2'	36:LA:2440:G:C8	2.48	0.49
81:EF:735:ILE:HD12	81:EF:905:VAL:HG22	1.92	0.49
16:D:81:ASP:HA	33:N:113:LYS:HD2	1.94	0.49
36:LA:551:A:O2'	36:LA:552:G:O4'	2.30	0.49
36:LA:936:A:OP1	64:LW:32:ARG:NH2	2.45	0.49
36:LA:2282:U:OP1	36:LA:2973:G:O2'	2.26	0.49
38:LC:13:A:O2'	53:LR:121:GLN:O	2.24	0.49
16:D:69:ALA:HA	16:D:72:ILE:HD13	1.95	0.49
36:LA:2216:G:OP1	72:Le:75:LYS:NZ	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:LA:2737:C:O2'	65:LX:36:ASP:OD1	2.30	0.49
38:LC:52:A:H62	75:Lh:27:ILE:HD13	1.76	0.49
41:LF:261:VAL:O	41:LF:271:LYS:NZ	2.45	0.49
6:R:174:ARG:HD2	13:W:94:ASP:HB2	1.94	0.49
36:LA:764:U:O2'	36:LA:766:U:OP2	2.27	0.49
36:LA:1813:A:O2'	36:LA:1816:A:N3	2.36	0.49
42:LG:41:LYS:NZ	57:Lp:30:TYR:O	2.45	0.49
55:Ln:25:ASP:OD1	55:Ln:25:ASP:N	2.45	0.49
1:2:174:U:O4	1:2:266:A:N7	2.46	0.49
1:2:1496:U:O2'	1:2:1519:U:O2'	2.21	0.49
8:S:141:THR:OG1	8:S:143:ASP:OD1	2.27	0.49
15:X:76:VAL:HA	15:X:119:VAL:HG13	1.95	0.49
36:LA:1410:U:H4'	68:La:75:LEU:HD11	1.93	0.49
36:LA:1521:G:O6	75:Lh:17:LYS:NZ	2.46	0.49
36:LA:1693:C:HO2'	36:LA:1772:U:HO2'	1.57	0.49
69:Lb:14:LEU:HD11	69:Lb:31:LYS:HB2	1.95	0.49
1:2:247:A:O2'	15:X:37:ASN:O	2.25	0.49
1:2:332:U:OP1	12:V:31:ARG:NH1	2.39	0.49
1:2:1312:A:OP1	20:G:2:GLY:N	2.45	0.49
8:S:193:GLY:O	8:S:211:LYS:N	2.40	0.49
19:F:41:PRO:HB2	19:F:44:LEU:HB2	1.94	0.49
21:H:45:LEU:HD21	21:H:81:ILE:HG23	1.93	0.49
36:LA:2876:C:O2'	80:Sm:75:C:O2	2.30	0.49
36:LA:3184:A:N3	36:LA:3187:A:O2'	2.42	0.49
74:Lg:65:LEU:O	74:Lg:68:SER:OG	2.29	0.49
1:2:872:G:H1'	30:f:68:GLY:H	1.78	0.49
1:2:974:A:O3'	17:Y:112:LYS:NZ	2.38	0.49
1:2:1564:U:OP1	22:I:38:LYS:NZ	2.35	0.49
6:R:140:ARG:NH2	6:R:226:THR:OG1	2.46	0.49
13:W:87:SER:OG	13:W:88:GLU:N	2.45	0.49
14:C:47:GLN:O	14:C:50:THR:OG1	2.28	0.49
33:N:123:ASN:ND2	33:N:144:CYS:SG	2.86	0.49
36:LA:598:A:H1'	41:LF:322:GLN:HE22	1.78	0.49
36:LA:1562:C:O2'	36:LA:1563:C:O4'	2.30	0.49
39:LD:117:GLU:OE2	39:LD:163:ARG:NE	2.41	0.49
66:LY:9:SER:OG	66:LY:10:ILE:N	2.45	0.49
75:Lh:5:LYS:HD2	75:Lh:10:LYS:HG3	1.95	0.49
1:2:554:C:N4	1:2:571:G:O6	2.46	0.48
4:Q:8:ARG:HD3	4:Q:11:LYS:HB2	1.95	0.48
4:Q:92:GLN:NE2	4:Q:229:MET:SD	2.86	0.48
36:LA:503:C:O2	43:LH:23:LYS:NZ	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:LA:3344:A:H2	36:LA:3361:G:H21	1.60	0.48
77:Lj:8:LYS:HD3	77:Lj:12:ARG:HH21	1.77	0.48
1:2:835:U:H2'	1:2:836:U:H5	1.77	0.48
3:P:105:GLY:N	3:P:135:GLU:OE2	2.46	0.48
49:LN:179:PHE:O	49:LN:183:ARG:NH1	2.46	0.48
52:LQ:126[A]:VAL:O	56:Lo:154:HIS:NE2	2.39	0.48
52:LQ:157[A]:GLU:OE1	52:LQ:160[A]:ARG:NH2	2.43	0.48
75:Lh:42:ARG:HG2	75:Lh:47:THR:HG23	1.94	0.48
1:2:471:A:OP1	13:W:10:LYS:NZ	2.45	0.48
37:LB:12:U:OP2	37:LB:68:C:O2'	2.30	0.48
57:Lp:68:THR:OG1	57:Lp:71:SER:OG	2.28	0.48
1:2:123:G:H21	8:S:146:THR:HG21	1.78	0.48
1:2:566:C:O2	32:g:13:LYS:NZ	2.43	0.48
8:S:139:VAL:HG13	8:S:150:PRO:HG3	1.96	0.48
14:C:37:THR:HG22	14:C:38:LYS:H	1.78	0.48
36:LA:538:G:H1	36:LA:553:U:H3	1.61	0.48
36:LA:1156:C:OP2	44:LI:94:LYS:NZ	2.43	0.48
36:LA:1268:G:O2'	36:LA:1269:U:O2	2.29	0.48
36:LA:2785:A:O2'	78:Lk:41:ARG:NH2	2.46	0.48
40:LE:346:THR:OG1	40:LE:347:SER:N	2.45	0.48
41:LF:8:VAL:HG23	41:LF:151:VAL:HG12	1.94	0.48
1:2:463:U:O2'	1:2:527:A:N6	2.47	0.48
1:2:1319:A:OP2	20:G:67:ARG:NH1	2.46	0.48
36:LA:1201:C:N4	36:LA:2857:C:OP1	2.36	0.48
36:LA:2890:A:O2'	36:LA:2933:A:N3	2.43	0.48
36:LA:3068:U:OP2	55:Ln:62:ARG:NH1	2.42	0.48
39:LD:96:LEU:HD23	79:Ll:83:ILE:HG23	1.94	0.48
81:EF:92:PRO:HA	81:EF:95:CYS:HB2	1.95	0.48
81:EF:275:LEU:HD21	81:EF:438:ALA:HB2	1.95	0.48
24:a:36:VAL:HB	24:a:51:VAL:HG23	1.95	0.48
43:LH:165:LEU:O	69:Lb:4:SER:OG	2.31	0.48
47:LL:30:LYS:HG2	47:LL:66:GLU:HG2	1.94	0.48
48:LM:61:ARG:NH2	80:Sn:56:C:OP1	2.44	0.48
69:Lb:47:LYS:NZ	69:Lb:102:LEU:O	2.45	0.48
7:A:116:ARG:HG2	7:A:150:MET:HE1	1.95	0.48
36:LA:92:G:O5'	78:Lk:46:LYS:NZ	2.47	0.48
52:LQ:37[A]:ARG:HH21	52:LQ:160[A]:ARG:HH22	1.62	0.48
69:Lb:37:THR:OG1	69:Lb:39:GLN:OE1	2.29	0.48
1:2:271:A:H62	10:T:182:GLN:HE22	1.61	0.48
1:2:765:G:N1	13:W:149:ARG:HD3	2.29	0.48
1:2:1255:G:N7	16:D:46:ARG:NH1	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:123:TYR:OH	21:H:126:ARG:NH1	2.47	0.48
36:LA:872:U:O2'	36:LA:1908:A:OP1	2.30	0.48
45:LJ:42:PRO:HD2	45:LJ:44:ARG:NH1	2.28	0.48
1:2:938:G:N2	1:2:941:A:OP2	2.42	0.48
1:2:1099:U:O4	6:R:168:ARG:NH1	2.47	0.48
6:R:59:HIS:NE2	6:R:237:VAL:O	2.47	0.48
19:F:79:TYR:HD1	19:F:82:ARG:HD3	1.79	0.48
36:LA:598:A:H4'	41:LF:325:LEU:HD13	1.96	0.48
36:LA:2941:A:OP2	40:LE:256:HIS:ND1	2.46	0.48
39:LD:116:VAL:HB	39:LD:126:LEU:HB2	1.94	0.48
47:LL:160:PRO:O	47:LL:163:GLN:NE2	2.45	0.48
73:Lf:64:MET:HB3	73:Lf:67:LEU:HB3	1.95	0.48
1:2:146:U:H2'	1:2:147:A:H8	1.78	0.48
17:Y:6:SER:OG	17:Y:7:ALA:N	2.46	0.48
19:F:64:ASP:OD1	19:F:64:ASP:N	2.45	0.48
36:LA:3042:U:OP2	36:LA:3092:C:N4	2.44	0.48
36:LA:3243:A:H4'	40:LE:95:THR:HG22	1.94	0.48
42:LG:184:ASP:OD2	42:LG:187:THR:OG1	2.31	0.48
1:2:1353:U:H3	1:2:1372:U:H3	1.61	0.47
36:LA:315:C:OP2	72:Le:28:TYR:OH	2.28	0.47
36:LA:1047:A:N3	36:LA:2633:U:O2'	2.43	0.47
37:LB:29:C:O2'	37:LB:51:A:N1	2.36	0.47
1:2:381:C:O2'	1:2:755:A:N1	2.44	0.47
17:Y:90:TYR:HA	17:Y:93:LYS:HG2	1.95	0.47
36:LA:427:C:OP2	68:La:15:LYS:NZ	2.39	0.47
39:LD:95:SER:OG	39:LD:97:ASN:OD1	2.32	0.47
41:LF:233:LEU:HD22	41:LF:238:LEU:HD11	1.96	0.47
50:LO:45:LEU:HD22	56:Lo:72:VAL:HG23	1.96	0.47
1:2:1688:U:H3	1:2:1713:G:H22	1.62	0.47
20:G:5:ARG:HG3	20:G:10:LYS:HE2	1.96	0.47
36:LA:884:A:OP2	36:LA:2139:A:N6	2.47	0.47
36:LA:1334:U:H5''	44:LI:206:LYS:HB3	1.96	0.47
38:LC:61:A:H3'	71:Ld:48:ARG:HH22	1.79	0.47
1:2:871:G:H2'	1:2:872:G:C8	2.49	0.47
20:G:5:ARG:HD3	20:G:9:VAL:HG11	1.97	0.47
36:LA:68:C:N4	36:LA:314:U:O2'	2.47	0.47
36:LA:264:G:O6	72:Le:29:LYS:NZ	2.45	0.47
36:LA:2722:U:OP1	65:LX:33:LYS:NZ	2.46	0.47
46:LK:77:ASN:HA	46:LK:80:THR:HG22	1.96	0.47
63:LV:78:ASN:OD1	66:LY:35:ARG:NH2	2.35	0.47
1:2:738:G:H3'	1:2:739:G:H5''	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1477:G:H2'	1:2:1478:G:H8	1.80	0.47
1:2:1667:A:HO2'	36:LA:1935:G:HO2'	1.63	0.47
6:R:81:MET:HB2	6:R:101:VAL:HG13	1.96	0.47
36:LA:339:C:OP1	36:LA:1380:G:O2'	2.33	0.47
40:LE:216:ASP:OD2	40:LE:339:ARG:NH2	2.48	0.47
79:LI:46:THR:OG1	79:LI:57:CYS:SG	2.70	0.47
81:EF:347:LEU:HD23	81:EF:402:ILE:HG23	1.95	0.47
81:EF:902:VAL:HA	81:EF:905:VAL:HG12	1.96	0.47
1:2:209:U:H2'	1:2:210:A:H8	1.79	0.47
1:2:1170:G:H21	1:2:1571:C:H4'	1.78	0.47
1:2:1684:U:H3	1:2:1717:G:H1	1.63	0.47
5:E:80:MET:HE2	5:E:83:MET:HB2	1.97	0.47
14:C:54:TYR:HB3	14:C:72:GLY:HA2	1.97	0.47
34:O:5:GLU:HB2	34:O:316:MET:HB3	1.97	0.47
36:LA:69:C:OP1	51:LP:178:HIS:ND1	2.36	0.47
36:LA:292:U:OP2	51:LP:68:ARG:NH1	2.47	0.47
36:LA:3212:C:OP2	50:LO:124:ARG:NH2	2.48	0.47
39:LD:6:ARG:HH12	39:LD:199:THR:H	1.62	0.47
41:LF:206:LEU:HD23	41:LF:248:VAL:HG22	1.96	0.47
81:EF:259:THR:HA	81:EF:262:LYS:HB2	1.95	0.47
1:2:1483:A:OP2	1:2:1521:G:N2	2.46	0.47
6:R:142:GLY:HA2	24:a:1:MET:HE1	1.96	0.47
14:C:30:ALA:HA	14:C:38:LYS:HA	1.96	0.47
20:G:5:ARG:HD2	20:G:53:TYR:CD1	2.50	0.47
34:O:305:TYR:HB2	34:O:309:VAL:HG23	1.96	0.47
36:LA:120:G:N2	45:LJ:123:GLN:O	2.47	0.47
36:LA:284:A:OP2	78:Lk:41:ARG:NH1	2.48	0.47
36:LA:664:U:H2'	36:LA:665:A:C8	2.50	0.47
36:LA:2482:U:H2'	36:LA:2483:G:H8	1.79	0.47
47:LL:54:SER:OG	47:LL:130:ASP:O	2.32	0.47
67:LZ:51:LEU:HB3	67:LZ:55:LEU:HD23	1.96	0.47
81:EF:346:GLU:HB3	81:EF:409:ARG:HH12	1.80	0.47
1:2:966:A:H5''	17:Y:4:MET:HE1	1.97	0.47
22:I:86:ARG:HD2	22:I:92:LYS:HE2	1.96	0.47
25:b:75:ILE:N	25:b:126:LEU:O	2.39	0.47
35:L:30:VAL:HG23	35:L:40:ILE:HG23	1.97	0.47
36:LA:910:G:O6	39:LD:3:ARG:NH1	2.46	0.47
36:LA:2875:U:OP2	36:LA:2945:G:N1	2.34	0.47
36:LA:3000:A:O2'	40:LE:118:PHE:O	2.33	0.47
40:LE:183:LEU:O	40:LE:191:LYS:NZ	2.48	0.47
42:LG:163:LEU:HD21	42:LG:175:HIS:CG	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:LJ:83:ASP:OD1	45:LJ:83:ASP:N	2.48	0.47
46:LK:57:VAL:HG12	46:LK:68:LEU:HD13	1.97	0.47
58:Lq:89:LEU:HB3	58:Lq:93:ILE:HD12	1.97	0.47
1:2:698:U:H3	1:2:741:C:H42	1.63	0.47
7:A:9:ARG:HA	7:A:12:VAL:HG22	1.97	0.47
32:g:35:TYR:HA	32:g:38:LEU:HD23	1.96	0.47
36:LA:1084:A:H5''	57:Lp:35:LYS:HZ1	1.80	0.47
47:LL:61:SER:OG	47:LL:63:GLU:OE1	2.25	0.47
50:LO:37:GLU:HG3	50:LO:75:GLY:H	1.79	0.47
53:LR:10:ASN:O	53:LR:14:SER:OG	2.26	0.47
66:LY:17:VAL:HG11	66:LY:92:ILE:HD12	1.97	0.47
1:2:229:U:O4	1:2:237:C:N3	2.48	0.47
7:A:162:GLN:OE1	7:A:165:ASN:ND2	2.47	0.47
7:A:224:ASP:OD2	34:O:228:LYS:NZ	2.48	0.47
36:LA:2549:G:N2	36:LA:2549:G:OP2	2.48	0.47
38:LC:103:G:OP1	38:LC:110:C:N4	2.48	0.47
1:2:924:A:O2'	1:2:987:G:OP1	2.28	0.46
1:2:1477:G:H4'	22:I:47:PRO:HA	1.97	0.46
9:B:58:LEU:HD12	9:B:138:THR:HG22	1.97	0.46
34:O:224:ASN:O	34:O:228:LYS:N	2.47	0.46
36:LA:2720:G:OP2	54:Lm:180:ARG:NH1	2.47	0.46
38:LC:63:G:H1	38:LC:97:A:H61	1.63	0.46
8:S:207:LEU:HD22	8:S:219:VAL:HG22	1.97	0.46
55:Ln:182:ASP:OD1	55:Ln:183:ALA:N	2.48	0.46
67:LZ:26:LYS:HA	67:LZ:64:VAL:HG11	1.96	0.46
81:EF:376:ILE:O	81:EF:382:TRP:NE1	2.46	0.46
1:2:886:U:OP2	4:Q:216:LYS:NZ	2.48	0.46
14:C:56:LYS:O	14:C:66:TYR:HA	2.14	0.46
26:c:111:GLY:HA2	26:c:121:ARG:HD3	1.98	0.46
36:LA:1178:G:N3	36:LA:1328:C:O2'	2.44	0.46
1:2:990:C:H1'	18:Z:127:ARG:HD3	1.98	0.46
19:F:99:GLU:HB2	34:O:57:PRO:O	2.15	0.46
34:O:117:LYS:HG3	34:O:118:LYS:HG2	1.97	0.46
36:LA:1512:U:O2'	55:Ln:5:ARG:NH2	2.46	0.46
36:LA:2854:U:OP2	47:LL:3:ARG:NH2	2.48	0.46
59:Lr:18:PRO:HA	59:Lr:51:ALA:HA	1.97	0.46
72:Le:57:LEU:HD11	72:Le:73:ALA:HB2	1.97	0.46
81:EF:598:ASP:HB3	81:EF:601:PHE:HB3	1.97	0.46
1:2:307:G:OP1	15:X:90:TYR:OH	2.33	0.46
36:LA:2514:U:OP2	36:LA:2586:G:N2	2.49	0.46
43:LH:35:VAL:O	43:LH:38:THR:OG1	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:EF:310:LEU:HD22	81:EF:314:LYS:HE2	1.98	0.46
81:EF:486:GLN:OE1	81:EF:491:THR:OG1	2.34	0.46
1:2:1175:U:H2'	1:2:1176:G:H8	1.80	0.46
7:A:67:ASN:O	7:A:70:THR:OG1	2.30	0.46
11:U:10:SER:OG	11:U:11:GLN:N	2.48	0.46
22:I:131:ASP:HB2	81:EF:181:THR:HG21	1.96	0.46
36:LA:2727:A:OP2	36:LA:2728:G:N2	2.43	0.46
36:LA:2767:U:O2'	78:Lk:30:ALA:O	2.26	0.46
41:LF:283:THR:OG1	41:LF:288:ARG:NH2	2.49	0.46
1:2:932:U:OP2	4:Q:155:TYR:OH	2.33	0.46
11:U:22:GLN:HA	11:U:25:VAL:HG22	1.98	0.46
36:LA:1190:A:H2'	52:LQ:49[A]:ARG:HH12	1.79	0.46
44:LI:110:ARG:HH21	54:Lm:3:ILE:HD12	1.81	0.46
45:LJ:54:GLU:HG3	45:LJ:57:ARG:HH21	1.81	0.46
51:LP:122:ASN:HB3	51:LP:129:TYR:HD2	1.81	0.46
1:2:1558:U:O4	5:E:81:ARG:NH2	2.49	0.46
3:P:150:ASP:OD2	3:P:165:ARG:NH2	2.48	0.46
4:Q:78:ASP:OD1	4:Q:79:HIS:ND1	2.48	0.46
21:H:53:ASP:OD2	21:H:56:LYS:N	2.49	0.46
25:b:73:GLY:O	25:b:127:GLY:CA	2.64	0.46
36:LA:1159:A:H5''	44:LI:93:ASN:HD21	1.80	0.46
1:2:477:A:H2'	1:2:478:A:H8	1.81	0.46
1:2:1334:U:O2'	23:J:85:ARG:NH2	2.49	0.46
8:S:98:ASN:HB2	8:S:114:ILE:O	2.16	0.46
36:LA:3181:C:HO2'	52:LQ:164[A]:SER:HG	1.60	0.46
41:LF:45:ASN:HA	41:LF:110:ASN:HD22	1.81	0.46
52:LQ:54[A]:TYR:OH	52:LQ:73[A]:PHE:O	2.32	0.46
54:Lm:80:THR:HG23	54:Lm:100:THR:HG23	1.97	0.46
67:LZ:75:ILE:HG12	67:LZ:93:VAL:HG22	1.98	0.46
1:2:551:G:H2'	1:2:552:G:H8	1.81	0.46
11:U:24:PHE:HE1	11:U:77:LEU:HD21	1.80	0.46
23:J:68:ARG:HH12	23:J:77:LYS:HG3	1.80	0.46
36:LA:36:C:OP2	51:LP:83:LYS:NZ	2.43	0.46
36:LA:1084:A:H5''	57:Lp:35:LYS:NZ	2.31	0.46
38:LC:72:A:H61	38:LC:79:A:H61	1.64	0.46
81:EF:204:ASP:HB3	81:EF:207:ARG:HH12	1.81	0.46
1:2:815:G:HO2'	55:Ln:162:ARG:NH2	2.12	0.45
5:E:22:LEU:HD23	5:E:22:LEU:HA	1.77	0.45
10:T:22:HIS:HA	10:T:25:ARG:HE	1.81	0.45
36:LA:1544:G:O2'	36:LA:2167:A:N3	2.47	0.45
36:LA:1601:U:OP1	55:Ln:42:ARG:NH2	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:LH:102:ASN:HD21	43:LH:104:GLU:HG3	1.81	0.45
67:LZ:23:VAL:HB	67:LZ:28:ARG:HE	1.81	0.45
10:T:47:GLY:O	10:T:115:LYS:NZ	2.43	0.45
13:W:151:ASP:O	13:W:155:HIS:ND1	2.41	0.45
16:D:31:VAL:HA	16:D:34:THR:HG22	1.98	0.45
21:H:17:LEU:HD12	21:H:22:VAL:HG21	1.98	0.45
36:LA:96:G:H5'	49:LN:15:ARG:HE	1.80	0.45
37:LB:64:A:N7	47:LL:209:ASN:ND2	2.64	0.45
7:A:109:LEU:HB3	7:A:177:MET:HE1	1.98	0.45
36:LA:2245:C:O2'	39:LD:220:GLY:O	2.34	0.45
36:LA:3329:U:H5''	40:LE:308:MET:HE2	1.97	0.45
81:EF:735:ILE:HD11	81:EF:909:GLY:HA3	1.98	0.45
1:2:219:A:H61	1:2:842:C:H42	1.64	0.45
1:2:738:G:H5'	8:S:200:ARG:HH12	1.81	0.45
1:2:1410:A:H5''	19:F:118:ILE:HG23	1.97	0.45
15:X:123:VAL:HG12	15:X:142:VAL:HG23	1.98	0.45
36:LA:113:C:OP1	51:LP:147:ARG:NE	2.38	0.45
36:LA:2947:G:OP1	36:LA:2982:A:N6	2.43	0.45
47:LL:181:TYR:CE2	47:LL:185:ARG:HD2	2.51	0.45
63:LV:73:LYS:HG3	63:LV:75:VAL:HG22	1.98	0.45
78:Lk:45:ARG:O	78:Lk:48:SER:OG	2.30	0.45
1:2:1029:U:OP2	29:e:12:LYS:NZ	2.49	0.45
1:2:1217:A:O3'	14:C:44:LYS:NZ	2.41	0.45
1:2:1226:A:H2'	16:D:116:VAL:HG11	1.99	0.45
15:X:33:ARG:NH2	15:X:51:GLY:O	2.49	0.45
26:c:68:ILE:HG22	26:c:70:LYS:HD3	1.98	0.45
36:LA:1369:A:H5''	64:LW:21:ARG:HH11	1.82	0.45
37:LB:39:C:H4'	48:LM:44:THR:HG23	1.98	0.45
40:LE:220:VAL:O	40:LE:334:ARG:NH1	2.50	0.45
46:LK:138:THR:OG1	46:LK:139:ASN:N	2.49	0.45
81:EF:792:THR:OG1	81:EF:794:ARG:NE	2.45	0.45
1:2:587:C:OP1	32:g:26:LYS:NZ	2.49	0.45
1:2:637:C:O2	11:U:114:ARG:NH2	2.38	0.45
1:2:1315:U:OP2	1:2:1328:G:N1	2.36	0.45
1:2:1345:A:H5'	23:J:53:LYS:HD2	1.98	0.45
1:2:1630:U:O2'	1:2:1764:C:O2'	2.30	0.45
1:2:1673:G:OP1	10:T:94:ARG:NH2	2.49	0.45
17:Y:13:SER:OG	17:Y:14:SER:N	2.50	0.45
27:d:23:PHE:HE1	27:d:75:VAL:HG13	1.81	0.45
36:LA:1590:G:OP1	70:Lc:17:SER:OG	2.34	0.45
36:LA:2703:A:N6	42:LG:28:THR:O	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:LA:3121:U:OP2	76:Li:111:ARG:NE	2.47	0.45
40:LE:10:ARG:NH1	40:LE:263:SER:O	2.49	0.45
42:LG:197:SER:O	42:LG:202:GLY:N	2.50	0.45
43:LH:2:THR:HG21	43:LH:5:GLN:HA	1.99	0.45
49:LN:106:GLN:NE2	49:LN:110:ASP:OD1	2.43	0.45
57:Lp:42:ILE:HD11	57:Lp:74:VAL:HG11	1.98	0.45
81:EF:549:MET:HE3	81:EF:571:ASN:HB2	1.98	0.45
18:Z:128:LYS:HE3	29:e:27:SER:HB2	1.99	0.45
36:LA:509:U:H3	36:LA:582:G:H1	1.64	0.45
36:LA:1621:A:H62	36:LA:1820:U:H3	1.65	0.45
41:LF:150:LEU:HD23	41:LF:249:ILE:HG12	1.99	0.45
44:LI:219:LYS:O	44:LI:221:LYS:N	2.50	0.45
61:LT:57:LEU:HG	61:LT:62:VAL:HG12	1.99	0.45
10:T:159:ARG:HE	10:T:170:THR:HG21	1.82	0.45
16:D:59:LEU:HD23	16:D:89:ILE:HD11	1.99	0.45
18:Z:78:ALA:HB2	18:Z:111:ARG:HB2	1.98	0.45
25:b:41:MET:HG2	25:b:129:VAL:HG21	1.97	0.45
30:f:33:LEU:HD23	30:f:81:ARG:HA	1.99	0.45
36:LA:675:C:O2'	36:LA:679:U:OP1	2.33	0.45
36:LA:1141:C:O2'	36:LA:1153:A:N3	2.50	0.45
37:LB:38:U:N3	37:LB:41:G:OP2	2.47	0.45
41:LF:233:LEU:HD23	41:LF:233:LEU:HA	1.88	0.45
4:Q:146:GLN:HE21	4:Q:206:PRO:HG3	1.82	0.45
17:Y:25:TRP:CE2	30:f:82:LYS:HD3	2.52	0.45
19:F:99:GLU:OE2	34:O:60:SER:OG	2.28	0.45
36:LA:439:C:H1'	36:LA:494:G:H21	1.82	0.45
36:LA:2439:A:H2'	36:LA:2440:G:H8	1.82	0.45
50:LO:19:ARG:NH2	50:LO:66:THR:O	2.50	0.45
63:LV:115:LYS:NZ	63:LV:119:GLU:OE2	2.48	0.45
1:2:312:A:H62	1:2:352:A:H1'	1.82	0.45
1:2:1680:G:H1'	1:2:1721:A:H61	1.82	0.45
4:Q:27:LYS:NZ	4:Q:49:ASN:OD1	2.50	0.45
13:W:82:ARG:HE	13:W:149:ARG:HG2	1.82	0.45
16:D:62:LEU:HD11	16:D:72:ILE:HG13	1.99	0.45
22:I:76:LEU:HD12	22:I:105:LEU:HD11	1.99	0.45
33:N:141:CYS:SG	33:N:144:CYS:N	2.88	0.45
36:LA:286:U:O2'	51:LP:179:LYS:O	2.35	0.45
36:LA:1243:G:O2'	36:LA:1271:A:O2'	2.35	0.45
36:LA:1686:U:OP1	58:Lq:42:LYS:NZ	2.34	0.45
42:LG:77:ALA:O	42:LG:108:ARG:NH1	2.50	0.45
64:LW:88:ASP:N	64:LW:88:ASP:OD1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:53:THR:HG22	3:P:161:PRO:HB2	1.99	0.44
4:Q:48:VAL:HG11	4:Q:61:LEU:HB2	1.99	0.44
6:R:157:LYS:HA	6:R:169:LEU:O	2.17	0.44
9:B:70:VAL:HG21	19:F:47:LYS:HB2	1.99	0.44
13:W:83:VAL:HA	13:W:149:ARG:HG3	1.99	0.44
14:C:9:ASN:ND2	14:C:79:TYR:OH	2.51	0.44
33:N:119:ARG:HH11	33:N:152:ALA:HB3	1.82	0.44
36:LA:52:A:H5''	73:Lf:48:ASN:HB2	1.99	0.44
36:LA:2654:C:OP2	78:Lk:2:VAL:N	2.50	0.44
36:LA:2660:G:O2'	36:LA:2744:U:O2	2.35	0.44
36:LA:3026:G:N2	36:LA:3029:A:OP2	2.44	0.44
78:Lk:71:ARG:HD3	78:Lk:80:ARG:HD3	2.00	0.44
81:EF:690:CYS:SG	81:EF:694:SER:OG	2.60	0.44
1:2:791:A:OP1	8:S:187:ARG:NH1	2.38	0.44
1:2:1202:A:O2'	1:2:1204:A:OP2	2.33	0.44
4:Q:33:LYS:HE2	4:Q:95:ASN:HB2	1.99	0.44
32:g:30:PRO:HG2	32:g:38:LEU:HD22	1.99	0.44
36:LA:1155:C:O2'	36:LA:1197:A:N1	2.45	0.44
36:LA:2947:G:N3	40:LE:250:ALA:HB1	2.31	0.44
36:LA:3268:A:OP1	43:LH:46:ARG:NH1	2.42	0.44
36:LA:3273:A:H4'	43:LH:44:ALA:HB1	1.99	0.44
38:LC:8:C:H2'	38:LC:9:A:H8	1.82	0.44
81:EF:607:GLU:O	81:EF:622:GLY:N	2.50	0.44
1:2:56:U:OP1	1:2:403:G:N1	2.40	0.44
1:2:1160:A:H2'	1:2:1161:C:C6	2.52	0.44
1:2:1474:G:H2'	1:2:1475:A:C8	2.53	0.44
3:P:155:PHE:HA	24:a:60:ARG:HG2	1.98	0.44
36:LA:80:G:OP1	51:LP:193:ARG:NH1	2.50	0.44
36:LA:873:C:H3'	36:LA:874:U:H4'	2.00	0.44
36:LA:1831:U:O2'	38:LC:114:G:OP1	2.23	0.44
36:LA:2718:U:OP1	78:Lk:13:LYS:NZ	2.50	0.44
40:LE:65:SER:OG	40:LE:66:LYS:N	2.49	0.44
41:LF:193:LYS:HA	41:LF:198:ARG:HA	1.99	0.44
42:LG:39:GLN:HE22	42:LG:43:LYS:HE2	1.82	0.44
52:LQ:127[A]:LEU:HD22	56:Lo:156:VAL:HG13	1.99	0.44
81:EF:805:PHE:N	81:EF:808:THR:O	2.37	0.44
81:EF:899:GLY:HA2	81:EF:925:TYR:HB3	1.98	0.44
1:2:698:U:H3	1:2:741:C:N4	2.15	0.44
10:T:98:ARG:NH1	10:T:101:ILE:O	2.51	0.44
23:J:27:THR:HG23	23:J:113:ASP:HB3	1.99	0.44
32:g:31:LYS:HD3	32:g:31:LYS:HA	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:O:292:LEU:HD13	34:O:301:LEU:HD11	1.98	0.44
36:LA:528:U:H2'	36:LA:529:A:C8	2.52	0.44
36:LA:1795:U:N3	79:Ll:50:GLY:O	2.48	0.44
38:LC:97:A:O2'	71:Ld:59:ASN:OD1	2.28	0.44
43:LH:170:LYS:HE3	69:Lb:34:GLY:HA2	1.98	0.44
45:LJ:139:VAL:HG21	45:LJ:197:VAL:HG21	2.00	0.44
1:2:843:U:H2'	1:2:844:A:H8	1.83	0.44
1:2:992:A:O2'	1:2:1785:U:O2	2.32	0.44
3:P:148:ASP:OD1	3:P:149:LEU:N	2.47	0.44
3:P:163:ASN:O	3:P:169:SER:OG	2.29	0.44
19:F:13:LYS:HE2	19:F:79:TYR:HD2	1.82	0.44
26:c:132:LEU:HD23	26:c:135:LEU:HD12	1.99	0.44
28:K:45:GLU:O	28:K:49:ARG:HB2	2.18	0.44
36:LA:329:U:O2	41:LF:55:LYS:NZ	2.43	0.44
40:LE:215:ILE:HD12	40:LE:338:LEU:HD12	1.98	0.44
41:LF:25:VAL:HG23	41:LF:276:LEU:HD21	1.99	0.44
48:LM:53:THR:HG22	48:LM:60:ARG:HA	1.99	0.44
55:Ln:115:ILE:HG22	55:Ln:119:LEU:HD23	1.99	0.44
66:LY:30:THR:HG23	66:LY:91:SER:HB2	1.99	0.44
81:EF:238:VAL:HG13	81:EF:243:LEU:HD21	1.99	0.44
1:2:541:A:O2'	1:2:542:A:OP1	2.35	0.44
1:2:1171:A:H2'	1:2:1172:G:H8	1.83	0.44
1:2:1549:C:OP1	5:E:42:ARG:NH2	2.47	0.44
36:LA:2339:C:P	59:Lr:48:ARG:HG3	2.58	0.44
39:LD:112:ILE:HG13	79:Ll:79:VAL:HG22	1.99	0.44
81:EF:492:VAL:HB	81:EF:555:ARG:HH12	1.83	0.44
81:EF:753:GLU:HA	81:EF:756:GLN:HB2	2.00	0.44
1:2:1366:U:P	19:F:66:ARG:HH22	2.40	0.44
6:R:116:LYS:HG2	6:R:127:ALA:HB3	1.99	0.44
16:D:62:LEU:HD21	16:D:72:ILE:HG23	2.00	0.44
20:G:30:THR:HG22	34:O:127:ARG:HH22	1.82	0.44
36:LA:1190:A:O2'	36:LA:1193:A:OP2	2.32	0.44
38:LC:155:A:H5'	45:LJ:185:ARG:HD2	1.98	0.44
41:LF:188:ARG:O	41:LF:193:LYS:NZ	2.47	0.44
44:Li:77:VAL:HG22	56:Lo:59:VAL:HA	1.99	0.44
49:LN:162:ASN:OD1	49:LN:162:ASN:N	2.51	0.44
64:LW:82:ILE:HD11	64:LW:102:ILE:HD11	1.99	0.44
1:2:67:A:N6	1:2:83:G:O2'	2.51	0.44
1:2:1367:G:P	19:F:68:ARG:HH22	2.40	0.44
15:X:99:ARG:HG3	26:c:12:ALA:HB2	2.00	0.44
19:F:16:ALA:HA	19:F:70:THR:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:F:44:LEU:HB3	19:F:78:VAL:HG11	2.00	0.44
23:J:70:THR:OG1	23:J:72:ASN:OD1	2.36	0.44
36:LA:90:C:O2'	36:LA:282:G:OP1	2.31	0.44
36:LA:151:A:H5''	71:Ld:102:GLU:CD	2.42	0.44
36:LA:2617:U:O2'	47:LL:116:ARG:NH2	2.51	0.44
38:LC:26:U:O2'	41:LF:51:ALA:O	2.32	0.44
42:LG:182:GLY:HA2	42:LG:194:LEU:HD23	2.00	0.44
52:LQ:45[A]:GLY:O	52:LQ:50[A]:ASN:ND2	2.50	0.44
63:LV:17:ARG:NH2	63:LV:18:TYR:OH	2.51	0.44
81:EF:81:PRO:HB2	81:EF:392:ILE:HD11	2.00	0.44
1:2:1003:A:O2'	1:2:1005:A:N7	2.47	0.44
1:2:1471:A:O2'	1:2:1472:C:OP1	2.33	0.44
15:X:77:SER:HB3	15:X:85:VAL:HB	2.00	0.44
21:H:107:SER:OG	21:H:108:LYS:N	2.51	0.44
34:O:144:LEU:HD13	34:O:144:LEU:HA	1.87	0.44
36:LA:837:A:OP2	79:Ll:4:ARG:HD2	2.18	0.44
45:LJ:162:LEU:HA	51:LP:7:LEU:HD11	2.00	0.44
47:LL:5:PRO:HB2	47:LL:7:ARG:HG2	2.00	0.44
47:LL:47:PRO:HB3	47:LL:171:TRP:CZ2	2.53	0.44
47:LL:61:SER:HA	47:LL:126:ALA:HA	1.99	0.44
69:Lb:48:ARG:HG2	69:Lb:104:PRO:HD3	2.00	0.44
81:EF:240:PRO:HG3	81:EF:281:VAL:HA	2.00	0.44
1:2:293:U:O2'	8:S:133:LYS:NZ	2.51	0.43
1:2:329:G:H2'	1:2:330:G:C8	2.52	0.43
1:2:959:U:OP2	30:f:20:LYS:NZ	2.50	0.43
4:Q:137:ILE:HG13	4:Q:215:VAL:HG23	2.00	0.43
5:E:20:VAL:HG12	5:E:25:LEU:HD23	1.99	0.43
7:A:96:LEU:HD23	7:A:96:LEU:HA	1.86	0.43
36:LA:199:A:H5''	62:LU:60:ARG:HD2	1.99	0.43
36:LA:2468:A:N3	36:LA:2477:G:N2	2.66	0.43
41:LF:290:ILE:O	41:LF:296:GLN:NE2	2.51	0.43
56:Lo:8:GLN:HB3	56:Lo:64:ILE:HD11	2.00	0.43
67:LZ:46:THR:HG22	67:LZ:48:ASP:H	1.83	0.43
71:Ld:8:GLU:O	71:Ld:11:THR:OG1	2.36	0.43
71:Ld:30:GLU:OE2	71:Ld:34:GLN:NE2	2.51	0.43
81:EF:371:LEU:HD12	81:EF:376:ILE:HB	1.99	0.43
81:EF:542:SER:HB3	82:EF:1101:ATP:N7	2.33	0.43
1:2:168:A:OP1	10:T:136:LYS:N	2.51	0.43
1:2:1546:G:OP1	21:H:123:ARG:NH2	2.36	0.43
1:2:1619:C:C2	35:L:22:ARG:HG2	2.53	0.43
1:2:1795:U:H5'	29:e:79:ILE:HD11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:144:TRP:CE2	6:R:173:PRO:HG3	2.53	0.43
20:G:36:ASP:OD1	20:G:37:GLU:N	2.52	0.43
36:LA:627:U:H2'	36:LA:628:A:C8	2.53	0.43
39:LD:36:GLU:HG3	39:LD:91:GLY:HA2	1.99	0.43
40:LE:205:VAL:HA	40:LE:208:VAL:HG12	1.99	0.43
68:La:19:ARG:HD3	68:La:33:ARG:HB2	2.00	0.43
12:V:48:THR:OG1	12:V:52:ASN:O	2.26	0.43
27:d:41:ARG:HH22	27:d:53:ASP:HA	1.84	0.43
36:LA:41:G:N2	36:LA:2803:A:N7	2.66	0.43
36:LA:1385:C:OP1	41:LF:141:ARG:NH2	2.42	0.43
36:LA:1637:A:H4'	63:LV:15:ARG:HB3	2.01	0.43
36:LA:2609:A:N3	51:LP:87:GLN:NE2	2.63	0.43
36:LA:3002:C:H5'	40:LE:178:LEU:HD23	2.00	0.43
43:LH:85:ILE:HG23	69:Lb:107:ILE:HG22	1.99	0.43
51:LP:51:LEU:HB3	51:LP:117:ASN:HD22	1.83	0.43
51:LP:140:LYS:HB3	51:LP:144:ARG:NH1	2.33	0.43
1:2:1182:U:H5	1:2:1185:U:H5''	1.83	0.43
1:2:1387:G:N7	20:G:44:LYS:HE3	2.34	0.43
7:A:32:GLU:HA	7:A:54:ARG:HD2	2.01	0.43
8:S:129:VAL:HG12	8:S:139:VAL:HG12	2.01	0.43
16:D:33:ARG:HD3	16:D:36:LEU:HD21	2.00	0.43
22:I:108:LEU:HA	22:I:111:ILE:HG22	1.99	0.43
34:O:210:LEU:HD11	34:O:222:LEU:HB3	2.00	0.43
36:LA:1184:A:H5''	50:LO:59:ASN:HD22	1.82	0.43
38:LC:8:C:H2'	38:LC:9:A:C8	2.52	0.43
81:EF:682:GLN:HG3	81:EF:683:ILE:HG23	1.98	0.43
1:2:401:A:O3'	8:S:3:ARG:NH1	2.51	0.43
1:2:913:G:N7	4:Q:12:GLY:HA2	2.34	0.43
1:2:1389:C:OP1	20:G:48:ASN:ND2	2.49	0.43
1:2:1697:G:O6	1:2:1704:U:O4	2.36	0.43
12:V:103:GLN:HE21	12:V:166:TYR:HE1	1.66	0.43
13:W:79:ARG:HH11	13:W:79:ARG:HD3	1.71	0.43
18:Z:81:VAL:HG11	18:Z:102:LEU:HD13	2.01	0.43
34:O:261:LYS:NZ	34:O:273:ASP:OD2	2.39	0.43
42:LG:146:LEU:HG	42:LG:163:LEU:HD12	2.00	0.43
62:LU:22:ALA:O	62:LU:27:ARG:NE	2.49	0.43
81:EF:124:ALA:HB1	81:EF:127:ALA:HB3	2.00	0.43
81:EF:395:HIS:CD2	81:EF:397:LYS:HG2	2.53	0.43
81:EF:445:LEU:HD22	81:EF:448:THR:HG21	2.01	0.43
81:EF:758:ARG:NH2	81:EF:764:ASP:OD2	2.52	0.43
1:2:1316:G:OP1	20:G:7:LYS:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:S:98:ASN:ND2	8:S:116:ASP:OD1	2.52	0.43
16:D:27:ALA:HA	16:D:30:VAL:HG22	2.00	0.43
25:b:27:ILE:HB	25:b:61:ILE:HB	2.01	0.43
36:LA:2901:G:O2'	36:LA:3024:A:N1	2.50	0.43
36:LA:3042:U:OP1	59:Lr:48:ARG:NH1	2.52	0.43
42:LG:55:PHE:HE2	42:LG:159:VAL:HG13	1.84	0.43
50:LO:36:VAL:HG11	50:LO:55:ARG:HH21	1.83	0.43
56:Lo:124:LEU:HD23	57:Lp:153:PRO:HB2	1.99	0.43
58:Lq:35:LYS:HA	58:Lq:38:ILE:HG12	2.00	0.43
64:LW:100:PRO:HG2	64:LW:123:VAL:HG22	2.00	0.43
81:EF:193:MET:HA	81:EF:196:ALA:HB3	2.01	0.43
81:EF:264:LYS:HE2	81:EF:268:ILE:HD11	2.00	0.43
1:2:590:C:P	32:g:42:ARG:HH22	2.41	0.43
1:2:990:C:H5''	18:Z:129:LYS:HB3	2.01	0.43
1:2:1672:G:H2'	1:2:1673:G:C8	2.54	0.43
24:a:28:ASP:O	24:a:31:SER:OG	2.27	0.43
36:LA:609:G:O6	41:LF:308:LYS:NZ	2.43	0.43
36:LA:1277:C:O2'	36:LA:1278:A:O5'	2.35	0.43
36:LA:2588:U:OP1	45:LJ:48:ARG:NH2	2.46	0.43
46:LK:88:TYR:HD2	46:LK:154:VAL:HG12	1.83	0.43
58:Lq:77:LYS:HG2	58:Lq:81:LYS:HG3	2.01	0.43
60:LS:20:LEU:HD21	60:LS:28:ILE:HG23	2.00	0.43
1:2:142:G:H22	1:2:173:A:H2	1.65	0.43
8:S:65:LEU:HD13	8:S:80:THR:HA	2.01	0.43
10:T:57:ASP:HB3	10:T:98:ARG:HD2	2.01	0.43
11:U:80:GLU:HA	11:U:83:LYS:HE3	2.00	0.43
19:F:22:VAL:HG13	19:F:65:ILE:HG13	2.00	0.43
21:H:91:ASP:OD1	21:H:95:GLY:N	2.52	0.43
23:J:70:THR:O	31:M:40:ARG:NH1	2.38	0.43
25:b:57:ARG:NE	30:f:26:GLN:HE21	2.17	0.43
34:O:266:ASP:CG	34:O:267:PRO:HD3	2.44	0.43
36:LA:129:U:H2'	36:LA:130:A:C8	2.54	0.43
36:LA:839:C:H4'	36:LA:1724:U:H2'	2.01	0.43
36:LA:990:U:H1'	57:Lp:101:CYS:HB3	2.00	0.43
36:LA:1253:U:N3	36:LA:1264:G:OP1	2.52	0.43
65:LX:11:ASN:HA	65:LX:14:ARG:HD3	2.01	0.43
73:Lf:21:ARG:HG3	73:Lf:39:TYR:CD1	2.53	0.43
1:2:387:A:H2'	1:2:402:C:H5'	2.01	0.43
1:2:513:U:H3	1:2:538:A:H62	1.66	0.43
1:2:780:A:C2	27:d:8:ARG:HD3	2.53	0.43
36:LA:209:A:H4'	36:LA:211:A:N7	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:LA:655:C:OP1	68:La:27:ARG:N	2.50	0.43
36:LA:1203:A:OP2	36:LA:1301:A:N6	2.51	0.43
36:LA:1246:G:H1'	36:LA:1264:G:H2'	1.99	0.43
54:Lm:176:ARG:HA	54:Lm:182:LYS:O	2.18	0.43
13:W:89:ASP:OD1	13:W:89:ASP:N	2.52	0.43
36:LA:341:G:O2'	38:LC:22:U:O4	2.26	0.43
36:LA:645:A:N6	36:LA:2869:U:OP1	2.51	0.43
36:LA:1119:C:H2'	36:LA:1120:A:H8	1.84	0.43
39:LD:181:LYS:HB3	39:LD:181:LYS:HE2	1.86	0.43
43:LH:40:LEU:HD11	43:LH:54:TYR:HB2	2.01	0.43
44:LI:160:ARG:HD2	44:LI:203:TRP:CG	2.54	0.43
44:LI:176:TYR:CZ	44:LI:197:GLN:HG2	2.54	0.43
45:LJ:83:ASP:OD1	45:LJ:86:THR:OG1	2.26	0.43
59:Lr:14:SER:O	59:Lr:81:GLN:NE2	2.52	0.43
81:EF:695:ARG:HH11	81:EF:945:VAL:HG12	1.84	0.43
1:2:1699:G:H8	1:2:1702:A:H62	1.67	0.42
10:T:12:SER:OG	10:T:123:GLY:O	2.37	0.42
13:W:59:LEU:HD23	13:W:59:LEU:HA	1.92	0.42
22:I:130:ARG:O	22:I:134:ARG:HB2	2.19	0.42
36:LA:1925:U:O2'	36:LA:1927:G:N7	2.52	0.42
36:LA:1940:G:HO2'	36:LA:3362:A:HO2'	1.61	0.42
36:LA:2756:C:O2	57:Lp:8:ARG:NH2	2.52	0.42
36:LA:3198:U:O2	46:LK:21:LYS:N	2.52	0.42
46:LK:50:ASN:HD21	50:LO:4:ASP:HA	1.84	0.42
81:EF:508:LEU:HD23	81:EF:519:LYS:HE3	2.00	0.42
1:2:765:G:O2'	1:2:767:U:O3'	2.35	0.42
1:2:1548:G:OP1	5:E:18:ARG:NH2	2.44	0.42
1:2:1727:G:H2'	1:2:1728:A:C8	2.53	0.42
4:Q:210:ILE:HG23	4:Q:210:ILE:HD12	1.74	0.42
12:V:67:TRP:HE3	12:V:72:ILE:HD11	1.84	0.42
13:W:64:GLU:OE2	13:W:69:ARG:NH2	2.51	0.42
36:LA:817:A:O2'	73:Lf:11:ARG:HG3	2.19	0.42
36:LA:1219:C:O2'	36:LA:1286:A:N1	2.47	0.42
42:LG:60:ILE:HB	42:LG:80:SER:HB3	2.00	0.42
42:LG:214:ASP:HB2	81:EF:664:ALA:HB2	2.00	0.42
43:LH:2:THR:OG1	43:LH:3:ALA:N	2.51	0.42
1:2:10:G:O2'	6:R:87:GLN:OE1	2.29	0.42
8:S:11:ARG:NH2	8:S:20:LEU:HB3	2.34	0.42
20:G:108:ASP:HA	20:G:111:LYS:HG2	2.01	0.42
36:LA:874:U:N3	36:LA:2978:U:OP1	2.46	0.42
36:LA:2509:U:H2'	36:LA:2510:U:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:LA:2894:C:OP1	46:LK:166:ARG:NH2	2.52	0.42
36:LA:2904:U:H2'	36:LA:2905:U:H6	1.84	0.42
40:LE:17:LEU:HD11	40:LE:233:TRP:HH2	1.84	0.42
40:LE:232:ARG:HH11	40:LE:232:ARG:HD3	1.69	0.42
47:LL:189:GLU:HB2	47:LL:200:LEU:HB3	2.01	0.42
50:LO:37:GLU:OE2	50:LO:74:ARG:NH2	2.52	0.42
64:LW:104:THR:HG21	64:LW:112:ILE:HD11	2.01	0.42
70:Lc:38:LEU:HA	70:Lc:38:LEU:HD23	1.80	0.42
80:Sn:56:C:N4	80:Sn:57:G:O6	2.52	0.42
81:EF:380:GLN:HA	81:EF:383:PHE:HD2	1.83	0.42
81:EF:547:TRP:HA	81:EF:550:LYS:HB3	2.01	0.42
1:2:311:U:P	26:c:24:TRP:HE1	2.42	0.42
1:2:496:G:H2'	1:2:497:G:C8	2.55	0.42
1:2:518:A:O2'	1:2:519:C:O5'	2.35	0.42
15:X:81:HIS:CE1	15:X:82:ARG:HD2	2.55	0.42
22:I:101:ASN:HA	22:I:104:VAL:HG12	2.01	0.42
34:O:219:GLU:HA	34:O:234:LEU:O	2.19	0.42
35:L:18:ARG:HH21	35:L:18:ARG:HD3	1.72	0.42
36:LA:2457:G:H5'	36:LA:2482:U:H1'	2.01	0.42
36:LA:3206:C:H2'	50:LO:99:TRP:CZ2	2.55	0.42
36:LA:3294:A:H5'	40:LE:128:LYS:HD3	2.02	0.42
46:LK:128:VAL:HG13	46:LK:157:ASN:HD21	1.85	0.42
56:Lo:87:THR:O	56:Lo:88:HIS:ND1	2.52	0.42
61:LT:105:VAL:HG11	61:LT:126:LEU:HD13	2.01	0.42
64:LW:77:LYS:O	64:LW:80:THR:OG1	2.26	0.42
79:Ll:58:SER:O	79:Ll:61:LYS:NZ	2.41	0.42
36:LA:217:U:O2	62:LU:103:LYS:NZ	2.39	0.42
36:LA:3214:U:OP2	50:LO:128:ARG:NH1	2.47	0.42
40:LE:261:MET:HG2	52:LQ:64[A]:PHE:HA	2.02	0.42
46:LK:128:VAL:HG21	46:LK:134:ILE:HD11	2.00	0.42
81:EF:468:LYS:N	82:EF:1102:ATP:O1A	2.52	0.42
1:2:38:C:H4'	13:W:6:ARG:NH2	2.35	0.42
1:2:209:U:H2'	1:2:210:A:C8	2.54	0.42
1:2:1163:A:N3	1:2:1613:U:O2'	2.49	0.42
1:2:1534:G:N7	28:K:77:ARG:NH2	2.66	0.42
3:P:125:ASP:HB3	3:P:128:SER:HB2	2.02	0.42
4:Q:207:LEU:HG	4:Q:210:ILE:HD11	2.00	0.42
6:R:219:GLY:O	24:a:25:LYS:NZ	2.53	0.42
17:Y:35:GLU:HA	17:Y:38:VAL:HG22	2.00	0.42
22:I:42:GLY:HA2	22:I:84:LYS:HD2	2.00	0.42
26:c:57:LEU:HD11	26:c:73:ARG:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:d:15:ASN:HD22	27:d:22:GLN:HE21	1.66	0.42
36:LA:209:A:O2'	36:LA:211:A:OP2	2.31	0.42
36:LA:2922:G:H1	80:Sm:75:C:H42	1.67	0.42
50:LO:60:LEU:HD13	56:Lo:152:LEU:HD11	2.01	0.42
52:LQ:46[A]:GLU:HB3	52:LQ:134[A]:LYS:HD2	2.01	0.42
81:EF:101:LYS:HD2	81:EF:101:LYS:HA	1.81	0.42
1:2:418:G:O2'	10:T:72:ARG:NH2	2.53	0.42
7:A:17:PHE:HE2	7:A:39:VAL:HG11	1.85	0.42
16:D:62:LEU:HD13	16:D:75:VAL:HG21	2.01	0.42
36:LA:1696:A:H2'	36:LA:1697:A:C8	2.54	0.42
36:LA:1751:G:O6	74:Lg:44:LYS:NZ	2.44	0.42
1:2:74:U:O2'	1:2:76:A:OP2	2.31	0.42
4:Q:136:ARG:O	4:Q:215:VAL:HA	2.20	0.42
23:J:87:HIS:HB3	23:J:89:ARG:NH2	2.35	0.42
34:O:197:SER:OG	34:O:198:ASN:N	2.53	0.42
36:LA:2116:G:OP1	36:LA:2118:C:N4	2.53	0.42
37:LB:97:A:O4'	44:LI:225:GLN:NE2	2.53	0.42
46:LK:71:VAL:HA	46:LK:74:LEU:HB2	2.02	0.42
51:LP:98:LEU:HA	51:LP:101:THR:HG22	2.02	0.42
56:Lo:79:VAL:HG21	56:Lo:106:LEU:HD21	2.02	0.42
64:LW:6:THR:HG22	64:LW:8:THR:H	1.85	0.42
73:Lf:18:LEU:HD22	75:Lh:12:LYS:HE3	2.02	0.42
81:EF:395:HIS:HD2	81:EF:397:LYS:HG2	1.85	0.42
81:EF:514:SER:HB3	81:EF:555:ARG:HE	1.85	0.42
1:2:1537:C:O4'	1:2:1572:G:N2	2.53	0.42
4:Q:35:PRO:HD2	4:Q:38:PHE:HD2	1.84	0.42
8:S:181:VAL:HA	8:S:227:VAL:HA	2.01	0.42
26:c:62:LYS:HD2	26:c:118:PRO:HB3	2.02	0.42
36:LA:221:A:O2'	36:LA:223:U:OP2	2.27	0.42
36:LA:2747:A:H5'	42:LG:175:HIS:HA	2.02	0.42
39:LD:6:ARG:HE	39:LD:6:ARG:HB2	1.75	0.42
39:LD:147:ARG:HG2	39:LD:157:VAL:HG22	2.00	0.42
40:LE:44:THR:HG21	40:LE:184:ASN:ND2	2.35	0.42
47:LL:80:SER:HB2	47:LL:147:VAL:HG21	2.02	0.42
50:LO:19:ARG:HB3	50:LO:35:ILE:HD12	2.02	0.42
59:Lr:69:LEU:HB3	59:Lr:74:MET:HE1	2.02	0.42
61:LT:142:ILE:HD12	61:LT:142:ILE:HA	1.87	0.42
76:Li:98:LYS:HD2	76:Li:118:THR:HG21	2.01	0.42
1:2:63:G:O2'	1:2:170:U:OP1	2.35	0.42
1:2:256:A:N3	12:V:73:SER:OG	2.44	0.42
1:2:1542:G:N2	1:2:1568:C:H1'	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:139:VAL:HG23	3:P:141:ILE:HD12	2.01	0.42
7:A:224:ASP:OD1	7:A:225:TYR:N	2.52	0.42
12:V:4:SER:HB2	12:V:24:LYS:HD3	2.01	0.42
23:J:57:ARG:HG2	23:J:89:ARG:NE	2.35	0.42
37:LB:39:C:O2'	48:LM:44:THR:O	2.27	0.42
42:LG:178:ASN:HA	42:LG:183:TRP:CD2	2.54	0.42
47:LL:35:ASP:OD1	47:LL:88:ARG:HG2	2.20	0.42
49:LN:179:PHE:HB2	49:LN:183:ARG:HH12	1.85	0.42
81:EF:91:VAL:O	81:EF:95:CYS:N	2.49	0.42
81:EF:655:LEU:HD23	81:EF:692:LEU:HD22	2.01	0.42
1:2:105:A:HO2'	12:V:8:ARG:HH12	1.67	0.41
1:2:838:G:H2'	1:2:839:U:C6	2.55	0.41
1:2:1175:U:H2'	1:2:1176:G:C8	2.55	0.41
1:2:1441:C:O2'	1:2:1447:C:N4	2.50	0.41
5:E:63:ALA:HB1	5:E:74:ALA:H	1.84	0.41
6:R:207:LEU:HA	6:R:210:THR:HG22	2.01	0.41
8:S:200:ARG:NE	8:S:202:ASP:OD2	2.53	0.41
10:T:77:LEU:HD12	10:T:95:LYS:HB2	2.01	0.41
22:I:76:LEU:HD23	22:I:76:LEU:HA	1.80	0.41
29:e:51:ARG:HH22	35:L:38:ARG:HG2	1.85	0.41
36:LA:198:A:N3	36:LA:218:G:O2'	2.50	0.41
36:LA:269:G:H5''	51:LP:14:LYS:HE3	2.02	0.41
36:LA:2440:G:H1	36:LA:2507:C:H42	1.66	0.41
36:LA:2765:C:O3'	78:Lk:39:GLY:HA3	2.20	0.41
42:LG:111:GLN:HE22	42:LG:252:ALA:HB2	1.85	0.41
45:LJ:213:LYS:O	45:LJ:216:SER:OG	2.32	0.41
1:2:1273:G:H4'	1:2:1274:C:H3'	2.01	0.41
3:P:189:VAL:O	24:a:44:ARG:NH2	2.53	0.41
10:T:32:ILE:HD12	10:T:65:GLN:HA	2.01	0.41
12:V:158:SER:O	12:V:161:SER:OG	2.35	0.41
27:d:112:LYS:HD2	27:d:116:LYS:HD3	2.02	0.41
30:f:11:THR:HG23	30:f:14:SER:H	1.85	0.41
36:LA:116:A:P	72:Le:36:ARG:HH21	2.44	0.41
39:LD:111:THR:HB	39:LD:136:ILE:HD13	2.01	0.41
42:LG:198:TYR:CE1	42:LG:203:HIS:HB3	2.55	0.41
47:LL:17:TYR:OH	47:LL:23:ASN:ND2	2.49	0.41
80:Sn:10:A:H61	80:Sn:25:C:H42	1.67	0.41
81:EF:226:VAL:HG11	81:EF:261:ILE:HG23	2.02	0.41
81:EF:642:ASN:ND2	81:EF:929:ASP:O	2.53	0.41
81:EF:779:ASP:O	81:EF:784:ASN:ND2	2.47	0.41
1:2:553:G:H3'	1:2:554:C:H2'	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:856:A:N6	11:U:116:ARG:HD3	2.36	0.41
1:2:859:A:O2'	17:Y:73:ARG:NH1	2.41	0.41
6:R:81:MET:HG3	6:R:211:LEU:HD11	2.02	0.41
9:B:57:SER:HA	35:L:53:ILE:HB	2.02	0.41
21:H:67:GLU:HA	21:H:70:VAL:HG22	2.02	0.41
30:f:20:LYS:HB3	30:f:29:ARG:HG2	2.02	0.41
34:O:123:ILE:HD13	34:O:169:ILE:HG21	2.01	0.41
36:LA:59:G:H2'	38:LC:33:A:H2'	2.02	0.41
36:LA:2484:A:H3'	36:LA:2485:A:H8	1.86	0.41
36:LA:3231:U:H2'	36:LA:3232:G:H8	1.85	0.41
46:LK:4:ILE:HG12	56:Lo:142:GLN:NE2	2.35	0.41
48:LM:7:ASN:OD1	48:LM:7:ASN:N	2.52	0.41
51:LP:46:ASP:OD1	51:LP:46:ASP:N	2.52	0.41
56:Lo:73:LYS:HD2	56:Lo:128:GLU:HG3	2.02	0.41
81:EF:563:ILE:HG12	81:EF:591:THR:HG23	2.03	0.41
81:EF:579:ALA:HA	81:EF:582:VAL:HB	2.03	0.41
1:2:632:U:H4'	26:c:11:SER:HB3	2.02	0.41
1:2:1400:A:H4'	20:G:60:ARG:NH2	2.35	0.41
9:B:72:HIS:CD2	9:B:107:LYS:HD2	2.55	0.41
12:V:26:LYS:O	12:V:29:LEU:HD22	2.20	0.41
34:O:106:HIS:NE2	34:O:132:LYS:HG3	2.36	0.41
36:LA:348:A:N3	36:LA:352:A:O2'	2.54	0.41
36:LA:1203:A:H2'	36:LA:1204:A:C8	2.56	0.41
36:LA:2745:G:N2	36:LA:2748:A:OP2	2.47	0.41
41:LF:138:ARG:HH12	41:LF:246:ARG:HD3	1.86	0.41
48:LM:26:SER:OG	48:LM:27:GLY:N	2.54	0.41
81:EF:431:CYS:HB3	81:EF:452:LEU:HB2	2.03	0.41
81:EF:922:PRO:HG2	81:EF:947:ILE:HD11	2.01	0.41
1:2:1522:U:O3'	22:I:78:LYS:NZ	2.54	0.41
11:U:138:LYS:HG2	11:U:152:VAL:HG12	2.02	0.41
17:Y:104:ARG:HE	17:Y:104:ARG:HB2	1.66	0.41
34:O:7:LEU:HD22	34:O:313:TRP:HB3	2.03	0.41
34:O:112:SER:HB3	34:O:154:VAL:HG22	2.02	0.41
36:LA:1322:U:O2	56:Lo:108:GLN:NE2	2.48	0.41
36:LA:2878:G:H5''	40:LE:5:LYS:HE2	2.03	0.41
36:LA:2899:C:O2'	36:LA:2901:G:OP2	2.30	0.41
57:Lp:136:ARG:HD3	57:Lp:139:ARG:HH12	1.85	0.41
64:LW:126:LYS:HE3	64:LW:126:LYS:HB2	1.86	0.41
68:La:94:ALA:HB3	68:La:119:VAL:HG22	2.03	0.41
81:EF:557:VAL:HG11	81:EF:584:TYR:HD2	1.86	0.41
1:2:142:G:P	10:T:139:ASN:HD21	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1553:G:N1	1:2:1556:A:OP2	2.53	0.41
5:E:18:ARG:NH1	21:H:90:ASN:O	2.53	0.41
34:O:274:LEU:HD23	34:O:274:LEU:HA	1.77	0.41
36:LA:26:A:N3	36:LA:328:U:O2'	2.45	0.41
36:LA:655:C:H2'	36:LA:656:A:C8	2.55	0.41
36:LA:1601:U:P	55:Ln:42:ARG:HH22	2.42	0.41
36:LA:2433:U:H1'	51:LP:125:SER:HB3	2.02	0.41
36:LA:3215:A:H8	50:LO:121:MET:HE2	1.85	0.41
41:LF:22:LEU:HD23	41:LF:22:LEU:HA	1.85	0.41
42:LG:150:LEU:HD12	48:LM:143:ARG:HG3	2.02	0.41
51:LP:97:SER:OG	51:LP:98:LEU:N	2.53	0.41
60:LS:56:ARG:HE	60:LS:61:LYS:HB2	1.85	0.41
74:Lg:12:LEU:O	74:Lg:15:THR:HG22	2.21	0.41
1:2:956:C:OP1	1:2:1072:C:O2'	2.37	0.41
1:2:1610:G:N7	19:F:14:LYS:NZ	2.69	0.41
1:2:1681:A:H2	1:2:1720:G:H21	1.68	0.41
1:2:1699:G:H2'	1:2:1701:A:H62	1.85	0.41
8:S:124:GLY:HA2	8:S:142:HIS:CE1	2.56	0.41
8:S:183:VAL:HG11	8:S:188:ASN:HB2	2.03	0.41
9:B:93:LEU:HD12	9:B:93:LEU:HA	1.92	0.41
12:V:5:ARG:N	12:V:28:GLU:O	2.54	0.41
36:LA:215:G:H5''	62:LU:12:ARG:HG3	2.03	0.41
36:LA:595:G:OP2	44:LI:30:ARG:NH2	2.50	0.41
36:LA:712:G:OP1	49:LN:174:ARG:NH1	2.53	0.41
36:LA:3111:U:OP1	46:LK:184:LYS:NZ	2.51	0.41
37:LB:37:G:N2	37:LB:41:G:N3	2.68	0.41
38:LC:29:U:H5''	49:LN:27:ASP:HB3	2.03	0.41
39:LD:142:ASP:OD1	39:LD:142:ASP:N	2.54	0.41
46:LK:41:ILE:HD13	46:LK:71:VAL:HB	2.03	0.41
53:LR:138:LYS:HD2	53:LR:140:GLU:CD	2.45	0.41
65:LX:18:ARG:HA	65:LX:18:ARG:HD2	1.78	0.41
1:2:911:U:OP2	4:Q:8:ARG:NH2	2.52	0.41
3:P:2:SER:OG	3:P:3:LEU:N	2.53	0.41
6:R:157:LYS:HG2	6:R:170:ILE:HA	2.03	0.41
13:W:65:LYS:HA	13:W:70:LEU:HD11	2.03	0.41
13:W:78:ARG:HH22	13:W:82:ARG:HH11	1.67	0.41
15:X:5:LEU:HD12	15:X:6:THR:HG22	2.03	0.41
34:O:220:ILE:O	34:O:233:THR:HA	2.20	0.41
36:LA:655:C:H2'	36:LA:656:A:H8	1.85	0.41
36:LA:2555:G:N7	70:Lc:95:ILE:HD11	2.35	0.41
42:LG:24:ARG:HH11	42:LG:24:ARG:HD2	1.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:EF:518:THR:H	81:EF:521:ALA:HB3	1.86	0.41
1:2:549:G:H2'	1:2:550:A:H8	1.86	0.41
1:2:614:C:OP2	26:c:5:LYS:NZ	2.41	0.41
3:P:167:LYS:HE3	3:P:167:LYS:HB3	1.93	0.41
4:Q:151:LYS:HE3	4:Q:154:SER:HA	2.02	0.41
14:C:22:VAL:O	14:C:32:HIS:NE2	2.49	0.41
16:D:33:ARG:HA	16:D:36:LEU:HG	2.03	0.41
21:H:11:PHE:HD1	21:H:60:GLU:HB3	1.85	0.41
21:H:101:LEU:HA	21:H:101:LEU:HD23	1.84	0.41
23:J:63:LEU:HD13	23:J:86:ILE:HD12	2.02	0.41
36:LA:307:A:H2'	36:LA:308:A:C8	2.56	0.41
36:LA:364:G:N7	73:Lf:56:ARG:NH2	2.69	0.41
36:LA:597:G:H4'	44:LI:41:ARG:HH22	1.85	0.41
36:LA:674:G:O6	54:Lm:56:LYS:NZ	2.53	0.41
36:LA:1093:A:N3	36:LA:1096:U:N3	2.68	0.41
36:LA:1178:G:OP2	52:LQ:25[A]:LYS:NZ	2.54	0.41
36:LA:1376:C:O2'	36:LA:1408:G:O2'	2.25	0.41
36:LA:2335:G:N2	36:LA:2339:C:O2'	2.54	0.41
36:LA:2820:A:O2'	80:Sn:76:A:O2'	2.29	0.41
36:LA:2945:G:O2'	36:LA:2948:C:OP2	2.26	0.41
36:LA:2960:C:H2'	36:LA:2961:G:C8	2.56	0.41
36:LA:3008:A:OP2	52:LQ:74[A]:ARG:NH1	2.54	0.41
36:LA:3269:U:H3	43:LH:134:ARG:NH1	2.18	0.41
39:LD:30:ARG:HD2	39:LD:63:PHE:CD2	2.56	0.41
41:LF:11:LEU:HD21	41:LF:156:LEU:HB2	2.02	0.41
43:LH:92:SER:OG	43:LH:148:GLU:OE2	2.36	0.41
46:LK:170:LYS:HG2	46:LK:175:PHE:CE2	2.56	0.41
53:LR:23:ARG:NH2	53:LR:141:SER:OG	2.52	0.41
54:Lm:174:ARG:HA	54:Lm:178:ARG:HG2	2.02	0.41
78:Lk:46:LYS:HE2	78:Lk:54:THR:HB	2.03	0.41
81:EF:50:PHE:HZ	81:EF:83:VAL:HG23	1.86	0.41
81:EF:491:THR:HG22	81:EF:563:ILE:HB	2.03	0.41
1:2:107:C:OP1	1:2:383:G:O2'	2.34	0.41
1:2:861:U:O2'	25:b:56:HIS:O	2.39	0.41
1:2:1383:G:O5'	23:J:89:ARG:NH1	2.53	0.41
1:2:1785:U:OP2	18:Z:133:ARG:NH2	2.54	0.41
5:E:118:GLU:O	21:H:122:HIS:N	2.54	0.41
6:R:148:LEU:HD11	13:W:92:LYS:HG2	2.03	0.41
9:B:58:LEU:HD21	9:B:167:ARG:HD3	2.02	0.41
10:T:57:ASP:HA	10:T:106:LEU:HA	2.03	0.41
16:D:70:ASN:O	16:D:74:LEU:HD23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Y:38:VAL:O	17:Y:42:ARG:HB2	2.20	0.41
22:I:40:SER:OG	22:I:41:SER:N	2.53	0.41
31:M:54:LYS:HE3	31:M:54:LYS:HB2	1.91	0.41
36:LA:90:C:H4'	36:LA:282:G:H5''	2.03	0.41
36:LA:98:G:N7	49:LN:13:HIS:NE2	2.64	0.41
36:LA:1186:G:O3'	56:Lo:113:ARG:NH2	2.54	0.41
36:LA:2482:U:H3	36:LA:2486:A:N6	2.18	0.41
45:LJ:72:PRO:HG3	51:LP:18:VAL:HA	2.02	0.41
48:LM:36:VAL:HG21	48:LM:123:PHE:HD2	1.85	0.41
50:LO:12:TRP:NE1	56:Lo:151:PRO:HB2	2.36	0.41
59:Lr:22:ILE:HG13	59:Lr:35:TYR:HD1	1.86	0.41
61:LT:53:HIS:CG	61:LT:56:ARG:HE	2.39	0.41
1:2:590:C:H5''	32:g:43:ARG:HH21	1.86	0.40
17:Y:5:HIS:CE1	17:Y:121:ARG:HG3	2.56	0.40
23:J:101:LYS:HA	23:J:104:THR:HG22	2.02	0.40
27:d:20:ARG:HE	27:d:22:GLN:NE2	2.19	0.40
36:LA:3086:A:H4'	40:LE:366:GLY:HA2	2.03	0.40
41:LF:22:LEU:HD23	41:LF:255:PHE:HZ	1.86	0.40
44:LI:160:ARG:HD2	44:LI:203:TRP:CD1	2.56	0.40
50:LO:114:ASP:HA	50:LO:117:ARG:HE	1.86	0.40
57:Lp:53:PRO:HB3	57:Lp:91:LEU:HD21	2.02	0.40
64:LW:64:GLN:C	64:LW:66:ALA:H	2.29	0.40
81:EF:47:GLU:HB3	81:EF:48:HIS:H	1.74	0.40
1:2:555:A:H8	1:2:590:C:O2'	2.04	0.40
5:E:52:LYS:HD2	5:E:52:LYS:HA	1.89	0.40
9:B:196:GLU:O	9:B:200:ASN:ND2	2.54	0.40
15:X:56:LYS:HE3	15:X:56:LYS:HB3	1.97	0.40
20:G:33:ARG:HA	20:G:33:ARG:HD3	1.83	0.40
21:H:29:VAL:O	21:H:33:THR:HG23	2.21	0.40
37:LB:77:G:H5''	56:Lo:46:GLN:O	2.21	0.40
39:LD:163:ARG:HD3	39:LD:163:ARG:H	1.86	0.40
53:LR:118:GLN:HG2	53:LR:147:GLU:HG2	2.03	0.40
53:LR:178:ALA:HA	53:LR:181:ARG:HH11	1.86	0.40
68:La:32:TRP:CZ2	68:La:53:PRO:HD2	2.56	0.40
68:La:82:LEU:HD21	68:La:112:ALA:HB2	2.03	0.40
1:2:1677:C:H42	1:2:1724:U:H3	1.69	0.40
4:Q:130:SER:HB2	4:Q:180:THR:HG22	2.03	0.40
5:E:26:LEU:HD23	5:E:26:LEU:HA	1.86	0.40
9:B:143:ARG:HG2	9:B:218:GLU:OE2	2.22	0.40
34:O:190:ALA:HB1	34:O:192:PHE:CE1	2.55	0.40
36:LA:744:A:P	54:Lm:66:ARG:HH22	2.44	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:LA:937:G:C6	36:LA:2410:U:H5''	2.57	0.40
43:LH:172:HIS:CD2	43:LH:173:LEU:HG	2.56	0.40
46:LK:70:THR:O	46:LK:73:SER:OG	2.34	0.40
47:LL:29:SER:OG	47:LL:30:LYS:N	2.54	0.40
54:Lm:64:VAL:HA	54:Lm:67:ILE:HD12	2.03	0.40
1:2:97:C:O2	1:2:425:A:O2'	2.32	0.40
17:Y:125:LEU:HA	17:Y:125:LEU:HD23	1.93	0.40
18:Z:107:ARG:NH1	35:L:60:GLU:OE2	2.55	0.40
20:G:105:GLN:OE1	20:G:105:GLN:N	2.54	0.40
29:e:12:LYS:HG3	29:e:15:ARG:HB2	2.03	0.40
34:O:127:ARG:HA	34:O:150:TRP:HB2	2.04	0.40
36:LA:1072:G:H21	65:LX:50:THR:HG21	1.86	0.40
36:LA:1244:A:O2'	36:LA:1247:U:OP1	2.39	0.40
36:LA:1477:A:OP1	36:LA:3075:G:O2'	2.30	0.40
36:LA:2836:C:H5	36:LA:2852:C:H42	1.67	0.40
41:LF:318:LEU:HA	41:LF:318:LEU:HD23	1.89	0.40
61:LT:141:TYR:HB3	71:Ld:33:VAL:HG22	2.03	0.40
77:Lj:8:LYS:HD3	77:Lj:12:ARG:NH2	2.37	0.40
81:EF:628:VAL:HG13	81:EF:635:LYS:HA	2.04	0.40
1:2:1182:U:C5	1:2:1185:U:H5''	2.56	0.40
10:T:1:MET:HE3	10:T:24:ILE:HD12	2.03	0.40
15:X:109:VAL:HG12	15:X:137:PHE:HB2	2.04	0.40
36:LA:299:G:C4	72:Le:31:GLY:HA3	2.56	0.40
36:LA:949:C:O2'	36:LA:971:G:OP1	2.31	0.40
36:LA:967:A:OP1	64:LW:47:LYS:NZ	2.54	0.40
40:LE:343:TYR:CE2	40:LE:345:ASN:HB2	2.57	0.40
53:LR:2:ALA:O	53:LR:18:ARG:NH2	2.53	0.40
63:LV:101:PHE:HA	63:LV:107:ARG:HE	1.86	0.40
72:Le:75:LYS:HD2	72:Le:75:LYS:HA	1.91	0.40
80:Sn:23:C:H2'	80:Sn:24:G: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	
3	P	204/206 (99%)	182 (89%)	22 (11%)	0	100	100
4	Q	222/232 (96%)	196 (88%)	26 (12%)	0	100	100
5	E	115/117 (98%)	100 (87%)	15 (13%)	0	100	100
6	R	214/216 (99%)	188 (88%)	26 (12%)	0	100	100
7	A	220/222 (99%)	209 (95%)	11 (5%)	0	100	100
8	S	256/258 (99%)	229 (90%)	27 (10%)	0	100	100
9	B	204/206 (99%)	188 (92%)	16 (8%)	0	100	100
10	T	226/228 (99%)	212 (94%)	14 (6%)	0	100	100
11	U	182/184 (99%)	162 (89%)	20 (11%)	0	100	100
12	V	183/198 (92%)	168 (92%)	15 (8%)	0	100	100
13	W	182/184 (99%)	165 (91%)	16 (9%)	1 (0%)	24	55
14	C	90/92 (98%)	79 (88%)	11 (12%)	0	100	100
15	X	140/142 (99%)	124 (89%)	16 (11%)	0	100	100
16	D	119/121 (98%)	90 (76%)	27 (23%)	2 (2%)	7	30
17	Y	148/150 (99%)	134 (90%)	14 (10%)	0	100	100
18	Z	125/127 (98%)	110 (88%)	15 (12%)	0	100	100
19	F	139/141 (99%)	127 (91%)	12 (9%)	0	100	100
20	G	117/125 (94%)	112 (96%)	5 (4%)	0	100	100
21	H	143/145 (99%)	130 (91%)	13 (9%)	0	100	100
22	I	141/143 (99%)	129 (92%)	10 (7%)	2 (1%)	9	33
23	J	98/100 (98%)	89 (91%)	9 (9%)	0	100	100
24	a	85/87 (98%)	71 (84%)	14 (16%)	0	100	100
25	b	127/129 (98%)	113 (89%)	14 (11%)	0	100	100
26	c	142/144 (99%)	125 (88%)	17 (12%)	0	100	100
27	d	132/134 (98%)	124 (94%)	8 (6%)	0	100	100
28	K	80/82 (98%)	70 (88%)	10 (12%)	0	100	100
29	e	95/97 (98%)	86 (90%)	9 (10%)	0	100	100
30	f	79/81 (98%)	70 (89%)	9 (11%)	0	100	100
31	M	51/53 (96%)	50 (98%)	1 (2%)	0	100	100
32	g	58/60 (97%)	49 (84%)	9 (16%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	N	71/73 (97%)	51 (72%)	20 (28%)	0	100	100
34	O	310/312 (99%)	269 (87%)	41 (13%)	0	100	100
35	L	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
39	LD	249/251 (99%)	222 (89%)	27 (11%)	0	100	100
40	LE	384/386 (100%)	357 (93%)	27 (7%)	0	100	100
41	LF	359/361 (99%)	324 (90%)	33 (9%)	2 (1%)	21	52
42	LG	292/294 (99%)	266 (91%)	26 (9%)	0	100	100
43	LH	163/175 (93%)	146 (90%)	17 (10%)	0	100	100
44	LI	220/222 (99%)	206 (94%)	14 (6%)	0	100	100
45	LJ	231/233 (99%)	210 (91%)	21 (9%)	0	100	100
46	LK	189/191 (99%)	172 (91%)	17 (9%)	0	100	100
47	LL	216/218 (99%)	190 (88%)	26 (12%)	0	100	100
48	LM	167/169 (99%)	153 (92%)	14 (8%)	0	100	100
49	LN	191/193 (99%)	171 (90%)	19 (10%)	1 (0%)	24	55
50	LO	134/136 (98%)	120 (90%)	13 (10%)	1 (1%)	18	49
51	LP	201/203 (99%)	181 (90%)	19 (10%)	1 (0%)	24	55
52	LQ	195/197 (99%)	187 (96%)	8 (4%)	0	100	100
53	LR	181/183 (99%)	168 (93%)	13 (7%)	0	100	100
54	Lm	183/185 (99%)	168 (92%)	15 (8%)	0	100	100
55	Ln	186/188 (99%)	180 (97%)	6 (3%)	0	100	100
56	Lo	169/171 (99%)	155 (92%)	14 (8%)	0	100	100
57	Lp	157/159 (99%)	143 (91%)	14 (9%)	0	100	100
58	Lq	98/100 (98%)	92 (94%)	6 (6%)	0	100	100
59	Lr	134/136 (98%)	128 (96%)	6 (4%)	0	100	100
60	LS	124/126 (98%)	109 (88%)	15 (12%)	0	100	100
61	LT	119/121 (98%)	111 (93%)	8 (7%)	0	100	100
62	LU	123/125 (98%)	117 (95%)	6 (5%)	0	100	100
63	LV	133/135 (98%)	117 (88%)	16 (12%)	0	100	100
64	LW	146/148 (99%)	127 (87%)	19 (13%)	0	100	100
65	LX	56/58 (97%)	48 (86%)	8 (14%)	0	100	100
66	LY	94/96 (98%)	92 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
67	LZ	107/109 (98%)	92 (86%)	15 (14%)	0	100	100
68	La	125/127 (98%)	115 (92%)	10 (8%)	0	100	100
69	Lb	104/106 (98%)	98 (94%)	6 (6%)	0	100	100
70	Lc	110/112 (98%)	105 (96%)	5 (4%)	0	100	100
71	Ld	117/119 (98%)	109 (93%)	8 (7%)	0	100	100
72	Le	97/99 (98%)	92 (95%)	5 (5%)	0	100	100
73	Lf	79/81 (98%)	70 (89%)	9 (11%)	0	100	100
74	Lg	75/77 (97%)	73 (97%)	2 (3%)	0	100	100
75	Lh	48/50 (96%)	45 (94%)	3 (6%)	0	100	100
76	Li	50/52 (96%)	44 (88%)	6 (12%)	0	100	100
77	Lj	23/25 (92%)	23 (100%)	0	0	100	100
78	Lk	101/103 (98%)	94 (93%)	7 (7%)	0	100	100
79	Ll	89/91 (98%)	87 (98%)	2 (2%)	0	100	100
81	EF	975/1044 (93%)	857 (88%)	117 (12%)	1 (0%)	48	75
All	All	11953/12207 (98%)	10821 (90%)	1121 (9%)	11 (0%)	49	75

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
81	EF	418	PRO
16	D	109	GLU
22	I	25	GLN
22	I	29	GLU
41	LF	4	PRO
41	LF	130	ALA
50	LO	135	LEU
51	LP	146	ALA
49	LN	61	PRO
16	D	127	GLY
13	W	18	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	P	170/173 (98%)	170 (100%)	0	100	100
4	Q	200/205 (98%)	198 (99%)	2 (1%)	68	76
5	E	95/98 (97%)	93 (98%)	2 (2%)	47	67
6	R	175/175 (100%)	171 (98%)	4 (2%)	44	66
7	A	182/182 (100%)	179 (98%)	3 (2%)	55	72
8	S	220/220 (100%)	218 (99%)	2 (1%)	70	78
9	B	172/173 (99%)	171 (99%)	1 (1%)	78	81
10	T	189/195 (97%)	186 (98%)	3 (2%)	55	72
11	U	163/165 (99%)	161 (99%)	2 (1%)	63	75
12	V	148/159 (93%)	148 (100%)	0	100	100
13	W	156/157 (99%)	155 (99%)	1 (1%)	78	81
14	C	77/85 (91%)	76 (99%)	1 (1%)	61	74
15	X	126/127 (99%)	126 (100%)	0	100	100
16	D	88/98 (90%)	85 (97%)	3 (3%)	32	59
17	Y	127/127 (100%)	125 (98%)	2 (2%)	55	72
18	Z	90/96 (94%)	88 (98%)	2 (2%)	45	66
19	F	117/117 (100%)	116 (99%)	1 (1%)	70	78
20	G	101/113 (89%)	100 (99%)	1 (1%)	68	76
21	H	127/128 (99%)	126 (99%)	1 (1%)	73	79
22	I	115/115 (100%)	115 (100%)	0	100	100
23	J	93/93 (100%)	92 (99%)	1 (1%)	65	76
24	a	71/74 (96%)	70 (99%)	1 (1%)	59	73
25	b	110/110 (100%)	110 (100%)	0	100	100
26	c	119/119 (100%)	118 (99%)	1 (1%)	73	79
27	d	112/112 (100%)	110 (98%)	2 (2%)	51	70
28	K	67/73 (92%)	65 (97%)	2 (3%)	36	61
29	e	82/83 (99%)	81 (99%)	1 (1%)	63	75
30	f	70/70 (100%)	69 (99%)	1 (1%)	59	73
31	M	47/47 (100%)	47 (100%)	0	100	100
32	g	50/51 (98%)	49 (98%)	1 (2%)	48	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	N	56/63 (89%)	55 (98%)	1 (2%)	51	70
34	O	250/257 (97%)	245 (98%)	5 (2%)	48	68
35	L	55/56 (98%)	54 (98%)	1 (2%)	51	70
39	LD	190/193 (98%)	189 (100%)	1 (0%)	81	83
40	LE	321/322 (100%)	316 (98%)	5 (2%)	55	72
41	LF	288/288 (100%)	285 (99%)	3 (1%)	68	76
42	LG	241/243 (99%)	240 (100%)	1 (0%)	84	84
43	LH	139/154 (90%)	138 (99%)	1 (1%)	76	80
44	LI	186/186 (100%)	185 (100%)	1 (0%)	81	83
45	LJ	187/191 (98%)	185 (99%)	2 (1%)	65	76
46	LK	168/171 (98%)	167 (99%)	1 (1%)	78	81
47	LL	185/185 (100%)	182 (98%)	3 (2%)	55	72
48	LM	145/147 (99%)	145 (100%)	0	100	100
49	LN	154/154 (100%)	154 (100%)	0	100	100
50	LO	107/107 (100%)	105 (98%)	2 (2%)	50	68
51	LP	175/175 (100%)	174 (99%)	1 (1%)	78	81
52	LQ	160/160 (100%)	158 (99%)	2 (1%)	61	74
53	LR	138/145 (95%)	137 (99%)	1 (1%)	76	80
54	Lm	150/150 (100%)	147 (98%)	3 (2%)	48	68
55	Ln	152/153 (99%)	150 (99%)	2 (1%)	61	74
56	Lo	155/155 (100%)	154 (99%)	1 (1%)	78	81
57	Lp	135/136 (99%)	134 (99%)	1 (1%)	76	80
58	Lq	87/87 (100%)	86 (99%)	1 (1%)	65	76
59	Lr	104/104 (100%)	104 (100%)	0	100	100
60	LS	56/108 (52%)	56 (100%)	0	100	100
61	LT	104/105 (99%)	102 (98%)	2 (2%)	50	68
62	LU	108/108 (100%)	107 (99%)	1 (1%)	70	78
63	LV	112/115 (97%)	111 (99%)	1 (1%)	70	78
64	LW	117/118 (99%)	116 (99%)	1 (1%)	70	78
65	LX	46/46 (100%)	46 (100%)	0	100	100
66	LY	81/81 (100%)	81 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
67	LZ	92/96 (96%)	90 (98%)	2 (2%)	45	66
68	La	107/109 (98%)	106 (99%)	1 (1%)	70	78
69	Lb	90/90 (100%)	89 (99%)	1 (1%)	65	76
70	Lc	95/95 (100%)	94 (99%)	1 (1%)	65	76
71	Ld	104/104 (100%)	102 (98%)	2 (2%)	50	68
72	Le	80/81 (99%)	80 (100%)	0	100	100
73	Lf	67/67 (100%)	67 (100%)	0	100	100
74	Lg	68/68 (100%)	68 (100%)	0	100	100
75	Lh	45/45 (100%)	45 (100%)	0	100	100
76	Li	45/47 (96%)	45 (100%)	0	100	100
77	Lj	22/23 (96%)	20 (91%)	2 (9%)	9	31
78	Lk	87/88 (99%)	86 (99%)	1 (1%)	65	76
79	Ll	71/71 (100%)	71 (100%)	0	100	100
81	EF	789/885 (89%)	785 (100%)	4 (0%)	81	83
All	All	9973/10272 (97%)	9874 (99%)	99 (1%)	65	76

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	Q	48	VAL
4	Q	174	LYS
5	E	36	LEU
5	E	64	LYS
6	R	39	THR
6	R	95	ARG
6	R	146	THR
6	R	159	THR
7	A	14	ASP
7	A	168	ILE
7	A	218	LEU
8	S	38	LEU
8	S	258	GLN
9	B	25	LEU
10	T	69	LEU
10	T	71	THR
10	T	116	LYS
11	U	91	ILE

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Mol	Chain	Res	Type
11	U	152	VAL
13	W	78	ARG
14	C	37	THR
16	D	60	VAL
16	D	74	LEU
16	D	138	GLU
17	Y	39	LYS
17	Y	70	LYS
18	Z	26	THR
18	Z	102	LEU
19	F	52	LEU
20	G	44	LYS
21	H	98	TYR
23	J	26	LEU
24	a	13	VAL
26	c	120	VAL
27	d	35	VAL
27	d	102	LYS
28	K	40	VAL
28	K	85	LYS
29	e	64	LEU
30	f	25	VAL
32	g	38	LEU
33	N	138	ARG
34	O	87	LYS
34	O	144	LEU
34	O	271	VAL
34	O	290	VAL
34	O	312	VAL
35	L	30	VAL
39	LD	92	LYS
40	LE	89	VAL
40	LE	90	VAL
40	LE	93	VAL
40	LE	104	THR
40	LE	202	THR
41	LF	6	VAL
41	LF	12	THR
41	LF	343	LYS
42	LG	110	LEU
43	LH	93	VAL
44	LI	168	ILE

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Mol	Chain	Res	Type
45	LJ	26	LEU
45	LJ	158	ASP
46	LK	47	LYS
47	LL	36	LEU
47	LL	147	VAL
47	LL	191	LYS
50	LO	65	LEU
50	LO	78	THR
51	LP	153	ASP
52	LQ	125[A]	ARG
52	LQ	155[A]	LYS
53	LR	79	THR
54	Lm	31	LYS
54	Lm	147	ARG
54	Lm	176	ARG
55	Ln	6	THR
55	Ln	164	LEU
56	Lo	79	VAL
57	Lp	50	LYS
58	Lq	74	LYS
61	LT	77	GLU
61	LT	107	VAL
62	LU	80	VAL
63	LV	75	VAL
64	LW	123	VAL
67	LZ	9	THR
67	LZ	107	VAL
68	La	10	VAL
69	Lb	20	LYS
70	Lc	56	THR
71	Ld	33	VAL
71	Ld	90	ARG
77	Lj	7	LYS
77	Lj	8	LYS
78	Lk	57	VAL
81	EF	212	LEU
81	EF	229	LEU
81	EF	364	ILE
81	EF	543	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (124) such sidechains are listed below:

Mol	Chain	Res	Type
3	P	23	HIS
3	P	33	GLN
4	Q	199	ASN
5	E	98	ASN
5	E	103	ASN
7	A	111	ASN
7	A	165	ASN
8	S	16	HIS
8	S	258	GLN
9	B	63	GLN
9	B	100	ASN
9	B	186	ASN
10	T	182	GLN
11	U	86	GLN
11	U	89	HIS
11	U	161	GLN
14	C	9	ASN
14	C	81	ASN
15	X	22	ASN
15	X	81	HIS
16	D	80	ASN
17	Y	58	HIS
17	Y	78	ASN
17	Y	105	ASN
17	Y	123	HIS
18	Z	12	GLN
19	F	83	GLN
21	H	13	HIS
22	I	12	GLN
22	I	70	GLN
23	J	105	GLN
24	a	29	HIS
25	b	92	ASN
26	c	18	HIS
27	d	22	GLN
27	d	29	HIS
27	d	63	GLN
27	d	110	GLN
28	K	98	GLN
29	e	94	ASN
33	N	123	ASN
34	O	198	ASN
34	O	299	GLN

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Mol	Chain	Res	Type
34	O	308	ASN
35	L	27	GLN
35	L	43	ASN
39	LD	47	GLN
39	LD	132	ASN
39	LD	216	HIS
40	LE	231	HIS
40	LE	293	ASN
40	LE	319	ASN
41	LF	110	ASN
41	LF	296	GLN
42	LG	296	GLN
43	LH	102	ASN
43	LH	172	HIS
44	LI	37	ASN
44	LI	93	ASN
44	LI	244	ASN
45	LJ	59	GLN
45	LJ	192	GLN
46	LK	51	GLN
46	LK	58	HIS
46	LK	64	HIS
46	LK	102	ASN
46	LK	125	ASN
46	LK	149	ASN
46	LK	163	GLN
47	LL	14	ASN
47	LL	23	ASN
47	LL	51	HIS
48	LM	39	GLN
48	LM	62	ASN
49	LN	19	GLN
49	LN	105	ASN
49	LN	137	GLN
51	LP	11	GLN
51	LP	117	ASN
53	LR	55	GLN
53	LR	97	ASN
53	LR	133	HIS
54	Lm	9	GLN
54	Lm	58	ASN
55	Ln	166	ASN

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Mol	Chain	Res	Type
55	Ln	175	GLN
56	Lo	49	HIS
56	Lo	138	GLN
56	Lo	142	GLN
57	Lp	131	GLN
60	LS	59	HIS
63	LV	122	HIS
64	LW	39	HIS
65	LX	43	HIS
68	La	6	HIS
68	La	13	HIS
68	La	49	ASN
68	La	104	ASN
69	Lb	26	ASN
70	Lc	11	ASN
71	Ld	34	GLN
73	Lf	20	ASN
73	Lf	57	HIS
75	Lh	43	ASN
76	Li	109	ASN
81	EF	68	GLN
81	EF	97	ASN
81	EF	100	ASN
81	EF	255	ASN
81	EF	271	ASN
81	EF	296	ASN
81	EF	395	HIS
81	EF	413	ASN
81	EF	464	ASN
81	EF	486	GLN
81	EF	496	HIS
81	EF	577	ASN
81	EF	604	ASN
81	EF	611	ASN
81	EF	729	ASN
81	EF	800	HIS
81	EF	848	HIS
81	EF	975	HIS
81	EF	976	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1768/1771 (99%)	534 (30%)	54 (3%)
2	1	6/7 (85%)	1 (16%)	0
36	LA	3220/3223 (99%)	751 (23%)	42 (1%)
37	LB	120/121 (99%)	15 (12%)	1 (0%)
38	LC	157/158 (99%)	32 (20%)	3 (1%)
80	Sm	74/75 (98%)	24 (32%)	0
80	Sn	74/75 (98%)	23 (31%)	0
All	All	5419/5430 (99%)	1380 (25%)	100 (1%)

All (1380) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	14	C
1	2	25	C
1	2	26	A
1	2	34	G
1	2	43	A
1	2	45	U
1	2	46	A
1	2	47	A
1	2	56	U
1	2	57	G
1	2	62	A
1	2	65	A
1	2	67	A
1	2	68	A
1	2	69	G
1	2	73	U
1	2	74	U
1	2	75	U
1	2	76	A
1	2	78	A
1	2	79	C
1	2	80	A
1	2	81	G
1	2	104	A
1	2	114	C
1	2	116	U
1	2	121	U
1	2	127	G
1	2	129	U

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Mol	Chain	Res	Type
1	2	130	C
1	2	131	C
1	2	132	U
1	2	133	U
1	2	134	U
1	2	135	A
1	2	136	C
1	2	137	U
1	2	138	A
1	2	140	A
1	2	141	U
1	2	142	G
1	2	153	G
1	2	155	U
1	2	156	A
1	2	158	U
1	2	161	U
1	2	168	A
1	2	171	A
1	2	172	C
1	2	174	U
1	2	176	C
1	2	178	U
1	2	179	A
1	2	182	A
1	2	185	U
1	2	186	C
1	2	187	G
1	2	188	A
1	2	189	C
1	2	191	C
1	2	193	U
1	2	194	U
1	2	195	G
1	2	201	G
1	2	203	U
1	2	204	G
1	2	216	U
1	2	217	A
1	2	218	A
1	2	223	U
1	2	224	C

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Mol	Chain	Res	Type
1	2	225	A
1	2	227	U
1	2	228	G
1	2	230	C
1	2	232	U
1	2	233	C
1	2	234	G
1	2	235	G
1	2	236	A
1	2	238	U
1	2	240	U
1	2	241	U
1	2	243	G
1	2	246	G
1	2	250	C
1	2	256	A
1	2	260	U
1	2	261	U
1	2	265	A
1	2	270	C
1	2	272	U
1	2	274	G
1	2	276	C
1	2	277	U
1	2	278	U
1	2	279	G
1	2	280	U
1	2	281	G
1	2	287	G
1	2	299	A
1	2	313	U
1	2	314	C
1	2	316	A
1	2	320	U
1	2	321	C
1	2	322	G
1	2	323	A
1	2	324	U
1	2	330	G
1	2	333	A
1	2	334	G
1	2	337	G

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Mol	Chain	Res	Type
1	2	338	C
1	2	352	A
1	2	353	A
1	2	359	A
1	2	360	A
1	2	361	C
1	2	369	A
1	2	370	A
1	2	373	G
1	2	378	A
1	2	380	U
1	2	388	G
1	2	390	G
1	2	400	A
1	2	401	A
1	2	402	C
1	2	404	G
1	2	406	U
1	2	411	C
1	2	415	C
1	2	417	A
1	2	419	G
1	2	423	G
1	2	424	C
1	2	425	A
1	2	426	G
1	2	434	G
1	2	435	C
1	2	438	A
1	2	439	U
1	2	444	C
1	2	446	A
1	2	448	C
1	2	454	U
1	2	460	A
1	2	468	A
1	2	482	U
1	2	483	A
1	2	485	A
1	2	487	G
1	2	489	C
1	2	491	C

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Mol	Chain	Res	Type
1	2	492	A
1	2	493	U
1	2	494	U
1	2	495	C
1	2	496	G
1	2	498	G
1	2	499	U
1	2	500	C
1	2	502	U
1	2	506	A
1	2	507	U
1	2	510	G
1	2	511	A
1	2	513	U
1	2	517	U
1	2	518	A
1	2	519	C
1	2	520	A
1	2	525	A
1	2	527	A
1	2	529	A
1	2	534	A
1	2	538	A
1	2	539	G
1	2	540	G
1	2	541	A
1	2	542	A
1	2	543	C
1	2	554	C
1	2	555	A
1	2	556	A
1	2	557	G
1	2	558	U
1	2	565	C
1	2	571	G
1	2	572	C
1	2	578	U
1	2	579	A
1	2	580	A
1	2	594	A
1	2	595	G
1	2	606	A

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Mol	Chain	Res	Type
1	2	609	U
1	2	610	G
1	2	611	U
1	2	617	U
1	2	619	A
1	2	620	A
1	2	622	A
1	2	623	A
1	2	624	G
1	2	635	A
1	2	638	U
1	2	639	U
1	2	640	U
1	2	641	G
1	2	643	G
1	2	645	C
1	2	651	G
1	2	653	C
1	2	654	C
1	2	655	G
1	2	656	G
1	2	677	G
1	2	678	A
1	2	680	U
1	2	684	A
1	2	687	G
1	2	693	U
1	2	694	U
1	2	696	C
1	2	697	C
1	2	698	U
1	2	700	C
1	2	702	G
1	2	703	G
1	2	704	C
1	2	705	U
1	2	706	A
1	2	707	A
1	2	708	C
1	2	709	C
1	2	710	U
1	2	711	U

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Mol	Chain	Res	Type
1	2	712	G
1	2	714	G
1	2	728	U
1	2	729	G
1	2	730	G
1	2	732	G
1	2	733	A
1	2	736	C
1	2	738	G
1	2	739	G
1	2	741	C
1	2	742	U
1	2	743	U
1	2	744	U
1	2	745	U
1	2	753	A
1	2	755	A
1	2	756	A
1	2	765	G
1	2	766	U
1	2	767	U
1	2	771	A
1	2	774	A
1	2	775	G
1	2	778	G
1	2	781	U
1	2	782	U
1	2	783	G
1	2	787	G
1	2	789	A
1	2	794	U
1	2	804	A
1	2	807	A
1	2	811	A
1	2	812	A
1	2	813	U
1	2	814	A
1	2	815	G
1	2	816	G
1	2	818	C
1	2	819	G
1	2	820	U

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Mol	Chain	Res	Type
1	2	821	U
1	2	823	G
1	2	832	U
1	2	833	U
1	2	836	U
1	2	837	G
1	2	839	U
1	2	840	U
1	2	841	U
1	2	846	G
1	2	851	U
1	2	852	C
1	2	855	A
1	2	856	A
1	2	857	U
1	2	863	A
1	2	865	A
1	2	873	U
1	2	876	G
1	2	886	U
1	2	898	A
1	2	899	G
1	2	901	G
1	2	902	G
1	2	904	G
1	2	912	U
1	2	913	G
1	2	929	A
1	2	932	U
1	2	933	A
1	2	934	C
1	2	935	U
1	2	940	A
1	2	945	U
1	2	960	U
1	2	964	U
1	2	966	A
1	2	970	A
1	2	973	A
1	2	977	A
1	2	988	A
1	2	989	U

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Mol	Chain	Res	Type
1	2	992	A
1	2	996	U
1	2	998	A
1	2	1001	A
1	2	1004	U
1	2	1024	U
1	2	1026	A
1	2	1028	C
1	2	1029	U
1	2	1032	G
1	2	1039	A
1	2	1040	G
1	2	1052	U
1	2	1053	G
1	2	1057	U
1	2	1058	U
1	2	1059	U
1	2	1060	U
1	2	1061	A
1	2	1062	A
1	2	1063	U
1	2	1074	G
1	2	1080	U
1	2	1081	A
1	2	1082	C
1	2	1092	A
1	2	1096	C
1	2	1099	U
1	2	1100	G
1	2	1109	G
1	2	1111	G
1	2	1113	A
1	2	1138	A
1	2	1139	A
1	2	1156	C
1	2	1158	C
1	2	1160	A
1	2	1164	G
1	2	1167	G
1	2	1170	G
1	2	1183	A
1	2	1185	U

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Mol	Chain	Res	Type
1	2	1186	U
1	2	1187	U
1	2	1191	U
1	2	1194	A
1	2	1196	A
1	2	1197	C
1	2	1199	G
1	2	1200	G
1	2	1208	A
1	2	1212	G
1	2	1214	U
1	2	1217	A
1	2	1218	G
1	2	1227	A
1	2	1229	G
1	2	1241	G
1	2	1243	G
1	2	1244	A
1	2	1245	G
1	2	1246	C
1	2	1252	C
1	2	1256	A
1	2	1257	U
1	2	1258	U
1	2	1263	G
1	2	1264	G
1	2	1265	G
1	2	1269	U
1	2	1273	G
1	2	1274	C
1	2	1275	A
1	2	1276	U
1	2	1285	U
1	2	1294	G
1	2	1301	U
1	2	1307	U
1	2	1314	U
1	2	1315	U
1	2	1318	G
1	2	1321	A
1	2	1322	A
1	2	1325	A

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Mol	Chain	Res	Type
1	2	1337	A
1	2	1341	A
1	2	1344	A
1	2	1345	A
1	2	1346	A
1	2	1348	A
1	2	1349	G
1	2	1354	G
1	2	1360	A
1	2	1361	U
1	2	1363	U
1	2	1367	G
1	2	1370	U
1	2	1371	A
1	2	1372	U
1	2	1373	C
1	2	1381	U
1	2	1382	A
1	2	1383	G
1	2	1385	G
1	2	1390	U
1	2	1398	U
1	2	1399	C
1	2	1400	A
1	2	1402	G
1	2	1414	U
1	2	1415	U
1	2	1421	A
1	2	1427	A
1	2	1431	C
1	2	1432	U
1	2	1433	G
1	2	1446	A
1	2	1447	C
1	2	1457	C
1	2	1459	C
1	2	1460	A
1	2	1469	A
1	2	1471	A
1	2	1472	C
1	2	1473	U
1	2	1479	A

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Mol	Chain	Res	Type
1	2	1482	C
1	2	1483	A
1	2	1488	G
1	2	1489	U
1	2	1490	C
1	2	1491	U
1	2	1492	A
1	2	1493	A
1	2	1496	U
1	2	1510	U
1	2	1514	U
1	2	1515	A
1	2	1516	A
1	2	1517	U
1	2	1518	C
1	2	1521	G
1	2	1523	G
1	2	1524	A
1	2	1528	U
1	2	1529	C
1	2	1531	G
1	2	1537	C
1	2	1540	G
1	2	1543	A
1	2	1545	A
1	2	1556	A
1	2	1557	U
1	2	1558	U
1	2	1559	A
1	2	1572	G
1	2	1573	A
1	2	1574	G
1	2	1575	G
1	2	1576	A
1	2	1583	A
1	2	1584	G
1	2	1585	U
1	2	1590	G
1	2	1592	A
1	2	1601	G
1	2	1607	G
1	2	1611	A

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Mol	Chain	Res	Type
1	2	1614	A
1	2	1616	G
1	2	1619	C
1	2	1622	G
1	2	1634	C
1	2	1637	C
1	2	1657	U
1	2	1658	G
1	2	1676	U
1	2	1682	U
1	2	1688	U
1	2	1689	A
1	2	1693	A
1	2	1700	C
1	2	1701	A
1	2	1702	A
1	2	1703	C
1	2	1709	C
1	2	1711	C
1	2	1715	G
1	2	1717	G
1	2	1736	G
1	2	1740	A
1	2	1755	A
1	2	1756	A
1	2	1757	G
1	2	1760	G
1	2	1762	A
1	2	1766	A
1	2	1767	G
1	2	1769	U
1	2	1770	U
1	2	1780	G
1	2	1782	A
1	2	1783	C
1	2	1788	G
1	2	1792	G
1	2	1793	G
1	2	1794	A
1	2	1796	C
1	2	1799	U
2	1	4	A

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Mol	Chain	Res	Type
36	LA	6	A
36	LA	11	A
36	LA	14	U
36	LA	21	G
36	LA	22	G
36	LA	26	A
36	LA	30	G
36	LA	40	A
36	LA	43	A
36	LA	44	U
36	LA	48	A
36	LA	49	A
36	LA	51	A
36	LA	59	G
36	LA	60	A
36	LA	65	A
36	LA	66	A
36	LA	73	C
36	LA	74	G
36	LA	76	G
36	LA	85	A
36	LA	89	A
36	LA	92	G
36	LA	109	A
36	LA	110	G
36	LA	111	C
36	LA	113	C
36	LA	120	G
36	LA	121	A
36	LA	122	A
36	LA	133	U
36	LA	136	G
36	LA	143	G
36	LA	150	A
36	LA	156	G
36	LA	157	A
36	LA	166	C
36	LA	173	G
36	LA	187	A
36	LA	190	U
36	LA	191	U
36	LA	200	C

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Mol	Chain	Res	Type
36	LA	206	G
36	LA	210	U
36	LA	211	A
36	LA	213	A
36	LA	218	G
36	LA	219	A
36	LA	221	A
36	LA	231	G
36	LA	234	G
36	LA	236	G
36	LA	239	G
36	LA	240	U
36	LA	243	G
36	LA	249	U
36	LA	252	U
36	LA	263	C
36	LA	269	G
36	LA	282	G
36	LA	283	G
36	LA	286	U
36	LA	295	A
36	LA	298	U
36	LA	315	C
36	LA	323	A
36	LA	329	U
36	LA	330	G
36	LA	334	A
36	LA	338	A
36	LA	339	C
36	LA	346	C
36	LA	350	C
36	LA	351	A
36	LA	376	G
36	LA	385	A
36	LA	390	G
36	LA	395	A
36	LA	397	A
36	LA	399	A
36	LA	401	U
36	LA	402	A
36	LA	403	C
36	LA	421	G

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Mol	Chain	Res	Type
36	LA	422	A
36	LA	438	A
36	LA	440	A
36	LA	441	U
36	LA	442	G
36	LA	443	G
36	LA	445	G
36	LA	446	U
36	LA	447	U
36	LA	448	U
36	LA	449	U
36	LA	450	G
36	LA	487	U
36	LA	488	U
36	LA	489	U
36	LA	490	C
36	LA	491	A
36	LA	492	C
36	LA	494	G
36	LA	498	A
36	LA	510	G
36	LA	515	C
36	LA	517	G
36	LA	520	U
36	LA	521	A
36	LA	535	G
36	LA	543	C
36	LA	544	C
36	LA	545	U
36	LA	546	C
36	LA	547	G
36	LA	552	G
36	LA	555	U
36	LA	557	A
36	LA	559	A
36	LA	568	G
36	LA	578	A
36	LA	579	G
36	LA	597	G
36	LA	600	G
36	LA	603	A
36	LA	604	G

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Mol	Chain	Res	Type
36	LA	609	G
36	LA	610	G
36	LA	611	A
36	LA	612	U
36	LA	619	A
36	LA	620	U
36	LA	621	A
36	LA	625	G
36	LA	637	C
36	LA	638	C
36	LA	642	U
36	LA	649	A
36	LA	650	C
36	LA	660	A
36	LA	667	C
36	LA	677	A
36	LA	681	U
36	LA	691	A
36	LA	699	A
36	LA	705	A
36	LA	712	G
36	LA	716	A
36	LA	720	A
36	LA	726	G
36	LA	737	G
36	LA	742	G
36	LA	758	C
36	LA	763	G
36	LA	764	U
36	LA	765	C
36	LA	766	U
36	LA	767	U
36	LA	771	A
36	LA	774	G
36	LA	776	U
36	LA	777	U
36	LA	780	A
36	LA	781	G
36	LA	785	G
36	LA	786	A
36	LA	806	A
36	LA	808	A

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Mol	Chain	Res	Type
36	LA	817	A
36	LA	830	A
36	LA	832	G
36	LA	848	A
36	LA	849	C
36	LA	850	U
36	LA	851	C
36	LA	861	C
36	LA	865	U
36	LA	868	C
36	LA	871	U
36	LA	874	U
36	LA	879	U
36	LA	894	G
36	LA	895	A
36	LA	896	A
36	LA	899	U
36	LA	906	A
36	LA	907	G
36	LA	908	G
36	LA	914	A
36	LA	916	G
36	LA	917	A
36	LA	921	A
36	LA	923	C
36	LA	932	U
36	LA	934	G
36	LA	937	G
36	LA	944	C
36	LA	959	C
36	LA	960	U
36	LA	971	G
36	LA	974	G
36	LA	981	U
36	LA	982	C
36	LA	991	G
36	LA	1002	A
36	LA	1015	U
36	LA	1018	G
36	LA	1020	G
36	LA	1021	G
36	LA	1024	G

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Mol	Chain	Res	Type
36	LA	1028	U
36	LA	1029	G
36	LA	1040	A
36	LA	1041	U
36	LA	1045	C
36	LA	1047	A
36	LA	1049	C
36	LA	1064	A
36	LA	1065	A
36	LA	1072	G
36	LA	1081	U
36	LA	1093	A
36	LA	1094	U
36	LA	1095	U
36	LA	1096	U
36	LA	1097	G
36	LA	1098	A
36	LA	1103	A
36	LA	1104	G
36	LA	1117	G
36	LA	1118	C
36	LA	1128	U
36	LA	1131	G
36	LA	1144	U
36	LA	1145	G
36	LA	1148	G
36	LA	1153	A
36	LA	1158	A
36	LA	1159	A
36	LA	1177	G
36	LA	1178	G
36	LA	1180	A
36	LA	1181	U
36	LA	1182	A
36	LA	1190	A
36	LA	1192	C
36	LA	1193	A
36	LA	1196	C
36	LA	1197	A
36	LA	1201	C
36	LA	1202	A
36	LA	1206	G

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Mol	Chain	Res	Type
36	LA	1208	U
36	LA	1217	A
36	LA	1218	U
36	LA	1222	G
36	LA	1223	A
36	LA	1227	C
36	LA	1229	G
36	LA	1234	G
36	LA	1236	G
36	LA	1237	G
36	LA	1238	C
36	LA	1239	C
36	LA	1240	A
36	LA	1241	U
36	LA	1242	G
36	LA	1243	G
36	LA	1244	A
36	LA	1245	A
36	LA	1246	G
36	LA	1248	C
36	LA	1251	A
36	LA	1253	U
36	LA	1258	U
36	LA	1262	G
36	LA	1263	A
36	LA	1264	G
36	LA	1266	G
36	LA	1267	U
36	LA	1269	U
36	LA	1270	A
36	LA	1271	A
36	LA	1272	C
36	LA	1278	A
36	LA	1279	C
36	LA	1280	C
36	LA	1282	G
36	LA	1285	G
36	LA	1286	A
36	LA	1287	A
36	LA	1295	G
36	LA	1307	G
36	LA	1308	A

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Mol	Chain	Res	Type
36	LA	1309	U
36	LA	1313	G
36	LA	1316	C
36	LA	1318	A
36	LA	1325	U
36	LA	1330	A
36	LA	1345	G
36	LA	1348	U
36	LA	1349	G
36	LA	1351	U
36	LA	1352	A
36	LA	1353	U
36	LA	1354	G
36	LA	1355	A
36	LA	1356	U
36	LA	1357	G
36	LA	1386	A
36	LA	1392	G
36	LA	1399	A
36	LA	1400	G
36	LA	1418	A
36	LA	1419	A
36	LA	1421	G
36	LA	1429	G
36	LA	1430	U
36	LA	1431	G
36	LA	1434	G
36	LA	1437	C
36	LA	1442	U
36	LA	1443	G
36	LA	1446	A
36	LA	1450	G
36	LA	1455	U
36	LA	1481	A
36	LA	1482	A
36	LA	1483	G
36	LA	1484	U
36	LA	1487	G
36	LA	1488	G
36	LA	1503	A
36	LA	1508	C
36	LA	1523	U

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Mol	Chain	Res	Type
36	LA	1528	G
36	LA	1533	U
36	LA	1536	G
36	LA	1542	G
36	LA	1549	U
36	LA	1555	U
36	LA	1556	C
36	LA	1557	A
36	LA	1559	A
36	LA	1560	G
36	LA	1562	C
36	LA	1563	C
36	LA	1565	G
36	LA	1566	A
36	LA	1567	U
36	LA	1568	U
36	LA	1569	U
36	LA	1572	U
36	LA	1573	G
36	LA	1574	C
36	LA	1575	A
36	LA	1576	G
36	LA	1580	A
36	LA	1581	C
36	LA	1582	C
36	LA	1583	A
36	LA	1587	A
36	LA	1588	A
36	LA	1589	A
36	LA	1590	G
36	LA	1602	A
36	LA	1605	A
36	LA	1607	U
36	LA	1621	A
36	LA	1629	U
36	LA	1632	A
36	LA	1639	C
36	LA	1642	A
36	LA	1643	A
36	LA	1645	U
36	LA	1658	G
36	LA	1677	G

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Mol	Chain	Res	Type
36	LA	1683	A
36	LA	1687	U
36	LA	1688	U
36	LA	1696	A
36	LA	1704	A
36	LA	1705	U
36	LA	1715	A
36	LA	1716	U
36	LA	1717	U
36	LA	1722	U
36	LA	1724	U
36	LA	1725	C
36	LA	1750	A
36	LA	1751	G
36	LA	1756	C
36	LA	1760	A
36	LA	1765	U
36	LA	1766	G
36	LA	1770	G
36	LA	1775	G
36	LA	1780	G
36	LA	1788	C
36	LA	1796	G
36	LA	1797	A
36	LA	1812	G
36	LA	1814	A
36	LA	1816	A
36	LA	1817	G
36	LA	1819	U
36	LA	1820	U
36	LA	1821	U
36	LA	1822	C
36	LA	1835	A
36	LA	1839	A
36	LA	1840	U
36	LA	1841	A
36	LA	1842	A
36	LA	1846	C
36	LA	1849	C
36	LA	1850	A
36	LA	1866	C
36	LA	1867	A

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Mol	Chain	Res	Type
36	LA	1874	A
36	LA	1880	U
36	LA	1881	A
36	LA	1893	A
36	LA	1897	G
36	LA	1906	G
36	LA	1908	A
36	LA	1930	A
36	LA	1935	G
36	LA	1943	C
36	LA	1951	C
36	LA	1952	G
36	LA	1953	G
36	LA	1954	G
36	LA	2101	C
36	LA	2102	U
36	LA	2111	G
36	LA	2113	A
36	LA	2121	G
36	LA	2122	G
36	LA	2131	A
36	LA	2139	A
36	LA	2149	A
36	LA	2158	A
36	LA	2169	G
36	LA	2170	U
36	LA	2187	G
36	LA	2188	A
36	LA	2201	G
36	LA	2205	U
36	LA	2206	G
36	LA	2207	A
36	LA	2209	U
36	LA	2223	A
36	LA	2228	A
36	LA	2244	A
36	LA	2249	G
36	LA	2250	G
36	LA	2252	A
36	LA	2256	A
36	LA	2257	C
36	LA	2262	A

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Mol	Chain	Res	Type
36	LA	2272	G
36	LA	2273	G
36	LA	2274	U
36	LA	2279	A
36	LA	2280	A
36	LA	2281	A
36	LA	2282	U
36	LA	2284	C
36	LA	2285	C
36	LA	2288	G
36	LA	2299	A
36	LA	2306	C
36	LA	2307	G
36	LA	2308	C
36	LA	2309	A
36	LA	2310	U
36	LA	2313	A
36	LA	2314	U
36	LA	2315	G
36	LA	2335	G
36	LA	2336	U
36	LA	2347	U
36	LA	2364	G
36	LA	2372	A
36	LA	2373	A
36	LA	2374	C
36	LA	2375	G
36	LA	2385	G
36	LA	2388	U
36	LA	2393	G
36	LA	2394	G
36	LA	2397	A
36	LA	2402	A
36	LA	2403	G
36	LA	2404	A
36	LA	2411	U
36	LA	2412	G
36	LA	2419	A
36	LA	2422	C
36	LA	2434	U
36	LA	2435	G
36	LA	2437	G

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Mol	Chain	Res	Type
36	LA	2438	A
36	LA	2439	A
36	LA	2440	G
36	LA	2452	G
36	LA	2453	U
36	LA	2454	G
36	LA	2455	U
36	LA	2456	A
36	LA	2457	G
36	LA	2458	A
36	LA	2459	A
36	LA	2461	A
36	LA	2462	A
36	LA	2463	G
36	LA	2466	G
36	LA	2467	G
36	LA	2468	A
36	LA	2469	G
36	LA	2471	U
36	LA	2474	G
36	LA	2477	G
36	LA	2480	A
36	LA	2484	A
36	LA	2487	U
36	LA	2488	A
36	LA	2489	C
36	LA	2491	A
36	LA	2492	C
36	LA	2493	U
36	LA	2494	A
36	LA	2496	C
36	LA	2497	U
36	LA	2498	U
36	LA	2499	U
36	LA	2500	A
36	LA	2501	U
36	LA	2503	G
36	LA	2505	U
36	LA	2506	U
36	LA	2507	C
36	LA	2510	U
36	LA	2514	U

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Mol	Chain	Res	Type
36	LA	2515	A
36	LA	2522	G
36	LA	2523	A
36	LA	2524	A
36	LA	2525	G
36	LA	2526	C
36	LA	2531	C
36	LA	2532	U
36	LA	2537	U
36	LA	2538	U
36	LA	2539	C
36	LA	2540	A
36	LA	2541	U
36	LA	2542	U
36	LA	2543	U
36	LA	2546	C
36	LA	2548	C
36	LA	2549	G
36	LA	2552	C
36	LA	2554	A
36	LA	2561	A
36	LA	2569	A
36	LA	2570	U
36	LA	2571	U
36	LA	2572	C
36	LA	2573	G
36	LA	2576	G
36	LA	2585	G
36	LA	2589	G
36	LA	2593	A
36	LA	2594	C
36	LA	2595	A
36	LA	2606	G
36	LA	2607	G
36	LA	2614	G
36	LA	2626	A
36	LA	2629	U
36	LA	2636	A
36	LA	2648	G
36	LA	2652	U
36	LA	2656	A
36	LA	2672	G

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Mol	Chain	Res	Type
36	LA	2674	A
36	LA	2677	G
36	LA	2689	A
36	LA	2691	A
36	LA	2694	A
36	LA	2696	A
36	LA	2703	A
36	LA	2704	A
36	LA	2714	G
36	LA	2719	U
36	LA	2728	G
36	LA	2748	A
36	LA	2749	G
36	LA	2752	U
36	LA	2753	G
36	LA	2755	C
36	LA	2777	G
36	LA	2778	G
36	LA	2796	G
36	LA	2800	G
36	LA	2801	A
36	LA	2802	A
36	LA	2803	A
36	LA	2804	A
36	LA	2805	G
36	LA	2810	C
36	LA	2817	A
36	LA	2818	U
36	LA	2821	C
36	LA	2838	A
36	LA	2842	U
36	LA	2844	C
36	LA	2845	A
36	LA	2847	A
36	LA	2849	C
36	LA	2856	G
36	LA	2861	U
36	LA	2867	C
36	LA	2871	G
36	LA	2872	A
36	LA	2873	U
36	LA	2875	U

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Mol	Chain	Res	Type
36	LA	2876	C
36	LA	2887	A
36	LA	2894	C
36	LA	2899	C
36	LA	2910	A
36	LA	2916	U
36	LA	2918	G
36	LA	2923	U
36	LA	2928	C
36	LA	2933	A
36	LA	2935	U
36	LA	2936	A
36	LA	2941	A
36	LA	2942	C
36	LA	2947	G
36	LA	2954	U
36	LA	2955	U
36	LA	2957	G
36	LA	2971	A
36	LA	2983	C
36	LA	2990	G
36	LA	2996	U
36	LA	2997	G
36	LA	3003	G
36	LA	3012	A
36	LA	3030	G
36	LA	3055	U
36	LA	3056	U
36	LA	3058	U
36	LA	3059	G
36	LA	3078	U
36	LA	3079	U
36	LA	3080	G
36	LA	3086	A
36	LA	3092	C
36	LA	3101	G
36	LA	3104	U
36	LA	3115	C
36	LA	3116	G
36	LA	3118	C
36	LA	3119	U
36	LA	3122	A

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Mol	Chain	Res	Type
36	LA	3129	A
36	LA	3130	A
36	LA	3131	U
36	LA	3142	A
36	LA	3143	C
36	LA	3151	U
36	LA	3154	C
36	LA	3155	U
36	LA	3156	U
36	LA	3157	U
36	LA	3158	G
36	LA	3165	A
36	LA	3170	A
36	LA	3172	A
36	LA	3173	G
36	LA	3174	A
36	LA	3175	U
36	LA	3176	G
36	LA	3180	A
36	LA	3181	C
36	LA	3187	A
36	LA	3196	U
36	LA	3199	G
36	LA	3207	U
36	LA	3210	A
36	LA	3216	G
36	LA	3217	C
36	LA	3218	A
36	LA	3219	G
36	LA	3222	U
36	LA	3229	G
36	LA	3235	C
36	LA	3239	G
36	LA	3242	G
36	LA	3243	A
36	LA	3244	A
36	LA	3245	A
36	LA	3247	G
36	LA	3259	U
36	LA	3260	G
36	LA	3263	G
36	LA	3269	U

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Mol	Chain	Res	Type
36	LA	3270	U
36	LA	3272	C
36	LA	3273	A
36	LA	3276	G
36	LA	3277	U
36	LA	3281	U
36	LA	3286	G
36	LA	3287	U
36	LA	3288	G
36	LA	3289	G
36	LA	3294	A
36	LA	3295	A
36	LA	3304	U
36	LA	3313	U
36	LA	3316	A
36	LA	3318	G
36	LA	3319	U
36	LA	3320	A
36	LA	3334	U
36	LA	3341	U
36	LA	3345	G
36	LA	3347	A
36	LA	3351	U
36	LA	3352	U
36	LA	3353	G
36	LA	3354	U
36	LA	3355	U
36	LA	3356	G
36	LA	3368	U
36	LA	3369	G
36	LA	3378	C
36	LA	3381	U
36	LA	3382	U
36	LA	3386	G
36	LA	3389	U
36	LA	3390	G
36	LA	3396	U
37	LB	7	G
37	LB	10	C
37	LB	17	A
37	LB	22	A
37	LB	35	C

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Mol	Chain	Res	Type
37	LB	52	G
37	LB	53	U
37	LB	54	U
37	LB	65	G
37	LB	74	C
37	LB	76	A
37	LB	99	G
37	LB	102	A
37	LB	112	G
37	LB	121	U
38	LC	16	G
38	LC	25	G
38	LC	34	U
38	LC	35	C
38	LC	38	U
38	LC	59	A
38	LC	62	C
38	LC	63	G
38	LC	80	A
38	LC	81	U
38	LC	82	U
38	LC	83	C
38	LC	84	C
38	LC	85	G
38	LC	86	U
38	LC	87	G
38	LC	90	U
38	LC	95	G
38	LC	97	A
38	LC	99	C
38	LC	104	A
38	LC	106	C
38	LC	111	A
38	LC	112	U
38	LC	113	U
38	LC	125	U
38	LC	126	A
38	LC	138	A
38	LC	148	G
38	LC	152	G
38	LC	157	U
38	LC	158	U

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Mol	Chain	Res	Type
80	Sn	8	U
80	Sn	9	G
80	Sn	11	C
80	Sn	14	A
80	Sn	19	G
80	Sn	20	A
80	Sn	21	A
80	Sn	25	C
80	Sn	27	C
80	Sn	36	U
80	Sn	45	U
80	Sn	46	G
80	Sn	47	U
80	Sn	48	C
80	Sn	49	C
80	Sn	54	A
80	Sn	57	G
80	Sn	59	A
80	Sn	61	C
80	Sn	63	G
80	Sn	64	A
80	Sn	66	C
80	Sn	76	A
80	Sm	8	U
80	Sm	9	G
80	Sm	11	C
80	Sm	14	A
80	Sm	19	G
80	Sm	20	A
80	Sm	21	A
80	Sm	25	C
80	Sm	27	C
80	Sm	36	U
80	Sm	45	U
80	Sm	46	G
80	Sm	47	U
80	Sm	48	C
80	Sm	49	C
80	Sm	54	A
80	Sm	57	G
80	Sm	59	A
80	Sm	61	C

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Mol	Chain	Res	Type
80	Sm	63	G
80	Sm	64	A
80	Sm	66	C
80	Sm	74	C
80	Sm	76	A

All (100) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	68	A
1	2	77	U
1	2	139	C
1	2	141	U
1	2	215	A
1	2	224	C
1	2	237	C
1	2	278	U
1	2	280	U
1	2	313	U
1	2	322	G
1	2	352	A
1	2	387	A
1	2	400	A
1	2	447	U
1	2	518	A
1	2	539	G
1	2	541	A
1	2	555	A
1	2	609	U
1	2	639	U
1	2	640	U
1	2	705	U
1	2	711	U
1	2	740	A
1	2	755	A
1	2	803	A
1	2	819	G
1	2	912	U
1	2	928	U
1	2	987	G
1	2	1023	A
1	2	1207	C

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Mol	Chain	Res	Type
1	2	1226	A
1	2	1245	G
1	2	1251	U
1	2	1256	A
1	2	1273	G
1	2	1274	C
1	2	1314	U
1	2	1344	A
1	2	1348	A
1	2	1382	A
1	2	1399	C
1	2	1430	U
1	2	1471	A
1	2	1556	A
1	2	1557	U
1	2	1573	A
1	2	1584	G
1	2	1633	A
1	2	1636	C
1	2	1700	C
1	2	1755	A
36	LA	13	A
36	LA	282	G
36	LA	439	C
36	LA	637	C
36	LA	763	G
36	LA	849	C
36	LA	873	C
36	LA	896	A
36	LA	916	G
36	LA	993	G
36	LA	1064	A
36	LA	1097	G
36	LA	1271	A
36	LA	1307	G
36	LA	1355	A
36	LA	1562	C
36	LA	1572	U
36	LA	1582	C
36	LA	1716	U
36	LA	1815	U
36	LA	1820	U

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Mol	Chain	Res	Type
36	LA	2101	C
36	LA	2112	U
36	LA	2227	C
36	LA	2256	A
36	LA	2500	A
36	LA	2504	U
36	LA	2505	U
36	LA	2509	U
36	LA	2525	G
36	LA	2537	U
36	LA	2538	U
36	LA	2541	U
36	LA	3055	U
36	LA	3078	U
36	LA	3121	U
36	LA	3218	A
36	LA	3228	C
36	LA	3269	U
36	LA	3275	U
36	LA	3319	U
36	LA	3350	C
37	LB	52	G
38	LC	82	U
38	LC	85	G
38	LC	125	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands 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
82	ATP	EF	1101	-	32,33,33	1.28	4 (12%)	48,52,52	1.91	13 (27%)
82	ATP	EF	1102	-	32,33,33	1.32	5 (15%)	48,52,52	1.86	8 (16%)

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
82	ATP	EF	1101	-	-	2/22/38/38	0/3/3/3
82	ATP	EF	1102	-	-	0/22/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	EF	1101	ATP	C5-C4	4.31	1.46	1.39
82	EF	1102	ATP	C5-C4	4.12	1.46	1.39
82	EF	1102	ATP	C5-N7	-2.73	1.34	1.39
82	EF	1101	ATP	C5-N7	-2.57	1.34	1.39
82	EF	1101	ATP	C5-C6	2.44	1.47	1.41
82	EF	1102	ATP	C5-C6	2.28	1.47	1.41
82	EF	1102	ATP	C4-N9	-2.20	1.33	1.37
82	EF	1101	ATP	C4-N9	-2.18	1.33	1.37
82	EF	1102	ATP	C8-N9	-2.02	1.34	1.37

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
82	EF	1102	ATP	C5-C4-N3	-5.72	118.85	126.72
82	EF	1101	ATP	C5-C4-N3	-5.66	118.92	126.72
82	EF	1102	ATP	N3-C4-N9	4.80	135.32	127.17
82	EF	1101	ATP	N3-C4-N9	4.72	135.19	127.17
82	EF	1102	ATP	C4-C5-N7	-3.67	106.38	110.58
82	EF	1102	ATP	C4-N9-C8	3.57	109.48	105.74
82	EF	1101	ATP	C2-N3-C4	3.57	120.55	111.83
82	EF	1102	ATP	C2-N3-C4	3.53	120.44	111.83
82	EF	1101	ATP	C4-C5-N7	-3.39	106.71	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
82	EF	1101	ATP	C2'-C1'-N9	-3.23	105.29	113.30
82	EF	1101	ATP	C4-N9-C8	3.19	109.08	105.74
82	EF	1101	ATP	N3-C2-N1	-3.17	123.78	128.58
82	EF	1102	ATP	N3-C2-N1	-3.09	123.91	128.58
82	EF	1102	ATP	C5-N7-C8	3.08	108.30	103.45
82	EF	1102	ATP	N9-C8-N7	-2.77	110.01	113.94
82	EF	1101	ATP	C3'-C2'-C1'	2.70	106.56	101.46
82	EF	1101	ATP	C5-N7-C8	2.65	107.61	103.45
82	EF	1101	ATP	O2A-PA-O3A	2.33	113.56	107.27
82	EF	1101	ATP	N9-C8-N7	-2.28	110.71	113.94
82	EF	1101	ATP	O2A-PA-O1A	2.19	122.65	112.44
82	EF	1101	ATP	C6-C5-N7	2.12	136.18	132.09

There are no chirality outliers.

All (2) torsion outliers are listed below:

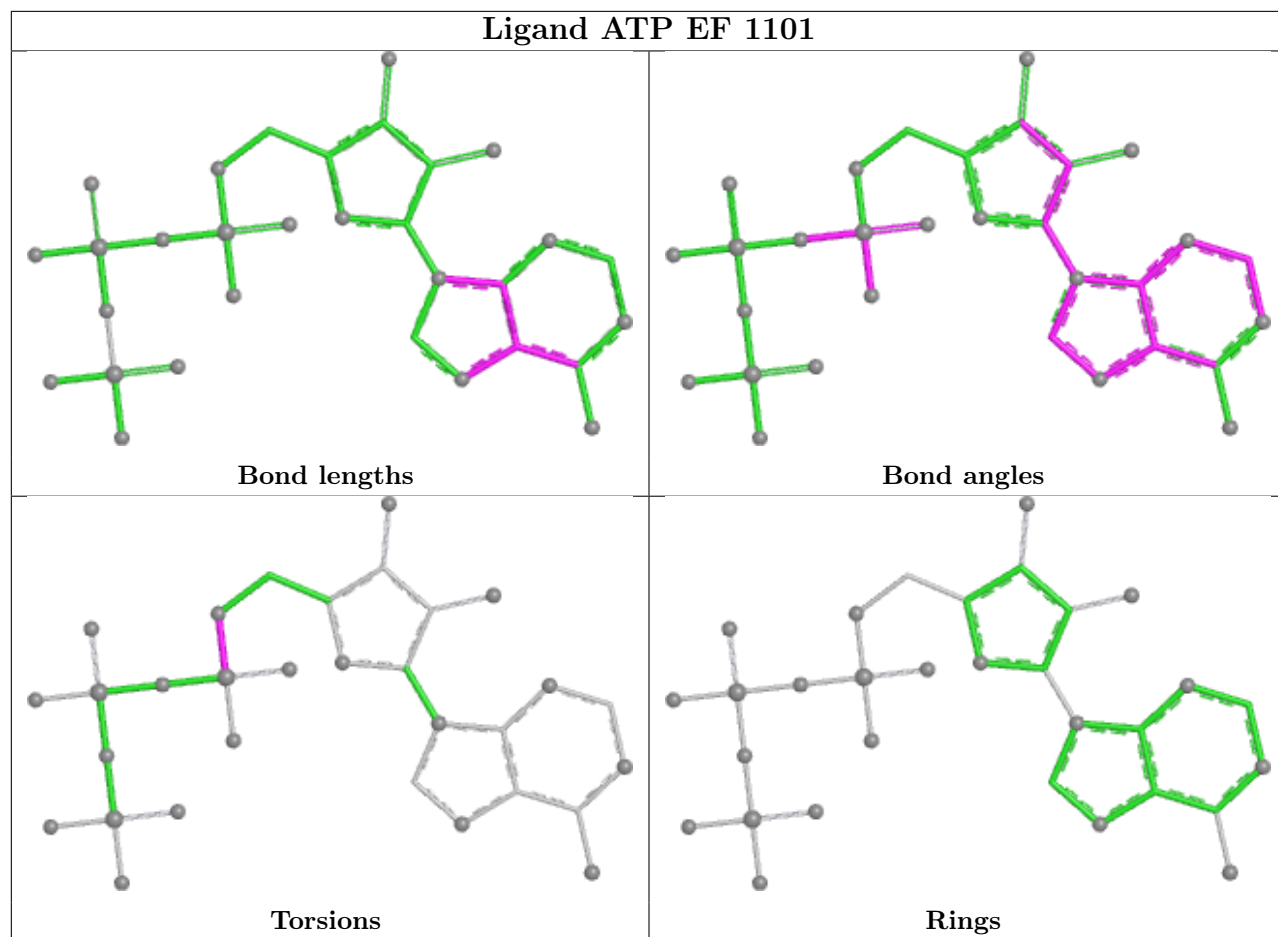
Mol	Chain	Res	Type	Atoms
82	EF	1101	ATP	C5'-O5'-PA-O2A
82	EF	1101	ATP	C5'-O5'-PA-O3A

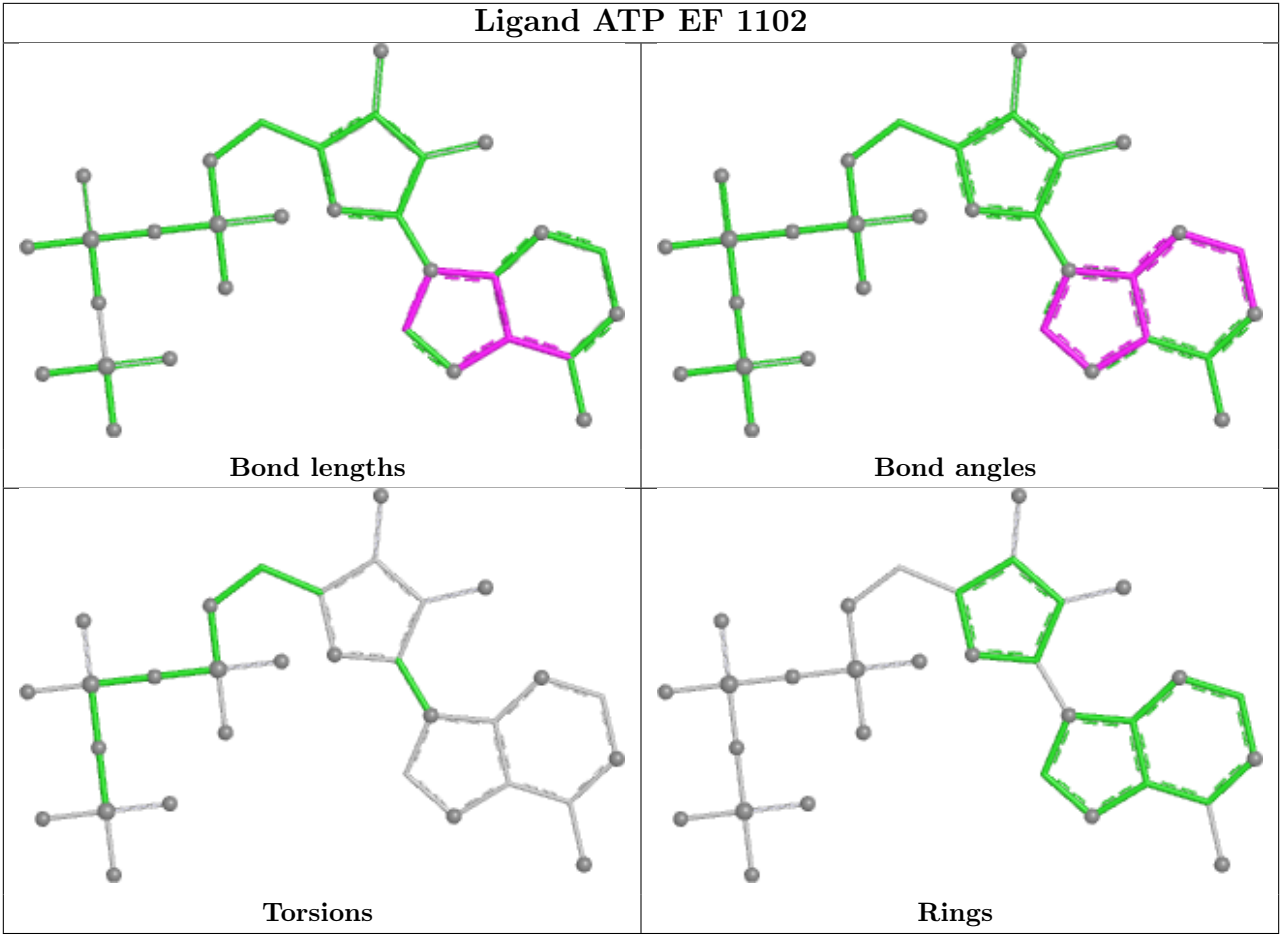
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	EF	1101	ATP	1	0
82	EF	1102	ATP	4	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
36	LA	2
1	2	2
6	R	1
45	LJ	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	LA	1955:U	O3'	2093:A	P	27.27
1	2	658:C	O3'	676:G	P	15.54

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	LA	451:U	O3'	486:A	P	11.17
1	2	714:G	O3'	726:C	P	10.44
1	R	60:SER	C	61:LEU	N	1.18
1	LJ	40:VAL	C	41:GLN	N	1.18

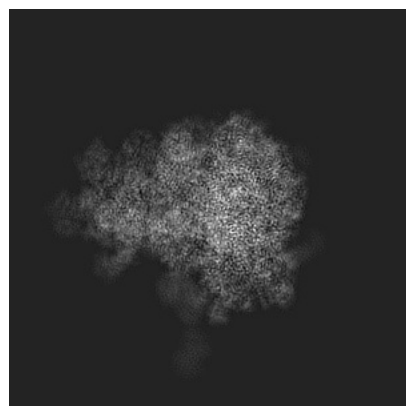
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12081. These allow visual inspection of the internal detail of the map and identification of artifacts.

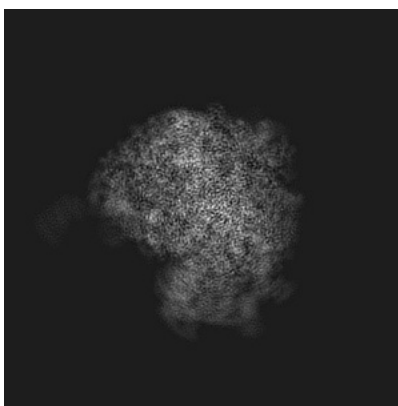
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

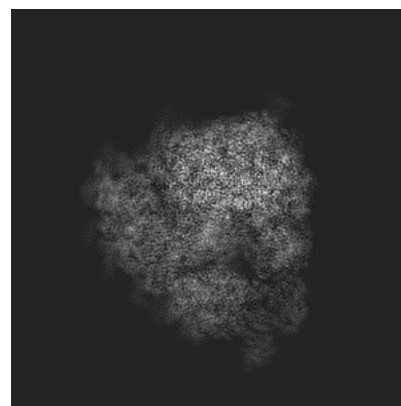
6.1.1 Primary map



X

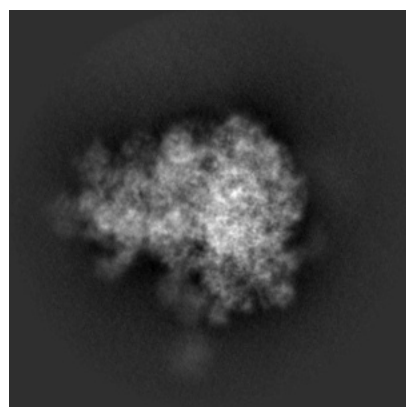


Y

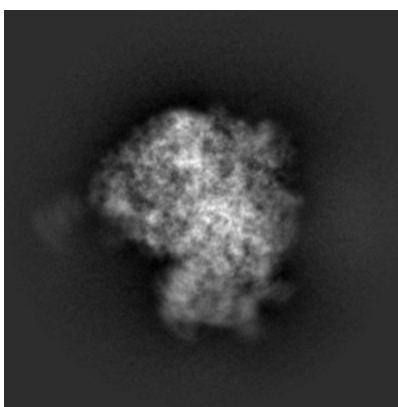


Z

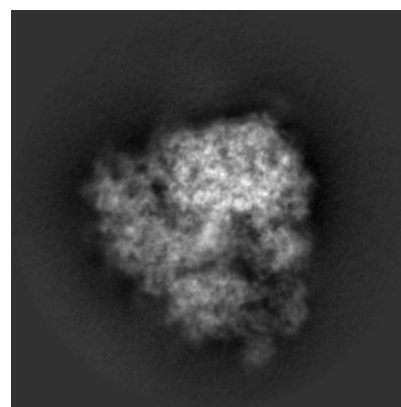
6.1.2 Raw map



X



Y

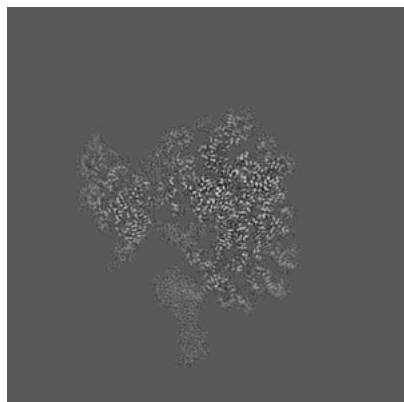


Z

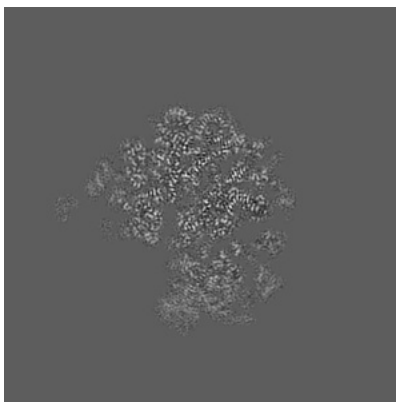
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

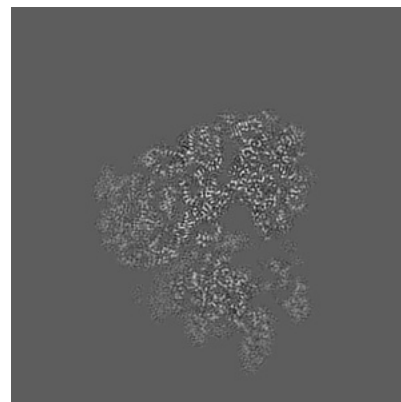
6.2.1 Primary map



X Index: 210

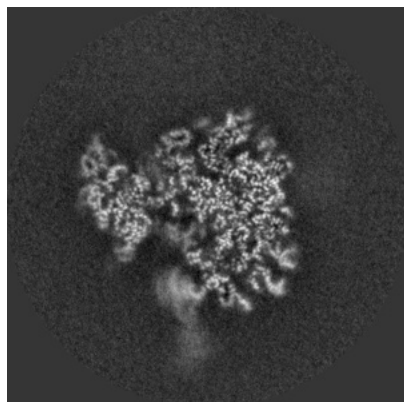


Y Index: 210

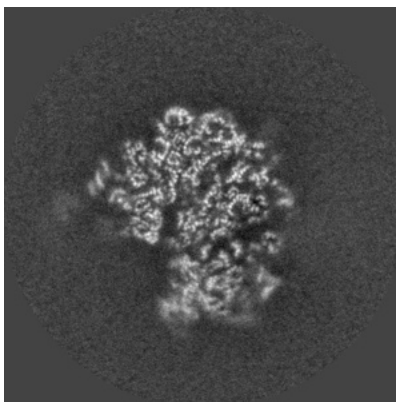


Z Index: 210

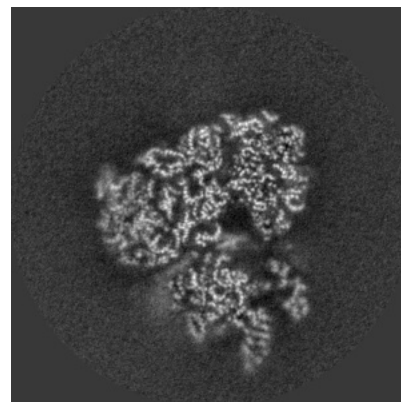
6.2.2 Raw map



X Index: 210



Y Index: 210

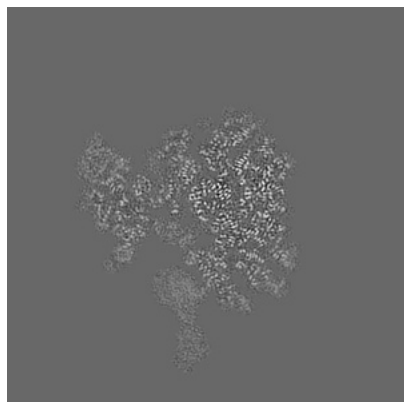


Z Index: 210

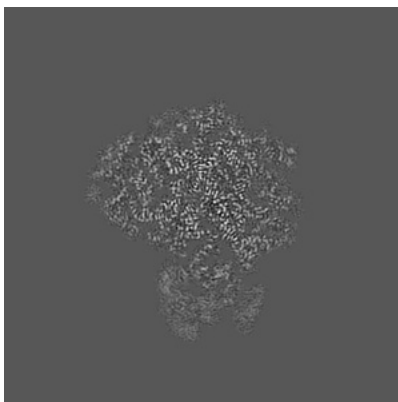
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

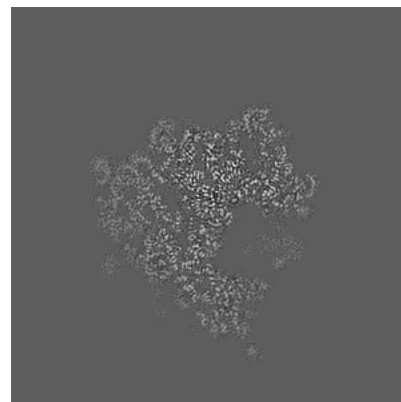
6.3.1 Primary map



X Index: 207

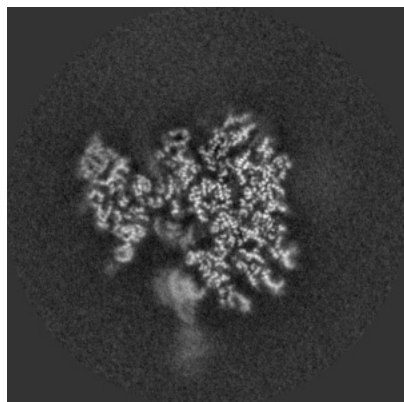


Y Index: 228

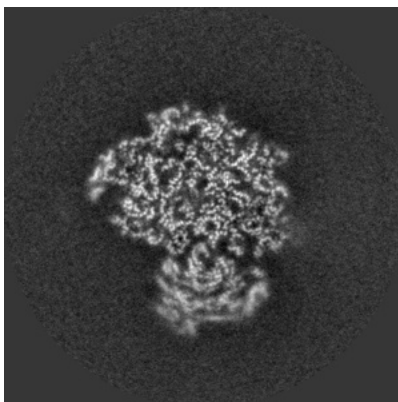


Z Index: 228

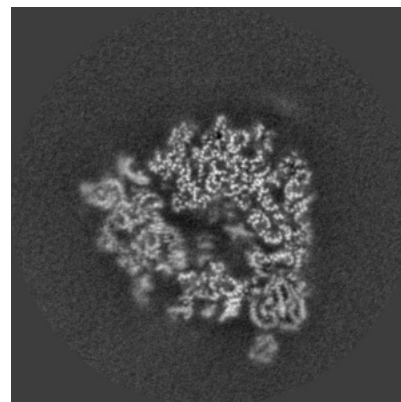
6.3.2 Raw map



X Index: 207



Y Index: 219

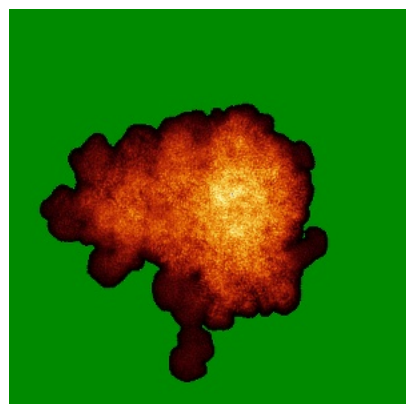


Z Index: 192

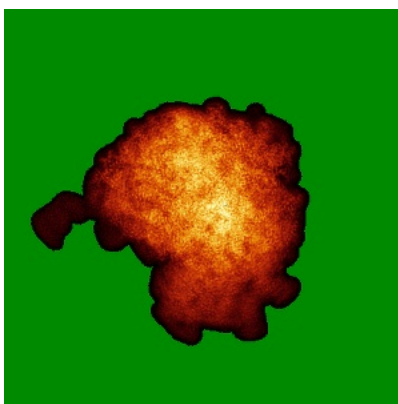
The images above show the largest variance slices of the map in three orthogonal directions.

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

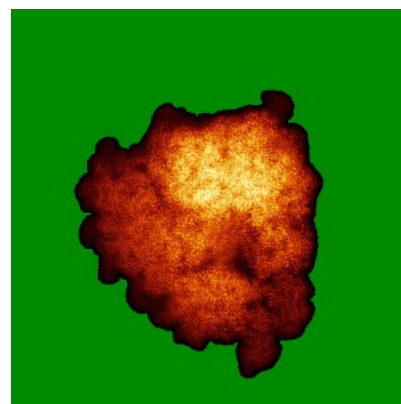
6.4.1 Primary map



X

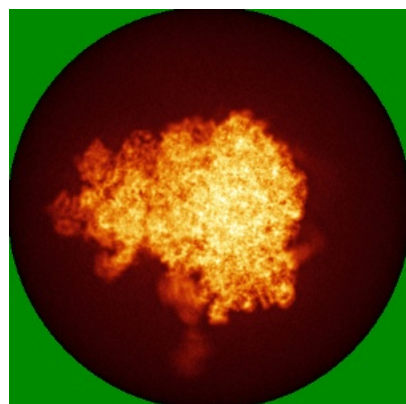


Y

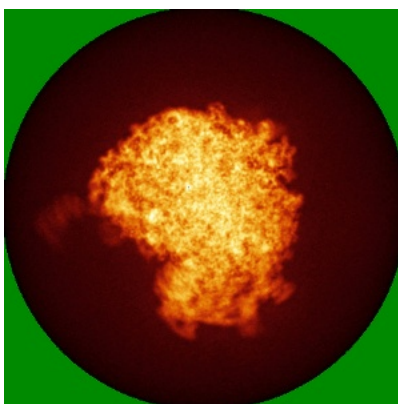


Z

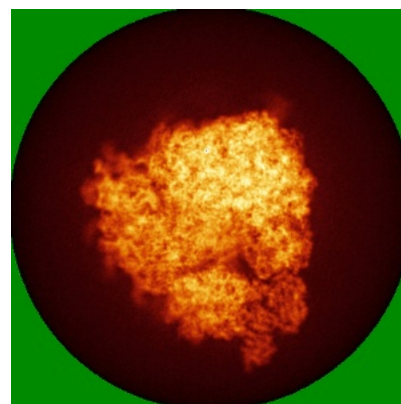
6.4.2 Raw map



X



Y

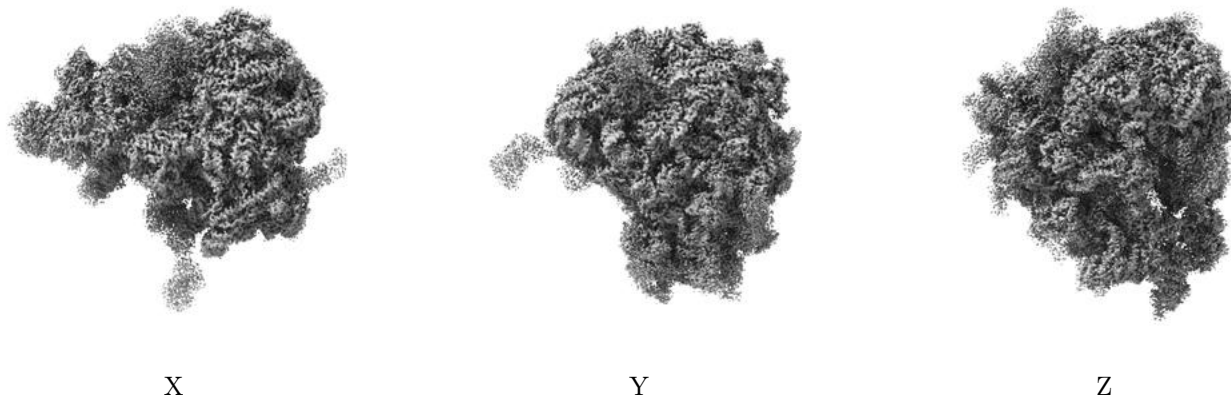


Z

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

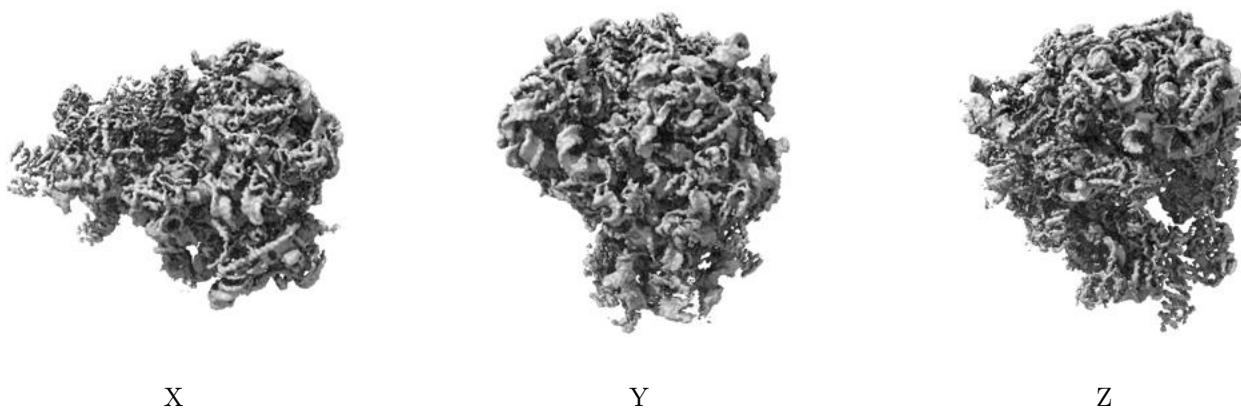
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

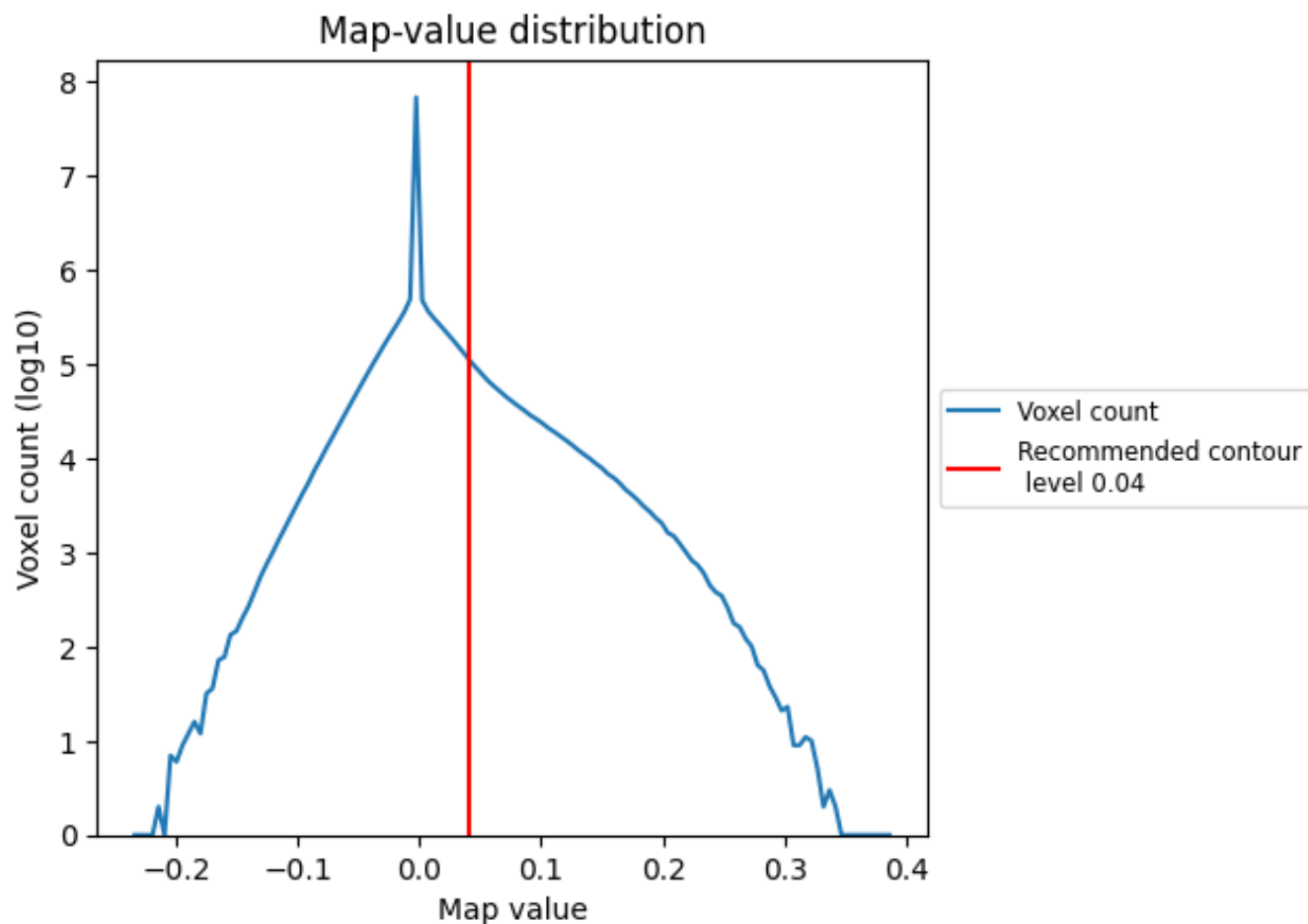
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

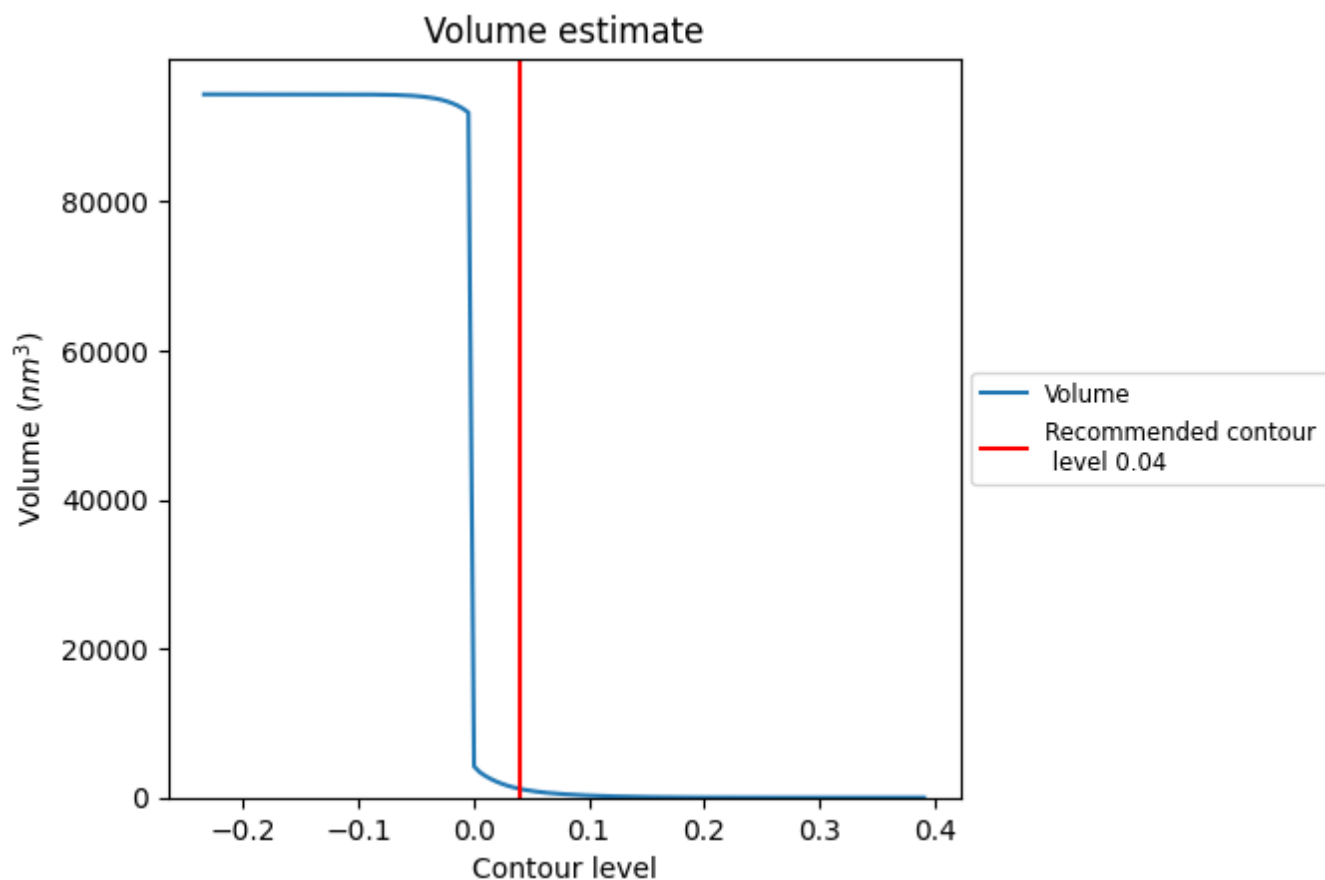
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

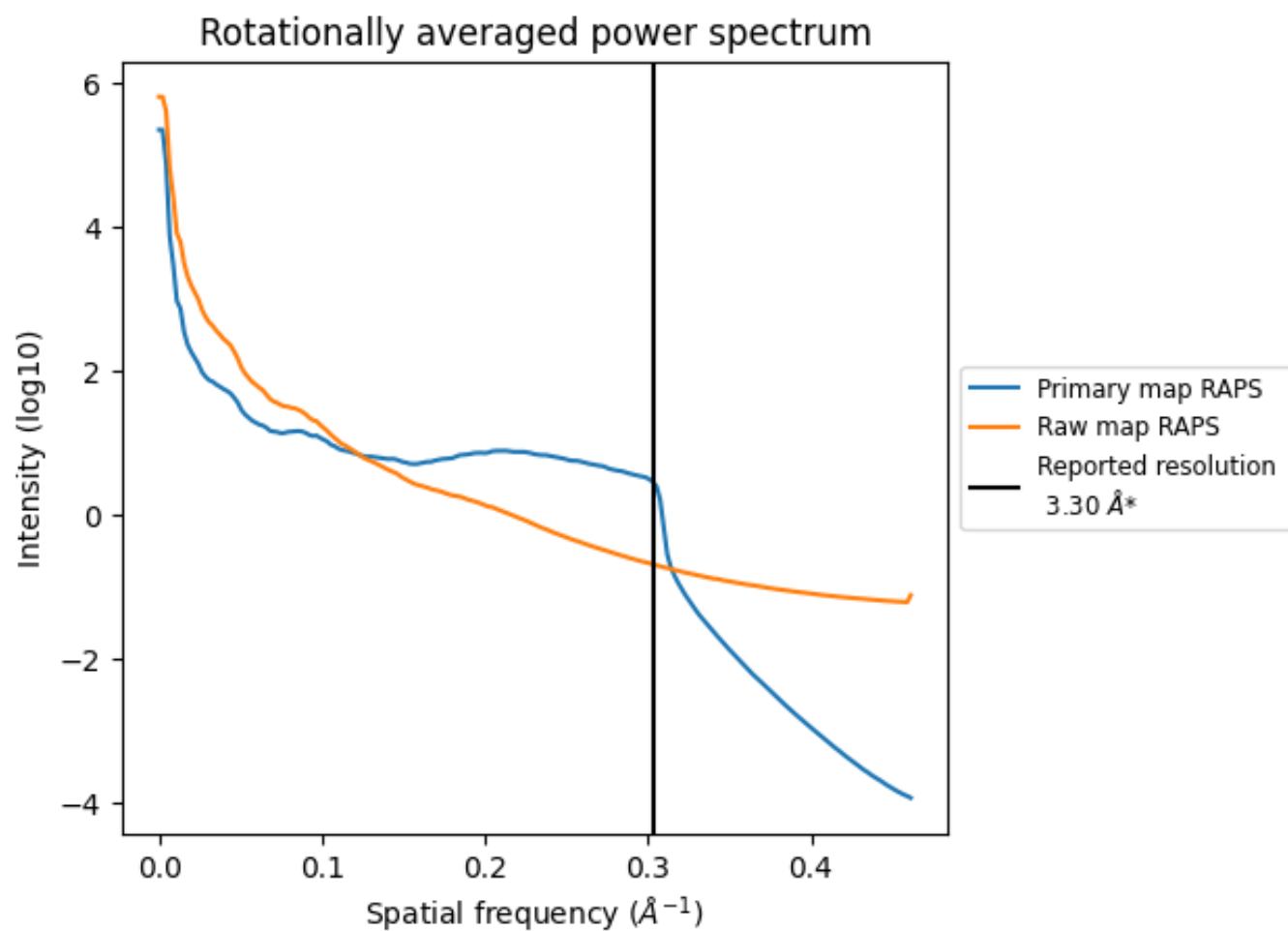
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1176 nm³; this corresponds to an approximate mass of 1062 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 ⓘ

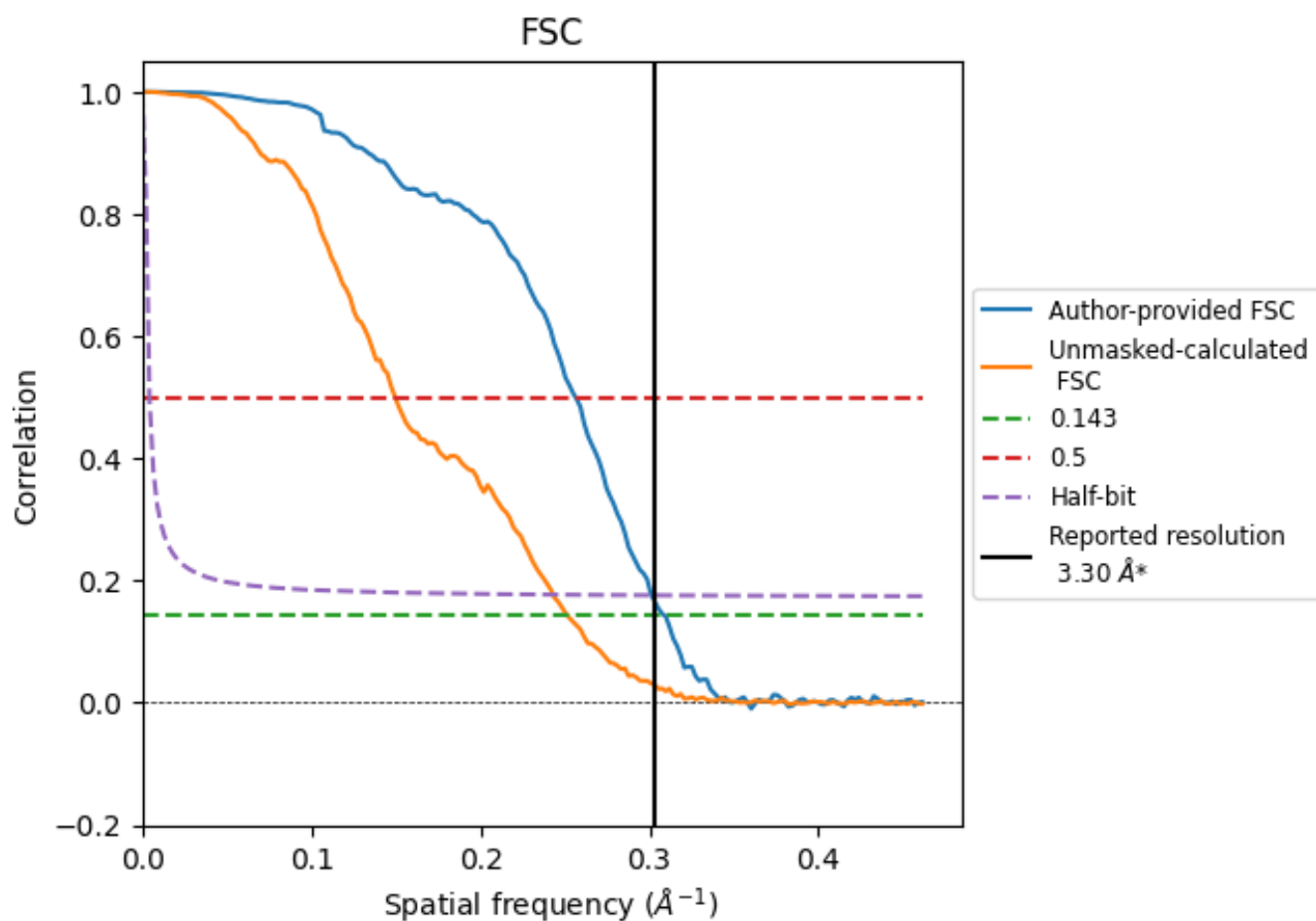


*Reported resolution corresponds to spatial frequency of $0.303 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

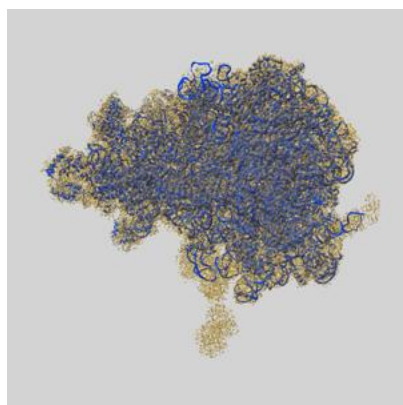
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.24	3.90	3.32
Unmasked-calculated*	3.98	6.68	4.12

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.98 differs from the reported value 3.3 by more than 10 %

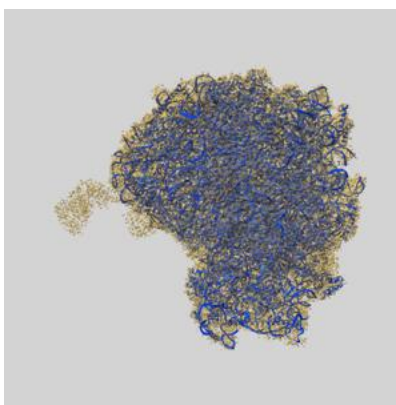
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12081 and PDB model 7B7D. Per-residue inclusion information can be found in [section 3](#) on [page 20](#).

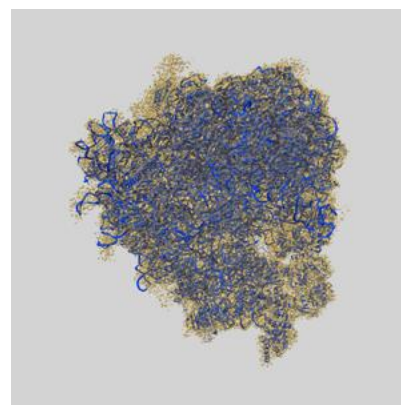
9.1 Map-model overlay [i](#)



X



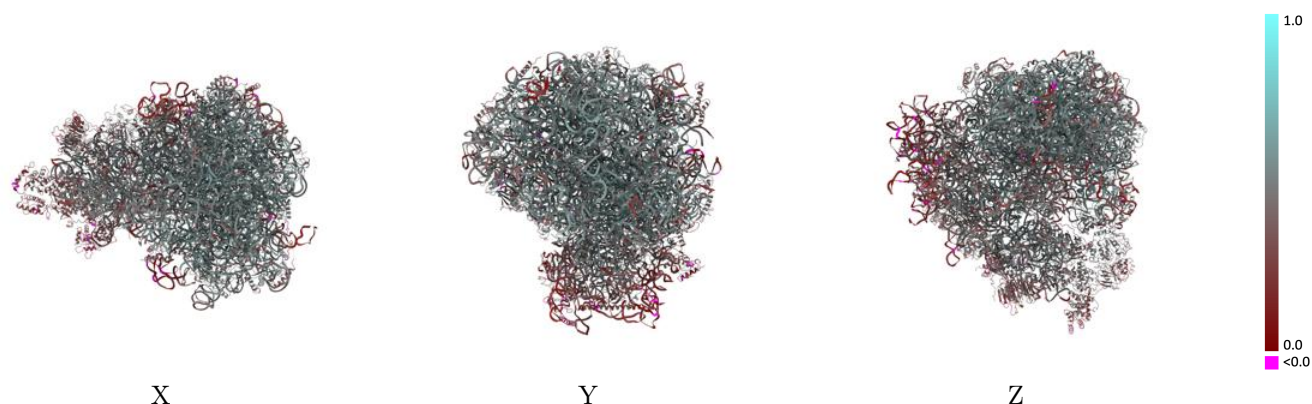
Y



Z

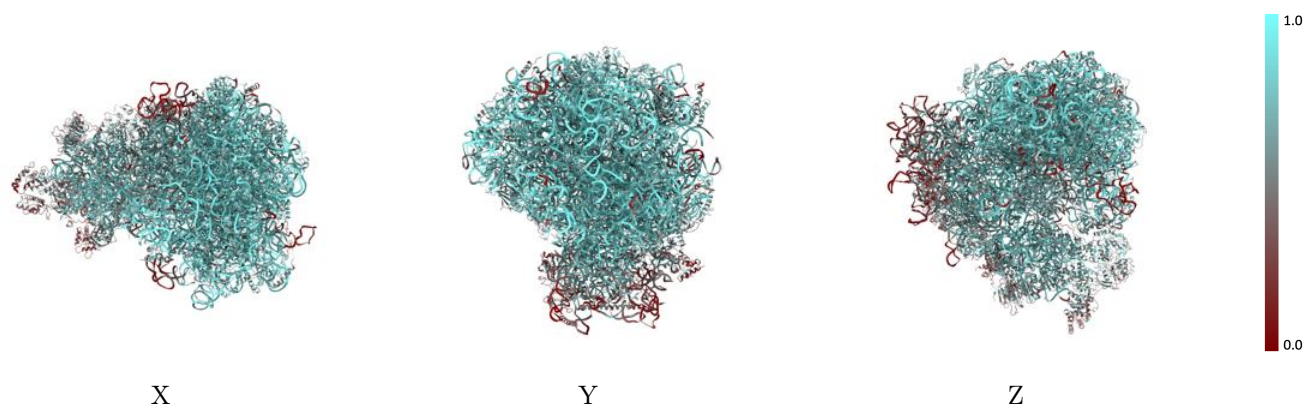
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



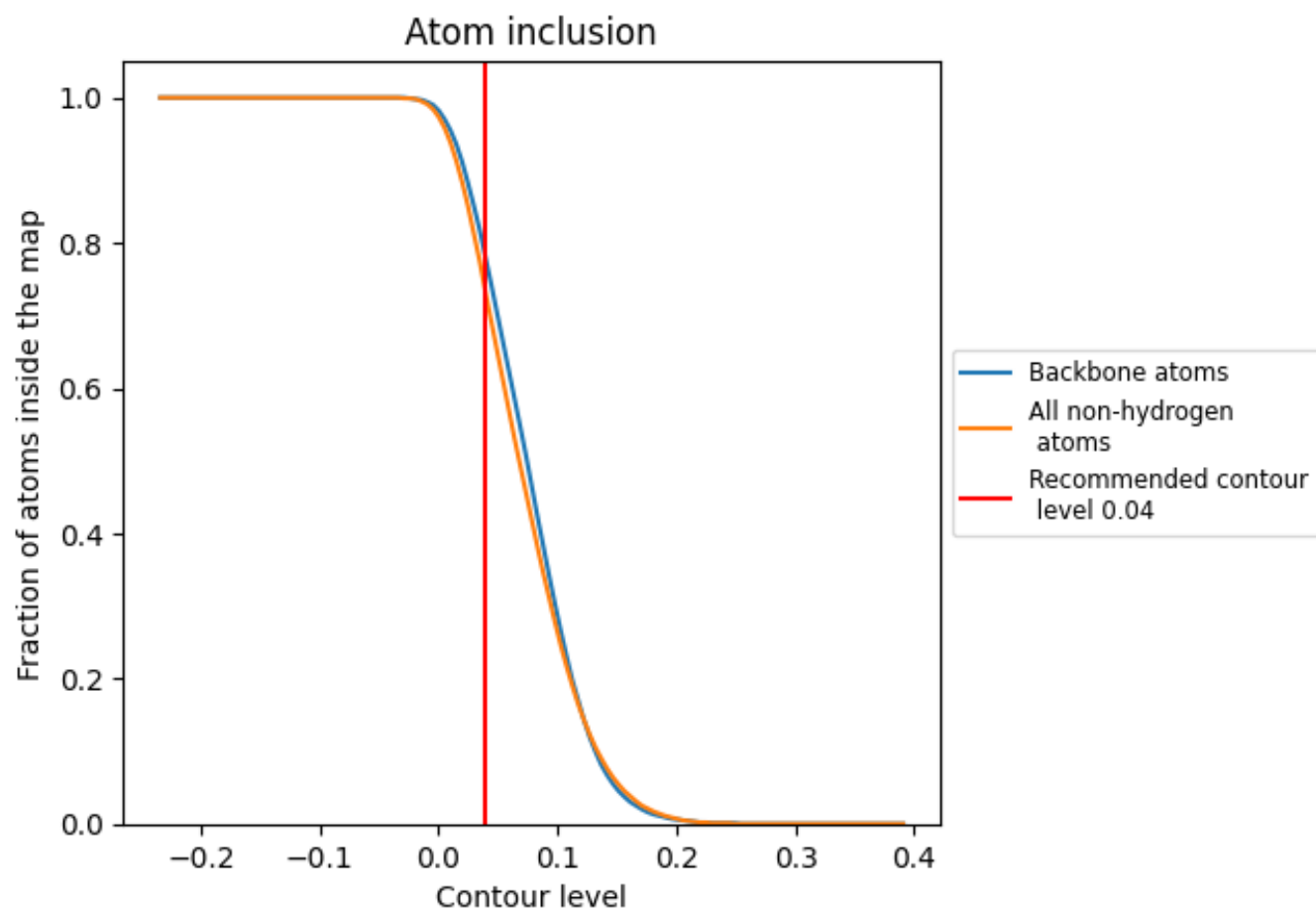
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 73% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7290	 0.4640
1	 0.7920	 0.5060
2	 0.7210	 0.4320
A	 0.5500	 0.3880
B	 0.6250	 0.4200
C	 0.5240	 0.3600
D	 0.1780	 0.1740
E	 0.5960	 0.3720
EF	 0.5300	 0.3800
F	 0.6830	 0.4600
G	 0.5620	 0.3970
H	 0.6630	 0.4310
I	 0.6900	 0.4610
J	 0.5550	 0.3880
K	 0.5510	 0.3510
L	 0.5730	 0.3960
LA	 0.8460	 0.5110
LB	 0.9010	 0.5280
LC	 0.8830	 0.5340
LD	 0.8060	 0.5400
LE	 0.7770	 0.5110
LF	 0.7670	 0.5080
LG	 0.7200	 0.4630
LH	 0.6570	 0.4420
LI	 0.7670	 0.5060
LJ	 0.6720	 0.4510
LK	 0.7140	 0.4790
LL	 0.6820	 0.4670
LM	 0.7090	 0.4590
LN	 0.7380	 0.5010
LO	 0.7240	 0.4810
LP	 0.8140	 0.5480
LQ	 0.7650	 0.5150
LR	 0.7690	 0.5070
LS	 0.5130	 0.3850



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Chain	Atom inclusion	Q-score
LT	 0.7530	 0.5070
LU	 0.7470	 0.5030
LV	 0.7140	 0.4740
LW	 0.7950	 0.5280
LX	 0.7210	 0.4960
LY	 0.6730	 0.4670
LZ	 0.7210	 0.4880
La	 0.7690	 0.5240
Lb	 0.7980	 0.5420
Lc	 0.7230	 0.5140
Ld	 0.7210	 0.4930
Le	 0.6820	 0.4630
Lf	 0.8400	 0.5520
Lg	 0.6330	 0.4260
Lh	 0.7660	 0.5160
Li	 0.7200	 0.4920
Lj	 0.6680	 0.4970
Lk	 0.7580	 0.5130
Ll	 0.7400	 0.5190
Lm	 0.7630	 0.5190
Ln	 0.7010	 0.4730
Lo	 0.7500	 0.5100
Lp	 0.7480	 0.5080
Lq	 0.6610	 0.4310
Lr	 0.7100	 0.4990
M	 0.7560	 0.4810
N	 0.2840	 0.2210
O	 0.4890	 0.3320
P	 0.6060	 0.4190
Q	 0.5690	 0.4120
R	 0.6370	 0.4490
S	 0.4670	 0.3650
Sm	 0.3710	 0.3140
Sn	 0.5750	 0.3680
T	 0.3780	 0.2810
U	 0.4310	 0.3330
V	 0.6210	 0.4270
W	 0.4410	 0.3450
X	 0.5830	 0.4370
Y	 0.6330	 0.4370
Z	 0.6660	 0.4590
a	 0.6100	 0.4220

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Chain	Atom inclusion	Q-score
b	 0.6780	 0.4810
c	 0.5630	 0.4070
d	 0.4090	 0.3280
e	 0.7120	 0.4760
f	 0.5490	 0.3830
g	 0.4100	 0.2890