



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 09:40 PM UTC

PDB ID : 6R84 / pdb_00006r84
EMDB ID : EMD-4751
Title : Yeast Vms1 (Q295L)-60S ribosomal subunit complex (pre-state with Arb1)
Authors : Su, T.; Izawa, T.; Cheng, J.; Yamashita, Y.; Berninghausen, O.; Inada, T.;
Neupert, W.; Beckmann, R.
Deposited on : 2019-03-31
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

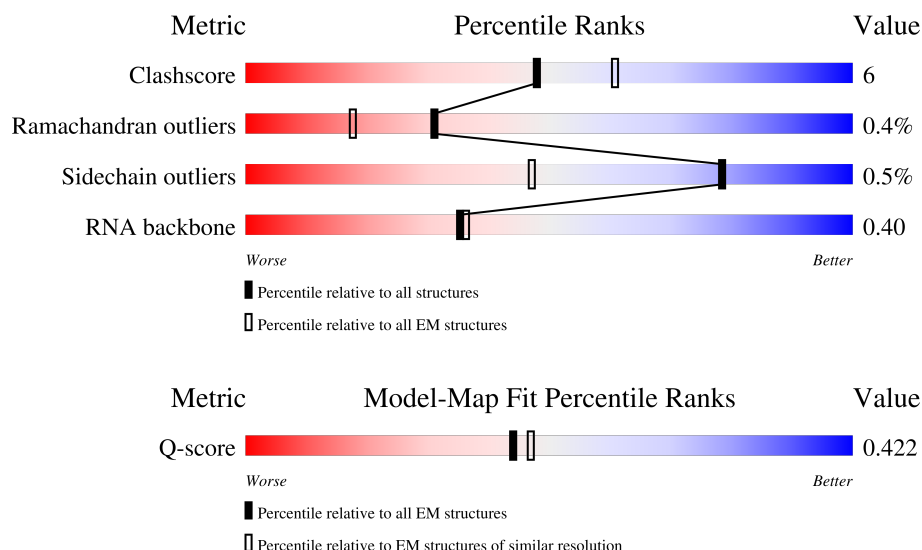
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.60 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.



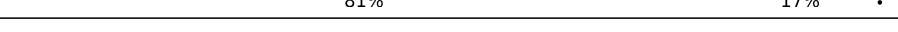
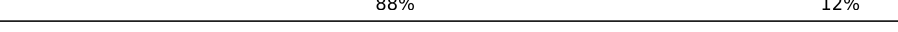
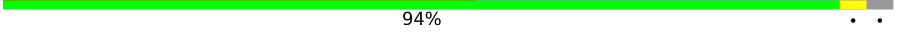
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	A	519	
2	R	433	
3	X	224	

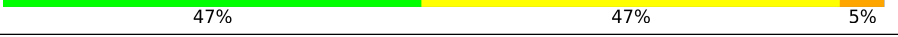
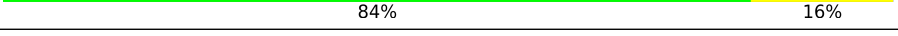
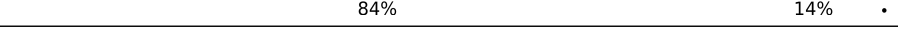
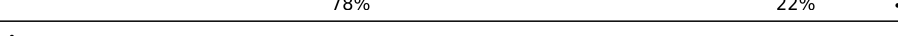
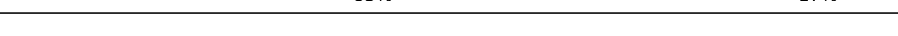
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Mol	Chain	Length	Quality of chain
4	i	112	 82% 17%
5	J	222	 83% 17%
6	j	119	 86% 12%
7	K	233	 88% 10%
8	k	99	 92% 8%
9	7	191	 84% 16%
10	l	87	 79% 21%
11	M	169	 81% 18%
12	m	77	 94% 6%
13	N	193	 78% 20%
14	n	50	 82% 18%
15	O	136	 86% 14%
16	o	52	 85% 15%
17	p	203	 72% 27%
18	Q	197	 87% 13%
19	5	183	 81% 17%
20	S	185	 88% 12%
21	s	220	 74% 22%
22	T	152	 85% 15%
23	U	172	 82% 17%
24	V	159	 86% 14%
25	W	100	 89% 10%
26	P	155	 53% 94%
27	r	197	 14% 49% 12% 39%
28	x	136	 76% 24%

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Mol	Chain	Length	Quality of chain
29	3	121	 56% 36% 7%
30	Y	62	 87% 13%
31	4	158	 52% 37% 11%
32	Z	121	 88% 12%
33	a	126	 84% 16%
34	B	76	 47% 47% 5%
35	b	135	 85% 13%
36	C	105	 88% 12%
37	c	148	 84% 16%
38	D	91	 81% 19%
39	d	58	 84% 14%
40	E	252	 80% 20%
41	e	97	 84% 16%
42	F	386	 78% 22%
43	f	109	 85% 15%
44	G	361	 84% 15%
45	g	127	 86% 14%
46	H	296	 83% 16%
47	h	106	 83% 17%
48	I	175	 77% 13% 11%
49	L	204	 41% 81% 19%
50	1	3316	 54% 37% 9%

2 Entry composition

There are 51 unique types of molecules in this entry. The entry contains 138804 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called ABC transporter ATP-binding protein ARB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	446	Total	C	N	O	S	0	0
			3522	2232	610	668	12		

- Molecule 2 is a protein called Protein VMS1,Vms1,Protein VMS1,Vms1.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	R	360	Total	C	N	O	S	Se	0	0
			2804	1788	499	504	12	1		

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	?	-	PHE	deletion	UNP Q04311
R	?	-	ASP	deletion	UNP Q04311
R	?	-	SER	deletion	UNP Q04311
R	?	-	THR	deletion	UNP Q04311
R	?	-	LEU	deletion	UNP Q04311
R	?	-	ARG	deletion	UNP Q04311
R	?	-	GLU	deletion	UNP Q04311
R	?	-	VAL	deletion	UNP Q04311
R	?	-	GLU	deletion	UNP Q04311
R	?	-	VAL	deletion	UNP Q04311
R	?	-	GLU	deletion	UNP Q04311
R	?	-	LYS	deletion	UNP Q04311
R	?	-	THR	deletion	UNP Q04311
R	?	-	SER	deletion	UNP Q04311
R	?	-	ASP	deletion	UNP Q04311
R	?	-	ASN	deletion	UNP Q04311
R	?	-	ASP	deletion	UNP Q04311
R	?	-	ARG	deletion	UNP Q04311
R	?	-	ASN	deletion	UNP Q04311
R	?	-	LYS	deletion	UNP Q04311
R	?	-	GLU	deletion	UNP Q04311

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Chain	Residue	Modelled	Actual	Comment	Reference
R	?	-	SER	deletion	UNP Q04311
R	?	-	GLY	deletion	UNP Q04311
R	?	-	ASP	deletion	UNP Q04311
R	?	-	LEU	deletion	UNP Q04311
R	?	-	GLN	deletion	UNP Q04311
R	?	-	ILE	deletion	UNP Q04311
R	?	-	ALA	deletion	UNP Q04311
R	?	-	ARG	deletion	UNP Q04311
R	?	-	LYS	deletion	UNP Q04311
R	?	-	LYS	deletion	UNP Q04311
R	?	-	VAL	deletion	UNP Q04311
R	?	-	THR	deletion	UNP Q04311
R	?	-	SER	deletion	UNP Q04311
R	?	-	ASN	deletion	UNP Q04311
R	?	-	VAL	deletion	UNP Q04311
R	?	-	MET	deletion	UNP Q04311
R	?	-	ARG	deletion	UNP Q04311
R	?	-	PHE	deletion	UNP Q04311
R	?	-	ASP	deletion	UNP Q04311
R	?	-	SER	deletion	UNP Q04311
R	?	-	ARG	deletion	UNP Q04311
R	?	-	ASN	deletion	UNP Q04311
R	?	-	GLU	deletion	UNP Q04311
R	?	-	GLN	deletion	UNP Q04311
R	?	-	LYS	deletion	UNP Q04311
R	?	-	ALA	deletion	UNP Q04311
R	187	SER	-	linker	UNP Q04311

- Molecule 3 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	X	224	Total	C	N	O	S	0	0
			1633	1019	279	328	7		

- Molecule 4 is a protein called 60S ribosomal protein L34-A.

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

- Molecule 5 is a protein called 60S ribosomal protein L7-A.

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

- Molecule 6 is a protein called 60S ribosomal protein L35-A.

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

- Molecule 7 is a protein called 60S ribosomal protein L8-A.

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

- Molecule 8 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	k	99	Total	C	N	O	S	0	0
			771	481	156	132	2		

- Molecule 9 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	7	191	Total	C	N	O	S	0	0
			1518	963	274	277	4		

- Molecule 10 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	l	87	Total	C	N	O	S	0	0
			681	414	148	114	5		

- Molecule 11 is a protein called 60S ribosomal protein L11-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	169	Total	C	N	O	S	0	0
			1353	847	253	249	4		

- Molecule 12 is a protein called 60S ribosomal protein L38.

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

- Molecule 13 is a protein called 60S ribosomal protein L13-A.

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

- Molecule 14 is a protein called 60S ribosomal protein L39.

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

- Molecule 15 is a protein called 60S ribosomal protein L14-A.

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

- Molecule 16 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	o	52	Total	C	N	O	S	0	0
			417	259	86	67	5		

- Molecule 17 is a protein called 60S ribosomal protein L15-A.

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

- Molecule 18 is a protein called 60S ribosomal protein L16-A.

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

- Molecule 19 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	5	183	Total	C	N	O	0	0
			1420	882	281	257		

- Molecule 20 is a protein called 60S ribosomal protein L18-A.

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

- Molecule 21 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	s	220	Total	C	N	O	S	0	0
			1770	1121	335	307	7		

- Molecule 22 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	T	152	Total	C	N	O	0	0
			1228	763	260	205		

- Molecule 23 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	172	Total	C	N	O	S	0	0
			1445	930	267	244	4		

- Molecule 24 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	V	159	Total	C	N	O	S	0	0
			1276	805	246	221	4		

- Molecule 25 is a protein called 60S ribosomal protein L22-A.

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

- Molecule 26 is a protein called 60S ribosomal protein L12-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	P	150	Total	C	N	O	0	0
			737	437	150	150		

- Molecule 27 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	r	121	Total	C	N	O	S	0	0
			967	621	170	173	3		

- Molecule 28 is a protein called 60S ribosomal protein L23-A.

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

- Molecule 29 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	3	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 30 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Y	62	Total	C	N	O	S	0	0
			513	330	101	81	1		

- Molecule 31 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	4	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 32 is a protein called 60S ribosomal protein L25.

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

- Molecule 33 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	a	126	Total	C	N	O	0	0
			993	625	192	176		

- Molecule 34 is a RNA chain called tRNA-Ala.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	B	76	Total	C	N	O	P	0	0
			1622	721	285	540	76		

- Molecule 35 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	b	135	Total	C	N	O	0	0
			1092	710	202	180		

- Molecule 36 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	C	105	Total	C	N	O	S	0	0
			847	534	170	138	5		

- Molecule 37 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	c	148	Total	C	N	O	S	0	0
			1173	749	231	190	3		

- Molecule 38 is a protein called 60S ribosomal protein L43-A.

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

- Molecule 39 is a protein called 60S ribosomal protein L29.

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

- Molecule 40 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	E	252	Total	C	N	O	S	0	0
			1914	1191	388	334	1		

- Molecule 41 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	e	97	Total	C	N	O	S	0	0
			743	479	124	139	1		

- Molecule 42 is a protein called 60S ribosomal protein L3.

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

- Molecule 43 is a protein called 60S ribosomal protein L31-A.

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

- Molecule 44 is a protein called 60S ribosomal protein L4-A.

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

- Molecule 45 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	g	127	Total	C	N	O	S	0	0
			1020	647	205	167	1		

- Molecule 46 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	H	296	Total	C	N	O	S	0	0
			2375	1501	414	458	2		

- Molecule 47 is a protein called 60S ribosomal protein L33-A.

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

- Molecule 48 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	I	156	Total	C	N	O	S	0	0
			1239	800	222	216	1		

- Molecule 49 is a protein called 60S ribosomal protein L1-A.

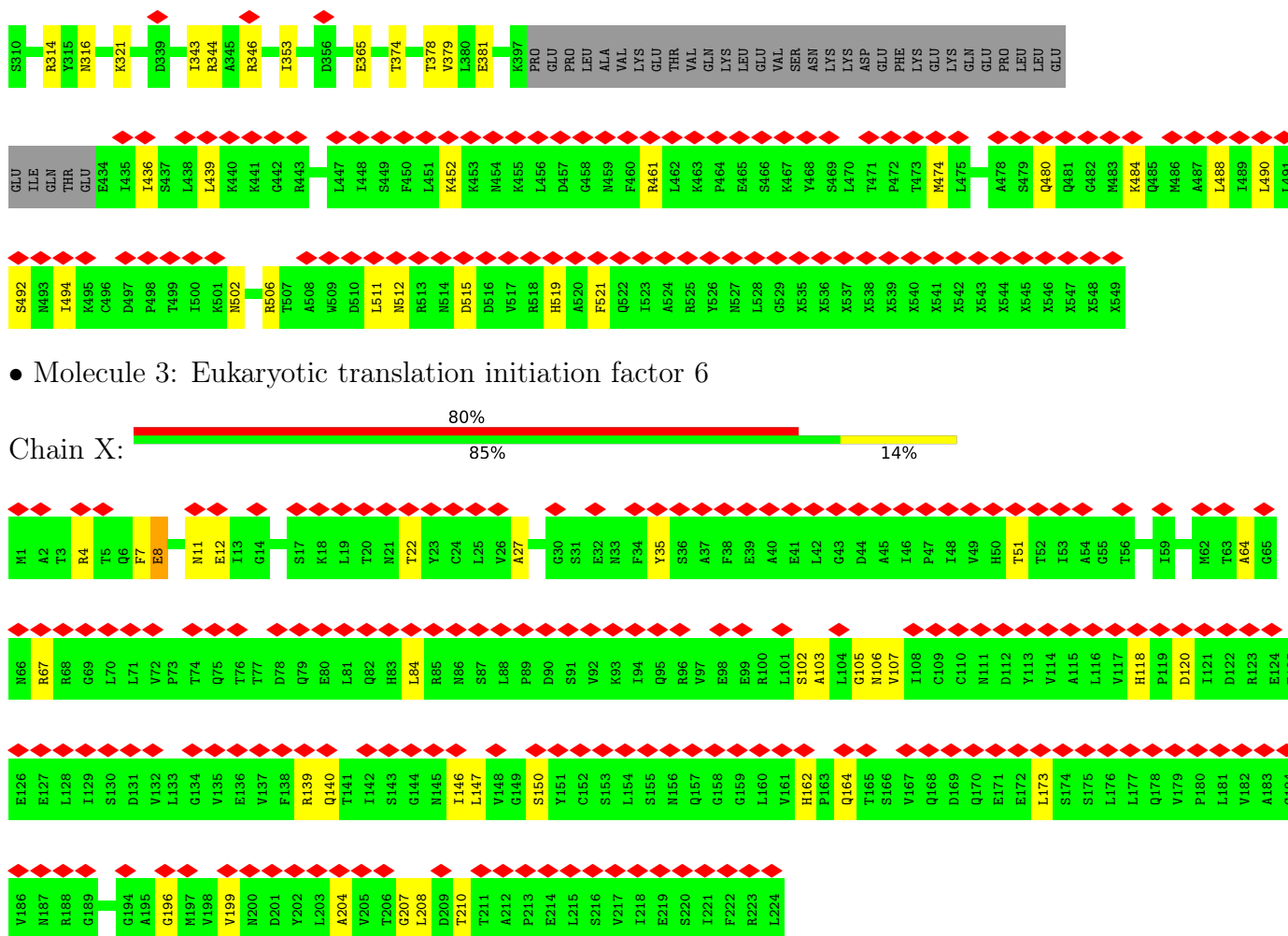
Mol	Chain	Residues	Atoms					AltConf	Trace
49	L	204	Total	C	N	O	S	0	0
			1609	1031	279	290	9		

- Molecule 50 is a RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	1	3316	Total	C	N	O	P	0	0
			70924	31675	12770	23163	3316		

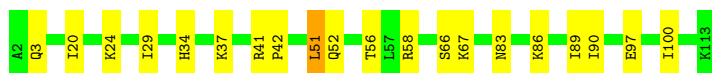
- Molecule 51 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
51	R	1	Total	Zn	0
			1	1	



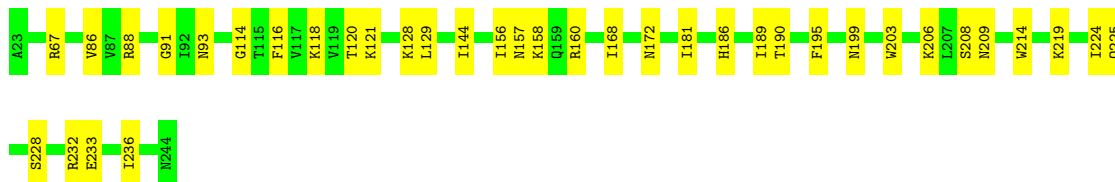
• Molecule 4: 60S ribosomal protein L34-A

Chain i: 82% 17%



• Molecule 5: 60S ribosomal protein L7-A

Chain J: 83% 17%

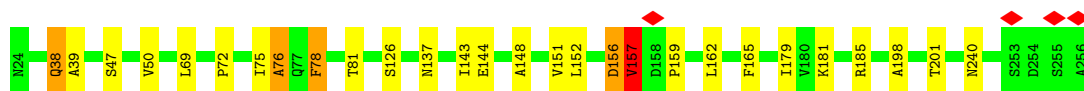
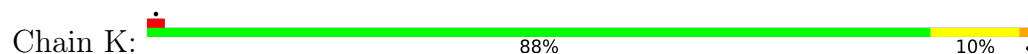


• Molecule 6: 60S ribosomal protein L35-A

Chain j: 86% 12%



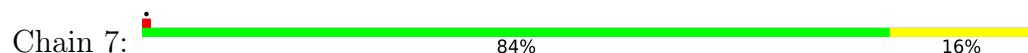
- Molecule 7: 60S ribosomal protein L8-A



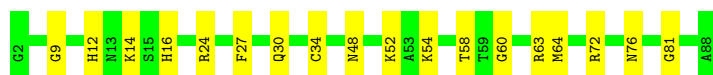
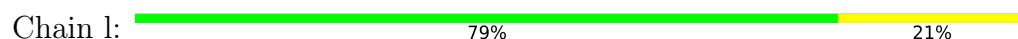
- Molecule 8: 60S ribosomal protein L36-A



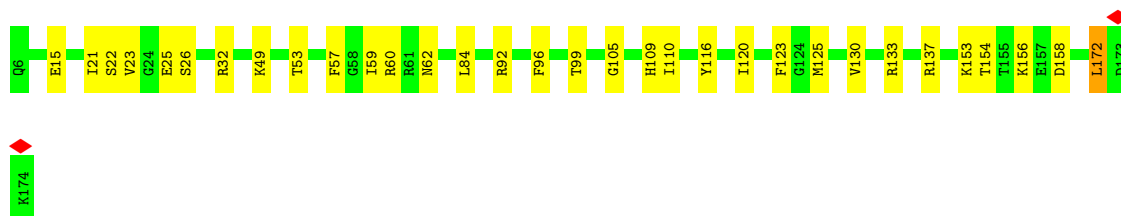
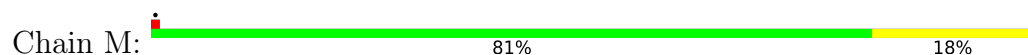
- Molecule 9: 60S ribosomal protein L9-A



- Molecule 10: 60S ribosomal protein L37-A



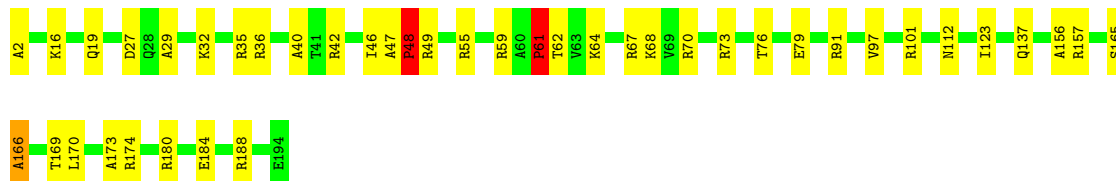
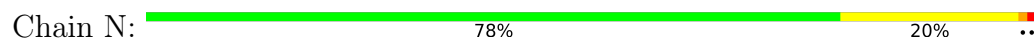
- Molecule 11: 60S ribosomal protein L11-B



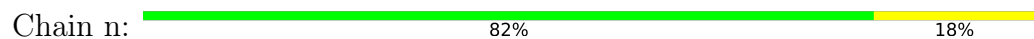
- Molecule 12: 60S ribosomal protein L38



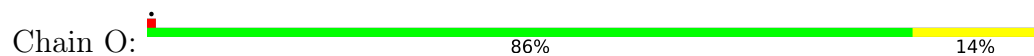
- Molecule 13: 60S ribosomal protein L13-A



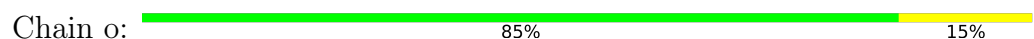
- Molecule 14: 60S ribosomal protein L39



- Molecule 15: 60S ribosomal protein L14-A



- Molecule 16: Ubiquitin-60S ribosomal protein L40



- Molecule 17: 60S ribosomal protein L15-A



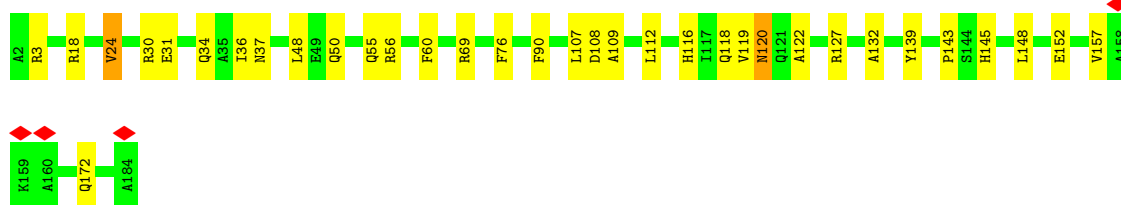
- Molecule 18: 60S ribosomal protein L16-A

Chain Q:  87% 13%



- Molecule 19: 60S ribosomal protein L17-A

Chain 5:  81% 17%



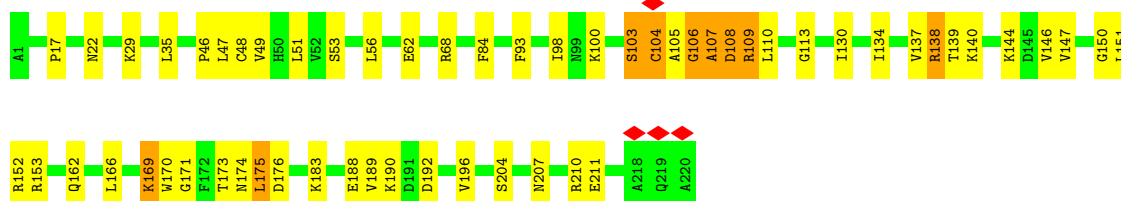
- Molecule 20: 60S ribosomal protein L18-A

Chain S:  88% 12%



- Molecule 21: 60S ribosomal protein L10

Chain s:  74% 22%



- Molecule 22: 60S ribosomal protein L19-A

Chain T:  85% 15%



- Molecule 23: 60S ribosomal protein L20-A

Chain U:  82% 17%



- Molecule 24: 60S ribosomal protein L21-A

Chain V:  86% 14%

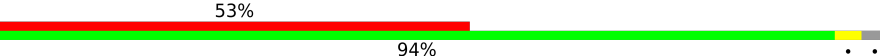


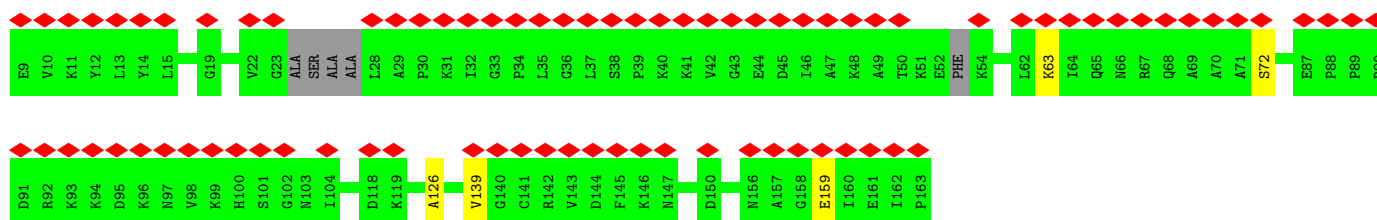
- Molecule 25: 60S ribosomal protein L22-A

Chain W:  89% 10%



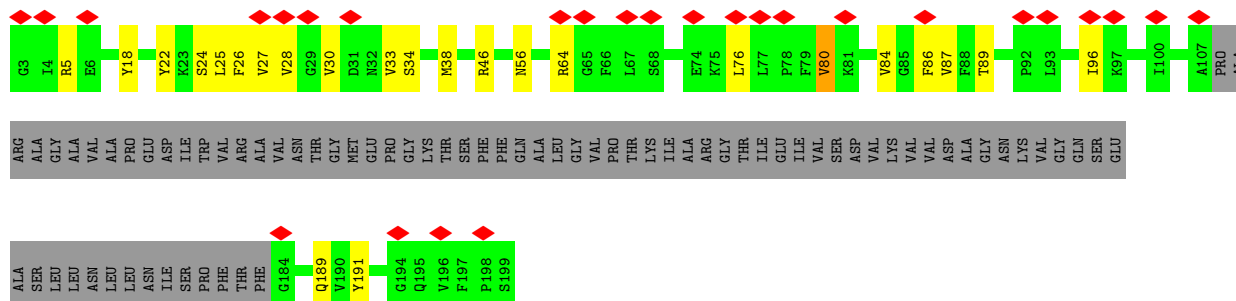
- Molecule 26: 60S ribosomal protein L12-A

Chain P:  53% 94%



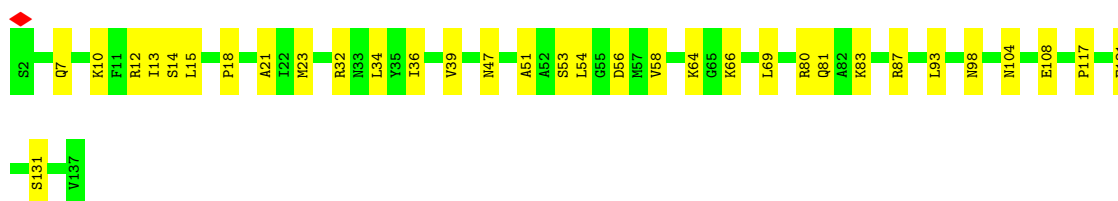
- Molecule 27: 60S acidic ribosomal protein P0

Chain r:  14% 49% 12% 39%



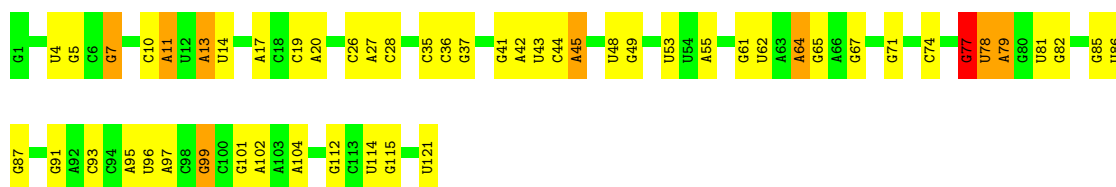
- Molecule 28: 60S ribosomal protein L23-A

Chain x:  76% 24%



- Molecule 29: 5S rRNA

Chain 3:  56% 36% 7%



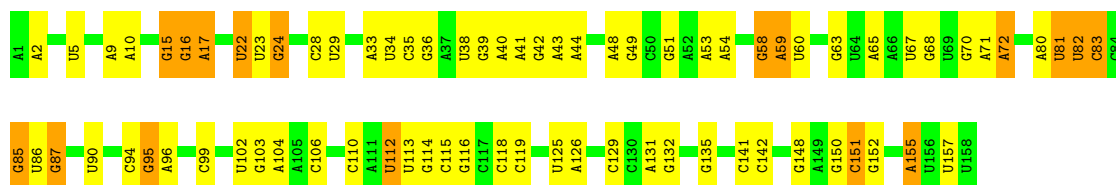
- Molecule 30: 60S ribosomal protein L24-A

Chain Y:  87% 13%



- Molecule 31: 5.8S rRNA

Chain 4:  52% 37% 11%



- Molecule 32: 60S ribosomal protein L25

Chain Z:  88% 12%



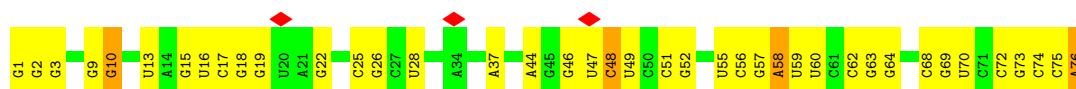
- Molecule 33: 60S ribosomal protein L26-A

Chain a:  84% 16%



- Molecule 34: tRNA-Ala

Chain B:  47% 47% 5%



- Molecule 35: 60S ribosomal protein L27-A

Chain b:  85% 13%



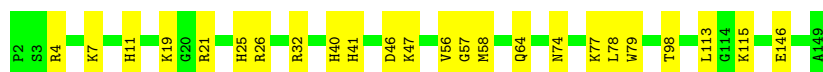
- Molecule 36: 60S ribosomal protein L42-A

Chain C:  88% 12%



- Molecule 37: 60S ribosomal protein L28

Chain c:  84% 16%



- Molecule 38: 60S ribosomal protein L43-A

Chain D:  81% 19%



- Molecule 39: 60S ribosomal protein L29

Chain d:  84% 14%



- Molecule 40: 60S ribosomal protein L2-A

Chain E:  80% 20%

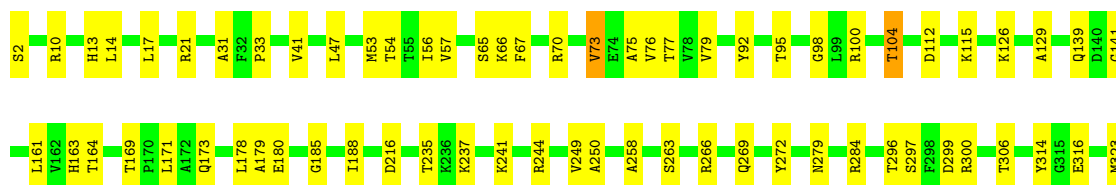
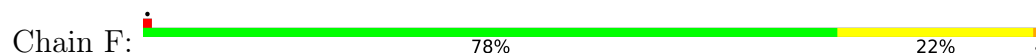


- Molecule 41: 60S ribosomal protein L30

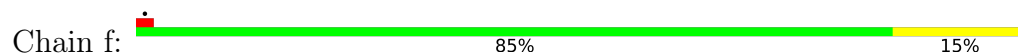
Chain e:  84% 16%



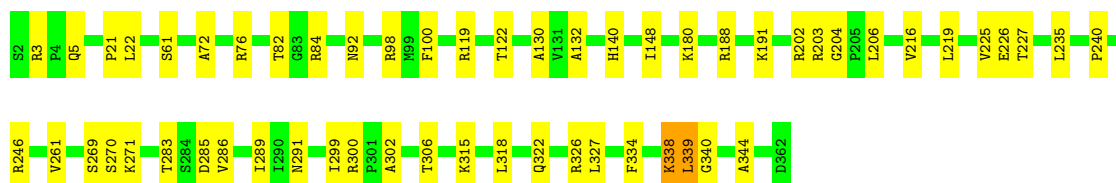
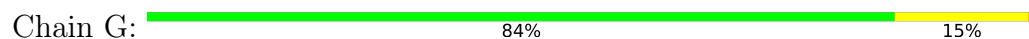
- Molecule 42: 60S ribosomal protein L3



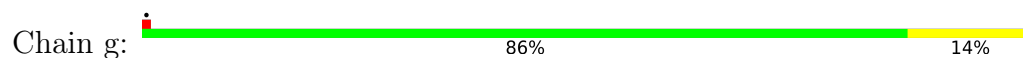
- Molecule 43: 60S ribosomal protein L31-A



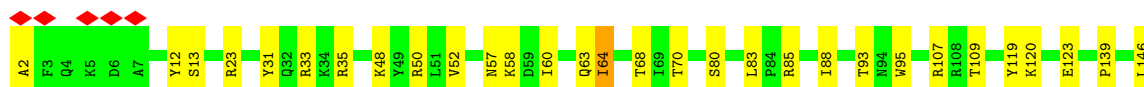
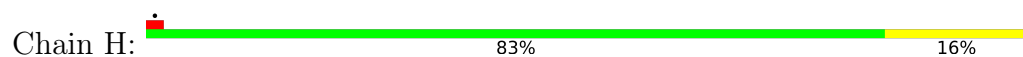
- Molecule 44: 60S ribosomal protein L4-A



- Molecule 45: 60S ribosomal protein L32



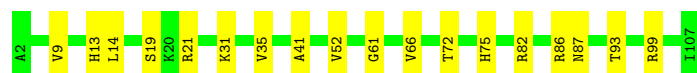
- Molecule 46: 60S ribosomal protein L5





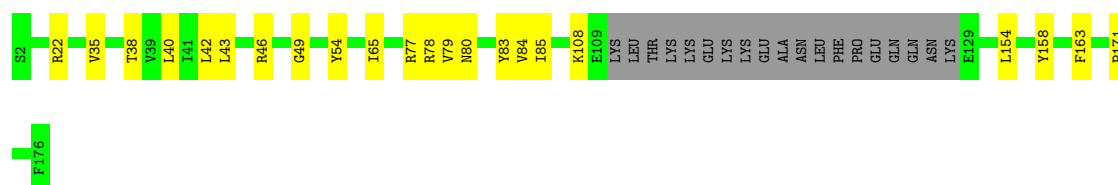
- Molecule 47: 60S ribosomal protein L33-A

Chain h: 83% 17%



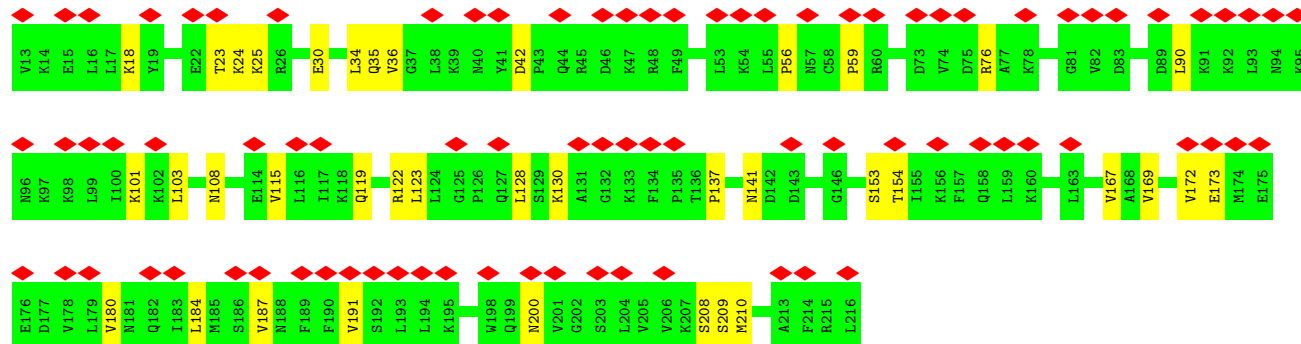
- Molecule 48: 60S ribosomal protein L6-A

Chain I: 77% 13% 11%



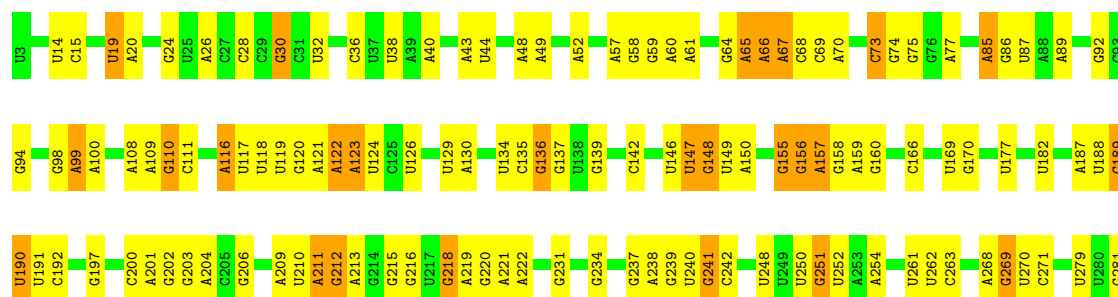
- Molecule 49: 60S ribosomal protein L1-A

Chain L: 41% 81% 19%



- Molecule 50: 25S rRNA

Chain 1: 54% 37% 9%



G1497	G1400	U1324	A1245	U1162	A1065	U986	C890	G799	C696	G616	A523	G371	G282
A1498	G1404	U1325	G1246	U1168	G1066	A989	G894	G800	A705	G617	A528	A372	G283
C1502	U1287	C1328	U1247	A1169	U1071	A989	A895	A801	A706	C618	U529	A373	A284
A1503	G1408	U1329	G1248	A1168	G1072	G994	A896	C804	U707	A619	A529	A374	A285
A1506	G1411	U1330	G1249	G1177	A1075	U995	G900	G805	G708	U620	G530	A375	U286
G1507	G1412	U1331	A1251	G1178	C1076	G999	A906	A806	U709	A621	G531	G376	G287
C1508	G1417	A1332	C1254	A1179	U1081	G999	G907	A807	A710	U623	A532	A385	C288
A1511	A1418	U1334	G1255	A1180	U1082	C1000	A908	A808	A711	U627	G535	A385	A289
U1512	A1419	U1336	C1256	A1181	U1083	G1001	G908	U811	G712	U628	U536	G394	U292
G1515	C1426	A1337	U1258	A1190	G1083	A1002	G908	U811	A716	U631	U540	A396	U294
U1523	C1432	C1342	A1259	U1191	A1093	A1006	C911	G815	A717	G632	U541	A397	A295
U1528	A1433	A1343	G1261	C1192	U1094	U1007	G912	A816	G717	C633	G542	A398	A296
G1529	G1434	G1344	G1262	A1193	U1095	U1008	A914	A817	G718	U719	C546	A399	U297
A1535	A1435	G1345	A1263	G1194	U1096	A1009	A915	C824	A720	G636	G547	G400	U298
U1530	U1436	G1346	G1264	A1195	U1097	G1010	G916	U825	U723	C637	G548	U401	G300
C1531	C1437	U1347	U1269	C1196	A1098	U1015	A917	G826	U723	C638	U549	C403	G301
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A1535	A1446	A1349	A1271	C1199	G1101	C1017	A921	A830	A738	C641	G552	A406	U305
G1536	G1447	U1351	C1272	A1200	A1102	G1018	U922	G835	C743	A645	U555	A307	A306
U1539	U1448	A1352	A1273	C1201	A1103	G1019	C923	A836	G750	A646	U556	U411	A308
G1542	A1451	U1353	A1274	A1202	G1104	G1020	A925	A837	A751	G647	U557	G412	U314
G1547	U1455	G1354	C1277	A1203	U1110	G1024	U932	G842	C752	C648	U558	G421	C315
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U1549	U1457	U1356	G1282	U1210	G1117	A1026	G934	G844	A755	A656	U570	G425	A317
C1550	A1461	C1357	C1283	U1211	U1128	A1027	U937	A846	C758	A657	U571	G426	A323
U1553	A1462	A1363	G1284	G1212	A1129	U1028	C938	U850	U759	A660	A578	U429	U329
U1554	U1467	C1364	G1285	U1213	A1130	G1032	U939	C851	G760	G661	A578	U430	G330
U1555	A1468	G1365	A1286	U1214	G1131	U1033	C944	U857	U764	U662	G579	G331	G332
C1556	U1469	A1366	A1287	G1215	C1132	U1034	U946	G857	C765	A665	C580	C439	G333
A1557	C1469	G1367	C1292	G1216	A1133	U1035	G947	A858	U766	A666	U581	A440	A494
A1558	U1470	U1368	U1293	A1217	G1134	G1036	G859	G859	U767	C667	A585	G495	C339
A1559	U1471	A1369	G1295	U1218	A1135	A1037	A952	G860	C768	G668	A589	C500	C340
G1560	U1474	U1369	G1295	C1219	A1138	C1037	G953	C861	G769	U671	G590	A501	G341
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C1562	U1477	G1380	A1301	A1221	G1142	U1041	U960	U870	U776	G674	A592	G505	A344
U1563	A1477	A1381	A1302	A1222	A1143	C1045	C961	G870	U777	A677	G595	G510	A349
U1564	U1482	G1382	A1303	A1223	U1144	A1046	A962	U871	G781	G678	C596	G511	C350
G1565	A1483	G1383	U1305	G1230	G1145	A1047	G963	U872	A784	U679	G597	U512	A351
U1566	U1484	U1384	A1306	A1231	G1149	A1048	U966	C873	G785	G680	A598	G513	A352
U1567	G1485	A1385	G1307	U1235	U1151	C1049	A967	U874	G786	U681	C599	G514	G353
U1568	U1486	A1386	A1308	G1236	G1152	A1053	G968	U879	A786	U682	G600	G515	U354
A1570	G1487	G1387	G1309	G1237	A1153	A1054	C969	G880	C788	U683	G604	A516	A355
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A2939	G2050
A2940	G2051
A2941	G2052
A2942	G2053
A2943	G2054
A2944	G2055
A2945	G2056
A2946	G2057
A2947	G2058
A2948	G2059
A2949	G2060
A2950	G2061
A2951	G2062
A2952	G2063
A2953	G2064
A2954	G2065
A2955	G2066
A2956	G2067
A2957	G2068
A2958	G2069
A2959	G2070
A2960	G2071
A2961	G2072
A2962	G2073
A2963	G2074
A2964	G2075
A2965	G2076
A2966	G2077
A2967	G2078
A2968	G2079
A2969	G2080
A2970	G2081
A2971	G2082
A2972	G2083
A2973	G2084
A2974	G2085
A2975	G2086
A2976	G2087
A2977	G2088
A2978	G2089
A2979	G2090
A2980	G2091
A2981	G2092
A2982	G2093
A2983	G2094
A2984	G2095
A2985	G2096
A2986	G2097
A2987	G2098
A2988	G2099
A2989	G2100
A2990	G2101
A2991	G2102
A2992	G2103
A2993	G2104
A2994	G2105
A2995	G2106
A2996	G2107
A2997	G2108
A2998	G2109
A2999	G2110
A3000	G2111
A3001	G2112
A3002	G2113
A3003	G2114
A3004	G2115
A3005	G2116
A3006	G2117
A3007	G2118
A3008	G2119
A3009	G2120
A3010	G2121
A3011	G2122
A3012	G2123
A3013	G2124
A3014	G2125
A3015	G2126
A3016	G2127
A3017	G2128
A3018	G2129
A3019	G2130
A3020	G2131
A3021	G2132
A3022	G2133
A3023	G2134
A3024	G2135
A3025	G2136
A3026	G2137
A3027	G2138
A3028	G2139
A3029	G2140
A3030	G2141
A3031	G2142
A3032	G2143
A3033	G2144
A3034	G2145
A3035	G2146
A3036	G2147
A3037	G2148
A3038	G2149
A3039	G2150
A3040	G2151
A3041	G2152
A3042	G2153
A3043	G2154
A3044	G2155
A3045	G2156
A3046	G2157
A3047	G2158
A3048	G2159
A3049	G2160
A3050	G2161
A3051	G2162
A3052	G2163
A3053	G2164
A3054	G2165
A3055	G2166
A3056	G2167
A3057	G2168
A3058	G2169
A3059	G2170
A3060	G2171
A3061	G2172
A3062	G2173
A3063	G2174
A3064	G2175
A3065	G2176
A3066	G2177
A3067	G2178
A3068	G2179
A3069	G2180
A3070	G2181
A3071	G2182
A3072	G2183
A3073	G2184
A3074	G2185
A3075	G2186
A3076	G2187
A3077	G2188
A3078	G2189
A3079	G2190
A3080	G2191
A3081	G2192
A3082	G2193
A3083	G2194
A3084	G2195
A3085	G2196
A3086	G2197
A3087	G2198
A3088	G2199
A3089	G2200
A3090	G2201
A3091	G2202
A3092	G2203
A3093	G2204
A3094	G2205
A3095	G2206
A3096	G2207
A3097	G2208
A3098	G2209
A3099	G2210
A3100	G2211
A3101	G2212
A3102	G2213
A3103	G2214
A3104	G2215
A3105	G2216
A3106	G2217
A3107	G2218
A3108	G2219
A3109	G2220
A3110	G2221
A3111	G2222
A3112	G2223
A3113	G2224
A3114	G2225
A3115	G2226
A3116	G2227
A3117	G2228
A3118	G2229
A3119	G2230
A3120	G2231
A3121	G2232
A3122	G2233
A3123	G2234
A3124	G2235
A3125	G2236
A3126	G2237
A3127	G2238
A3128	G2239
A3129	G2240
A3130	G2241
A3131	G2242
A3132	G2243
A3133	G2244
A3134	G2245
A3135	G2246
A3136	G2247
A3137	G2248
A3138	G2249
A3139	G2250
A3140	G2251
A3141	G2252
A3142	G2253
A3143	G2254
A3144	G2255
A3145	G2256
A3146	G2257
A3147	G2258
A3148	G2259
A3149	G2260
A3150	G2261
A3151	G2262
A3152	G2263
A3153	G2264
A3154	G2265
A3155	G2266
A3156	G2267
A3157	G2268
A3158	G2269
A3159	G2270
A3160	G2271
A3161	G2272
A3162	G2273
A3163	G2274
A3164	G2275
A3165	G2276
A3166	G2277
A3167	G2278
A3168	G2279
A3169	G2280
A3170	G2281</



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31832	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2.8	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	0.560	Depositor
Minimum map value	-0.382	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.025	Depositor
Map size ($\text{\AA}$)	429.264, 429.264, 429.264	wwPDB
Map dimensions	396, 396, 396	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:
ZN

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	A	0.22	0/3583	0.58	0/4831
2	R	0.25	0/2631	0.56	0/3532
3	X	0.20	0/1653	0.55	0/2255
4	i	0.53	0/890	0.85	3/1189 (0.3%)
5	J	0.44	0/1821	0.70	0/2451
6	j	0.35	0/978	0.86	8/1301 (0.6%)
7	K	0.37	0/1836	0.75	8/2481 (0.3%)
8	k	0.38	0/778	0.74	0/1034
9	7	0.42	0/1539	0.68	1/2073 (0.0%)
10	l	0.56	0/696	0.90	0/923
11	M	0.29	0/1374	0.76	2/1842 (0.1%)
12	m	0.35	0/618	0.64	0/826
13	N	0.43	0/1568	0.84	4/2106 (0.2%)
14	n	0.60	0/443	0.84	0/588
15	O	0.39	0/1068	0.70	0/1438
16	o	0.42	0/423	0.78	1/562 (0.2%)
17	p	0.56	0/1757	0.89	4/2354 (0.2%)
18	Q	0.51	0/1585	0.77	0/2128
19	5	0.49	0/1443	0.83	2/1944 (0.1%)
20	S	0.38	0/1465	0.74	0/1965
21	s	0.41	0/1807	0.82	5/2425 (0.2%)
22	T	0.45	0/1245	0.79	0/1661
23	U	0.49	0/1481	0.80	1/1990 (0.1%)
24	V	0.41	0/1300	0.73	0/1743
25	W	0.34	0/812	0.71	1/1099 (0.1%)
26	P	0.24	0/734	0.84	1/1015 (0.1%)
27	r	0.21	0/982	0.64	1/1320 (0.1%)
28	x	0.44	0/1018	0.71	0/1369
29	3	0.36	0/2883	0.49	1/4491 (0.0%)
30	Y	0.41	0/525	0.70	0/696
31	4	0.47	0/3746	0.53	0/5832
32	Z	0.46	0/979	0.71	0/1321

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	a	0.39	0/1004	0.73	0/1341
34	B	0.22	0/1810	0.39	0/2821
35	b	0.39	0/1118	0.73	1/1497 (0.1%)
36	C	0.39	0/860	0.78	0/1136
37	c	0.44	0/1204	0.78	0/1612
38	D	0.48	0/701	0.76	0/934
39	d	0.40	0/473	0.68	0/629
40	E	0.56	0/1948	0.81	4/2617 (0.2%)
41	e	0.34	0/751	0.68	0/1008
42	F	0.57	1/3146 (0.0%)	0.79	0/4228
43	f	0.50	0/890	0.74	0/1196
44	G	0.44	0/2800	0.80	0/3790
45	g	0.45	0/1041	0.73	0/1394
46	H	0.31	0/2425	0.64	0/3271
47	h	0.51	0/868	0.71	0/1168
48	I	0.33	0/1260	0.65	0/1694
49	L	0.24	0/1634	0.74	1/2195 (0.0%)
50	l	0.46	0/79382	0.57	17/123763 (0.0%)
All	All	0.44	1/148976 (0.0%)	0.63	66/219079 (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
1	A	0	1
3	X	0	1
5	J	0	2
6	j	0	2
7	K	0	3
9	7	0	1
11	M	0	1
12	m	0	1
13	N	0	3
21	s	0	2
23	U	0	1
35	b	0	1
37	c	0	1
39	d	0	1
42	F	0	1
44	G	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
46	H	0	1
All	All	0	27

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	F	237	LYS	C-N	-13.03	1.13	1.33

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	N	48	PRO	CA-C-N	9.06	139.97	121.48
13	N	48	PRO	C-N-CA	9.06	139.97	121.48
49	L	191	VAL	N-CA-C	-6.59	106.31	112.83
13	N	61	PRO	CA-C-N	6.52	133.99	121.54
13	N	61	PRO	C-N-CA	6.52	133.99	121.54
4	i	24	LYS	CA-C-N	6.49	131.90	122.29
4	i	24	LYS	C-N-CA	6.49	131.90	122.29
19	5	157	VAL	CA-C-N	6.49	130.98	121.31
19	5	157	VAL	C-N-CA	6.49	130.98	121.31
50	1	1900	A	C2'-C3'-O3'	6.42	119.13	109.50
17	p	184	LYS	N-CA-C	-6.35	104.74	113.18
17	p	75	VAL	CA-CB-CG2	6.24	121.01	110.40
6	j	46	THR	CA-C-N	-6.21	114.82	121.84
6	j	46	THR	C-N-CA	-6.21	114.82	121.84
6	j	91	ALA	CA-C-N	6.20	130.54	121.31
6	j	91	ALA	C-N-CA	6.20	130.54	121.31
27	r	80	VAL	N-CA-C	-6.18	106.72	112.83
7	K	38	GLN	CA-C-N	6.06	130.34	121.31
7	K	38	GLN	C-N-CA	6.06	130.34	121.31
17	p	120	TRP	CA-C-N	-6.02	116.45	122.77
17	p	120	TRP	C-N-CA	-6.02	116.45	122.77
16	o	78	ILE	N-CA-C	-6.01	107.64	113.53
50	1	933	A	P-O3'-C3'	6.01	129.22	120.20
29	3	77	G	C2'-C3'-O3'	5.93	118.40	109.50
50	1	1391	C	C2'-C3'-O3'	5.91	118.37	109.50
9	7	21	LYS	N-CA-C	-5.91	101.71	110.46
6	j	84	LYS	CA-C-N	5.88	132.76	121.54
6	j	84	LYS	C-N-CA	5.88	132.76	121.54
23	U	12	ARG	N-CA-C	5.88	118.46	110.06
50	1	2046	U	N1-C1'-C2'	5.82	120.72	112.00
50	1	1483	G	C2'-C3'-O3'	5.75	118.12	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	j	90	ARG	CA-C-N	5.72	132.46	121.54
6	j	90	ARG	C-N-CA	5.72	132.46	121.54
50	1	2541	U	P-O3'-C3'	5.71	128.77	120.20
50	1	282	G	C2'-C3'-O3'	5.63	122.15	113.70
11	M	26	SER	CA-C-N	5.61	132.40	121.41
11	M	26	SER	C-N-CA	5.61	132.40	121.41
4	i	89	ILE	N-CA-C	-5.51	106.33	111.45
21	s	169	LYS	CA-CB-CG	5.48	125.06	114.10
50	1	2177	G	P-O3'-C3'	5.46	128.38	120.20
50	1	2509	U	P-O3'-C3'	5.41	128.31	120.20
21	s	134	ILE	CA-C-N	5.40	131.86	121.54
21	s	134	ILE	C-N-CA	5.40	131.86	121.54
50	1	1329	U	C2'-C3'-O3'	5.40	117.60	109.50
50	1	2468	A	P-O3'-C3'	5.40	128.31	120.20
50	1	906	A	P-O3'-C3'	5.37	128.25	120.20
50	1	2447	A	P-O3'-C3'	5.37	128.25	120.20
40	E	143	GLU	CA-C-N	5.36	131.78	121.54
40	E	143	GLU	C-N-CA	5.36	131.78	121.54
7	K	78	PHE	CA-C-N	5.30	131.66	121.54
7	K	78	PHE	C-N-CA	5.30	131.66	121.54
50	1	906	A	C2'-C3'-O3'	5.28	121.62	113.70
40	E	179	LEU	CA-C-N	5.20	128.61	120.82
40	E	179	LEU	C-N-CA	5.20	128.61	120.82
50	1	1840	U	P-O3'-C3'	5.15	127.92	120.20
7	K	156	ASP	CA-C-N	5.13	131.20	121.97
7	K	156	ASP	C-N-CA	5.13	131.20	121.97
7	K	39	ALA	CA-C-N	5.07	128.09	120.69
7	K	39	ALA	C-N-CA	5.07	128.09	120.69
50	1	933	A	C2'-C3'-O3'	5.04	117.06	109.50
25	W	59	ASP	N-CA-C	-5.03	108.41	114.75
50	1	2158	A	C4'-C3'-O3'	5.03	116.94	109.40
21	s	175	LEU	CA-C-N	5.03	128.80	121.31
21	s	175	LEU	C-N-CA	5.03	128.80	121.31
26	P	139	VAL	N-CA-C	-5.02	108.94	113.71
35	b	26	VAL	N-CA-C	-5.02	107.55	113.42

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	7	21	LYS	Peptide
1	A	289	VAL	Peptide

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Mol	Chain	Res	Type	Group
42	F	385	LYS	Peptide
44	G	130	ALA	Peptide
44	G	291	ASN	Peptide
44	G	318	LEU	Peptide
44	G	338	LYS	Peptide
46	H	259	LYS	Peptide
5	J	157	ASN	Peptide
5	J	232	ARG	Peptide
7	K	156	ASP	Peptide
7	K	38	GLN	Peptide
7	K	76	ALA	Peptide
11	M	172	LEU	Peptide
13	N	165	SER	Peptide
13	N	47	ALA	Peptide
13	N	61	PRO	Peptide
23	U	12	ARG	Peptide
3	X	8	GLU	Peptide
35	b	102	GLU	Peptide
37	c	46	ASP	Peptide
39	d	19	ASN	Peptide
6	j	90	ARG	Peptide
6	j	91	ALA	Peptide
12	m	32	ASN	Peptide
21	s	170	TRP	Peptide
21	s	171	GLY	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	A	3522	0	3534	74	0
2	R	2804	0	2687	46	0
3	X	1633	0	1596	21	0
4	i	880	0	945	11	0
5	J	1784	0	1862	24	0
6	j	969	0	1078	10	0
7	K	1804	0	1877	19	0
8	k	771	0	849	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	7	1518	0	1587	21	0
10	l	681	0	687	17	0
11	M	1353	0	1383	19	0
12	m	612	0	682	3	0
13	N	1543	0	1608	29	0
14	n	436	0	475	5	0
15	O	1053	0	1149	15	0
16	o	417	0	459	7	0
17	p	1720	0	1779	45	0
18	Q	1555	0	1659	16	0
19	5	1420	0	1437	21	0
20	S	1441	0	1543	20	0
21	s	1770	0	1808	57	0
22	T	1228	0	1314	17	0
23	U	1445	0	1487	19	0
24	V	1276	0	1323	18	0
25	W	796	0	812	6	0
26	P	737	0	341	2	0
27	r	967	0	991	17	0
28	x	1003	0	1048	24	0
29	3	2579	0	1304	32	0
30	Y	513	0	540	6	0
31	4	3353	0	1695	40	0
32	Z	964	0	1025	12	0
33	a	993	0	1081	16	0
34	B	1622	0	820	44	0
35	b	1092	0	1155	16	0
36	C	847	0	918	8	0
37	c	1173	0	1215	17	0
38	D	694	0	738	13	0
39	d	462	0	491	7	0
40	E	1914	0	1981	38	0
41	e	743	0	797	12	0
42	F	3075	0	3141	59	0
43	f	876	0	912	12	0
44	G	2748	0	2859	39	0
45	g	1020	0	1090	13	0
46	H	2375	0	2325	31	0
47	h	850	0	880	15	0
48	I	1239	0	1326	14	0
49	L	1609	0	1701	24	0
50	1	70924	0	35641	632	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	R	1	0	0	0	0
All	All	138804	0	101635	1339	0

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

All (1339) 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)
1:A:345:THR:HG21	21:s:109:ARG:NH1	1.62	1.14
2:R:286:THR:HG22	2:R:316:ASN:HB3	1.35	1.06
2:R:286:THR:HG22	2:R:316:ASN:CB	1.86	1.05
1:A:345:THR:CG2	21:s:109:ARG:NH1	2.22	1.03
2:R:284:ARG:NH1	34:B:1:G:C8	2.31	0.99
50:1:160:G:H1	50:1:261:U:H3	1.01	0.97
1:A:345:THR:OG1	21:s:109:ARG:NH1	1.96	0.97
21:s:106:GLY:H	34:B:1:G:N2	1.61	0.97
50:1:129:U:H3	50:1:139:G:H1	1.13	0.96
50:1:3231:U:H3	50:1:3256:G:H1	0.96	0.95
1:A:345:THR:CB	21:s:109:ARG:HH12	1.81	0.94
50:1:170:G:H1	50:1:248:U:H3	0.99	0.93
50:1:1958:U:C2	50:1:2083:G:O6	2.20	0.93
21:s:106:GLY:N	34:B:1:G:H21	1.65	0.93
21:s:106:GLY:H	34:B:1:G:H21	0.96	0.93
2:R:286:THR:CG2	2:R:316:ASN:HB3	2.01	0.91
50:1:1966:U:H3	50:1:2057:G:H1	0.96	0.91
2:R:284:ARG:NH2	34:B:1:G:OP2	2.04	0.90
34:B:15:G:H22	34:B:48:C:H42	1.16	0.89
50:1:1257:C:H42	50:1:1261:G:N2	1.70	0.89
50:1:1257:C:H42	50:1:1261:G:H22	1.20	0.89
1:A:345:THR:CB	21:s:109:ARG:NH1	2.37	0.88
1:A:345:THR:CG2	21:s:109:ARG:HH12	1.85	0.87
50:1:3348:G:H1	50:1:3357:U:H3	1.21	0.87
21:s:105:ALA:HB3	34:B:1:G:C2	2.10	0.86
50:1:1958:U:O2	50:1:2083:G:C6	2.29	0.85
21:s:106:GLY:N	34:B:1:G:N2	2.22	0.84
50:1:1257:C:N4	50:1:1261:G:H22	1.77	0.83
34:B:15:G:N2	34:B:48:C:H42	1.77	0.82
1:A:345:THR:HG21	21:s:109:ARG:HH12	1.36	0.82
21:s:106:GLY:HA2	34:B:72:C:O2	1.81	0.80
36:C:10:THR:O	36:C:20:HIS:HA	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:1:542:G:H1	50:1:549:U:H3	1.27	0.79
34:B:3:G:H1	34:B:70:U:H3	0.85	0.79
34:B:15:G:H22	34:B:48:C:N4	1.81	0.77
34:B:46:G:O2'	34:B:48:C:OP2	2.02	0.77
1:A:153:SER:O	1:A:157:TYR:HB2	1.86	0.75
17:p:53:TYR:HB2	17:p:133:ILE:HD11	1.69	0.74
50:1:1018:G:H1	50:1:1034:U:H3	1.34	0.73
50:1:3047:U:O4	50:1:3094:A:N1	2.21	0.73
31:4:72:A:H8	33:a:52:ARG:HH22	1.33	0.73
45:g:42:VAL:HG12	45:g:52:GLN:HE21	1.54	0.72
2:R:283:HIS:HE1	34:B:72:C:H41	1.38	0.72
2:R:286:THR:HG22	2:R:316:ASN:HB2	1.74	0.70
5:J:86:VAL:O	5:J:114:GLY:HA2	1.92	0.69
13:N:67:ARG:HG3	13:N:68:LYS:HG2	1.74	0.69
2:R:452:LYS:HG3	2:R:494:ILE:HG12	1.75	0.69
50:1:512:U:H3	50:1:579:G:H1	1.39	0.69
34:B:58:A:O2'	34:B:60:U:OP2	2.04	0.69
2:R:245:HIS:CE1	2:R:283:HIS:CD2	2.81	0.68
16:o:97:ARG:HE	16:o:122:ARG:HB3	1.58	0.68
28:x:12:ARG:NH1	50:1:3041:U:OP1	2.27	0.68
22:T:103:ARG:NH1	22:T:124:TYR:OH	2.27	0.68
50:1:718:G:H1	50:1:750:G:H21	1.42	0.68
38:D:56:THR:HG22	38:D:63:THR:HG23	1.76	0.67
2:R:77:CYS:SG	2:R:90:HIS:NE2	2.59	0.67
2:R:284:ARG:NH1	34:B:1:G:N9	2.41	0.67
40:E:117:GLU:HG2	40:E:124:GLY:H	1.61	0.66
27:r:27:VAL:HB	27:r:189:GLN:HB2	1.77	0.66
49:L:209:SER:HB2	50:1:2466:G:H21	1.59	0.66
50:1:2693:C:H5'	50:1:2694:A:H5''	1.77	0.66
50:1:1564:U:N3	50:1:1576:G:N1	2.42	0.66
35:b:51:LEU:HB2	35:b:65:ARG:HD2	1.77	0.66
2:R:283:HIS:CE1	34:B:72:C:H41	2.14	0.65
21:s:109:ARG:HE	21:s:109:ARG:HA	1.60	0.65
17:p:178:HIS:ND1	50:1:69:C:OP1	2.26	0.65
29:3:96:U:H2'	29:3:97:A:H8	1.61	0.65
48:I:54:TYR:HA	48:I:65:ILE:HG22	1.78	0.65
13:N:29:ALA:O	13:N:32:LYS:HB3	1.97	0.65
42:F:384:LYS:NZ	50:1:3368:U:OP1	2.30	0.65
45:g:33:ARG:NH2	50:1:1408:G:OP1	2.30	0.65
1:A:345:THR:HG21	21:s:109:ARG:CZ	2.27	0.65
19:5:119:VAL:HA	19:5:145:HIS:O	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:7:3:TYR:HA	23:U:142:GLN:HE22	1.61	0.64
10:l:52:LYS:NZ	50:1:353:G:O6	2.30	0.64
20:S:141:ARG:NH1	50:1:743:C:N3	2.45	0.64
6:j:47:VAL:O	6:j:50:SER:HB2	1.97	0.64
50:1:3172:A:N3	50:1:3173:G:N2	2.46	0.64
50:1:3344:A:N7	50:1:3362:A:N6	2.46	0.64
27:r:24:SER:HB2	27:r:89:THR:O	1.98	0.64
44:G:92:ASN:HD22	44:G:100:PHE:HB2	1.59	0.64
21:s:106:GLY:O	34:B:72:C:O2'	2.16	0.64
50:1:1966:U:O2	50:1:2057:G:N2	2.29	0.64
19:5:69:ARG:HD3	50:1:3309:G:H1'	1.78	0.64
27:r:46:ARG:HH22	50:1:1257:C:H4'	1.61	0.64
27:r:25:LEU:HB3	27:r:191:TYR:HB3	1.80	0.64
36:C:100:LYS:HB2	36:C:102:GLN:HE21	1.62	0.64
50:1:3047:U:C4	50:1:3094:A:N1	2.66	0.64
11:M:22:SER:HB2	50:1:2675:C:H42	1.63	0.63
22:T:82:LYS:HD3	50:1:1863:G:H4'	1.79	0.63
15:O:23:ILE:O	15:O:30:GLY:N	2.30	0.63
50:1:571:U:H2'	50:1:572:A:H8	1.64	0.63
27:r:34:SER:HA	50:1:1230:G:H4'	1.79	0.63
44:G:98:ARG:NH2	50:1:804:C:OP1	2.32	0.63
19:5:31:GLU:HG2	19:5:60:PHE:HA	1.80	0.63
49:L:42:ASP:OD2	49:L:200:ASN:ND2	2.32	0.62
1:A:297:ARG:NH2	1:A:311:TYR:OH	2.32	0.62
24:V:17:ARG:NH1	24:V:45:ASN:OD1	2.33	0.62
34:B:15:G:N1	34:B:48:C:N3	2.47	0.62
50:1:2149:A:N6	50:1:2187:G:O2'	2.32	0.62
50:1:1635:G:N2	50:1:1638:A:OP2	2.31	0.62
1:A:582:ILE:HB	1:A:593:TRP:HB3	1.81	0.62
18:Q:164:SER:O	18:Q:167:TYR:HB3	2.00	0.62
47:h:99:ARG:NH1	50:1:3275:U:O2'	2.32	0.62
31:4:150:G:OP1	32:Z:27:ARG:NH2	2.33	0.62
50:1:1240:A:N1	50:1:1248:C:N4	2.48	0.62
20:S:170:ARG:HD2	37:c:57:GLY:HA3	1.81	0.62
50:1:920:A:OP1	50:1:923:C:N4	2.31	0.62
7:K:137:ASN:ND2	50:1:148:G:N7	2.48	0.62
13:N:16:LYS:NZ	50:1:98:G:OP1	2.33	0.61
50:1:920:A:H5''	50:1:922:U:H3	1.65	0.61
50:1:1846:C:OP1	50:1:1849:C:N4	2.31	0.61
50:1:1900:A:H61	50:1:1908:A:H61	1.48	0.61
2:R:74:CYS:SG	2:R:77:CYS:HB2	2.41	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:p:163:GLY:O	17:p:172:ARG:NH1	2.31	0.61
45:g:33:ARG:NH1	50:1:944:C:O2'	2.33	0.61
5:J:206:LYS:NZ	50:1:1334:U:OP1	2.32	0.61
27:r:28:VAL:O	27:r:84:VAL:HA	2.00	0.61
42:F:244:ARG:NH2	50:1:2948:C:OP1	2.34	0.61
44:G:188:ARG:NH1	50:1:1382:G:OP2	2.34	0.61
50:1:962:A:N6	50:1:2408:U:O2	2.33	0.61
50:1:1064:A:OP2	50:1:1097:G:N2	2.34	0.61
50:1:589:A:N6	50:1:610:G:O2'	2.34	0.61
50:1:1493:G:N2	50:1:1493:G:OP2	2.33	0.61
14:n:27:ILE:O	14:n:33:ASN:ND2	2.34	0.61
31:4:81:U:H5''	31:4:82:U:H5'	1.81	0.61
13:N:91:ARG:HE	13:N:97:VAL:HB	1.65	0.61
50:1:373:A:C6	50:1:375:A:C6	2.89	0.61
50:1:1003:A:N1	50:1:1049:C:O2'	2.32	0.61
50:1:3042:U:OP2	50:1:3092:C:N4	2.34	0.61
2:R:285:TYR:HB2	34:B:72:C:C5	2.36	0.60
1:A:465:GLN:HE22	1:A:541:GLU:HB2	1.66	0.60
17:p:68:ARG:NH2	50:1:292:U:OP2	2.33	0.60
50:1:394:G:N1	50:1:397:A:OP2	2.33	0.60
2:R:379:VAL:HG21	34:B:68:C:H5''	1.82	0.60
13:N:59:ARG:NH1	50:1:73:C:N3	2.50	0.60
28:x:14:SER:O	28:x:81:GLN:NE2	2.34	0.60
42:F:241:LYS:NZ	50:1:874:U:OP2	2.34	0.60
21:s:108:ASP:O	21:s:109:ARG:HB2	2.00	0.60
42:F:364:LYS:HD2	50:1:3049:A:H4'	1.82	0.60
27:r:89:THR:HG21	27:r:96:ILE:HG13	1.82	0.60
46:H:64:ILE:HD13	46:H:109:THR:HG21	1.82	0.60
42:F:266:ARG:NH2	50:1:2392:C:O2'	2.34	0.60
44:G:82:THR:HG23	44:G:84:ARG:H	1.65	0.60
9:7:16:VAL:HG12	9:7:29:GLY:HA3	1.82	0.60
34:B:25:C:H2'	34:B:26:G:H8	1.67	0.60
50:1:512:U:O2	50:1:579:G:N2	2.31	0.60
50:1:1204:A:N6	50:1:1300:G:O2'	2.33	0.60
22:T:98:ARG:NH2	22:T:132:PHE:O	2.35	0.60
28:x:80:ARG:HD3	28:x:117:PRO:HG2	1.83	0.60
7:K:162:LEU:HA	17:p:7:LEU:HD11	1.83	0.60
50:1:1627:U:O2	50:1:1817:G:N2	2.33	0.60
50:1:1958:U:O2	50:1:2083:G:O6	2.15	0.60
50:1:2036:U:H2'	50:1:2037:G:H8	1.67	0.60
10:l:9:GLY:HA3	50:1:1852:G:H1'	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:F:57:VAL:HG22	42:F:73:VAL:HG12	1.83	0.59
50:1:2193:U:H5'	50:1:2194:G:H5'	1.83	0.59
42:F:139:GLN:HG3	42:F:141:GLY:H	1.65	0.59
50:1:518:G:N2	50:1:520:U:O2'	2.35	0.59
50:1:908:G:N2	50:1:925:A:N7	2.49	0.59
50:1:2116:G:OP1	50:1:2118:C:N4	2.36	0.59
19:5:127:ARG:NH2	50:1:1508:C:OP1	2.36	0.59
35:b:48:ARG:NH2	50:1:1631:C:OP2	2.36	0.59
50:1:907:G:N2	50:1:925:A:O2'	2.36	0.59
43:f:26:LYS:NZ	50:1:1455:U:O2	2.36	0.59
49:L:18:LYS:HG3	49:L:24:LYS:H	1.66	0.59
8:k:30:LYS:NZ	50:1:317:A:OP2	2.34	0.59
17:p:201:ARG:NH2	50:1:692:A:OP1	2.34	0.59
15:O:36:VAL:HG11	15:O:55:ARG:HH12	1.66	0.59
31:4:135:G:H5''	32:Z:49:LYS:HD3	1.83	0.59
50:1:2761:G:O2'	50:1:2800:G:N2	2.35	0.59
13:N:64:LYS:O	13:N:67:ARG:NH1	2.35	0.59
21:s:190:LYS:NZ	21:s:211:GLU:OE1	2.35	0.59
1:A:356:ARG:NH2	50:1:2964:G:O2'	2.35	0.59
3:X:7:PHE:O	28:x:7:GLN:NE2	2.36	0.59
10:l:14:LYS:NZ	50:1:1491:A:OP1	2.36	0.59
13:N:169:THR:O	13:N:173:ALA:N	2.36	0.59
17:p:112:ASN:ND2	31:4:141:C:O2	2.36	0.59
23:U:6:GLU:O	23:U:64:ILE:HB	2.02	0.59
50:1:753:C:H2'	50:1:754:G:H8	1.67	0.59
43:f:57:GLN:NE2	50:1:1474:A:O2'	2.36	0.58
17:p:99:ARG:NH2	17:p:118:SER:O	2.36	0.58
2:R:436:ILE:HG12	2:R:461:ARG:HH11	1.68	0.58
19:5:30:ARG:NH1	19:5:31:GLU:OE1	2.36	0.58
21:s:207:ASN:HA	21:s:210:ARG:HG2	1.86	0.58
50:1:177:U:O2	50:1:241:G:N2	2.35	0.58
50:1:807:A:H61	50:1:934:G:H22	1.52	0.58
7:K:157:VAL:HG12	7:K:159:PRO:HD2	1.85	0.58
10:l:76:ASN:HD21	31:4:94:C:H5''	1.69	0.58
17:p:108:ARG:NH2	50:1:1547:G:OP1	2.36	0.58
20:S:92:ARG:NH1	50:1:784:A:O2'	2.36	0.58
21:s:107:ALA:HA	21:s:110:LEU:HD23	1.84	0.58
24:V:88:ARG:NH2	39:d:31:SER:OG	2.36	0.58
45:g:16:LYS:NZ	50:1:1404:G:O6	2.37	0.58
46:H:85:ARG:HE	46:H:254:LYS:HE3	1.68	0.58
5:J:67:ARG:NH2	50:1:517:G:OP1	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:7:62:ARG:NH2	50:1:3115:C:OP1	2.35	0.58
11:M:137:ARG:NH1	29:3:28:C:OP1	2.36	0.58
13:N:166:ALA:O	13:N:169:THR:HB	2.02	0.58
30:Y:48:ARG:NH2	50:1:2111:G:OP2	2.36	0.58
42:F:126:LYS:HG3	50:1:3294:A:H5'	1.85	0.58
17:p:144:ARG:NH1	50:1:126:U:OP1	2.37	0.58
42:F:115:LYS:NZ	42:F:129:ALA:O	2.36	0.58
7:K:148:ALA:HA	7:K:201:THR:HG22	1.86	0.58
50:1:2816:G:N2	50:1:2819:A:OP2	2.37	0.58
28:x:15:LEU:HD23	28:x:53:SER:HB3	1.85	0.58
49:L:30:GLU:HB2	49:L:34:LEU:HD11	1.85	0.58
50:1:2955:U:OP2	50:1:2977:G:N1	2.31	0.58
50:1:3234:A:C2	50:1:3253:G:N1	2.69	0.58
20:S:69:ARG:HH12	50:1:720:A:H5''	1.67	0.58
44:G:216:VAL:HA	44:G:227:THR:HG21	1.86	0.58
50:1:2745:G:N2	50:1:2748:A:OP2	2.36	0.58
50:1:1896:A:H61	50:1:2339:C:H42	1.50	0.57
6:j:10:ARG:NH2	31:4:65:A:O2'	2.37	0.57
29:3:17:A:OP1	46:H:2:ALA:N	2.37	0.57
33:a:2:ALA:N	50:1:212:G:OP2	2.37	0.57
36:C:74:CYS:SG	36:C:75:VAL:N	2.77	0.57
20:S:56:LYS:NZ	50:1:674:G:O6	2.35	0.57
27:r:38:MET:HE2	50:1:1259:A:H62	1.69	0.57
33:a:12:ARG:NH1	50:1:215:G:OP1	2.31	0.57
38:D:66:GLY:HA2	40:E:80:GLU:HG3	1.85	0.57
50:1:1231:A:O2'	50:1:1278:A:N6	2.37	0.57
1:A:243:VAL:HG12	1:A:245:PRO:HD3	1.85	0.57
16:o:100:TYR:O	50:1:2895:G:O2'	2.21	0.57
17:p:2:GLY:N	50:1:116:A:OP2	2.37	0.57
24:V:130:ARG:NH2	50:1:1062:A:N3	2.47	0.57
29:3:7:G:OP1	46:H:33:ARG:NH1	2.38	0.57
50:1:1210:U:H3	50:1:1295:G:H1	1.53	0.57
50:1:2137:U:OP2	50:1:2142:A:N6	2.36	0.57
50:1:2396:G:H5''	50:1:2397:A:H4'	1.86	0.57
50:1:1492:G:H1'	50:1:1843:C:H5''	1.87	0.57
1:A:476:SER:HA	1:A:512:GLN:HA	1.86	0.57
50:1:371:G:N1	50:1:374:A:OP2	2.37	0.57
46:H:210:GLU:O	46:H:214:ASP:HB2	2.04	0.57
2:R:502:ASN:HD21	2:R:506:ARG:HE	1.53	0.57
17:p:4:TYR:OH	50:1:148:G:OP2	2.22	0.57
28:x:47:ASN:ND2	50:1:2880:U:OP1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:H:60:ILE:HB	46:H:80:SER:HB3	1.87	0.57
47:h:86:ARG:NH1	47:h:87:ASN:OD1	2.38	0.57
50:1:3305:A:O2'	50:1:3310:A:N1	2.36	0.57
1:A:423:ARG:HH11	1:A:580:GLN:HE21	1.53	0.57
27:r:26:PHE:HB2	27:r:87:VAL:HB	1.86	0.57
50:1:1564:U:O2	50:1:1576:G:N2	2.37	0.57
7:K:69:LEU:HD21	17:p:24:ARG:HD2	1.87	0.56
25:W:15:PHE:HB2	25:W:65:VAL:HB	1.87	0.56
40:E:200:ARG:NH1	50:1:2146:C:OP1	2.38	0.56
44:G:300:ARG:NH2	50:1:1347:U:OP2	2.34	0.56
1:A:488:ILE:HD12	1:A:531:LEU:HD22	1.86	0.56
9:7:58:HIS:O	50:1:3186:A:N6	2.34	0.56
48:I:43:LEU:HD11	48:I:85:ILE:HG13	1.87	0.56
50:1:3344:A:N6	50:1:3361:G:O2'	2.36	0.56
3:X:107:VAL:HG13	3:X:118:HIS:H	1.69	0.56
7:K:50:VAL:HG12	32:Z:30:ALA:HA	1.85	0.56
9:7:8:GLN:HB3	9:7:72:LYS:HD2	1.87	0.56
17:p:193:ARG:NH2	50:1:100:A:OP1	2.38	0.56
23:U:109:ASP:OD1	23:U:113:ARG:NH1	2.38	0.56
31:4:114:G:OP1	50:1:1831:U:O2'	2.23	0.56
40:E:47:GLN:HB3	40:E:60:LYS:HD2	1.87	0.56
50:1:2534:G:H2'	50:1:2535:A:H8	1.70	0.56
50:1:2874:G:N2	50:1:2979:U:O2	2.35	0.56
31:4:24:G:O6	33:a:13:ARG:NH2	2.38	0.56
3:X:4:ARG:HB3	3:X:208:LEU:HA	1.88	0.56
18:Q:32:LYS:NZ	50:1:3173:G:OP2	2.37	0.56
29:3:44:C:H2'	29:3:45:A:H8	1.71	0.56
31:4:41:A:N6	31:4:103:G:O2'	2.37	0.56
37:c:58:MET:SD	50:1:2786:G:N2	2.78	0.56
7:K:126:SER:O	50:1:120:G:N2	2.38	0.56
40:E:21:ARG:HD3	50:1:824:C:H5''	1.86	0.56
44:G:203:ARG:NH2	44:G:226:GLU:OE1	2.38	0.56
46:H:68:THR:HG22	46:H:70:THR:H	1.71	0.56
47:h:13:HIS:ND1	47:h:93:THR:O	2.38	0.56
44:G:72:ALA:O	44:G:76:ARG:NH2	2.37	0.56
49:L:56:PRO:HG3	49:L:187:VAL:HG21	1.86	0.56
50:1:952:A:N3	50:1:1114:U:O2'	2.39	0.56
17:p:169:LYS:NZ	50:1:64:G:OP2	2.39	0.56
23:U:66:GLU:HG3	23:U:68:HIS:H	1.71	0.56
1:A:89:LEU:HB2	1:A:97:ILE:HD11	1.87	0.56
2:R:77:CYS:SG	2:R:99:ASN:ND2	2.76	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:s:29:LYS:HG3	21:s:62:GLU:HG3	1.86	0.56
42:F:126:LYS:NZ	50:1:3294:A:OP2	2.39	0.56
46:H:50:ARG:NH1	46:H:147:ASP:OD2	2.39	0.56
50:1:1986:U:H3	50:1:2035:G:H1	1.52	0.56
50:1:2437:G:H1	50:1:2510:U:H3	1.52	0.56
50:1:2946:A:H5''	50:1:2947:G:H5'	1.88	0.56
50:1:3277:U:OP1	50:1:3278:C:N4	2.39	0.56
15:O:60:LEU:HD13	23:U:152:LEU:HD11	1.89	0.55
19:5:109:ALA:HA	19:5:112:LEU:HD13	1.88	0.55
40:E:117:GLU:HB2	40:E:162:ALA:HB1	1.88	0.55
49:L:101:LYS:NZ	49:L:122:ARG:O	2.39	0.55
31:4:70:G:OP1	33:a:121:ARG:NH1	2.34	0.55
33:a:24:SER:OG	33:a:75:ARG:NH1	2.37	0.55
46:H:235:SER:O	46:H:238:ASP:HB2	2.05	0.55
50:1:2448:G:H1	50:1:2498:U:H3	1.54	0.55
50:1:2535:A:H61	50:1:2544:U:H3	1.55	0.55
50:1:3150:A:O2'	50:1:3294:A:O2'	2.23	0.55
10:l:72:ARG:NH1	31:4:95:G:OP2	2.40	0.55
40:E:209:HIS:HD2	40:E:211:HIS:H	1.54	0.55
50:1:655:C:H2'	50:1:656:A:C8	2.41	0.55
9:7:182:SER:HA	16:o:85:LEU:HD11	1.88	0.55
11:M:133:ARG:NH2	11:M:158:ASP:OD2	2.39	0.55
22:T:59:SER:N	50:1:3068:U:OP1	2.40	0.55
50:1:1959:G:O6	50:1:2082:U:O2	2.25	0.55
1:A:385:VAL:HG22	1:A:562:ASN:HD22	1.70	0.55
18:Q:59:ARG:NH1	50:1:1307:G:OP1	2.39	0.55
23:U:22:PRO:O	24:V:146:ASN:ND2	2.39	0.55
42:F:53:MET:HG2	42:F:77:THR:HG22	1.87	0.55
1:A:383:PRO:HB2	1:A:534:PRO:HG2	1.88	0.55
13:N:48:PRO:HB2	13:N:137:GLN:HB3	1.88	0.55
13:N:79:GLU:OE2	13:N:112:ASN:ND2	2.40	0.55
18:Q:68:ARG:NH2	50:1:2365:C:O2'	2.40	0.55
24:V:104:GLU:OE1	50:1:989:A:O2'	2.23	0.55
44:G:140:HIS:H	44:G:180:LYS:HE2	1.71	0.55
23:U:170:THR:OG1	50:1:3186:A:OP2	2.24	0.55
50:1:3155:U:H5'	50:1:3156:U:H4'	1.89	0.55
20:S:164:ARG:NH2	50:1:1110:U:OP1	2.36	0.55
21:s:106:GLY:CA	34:B:1:G:H21	2.19	0.55
48:I:77:ARG:NH2	50:1:3273:A:OP2	2.40	0.55
50:1:908:G:H22	50:1:2414:G:H5''	1.71	0.55
50:1:1778:G:O2'	50:1:1780:G:OP2	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:239:PHE:HB2	2:R:343:ILE:HG12	1.89	0.55
36:C:8:ARG:NH1	50:1:2655:U:O4	2.40	0.55
7:K:144:GLU:OE1	8:k:36:ARG:NH1	2.40	0.54
50:1:2150:G:O2'	50:1:2189:U:OP1	2.24	0.54
50:1:2890:A:O2'	50:1:2933:A:N3	2.40	0.54
1:A:294:ILE:HA	1:A:302:THR:O	2.06	0.54
10:l:27:PHE:HA	10:l:34:CYS:HA	1.89	0.54
24:V:4:SER:OG	50:1:2631:U:OP2	2.24	0.54
41:e:30:THR:HG22	41:e:91:SER:HB2	1.89	0.54
3:X:12:GLU:HG2	3:X:196:GLY:HA2	1.89	0.54
35:b:133:LYS:NZ	50:1:1808:G:OP2	2.38	0.54
44:G:119:ARG:NE	50:1:695:C:OP1	2.38	0.54
11:M:15:GLU:HB3	11:M:130:VAL:HG13	1.88	0.54
24:V:39:ILE:HG12	24:V:63:VAL:HG22	1.89	0.54
40:E:9:ARG:NH2	50:1:912:G:N7	2.56	0.54
42:F:13:HIS:HB2	50:1:3044:G:H4'	1.89	0.54
50:1:1302:A:N7	50:1:2857:C:O2'	2.37	0.54
50:1:3234:A:N1	50:1:3253:G:O6	2.41	0.54
21:s:183:LYS:NZ	21:s:188:GLU:OE1	2.38	0.54
40:E:28:LYS:HB3	40:E:123:ARG:HB3	1.90	0.54
44:G:119:ARG:NH2	50:1:696:C:OP2	2.39	0.54
50:1:2458:A:N6	50:1:2477:G:OP2	2.37	0.54
8:k:26:ILE:HD13	50:1:157:A:C8	2.43	0.54
12:m:2:ALA:N	50:1:1613:A:OP1	2.41	0.54
40:E:9:ARG:HH11	40:E:16:PHE:HZ	1.55	0.54
50:1:2043:U:O4	50:1:2045:G:N2	2.41	0.54
37:c:19:LYS:HB3	37:c:25:HIS:HB2	1.90	0.54
50:1:1569:U:H5''	50:1:1570:U:H6	1.72	0.54
1:A:394:ALA:HB3	1:A:453:SER:HB3	1.89	0.54
4:i:58:ARG:NH2	50:1:1592:G:OP1	2.40	0.54
18:Q:160:ARG:O	18:Q:164:SER:N	2.41	0.54
29:3:5:G:O2'	46:H:63:GLN:NE2	2.41	0.54
40:E:93:LYS:NZ	50:1:2548:C:OP2	2.40	0.54
47:h:75:HIS:HB2	47:h:82:ARG:HG3	1.90	0.54
50:1:3255:U:H2'	50:1:3256:G:H8	1.73	0.54
10:l:48:ASN:OD1	10:l:54:LYS:NZ	2.40	0.54
21:s:109:ARG:HA	21:s:109:ARG:NE	2.20	0.54
44:G:340:GLY:O	50:1:514:G:N2	2.37	0.54
18:Q:173:ALA:O	18:Q:176:LYS:HB3	2.08	0.54
50:1:197:G:N2	50:1:218:G:O2'	2.40	0.54
11:M:92:ARG:HA	11:M:172:LEU:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M:105:GLY:HA3	50:1:2674:A:H5''	1.90	0.53
13:N:42:ARG:NH2	50:1:108:A:OP2	2.42	0.53
34:B:1:G:H2'	34:B:2:G:H8	1.73	0.53
42:F:235:THR:HG21	42:F:249:VAL:HG22	1.90	0.53
50:1:2768:U:H2'	50:1:2769:A:H8	1.73	0.53
21:s:107:ALA:O	21:s:109:ARG:N	2.35	0.53
49:L:18:LYS:HB2	49:L:23:THR:HB	1.91	0.53
1:A:109:ARG:HH11	1:A:289:VAL:HG22	1.73	0.53
3:X:27:ALA:O	3:X:35:TYR:OH	2.27	0.53
21:s:105:ALA:HB3	34:B:1:G:N2	2.22	0.53
13:N:55:ARG:NH1	13:N:73:ARG:O	2.35	0.53
49:L:76:ARG:O	49:L:141:ASN:ND2	2.41	0.53
34:B:17:C:O2'	34:B:57:G:N2	2.42	0.53
50:1:716:A:OP1	50:1:752:C:O2'	2.26	0.53
50:1:1529:A:OP2	50:1:1592:G:N2	2.33	0.53
50:1:3190:C:H2'	50:1:3191:G:H8	1.74	0.53
11:M:137:ARG:NE	29:3:43:U:OP1	2.35	0.53
21:s:105:ALA:HB3	34:B:1:G:N3	2.23	0.53
38:D:4:ARG:NH2	50:1:837:A:OP2	2.40	0.53
3:X:64:ALA:HB2	3:X:105:GLY:HA2	1.90	0.53
21:s:192:ASP:OD2	50:1:1010:G:N2	2.42	0.53
31:4:15:G:N1	50:1:407:A:OP2	2.38	0.53
46:H:31:TYR:O	46:H:35:ARG:NH1	2.42	0.53
46:H:107:ARG:NH2	46:H:120:LYS:O	2.42	0.53
50:1:3234:A:N1	50:1:3253:G:C6	2.76	0.53
28:x:81:GLN:O	28:x:98:ASN:ND2	2.42	0.53
8:k:5:THR:HG23	8:k:12:ASN:HB2	1.91	0.53
17:p:119:TYR:OH	17:p:131:GLU:OE1	2.25	0.53
5:J:160:ARG:NH1	50:1:1363:A:OP1	2.42	0.53
9:7:124:ARG:NH1	9:7:164:ILE:O	2.42	0.53
17:p:115:VAL:HG22	17:p:134:LEU:HG	1.89	0.53
19:5:3:ARG:O	19:5:18:ARG:NH2	2.40	0.53
41:e:50:VAL:HG11	50:1:2552:C:H2'	1.90	0.53
50:1:1564:U:O4	50:1:1576:G:O6	2.26	0.53
50:1:2941:A:H5''	50:1:2943:G:H4'	1.91	0.53
50:1:1899:G:O2'	50:1:1901:A:N6	2.43	0.52
50:1:2144:A:O2'	50:1:2281:A:N6	2.39	0.52
16:o:113:ARG:NH2	50:1:1192:C:OP1	2.43	0.52
18:Q:4:GLU:O	18:Q:31:GLN:NE2	2.37	0.52
26:P:126:ALA:HB3	26:P:159:GLU:HA	1.90	0.52
49:L:59:PRO:HG2	49:L:180:VAL:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:1:1628:C:O5'	50:1:1814:A:N6	2.43	0.52
50:1:2171:G:H2'	50:1:2172:A:H8	1.74	0.52
48:I:42:LEU:HD22	48:I:79:VAL:HG11	1.91	0.52
50:1:2901:G:O2'	50:1:3024:A:N1	2.42	0.52
17:p:37:HIS:HE1	17:p:63:ARG:HH11	1.57	0.52
28:x:18:PRO:HA	28:x:51:ALA:HA	1.91	0.52
13:N:184:GLU:O	13:N:188:ARG:N	2.42	0.52
35:b:107:ARG:NH1	50:1:1634:G:OP1	2.35	0.52
39:d:19:ASN:ND2	50:1:969:C:OP1	2.35	0.52
42:F:244:ARG:NH1	50:1:2946:A:O2'	2.41	0.52
50:1:1959:G:C6	50:1:2082:U:O2	2.62	0.52
5:J:181:ILE:HG21	44:G:327:LEU:HD23	1.91	0.52
33:a:16:ARG:NH1	50:1:216:G:OP1	2.43	0.52
50:1:1155:C:O2'	50:1:1197:A:N1	2.40	0.52
13:N:46:ILE:HG13	13:N:49:ARG:HB2	1.92	0.52
19:5:120:ASN:OD1	19:5:120:ASN:N	2.39	0.52
20:S:164:ARG:NH1	50:1:668:G:O2'	2.43	0.52
50:1:1398:U:O2	50:1:1412:G:O6	2.27	0.52
1:A:115:GLU:O	1:A:120:LYS:NZ	2.42	0.52
1:A:324:LYS:NZ	50:1:2238:G:OP1	2.39	0.52
2:R:484:LYS:HD2	2:R:519:HIS:HB3	1.92	0.52
2:R:512:ASN:HB3	2:R:521:PHE:HB2	1.90	0.52
21:s:51:LEU:HD12	21:s:151:LEU:HB3	1.91	0.52
29:3:19:C:H2'	29:3:20:A:H8	1.75	0.52
50:1:946:U:H2'	50:1:947:G:H8	1.75	0.52
50:1:1958:U:C2	50:1:2083:G:C6	2.90	0.52
50:1:2483:G:N2	50:1:2486:A:OP2	2.43	0.52
11:M:49:LYS:HB3	11:M:62:ASN:HA	1.91	0.52
46:H:123:GLU:HA	46:H:248:ARG:HH12	1.74	0.52
50:1:1222:G:O2'	50:1:1285:G:N1	2.41	0.52
50:1:2442:G:N2	50:1:2505:U:O2	2.42	0.52
1:A:462:VAL:HG22	1:A:538:LEU:HD12	1.92	0.52
13:N:73:ARG:NH1	50:1:110:G:OP2	2.35	0.52
13:N:76:THR:HG22	13:N:101:ARG:HG3	1.92	0.52
1:A:414:LEU:HD13	1:A:590:ALA:HB3	1.92	0.51
4:i:3:GLN:HE22	4:i:29:ILE:HG22	1.74	0.51
21:s:106:GLY:O	21:s:107:ALA:HB3	2.10	0.51
48:I:22:ARG:NH2	50:1:595:G:O6	2.33	0.51
11:M:32:ARG:NH1	11:M:120:ILE:O	2.37	0.51
17:p:203:ARG:NH1	50:1:665:A:OP1	2.38	0.51
22:T:148:ASP:OD1	22:T:151:ARG:NH2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:b:54:THR:H	35:b:57:HIS:CD2	2.28	0.51
41:e:29:SER:N	50:1:1730:G:O6	2.35	0.51
50:1:1190:A:C8	50:1:1193:A:H1'	2.46	0.51
50:1:1308:A:H61	50:1:2367:A:H2	1.57	0.51
50:1:2810:C:OP2	50:1:2955:U:O2'	2.28	0.51
15:O:19:ARG:HG2	15:O:65:LEU:HD22	1.92	0.51
19:5:122:ALA:HB3	19:5:143:PRO:HG2	1.92	0.51
21:s:46:PRO:HD2	21:s:140:LYS:HA	1.91	0.51
35:b:22:LYS:HE3	35:b:134:LEU:HB2	1.93	0.51
50:1:85:A:H61	50:1:99:A:H3'	1.76	0.51
1:A:233:MET:HE3	1:A:255:ALA:HB3	1.93	0.51
6:j:77:PRO:HD2	6:j:80:LEU:HD12	1.93	0.51
45:g:101:SER:HB3	50:1:1389:G:H5''	1.93	0.51
50:1:1714:A:H61	50:1:1730:G:H1'	1.74	0.51
1:A:399:SER:HB2	1:A:449:SER:HB3	1.91	0.51
5:J:88:ARG:NH2	5:J:91:GLY:O	2.43	0.51
21:s:106:GLY:CA	34:B:1:G:N2	2.72	0.51
23:U:9:VAL:O	23:U:26:ARG:HA	2.11	0.51
38:D:49:ARG:HH21	38:D:52:ALA:HB2	1.75	0.51
48:I:80:ASN:HB3	48:I:83:TYR:HD2	1.75	0.51
50:1:542:G:O6	50:1:549:U:O4	2.28	0.51
50:1:1555:U:O4	50:1:1557:A:N6	2.44	0.51
5:J:116:PHE:O	5:J:199:ASN:ND2	2.41	0.51
29:3:35:C:O2	29:3:45:A:O2'	2.27	0.51
33:a:111:LEU:HD23	33:a:116:LYS:HG2	1.93	0.51
42:F:10:ARG:NH2	42:F:263:SER:O	2.43	0.51
50:1:2085:U:H2'	50:1:2086:A:C8	2.46	0.51
33:a:63:LYS:HG2	33:a:85:VAL:HG13	1.93	0.51
45:g:54:LYS:HE3	50:1:1162:U:H5'	1.92	0.51
49:L:36:VAL:HA	49:L:208:SER:HA	1.91	0.51
41:e:57:GLU:OE2	41:e:69:TYR:OH	2.29	0.51
42:F:269:GLN:NE2	50:1:3306:U:OP1	2.40	0.51
50:1:1717:U:H2'	50:1:1718:G:C8	2.45	0.51
50:1:536:U:O4	50:1:557:A:N6	2.44	0.51
50:1:542:G:N2	50:1:549:U:O2	2.41	0.51
50:1:1018:G:O6	50:1:1034:U:O4	2.28	0.51
1:A:438:LEU:HD22	1:A:538:LEU:HB3	1.93	0.51
4:i:41:ARG:HG2	4:i:56:THR:HG21	1.93	0.51
44:G:132:ALA:HB2	44:G:148:ILE:HD13	1.92	0.51
50:1:510:G:H1	50:1:581:U:H3	1.58	0.51
50:1:1255:C:H2'	50:1:1256:G:H8	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:1:1870:C:O2	50:1:3066:U:O2'	2.29	0.51
9:7:141:LYS:NZ	9:7:142:ASP:OD2	2.41	0.50
15:O:128:ARG:NH1	50:1:3214:U:OP2	2.44	0.50
21:s:47:LEU:HD11	21:s:166:LEU:HD21	1.93	0.50
21:s:204:SER:HA	29:3:64:A:H5''	1.92	0.50
30:Y:14:TYR:OH	42:F:375:GLU:OE2	2.29	0.50
35:b:54:THR:HG23	35:b:56:LYS:H	1.75	0.50
50:1:1506:A:H5''	50:1:1507:G:H5''	1.93	0.50
50:1:2617:U:O2'	50:1:2644:C:N4	2.44	0.50
19:5:107:LEU:HD23	19:5:152:GLU:HG3	1.93	0.50
26:P:63:LYS:HA	26:P:72:SER:HA	1.93	0.50
45:g:63:THR:HA	45:g:66:LEU:HD12	1.93	0.50
50:1:2689:A:O2'	50:1:2691:A:N7	2.43	0.50
23:U:141:LYS:HA	23:U:144:LEU:HD12	1.92	0.50
27:r:64:ARG:NH1	50:1:1221:A:OP2	2.44	0.50
28:x:87:ARG:NE	28:x:121:GLU:OE2	2.44	0.50
44:G:326:ARG:NH1	50:1:608:A:O2'	2.45	0.50
50:1:1273:A:H3'	50:1:1274:A:H8	1.77	0.50
37:c:32:ARG:HG3	50:1:38:U:H4'	1.93	0.50
18:Q:171:LYS:O	18:Q:174:PHE:HB3	2.11	0.50
22:T:92:GLN:NE2	50:1:1662:G:O2'	2.44	0.50
35:b:54:THR:H	35:b:57:HIS:HD2	1.59	0.50
36:C:23:HIS:HA	36:C:73:GLU:O	2.11	0.50
42:F:173:GLN:HG3	50:1:3313:U:H4'	1.94	0.50
50:1:68:C:OP2	50:1:301:G:N2	2.44	0.50
50:1:806:A:N3	50:1:2812:C:O2'	2.38	0.50
27:r:27:VAL:HG21	27:r:76:LEU:HD21	1.93	0.50
39:d:28:LYS:HD3	50:1:1065:A:H1'	1.93	0.50
50:1:3348:G:O6	50:1:3357:U:O4	2.28	0.50
1:A:336:ILE:HD11	50:1:2418:G:H22	1.77	0.50
1:A:390:PRO:HA	1:A:420:MET:HB2	1.94	0.50
10:l:30:GLN:NE2	50:1:817:A:OP1	2.43	0.50
17:p:65:ARG:HG2	17:p:129:TYR:CE1	2.47	0.50
29:3:10:C:O2'	29:3:13:A:N1	2.43	0.50
50:1:85:A:N6	50:1:100:A:OP2	2.44	0.50
5:J:208:SER:OG	5:J:209:ASN:N	2.45	0.49
15:O:19:ARG:HB3	15:O:35:ILE:HD12	1.94	0.49
22:T:5:ARG:NH1	50:1:1471:U:OP1	2.45	0.49
23:U:137:ARG:NH2	50:1:1214:U:OP2	2.41	0.49
24:V:66:ASN:ND2	39:d:34:GLY:O	2.45	0.49
29:3:77:G:O2'	29:3:78:U:OP2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:4:110:C:O2'	31:4:112:U:OP2	2.30	0.49
44:G:240:PRO:HB2	50:1:1383:G:H4'	1.94	0.49
50:1:1255:C:H2'	50:1:1256:G:C8	2.47	0.49
50:1:2141:U:O2'	50:1:2976:A:O2'	2.26	0.49
28:x:66:LYS:HB2	28:x:69:LEU:HD13	1.93	0.49
32:Z:108:LEU:HG	32:Z:127:THR:HG22	1.94	0.49
42:F:76:VAL:HG12	42:F:325:LYS:HA	1.94	0.49
42:F:161:LEU:HA	42:F:179:ALA:O	2.12	0.49
43:f:10:ARG:HH11	43:f:44:MET:HE1	1.77	0.49
50:1:3322:A:H2'	50:1:3323:A:C8	2.47	0.49
7:K:72:PRO:HG3	17:p:18:VAL:HA	1.94	0.49
9:7:44:THR:OG1	50:1:3186:A:N3	2.44	0.49
24:V:119:ALA:HA	24:V:122:GLN:HB3	1.94	0.49
25:W:59:ASP:HB3	25:W:62:VAL:H	1.77	0.49
28:x:23:MET:HG3	28:x:34:LEU:HB2	1.94	0.49
42:F:65:SER:OG	42:F:66:LYS:N	2.45	0.49
50:1:67:A:N6	50:1:271:C:O2'	2.45	0.49
50:1:1157:G:O2'	50:1:1169:A:N3	2.43	0.49
50:1:1235:U:H4'	50:1:1236:G:H5'	1.94	0.49
50:1:2213:A:H2'	50:1:2214:A:C8	2.48	0.49
1:A:423:ARG:NH2	1:A:577:LYS:O	2.46	0.49
38:D:36:ARG:HG2	38:D:45:LYS:HG2	1.94	0.49
42:F:284:ARG:HB2	42:F:323:MET:HB3	1.94	0.49
44:G:334:PHE:HA	44:G:339:LEU:HD12	1.93	0.49
1:A:213:LEU:O	1:A:234:ARG:NH1	2.45	0.49
1:A:379:SER:OG	1:A:380:PHE:N	2.45	0.49
2:R:439:LEU:HG	2:R:474:MET:HB2	1.94	0.49
19:5:132:ALA:HB3	50:1:879:U:H4'	1.94	0.49
39:d:29:TYR:OH	50:1:723:U:O2'	2.27	0.49
50:1:1447:G:N2	50:1:2356:A:OP2	2.42	0.49
50:1:1534:A:H1'	50:1:1797:A:H2	1.77	0.49
1:A:398:ILE:HA	1:A:450:GLY:HA3	1.94	0.49
28:x:23:MET:HE3	28:x:36:ILE:HD11	1.95	0.49
47:h:9:VAL:HG22	48:I:171:PRO:HG2	1.94	0.49
49:L:103:LEU:HG	49:L:128:LEU:HD22	1.94	0.49
50:1:296:A:N3	50:1:299:G:O2'	2.44	0.49
50:1:1239:C:N4	50:1:1244:A:O2'	2.45	0.49
50:1:2618:G:H8	50:1:2865:U:H5''	1.77	0.49
1:A:551:ILE:HG23	1:A:574:LEU:HD11	1.95	0.49
1:A:575:LEU:HD23	1:A:578:ILE:HD11	1.95	0.49
35:b:59:ALA:O	35:b:62:VAL:HB	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:G:3:ARG:HB3	44:G:22:LEU:H	1.77	0.49
1:A:209:ILE:HD12	1:A:241:LEU:HD13	1.95	0.49
2:R:212:ASN:ND2	2:R:365:GLU:OE2	2.46	0.49
11:M:137:ARG:NH2	29:3:44:C:OP2	2.45	0.49
50:1:155:G:H5''	50:1:156:G:H2'	1.95	0.49
1:A:489:SER:HB2	1:A:533:GLN:HG3	1.94	0.49
6:j:7:TYR:OH	31:4:87:G:OP2	2.23	0.49
42:F:104:THR:HG1	50:1:3147:G:HO2'	1.54	0.49
1:A:540:ASP:HA	1:A:568:VAL:HB	1.95	0.49
10:l:16:HIS:NE2	50:1:815:G:OP1	2.37	0.49
17:p:38:ARG:NH1	31:4:142:C:OP1	2.46	0.49
20:S:39:ARG:NH1	50:1:1348:U:OP2	2.46	0.49
21:s:169:LYS:HB3	21:s:176:ASP:HA	1.95	0.49
29:3:27:A:H2'	29:3:28:C:H6	1.77	0.49
42:F:169:THR:HG22	42:F:171:LEU:H	1.77	0.49
44:G:206:LEU:HB2	44:G:246:ARG:HE	1.78	0.49
50:1:279:U:O2	50:1:287:G:C6	2.65	0.49
50:1:1392:G:O2'	50:1:1418:A:N6	2.45	0.49
50:1:1929:G:H4'	50:1:2321:A:H5''	1.95	0.49
17:p:46:ASP:OD1	17:p:46:ASP:N	2.44	0.48
34:B:13:U:O2	34:B:22:G:O6	2.30	0.48
37:c:26:ARG:HH12	50:1:938:C:H3'	1.76	0.48
40:E:79:ASN:ND2	40:E:166:ILE:O	2.45	0.48
45:g:3:SER:HA	45:g:90:LYS:HB3	1.95	0.48
50:1:1816:A:O2'	50:1:1817:G:O5'	2.31	0.48
1:A:112:LEU:HD23	1:A:294:ILE:HB	1.95	0.48
2:R:191:ILE:HG13	2:R:208:LYS:HG2	1.94	0.48
4:i:52:GLN:NE2	50:1:1638:A:O2'	2.47	0.48
10:l:58:THR:HG22	50:1:24:G:H5''	1.94	0.48
21:s:146:VAL:O	21:s:150:GLY:N	2.46	0.48
29:3:45:A:OP1	46:H:151:GLN:NE2	2.36	0.48
48:I:78:ARG:HB2	50:1:3272:C:H5'	1.96	0.48
50:1:1236:G:N1	50:1:1244:A:OP2	2.46	0.48
7:K:240:ASN:ND2	50:1:2584:G:O2'	2.47	0.48
21:s:113:GLY:HA2	50:1:2864:A:H5''	1.94	0.48
25:W:74:LYS:NZ	50:1:1678:G:O6	2.45	0.48
41:e:16:LEU:HD23	41:e:98:SER:HB2	1.96	0.48
50:1:28:C:O2'	50:1:61:A:N3	2.41	0.48
7:K:47:SER:OG	50:1:2585:G:O6	2.29	0.48
10:l:63:ARG:NH2	31:4:58:G:O6	2.45	0.48
21:s:173:THR:OG1	21:s:174:ASN:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:8:GLN:HG2	23:U:62:ASN:HB2	1.95	0.48
24:V:127:GLN:OE1	50:1:1095:U:N3	2.38	0.48
32:Z:86:VAL:HG21	32:Z:95:ILE:HG12	1.95	0.48
41:e:10:ILE:HD12	41:e:13:LYS:HD2	1.94	0.48
50:1:52:A:N3	50:1:811:U:O2'	2.47	0.48
50:1:1024:G:N2	50:1:1027:A:OP2	2.40	0.48
50:1:3141:A:OP1	50:1:3142:A:O2'	2.31	0.48
50:1:3258:U:O2'	50:1:3260:G:OP1	2.24	0.48
34:B:15:G:O6	34:B:48:C:O2	2.31	0.48
40:E:209:HIS:CD2	40:E:211:HIS:H	2.31	0.48
45:g:25:TYR:OH	50:1:2361:A:O2'	2.30	0.48
45:g:125:ARG:NH2	50:1:1393:A:OP1	2.44	0.48
49:L:18:LYS:NZ	49:L:24:LYS:O	2.46	0.48
1:A:108:ARG:HD2	1:A:291:THR:HG21	1.95	0.48
6:j:118:ILE:HG12	13:N:123:ILE:HG22	1.94	0.48
28:x:10:LYS:NZ	28:x:54:LEU:O	2.38	0.48
34:B:3:G:O6	34:B:70:U:O4	2.32	0.48
42:F:2:SER:HB3	50:1:2943:G:C8	2.49	0.48
42:F:163:HIS:ND1	42:F:164:THR:O	2.40	0.48
50:1:122:A:N6	50:1:148:G:O2'	2.46	0.48
50:1:1740:U:H1'	50:1:1741:A:H2	1.79	0.48
50:1:1956:A:H2'	50:1:1957:G:C8	2.49	0.48
2:R:480:GLN:HG3	2:R:511:LEU:HD13	1.96	0.48
44:G:283:THR:HB	44:G:289:ILE:HD11	1.96	0.48
50:1:1194:G:H2'	50:1:1195:A:C8	2.49	0.48
50:1:1433:A:O2'	50:1:1434:G:O4'	2.32	0.48
50:1:1717:U:H2'	50:1:1718:G:H8	1.78	0.48
50:1:2892:A:N3	50:1:3129:A:O2'	2.45	0.48
50:1:3233:C:H2'	50:1:3234:A:C8	2.48	0.48
11:M:57:PHE:HB2	11:M:59:ILE:HG12	1.95	0.48
21:s:17:PRO:O	21:s:22:ASN:ND2	2.41	0.48
31:4:83:C:O2'	31:4:85:G:N2	2.36	0.48
40:E:221:LYS:NZ	50:1:2965:U:O2	2.44	0.48
50:1:1203:A:H2'	50:1:1204:A:H8	1.79	0.48
50:1:2677:G:O6	50:1:2680:A:N7	2.47	0.48
18:Q:98:ALA:HA	18:Q:101:ARG:HH11	1.79	0.48
20:S:179:ARG:NH2	50:1:709:A:OP1	2.43	0.48
24:V:44:ALA:H	24:V:58:GLN:HE22	1.62	0.48
25:W:20:SER:HB3	25:W:61:THR:HA	1.95	0.48
42:F:41:VAL:HG22	42:F:185:GLY:HA3	1.94	0.48
44:G:61:SER:O	44:G:61:SER:OG	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:G:82:THR:OG1	50:1:364:G:O2'	2.28	0.48
47:h:14:LEU:HD11	47:h:31:LYS:HB2	1.96	0.48
50:1:627:U:H2'	50:1:628:A:C8	2.48	0.48
50:1:3060:C:O2	50:1:3332:U:O2'	2.32	0.48
13:N:35:ARG:HH22	50:1:684:G:H5''	1.77	0.48
42:F:334:ARG:NH2	50:1:3305:A:OP1	2.46	0.48
50:1:1539:A:N7	50:1:1553:U:O2	2.47	0.48
50:1:2007:G:H1	50:1:2014:U:H3	1.61	0.48
1:A:478:LEU:HB2	1:A:509:GLN:HB3	1.95	0.47
3:X:4:ARG:NE	3:X:210:THR:O	2.42	0.47
13:N:174:ARG:NH1	50:1:712:G:OP1	2.47	0.47
19:5:108:ASP:N	19:5:152:GLU:OE2	2.45	0.47
21:s:53:SER:HA	21:s:162:GLN:HB2	1.95	0.47
29:3:28:C:OP2	46:H:57:ASN:ND2	2.48	0.47
29:3:81:U:O2'	50:1:1055:A:N3	2.43	0.47
44:G:322:GLN:HE22	50:1:598:A:H1'	1.78	0.47
50:1:649:A:OP2	50:1:2868:U:O2'	2.30	0.47
50:1:655:C:H2'	50:1:656:A:H8	1.78	0.47
50:1:2945:G:O2'	50:1:2948:C:OP2	2.25	0.47
2:R:97:LEU:HD21	3:X:139:ARG:HD3	1.96	0.47
2:R:490:LEU:HD23	2:R:494:ILE:HD12	1.96	0.47
11:M:21:ILE:HD11	11:M:125:MET:HE2	1.95	0.47
11:M:133:ARG:NH1	11:M:153:LYS:O	2.45	0.47
21:s:56:LEU:HB2	21:s:130:ILE:HG13	1.96	0.47
32:Z:86:VAL:O	32:Z:120:LYS:HB3	2.13	0.47
44:G:219:LEU:HD22	44:G:225:VAL:HG11	1.95	0.47
47:h:21:ARG:O	50:1:633:C:O2'	2.26	0.47
50:1:900:G:N3	50:1:1589:A:N6	2.63	0.47
50:1:1203:A:H2'	50:1:1204:A:C8	2.49	0.47
50:1:1381:A:H2'	50:1:1382:G:H8	1.79	0.47
50:1:2385:G:O2'	50:1:2386:A:O5'	2.29	0.47
50:1:2668:U:H2'	50:1:2669:G:H8	1.78	0.47
50:1:3015:G:H2'	50:1:3016:A:H8	1.79	0.47
1:A:153:SER:O	1:A:157:TYR:CB	2.58	0.47
31:4:9:A:H2'	31:4:10:A:C8	2.50	0.47
46:H:173:VAL:O	46:H:175:HIS:ND1	2.34	0.47
46:H:211:LEU:HB3	46:H:219:PHE:HB2	1.95	0.47
48:I:46:ARG:NH2	50:1:3218:A:OP1	2.35	0.47
49:L:122:ARG:NH1	50:1:2483:G:OP2	2.47	0.47
50:1:536:U:H3	50:1:557:A:H62	1.61	0.47
50:1:1149:G:H21	50:1:1199:C:H42	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:LYS:HE3	1:A:480:PHE:HA	1.96	0.47
9:7:18:VAL:HG21	9:7:53:ILE:HD11	1.95	0.47
9:7:77:ASN:HB3	9:7:151:VAL:HG21	1.97	0.47
29:3:85:G:O2'	29:3:87:G:OP1	2.28	0.47
34:B:62:C:H2'	34:B:63:G:H8	1.79	0.47
40:E:117:GLU:OE1	40:E:121:GLY:N	2.40	0.47
42:F:57:VAL:HB	42:F:358:TRP:HB3	1.97	0.47
44:G:202:ARG:HH21	50:1:1385:C:H41	1.63	0.47
44:G:338:LYS:O	44:G:340:GLY:N	2.47	0.47
48:I:154:LEU:O	48:I:158:TYR:N	2.48	0.47
50:1:2526:C:H2'	50:1:2527:G:H8	1.79	0.47
18:Q:181:ALA:HA	18:Q:184:THR:HG22	1.97	0.47
22:T:79:GLY:N	50:1:1938:U:O2'	2.47	0.47
27:r:30:VAL:HB	27:r:33:VAL:HG21	1.96	0.47
29:3:4:U:H2'	29:3:5:G:C8	2.49	0.47
32:Z:103:TYR:HB3	32:Z:135:ILE:HD11	1.96	0.47
50:1:1549:U:H2'	50:1:1550:C:H6	1.80	0.47
50:1:1940:G:H21	50:1:3362:A:H8	1.62	0.47
30:Y:17:ARG:NH1	42:F:368:GLY:O	2.47	0.47
19:5:36:ILE:HD12	19:5:48:LEU:HD11	1.97	0.47
29:3:61:G:H5''	46:H:276:LYS:HA	1.96	0.47
31:4:72:A:OP2	33:a:52:ARG:NH2	2.48	0.47
40:E:14:SER:OG	40:E:15:ILE:N	2.46	0.47
40:E:211:HIS:NE2	40:E:235:ALA:O	2.47	0.47
46:H:58:LYS:HA	46:H:93:THR:HG21	1.97	0.47
50:1:218:G:H1'	50:1:372:A:H1'	1.96	0.47
50:1:1250:G:H2'	50:1:1251:A:C8	2.50	0.47
50:1:1945:A:H2'	50:1:1946:A:C8	2.50	0.47
5:J:186:HIS:O	5:J:190:THR:OG1	2.26	0.47
12:m:46:ARG:HH11	12:m:51:LEU:HB2	1.80	0.47
13:N:36:ARG:O	13:N:40:ALA:N	2.48	0.47
46:H:107:ARG:HG3	46:H:251:PRO:HG3	1.96	0.47
2:R:283:HIS:C	2:R:283:HIS:ND1	2.72	0.47
2:R:344:ARG:HH11	2:R:346:ARG:HG3	1.79	0.47
5:J:128:LYS:HE3	29:3:99:G:H4'	1.96	0.47
5:J:224:ILE:HA	23:U:36:ILE:HG12	1.96	0.47
40:E:3:ARG:HD3	50:1:911:C:H42	1.79	0.47
42:F:21:ARG:HB3	42:F:272:TYR:HD2	1.80	0.47
46:H:261:THR:OG1	46:H:264:GLN:OE1	2.26	0.47
50:1:332:C:H2'	50:1:333:G:H8	1.80	0.47
2:R:193:PHE:O	2:R:203:VAL:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:p:112:ASN:N	17:p:112:ASN:OD1	2.41	0.47
20:S:32:LEU:HD12	44:G:286:VAL:HG13	1.95	0.47
22:T:88:ARG:NH1	50:1:1864:A:OP1	2.48	0.47
34:B:76:A:N1	50:1:2819:A:O2'	2.41	0.46
42:F:14:LEU:O	50:1:3009:G:O2'	2.28	0.46
44:G:204:GLY:O	44:G:246:ARG:NH2	2.48	0.46
50:1:1965:C:O2	50:1:2059:U:O2'	2.30	0.46
6:j:31:LEU:O	6:j:35:LYS:HB2	2.14	0.46
40:E:241:ARG:NH1	50:1:2155:G:OP1	2.49	0.46
50:1:881:C:O2'	50:1:1850:A:OP1	2.31	0.46
1:A:395:PHE:HE1	1:A:452:VAL:HG23	1.80	0.46
5:J:168:ILE:O	5:J:172:ASN:ND2	2.48	0.46
16:o:122:ARG:NH2	50:1:2896:A:O2'	2.49	0.46
17:p:179:LYS:O	50:1:286:U:O2'	2.33	0.46
43:f:47:ASP:HB2	43:f:87:ASN:HD21	1.80	0.46
44:G:5:GLN:HE22	44:G:21:PRO:HG3	1.80	0.46
50:1:2223:A:H2'	50:1:2224:A:C8	2.51	0.46
50:1:2468:A:N1	50:1:2477:G:O2'	2.47	0.46
50:1:2618:G:O2'	50:1:2866:U:OP2	2.29	0.46
1:A:280:SER:HB3	1:A:286:LEU:HD13	1.97	0.46
15:O:125:LYS:HA	15:O:128:ARG:HG2	1.96	0.46
20:S:39:ARG:HH12	44:G:302:ALA:HA	1.79	0.46
47:h:86:ARG:NH2	50:1:623:U:O2'	2.49	0.46
50:1:528:U:H2'	50:1:529:A:C8	2.50	0.46
14:n:5:LYS:HD2	14:n:13:MET:HE1	1.97	0.46
19:5:56:ARG:HH11	19:5:76:PHE:HZ	1.62	0.46
23:U:77:VAL:HA	23:U:125:LYS:O	2.16	0.46
34:B:9:G:O2'	34:B:10:G:N7	2.48	0.46
50:1:1411:C:H2'	50:1:1412:G:H8	1.80	0.46
50:1:1596:C:OP2	50:1:1606:U:N3	2.49	0.46
50:1:2007:G:N2	50:1:2014:U:O2	2.41	0.46
2:R:502:ASN:OD1	2:R:506:ARG:N	2.46	0.46
3:X:51:THR:HG21	3:X:84:LEU:HD21	1.98	0.46
10:l:81:GLY:O	31:4:95:G:O2'	2.32	0.46
20:S:171:LYS:NZ	50:1:89:A:N7	2.64	0.46
35:b:54:THR:HG22	35:b:57:HIS:CD2	2.51	0.46
40:E:136:ILE:HA	40:E:148:VAL:HG12	1.97	0.46
50:1:1129:A:H61	50:1:2864:A:H1'	1.81	0.46
50:1:1626:U:H3	50:1:1818:U:H3	1.64	0.46
50:1:2697:A:H2'	50:1:2698:G:C8	2.51	0.46
50:1:3162:C:H2'	50:1:3163:A:H8	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:LEU:HD22	1:A:249:LEU:HD13	1.97	0.46
2:R:285:TYR:CD2	34:B:72:C:H5''	2.50	0.46
3:X:8:GLU:HB3	50:1:3018:C:H5''	1.97	0.46
11:M:96:PHE:HB2	11:M:156:LYS:HE3	1.97	0.46
17:p:93:LYS:O	50:1:289:A:O2'	2.24	0.46
28:x:18:PRO:HD2	50:1:1898:G:H1'	1.98	0.46
40:E:79:ASN:HD21	40:E:165:VAL:HG13	1.80	0.46
40:E:181:LYS:NZ	50:1:860:G:OP2	2.39	0.46
46:H:146:LEU:HD11	46:H:163:LEU:HD12	1.98	0.46
50:1:1446:A:H5'	50:1:1448:U:H1'	1.97	0.46
50:1:2449:A:H61	50:1:2497:U:H3	1.62	0.46
1:A:245:PRO:O	1:A:274:ARG:NH2	2.49	0.46
6:j:86:ARG:N	31:4:36:G:OP2	2.40	0.46
9:7:89:LYS:HB2	9:7:183:HIS:HB3	1.97	0.46
28:x:12:ARG:HB2	50:1:3040:A:H5''	1.98	0.46
35:b:23:VAL:HG12	35:b:45:GLY:HA3	1.97	0.46
42:F:314:TYR:HD1	42:F:333:LYS:HG2	1.80	0.46
44:G:344:ALA:HB2	50:1:516:A:H5''	1.97	0.46
46:H:12:TYR:OH	50:1:2688:U:OP1	2.34	0.46
50:1:3353:G:O2'	50:1:3356:G:OP2	2.33	0.46
17:p:44:ARG:NH1	50:1:269:G:OP2	2.48	0.46
21:s:98:ILE:HD12	21:s:100:LYS:HG3	1.96	0.46
21:s:152:ARG:NH1	50:1:1206:G:OP1	2.48	0.46
42:F:67:PHE:HD1	42:F:70:ARG:HD2	1.80	0.46
42:F:77:THR:HG21	42:F:328:ILE:HG22	1.98	0.46
47:h:21:ARG:NH1	50:1:1151:U:OP1	2.43	0.46
49:L:130:LYS:HG3	49:L:137:PRO:HD3	1.98	0.46
50:1:616:G:H2'	50:1:617:G:H8	1.81	0.46
50:1:1101:G:H2'	50:1:1102:A:H8	1.81	0.46
50:1:1131:G:O2'	50:1:2373:A:N1	2.45	0.46
1:A:423:ARG:H	1:A:580:GLN:HB2	1.80	0.46
1:A:584:VAL:HB	1:A:591:THR:HB	1.98	0.46
5:J:129:LEU:HD11	50:1:986:U:H5'	1.98	0.46
13:N:157:ARG:NH2	37:c:146:GLU:OE1	2.49	0.46
17:p:78:GLY:HA2	17:p:89:VAL:HG21	1.97	0.46
37:c:64:GLN:HE22	50:1:70:A:H5'	1.81	0.46
46:H:119:TYR:OH	46:H:139:PRO:O	2.31	0.46
47:h:72:THR:HG22	50:1:585:A:H4'	1.98	0.46
1:A:210:LEU:HB3	1:A:216:ASN:HB3	1.98	0.45
17:p:94:TYR:CZ	17:p:96:ARG:HB2	2.51	0.45
21:s:189:VAL:HG13	21:s:196:VAL:HG11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Y:6:ASP:HB3	30:Y:10:GLY:H	1.80	0.45
42:F:216:ASP:OD2	42:F:339:ARG:NH2	2.35	0.45
2:R:245:HIS:CE1	2:R:283:HIS:CG	3.03	0.45
2:R:285:TYR:HD2	34:B:72:C:C6	2.35	0.45
5:J:156:ILE:HD11	5:J:168:ILE:HG23	1.97	0.45
20:S:86:THR:HG22	20:S:105:ARG:HB2	1.97	0.45
24:V:17:ARG:HG2	24:V:22:HIS:HA	1.97	0.45
31:4:71:A:N6	31:4:87:G:O2'	2.50	0.45
31:4:115:C:P	50:1:1830:G:H22	2.39	0.45
44:G:306:THR:HG1	50:1:1359:C:HO2'	1.63	0.45
50:1:1024:G:O2'	50:1:1026:A:N6	2.48	0.45
50:1:1071:U:H2'	50:1:1072:G:H8	1.80	0.45
1:A:227:MET:HA	1:A:231:TRP:HE3	1.80	0.45
50:1:1243:G:O6	50:1:1248:C:N4	2.50	0.45
20:S:185:LYS:HG2	20:S:186:VAL:HG23	1.98	0.45
28:x:104:ASN:OD1	28:x:108:GLU:N	2.42	0.45
31:4:22:U:OP1	33:a:12:ARG:NH2	2.40	0.45
42:F:31:ALA:O	42:F:339:ARG:NH1	2.50	0.45
50:1:1018:G:H2'	50:1:1019:G:H8	1.81	0.45
50:1:1260:A:H2'	50:1:1261:G:C4	2.51	0.45
50:1:2538:U:O2'	50:1:2541:U:O4	2.33	0.45
50:1:3190:C:H2'	50:1:3191:G:C8	2.52	0.45
14:n:9:ILE:HD12	14:n:51:ILE:HG21	1.98	0.45
15:O:20:VAL:O	15:O:66:THR:OG1	2.28	0.45
17:p:49:ARG:HH12	50:1:149:U:P	2.39	0.45
27:r:25:LEU:HD11	27:r:86:PHE:HD1	1.81	0.45
42:F:100:ARG:NH2	50:1:3244:A:OP2	2.47	0.45
50:1:373:A:C6	50:1:375:A:N6	2.84	0.45
50:1:1144:U:H6	50:1:1144:U:H2'	1.58	0.45
50:1:3346:U:H2'	50:1:3347:A:H8	1.81	0.45
3:X:150:SER:OG	28:x:131:SER:O	2.34	0.45
22:T:25:ASP:N	22:T:25:ASP:OD1	2.48	0.45
28:x:21:ALA:HB3	28:x:36:ILE:HD12	1.99	0.45
50:1:2457:G:O2'	50:1:2481:G:N2	2.49	0.45
50:1:2697:A:H2'	50:1:2698:G:H8	1.82	0.45
50:1:3231:U:O4	50:1:3256:G:O6	2.35	0.45
1:A:455:HIS:HB3	1:A:458:VAL:HG23	1.97	0.45
2:R:378:THR:H	2:R:381:GLU:HB3	1.82	0.45
13:N:70:ARG:NH2	50:1:75:G:O3'	2.50	0.45
19:5:24:VAL:HG22	19:5:90:PHE:HD2	1.82	0.45
40:E:244:GLY:HA3	50:1:2242:A:H5''	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:F:95:THR:OG1	42:F:98:GLY:O	2.26	0.45
50:1:2281:A:O2'	50:1:2973:G:N2	2.40	0.45
50:1:2631:U:OP1	50:1:2757:U:O2'	2.29	0.45
1:A:304:TYR:HB2	1:A:311:TYR:HD1	1.81	0.45
11:M:110:ILE:HG21	11:M:116:TYR:HA	1.98	0.45
42:F:258:ALA:O	50:1:2394:G:N2	2.25	0.45
44:G:191:LYS:NZ	50:1:1379:G:O2'	2.45	0.45
50:1:36:C:O2'	50:1:808:A:N1	2.45	0.45
50:1:411:U:H2'	50:1:412:G:H8	1.82	0.45
50:1:1303:A:O2'	50:1:1304:A:O4'	2.30	0.45
50:1:2655:U:H1'	50:1:2656:A:C2	2.52	0.45
50:1:2842:U:OP1	50:1:2844:C:N4	2.48	0.45
1:A:237:LEU:HD13	1:A:265:LEU:HD21	1.99	0.45
3:X:102:SER:OG	3:X:103:ALA:N	2.50	0.45
3:X:146:ILE:HG13	3:X:147:LEU:HD12	1.99	0.45
42:F:92:TYR:OH	42:F:180:GLU:OE1	2.33	0.45
45:g:76:VAL:HG11	45:g:82:LEU:HD12	1.98	0.45
50:1:2157:G:N2	50:1:2178:A:OP2	2.47	0.45
9:7:152:GLU:O	9:7:156:GLN:HB2	2.16	0.45
11:M:23:VAL:HG12	11:M:25:GLU:H	1.82	0.45
50:1:2428:U:H2'	50:1:2429:G:C8	2.52	0.45
6:j:44:ILE:HA	6:j:47:VAL:HG12	1.99	0.44
6:j:86:ARG:NH2	50:1:20:A:OP2	2.50	0.44
14:n:43:ASN:HD22	14:n:46:ARG:NH1	2.15	0.44
16:o:120:GLN:NE2	50:1:2836:C:OP1	2.50	0.44
27:r:56:ASN:N	50:1:1282:G:OP1	2.37	0.44
33:a:62:SER:N	50:1:218:G:O6	2.40	0.44
46:H:52:VAL:HA	46:H:147:ASP:HB3	1.99	0.44
49:L:90:LEU:HD22	49:L:115:VAL:HG21	1.97	0.44
50:1:359:U:H4'	50:1:817:A:H62	1.82	0.44
50:1:679:U:O2'	50:1:788:C:O2	2.36	0.44
50:1:1277:C:H2'	50:1:1278:A:H8	1.81	0.44
3:X:11:ASN:HB3	3:X:207:GLY:HA3	1.99	0.44
17:p:187:ARG:HH21	17:p:188:ARG:HE	1.65	0.44
50:1:19:U:H2'	50:1:20:A:C8	2.53	0.44
50:1:792:G:H2'	50:1:793:C:H6	1.81	0.44
50:1:2312:A:O2'	50:1:2315:G:N3	2.47	0.44
1:A:345:THR:HG1	21:s:109:ARG:NH1	2.11	0.44
4:i:83:ASN:O	4:i:86:LYS:HB3	2.17	0.44
11:M:109:HIS:CD2	11:M:123:PHE:H	2.35	0.44
19:5:118:GLN:OE1	50:1:412:G:N2	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:128:LYS:NZ	50:1:1723:A:OP1	2.51	0.44
44:G:261:VAL:O	44:G:270:SER:OG	2.35	0.44
47:h:82:ARG:NH2	50:1:1328:C:OP1	2.51	0.44
50:1:2448:G:H2'	50:1:2449:A:C8	2.52	0.44
50:1:2660:G:OP1	50:1:2750:U:O2'	2.36	0.44
5:J:144:ILE:HD12	5:J:189:ILE:HD12	1.99	0.44
9:7:87:LYS:HA	9:7:146:LEU:O	2.18	0.44
17:p:155:VAL:HG12	50:1:58:G:H4'	1.99	0.44
22:T:46:LYS:NZ	50:1:1765:U:O4	2.43	0.44
37:c:4:ARG:HH22	50:1:1426:C:P	2.41	0.44
37:c:7:LYS:O	37:c:11:HIS:ND1	2.50	0.44
46:H:175:HIS:HA	50:1:2747:A:H5'	1.99	0.44
49:L:210:MET:SD	50:1:2489:C:O2'	2.74	0.44
50:1:1580:A:O2'	50:1:1581:C:O5'	2.32	0.44
50:1:2219:A:H2'	50:1:2220:A:C8	2.53	0.44
50:1:2526:C:H2'	50:1:2527:G:C8	2.53	0.44
1:A:539:LEU:HD12	1:A:567:VAL:HG22	2.00	0.44
21:s:47:LEU:HD21	21:s:144:LYS:HD3	1.99	0.44
29:3:11:A:N6	46:H:13:SER:O	2.48	0.44
43:f:44:MET:O	43:f:77:ARG:NH1	2.51	0.44
50:1:129:U:O2	50:1:139:G:N2	2.42	0.44
50:1:985:U:H2'	50:1:986:U:H6	1.82	0.44
50:1:1529:A:H5'	50:1:1588:A:H1'	1.98	0.44
50:1:2886:U:H2'	50:1:2911:A:H62	1.83	0.44
1:A:267:GLU:HG2	1:A:271:ARG:HH12	1.83	0.44
4:i:97:GLU:O	4:i:100:ILE:HB	2.17	0.44
11:M:99:THR:O	11:M:154:THR:OG1	2.27	0.44
18:Q:34:VAL:HA	18:Q:103:LYS:O	2.17	0.44
20:S:39:ARG:HB3	44:G:299:ILE:HG23	1.99	0.44
42:F:33:PRO:HA	42:F:342:LEU:HD23	2.00	0.44
42:F:297:SER:HA	42:F:300:ARG:HE	1.83	0.44
50:1:68:C:N4	50:1:314:U:O2'	2.50	0.44
50:1:952:A:OP2	50:1:1143:A:N6	2.36	0.44
50:1:994:G:H2'	50:1:1053:A:H61	1.82	0.44
50:1:1982:G:N2	50:1:2040:U:H3	2.15	0.44
50:1:3047:U:O4	50:1:3094:A:C6	2.70	0.44
1:A:455:HIS:HE1	1:A:457:HIS:HD2	1.65	0.44
1:A:479:GLU:HA	1:A:482:ARG:HG2	1.99	0.44
2:R:488:LEU:O	2:R:492:SER:OG	2.32	0.44
3:X:118:HIS:HD1	3:X:120:ASP:H	1.65	0.44
5:J:225:GLN:NE2	29:3:97:A:O4'	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:143:ILE:HD11	7:K:151:VAL:HG21	1.98	0.44
17:p:178:HIS:O	17:p:181:ASN:ND2	2.51	0.44
28:x:13:ILE:HD12	28:x:54:LEU:HB3	1.99	0.44
41:e:74:ASN:N	41:e:74:ASN:OD1	2.49	0.44
49:L:18:LYS:HZ2	49:L:24:LYS:HB3	1.81	0.44
49:L:35:GLN:HG3	49:L:169:VAL:HG22	1.99	0.44
50:1:2234:G:O2'	50:1:2603:G:O2'	2.29	0.44
50:1:2999:U:H2'	50:1:3000:A:C8	2.53	0.44
2:R:240:MET:HE1	2:R:374:THR:HB	2.00	0.44
13:N:156:ALA:HB1	37:c:98:THR:HA	2.00	0.44
18:Q:22:VAL:HG21	18:Q:120:VAL:HG11	1.99	0.44
22:T:106:LEU:HB3	22:T:120:TYR:HE1	1.83	0.44
29:3:27:A:H2'	29:3:28:C:C6	2.53	0.44
29:3:36:C:H2'	29:3:37:G:C8	2.53	0.44
33:a:39:LEU:HD22	33:a:43:TYR:HE2	1.82	0.44
40:E:101:VAL:HA	40:E:165:VAL:HA	2.00	0.44
50:1:306:A:N6	50:1:2784:G:C2	2.86	0.44
50:1:737:G:H2'	50:1:738:A:H8	1.83	0.44
50:1:2565:U:O2	50:1:2576:G:N2	2.44	0.44
9:7:173:ARG:NH1	50:1:2899:C:N3	2.45	0.44
15:O:88:ALA:O	15:O:93:LYS:NZ	2.42	0.44
17:p:31:ARG:HH21	50:1:2516:U:H5'	1.83	0.44
20:S:148:GLU:N	50:1:787:G:OP1	2.51	0.44
27:r:5:ARG:NH2	50:1:1219:C:OP2	2.47	0.44
36:C:10:THR:OG1	36:C:11:TYR:N	2.51	0.44
50:1:425:G:H2'	50:1:426:G:H8	1.83	0.44
50:1:707:U:O2'	50:1:754:G:N3	2.51	0.44
50:1:829:U:O4	50:1:894:G:N2	2.51	0.44
50:1:1018:G:H2'	50:1:1019:G:C8	2.53	0.44
50:1:1615:C:H2'	50:1:1616:U:C6	2.53	0.44
50:1:1886:A:H1'	50:1:3307:A:H5'	1.99	0.44
50:1:2049:A:H8	50:1:2050:C:H4'	1.82	0.44
4:i:42:PRO:HB2	4:i:51:LEU:HD11	2.00	0.43
34:B:68:C:H2'	34:B:69:G:C8	2.52	0.43
36:C:60:LYS:NZ	50:1:2797:C:N3	2.64	0.43
37:c:74:ASN:ND2	37:c:113:LEU:O	2.43	0.43
39:d:6:ASN:N	50:1:1135:A:OP1	2.42	0.43
50:1:122:A:O2'	50:1:123:A:O5'	2.34	0.43
50:1:158:G:H2'	50:1:159:A:H8	1.83	0.43
50:1:170:G:O6	50:1:248:U:O4	2.35	0.43
50:1:429:U:H2'	50:1:430:U:H6	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:1:792:G:H2'	50:1:793:C:C6	2.53	0.43
50:1:1351:U:H2'	50:1:1352:A:H2'	1.99	0.43
50:1:2433:U:H3'	50:1:2434:U:H2'	2.00	0.43
50:1:2899:C:O2'	50:1:2901:G:OP2	2.27	0.43
50:1:3086:A:O2'	50:1:3330:A:O2'	2.33	0.43
1:A:112:LEU:HB2	1:A:279:VAL:HG22	2.00	0.43
10:l:24:ARG:NH2	50:1:362:U:O4	2.51	0.43
20:S:176:ARG:HG3	20:S:183:GLY:HA3	2.00	0.43
23:U:12:ARG:HD3	23:U:59:VAL:HG22	1.99	0.43
40:E:218:HIS:HE1	50:1:2966:G:H5'	1.82	0.43
40:E:223:SER:OG	50:1:2244:A:O2'	2.33	0.43
50:1:638:C:N4	50:1:639:G:O6	2.51	0.43
50:1:1342:C:H2'	50:1:1343:A:C8	2.54	0.43
50:1:3222:U:H3	50:1:3263:G:H1	1.65	0.43
6:j:85:THR:HG23	6:j:88:LEU:H	1.84	0.43
9:7:94:TYR:OH	9:7:141:LYS:NZ	2.51	0.43
18:Q:49:ARG:HH22	50:1:1193:A:H8	1.66	0.43
21:s:137:VAL:HG21	21:s:147:VAL:HB	2.00	0.43
24:V:6:GLY:H	24:V:9:SER:HB2	1.83	0.43
35:b:34:LYS:NZ	50:1:1967:U:OP2	2.50	0.43
43:f:31:ARG:NH2	50:1:1884:A:OP1	2.31	0.43
48:I:49:GLY:O	48:I:163:PHE:N	2.43	0.43
50:1:340:C:O2'	50:1:344:A:N3	2.42	0.43
50:1:531:G:H2'	50:1:532:A:C8	2.53	0.43
15:O:50:LYS:HD3	15:O:85:TRP:HD1	1.82	0.43
21:s:93:PHE:HD2	50:1:1045:C:H1'	1.83	0.43
42:F:332:ARG:H	42:F:332:ARG:HG2	1.64	0.43
45:g:73:THR:OG1	45:g:95:GLU:OE1	2.37	0.43
50:1:1209:G:H2'	50:1:1210:U:C6	2.53	0.43
50:1:2397:A:H8	50:1:2941:A:N1	2.16	0.43
50:1:3051:U:H2'	50:1:3052:G:H8	1.82	0.43
3:X:106:ASN:ND2	28:x:131:SER:O	2.51	0.43
18:Q:133:ARG:NE	50:1:1316:C:OP2	2.51	0.43
21:s:48:CYS:SG	21:s:49:VAL:N	2.92	0.43
31:4:9:A:H2'	31:4:10:A:H8	1.84	0.43
40:E:9:ARG:NH1	50:1:912:G:OP2	2.52	0.43
42:F:47:LEU:HD23	42:F:335:ILE:HD11	2.00	0.43
50:1:504:A:H2'	50:1:505:G:C8	2.53	0.43
50:1:1977:C:N3	50:1:2046:U:O2'	2.49	0.43
15:O:50:LYS:HD3	15:O:85:TRP:CD1	2.54	0.43
41:e:25:LEU:HD22	41:e:87:VAL:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:f:24:SER:OG	50:1:2345:A:OP1	2.35	0.43
50:1:209:A:H4'	50:1:211:A:N7	2.34	0.43
50:1:636:C:O2	50:1:2375:G:N2	2.37	0.43
50:1:754:G:H2'	50:1:755:A:H8	1.83	0.43
50:1:2213:A:H2'	50:1:2214:A:H8	1.84	0.43
50:1:2428:U:H2'	50:1:2429:G:H8	1.83	0.43
2:R:276:PHE:HE2	2:R:379:VAL:HG13	1.82	0.43
7:K:152:LEU:HB2	7:K:198:ALA:HB3	2.01	0.43
17:p:75:VAL:HA	17:p:76:PRO:HD3	1.85	0.43
19:5:116:HIS:O	19:5:148:LEU:HA	2.18	0.43
27:r:56:ASN:HB3	27:r:80:VAL:HG22	1.99	0.43
34:B:62:C:H2'	34:B:63:G:C8	2.54	0.43
37:c:77:LYS:O	37:c:79:TRP:N	2.51	0.43
42:F:54:THR:OG1	42:F:360:ASP:O	2.31	0.43
50:1:411:U:H2'	50:1:412:G:C8	2.53	0.43
50:1:843:A:H2'	50:1:844:G:C8	2.54	0.43
50:1:908:G:N3	50:1:925:A:N6	2.66	0.43
50:1:1149:G:H21	50:1:1199:C:N4	2.16	0.43
50:1:1981:G:N2	50:1:2042:G:H22	2.17	0.43
50:1:2323:G:O2'	50:1:2325:G:OP2	2.31	0.43
50:1:2510:U:H2'	50:1:2511:A:C8	2.53	0.43
10:l:54:LYS:O	10:l:58:THR:N	2.52	0.43
23:U:24:LEU:HD22	23:U:59:VAL:HG21	2.00	0.43
29:3:4:U:H2'	29:3:5:G:H8	1.83	0.43
38:D:16:VAL:HA	50:1:1927:G:C8	2.53	0.43
38:D:22:LEU:HD21	50:1:2150:G:H4'	2.01	0.43
42:F:296:THR:H	42:F:299:ASP:HB3	1.83	0.43
43:f:19:ARG:NH1	50:1:3324:C:OP1	2.43	0.43
46:H:83:LEU:HB3	46:H:88:ILE:HB	2.01	0.43
50:1:707:U:H1'	50:1:754:G:H1'	2.00	0.43
9:7:152:GLU:O	9:7:156:GLN:CB	2.66	0.43
11:M:53:THR:HG23	11:M:60:ARG:HA	2.01	0.43
31:4:28:C:O2'	50:1:691:A:N6	2.52	0.43
34:B:55:U:O2'	34:B:57:G:N7	2.36	0.43
38:D:29:LEU:HD23	38:D:29:LEU:HA	1.89	0.43
40:E:134:VAL:HG12	40:E:150:LEU:HA	2.00	0.43
49:L:25:LYS:NZ	49:L:173:GLU:OE2	2.51	0.43
50:1:2744:U:H2'	50:1:2745:G:C8	2.53	0.43
1:A:393:LEU:HD13	1:A:441:MET:HE3	2.00	0.43
5:J:118:LYS:HB2	5:J:195:PHE:CE2	2.54	0.43
9:7:164:ILE:HD12	9:7:164:ILE:HA	1.93	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:l:60:GLY:HA2	10:l:64:MET:HE2	2.01	0.43
21:s:48:CYS:HA	21:s:138:ARG:HA	2.01	0.43
22:T:38:ARG:HG3	50:1:1602:A:H5''	2.00	0.43
37:c:26:ARG:NH1	50:1:939:U:OP2	2.43	0.43
45:g:37:GLY:O	45:g:43:ARG:NE	2.52	0.43
50:1:999:G:H2'	50:1:1000:C:C6	2.54	0.43
50:1:1132:C:H2'	50:1:1133:A:H8	1.84	0.43
50:1:1216:C:H2'	50:1:1217:A:C8	2.53	0.43
50:1:3231:U:O2	50:1:3256:G:N2	2.35	0.43
50:1:3375:A:O2'	50:1:3376:A:O4'	2.33	0.43
1:A:104:LEU:HB3	1:A:275:THR:HG21	2.00	0.42
1:A:403:GLU:HB2	1:A:408:GLU:H	1.84	0.42
3:X:140:GLN:HG2	3:X:173:LEU:HD21	2.01	0.42
14:n:2:ALA:HB2	50:1:1493:G:O6	2.19	0.42
17:p:56:LYS:NZ	50:1:150:A:OP1	2.47	0.42
17:p:190:THR:HA	17:p:193:ARG:HG2	2.01	0.42
18:Q:39:GLU:OE1	18:Q:107:GLY:N	2.50	0.42
29:3:11:A:N1	29:3:67:G:O2'	2.42	0.42
31:4:40:A:OP2	31:4:103:G:N1	2.46	0.42
31:4:67:U:H2'	31:4:68:G:H8	1.84	0.42
32:Z:45:LYS:NZ	50:1:129:U:OP1	2.52	0.42
35:b:5:LEU:HD11	41:e:35:ARG:HD2	2.01	0.42
38:D:79:VAL:HG22	40:E:112:ILE:HD13	2.00	0.42
50:1:1621:A:H2'	50:1:1622:U:C6	2.54	0.42
50:1:2085:U:H2'	50:1:2086:A:H8	1.83	0.42
29:3:81:U:H2'	29:3:82:G:H8	1.84	0.42
40:E:236:GLY:O	50:1:2183:A:O2'	2.28	0.42
42:F:279:ASN:OD1	42:F:345:ASN:ND2	2.52	0.42
44:G:122:THR:HG22	44:G:235:LEU:HB2	2.01	0.42
50:1:354:U:H2'	50:1:355:A:H8	1.84	0.42
50:1:616:G:H2'	50:1:617:G:C8	2.54	0.42
50:1:1663:C:H2'	50:1:1664:G:H8	1.84	0.42
7:K:81:THR:HG21	7:K:181:LYS:HD2	2.01	0.42
13:N:2:ALA:HB3	37:c:41:HIS:CE1	2.54	0.42
23:U:13:ARG:HG2	23:U:51:VAL:HG21	2.01	0.42
29:3:19:C:H2'	29:3:20:A:C8	2.52	0.42
38:D:80:ARG:O	38:D:84:ARG:N	2.44	0.42
41:e:30:THR:O	41:e:34:LEU:HB2	2.19	0.42
42:F:14:LEU:HA	42:F:17:LEU:HD13	2.01	0.42
50:1:708:G:N2	50:1:711:A:OP2	2.46	0.42
50:1:1015:U:H3	50:1:1035:G:H22	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:1:1863:G:N1	50:1:1866:C:OP2	2.50	0.42
50:1:2403:G:H21	50:1:2404:A:H2	1.66	0.42
50:1:2923:U:H2'	50:1:2924:U:H6	1.84	0.42
2:R:74:CYS:SG	2:R:77:CYS:CB	3.08	0.42
5:J:93:ASN:OD1	5:J:93:ASN:N	2.49	0.42
17:p:55:ALA:HB3	50:1:148:G:H5''	2.00	0.42
31:4:53:A:H2'	31:4:54:A:H8	1.84	0.42
33:a:97:ILE:HD13	33:a:97:ILE:HA	1.89	0.42
40:E:8:GLN:HA	50:1:2163:C:H4'	2.01	0.42
50:1:129:U:H2'	50:1:130:A:C8	2.55	0.42
50:1:3295:A:H2'	50:1:3296:A:C8	2.53	0.42
1:A:537:LEU:HB2	1:A:565:VAL:HG23	2.00	0.42
2:R:101:LYS:NZ	3:X:120:ASP:OD1	2.45	0.42
10:l:76:ASN:ND2	31:4:95:G:OP1	2.45	0.42
32:Z:108:LEU:HB3	32:Z:109:LYS:H	1.64	0.42
40:E:126:LEU:HD13	40:E:150:LEU:HD21	2.00	0.42
42:F:75:ALA:HB2	50:1:3049:A:C6	2.54	0.42
42:F:98:GLY:HA3	50:1:3005:A:H5'	2.01	0.42
48:I:35:VAL:O	48:I:38:THR:OG1	2.25	0.42
50:1:1015:U:O4	50:1:1035:G:N1	2.35	0.42
50:1:2344:U:H1'	50:1:3079:U:H3	1.84	0.42
50:1:3332:U:H2'	50:1:3333:G:O4'	2.19	0.42
7:K:75:ILE:HG22	7:K:76:ALA:H	1.85	0.42
7:K:165:PHE:HZ	17:p:3:ALA:HB1	1.84	0.42
13:N:19:GLN:HE22	50:1:801:A:H61	1.67	0.42
19:5:50:GLN:HB3	19:5:55:GLN:HB3	2.01	0.42
19:5:172:GLN:NE2	47:h:61:GLY:O	2.51	0.42
28:x:53:SER:OG	28:x:56:ASP:OD2	2.36	0.42
34:B:26:G:H1	34:B:44:A:H2	1.66	0.42
44:G:269:SER:OG	44:G:271:LYS:O	2.28	0.42
47:h:52:VAL:HG22	47:h:66:VAL:HG22	2.01	0.42
50:1:250:U:OP2	50:1:251:G:O2'	2.34	0.42
50:1:540:U:H2'	50:1:541:U:C6	2.55	0.42
50:1:1336:U:H2'	50:1:1337:A:C8	2.55	0.42
50:1:1549:U:H2'	50:1:1550:C:C6	2.54	0.42
4:i:86:LYS:O	4:i:90:ILE:HG12	2.20	0.42
24:V:102:ARG:HD2	24:V:102:ARG:HA	1.89	0.42
41:e:25:LEU:O	41:e:29:SER:OG	2.38	0.42
42:F:95:THR:HG22	50:1:3243:A:H5'	2.00	0.42
50:1:631:U:H2'	50:1:632:G:C8	2.54	0.42
50:1:797:U:H2'	50:1:798:G:H8	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:89:ASP:OD1	20:S:90:ASP:N	2.52	0.42
38:D:26:VAL:HG21	40:E:180:LEU:HD11	2.01	0.42
38:D:78:THR:O	38:D:81:SER:OG	2.26	0.42
40:E:234:LYS:NZ	50:1:2162:U:OP1	2.46	0.42
50:1:147:U:O2'	50:1:148:G:OP1	2.36	0.42
50:1:2502:A:H2'	50:1:2503:G:C8	2.55	0.42
2:R:284:ARG:HH12	34:B:1:G:C1'	2.33	0.42
5:J:219:LYS:O	5:J:228:SER:N	2.50	0.42
29:3:79:A:H62	29:3:101:G:H21	1.68	0.42
31:4:43:A:H2'	31:4:44:A:C8	2.55	0.42
35:b:62:VAL:O	35:b:65:ARG:HB2	2.20	0.42
40:E:190:ARG:HG3	40:E:191:LEU:HD12	2.01	0.42
50:1:528:U:H2'	50:1:529:A:H8	1.85	0.42
50:1:797:U:H2'	50:1:798:G:C8	2.55	0.42
50:1:2597:U:H2'	50:1:2598:G:H8	1.84	0.42
5:J:120:THR:HB	24:V:132:PRO:HB2	2.02	0.42
7:K:78:PHE:HD1	7:K:179:ILE:HD13	1.85	0.42
21:s:153:ARG:NH1	50:1:2837:A:O3'	2.53	0.42
29:3:11:A:O2'	29:3:13:A:OP2	2.29	0.42
34:B:63:G:H2'	34:B:64:G:C8	2.55	0.42
37:c:74:ASN:HD21	50:1:705:A:H62	1.67	0.42
41:e:30:THR:HG21	41:e:89:VAL:HG22	2.02	0.42
50:1:656:A:H2'	50:1:657:A:C8	2.55	0.42
50:1:1786:G:H2'	50:1:1787:A:C8	2.55	0.42
21:s:107:ALA:C	21:s:109:ARG:N	2.78	0.41
21:s:175:LEU:HD21	21:s:183:LYS:HD2	2.02	0.41
28:x:32:ARG:HB2	28:x:64:LYS:HB2	2.02	0.41
28:x:39:VAL:HG22	28:x:58:VAL:HG12	2.02	0.41
42:F:306:THR:O	42:F:361:THR:OG1	2.38	0.41
47:h:19:SER:OG	50:1:1330:A:OP1	2.27	0.41
50:1:307:A:H2'	50:1:308:A:C8	2.55	0.41
50:1:627:U:H2'	50:1:628:A:H8	1.85	0.41
50:1:1956:A:H2'	50:1:1957:G:H8	1.84	0.41
50:1:1982:G:H2'	50:1:1983:G:C8	2.55	0.41
50:1:3334:U:O2	50:1:3368:U:O2'	2.31	0.41
2:R:314:ARG:NH1	50:1:2861:U:O2'	2.51	0.41
3:X:162:HIS:HE1	3:X:164:GLN:HB2	1.85	0.41
8:k:11:LEU:HD11	13:N:180:ARG:HH11	1.84	0.41
20:S:127:LEU:O	20:S:131:ALA:N	2.53	0.41
21:s:35:LEU:HD23	21:s:68:ARG:HH11	1.85	0.41
34:B:51:C:H2'	34:B:52:G:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:L:103:LEU:HD11	49:L:128:LEU:HB3	2.01	0.41
49:L:167:VAL:HG22	49:L:184:LEU:HD13	2.01	0.41
50:1:160:G:O6	50:1:261:U:O4	2.38	0.41
50:1:237:G:H2'	50:1:238:A:H8	1.85	0.41
50:1:1709:C:H2'	50:1:1710:C:H6	1.85	0.41
50:1:3015:G:H2'	50:1:3016:A:C8	2.55	0.41
50:1:3157:U:H4'	50:1:3158:G:C8	2.55	0.41
50:1:3291:G:H2'	50:1:3292:A:C8	2.55	0.41
1:A:470:GLN:HE21	1:A:473:LEU:HD23	1.85	0.41
2:R:74:CYS:SG	2:R:77:CYS:SG	3.18	0.41
2:R:439:LEU:HD11	2:R:490:LEU:HD11	2.02	0.41
2:R:511:LEU:O	2:R:515:ASP:HB2	2.20	0.41
3:X:22:THR:HG23	3:X:67:ARG:HG3	2.01	0.41
16:o:104:PRO:HG2	50:1:3119:U:H4'	2.02	0.41
19:5:34:GLN:HE22	19:5:37:ASN:HD22	1.69	0.41
20:S:152:HIS:ND1	20:S:162:ALA:O	2.54	0.41
22:T:84:THR:HG22	50:1:1915:A:H5''	2.02	0.41
23:U:93:GLU:OE2	23:U:136:LYS:N	2.53	0.41
28:x:81:GLN:HG2	28:x:83:LYS:H	1.86	0.41
33:a:82:VAL:HB	33:a:85:VAL:HB	2.02	0.41
38:D:22:LEU:HD22	40:E:178:PRO:HB3	2.02	0.41
39:d:47:LEU:HA	39:d:50:THR:HG22	2.01	0.41
42:F:112:ASP:HA	42:F:115:LYS:HB2	2.02	0.41
44:G:283:THR:HG22	44:G:285:ASP:H	1.85	0.41
50:1:540:U:H2'	50:1:541:U:H6	1.86	0.41
50:1:3216:G:H22	50:1:3258:U:H5''	1.84	0.41
1:A:215:PHE:HA	1:A:219:THR:HB	2.01	0.41
4:i:37:LYS:NZ	50:1:1592:G:OP2	2.46	0.41
9:7:20:ILE:HD13	15:O:7:VAL:HG22	2.02	0.41
9:7:73:SER:O	9:7:77:ASN:ND2	2.53	0.41
12:m:4:GLU:OE1	50:1:1746:U:O2'	2.38	0.41
13:N:170:LEU:O	13:N:173:ALA:HB3	2.21	0.41
37:c:115:LYS:HG3	50:1:715:A:H3'	2.02	0.41
49:L:169:VAL:HB	49:L:172:VAL:HG23	2.02	0.41
50:1:261:U:H2'	50:1:262:U:C6	2.55	0.41
50:1:500:C:H2'	50:1:501:A:H8	1.84	0.41
50:1:513:G:H2'	50:1:514:G:H8	1.84	0.41
50:1:1497:C:H2'	50:1:1498:A:C8	2.55	0.41
1:A:231:TRP:CD1	1:A:234:ARG:HH21	2.39	0.41
9:7:8:GLN:HB2	9:7:55:VAL:HG22	2.03	0.41
13:N:27:ASP:HB3	31:4:29:U:H5''	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:124:ARG:NH1	50:1:3214:U:O4	2.54	0.41
17:p:120:TRP:HZ2	17:p:123:GLN:HG2	1.84	0.41
31:4:135:G:OP1	32:Z:49:LYS:NZ	2.47	0.41
37:c:21:ARG:HB2	50:1:1369:A:H4'	2.02	0.41
49:L:153:SER:OG	49:L:154:THR:N	2.53	0.41
50:1:504:A:H2'	50:1:505:G:H8	1.86	0.41
50:1:1144:U:OP1	50:1:1367:G:O2'	2.37	0.41
50:1:3153:U:O4	50:1:3293:U:N3	2.54	0.41
5:J:160:ARG:HD2	5:J:203:TRP:CE2	2.55	0.41
17:p:133:ILE:HD13	17:p:133:ILE:HG21	1.90	0.41
42:F:56:ILE:HD13	42:F:56:ILE:HA	1.88	0.41
50:1:65:A:H5''	50:1:66:A:H4'	2.03	0.41
50:1:1269:U:H1'	50:1:1272:C:H5	1.86	0.41
50:1:1497:C:H2'	50:1:1498:A:H8	1.85	0.41
50:1:1627:U:O2'	50:1:1630:U:O2'	2.33	0.41
50:1:2668:U:H2'	50:1:2669:G:C8	2.54	0.41
15:O:23:ILE:HA	15:O:63:VAL:HG23	2.01	0.41
21:s:84:PHE:HA	21:s:139:THR:HG22	2.03	0.41
23:U:112:ALA:HB2	50:1:1321:G:N2	2.36	0.41
24:V:75:ILE:HG22	24:V:88:ARG:HG2	2.02	0.41
25:W:33:TYR:HE2	25:W:63:VAL:HG11	1.85	0.41
30:Y:56:ARG:HB3	30:Y:61:LYS:HB2	2.02	0.41
35:b:33:SER:OG	35:b:34:LYS:N	2.54	0.41
42:F:306:THR:HG21	42:F:316:GLU:HG2	2.03	0.41
46:H:95:TRP:CD1	46:H:158:ARG:HA	2.55	0.41
48:I:108:LYS:HE2	50:1:3271:G:C8	2.56	0.41
50:1:966:U:H2'	50:1:967:A:C8	2.55	0.41
50:1:1381:A:H2'	50:1:1382:G:C8	2.56	0.41
17:p:71:ARG:NH2	50:1:32:U:O3'	2.53	0.41
29:3:114:U:H2'	29:3:115:G:H8	1.86	0.41
30:Y:6:ASP:OD1	30:Y:32:GLN:N	2.54	0.41
31:4:16:G:N2	50:1:406:G:H2'	2.36	0.41
31:4:151:C:H5	32:Z:24:LEU:HD11	1.85	0.41
34:B:51:C:H2'	34:B:52:G:H8	1.85	0.41
40:E:206:PRO:HG3	40:E:213:GLY:HA3	2.01	0.41
42:F:178:LEU:HD23	50:1:3002:C:H5'	2.03	0.41
50:1:1216:C:H2'	50:1:1217:A:H8	1.85	0.41
50:1:1284:C:H2'	50:1:1285:G:C4	2.56	0.41
50:1:1792:C:O2'	50:1:1794:G:OP1	2.30	0.41
1:A:207:ALA:HA	1:A:210:LEU:HD12	2.03	0.41
1:A:409:ASN:HB2	1:A:588:LYS:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:321:LYS:HG3	2:R:353:ILE:HG12	2.03	0.41
4:i:66:SER:OG	4:i:67:LYS:N	2.54	0.41
5:J:236:ILE:HD12	5:J:236:ILE:HA	1.95	0.41
8:k:76:ARG:O	50:1:293:C:O2'	2.34	0.41
13:N:27:ASP:OD1	13:N:27:ASP:N	2.49	0.41
15:O:60:LEU:HD23	15:O:60:LEU:HA	1.95	0.41
19:5:127:ARG:O	19:5:139:TYR:N	2.50	0.41
22:T:78:TYR:O	50:1:1914:G:N2	2.51	0.41
22:T:81:ARG:HH11	22:T:81:ARG:HD3	1.72	0.41
24:V:88:ARG:O	50:1:2722:U:O2'	2.29	0.41
42:F:56:ILE:HD11	42:F:323:MET:HE2	2.03	0.41
42:F:250:ALA:HB1	50:1:2947:G:N3	2.35	0.41
43:f:16:LEU:N	43:f:69:TYR:O	2.48	0.41
46:H:23:ARG:HA	46:H:23:ARG:HD2	1.87	0.41
49:L:119:GLN:HB3	49:L:123:LEU:HD12	2.03	0.41
50:1:1660:C:H2'	50:1:1661:G:C8	2.55	0.41
50:1:2371:G:N2	50:1:2375:G:OP1	2.48	0.41
50:1:2376:G:H2'	50:1:2377:G:C8	2.56	0.41
50:1:3255:U:H2'	50:1:3256:G:C8	2.53	0.41
1:A:292:ASN:HA	1:A:305:GLY:HA2	2.03	0.41
21:s:103:SER:O	21:s:104:CYS:SG	2.79	0.41
32:Z:37:THR:OG1	32:Z:38:LEU:N	2.54	0.41
36:C:35:LEU:HD23	36:C:40:LYS:HG2	2.03	0.41
48:I:40:LEU:HD13	48:I:84:VAL:HG11	2.02	0.41
50:1:1461:A:H2'	50:1:1462:A:H8	1.85	0.41
50:1:1915:A:H2'	50:1:1916:U:C6	2.56	0.41
50:1:2273:G:N2	50:1:2312:A:OP2	2.47	0.41
50:1:2464:U:H2'	50:1:2465:G:H8	1.86	0.41
3:X:199:VAL:HG23	3:X:204:ALA:HB2	2.04	0.40
7:K:137:ASN:HD21	17:p:4:TYR:HE2	1.68	0.40
7:K:185:ARG:CZ	31:4:155:A:H4'	2.50	0.40
31:4:58:G:O2'	31:4:59:A:O5'	2.36	0.40
43:f:72:ARG:HG3	43:f:98:VAL:HG11	2.02	0.40
50:1:201:A:H2'	50:1:202:G:H8	1.84	0.40
50:1:835:G:H2'	50:1:857:G:N2	2.36	0.40
50:1:1362:G:H2'	50:1:1363:A:C8	2.56	0.40
1:A:520:GLN:HG2	1:A:523:ARG:HH21	1.86	0.40
18:Q:22:VAL:HG11	18:Q:122:GLN:HE21	1.86	0.40
50:1:1058:U:H2'	50:1:1059:G:H8	1.85	0.40
50:1:1604:G:H4'	50:1:1835:A:H4'	2.03	0.40
50:1:1660:C:H2'	50:1:1661:G:H8	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:1:1920:U:O2'	50:1:1932:A:N7	2.52	0.40
50:1:2158:A:H1'	50:1:2160:G:C8	2.56	0.40
50:1:2467:G:N1	50:1:2487:U:OP1	2.44	0.40
5:J:214:TRP:NE1	50:1:1168:U:O2'	2.38	0.40
10:l:12:HIS:O	10:l:12:HIS:ND1	2.53	0.40
17:p:89:VAL:HB	50:1:2424:A:H5'	2.03	0.40
27:r:18:TYR:HD1	27:r:22:TYR:HE2	1.69	0.40
31:4:118:C:H2'	31:4:119:C:H6	1.86	0.40
43:f:77:ARG:HG2	43:f:89:LEU:HD23	2.03	0.40
46:H:48:LYS:HE2	46:H:48:LYS:HB2	1.90	0.40
50:1:136:G:H2'	50:1:137:G:H8	1.86	0.40
50:1:189:G:O2'	50:1:190:U:OP1	2.38	0.40
50:1:842:G:H2'	50:1:843:A:H8	1.86	0.40
50:1:1455:U:OP1	50:1:1879:A:N6	2.54	0.40
4:i:20:ILE:HD11	4:i:34:HIS:CE1	2.57	0.40
5:J:121:LYS:HB2	24:V:133:ALA:HB3	2.03	0.40
8:k:57:LEU:HD23	8:k:57:LEU:HA	1.95	0.40
21:s:103:SER:O	21:s:104:CYS:CB	2.70	0.40
23:U:80:ARG:HB3	23:U:122:HIS:HB2	2.03	0.40
31:4:17:A:N6	50:1:406:G:H1'	2.35	0.40
40:E:204:MET:SD	40:E:209:HIS:HB2	2.62	0.40
47:h:35:VAL:HG11	47:h:41:ALA:HB2	2.04	0.40
50:1:203:G:H2'	50:1:204:A:H8	1.85	0.40
50:1:1900:A:O2'	50:1:1902:G:N7	2.52	0.40
50:1:2129:U:H2'	50:1:2130:G:C8	2.56	0.40
17:p:172:ARG:HG2	50:1:30:G:H5'	2.03	0.40
25:W:97:SER:OG	25:W:98:THR:N	2.55	0.40
33:a:59:VAL:HG13	33:a:60:ARG:HG2	2.03	0.40
35:b:26:VAL:HG21	35:b:96:VAL:HB	2.04	0.40
43:f:72:ARG:HB3	43:f:96:VAL:HG23	2.04	0.40
44:G:315:LYS:HG2	50:1:505:G:H5'	2.04	0.40
50:1:1009:A:H2'	50:1:1010:G:C8	2.57	0.40
50:1:1342:C:H2'	50:1:1343:A:H8	1.84	0.40
50:1:1724:U:H1'	50:1:1725:C:C6	2.57	0.40
50:1:1945:A:H2'	50:1:1946:A:H8	1.86	0.40
50:1:2516:U:H3	50:1:2591:A:H2	1.69	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	
1	A	438/519 (84%)	411 (94%)	27 (6%)	0	100	100
2	R	300/433 (69%)	286 (95%)	14 (5%)	0	100	100
3	X	222/224 (99%)	206 (93%)	16 (7%)	0	100	100
4	i	110/112 (98%)	104 (94%)	6 (6%)	0	100	100
5	J	220/222 (99%)	205 (93%)	13 (6%)	2 (1%)	14	46
6	j	117/119 (98%)	110 (94%)	4 (3%)	3 (3%)	4	27
7	K	231/233 (99%)	211 (91%)	19 (8%)	1 (0%)	30	61
8	k	97/99 (98%)	87 (90%)	10 (10%)	0	100	100
9	7	189/191 (99%)	176 (93%)	13 (7%)	0	100	100
10	l	85/87 (98%)	75 (88%)	10 (12%)	0	100	100
11	M	167/169 (99%)	148 (89%)	19 (11%)	0	100	100
12	m	75/77 (97%)	71 (95%)	4 (5%)	0	100	100
13	N	191/193 (99%)	171 (90%)	16 (8%)	4 (2%)	5	31
14	n	48/50 (96%)	43 (90%)	5 (10%)	0	100	100
15	O	134/136 (98%)	119 (89%)	15 (11%)	0	100	100
16	o	50/52 (96%)	47 (94%)	3 (6%)	0	100	100
17	p	201/203 (99%)	179 (89%)	19 (10%)	3 (2%)	8	37
18	Q	195/197 (99%)	187 (96%)	8 (4%)	0	100	100
19	5	181/183 (99%)	164 (91%)	17 (9%)	0	100	100
20	S	183/185 (99%)	169 (92%)	14 (8%)	0	100	100
21	s	218/220 (99%)	187 (86%)	26 (12%)	5 (2%)	5	30
22	T	150/152 (99%)	142 (95%)	7 (5%)	1 (1%)	18	51
23	U	170/172 (99%)	156 (92%)	13 (8%)	1 (1%)	21	54
24	V	157/159 (99%)	144 (92%)	13 (8%)	0	100	100
25	W	98/100 (98%)	91 (93%)	7 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	P	144/155 (93%)	122 (85%)	22 (15%)	0	100	100
27	r	117/197 (59%)	110 (94%)	7 (6%)	0	100	100
28	x	134/136 (98%)	128 (96%)	6 (4%)	0	100	100
30	Y	60/62 (97%)	56 (93%)	4 (7%)	0	100	100
32	Z	119/121 (98%)	109 (92%)	10 (8%)	0	100	100
33	a	124/126 (98%)	116 (94%)	8 (6%)	0	100	100
35	b	133/135 (98%)	117 (88%)	15 (11%)	1 (1%)	16	49
36	C	103/105 (98%)	92 (89%)	11 (11%)	0	100	100
37	c	146/148 (99%)	129 (88%)	14 (10%)	3 (2%)	5	31
38	D	89/91 (98%)	81 (91%)	8 (9%)	0	100	100
39	d	56/58 (97%)	49 (88%)	6 (11%)	1 (2%)	6	34
40	E	250/252 (99%)	223 (89%)	27 (11%)	0	100	100
41	e	95/97 (98%)	91 (96%)	4 (4%)	0	100	100
42	F	384/386 (100%)	349 (91%)	34 (9%)	1 (0%)	36	65
43	f	107/109 (98%)	97 (91%)	10 (9%)	0	100	100
44	G	359/361 (99%)	324 (90%)	34 (10%)	1 (0%)	36	65
45	g	125/127 (98%)	119 (95%)	6 (5%)	0	100	100
46	H	294/296 (99%)	271 (92%)	23 (8%)	0	100	100
47	h	104/106 (98%)	97 (93%)	7 (7%)	0	100	100
48	I	152/175 (87%)	143 (94%)	9 (6%)	0	100	100
49	L	202/204 (99%)	165 (82%)	37 (18%)	0	100	100
All	All	7524/7934 (95%)	6877 (91%)	620 (8%)	27 (0%)	31	61

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	s	104	CYS
21	s	106	GLY
37	c	47	LYS
44	G	339	LEU
5	J	158	LYS
6	j	85	THR
21	s	107	ALA
21	s	109	ARG
22	T	131	ALA

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Mol	Chain	Res	Type
6	j	90	ARG
13	N	62	THR
13	N	166	ALA
23	U	13	ARG
35	b	102	GLU
37	c	78	LEU
5	J	233	GLU
7	K	157	VAL
17	p	146	ALA
21	s	108	ASP
37	c	40	HIS
6	j	91	ALA
13	N	48	PRO
13	N	61	PRO
17	p	74	PRO
42	F	188	ILE
17	p	75	VAL
39	d	21	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	386/456 (85%)	385 (100%)	1 (0%)	86	83
2	R	288/349 (82%)	286 (99%)	2 (1%)	76	78
3	X	177/192 (92%)	177 (100%)	0	100	100
4	i	95/95 (100%)	94 (99%)	1 (1%)	65	74
5	J	186/186 (100%)	186 (100%)	0	100	100
6	j	104/104 (100%)	104 (100%)	0	100	100
7	K	187/191 (98%)	186 (100%)	1 (0%)	81	80
8	k	81/81 (100%)	81 (100%)	0	100	100
9	7	171/171 (100%)	169 (99%)	2 (1%)	63	73
10	l	70/70 (100%)	70 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	M	147/147 (100%)	146 (99%)	1 (1%)	76	78
12	m	68/68 (100%)	68 (100%)	0	100	100
13	N	154/154 (100%)	154 (100%)	0	100	100
14	n	45/45 (100%)	45 (100%)	0	100	100
15	O	107/107 (100%)	107 (100%)	0	100	100
16	o	47/47 (100%)	47 (100%)	0	100	100
17	p	175/175 (100%)	172 (98%)	3 (2%)	53	69
18	Q	160/160 (100%)	158 (99%)	2 (1%)	61	72
19	5	140/145 (97%)	138 (99%)	2 (1%)	59	71
20	S	150/150 (100%)	150 (100%)	0	100	100
21	s	184/186 (99%)	182 (99%)	2 (1%)	65	74
22	T	126/126 (100%)	125 (99%)	1 (1%)	73	77
23	U	156/156 (100%)	155 (99%)	1 (1%)	78	79
24	V	136/136 (100%)	136 (100%)	0	100	100
25	W	87/87 (100%)	87 (100%)	0	100	100
27	r	105/166 (63%)	105 (100%)	0	100	100
28	x	104/104 (100%)	103 (99%)	1 (1%)	68	75
30	Y	54/54 (100%)	54 (100%)	0	100	100
32	Z	104/105 (99%)	104 (100%)	0	100	100
33	a	109/109 (100%)	108 (99%)	1 (1%)	70	76
35	b	115/115 (100%)	115 (100%)	0	100	100
36	C	90/90 (100%)	90 (100%)	0	100	100
37	c	118/118 (100%)	117 (99%)	1 (1%)	73	77
38	D	71/71 (100%)	71 (100%)	0	100	100
39	d	46/46 (100%)	46 (100%)	0	100	100
40	E	193/194 (100%)	189 (98%)	4 (2%)	47	65
41	e	81/81 (100%)	81 (100%)	0	100	100
42	F	319/322 (99%)	315 (99%)	4 (1%)	61	72
43	f	92/96 (96%)	92 (100%)	0	100	100
44	G	288/288 (100%)	288 (100%)	0	100	100
45	g	109/109 (100%)	109 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	H	244/244 (100%)	243 (100%)	1 (0%)	84	81
47	h	90/90 (100%)	90 (100%)	0	100	100
48	I	134/152 (88%)	134 (100%)	0	100	100
49	L	185/185 (100%)	184 (100%)	1 (0%)	81	80
All	All	6278/6523 (96%)	6246 (100%)	32 (0%)	78	80

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	359	ILE
2	R	212	ASN
2	R	285	TYR
4	i	51	LEU
7	K	157	VAL
9	7	68	LEU
9	7	132	VAL
11	M	84	LEU
17	p	64	VAL
17	p	142	ILE
17	p	193	ARG
18	Q	34	VAL
18	Q	84	LEU
19	5	24	VAL
19	5	120	ASN
21	s	103	SER
21	s	138	ARG
22	T	104	ARG
23	U	100	VAL
28	x	93	LEU
33	a	80	VAL
37	c	56	VAL
40	E	45	VAL
40	E	101	VAL
40	E	202	VAL
40	E	230	VAL
42	F	73	VAL
42	F	79	VAL
42	F	104	THR
42	F	324	VAL
46	H	64	ILE
49	L	108	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (108) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	256	HIS
1	A	348	ASN
1	A	352	GLN
1	A	384	GLN
1	A	401	HIS
1	A	413	HIS
1	A	457	HIS
1	A	465	GLN
1	A	535	ASN
1	A	562	ASN
1	A	580	GLN
2	R	29	ASN
2	R	212	ASN
2	R	283	HIS
2	R	316	ASN
3	X	11	ASN
3	X	50	HIS
3	X	140	GLN
3	X	145	ASN
4	i	52	GLN
5	J	172	ASN
5	J	186	HIS
6	j	59	ASN
6	j	99	GLN
7	K	77	GLN
7	K	192	GLN
7	K	243	GLN
8	k	100	HIS
9	7	40	HIS
9	7	77	ASN
9	7	125	ASN
10	l	57	HIS
11	M	109	HIS
12	m	10	GLN
13	N	112	ASN
13	N	149	GLN
14	n	19	GLN
15	O	41	GLN
15	O	126	GLN
16	o	90	ASN
17	p	15	GLN

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Mol	Chain	Res	Type
17	p	37	HIS
17	p	95	GLN
17	p	156	HIS
18	Q	193	GLN
19	5	34	GLN
19	5	54	HIS
19	5	72	GLN
19	5	97	ASN
19	5	116	HIS
20	S	5	HIS
21	s	72	ASN
22	T	75	HIS
22	T	92	GLN
22	T	121	HIS
23	U	49	HIS
23	U	74	ASN
23	U	122	HIS
23	U	142	GLN
24	V	5	HIS
24	V	26	HIS
24	V	122	GLN
24	V	131	GLN
25	W	87	ASN
25	W	101	ASN
27	r	32	ASN
27	r	36	GLN
28	x	98	ASN
28	x	132	ASN
30	Y	59	HIS
32	Z	53	HIS
35	b	29	HIS
35	b	57	HIS
35	b	127	ASN
36	C	22	GLN
36	C	102	GLN
37	c	40	HIS
37	c	64	GLN
37	c	74	ASN
40	E	79	ASN
40	E	205	ASN
40	E	209	HIS
40	E	218	HIS

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Mol	Chain	Res	Type
42	F	3	HIS
42	F	109	HIS
42	F	198	HIS
42	F	319	ASN
42	F	345	ASN
43	f	15	ASN
43	f	43	HIS
43	f	57	GLN
43	f	87	ASN
44	G	5	GLN
44	G	114	ASN
44	G	260	GLN
44	G	320	ASN
45	g	20	HIS
45	g	49	ASN
45	g	104	ASN
46	H	63	GLN
47	h	5	HIS
47	h	42	GLN
49	L	21	ASN
49	L	44	GLN
49	L	57	ASN
49	L	96	ASN
49	L	108	ASN
49	L	127	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
29	3	120/121 (99%)	29 (24%)	1 (0%)
31	4	157/158 (99%)	47 (29%)	4 (2%)
34	B	75/76 (98%)	16 (21%)	0
50	1	3312/3316 (99%)	967 (29%)	155 (4%)
All	All	3664/3671 (99%)	1059 (28%)	160 (4%)

All (1059) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
29	3	7	G
29	3	11	A
29	3	13	A

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Mol	Chain	Res	Type
29	3	14	U
29	3	26	C
29	3	41	G
29	3	42	A
29	3	45	A
29	3	48	U
29	3	49	G
29	3	53	U
29	3	55	A
29	3	62	U
29	3	64	A
29	3	65	G
29	3	71	G
29	3	74	C
29	3	77	G
29	3	78	U
29	3	79	A
29	3	86	U
29	3	91	G
29	3	93	C
29	3	95	A
29	3	99	G
29	3	102	A
29	3	104	A
29	3	112	G
29	3	121	U
31	4	2	A
31	4	5	U
31	4	15	G
31	4	16	G
31	4	17	A
31	4	22	U
31	4	23	U
31	4	24	G
31	4	33	A
31	4	34	U
31	4	35	C
31	4	38	U
31	4	39	G
31	4	42	G
31	4	49	G
31	4	51	G

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Mol	Chain	Res	Type
31	4	59	A
31	4	60	U
31	4	63	G
31	4	72	A
31	4	80	A
31	4	81	U
31	4	82	U
31	4	83	C
31	4	85	G
31	4	86	U
31	4	87	G
31	4	90	U
31	4	95	G
31	4	96	A
31	4	99	C
31	4	102	U
31	4	104	A
31	4	106	C
31	4	112	U
31	4	113	U
31	4	116	G
31	4	125	U
31	4	126	A
31	4	129	C
31	4	131	A
31	4	132	G
31	4	148	G
31	4	151	C
31	4	152	G
31	4	155	A
31	4	157	U
34	B	10	G
34	B	16	U
34	B	18	G
34	B	19	G
34	B	28	U
34	B	37	A
34	B	47	U
34	B	48	C
34	B	49	U
34	B	56	C
34	B	58	A

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Mol	Chain	Res	Type
34	B	59	U
34	B	73	G
34	B	74	C
34	B	75	C
34	B	76	A
50	1	14	U
50	1	15	C
50	1	19	U
50	1	26	A
50	1	30	G
50	1	40	A
50	1	44	U
50	1	48	A
50	1	49	A
50	1	57	A
50	1	59	G
50	1	60	A
50	1	65	A
50	1	66	A
50	1	67	A
50	1	74	G
50	1	77	A
50	1	85	A
50	1	86	G
50	1	87	U
50	1	92	G
50	1	94	G
50	1	99	A
50	1	109	A
50	1	110	G
50	1	111	C
50	1	116	A
50	1	117	U
50	1	118	U
50	1	119	U
50	1	121	A
50	1	122	A
50	1	123	A
50	1	124	U
50	1	134	U
50	1	135	C
50	1	136	G

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Mol	Chain	Res	Type
50	1	142	C
50	1	146	U
50	1	147	U
50	1	148	G
50	1	155	G
50	1	156	G
50	1	157	A
50	1	166	C
50	1	169	U
50	1	182	U
50	1	187	A
50	1	188	U
50	1	189	G
50	1	190	U
50	1	191	U
50	1	192	C
50	1	200	C
50	1	206	G
50	1	210	U
50	1	211	A
50	1	212	G
50	1	213	A
50	1	218	G
50	1	219	A
50	1	220	G
50	1	221	A
50	1	222	A
50	1	231	G
50	1	234	G
50	1	240	U
50	1	241	G
50	1	242	C
50	1	251	G
50	1	252	U
50	1	254	A
50	1	263	C
50	1	268	A
50	1	269	G
50	1	270	U
50	1	281	G
50	1	283	G
50	1	286	U

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Mol	Chain	Res	Type
50	1	295	A
50	1	297	G
50	1	298	U
50	1	304	G
50	1	305	U
50	1	306	A
50	1	316	U
50	1	323	A
50	1	329	U
50	1	330	G
50	1	339	C
50	1	340	C
50	1	342	A
50	1	344	A
50	1	349	A
50	1	350	C
50	1	351	A
50	1	353	G
50	1	354	U
50	1	375	A
50	1	376	G
50	1	385	A
50	1	395	A
50	1	397	A
50	1	398	A
50	1	399	A
50	1	401	U
50	1	402	A
50	1	403	C
50	1	404	G
50	1	405	U
50	1	406	G
50	1	421	G
50	1	422	A
50	1	439	C
50	1	495	G
50	1	517	G
50	1	518	G
50	1	520	U
50	1	521	A
50	1	523	A
50	1	535	G

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Mol	Chain	Res	Type
50	1	536	U
50	1	546	C
50	1	547	G
50	1	548	G
50	1	550	A
50	1	552	G
50	1	555	U
50	1	556	U
50	1	558	U
50	1	559	A
50	1	569	A
50	1	578	A
50	1	579	G
50	1	581	U
50	1	589	A
50	1	590	G
50	1	591	G
50	1	592	A
50	1	597	G
50	1	600	G
50	1	604	G
50	1	609	G
50	1	610	G
50	1	611	A
50	1	619	A
50	1	620	U
50	1	621	A
50	1	622	A
50	1	623	U
50	1	637	C
50	1	641	C
50	1	645	A
50	1	646	A
50	1	648	C
50	1	649	A
50	1	660	A
50	1	661	G
50	1	662	U
50	1	667	C
50	1	671	U
50	1	677	A
50	1	678	G

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Mol	Chain	Res	Type
50	1	681	U
50	1	682	U
50	1	683	U
50	1	684	G
50	1	690	A
50	1	691	A
50	1	692	A
50	1	705	A
50	1	708	G
50	1	712	G
50	1	716	A
50	1	719	U
50	1	720	A
50	1	750	G
50	1	758	C
50	1	759	U
50	1	760	G
50	1	764	U
50	1	765	C
50	1	766	U
50	1	767	U
50	1	768	C
50	1	770	G
50	1	776	U
50	1	777	U
50	1	781	G
50	1	784	A
50	1	786	A
50	1	799	G
50	1	801	A
50	1	806	A
50	1	808	A
50	1	815	G
50	1	817	A
50	1	826	G
50	1	830	A
50	1	837	A
50	1	849	C
50	1	851	C
50	1	858	A
50	1	859	G
50	1	860	G

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Mol	Chain	Res	Type
50	1	861	C
50	1	867	G
50	1	871	U
50	1	872	U
50	1	874	U
50	1	879	U
50	1	881	C
50	1	884	A
50	1	885	U
50	1	888	A
50	1	890	C
50	1	894	G
50	1	895	A
50	1	906	A
50	1	907	G
50	1	914	A
50	1	915	A
50	1	916	G
50	1	917	A
50	1	921	A
50	1	923	C
50	1	925	A
50	1	932	U
50	1	933	A
50	1	934	G
50	1	937	G
50	1	939	U
50	1	944	C
50	1	953	G
50	1	959	C
50	1	960	U
50	1	962	A
50	1	963	G
50	1	980	A
50	1	981	U
50	1	982	C
50	1	995	U
50	1	1001	G
50	1	1002	A
50	1	1006	A
50	1	1008	U
50	1	1015	U

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Mol	Chain	Res	Type
50	1	1016	C
50	1	1017	C
50	1	1018	G
50	1	1021	G
50	1	1025	A
50	1	1026	A
50	1	1029	G
50	1	1032	C
50	1	1036	A
50	1	1037	C
50	1	1038	C
50	1	1041	U
50	1	1045	C
50	1	1047	A
50	1	1049	C
50	1	1054	A
50	1	1063	G
50	1	1065	A
50	1	1066	G
50	1	1075	A
50	1	1076	C
50	1	1080	A
50	1	1081	U
50	1	1082	U
50	1	1083	G
50	1	1093	A
50	1	1094	U
50	1	1095	U
50	1	1096	U
50	1	1097	G
50	1	1098	A
50	1	1103	A
50	1	1104	G
50	1	1117	G
50	1	1128	U
50	1	1131	G
50	1	1132	C
50	1	1135	A
50	1	1138	U
50	1	1142	G
50	1	1143	A
50	1	1144	U

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Mol	Chain	Res	Type
50	1	1145	G
50	1	1150	A
50	1	1151	U
50	1	1152	G
50	1	1153	A
50	1	1155	C
50	1	1156	C
50	1	1159	A
50	1	1177	G
50	1	1178	G
50	1	1180	A
50	1	1181	U
50	1	1182	A
50	1	1191	U
50	1	1192	C
50	1	1193	A
50	1	1196	C
50	1	1199	C
50	1	1200	A
50	1	1201	C
50	1	1202	A
50	1	1209	G
50	1	1212	A
50	1	1219	C
50	1	1220	U
50	1	1221	A
50	1	1222	G
50	1	1223	A
50	1	1232	C
50	1	1235	U
50	1	1236	G
50	1	1237	G
50	1	1239	C
50	1	1241	U
50	1	1242	G
50	1	1244	A
50	1	1245	A
50	1	1246	G
50	1	1254	C
50	1	1258	U
50	1	1259	A
50	1	1262	G

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Mol	Chain	Res	Type
50	1	1263	A
50	1	1264	G
50	1	1282	G
50	1	1285	G
50	1	1287	A
50	1	1292	C
50	1	1294	A
50	1	1300	G
50	1	1301	A
50	1	1303	A
50	1	1306	G
50	1	1307	G
50	1	1308	A
50	1	1313	G
50	1	1315	U
50	1	1316	C
50	1	1322	U
50	1	1323	G
50	1	1325	U
50	1	1329	U
50	1	1330	A
50	1	1331	U
50	1	1332	A
50	1	1345	G
50	1	1349	G
50	1	1351	U
50	1	1352	A
50	1	1353	U
50	1	1355	A
50	1	1356	U
50	1	1357	G
50	1	1366	A
50	1	1380	G
50	1	1386	A
50	1	1387	G
50	1	1390	A
50	1	1391	C
50	1	1392	G
50	1	1399	A
50	1	1400	G
50	1	1418	A
50	1	1419	A

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Mol	Chain	Res	Type
50	1	1432	C
50	1	1433	A
50	1	1434	G
50	1	1435	A
50	1	1436	U
50	1	1437	C
50	1	1443	G
50	1	1446	A
50	1	1447	G
50	1	1448	U
50	1	1450	G
50	1	1451	C
50	1	1455	U
50	1	1456	A
50	1	1467	A
50	1	1468	A
50	1	1470	U
50	1	1477	A
50	1	1481	A
50	1	1482	A
50	1	1483	G
50	1	1484	U
50	1	1485	G
50	1	1486	G
50	1	1487	G
50	1	1496	C
50	1	1502	C
50	1	1503	A
50	1	1508	C
50	1	1511	U
50	1	1512	U
50	1	1515	A
50	1	1523	U
50	1	1528	G
50	1	1531	C
50	1	1535	A
50	1	1536	G
50	1	1542	G
50	1	1549	U
50	1	1554	U
50	1	1555	U
50	1	1556	C

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Mol	Chain	Res	Type
50	1	1557	A
50	1	1558	A
50	1	1559	A
50	1	1560	G
50	1	1561	G
50	1	1563	C
50	1	1565	G
50	1	1567	U
50	1	1568	U
50	1	1569	U
50	1	1570	U
50	1	1571	A
50	1	1572	U
50	1	1573	G
50	1	1575	A
50	1	1578	C
50	1	1579	C
50	1	1580	A
50	1	1581	C
50	1	1582	C
50	1	1583	A
50	1	1588	A
50	1	1589	A
50	1	1590	G
50	1	1593	A
50	1	1595	U
50	1	1603	A
50	1	1604	G
50	1	1605	A
50	1	1613	A
50	1	1620	U
50	1	1623	G
50	1	1629	U
50	1	1630	U
50	1	1631	C
50	1	1638	A
50	1	1644	C
50	1	1645	U
50	1	1646	G
50	1	1656	A
50	1	1657	C
50	1	1662	G

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Mol	Chain	Res	Type
50	1	1683	A
50	1	1688	U
50	1	1696	A
50	1	1713	G
50	1	1715	A
50	1	1717	U
50	1	1719	G
50	1	1722	U
50	1	1724	U
50	1	1730	G
50	1	1741	A
50	1	1742	U
50	1	1749	A
50	1	1750	A
50	1	1752	A
50	1	1756	C
50	1	1760	A
50	1	1762	C
50	1	1763	U
50	1	1765	U
50	1	1766	G
50	1	1769	G
50	1	1770	G
50	1	1771	C
50	1	1773	C
50	1	1775	G
50	1	1780	G
50	1	1785	U
50	1	1788	C
50	1	1794	G
50	1	1796	G
50	1	1797	A
50	1	1813	A
50	1	1814	A
50	1	1815	U
50	1	1816	A
50	1	1817	G
50	1	1818	U
50	1	1819	U
50	1	1820	U
50	1	1821	U
50	1	1822	C

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Mol	Chain	Res	Type
50	1	1835	A
50	1	1839	A
50	1	1840	U
50	1	1841	A
50	1	1843	C
50	1	1846	C
50	1	1847	A
50	1	1848	G
50	1	1849	C
50	1	1850	A
50	1	1851	G
50	1	1854	C
50	1	1855	U
50	1	1866	C
50	1	1867	A
50	1	1869	C
50	1	1876	U
50	1	1878	G
50	1	1879	A
50	1	1880	U
50	1	1881	A
50	1	1886	A
50	1	1887	A
50	1	1889	G
50	1	1892	G
50	1	1893	A
50	1	1901	A
50	1	1906	G
50	1	1909	A
50	1	1926	C
50	1	1927	G
50	1	1930	A
50	1	1931	U
50	1	1932	A
50	1	1935	G
50	1	1939	G
50	1	1948	G
50	1	1953	G
50	1	1954	G
50	1	1955	U
50	1	1959	G
50	1	1960	A

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Mol	Chain	Res	Type
50	1	1961	G
50	1	1962	A
50	1	1963	G
50	1	1964	C
50	1	1972	A
50	1	1973	G
50	1	1979	G
50	1	1981	G
50	1	1986	U
50	1	1994	G
50	1	1999	C
50	1	2001	U
50	1	2002	G
50	1	2004	U
50	1	2005	G
50	1	2006	G
50	1	2010	U
50	1	2013	C
50	1	2017	G
50	1	2020	A
50	1	2022	G
50	1	2024	G
50	1	2026	A
50	1	2032	U
50	1	2033	G
50	1	2034	C
50	1	2035	G
50	1	2038	C
50	1	2039	C
50	1	2044	U
50	1	2045	G
50	1	2046	U
50	1	2047	A
50	1	2048	G
50	1	2049	A
50	1	2050	C
50	1	2053	C
50	1	2055	U
50	1	2056	U
50	1	2058	G
50	1	2059	U
50	1	2081	U

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Mol	Chain	Res	Type
50	1	2082	U
50	1	2085	U
50	1	2087	C
50	1	2101	C
50	1	2102	U
50	1	2107	A
50	1	2111	G
50	1	2112	U
50	1	2113	A
50	1	2114	C
50	1	2121	G
50	1	2122	G
50	1	2131	A
50	1	2134	G
50	1	2138	A
50	1	2139	A
50	1	2140	U
50	1	2142	A
50	1	2144	A
50	1	2145	A
50	1	2158	A
50	1	2159	U
50	1	2160	G
50	1	2169	G
50	1	2170	U
50	1	2175	U
50	1	2176	U
50	1	2177	G
50	1	2178	A
50	1	2179	C
50	1	2184	U
50	1	2187	G
50	1	2188	A
50	1	2205	U
50	1	2206	G
50	1	2209	U
50	1	2210	G
50	1	2211	U
50	1	2218	G
50	1	2228	A
50	1	2243	A
50	1	2244	A

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Mol	Chain	Res	Type
50	1	2248	C
50	1	2249	G
50	1	2250	G
50	1	2253	G
50	1	2254	U
50	1	2256	A
50	1	2257	C
50	1	2258	U
50	1	2261	G
50	1	2262	A
50	1	2263	C
50	1	2268	U
50	1	2270	A
50	1	2272	G
50	1	2273	G
50	1	2274	U
50	1	2279	A
50	1	2281	A
50	1	2282	U
50	1	2283	G
50	1	2284	C
50	1	2285	C
50	1	2288	G
50	1	2298	U
50	1	2299	A
50	1	2306	C
50	1	2307	G
50	1	2308	C
50	1	2309	A
50	1	2313	A
50	1	2314	U
50	1	2315	G
50	1	2319	U
50	1	2334	U
50	1	2336	U
50	1	2339	C
50	1	2340	U
50	1	2363	A
50	1	2365	C
50	1	2372	A
50	1	2373	A
50	1	2374	C

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Mol	Chain	Res	Type
50	1	2375	G
50	1	2377	G
50	1	2385	G
50	1	2386	A
50	1	2388	U
50	1	2393	G
50	1	2394	G
50	1	2397	A
50	1	2402	A
50	1	2403	G
50	1	2404	A
50	1	2411	U
50	1	2412	G
50	1	2418	G
50	1	2419	A
50	1	2424	A
50	1	2434	U
50	1	2435	G
50	1	2440	G
50	1	2441	A
50	1	2444	C
50	1	2447	A
50	1	2448	G
50	1	2453	U
50	1	2454	G
50	1	2459	A
50	1	2462	A
50	1	2469	G
50	1	2471	U
50	1	2482	U
50	1	2486	A
50	1	2487	U
50	1	2488	A
50	1	2496	C
50	1	2500	A
50	1	2504	U
50	1	2505	U
50	1	2506	U
50	1	2507	C
50	1	2509	U
50	1	2510	U
50	1	2513	U

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Mol	Chain	Res	Type
50	1	2514	U
50	1	2515	A
50	1	2522	G
50	1	2523	A
50	1	2531	C
50	1	2532	U
50	1	2533	G
50	1	2534	G
50	1	2537	U
50	1	2538	U
50	1	2539	C
50	1	2540	A
50	1	2541	U
50	1	2542	U
50	1	2543	U
50	1	2547	A
50	1	2549	G
50	1	2552	C
50	1	2554	A
50	1	2561	A
50	1	2569	A
50	1	2570	U
50	1	2571	U
50	1	2572	C
50	1	2573	G
50	1	2585	G
50	1	2593	A
50	1	2594	C
50	1	2595	A
50	1	2606	G
50	1	2607	G
50	1	2613	U
50	1	2614	G
50	1	2617	U
50	1	2618	G
50	1	2619	G
50	1	2626	A
50	1	2628	A
50	1	2629	U
50	1	2635	A
50	1	2636	A
50	1	2642	A

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Mol	Chain	Res	Type
50	1	2644	C
50	1	2652	U
50	1	2655	U
50	1	2657	A
50	1	2666	C
50	1	2674	A
50	1	2676	A
50	1	2678	A
50	1	2681	U
50	1	2688	U
50	1	2689	A
50	1	2691	A
50	1	2694	A
50	1	2703	A
50	1	2704	A
50	1	2707	C
50	1	2713	U
50	1	2716	U
50	1	2720	G
50	1	2728	G
50	1	2729	U
50	1	2737	C
50	1	2742	C
50	1	2752	U
50	1	2753	G
50	1	2754	G
50	1	2755	C
50	1	2762	A
50	1	2773	C
50	1	2777	G
50	1	2778	G
50	1	2797	C
50	1	2798	C
50	1	2799	A
50	1	2800	G
50	1	2801	A
50	1	2802	A
50	1	2804	A
50	1	2805	G
50	1	2808	A
50	1	2810	C
50	1	2814	G

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Mol	Chain	Res	Type
50	1	2816	G
50	1	2817	A
50	1	2827	U
50	1	2829	U
50	1	2830	G
50	1	2842	U
50	1	2845	A
50	1	2849	C
50	1	2856	G
50	1	2860	U
50	1	2861	U
50	1	2866	U
50	1	2867	C
50	1	2871	G
50	1	2872	A
50	1	2873	U
50	1	2874	G
50	1	2875	U
50	1	2876	C
50	1	2887	A
50	1	2888	U
50	1	2889	C
50	1	2904	U
50	1	2912	G
50	1	2919	A
50	1	2920	U
50	1	2922	G
50	1	2923	U
50	1	2935	U
50	1	2936	A
50	1	2941	A
50	1	2942	C
50	1	2946	A
50	1	2947	G
50	1	2950	G
50	1	2951	G
50	1	2954	U
50	1	2965	U
50	1	2971	A
50	1	2972	G
50	1	2977	G
50	1	2978	U

Continued on next page...

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Mol	Chain	Res	Type
50	1	2979	U
50	1	2983	C
50	1	2992	U
50	1	2996	U
50	1	2997	G
50	1	3011	A
50	1	3012	A
50	1	3021	A
50	1	3022	G
50	1	3023	U
50	1	3026	G
50	1	3047	U
50	1	3056	U
50	1	3058	U
50	1	3059	G
50	1	3078	U
50	1	3079	U
50	1	3080	G
50	1	3086	A
50	1	3088	G
50	1	3092	C
50	1	3098	G
50	1	3109	G
50	1	3111	U
50	1	3113	A
50	1	3115	C
50	1	3117	C
50	1	3118	C
50	1	3119	U
50	1	3122	A
50	1	3130	A
50	1	3131	U
50	1	3139	A
50	1	3142	A
50	1	3143	C
50	1	3144	G
50	1	3151	U
50	1	3153	U
50	1	3154	C
50	1	3155	U
50	1	3156	U
50	1	3157	U

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Mol	Chain	Res	Type
50	1	3158	G
50	1	3170	A
50	1	3172	A
50	1	3173	G
50	1	3174	A
50	1	3176	G
50	1	3179	U
50	1	3180	A
50	1	3181	C
50	1	3185	U
50	1	3186	A
50	1	3187	A
50	1	3194	C
50	1	3196	U
50	1	3197	G
50	1	3198	U
50	1	3205	G
50	1	3206	C
50	1	3207	U
50	1	3208	G
50	1	3209	A
50	1	3210	A
50	1	3217	C
50	1	3218	A
50	1	3219	G
50	1	3220	G
50	1	3222	U
50	1	3227	A
50	1	3228	C
50	1	3237	U
50	1	3243	A
50	1	3244	A
50	1	3245	A
50	1	3246	G
50	1	3247	G
50	1	3253	G
50	1	3259	U
50	1	3260	G
50	1	3263	G
50	1	3268	A
50	1	3269	U
50	1	3270	U

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Mol	Chain	Res	Type
50	1	3271	G
50	1	3272	C
50	1	3273	A
50	1	3274	A
50	1	3275	U
50	1	3276	G
50	1	3277	U
50	1	3278	C
50	1	3279	A
50	1	3286	G
50	1	3287	U
50	1	3288	G
50	1	3289	G
50	1	3290	G
50	1	3292	A
50	1	3293	U
50	1	3294	A
50	1	3295	A
50	1	3296	A
50	1	3305	A
50	1	3307	A
50	1	3313	U
50	1	3316	A
50	1	3317	U
50	1	3318	G
50	1	3319	U
50	1	3335	A
50	1	3340	G
50	1	3341	U
50	1	3345	G
50	1	3351	U
50	1	3352	U
50	1	3353	G
50	1	3354	U
50	1	3355	U
50	1	3357	U
50	1	3358	U
50	1	3362	A
50	1	3363	U
50	1	3368	U
50	1	3369	G
50	1	3370	A

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Mol	Chain	Res	Type
50	1	3375	A
50	1	3378	C
50	1	3382	U
50	1	3383	G
50	1	3386	G
50	1	3390	G

All (160) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
29	3	77	G
31	4	22	U
31	4	38	U
31	4	48	A
31	4	58	G
50	1	14	U
50	1	43	A
50	1	73	C
50	1	86	G
50	1	116	A
50	1	122	A
50	1	147	U
50	1	155	G
50	1	156	G
50	1	189	G
50	1	211	A
50	1	218	G
50	1	219	A
50	1	239	G
50	1	268	A
50	1	269	G
50	1	282	G
50	1	285	A
50	1	341	G
50	1	353	G
50	1	374	A
50	1	375	A
50	1	400	G
50	1	494	G
50	1	547	G
50	1	558	U
50	1	621	A

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Mol	Chain	Res	Type
50	1	645	A
50	1	648	C
50	1	661	G
50	1	677	A
50	1	715	A
50	1	764	U
50	1	767	U
50	1	870	G
50	1	884	A
50	1	896	A
50	1	906	A
50	1	914	A
50	1	916	G
50	1	923	C
50	1	924	G
50	1	933	A
50	1	962	A
50	1	979	U
50	1	994	G
50	1	1064	A
50	1	1065	A
50	1	1075	A
50	1	1103	A
50	1	1144	U
50	1	1177	G
50	1	1192	C
50	1	1196	C
50	1	1199	C
50	1	1241	U
50	1	1307	G
50	1	1329	U
50	1	1348	U
50	1	1352	A
50	1	1365	G
50	1	1391	C
50	1	1417	G
50	1	1418	A
50	1	1432	C
50	1	1433	A
50	1	1434	G
50	1	1455	U
50	1	1482	A

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Mol	Chain	Res	Type
50	1	1483	G
50	1	1553	U
50	1	1554	U
50	1	1557	A
50	1	1568	U
50	1	1580	A
50	1	1589	A
50	1	1695	U
50	1	1716	U
50	1	1740	U
50	1	1815	U
50	1	1816	A
50	1	1840	U
50	1	1849	C
50	1	1850	A
50	1	1900	A
50	1	1913	A
50	1	1931	U
50	1	1938	U
50	1	1953	G
50	1	1959	G
50	1	1971	C
50	1	2047	A
50	1	2086	A
50	1	2101	C
50	1	2111	G
50	1	2112	U
50	1	2139	A
50	1	2144	A
50	1	2158	A
50	1	2175	U
50	1	2177	G
50	1	2178	A
50	1	2187	G
50	1	2208	A
50	1	2262	A
50	1	2267	C
50	1	2271	A
50	1	2273	G
50	1	2313	A
50	1	2372	A
50	1	2385	G

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Mol	Chain	Res	Type
50	1	2393	G
50	1	2402	A
50	1	2403	G
50	1	2447	A
50	1	2468	A
50	1	2487	U
50	1	2509	U
50	1	2513	U
50	1	2537	U
50	1	2541	U
50	1	2593	A
50	1	2635	A
50	1	2656	A
50	1	2715	A
50	1	2727	A
50	1	2728	G
50	1	2761	G
50	1	2772	C
50	1	2797	C
50	1	2803	A
50	1	2816	G
50	1	2866	U
50	1	2911	A
50	1	2941	A
50	1	2950	G
50	1	2983	C
50	1	3021	A
50	1	3022	G
50	1	3078	U
50	1	3121	U
50	1	3152	U
50	1	3156	U
50	1	3172	A
50	1	3175	U
50	1	3179	U
50	1	3186	A
50	1	3208	G
50	1	3216	G
50	1	3218	A
50	1	3219	G
50	1	3246	G
50	1	3259	U

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Mol	Chain	Res	Type
50	1	3269	U
50	1	3334	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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	R	5
50	1	4
42	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	R	35:SER	C	74:CYS	N	41.41
1	1	2087:C	O3'	2093:A	P	28.40
1	R	529:GLY	C	535:UNK	N	19.42
1	R	105:ARG	C	113:UNK	N	18.44
1	R	123:UNK	C	156:UNK	N	13.45
1	1	440:A	O3'	494:G	P	13.22
1	1	2059:U	O3'	2080:C	P	11.99
1	R	80:SER	C	90:HIS	N	8.91
1	1	1984:C	O3'	1985:G	P	6.66
1	F	237:LYS	C	238:LEU	N	1.13

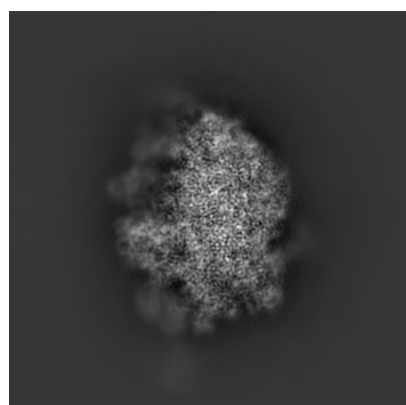
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4751. These allow visual inspection of the internal detail of the map and identification of artifacts.

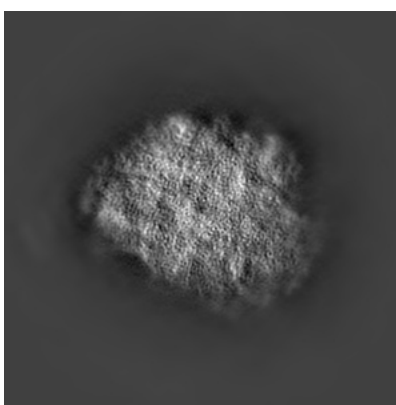
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

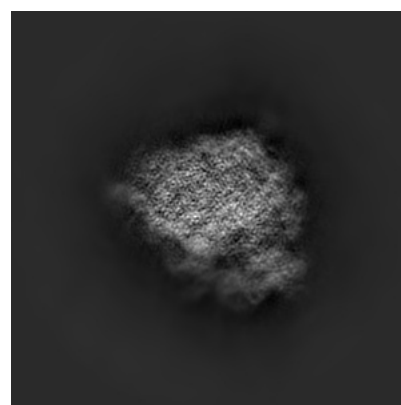
6.1.1 Primary map



X



Y

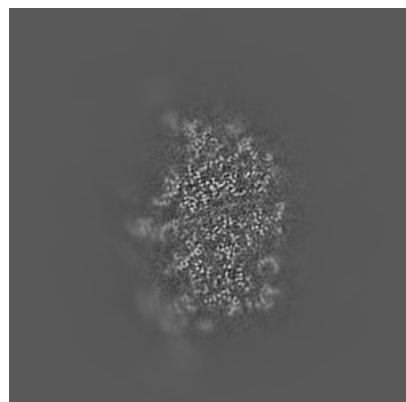


Z

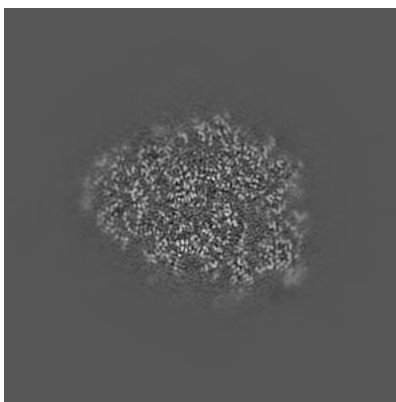
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

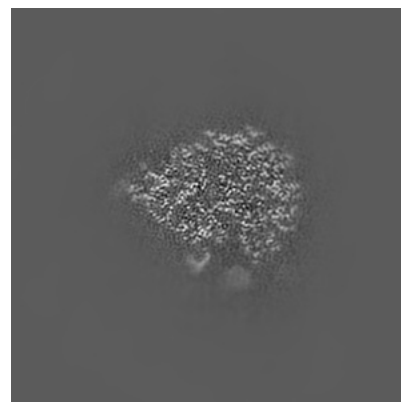
6.2.1 Primary map



X Index: 198



Y Index: 198

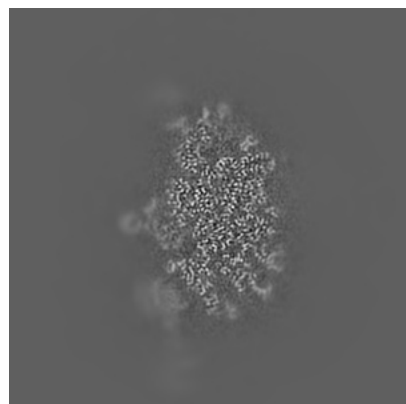


Z Index: 198

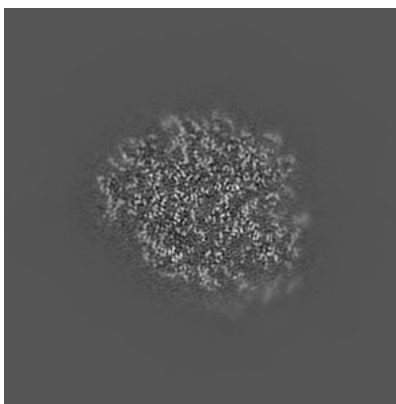
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

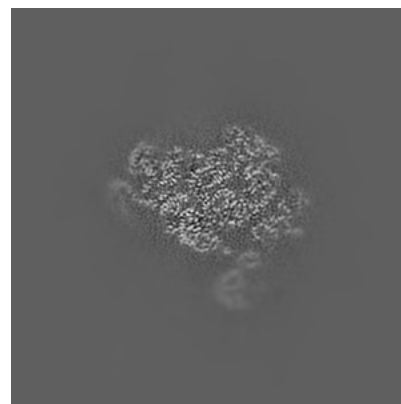
6.3.1 Primary map



X Index: 183



Y Index: 209

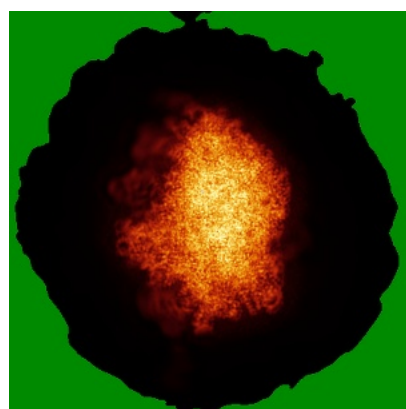


Z Index: 214

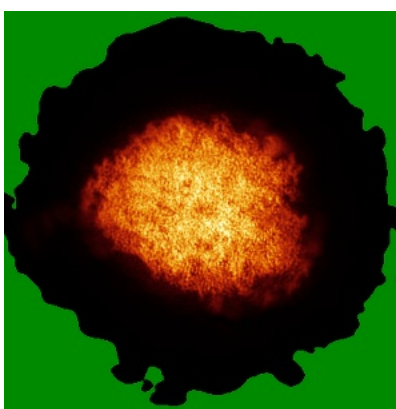
The images above show the largest variance slices of the map in three orthogonal directions.

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

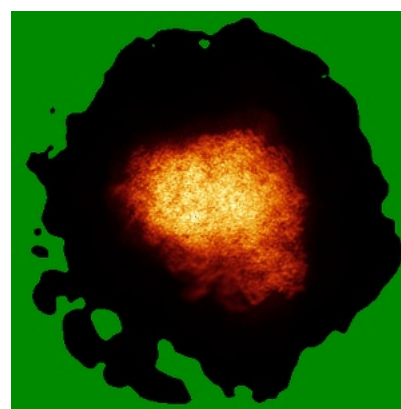
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

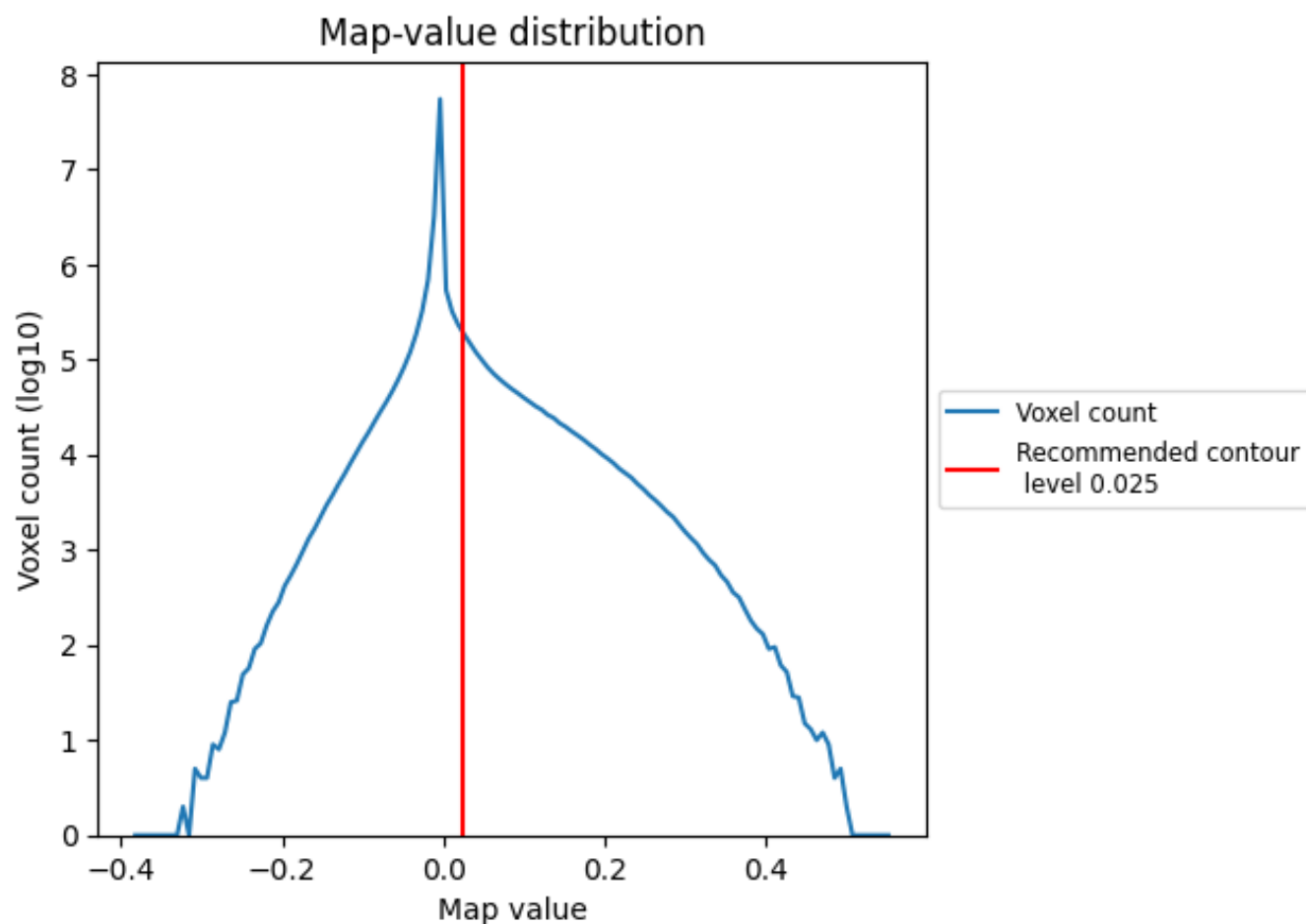
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

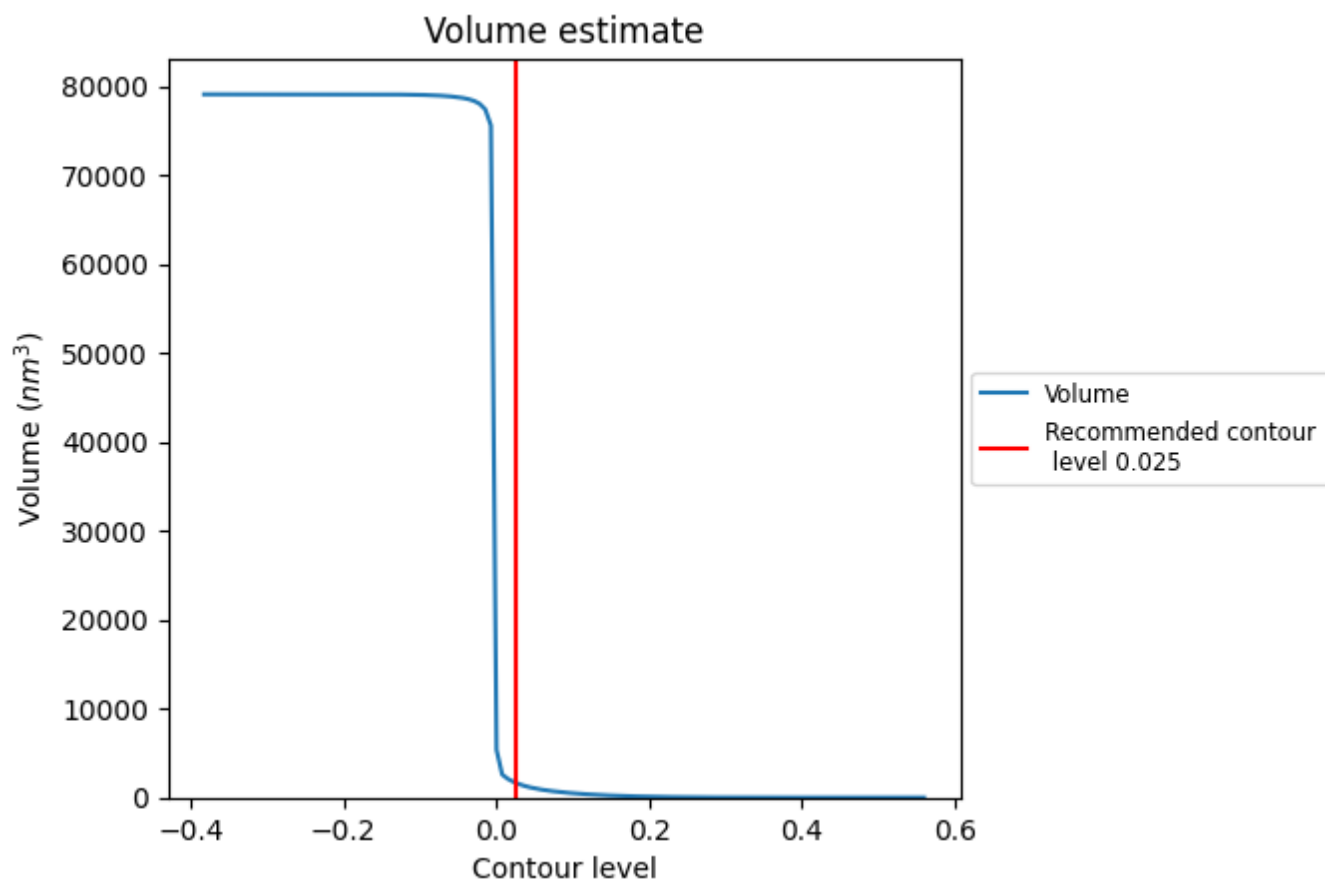
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

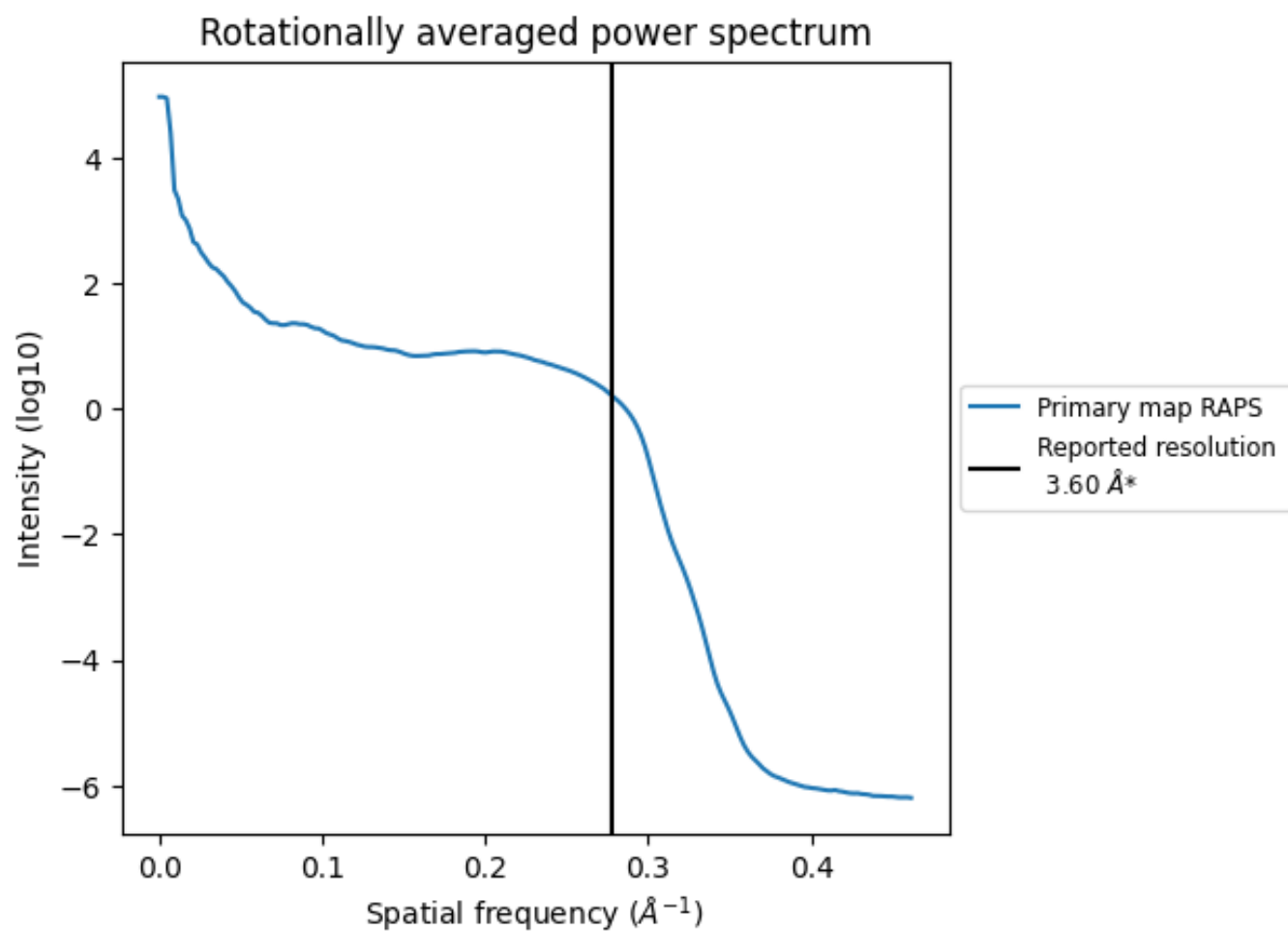
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1693 nm³; this corresponds to an approximate mass of 1530 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 0.278 Å⁻¹

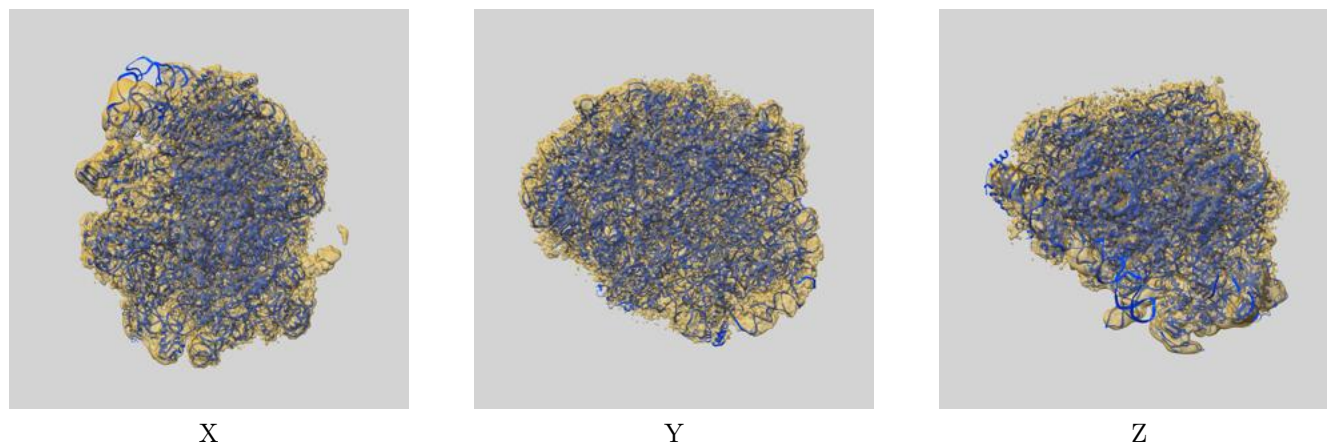
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

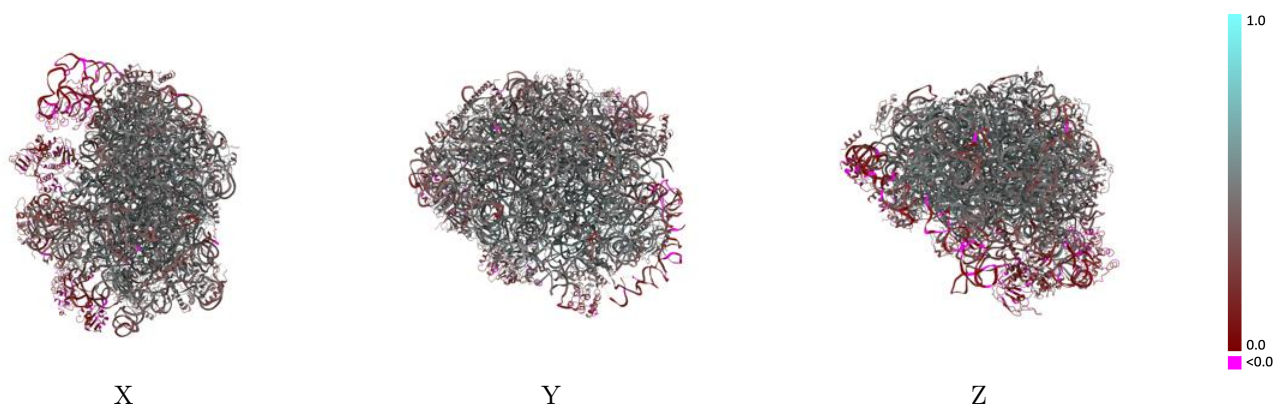
This section contains information regarding the fit between EMDB map EMD-4751 and PDB model 6R84. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

9.1 Map-model overlay [i](#)



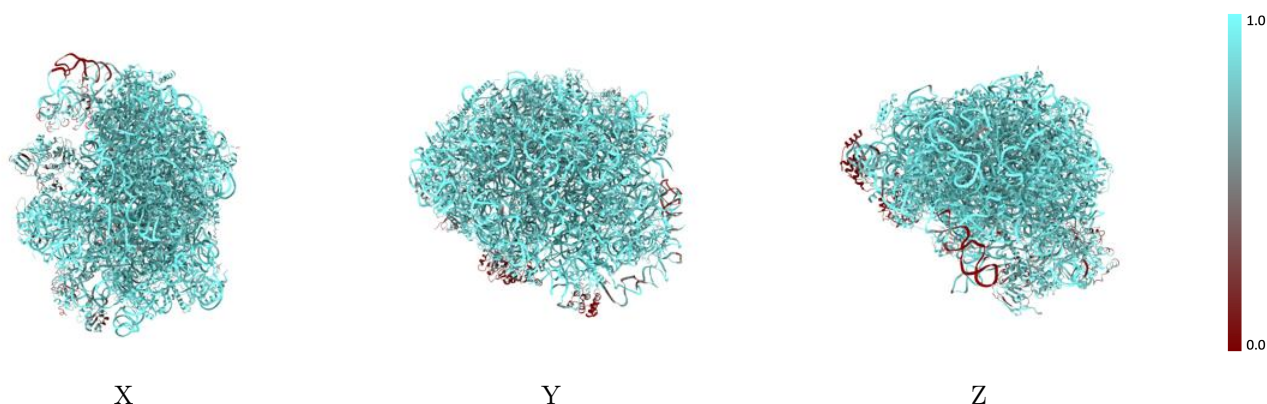
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



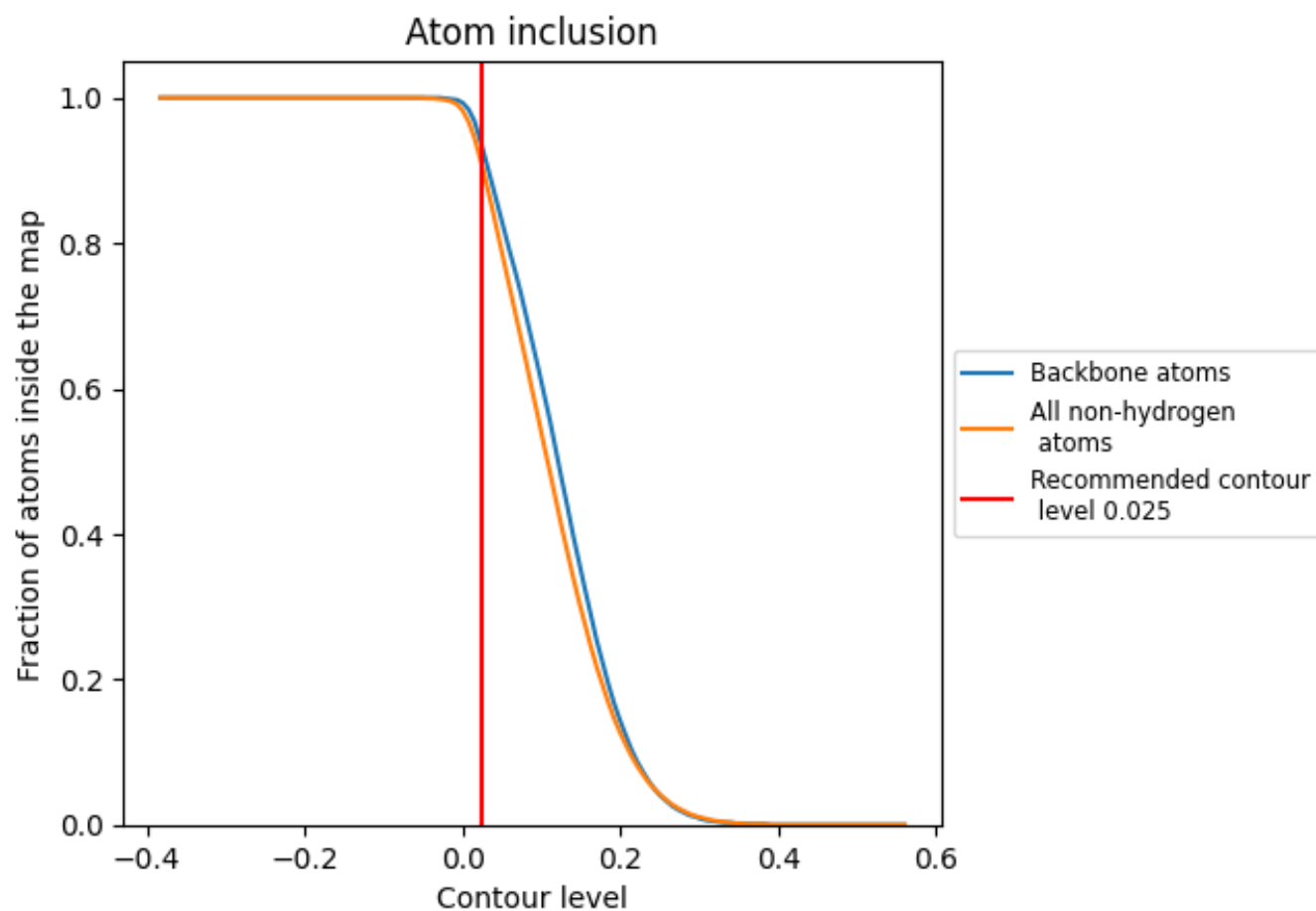
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 91% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9070	 0.4220
1	 0.9510	 0.4380
3	 0.9850	 0.4350
4	 0.9810	 0.4760
5	 0.9190	 0.4750
7	 0.9030	 0.4520
A	 0.7480	 0.1760
B	 0.9240	 0.2640
C	 0.8840	 0.4570
D	 0.9310	 0.4890
E	 0.9220	 0.5030
F	 0.9320	 0.4880
G	 0.9150	 0.4590
H	 0.8750	 0.3560
I	 0.8810	 0.4160
J	 0.9060	 0.4460
K	 0.8950	 0.4130
L	 0.5220	 0.0610
M	 0.8660	 0.3550
N	 0.9140	 0.4410
O	 0.9270	 0.4450
P	 0.4630	 0.1180
Q	 0.9390	 0.4920
R	 0.5590	 0.2560
S	 0.9210	 0.4640
T	 0.9250	 0.4730
U	 0.9140	 0.4760
V	 0.9010	 0.4590
W	 0.9080	 0.4110
X	 0.2340	 0.2510
Y	 0.9340	 0.4640
Z	 0.9200	 0.4840
a	 0.9180	 0.4570
b	 0.9010	 0.4480
c	 0.9300	 0.4670



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Chain	Atom inclusion	Q-score
d	 0.8940	 0.4180
e	 0.9040	 0.4300
f	 0.9120	 0.4770
g	 0.9110	 0.4850
h	 0.9270	 0.4970
i	 0.9200	 0.4920
j	 0.9140	 0.4500
k	 0.8750	 0.4260
l	 0.9560	 0.5230
m	 0.8480	 0.4190
n	 0.9420	 0.5110
o	 0.9330	 0.4730
p	 0.9340	 0.5050
r	 0.7010	 0.0920
s	 0.8790	 0.4360
x	 0.9180	 0.4790