Full wwPDB EM Validation Report ⓘ

Oct 26, 2026 – 10:57 AM EDT

PDB ID	:	9YWB / pdb_00009ywb
EMDB ID	:	EMD-73543
Title	:	Hypomethylated nucleoplasmic pre-60S intermediate containing Nog2 at Rsa4-arrested 5S post-rotation state
Authors	:	Zhao, Y.; Li, H.
Deposited on	:	2025-10-24
Resolution	:	2.85 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:

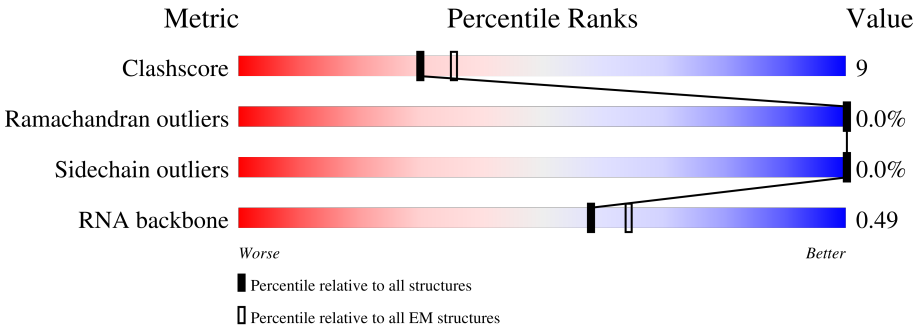
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

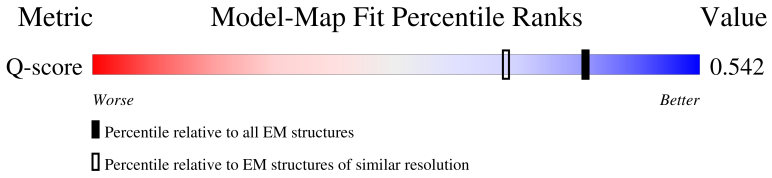
1 Overall quality at a glance

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

The reported resolution of this entry is 2.85 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.





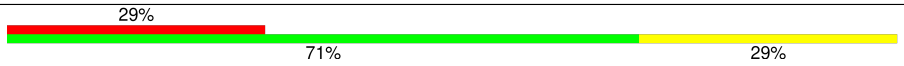
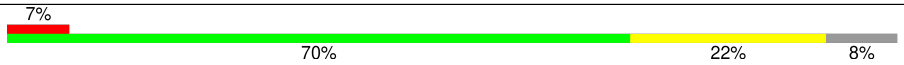
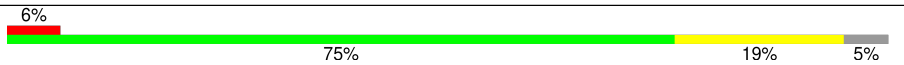
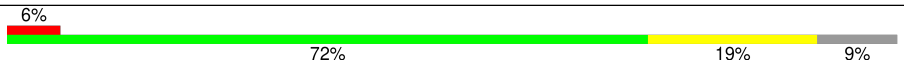
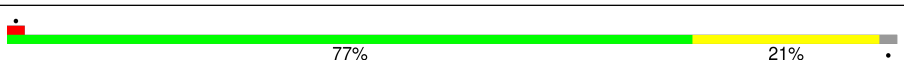
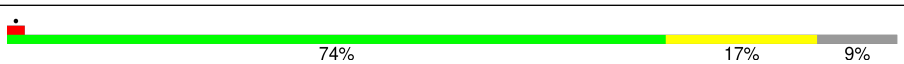
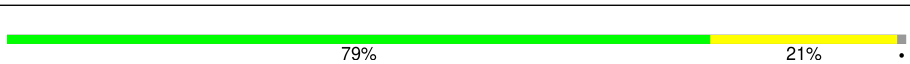
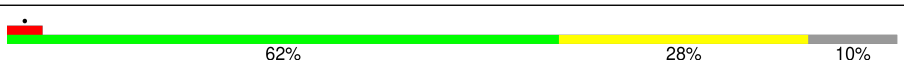
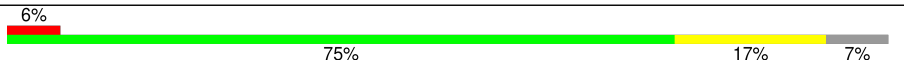
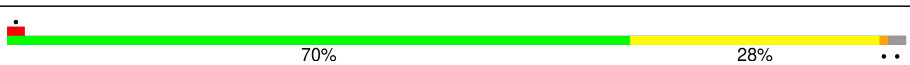
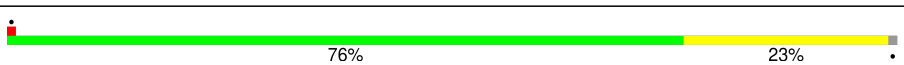
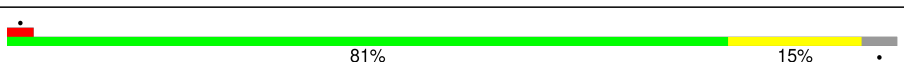
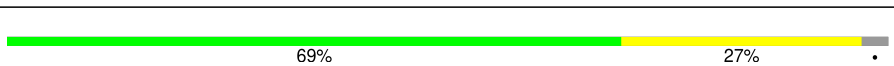
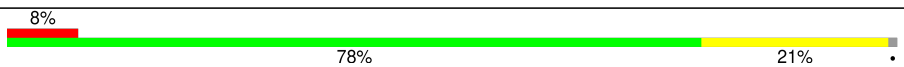
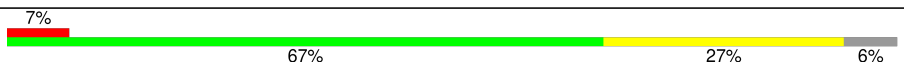
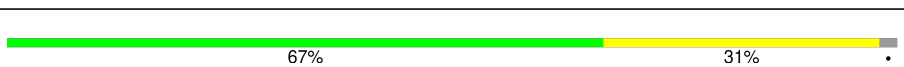
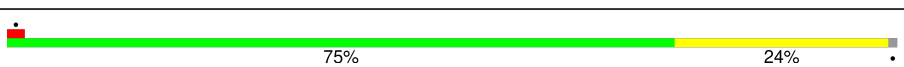
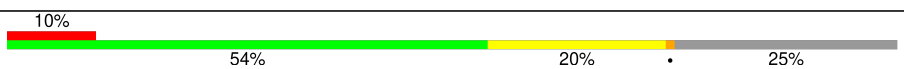
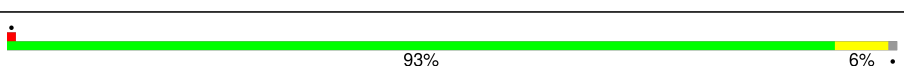
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11965 (2.35 - 3.35)

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 <=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	D	297	27% 61% 25% 14%
2	J	174	11% 66% 26% 7%
3	A	254	75% 22%

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Mol	Chain	Length	Quality of chain
4	a	149	
5	B	387	
6	b	647	
7	C	362	
8	c	105	
9	d	113	
10	E	176	
11	e	130	
12	F	244	
13	f	107	
14	G	256	
15	g	121	
16	I	166	
17	H	191	
18	h	120	
19	i	100	
20	j	88	
21	k	78	
22	L	199	
23	l	51	
24	M	138	
25	p	92	
26	N	204	
27	u	199	
28	O	199	

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Mol	Chain	Length	Quality of chain
29	P	184	8% 78% 21%
30	Q	186	5% 63% 11% 25%
31	R	189	63% 19% 19%
32	r	261	56% 26% 18%
33	S	172	72% 27%
34	T	160	21% 64% 26% 9%
35	U	121	10% 61% 25% 14%
36	V	137	77% 23%
37	W	236	7% 75% 22%
38	X	142	63% 22% 15%
39	Y	127	65% 35%
40	y	245	8% 65% 33%
41	Z	136	73% 26%
42	z	106	11% 42% 9% 48%
43	K	165	31% 76% 13% 11%
44	1	3396	6% 54% 29% 8% 8%
45	3	158	60% 34% 5%
46	5	120	17% 60% 31% 8%
47	x	515	6% 55% 21% 24%
48	m	486	15% 67% 26% 7%
49	2	121	54% 37% 5%
50	t	767	21% 36% 18% 46%
51	n	334	10% 88%
52	4	593	40% 62% 24% 14%
53	o	175	16% 50% 13% 38%

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Mol	Chain	Length	Quality of chain
54	s	217	
55	q	520	
56	Lr	25	

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 148851 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 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	D	255	2047	1303	354	388	2	0	0

- Molecule 2 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	J	161	1283	808	240	231	4	0	0

- Molecule 3 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	A	245	1863	1162	376	324	1	0	0

- Molecule 4 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	a	94	742	484	131	126	1	0	0

- Molecule 5 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	B	386	3081	1956	584	533	8	0	0

- Molecule 6 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	b	647	5219	3269	940	984	26	0	0

- Molecule 7 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	361	Total	C	N	O	S	0	0
			2749	1730	522	494	3		

- Molecule 8 is a protein called 60S ribosomal protein L30.

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

- Molecule 9 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	d	107	Total	C	N	O	S	0	0
			873	553	165	154	1		

- Molecule 10 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	E	160	Total	C	N	O	S	0	0
			1274	820	230	223	1		

- Molecule 11 is a protein called 60S ribosomal protein L32.

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

- Molecule 12 is a protein called 60S ribosomal protein L7-A.

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

- Molecule 13 is a protein called 60S ribosomal protein L33-A.

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

- Molecule 14 is a protein called Large ribosomal subunit protein eL8A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	230	Total	C	N	O	S	0	0
			1798	1149	323	323	3		

- Molecule 15 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	g	112	Total	C	N	O	S	0	0
			881	546	179	152	4		

- Molecule 16 is a protein called Bud site selection protein 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	131	Total	C	N	O	S	0	0
			1056	660	195	198	3		

- Molecule 17 is a protein called Large ribosomal subunit protein uL6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	H	188	Total	C	N	O	S	0	0
			1493	948	271	270	4		

- Molecule 18 is a protein called 60S ribosomal protein L35-A.

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

- Molecule 19 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	i	96	Total	C	N	O	S	0	0
			743	465	148	128	2		

- Molecule 20 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	j	85	Total	C	N	O	S	0	0
			670	408	146	111	5		

- Molecule 21 is a protein called 60S ribosomal protein L38.

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

- Molecule 22 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	L	187	Total	C	N	O	0	0
			1491	929	306	256		

- Molecule 23 is a protein called 60S ribosomal protein L39.

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

- Molecule 24 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	M	137	Total	C	N	O	S	0	0
			1059	678	200	179	2		

- Molecule 25 is a protein called 60S ribosomal protein L43-A.

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

- Molecule 26 is a protein called Large ribosomal subunit protein eL15A.

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

- Molecule 27 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	u	149	Total	C	N	O	S	0	0
			1256	788	252	207	9		

- Molecule 28 is a protein called Large ribosomal subunit protein uL13A.

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

- Molecule 29 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	P	183	Total	C	N	O	0	0
			1438	893	286	259		

- Molecule 30 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Q	139	Total	C	N	O	S	0	0
			1069	683	201	183	2		

- Molecule 31 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	R	154	Total	C	N	O	0	0
			1241	772	262	207		

- Molecule 32 is a protein called Ribosome biogenesis protein NSA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	r	213	Total	C	N	O	S	0	0
			1719	1088	328	296	7		

- Molecule 33 is a protein called Large ribosomal subunit protein eL20A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	S	170	Total	C	N	O	S	0	0
			1425	916	265	241	3		

- Molecule 34 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	T	145	Total	C	N	O	S	0	0
			1161	734	223	200	4		

- Molecule 35 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	U	104	Total 826	C 535	N 136	O 155	0	0

- Molecule 36 is a protein called 60S ribosomal protein L23-A.

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

- Molecule 37 is a protein called Ribosome assembly factor MRT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	W	227	Total 1814	C 1149	N 310	O 350	S 5	0	0

- Molecule 38 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	X	120	Total 959	C 617	N 168	O 172	S 2	0	0

- Molecule 39 is a protein called 60S ribosomal protein L26-A.

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

- Molecule 40 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	y	242	Total 1826	C 1131	N 317	O 372	S 6	0	0

- Molecule 41 is a protein called 60S ribosomal protein L27-A.

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

- Molecule 42 is a protein called UPF0642 protein YBL028C.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	z	55	Total	C	N	O	0	0
			444	273	88	83		

- Molecule 43 is a protein called 60S ribosomal protein L12.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	K	147	Total	C	N	O	0	0
			821	501	159	161		

- Molecule 44 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	1	3116	Total	C	N	O	P	0	0
			66660	29773	12017	21754	3116		

- Molecule 45 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	3	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 46 is a protein called rRNA-processing protein CGR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	5	110	Total	C	N	O	S	0	0
			934	579	191	161	3		

- Molecule 47 is a protein called Ribosome assembly protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	x	390	Total	C	N	O	S	0	0
			3051	1914	551	566	20		

- Molecule 48 is a protein called Nucleolar GTP-binding protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	m	453	Total	C	N	O	S	0	0
			3647	2309	656	672	10		

- Molecule 49 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	2	117	Total	C	N	O	P	0	0
			2494	1114	446	817	117		

- Molecule 50 is a protein called Protein SDA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	t	414	Total	C	N	O	S	0	0
			3289	2098	568	602	21		

- Molecule 51 is a protein called Pre-rRNA-processing protein IPI1.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	n	41	Total	C	N	O	0	0
			335	208	66	61		

- Molecule 52 is a protein called Probable metalloprotease ARX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	4	509	Total	C	N	O	S	0	0
			3945	2503	673	754	15		

- Molecule 53 is a protein called Ribosome biogenesis protein ALB1.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	o	109	Total	C	N	O	0	0
			872	543	171	158		

- Molecule 54 is a protein called Large ribosomal subunit protein uL1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	s	217	Total	C	N	O	S	0	0
			1718	1097	299	312	10		

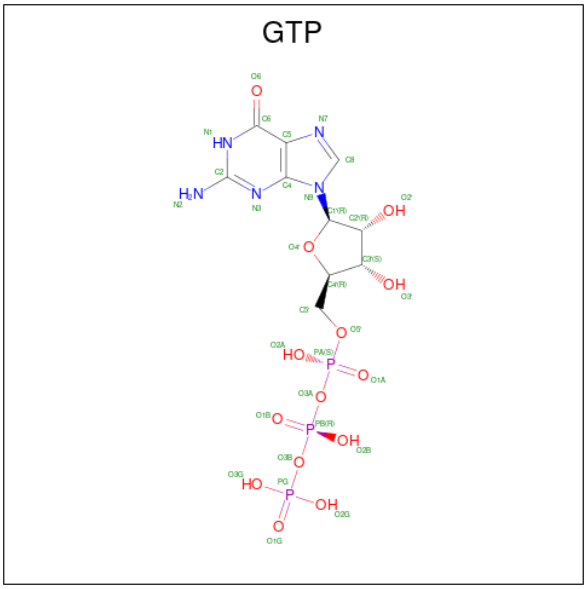
- Molecule 55 is a protein called Nuclear GTP-binding protein NUG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	q	64	Total	C	N	O	S	0	0
			533	333	109	90	1		

- Molecule 56 is a protein called Small ribosomal subunit protein eS32A.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	Lr	20	Total	C	N	O	S	0	0
			191	118	51	21	1		

- Molecule 57 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
57	m	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 58 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
58	m	1	Total	Mg	0
			1	1	

- Molecule 59 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
59	m	1	Total	K	0
			1	1	

- Molecule 60 is water.

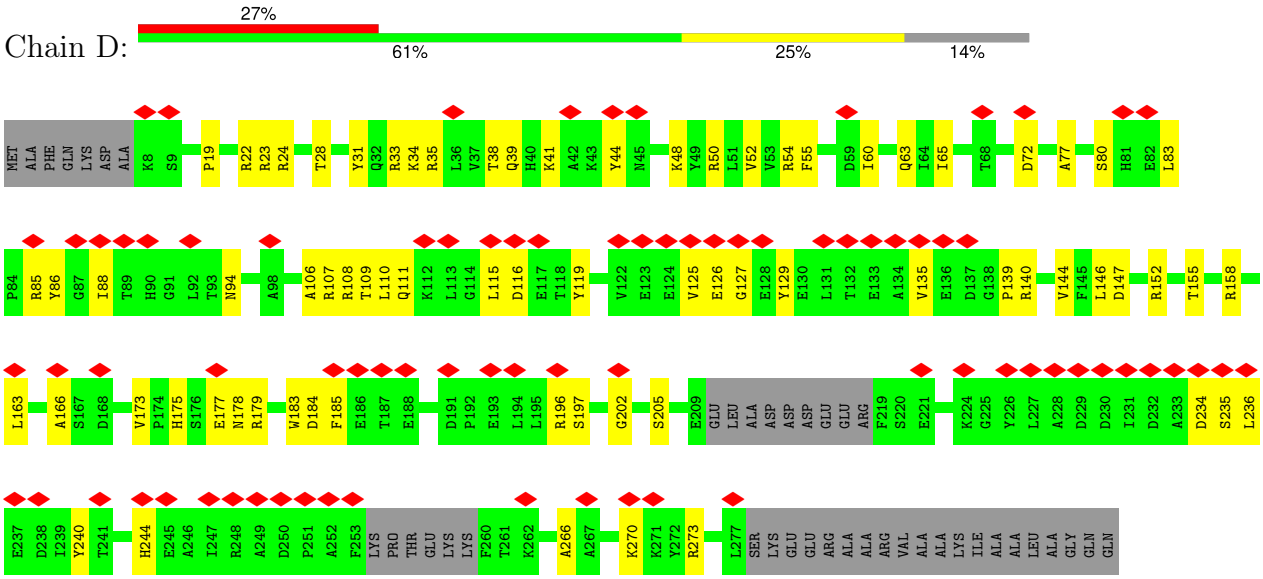
Mol	Chain	Residues	Atoms		AltConf
60	m	3	Total	O	0
			3	3	

3 Residue-property plots (i)

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

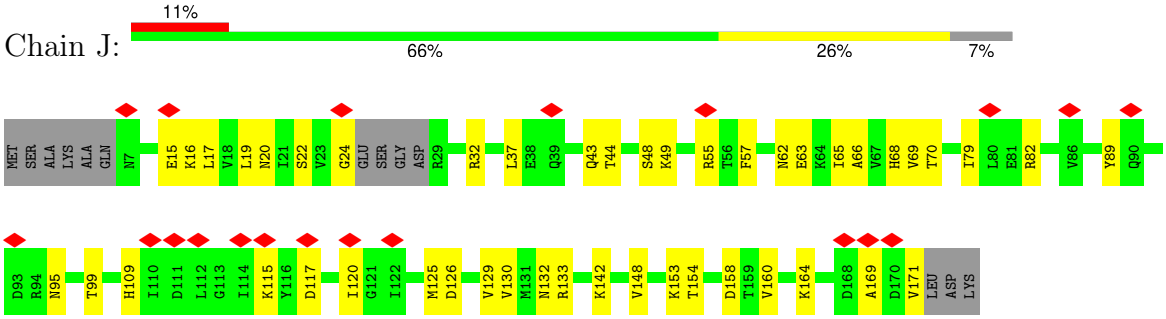
• Molecule 1: 60S ribosomal protein L5

Chain D:



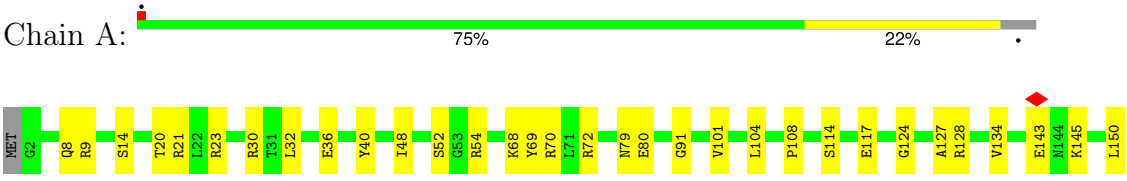
• Molecule 2: 60S ribosomal protein L11-A

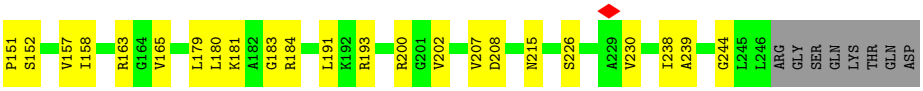
Chain J:



• Molecule 3: 60S ribosomal protein L2-A

Chain A:



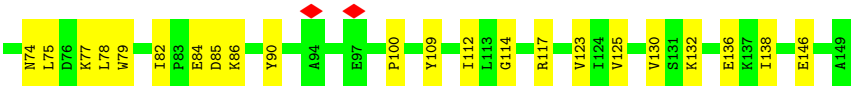


• Molecule 4: 60S ribosomal protein L28

Chain a:





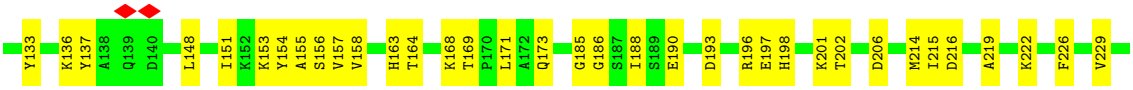


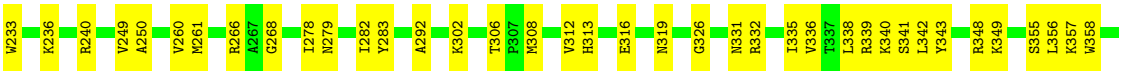
• Molecule 5: 60S ribosomal protein L3

Chain B:









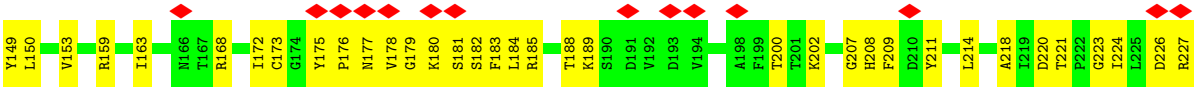


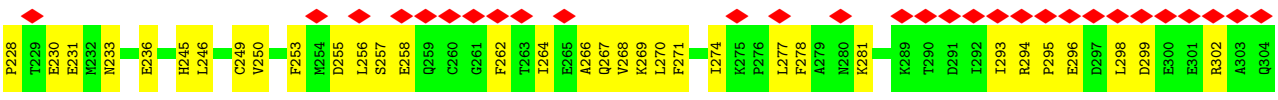
• Molecule 6: Nucleolar GTP-binding protein 1

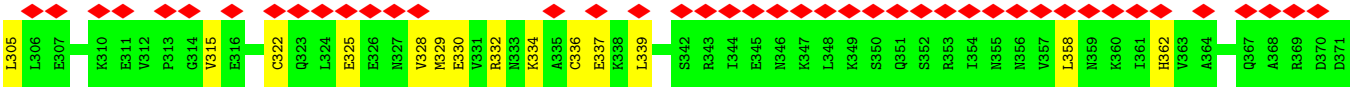
Chain b:

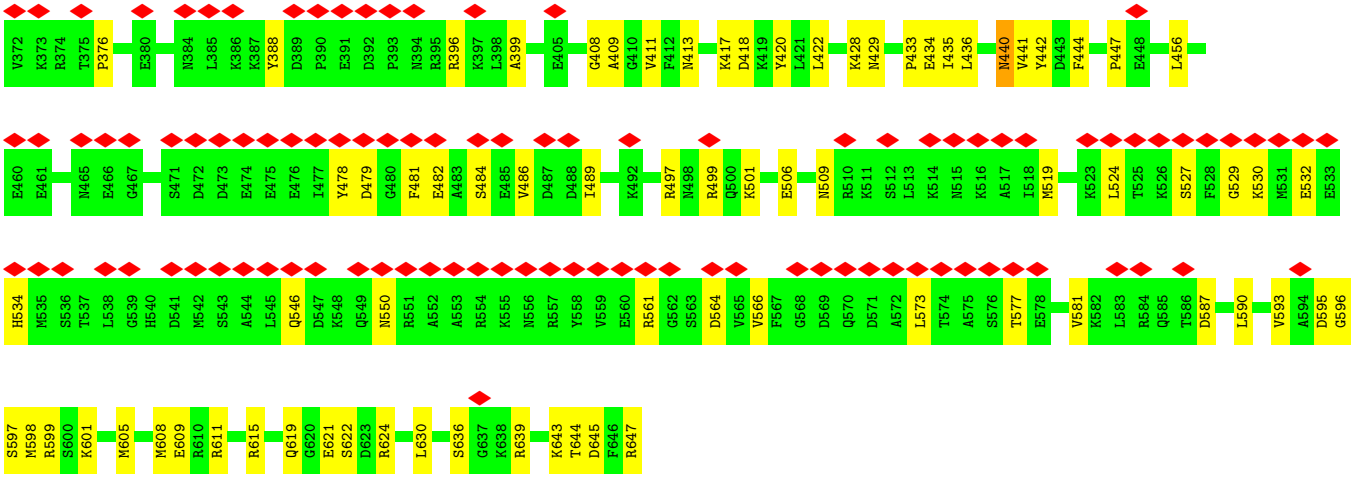












• Molecule 7: 60S ribosomal protein L4-A

Chain C:

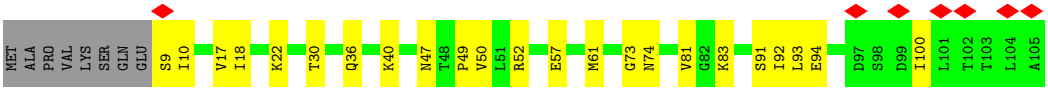




• Molecule 8: 60S ribosomal protein L30

Chain c:

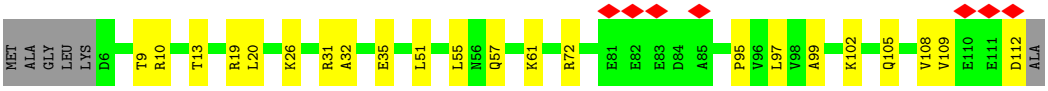




• Molecule 9: 60S ribosomal protein L31-A

Chain d:

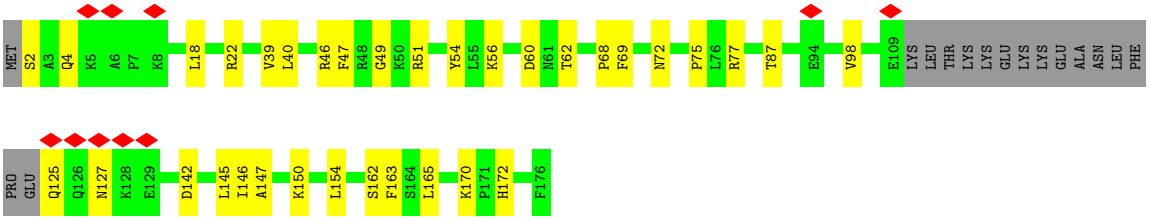




• Molecule 10: 60S ribosomal protein L6-A

Chain E:





• Molecule 11: 60S ribosomal protein L32

Chain e:

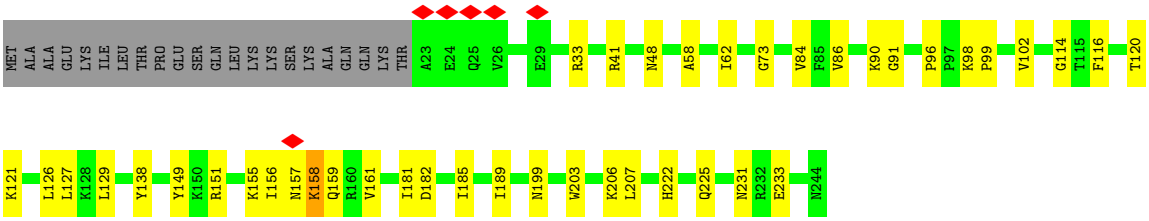




• Molecule 12: 60S ribosomal protein L7-A

Chain F:

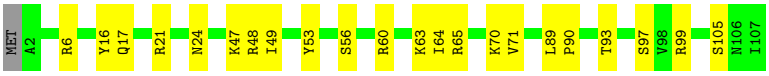




• Molecule 13: 60S ribosomal protein L33-A

Chain f:

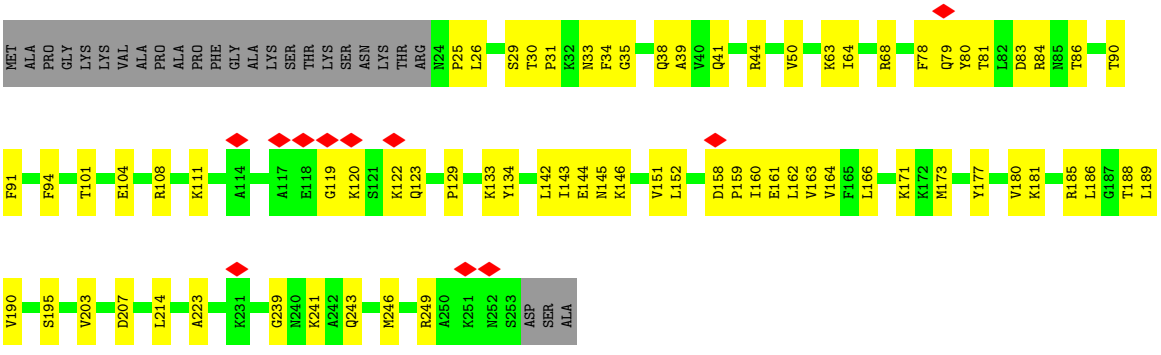




• Molecule 14: Large ribosomal subunit protein eL8A

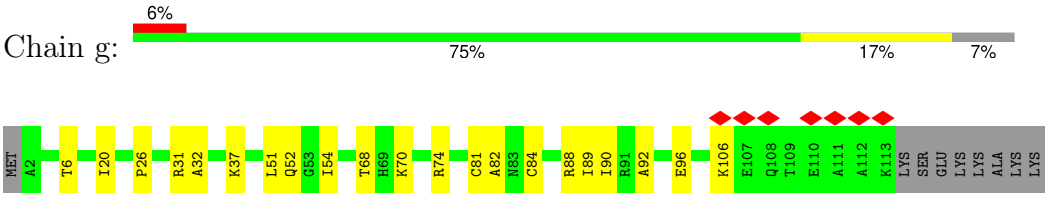
Chain G:





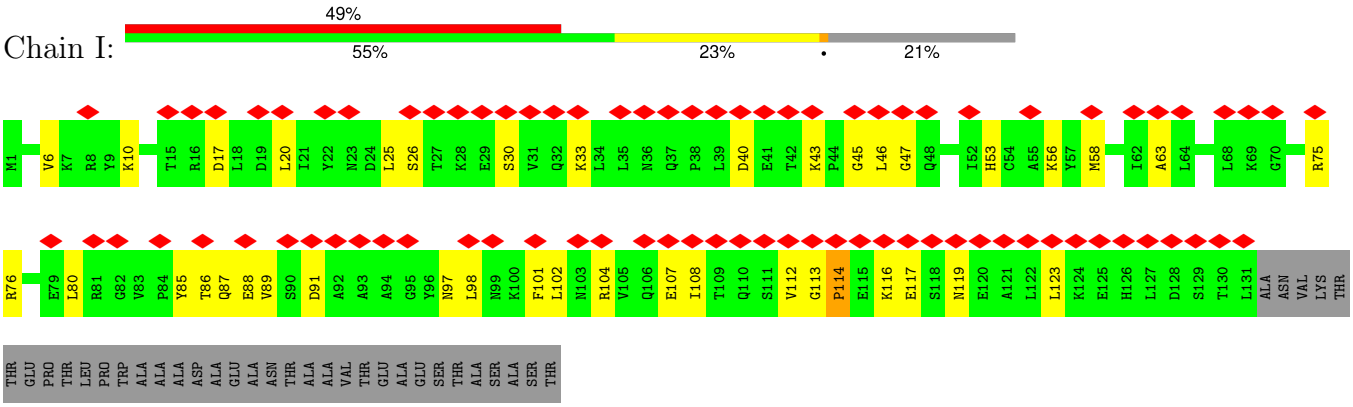
• Molecule 15: 60S ribosomal protein L34-A

Chain g:



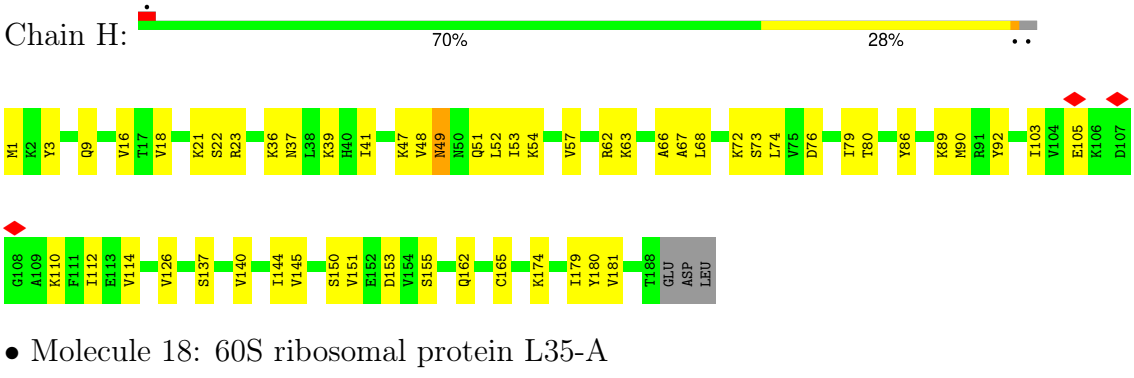
• Molecule 16: Bud site selection protein 20

Chain I:



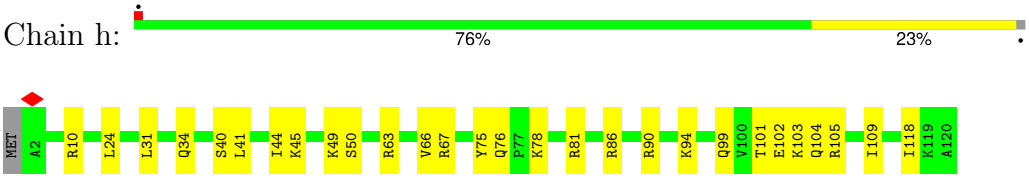
• Molecule 17: Large ribosomal subunit protein uL6A

Chain H:



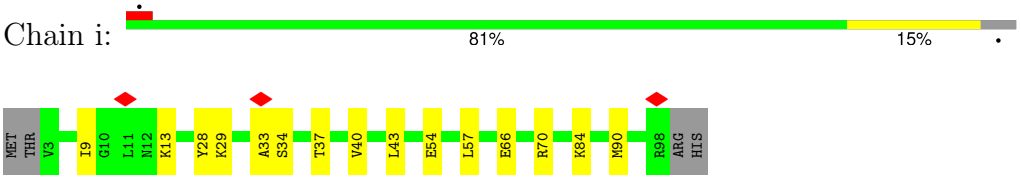
• Molecule 18: 60S ribosomal protein L35-A

Chain h:



• Molecule 19: 60S ribosomal protein L36-A

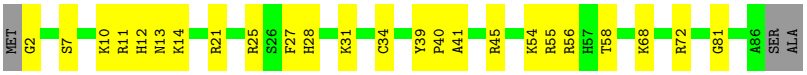
Chain i:



• Molecule 20: 60S ribosomal protein L37-A

Chain j:

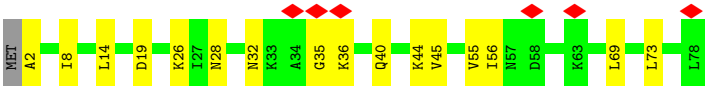




• Molecule 21: 60S ribosomal protein L38

Chain k:



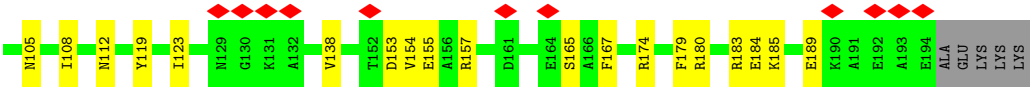


• Molecule 22: 60S ribosomal protein L13-A

Chain L:







• Molecule 23: 60S ribosomal protein L39

Chain l:

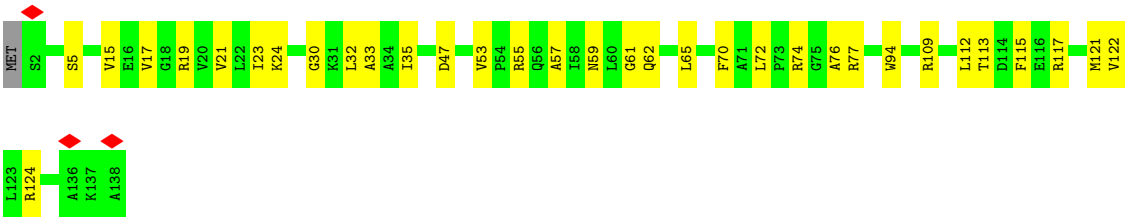




• Molecule 24: 60S ribosomal protein L14-A

Chain M:

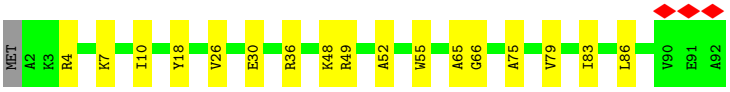




• Molecule 25: 60S ribosomal protein L43-A

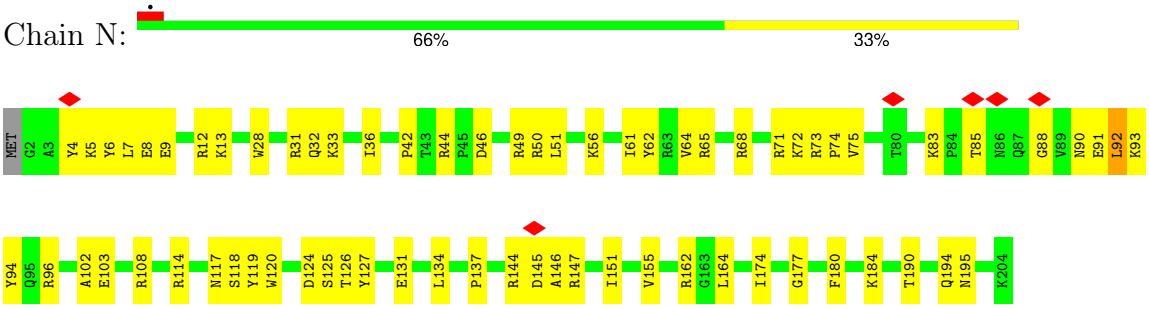
Chain p:





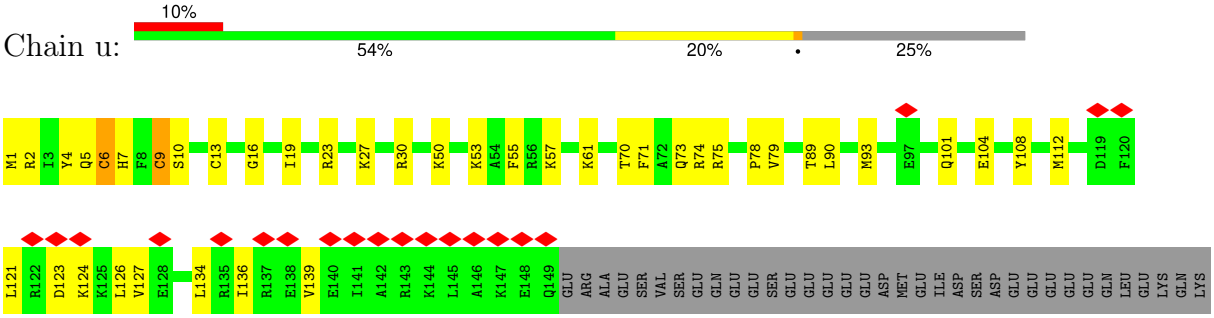
• Molecule 26: Large ribosomal subunit protein eL15A

Chain N:



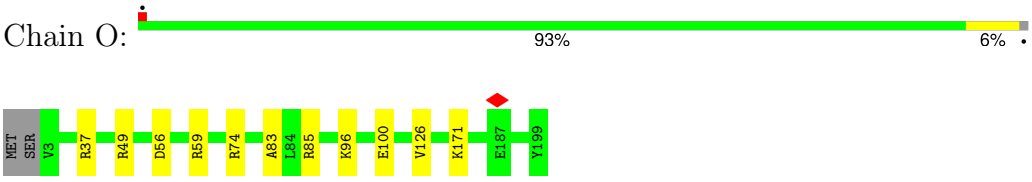
• Molecule 27: Ribosome biogenesis protein RLP24

Chain u:



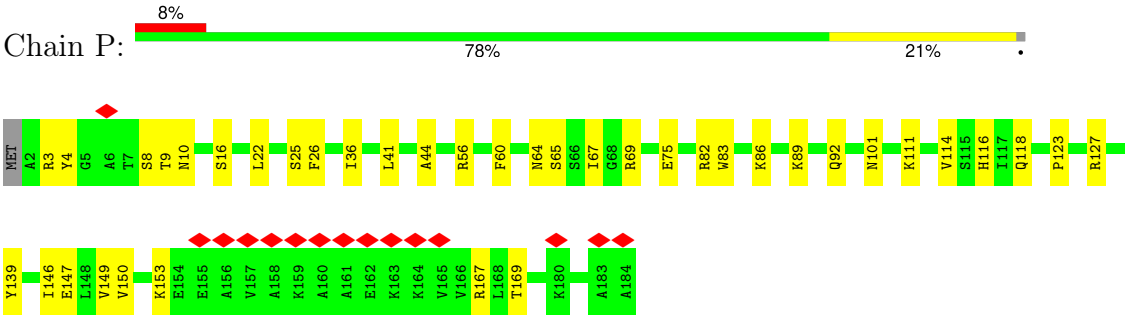
• Molecule 28: Large ribosomal subunit protein uL13A

Chain O:



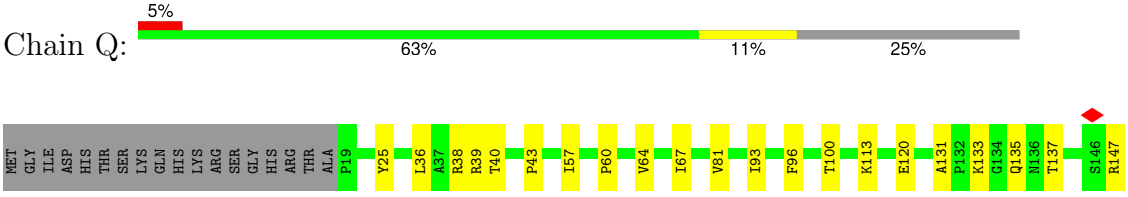
• Molecule 29: 60S ribosomal protein L17-A

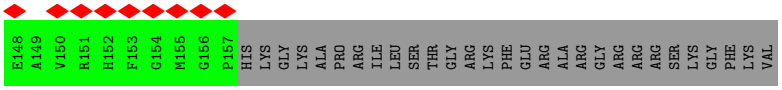
Chain P:



• Molecule 30: 60S ribosomal protein L18-A

Chain Q:

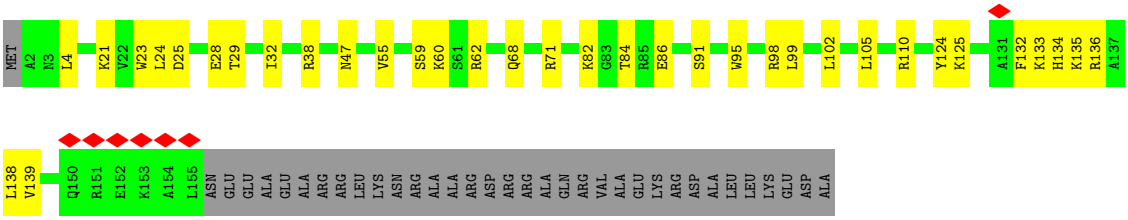




• Molecule 31: 60S ribosomal protein L19-A

Chain R:

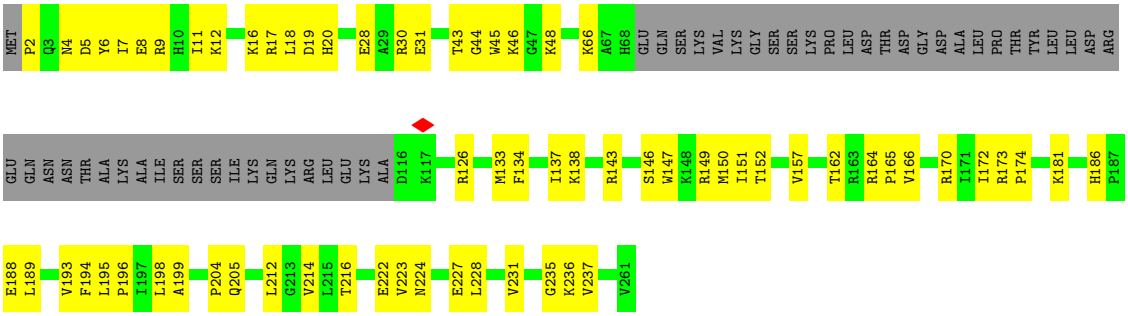




• Molecule 32: Ribosome biogenesis protein NSA2

Chain r:

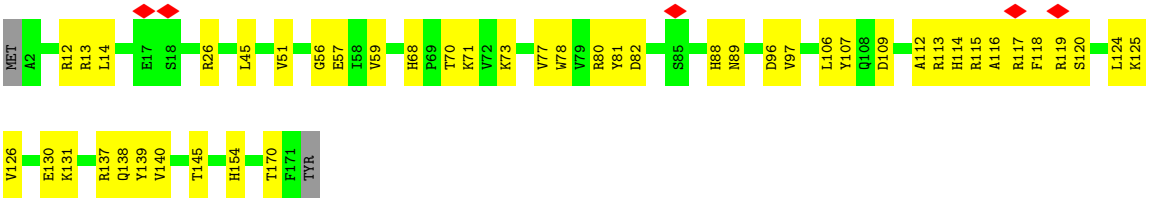




• Molecule 33: Large ribosomal subunit protein eL20A

Chain S:

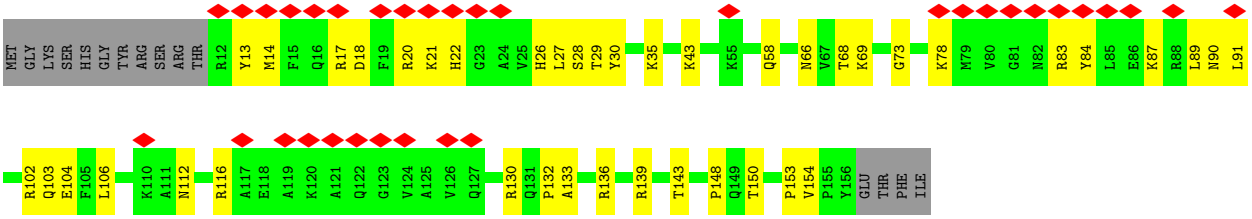




• Molecule 34: 60S ribosomal protein L21-A

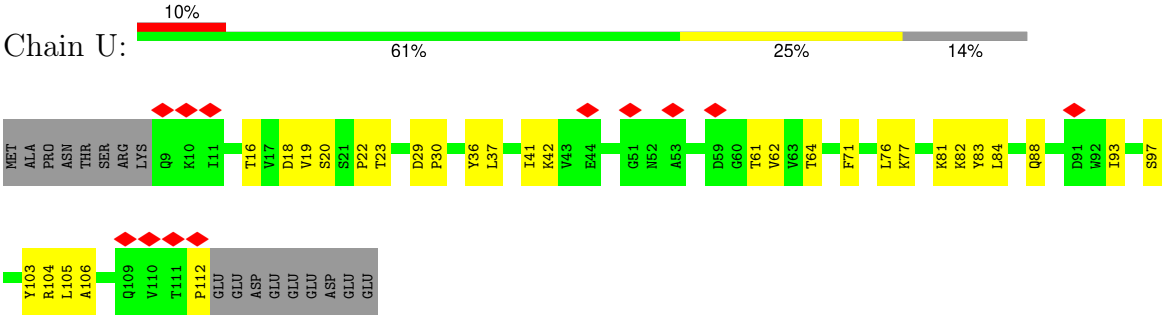
Chain T:





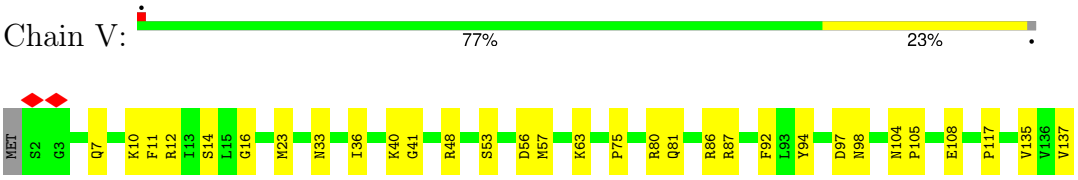
• Molecule 35: 60S ribosomal protein L22-A

Chain U:



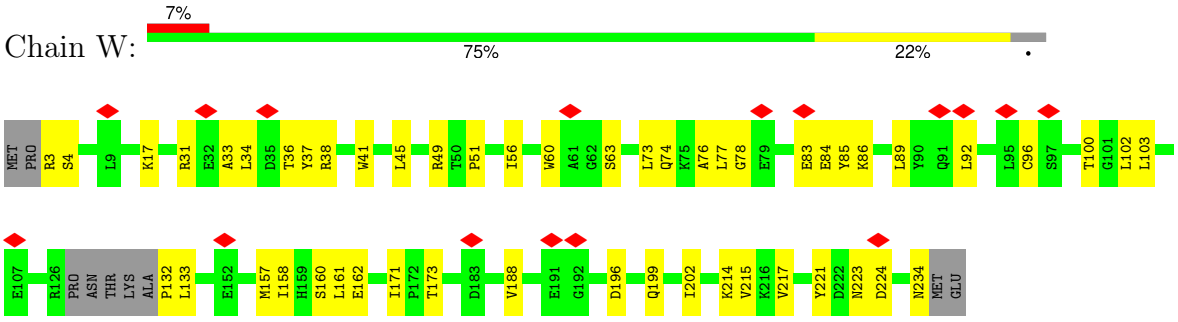
• Molecule 36: 60S ribosomal protein L23-A

Chain V:



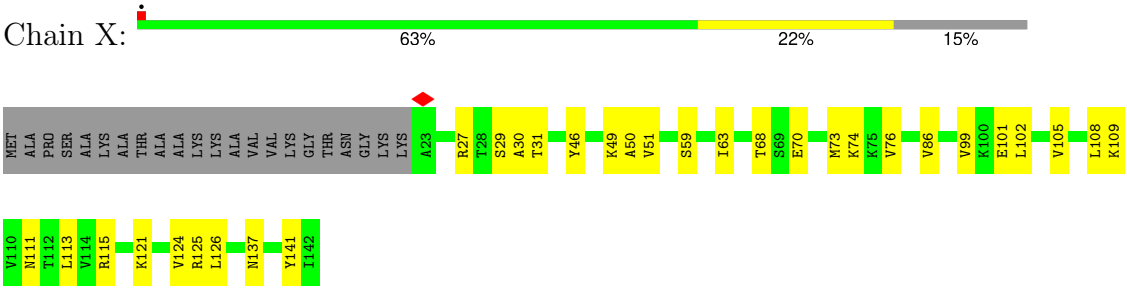
• Molecule 37: Ribosome assembly factor MRT4

Chain W:



• Molecule 38: 60S ribosomal protein L25

Chain X:



• Molecule 39: 60S ribosomal protein L26-A

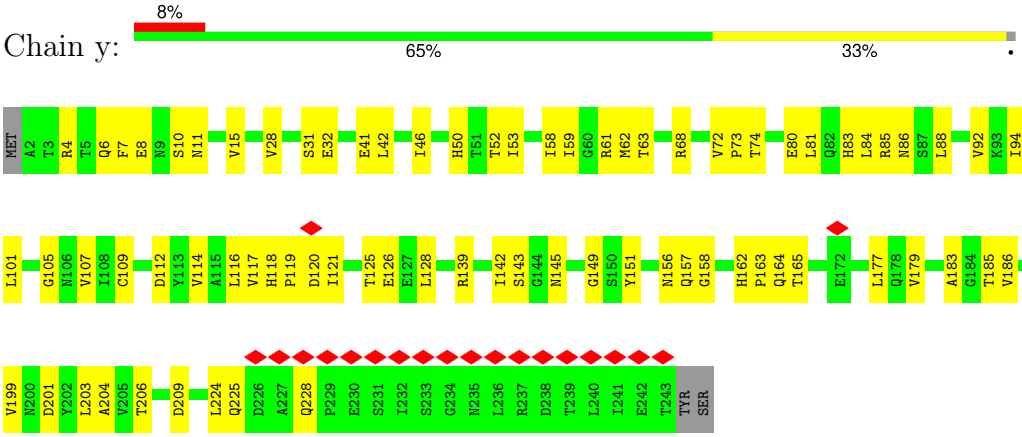
Chain Y:





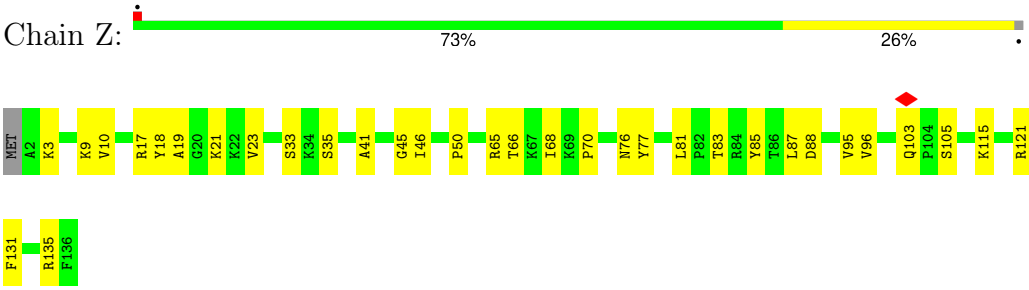
• Molecule 40: Eukaryotic translation initiation factor 6

Chain y:



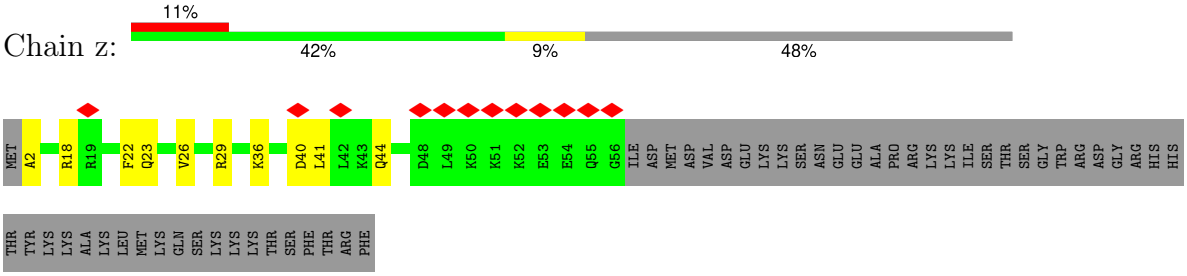
• Molecule 41: 60S ribosomal protein L27-A

Chain Z:



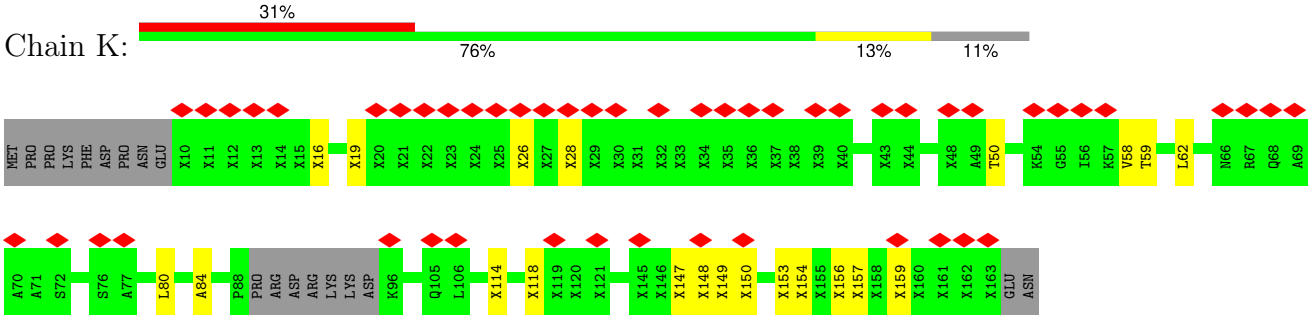
• Molecule 42: UPF0642 protein YBL028C

Chain z:



• Molecule 43: 60S ribosomal protein L12

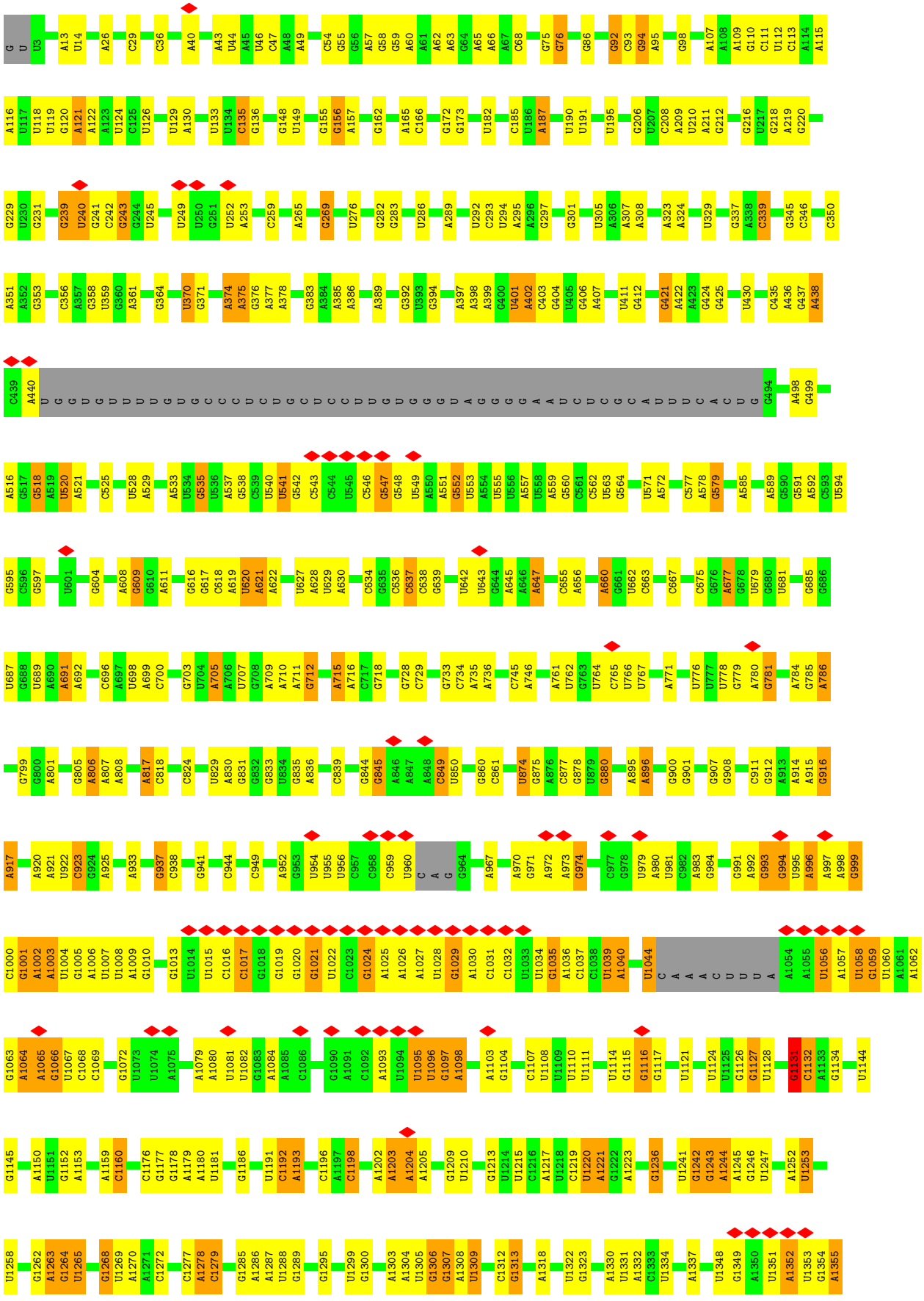
Chain K:

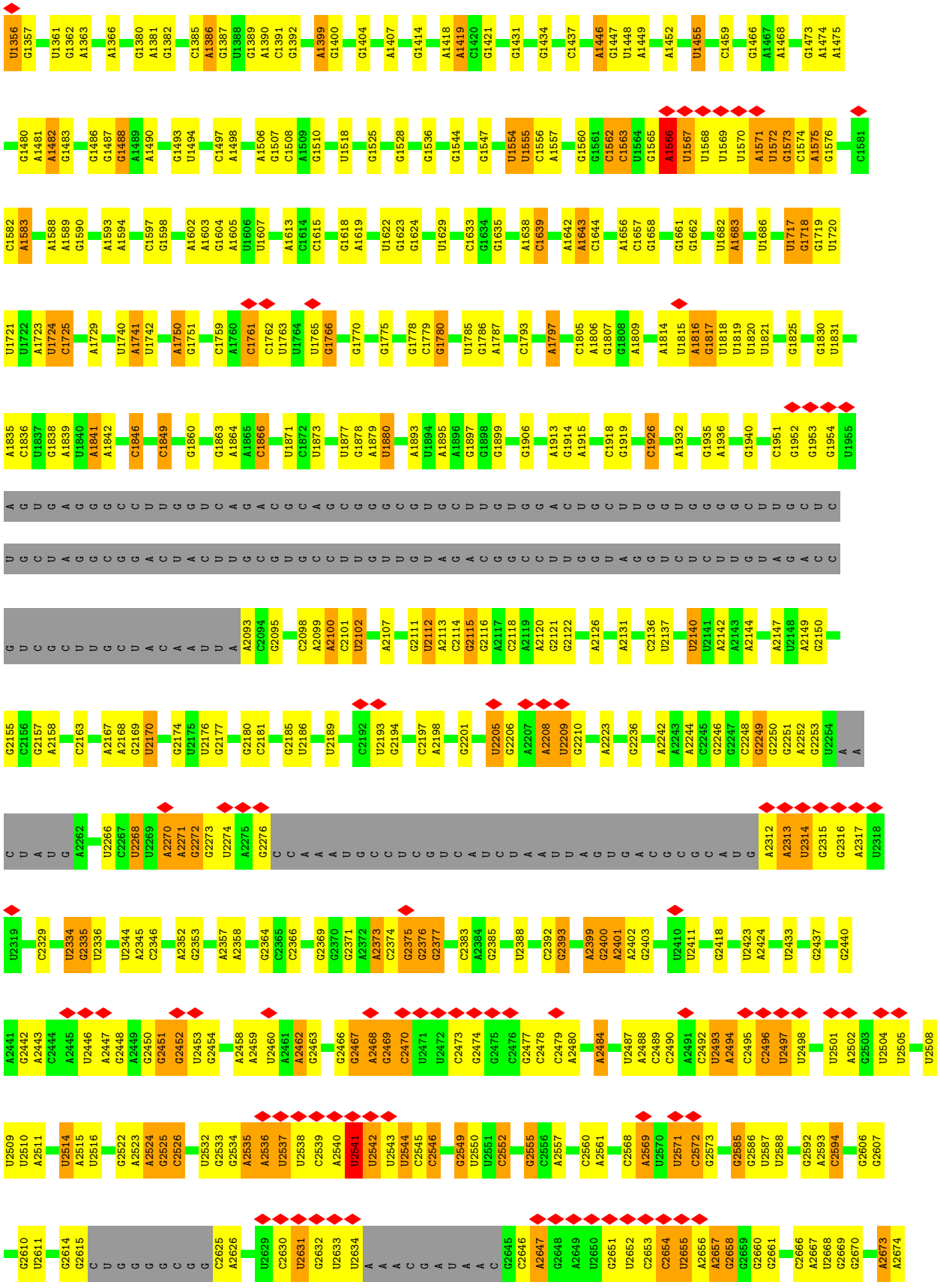


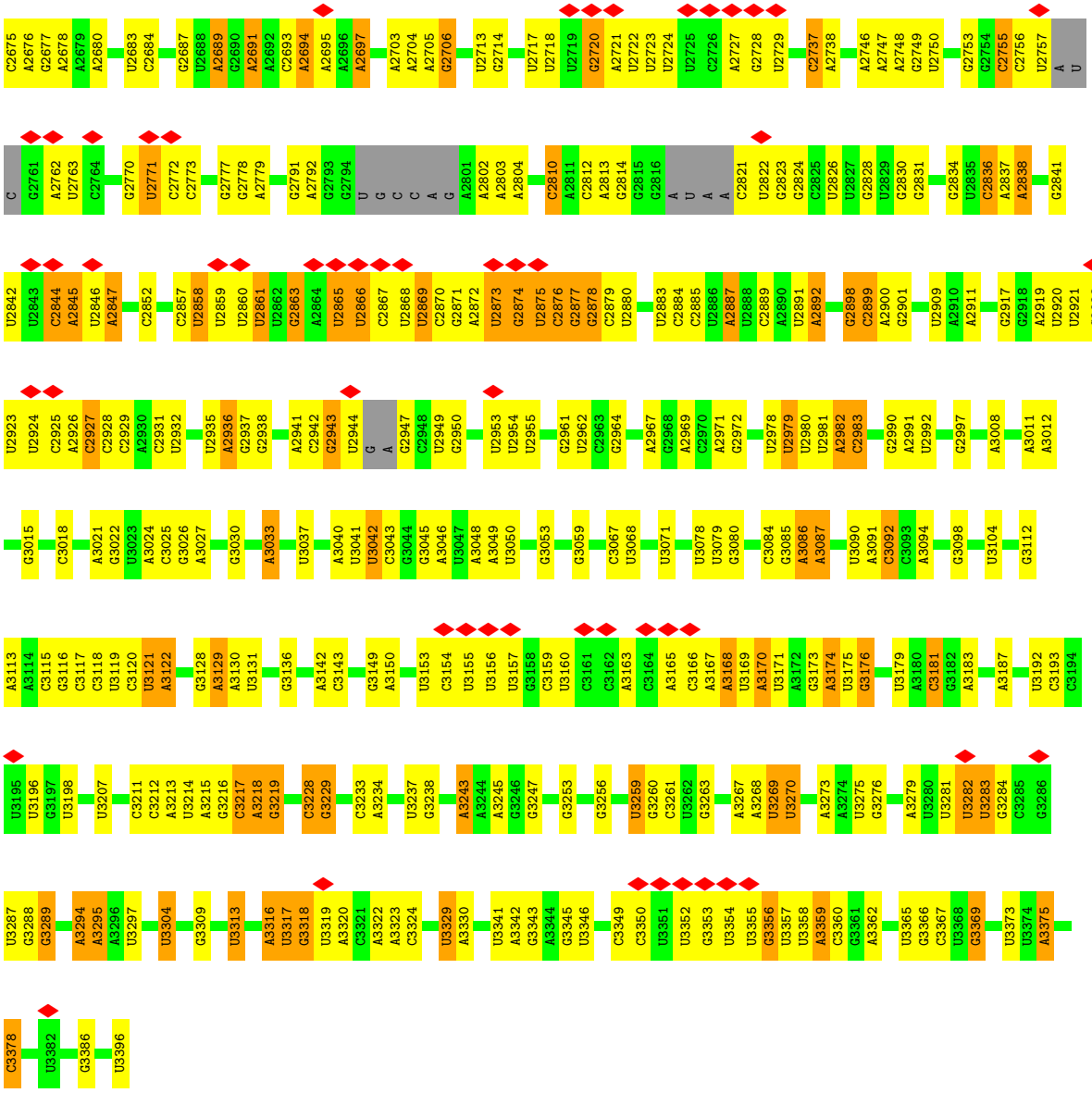
• Molecule 44: 25S ribosomal RNA

Chain 1:





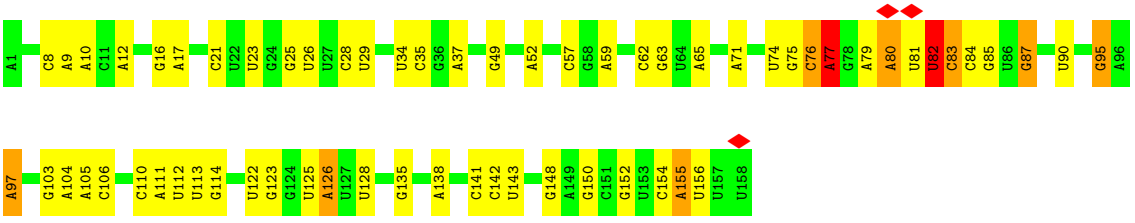




• Molecule 45: 5.8S rRNA

Chain 3:

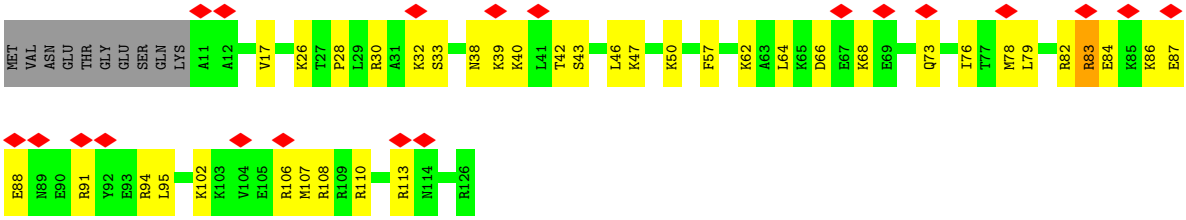




• Molecule 46: rRNA-processing protein CGR1

Chain 5:

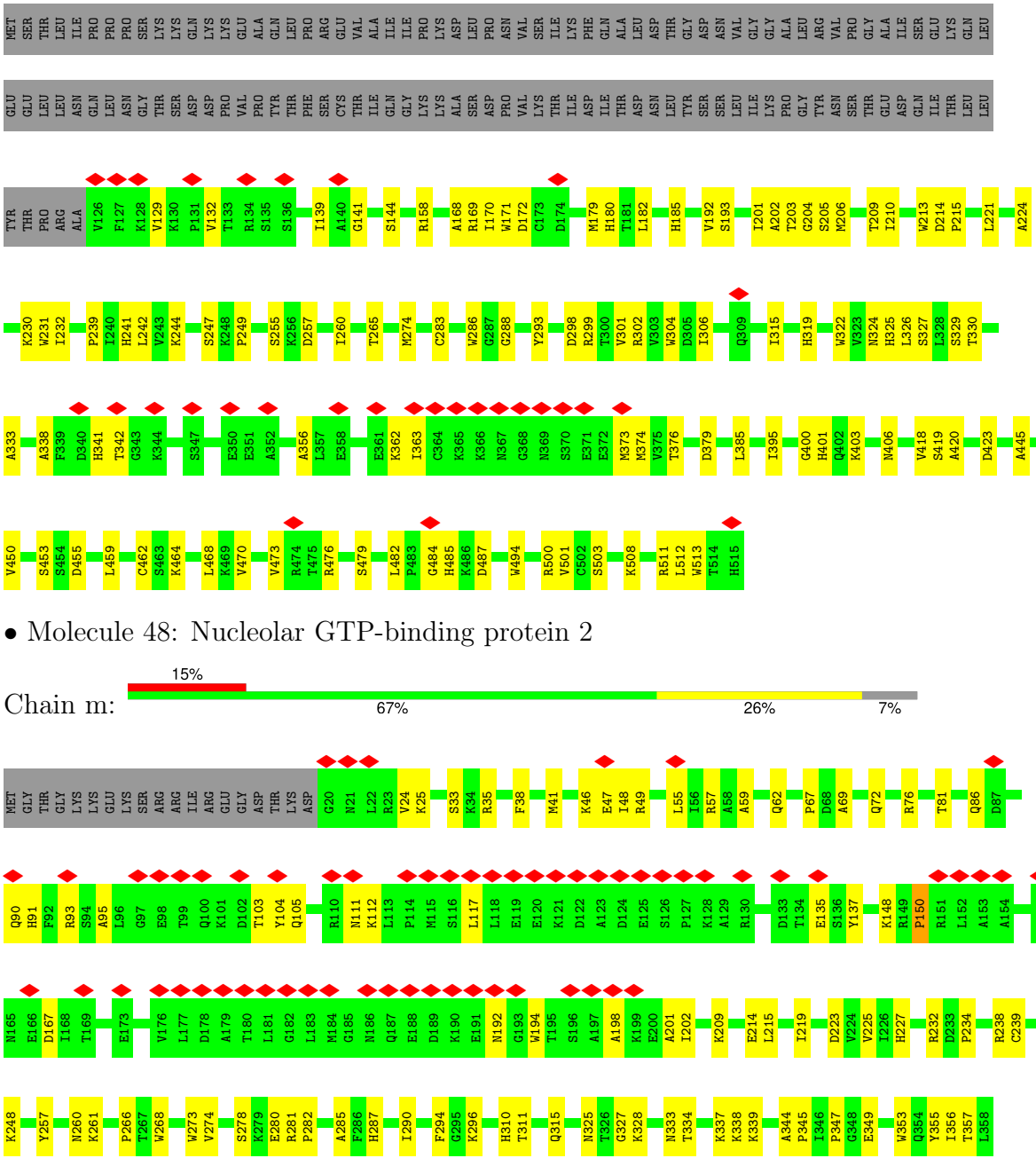




• Molecule 47: Ribosome assembly protein 4

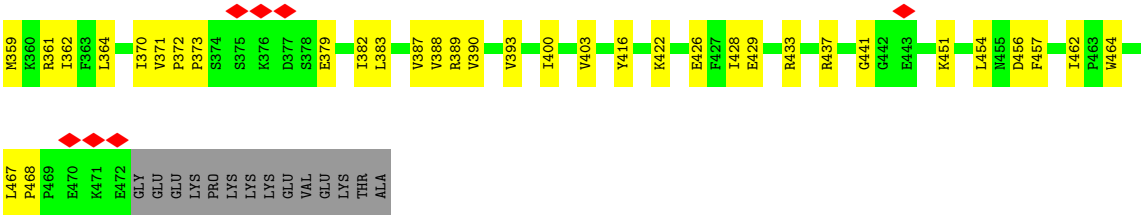
Chain x:





• Molecule 48: Nucleolar GTP-binding protein 2

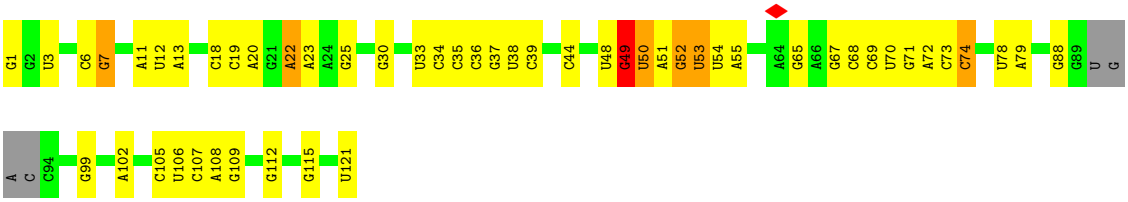
Chain m:



• Molecule 49: 5S rRNA

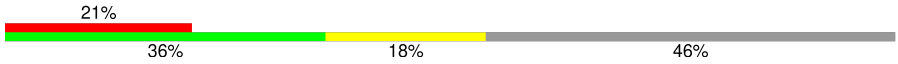
Chain 2:

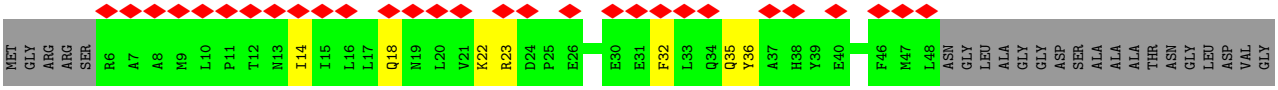


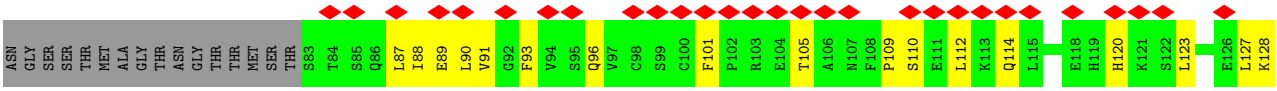


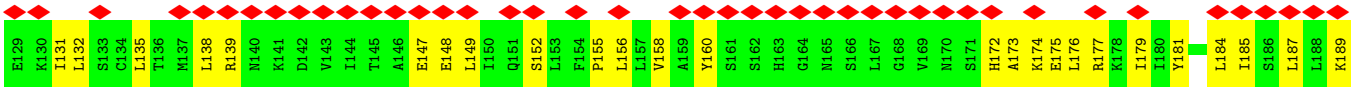
• Molecule 50: Protein SDA1

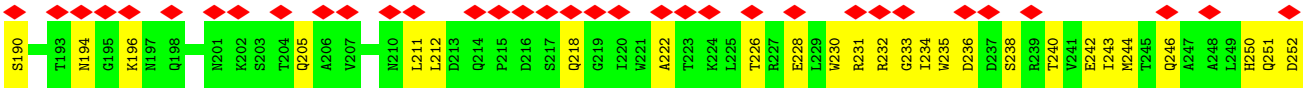
Chain t:

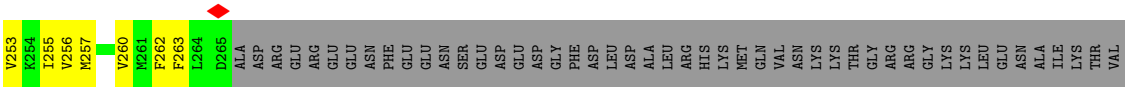


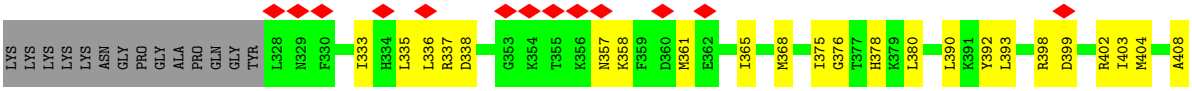


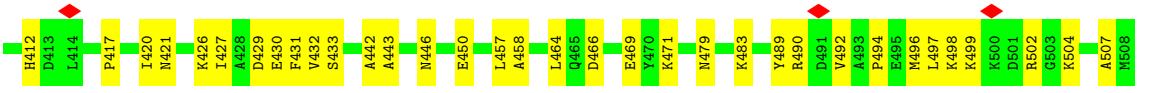


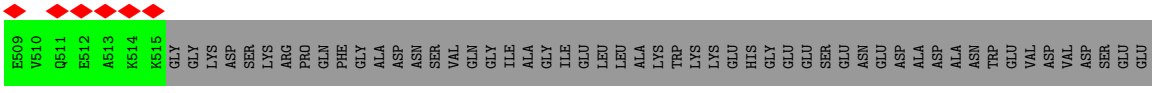


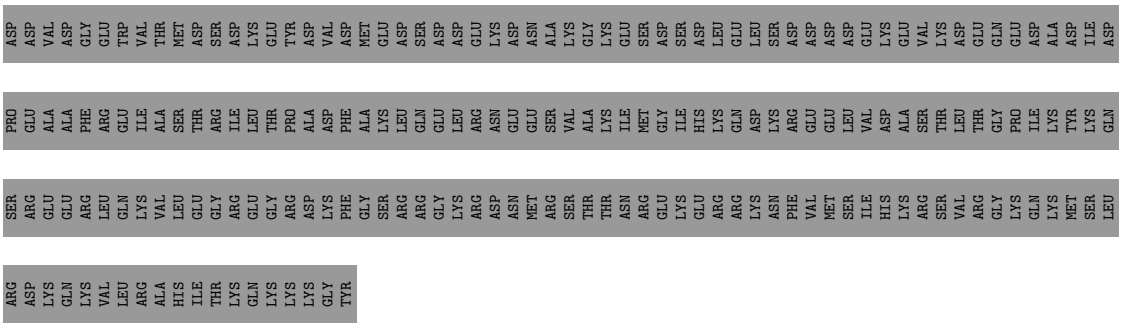








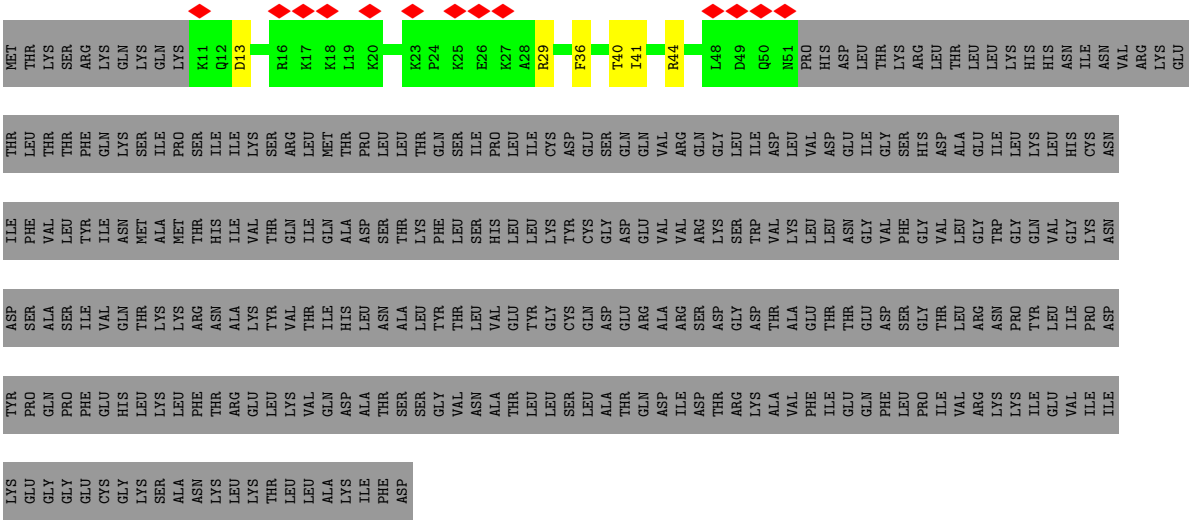




• Molecule 51: Pre-rRNA-processing protein IPI1

Chain n:

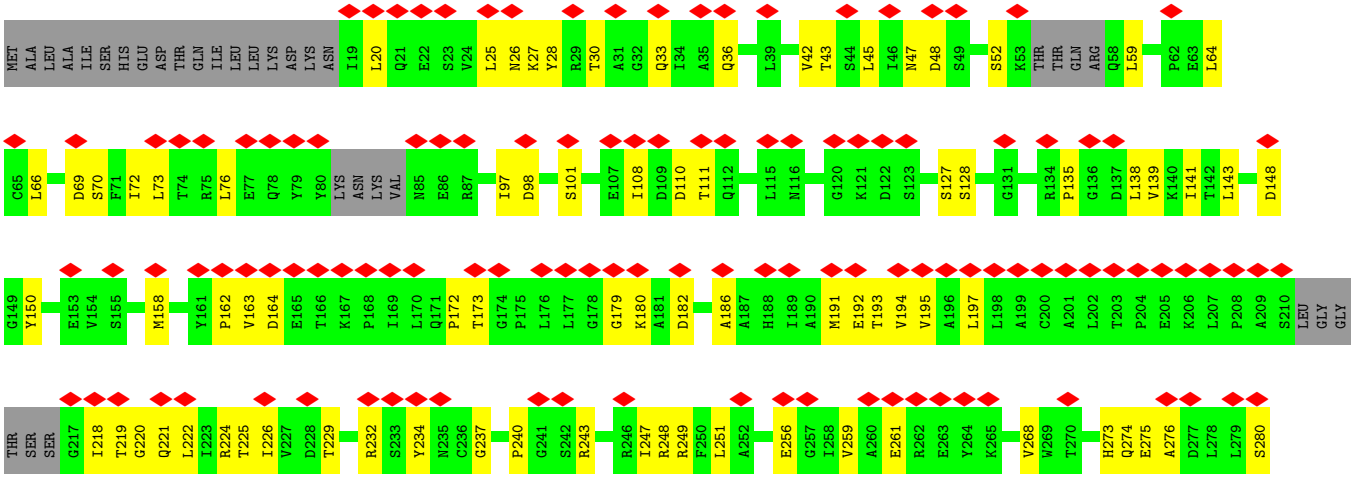


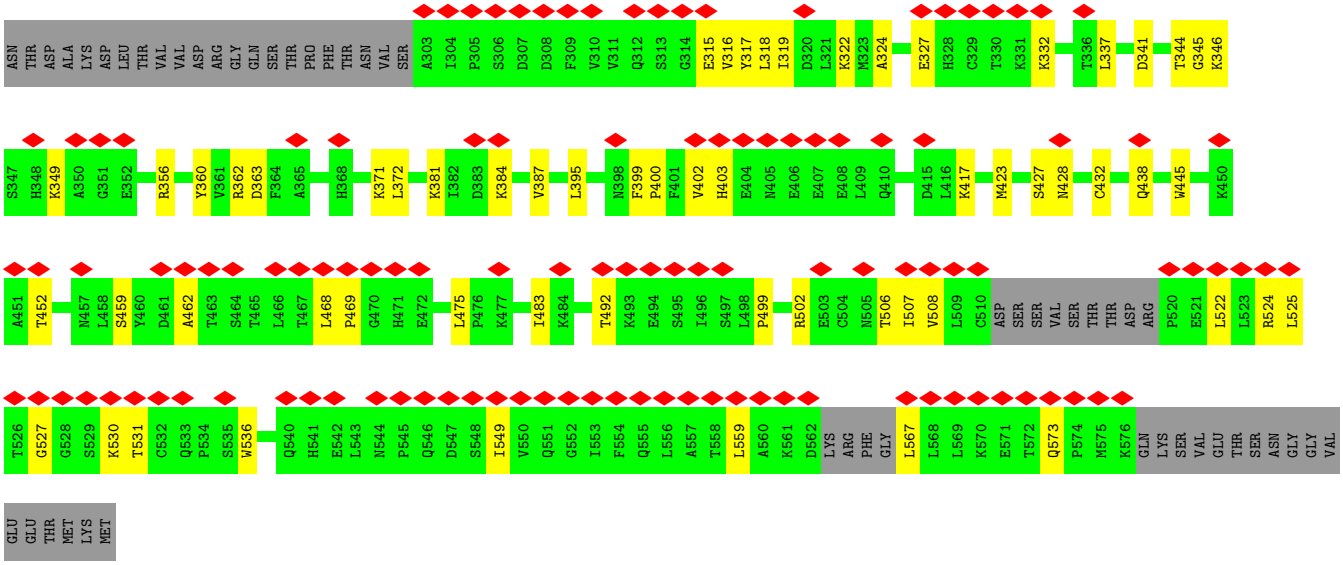


• Molecule 52: Probable metalloprotease ARX1

Chain 4:



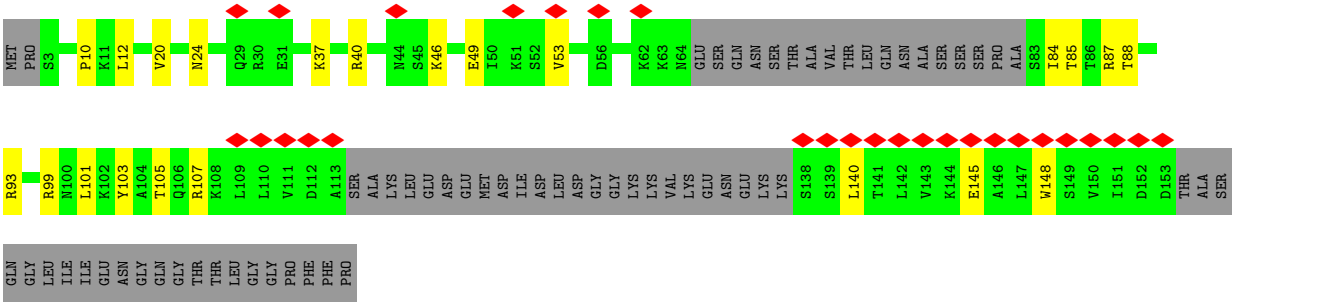




• Molecule 53: Ribosome biogenesis protein ALB1

Chain o:

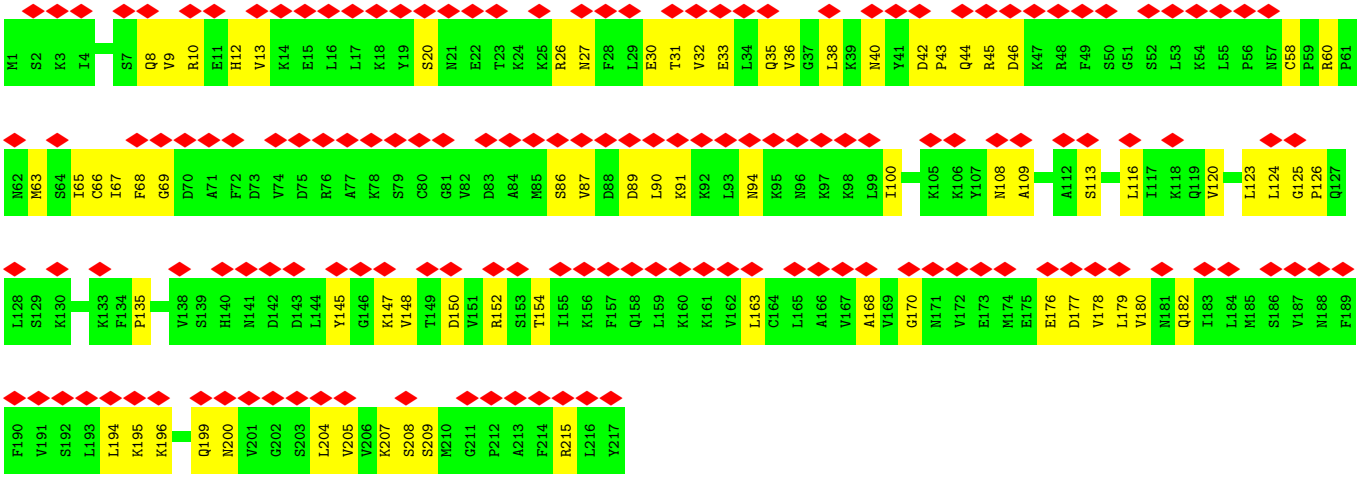




• Molecule 54: Large ribosomal subunit protein uL1A

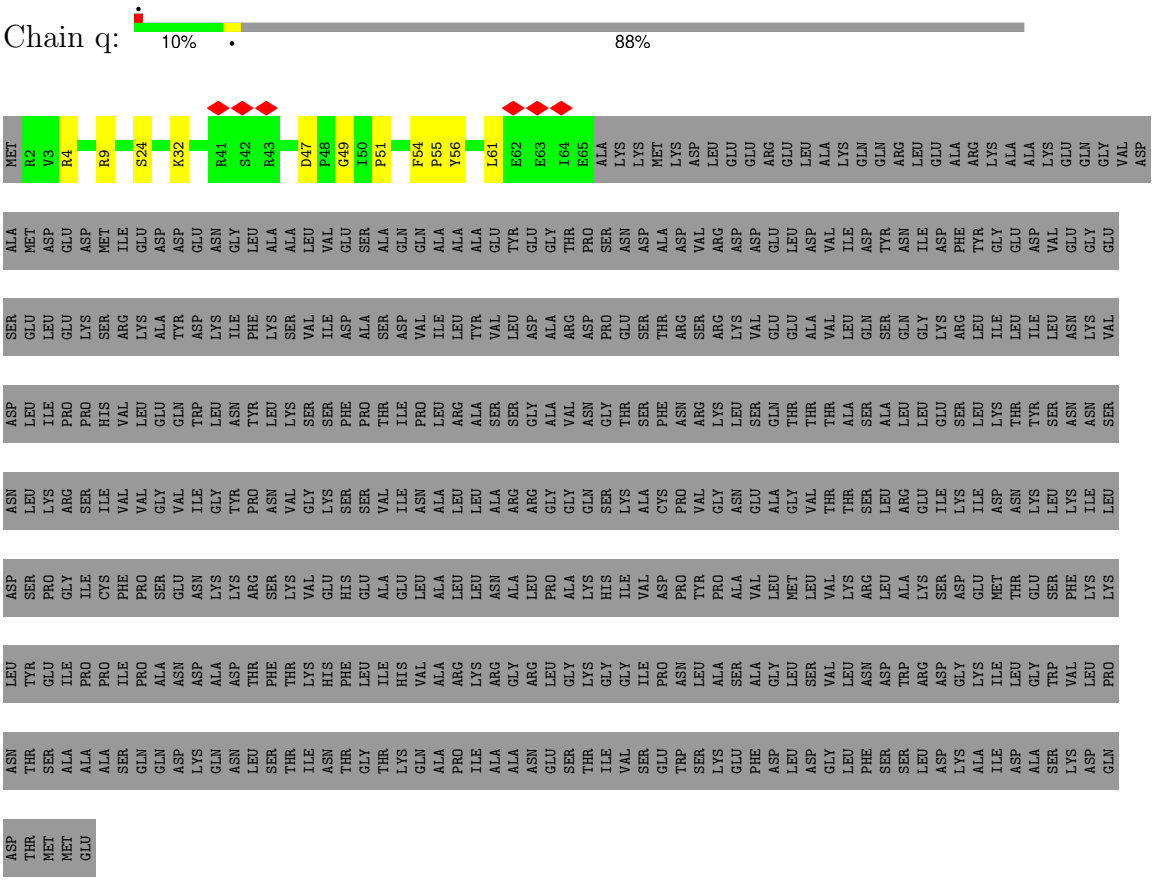
Chain s:





• Molecule 55: Nuclear GTP-binding protein NUG1

Chain q:



• Molecule 56: Small ribosomal subunit protein eS32A

Chain Lr:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	29051	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.891	Depositor
Minimum map value	-1.983	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.140	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	D	0.09	0/2093	0.28	0/2827
2	J	0.11	0/1303	0.30	0/1747
3	A	0.16	0/1897	0.37	0/2550
4	a	0.16	0/758	0.31	0/1023
5	B	0.20	1/3152 (0.0%)	0.38	0/4239
6	b	0.13	0/5305	0.35	0/7130
7	C	0.14	0/2801	0.34	0/3792
8	c	0.14	0/751	0.30	0/1008
9	d	0.13	0/887	0.29	0/1191
10	E	0.13	0/1295	0.33	0/1740
11	e	0.13	0/1041	0.29	0/1394
12	F	0.14	0/1821	0.36	0/2451
13	f	0.16	0/868	0.31	0/1168
14	G	0.16	0/1830	0.41	0/2469
15	g	0.15	0/891	0.32	0/1191
16	I	0.30	1/1072 (0.1%)	0.55	3/1440 (0.2%)
17	H	0.15	0/1514	0.32	0/2039
18	h	0.13	0/978	0.27	0/1301
19	i	0.14	0/749	0.38	1/995 (0.1%)
20	j	0.14	0/685	0.29	0/908
21	k	0.14	0/618	0.35	0/826
22	L	0.14	0/1516	0.37	0/2037
23	l	0.14	0/443	0.29	0/588
24	M	0.14	0/1074	0.31	0/1446
25	p	0.14	0/701	0.34	0/934
26	N	0.16	0/1757	0.34	0/2354
27	u	0.16	0/1278	0.44	2/1699 (0.1%)
28	O	0.14	0/1585	0.27	0/2128
29	P	0.14	0/1461	0.32	0/1964
30	Q	0.22	1/1086 (0.1%)	0.30	0/1466
31	R	0.14	0/1258	0.34	0/1679
32	r	0.16	0/1750	0.42	0/2338

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	S	0.15	0/1460	0.39	0/1962
34	T	0.10	0/1182	0.29	0/1586
35	U	0.13	0/843	0.37	0/1143
36	V	0.13	0/1018	0.33	0/1369
37	W	0.10	0/1843	0.28	0/2483
38	X	0.15	0/974	0.30	0/1314
39	Y	0.14	0/1004	0.30	0/1341
40	y	0.13	0/1848	0.34	0/2516
41	Z	0.15	0/1118	0.36	0/1497
42	z	0.08	0/445	0.20	0/585
43	K	0.11	0/363	0.35	0/494
44	1	0.26	0/74608	0.63	17/116301 (0.0%)
45	3	0.28	0/3746	0.66	4/5832 (0.1%)
46	5	0.15	0/941	0.40	0/1233
47	x	0.12	0/3130	0.31	0/4244
48	m	0.40	2/3722 (0.1%)	0.63	4/5019 (0.1%)
49	2	0.19	0/2787	0.61	1/4339 (0.0%)
50	t	0.14	0/3341	0.42	0/4500
51	n	0.15	0/338	0.38	0/448
52	4	0.16	0/4015	0.43	0/5447
53	o	0.11	0/879	0.28	0/1171
54	s	0.14	0/1745	0.38	0/2342
55	q	0.13	0/540	0.33	0/710
56	Lr	0.11	0/192	0.26	0/246
All	All	0.22	5/158300 (0.0%)	0.53	32/230184 (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
12	F	0	1
14	G	0	1
26	N	0	1
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	m	150	PRO	CG-CD	-20.23	0.81	1.50
16	I	114	PRO	CG-CD	-8.27	1.22	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	m	150	PRO	CB-CG	7.07	1.84	1.49
5	B	185	GLY	C-N	-6.59	1.30	1.33
30	Q	60	PRO	CA-C	5.49	1.54	1.51

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	m	150	PRO	N-CD-CG	-29.10	59.56	103.20
48	m	150	PRO	CA-CB-CG	-21.58	63.50	104.50
16	I	114	PRO	N-CD-CG	-11.55	85.88	103.20
48	m	150	PRO	N-CA-CB	-10.57	93.90	103.31
16	I	114	PRO	CA-CB-CG	-10.52	84.52	104.50
45	3	76	C	OP1-P-O3'	-9.08	80.76	108.00
44	1	3217	C	N1-C2-O2	7.53	123.42	118.90
45	3	76	C	OP2-P-O3'	-7.09	86.74	108.00
44	1	3217	C	C2-N1-C1'	7.02	126.53	118.80
48	m	150	PRO	CA-N-CD	-6.60	102.76	112.00
44	1	2861	U	C2-N1-C1'	6.40	125.38	117.70
44	1	922	U	C2-N1-C1'	6.34	125.31	117.70
27	u	9	CYS	CA-CB-SG	6.26	128.81	114.40
16	I	114	PRO	N-CA-CB	-6.26	97.22	103.48
44	1	3217	C	N3-C2-O2	-6.09	117.64	121.90
44	1	2869	U	C2-N1-C1'	5.88	124.75	117.70
45	3	82	U	N3-C2-O2	-5.82	118.13	122.20
19	i	28	TYR	N-CA-C	-5.78	107.22	114.56
44	1	2861	U	N1-C2-O2	5.67	126.77	122.80
45	3	77	A	O5'-C5'-C4'	5.51	113.81	109.40
27	u	6	CYS	CA-CB-SG	5.44	126.91	114.40
44	1	2268	U	C2-N1-C1'	5.34	124.11	117.70
44	1	1198	C	N1-C2-O2	5.22	122.03	118.90
44	1	1566	A	P-O3'-C3'	5.13	125.85	119.70
44	1	2541	U	P-O3'-C3'	5.11	125.83	119.70
44	1	1198	C	C2-N1-C1'	5.08	124.39	118.80
44	1	922	U	N1-C2-O2	5.08	126.35	122.80
44	1	1131	G	P-O3'-C3'	5.06	125.77	119.70
44	1	2869	U	N1-C2-O2	5.05	126.34	122.80
44	1	2836	C	C2-N1-C1'	5.05	124.36	118.80
49	2	49	G	P-O3'-C3'	5.01	125.72	119.70
44	1	2861	U	N3-C2-O2	-5.01	118.69	122.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	F	158	LYS	Peptide
14	G	30	THR	Peptide
26	N	92	LEU	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	D	2047	0	1988	55	0
2	J	1283	0	1315	34	0
3	A	1863	0	1930	44	0
4	a	742	0	785	17	0
5	B	3081	0	3165	89	0
6	b	5219	0	5266	167	0
7	C	2749	0	2863	64	0
8	c	743	0	797	16	0
9	d	873	0	914	17	0
10	E	1274	0	1361	24	0
11	e	1020	0	1090	21	0
12	F	1784	0	1862	32	0
13	f	850	0	880	18	0
14	G	1798	0	1894	52	0
15	g	881	0	945	21	0
16	I	1056	0	1084	30	0
17	H	1493	0	1566	45	0
18	h	969	0	1078	29	0
19	i	743	0	822	13	0
20	j	670	0	675	18	0
21	k	612	0	682	11	0
22	L	1491	0	1543	48	0
23	l	436	0	475	16	0
24	M	1059	0	1154	25	0
25	p	694	0	734	14	0
26	N	1720	0	1779	58	0
27	u	1256	0	1308	40	0
28	O	1555	0	1659	13	0
29	P	1438	0	1474	33	0
30	Q	1069	0	1149	15	0
31	R	1241	0	1330	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	r	1719	0	1820	59	0
33	S	1425	0	1466	50	0
34	T	1161	0	1212	38	0
35	U	826	0	843	23	0
36	V	1003	0	1048	23	0
37	W	1814	0	1833	33	0
38	X	959	0	1023	22	0
39	Y	993	0	1081	36	0
40	y	1826	0	1813	60	0
41	Z	1092	0	1155	26	0
42	z	444	0	478	10	0
43	K	821	0	438	12	0
44	1	66660	0	33500	757	0
45	3	3353	0	1695	45	0
46	5	934	0	1022	36	0
47	x	3051	0	3000	67	0
48	m	3647	0	3704	106	0
49	2	2494	0	1262	25	0
50	t	3289	0	3400	104	0
51	n	335	0	356	8	0
52	4	3945	0	4016	98	0
53	o	872	0	940	21	0
54	s	1718	0	1811	55	0
55	q	533	0	589	11	0
56	Lr	191	0	235	4	0
57	m	32	0	12	1	0
58	m	1	0	0	0	0
59	m	1	0	0	0	0
60	m	3	0	0	0	0
All	All	148851	0	115319	2272	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (2272) 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)
45:3:79:A:H3'	45:3:80:A:H4'	1.54	0.89
6:b:645:ASP:H	44:1:2401:A:H61	1.20	0.88
14:G:68:ARG:NH1	44:1:2514:U:OP1	2.07	0.87
42:z:2:ALA:N	44:1:2891:U:HO2'	1.75	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:x:204:GLY:HA3	47:x:232:ILE:HD11	1.59	0.85
12:F:156:ILE:HD13	12:F:161:VAL:HB	1.57	0.84
6:b:233:ASN:ND2	44:1:1242:G:OP1	2.10	0.83
5:B:266:ARG:NH1	44:1:2392:C:O2'	2.12	0.82
50:t:139:ARG:HH12	50:t:190:SER:HB2	1.43	0.82
28:O:100:GLU:HG2	53:o:10:PRO:HA	1.64	0.80
25:p:49:ARG:HH21	25:p:52:ALA:HB2	1.46	0.80
44:1:2467:G:H21	44:1:2488:A:H62	1.31	0.79
7:C:132:ALA:HB2	7:C:148:ILE:HG21	1.63	0.79
32:r:137:ILE:HD11	32:r:150:MET:HE3	1.65	0.79
54:s:8:GLN:O	54:s:12:HIS:ND1	2.15	0.79
44:1:967:A:H62	44:1:1115:G:H21	1.30	0.79
5:B:57:VAL:HG22	5:B:73:VAL:HG22	1.65	0.78
45:3:81:U:H4'	45:3:82:U:H5'	1.66	0.78
19:i:34:SER:HB2	19:i:37:THR:H	1.48	0.78
14:G:26:LEU:HD21	41:Z:66:THR:HG21	1.66	0.78
16:I:75:ARG:HE	44:1:2112:U:H2'	1.49	0.78
44:1:627:U:H4'	44:1:1399:A:H1'	1.64	0.78
47:x:501:VAL:HB	47:x:513:TRP:HB2	1.65	0.78
52:4:135:PRO:HB3	52:4:162:PRO:HD3	1.65	0.78
22:L:36:ARG:NH2	44:1:687:U:OP2	2.17	0.77
36:V:81:GLN:O	36:V:98:ASN:ND2	2.17	0.77
5:B:214:MET:HE1	5:B:349:LYS:HE3	1.66	0.77
2:J:20:ASN:HB3	2:J:126:ASP:HB3	1.67	0.77
14:G:81:THR:HG21	14:G:181:LYS:HB2	1.67	0.77
14:G:34:PHE:HA	14:G:39:ALA:HB3	1.66	0.76
17:H:23:ARG:HB2	17:H:39:LYS:HD2	1.66	0.76
6:b:434:GLU:HA	6:b:441:VAL:HG22	1.67	0.76
44:1:2919:A:H61	44:1:2927:C:H42	1.33	0.76
31:R:47:ASN:HB3	44:1:1761:C:H41	1.51	0.76
22:L:53:LEU:HB2	22:L:55:ARG:HH12	1.50	0.75
22:L:62:THR:HG22	22:L:64:LYS:H	1.51	0.75
15:g:96:GLU:OE1	44:1:2555:G:N1	2.19	0.75
44:1:2678:A:H4'	46:5:110:ARG:HG2	1.69	0.75
2:J:133:ARG:NH2	2:J:158:ASP:OD2	2.20	0.75
13:f:56:SER:OG	53:o:24:ASN:ND2	2.20	0.74
15:g:90:ILE:HG12	41:Z:81:LEU:HD11	1.69	0.74
40:y:8:GLU:HB3	44:1:3018:C:H5"	1.67	0.74
47:x:244:LYS:HE3	47:x:247:SER:HB3	1.69	0.74
3:A:21:ARG:HD3	44:1:824:C:H5"	1.69	0.74
44:1:974:G:H1	44:1:1108:U:H3	1.32	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:r:195:LEU:HD11	32:r:223:VAL:HG13	1.67	0.74
14:G:144:GLU:HA	14:G:173:MET:HE2	1.70	0.74
44:1:542:G:H1	44:1:549:U:H3	1.36	0.74
52:4:381:LYS:HB3	52:4:395:LEU:HD12	1.70	0.73
27:u:16:GLY:O	44:1:3050:U:O2'	2.06	0.73
48:m:311:THR:HA	48:m:361:ARG:HH22	1.52	0.73
5:B:10:ARG:NH1	5:B:11:HIS:O	2.21	0.73
5:B:36:ASP:HB3	5:B:39:LYS:HD3	1.71	0.73
16:I:80:LEU:O	16:I:116:LYS:NZ	2.17	0.73
39:Y:91:ASN:OD1	44:1:378:A:O2'	2.05	0.73
44:1:1683:A:H61	44:1:3071:U:H3	1.35	0.73
5:B:229:VAL:HG11	5:B:249:VAL:HG23	1.71	0.73
44:1:1414:G:OP1	53:o:93:ARG:NH2	2.22	0.73
53:o:53:VAL:HG13	53:o:87:ARG:HE	1.53	0.72
3:A:193:ARG:HH21	44:1:2174:G:P	2.12	0.72
6:b:41:ARG:HD2	44:1:2942:C:H2'	1.71	0.72
5:B:215:ILE:HD12	5:B:338:LEU:HD12	1.69	0.72
50:t:242:GLU:O	50:t:246:GLN:NE2	2.22	0.72
27:u:6:CYS:HB3	27:u:10:SER:N	2.05	0.72
15:g:74:ARG:NH2	44:1:1639:C:OP2	2.22	0.72
48:m:310:HIS:O	48:m:361:ARG:NH2	2.23	0.72
50:t:238:SER:HA	50:t:335:LEU:HD21	1.71	0.72
44:1:1940:G:H21	44:1:3362:A:H8	1.38	0.71
3:A:200:ARG:NH1	44:1:2147:A:OP2	2.22	0.71
22:L:64:LYS:O	22:L:67:ARG:NH1	2.23	0.71
54:s:38:LEU:HB2	54:s:163:LEU:HD12	1.72	0.71
48:m:225:VAL:HG11	48:m:246:MET:HE1	1.70	0.71
48:m:403:VAL:HG13	48:m:457:PHE:CE2	2.25	0.71
5:B:236:LYS:HD3	44:1:2880:U:H5"	1.72	0.71
4:a:75:LEU:HD22	4:a:78:LEU:HD22	1.70	0.71
44:1:3092:C:O2'	44:1:3094:A:OP2	2.09	0.71
5:B:47:LEU:HD12	5:B:335:ILE:HD11	1.73	0.71
22:L:18:TRP:NE1	44:1:799:G:O2'	2.19	0.71
24:M:124:ARG:NH2	44:1:3212:C:OP2	2.23	0.71
6:b:65:LEU:HD12	44:1:2863:G:H1'	1.70	0.71
4:a:117:ARG:NH2	44:1:718:G:OP1	2.23	0.71
34:T:78:LYS:NZ	44:1:2724:U:OP1	2.24	0.70
9:d:9:THR:HG23	9:d:109:VAL:HB	1.71	0.70
44:1:2400:G:HO2'	44:1:2979:U:H3	1.37	0.70
11:e:101:SER:OG	44:1:1391:C:O2'	2.09	0.70
44:1:1831:U:O2'	45:3:114:G:OP1	2.09	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:1:2137:U:OP2	44:1:2142:A:N6	2.24	0.70
32:r:11:ILE:HD12	32:r:16:LYS:HD2	1.73	0.70
44:1:2492:C:OP1	54:s:35:GLN:NE2	2.24	0.70
44:1:3021:A:H62	44:1:3033:A:H2	1.40	0.70
10:E:46:ARG:NH2	44:1:3268:A:OP1	2.25	0.69
40:y:143:SER:HB2	40:y:165:THR:HA	1.72	0.69
6:b:478:TYR:HB2	6:b:481:PHE:HB2	1.74	0.69
14:G:101:THR:HG22	14:G:104:GLU:HG2	1.74	0.69
33:S:130:GLU:OE1	55:q:56:TYR:OH	2.07	0.69
20:j:13:ASN:ND2	44:1:901:G:OP1	2.22	0.69
17:H:21:LYS:HG3	17:H:22:SER:H	1.57	0.69
34:T:18:ASP:HB2	34:T:21:LYS:HD2	1.74	0.69
18:h:104:GLN:NE2	44:1:112:U:OP1	2.22	0.69
32:r:17:ARG:HB2	32:r:20:HIS:HB2	1.75	0.69
25:p:49:ARG:NH2	44:1:1793:C:OP2	2.24	0.69
3:A:69:TYR:OH	44:1:2557:A:OP1	2.10	0.69
37:W:157:MET:HE2	37:W:161:LEU:HD11	1.74	0.69
44:1:2198:A:H62	44:1:2246:G:H21	1.38	0.69
3:A:215:ASN:ND2	44:1:2969:A:N7	2.41	0.69
18:h:34:GLN:NE2	52:4:344:THR:O	2.26	0.69
40:y:121:ILE:O	40:y:139:ARG:NH2	2.26	0.69
2:J:79:ILE:HG12	2:J:82:ARG:HH21	1.58	0.68
20:j:21:ARG:NH2	20:j:41:ALA:O	2.19	0.68
52:4:248:ARG:HE	52:4:249:ARG:H	1.41	0.68
26:N:155:VAL:O	26:N:162:ARG:NH2	2.22	0.68
44:1:1131:G:O2'	44:1:1132:C:O4'	2.11	0.68
44:1:2375:G:N2	44:1:2377:G:N7	2.40	0.68
6:b:644:THR:OG1	44:1:2401:A:N6	2.27	0.68
44:1:2451:G:N2	44:1:2495:C:O2	2.26	0.68
47:x:406:ASN:ND2	47:x:448:TYR:O	2.26	0.68
5:B:214:MET:O	5:B:341:SER:OG	2.12	0.68
2:J:48:SER:HB2	2:J:66:ALA:HB3	1.76	0.68
44:1:2964:G:OP1	48:m:35:ARG:NH2	2.25	0.68
50:t:376:GLY:HA2	50:t:412:HIS:CE1	2.29	0.68
5:B:37:ARG:NH2	5:B:156:SER:O	2.26	0.68
18:h:118:ILE:HG12	22:L:123:ILE:HG22	1.75	0.68
5:B:168:LYS:O	5:B:319:ASN:ND2	2.26	0.68
6:b:587:ASP:HB2	44:1:1518:U:H4'	1.76	0.68
8:c:52:ARG:NH1	44:1:1729:A:O4'	2.26	0.68
44:1:2962:U:H5"	48:m:357:THR:HG23	1.76	0.67
26:N:62:TYR:HD2	26:N:134:LEU:HD13	1.57	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:1:3042:U:OP2	44:1:3092:C:N4	2.27	0.67
52:4:337:LEU:HD13	52:4:438:GLN:HG3	1.77	0.67
27:u:112:MET:HE1	44:1:3367:C:H5"	1.76	0.67
16:I:58:MET:HE3	16:I:63:ALA:HB1	1.77	0.67
16:I:108:ILE:HA	16:I:112:VAL:HB	1.76	0.67
31:R:68:GLN:OE1	31:R:71:ARG:NH2	2.26	0.67
52:4:173:THR:HA	52:4:536:TRP:HZ3	1.59	0.67
6:b:509:ASN:HA	9:d:61:LYS:HE3	1.76	0.67
44:1:2872:A:O2'	44:1:2873:U:O2	2.11	0.67
22:L:100:ARG:NH1	44:1:76:G:O2'	2.28	0.67
43:K:19:UNK:HA	43:K:58:VAL:HG13	1.76	0.67
39:Y:16:ARG:NH1	44:1:216:G:OP1	2.27	0.67
44:1:920:A:OP1	44:1:923:C:N4	2.28	0.67
2:J:22:SER:OG	44:1:2675:C:N4	2.28	0.67
50:t:251:GLN:O	50:t:358:LYS:NZ	2.28	0.67
1:D:240:TYR:O	1:D:244:HIS:ND1	2.28	0.66
36:V:80:ARG:NH1	36:V:117:PRO:O	2.29	0.66
30:Q:39:ARG:NH1	44:1:1348:U:OP1	2.28	0.66
34:T:83:ARG:NH1	34:T:84:TYR:O	2.29	0.66
36:V:14:SER:O	36:V:81:GLN:NE2	2.26	0.66
6:b:595:ASP:HB3	52:4:483:ILE:HD13	1.76	0.66
10:E:60:ASP:OD1	10:E:62:THR:OG1	2.12	0.66
17:H:41:ILE:HD11	17:H:67:ALA:HB1	1.77	0.66
20:j:72:ARG:NH1	45:3:95:G:OP2	2.29	0.66
44:1:1778:G:O2'	44:1:1780:G:OP2	2.13	0.66
3:A:80:GLU:HG3	25:p:66:GLY:HA2	1.76	0.66
7:C:64:SER:OG	44:1:806:A:OP1	2.12	0.66
17:H:80:THR:OG1	17:H:86:TYR:OH	2.14	0.66
47:x:232:ILE:HA	47:x:255:SER:HA	1.78	0.66
6:b:609:GLU:OE2	44:1:401:U:O2'	2.13	0.66
26:N:114:ARG:HD3	26:N:137:PRO:HG3	1.76	0.66
4:a:125:VAL:HG11	4:a:138:ILE:HD13	1.78	0.66
32:r:134:PHE:O	48:m:62:GLN:NE2	2.28	0.66
54:s:196:LYS:HB3	54:s:199:GLN:HB3	1.77	0.66
5:B:260:VAL:HG11	5:B:266:ARG:HH21	1.59	0.66
5:B:124:LYS:NZ	44:1:3297:U:O4	2.29	0.66
15:g:54:ILE:HG23	15:g:70:LYS:HA	1.77	0.66
37:W:33:ALA:HA	37:W:36:THR:HG22	1.78	0.66
6:b:184:LEU:HD22	6:b:220:ASP:HB2	1.78	0.65
39:Y:2:ALA:N	44:1:212:G:OP2	2.28	0.65
47:x:193:SER:HB3	47:x:202:ALA:HB3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:t:365:ILE:HA	50:t:368:MET:HE2	1.76	0.65
9:d:55:LEU:HB2	9:d:95:PRO:HD3	1.78	0.65
1:D:109:THR:HG23	1:D:110:LEU:HD12	1.77	0.65
6:b:149:TYR:HB2	48:m:137:TYR:HB3	1.76	0.65
6:b:277:LEU:HA	48:m:161:VAL:HG21	1.79	0.65
6:b:622:SER:OG	23:l:46:ARG:NH1	2.30	0.65
30:Q:43:PRO:HB2	44:1:728:G:H5"	1.78	0.65
52:4:36:GLN:HE22	52:4:527:GLY:H	1.42	0.65
11:e:104:ASN:ND2	44:1:1389:G:OP1	2.27	0.65
13:f:21:ARG:NH2	44:1:1150:A:O3'	2.29	0.65
17:H:9:GLN:OE1	17:H:52:LEU:HD21	1.97	0.65
43:K:59:THR:HA	43:K:80:LEU:HD11	1.78	0.65
44:1:1657:C:O2'	44:1:1797:A:OP2	2.13	0.65
37:W:49:ARG:HG2	37:W:51:PRO:HD2	1.79	0.65
26:N:114:ARG:NH1	26:N:151:ILE:O	2.30	0.65
29:P:8:SER:H	53:o:84:ILE:HG13	1.61	0.65
13:f:16:TYR:OH	13:f:89:LEU:O	2.10	0.65
50:t:375:ILE:HA	50:t:380:LEU:HB2	1.78	0.65
6:b:577:THR:HG21	6:b:581:VAL:HG22	1.78	0.65
13:f:56:SER:O	13:f:63:LYS:NZ	2.25	0.65
19:i:9:ILE:HA	19:i:13:LYS:HE3	1.79	0.65
44:1:952:A:N3	44:1:1114:U:O2'	2.26	0.65
48:m:325:ASN:ND2	48:m:345:PRO:O	2.30	0.65
16:I:97:ASN:H	27:u:73:GLN:HA	1.62	0.65
26:N:93:LYS:O	44:1:289:A:O2'	2.14	0.65
39:Y:74:TYR:HE2	39:Y:77:LYS:HG3	1.62	0.65
44:1:2197:C:H4'	44:1:2198:A:H5'	1.79	0.65
14:G:38:GLN:NE2	44:1:2549:G:O2'	2.30	0.64
32:r:196:PRO:HG2	32:r:224:ASN:HD21	1.62	0.64
34:T:136:ARG:HD3	34:T:139:ARG:HH12	1.61	0.64
44:1:2205:U:H3	50:t:96:GLN:CD	2.06	0.64
54:s:10:ARG:HH21	54:s:180:VAL:HG11	1.61	0.64
5:B:173:GLN:NE2	44:1:3313:U:O5'	2.30	0.64
11:e:42:VAL:O	11:e:52:GLN:NE2	2.30	0.64
21:k:8:ILE:HD11	21:k:56:ILE:HD11	1.78	0.64
37:W:3:ARG:HG2	44:1:1210:U:H5	1.63	0.64
54:s:65:ILE:HG22	54:s:109:ALA:HB3	1.79	0.64
14:G:133:LYS:HG2	14:G:142:LEU:HD11	1.79	0.64
33:S:13:ARG:HA	33:S:56:GLY:HA2	1.78	0.64
14:G:246:MET:HA	14:G:249:ARG:HE	1.63	0.64
22:L:75:PHE:O	22:L:76:THR:OG1	2.14	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:1:2982:A:H4'	44:1:2983:C:H2'	1.79	0.64
47:x:286:TRP:HZ2	47:x:306:ILE:HD13	1.63	0.64
21:k:26:LYS:NZ	21:k:28:ASN:OD1	2.29	0.64
2:J:16:LYS:HE3	2:J:130:VAL:HG21	1.78	0.64
17:H:36:LYS:HZ3	17:H:74:LEU:HD13	1.61	0.64
44:1:2469:G:H5'	54:s:27:ASN:HB3	1.80	0.64
5:B:13:HIS:CD2	5:B:15:GLY:H	2.15	0.64
5:B:85:VAL:HB	5:B:202:THR:HG22	1.79	0.64
7:C:329:PRO:HB3	12:F:41:ARG:HH21	1.62	0.64
30:Q:57:ILE:HD11	30:Q:147:ARG:CZ	2.28	0.64
31:R:110:ARG:NH1	44:1:1719:G:OP1	2.31	0.64
6:b:418:ASP:HA	6:b:428:LYS:HD3	1.80	0.64
44:1:2253:G:OP1	50:t:177:ARG:NH2	2.31	0.64
50:t:128:LYS:HE3	50:t:176:LEU:HD11	1.79	0.64
50:t:88:ILE:HD11	50:t:127:LEU:HA	1.78	0.63
54:s:46:ASP:OD2	54:s:195:LYS:NZ	2.30	0.63
9:d:51:LEU:HB2	9:d:55:LEU:HD23	1.80	0.63
22:L:75:PHE:O	22:L:101:ARG:NH2	2.31	0.63
41:Z:88:ASP:H	41:Z:121:ARG:HH22	1.45	0.63
44:1:2615:G:H1	48:m:57:ARG:HH12	1.44	0.63
47:x:324:ASN:ND2	47:x:379:ASP:OD1	2.30	0.63
48:m:290:ILE:HG22	48:m:334:THR:HA	1.81	0.63
4:a:71:PRO:HG2	4:a:109:TYR:HA	1.80	0.63
44:1:3167:A:H61	44:1:3283:U:H3	1.45	0.63
13:f:97:SER:OG	44:1:3174:A:OP1	2.17	0.63
50:t:368:MET:HE1	50:t:403:ILE:HG12	1.80	0.63
6:b:25:THR:O	6:b:29:THR:OG1	2.15	0.63
14:G:91:PHE:HE1	14:G:180:VAL:HG21	1.64	0.63
44:1:2446:U:H2'	44:1:2447:A:H8	1.63	0.63
33:S:117:ARG:HG3	33:S:118:PHE:H	1.62	0.63
44:1:2469:G:O2'	54:s:26:ARG:NH1	2.30	0.63
44:1:1846:C:OP1	44:1:1849:C:N4	2.30	0.63
4:a:74:ASN:ND2	44:1:705:A:N7	2.45	0.63
27:u:73:GLN:HG3	27:u:74:ARG:H	1.64	0.63
31:R:125:LYS:NZ	44:1:1720:U:O4	2.32	0.63
38:X:59:SER:OG	38:X:101:GLU:OE2	2.17	0.63
52:4:362:ARG:NH1	52:4:363:ASP:O	2.32	0.63
6:b:99:SER:OG	44:1:2865:U:O4	2.17	0.62
15:g:37:LYS:NZ	44:1:1656:A:OP2	2.32	0.62
18:h:102:GLU:HG3	18:h:105:ARG:HH21	1.63	0.62
12:F:121:LYS:HB2	34:T:133:ALA:HB3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:I:104:ARG:NH1	16:I:107:GLU:OE1	2.32	0.62
52:4:43:THR:O	52:4:47:ASN:ND2	2.28	0.62
3:A:101:VAL:HG22	3:A:165:VAL:HG22	1.80	0.62
47:x:329:SER:OG	47:x:373:MET:O	2.18	0.62
48:m:76:ARG:HG2	51:n:29:ARG:HH12	1.64	0.62
48:m:416:TYR:OH	48:m:456:ASP:OD2	2.17	0.62
3:A:238:ILE:HD12	44:1:2155:G:H1'	1.81	0.62
6:b:619:GLN:O	23:l:46:ARG:NH2	2.32	0.62
27:u:6:CYS:SG	27:u:9:CYS:N	2.72	0.62
39:Y:86:THR:HG22	39:Y:96:PRO:HA	1.82	0.62
44:1:2443:A:H61	44:1:2504:U:H3	1.47	0.62
29:P:167:ARG:NH1	44:1:620:U:OP1	2.30	0.62
6:b:645:ASP:H	44:1:2401:A:N6	1.96	0.62
22:L:180:ARG:NH2	44:1:2779:A:O2'	2.32	0.62
3:A:36:GLU:OE1	3:A:163:ARG:NH1	2.27	0.62
6:b:168:ARG:HB2	6:b:339:LEU:HD22	1.82	0.62
6:b:506:GLU:HG2	9:d:97:LEU:HD13	1.82	0.62
44:1:394:G:N1	44:1:397:A:OP2	2.31	0.62
45:3:103:G:OP2	45:3:105:A:O2'	2.18	0.62
48:m:403:VAL:HG13	48:m:457:PHE:CZ	2.35	0.62
17:H:162:GLN:NE2	32:r:19:ASP:OD1	2.33	0.62
39:Y:126:LEU:HD12	39:Y:127:GLU:HG2	1.82	0.62
44:1:900:G:H1'	44:1:1589:A:N6	2.15	0.62
44:1:2270:A:OP2	51:n:44:ARG:NH1	2.33	0.62
47:x:473:VAL:O	47:x:476:ARG:NH1	2.32	0.62
5:B:93:VAL:HG12	5:B:155:ALA:H	1.63	0.62
17:H:18:VAL:HG21	17:H:53:ILE:HD11	1.82	0.62
33:S:12:ARG:HH22	34:T:139:ARG:HD2	1.65	0.62
44:1:2205:U:C4	50:t:18:GLN:HG3	2.35	0.62
18:h:67:ARG:NH2	45:3:97:A:OP1	2.33	0.61
40:y:186:VAL:HG23	40:y:193:VAL:HG12	1.80	0.61
44:1:972:A:N1	44:1:973:A:N6	2.47	0.61
44:1:1247:U:N3	44:1:1268:G:O6	2.33	0.61
46:5:83:ARG:HG3	46:5:84:GLU:H	1.65	0.61
48:m:344:ALA:HB3	48:m:349:GLU:HG3	1.81	0.61
52:4:36:GLN:NE2	52:4:527:GLY:H	1.97	0.61
4:a:146:GLU:OE2	22:L:157:ARG:NH2	2.33	0.61
5:B:342:LEU:HD21	44:1:3136:G:H4'	1.82	0.61
44:1:358:G:N2	44:1:361:A:OP2	2.31	0.61
46:5:94:ARG:NH1	47:x:487:ASP:OD2	2.33	0.61
5:B:129:ALA:O	44:1:3149:G:O2'	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:Z:135:ARG:HH12	44:1:1807:G:H5”	1.65	0.61
47:x:453:SER:HA	47:x:494:TRP:CD1	2.36	0.61
52:4:72:ILE:HD11	52:4:143:LEU:HD12	1.81	0.61
34:T:130:ARG:O	44:1:1098:A:O2’	2.18	0.61
44:1:1013:G:N2	44:1:1037:C:O2	2.34	0.61
44:1:1863:G:N1	44:1:1866:C:OP2	2.34	0.61
44:1:2657:A:H1’	44:1:2658:G:C8	2.36	0.61
48:m:232:ARG:NH1	48:m:457:PHE:O	2.28	0.61
2:J:95:ASN:ND2	44:1:2673:A:O5’	2.34	0.61
20:j:14:LYS:HD2	23:l:51:ILE:HD11	1.82	0.61
44:1:2841:G:O2’	44:1:2847:A:N6	2.34	0.61
45:3:8:C:H2’	45:3:9:A:C8	2.36	0.61
54:s:20:SER:OG	54:s:30:GLU:OE1	2.16	0.61
6:b:5:TRP:CD1	6:b:69:PRO:HB3	2.36	0.61
14:G:185:ARG:O	14:G:188:THR:OG1	2.17	0.61
44:1:1779:C:N4	44:1:2102:U:OP2	2.34	0.61
44:1:3259:U:H5”	44:1:3261:C:H5	1.65	0.61
46:5:82:ARG:HG2	46:5:83:ARG:H	1.64	0.61
52:4:559:LEU:O	52:4:567:LEU:N	2.33	0.61
26:N:73:ARG:NH2	26:N:88:GLY:O	2.34	0.61
28:O:85:ARG:NH2	44:1:2383:C:OP2	2.33	0.61
48:m:456:ASP:HB3	48:m:462:ILE:HG13	1.82	0.61
32:r:204:PRO:O	32:r:205:GLN:HG2	2.01	0.61
44:1:2185:G:O2’	44:1:2314:U:OP2	2.16	0.61
47:x:132:VAL:HG11	47:x:513:TRP:HB3	1.81	0.61
50:t:263:PHE:HB3	50:t:333:ILE:HD11	1.82	0.61
52:4:192:GLU:HA	52:4:195:VAL:HG12	1.82	0.61
44:1:2463:G:N1	44:1:2492:C:O2	2.32	0.61
48:m:371:VAL:HG21	48:m:387:VAL:HG21	1.83	0.61
2:J:89:TYR:HB2	2:J:169:ALA:HB3	1.82	0.60
33:S:117:ARG:HG3	33:S:118:PHE:HD1	1.66	0.60
44:1:2717:U:O4	44:1:2738:A:N6	2.34	0.60
44:1:2964:G:N2	44:1:2967:A:OP2	2.30	0.60
6:b:43:ARG:O	6:b:47:MET:HG3	2.01	0.60
11:e:118:LYS:NZ	44:1:438:A:OP1	2.31	0.60
6:b:546:GLN:NE2	6:b:550:ASN:OD1	2.34	0.60
44:1:2568:C:OP1	44:1:2569:A:N6	2.34	0.60
44:1:3375:A:O2’	44:1:3378:C:OP2	2.19	0.60
50:t:417:PRO:HA	50:t:420:ILE:HB	1.84	0.60
1:D:178:ASN:OD1	1:D:179:ARG:N	2.35	0.60
6:b:227:ARG:HG2	6:b:228:PRO:HD3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:R:38:ARG:NH1	44:1:1603:A:OP1	2.34	0.60
44:1:1020:G:H2'	44:1:1021:G:H8	1.65	0.60
50:t:390:LEU:O	50:t:426:LYS:NZ	2.32	0.60
52:4:73:LEU:HD12	52:4:399:PHE:HE2	1.66	0.60
22:L:53:LEU:HB2	22:L:55:ARG:NH1	2.16	0.60
24:M:113:THR:HG22	24:M:115:PHE:H	1.64	0.60
38:X:113:LEU:HD11	38:X:121:LYS:HE2	1.84	0.60
41:Z:65:ARG:NH1	44:1:1809:A:OP2	2.34	0.60
1:D:111:GLN:HA	1:D:116:ASP:HB2	1.82	0.60
6:b:175:TYR:HD2	6:b:262:PHE:CD1	2.20	0.60
26:N:125:SER:HB3	44:1:2433:U:H1'	1.81	0.60
29:P:116:HIS:HB3	29:P:149:VAL:HG22	1.83	0.60
40:y:126:GLU:OE2	40:y:139:ARG:NE	2.34	0.60
44:1:86:G:O2'	44:1:98:G:O6	2.18	0.60
49:2:11:A:N1	49:2:67:G:O2'	2.32	0.60
2:J:43:GLN:NE2	2:J:70:THR:O	2.34	0.60
4:a:84:GLU:N	4:a:84:GLU:OE2	2.31	0.60
5:B:216:ASP:OD2	5:B:339:ARG:NH2	2.34	0.60
6:b:433:PRO:O	6:b:434:GLU:HG2	2.01	0.60
29:P:25:SER:OG	44:1:1447:G:N7	2.32	0.60
54:s:40:ASN:O	54:s:196:LYS:NZ	2.34	0.60
23:l:27:ILE:HG23	23:l:30:ARG:HH21	1.67	0.60
32:r:189:LEU:HA	47:x:322:TRP:HE1	1.67	0.60
44:1:437:G:O6	53:o:40:ARG:NH1	2.35	0.60
44:1:1391:C:O2	53:o:107:ARG:NH2	2.34	0.60
44:1:68:C:OP2	44:1:301:G:N2	2.32	0.60
33:S:154:HIS:HA	33:S:170:THR:HG21	1.84	0.60
44:1:2821:C:H5"	44:1:2943:G:H2'	1.84	0.60
7:C:33:ASP:OD1	7:C:34:ILE:N	2.35	0.59
9:d:26:LYS:HE3	44:1:1455:U:H1'	1.84	0.59
47:x:341:HIS:CE1	47:x:342:THR:HG23	2.36	0.59
48:m:328:LYS:N	57:m:501:GTP:O1B	2.34	0.59
54:s:8:GLN:NE2	54:s:9:VAL:HG13	2.17	0.59
9:d:72:ARG:NH2	9:d:105:GLN:O	2.33	0.59
37:W:34:LEU:O	37:W:223:ASN:ND2	2.33	0.59
44:1:2466:G:O3'	54:s:60:ARG:NH1	2.35	0.59
4:a:90:TYR:OH	22:L:155:GLU:OE1	2.16	0.59
6:b:31:THR:OG1	44:1:2887:A:N7	2.34	0.59
17:H:174:LYS:NZ	44:1:3026:G:OP1	2.26	0.59
44:1:1242:G:N7	48:m:148:LYS:NZ	2.34	0.59
50:t:393:LEU:HD13	50:t:427:ILE:HG13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:157:ASN:O	12:F:158:LYS:HG2	2.02	0.59
44:1:2466:G:O2'	54:s:33:GLU:OE2	2.16	0.59
44:1:2720:G:H2'	44:1:2721:A:H8	1.67	0.59
44:1:2899:C:O2'	44:1:2901:G:OP2	2.19	0.59
29:P:16:SER:O	29:P:101:ASN:ND2	2.32	0.59
50:t:211:LEU:HD22	50:t:218:GLN:HB3	1.84	0.59
6:b:433:PRO:HG2	27:u:90:LEU:HD21	1.85	0.59
11:e:23:ASP:OD1	11:e:24:ARG:N	2.36	0.59
14:G:162:LEU:HD23	26:N:7:LEU:HD11	1.84	0.59
14:G:171:LYS:NZ	14:G:223:ALA:O	2.35	0.59
17:H:89:LYS:HG2	17:H:145:VAL:HG22	1.85	0.59
32:r:166:VAL:HG11	48:m:353:TRP:HH2	1.68	0.59
44:1:1097:G:H4'	44:1:1098:A:O5'	2.02	0.59
7:C:34:ILE:HG21	7:C:120:TYR:HD2	1.68	0.59
15:g:51:LEU:CD1	15:g:54:ILE:HD13	2.33	0.59
28:O:56:ASP:OD1	44:1:1192:C:N4	2.30	0.59
44:1:1390:A:N6	44:1:1418:A:O2'	2.35	0.59
48:m:72:GLN:NE2	51:n:13:ASP:OD2	2.33	0.59
50:t:231:ARG:HH21	50:t:232:ARG:HH12	1.50	0.59
50:t:376:GLY:HA2	50:t:412:HIS:HE1	1.68	0.59
12:F:96:PRO:HB2	12:F:99:PRO:HD2	1.85	0.59
29:P:118:GLN:NE2	29:P:147:GLU:OE2	2.35	0.59
48:m:347:PRO:HD2	48:m:389:ARG:HG2	1.85	0.59
5:B:250:ALA:HB1	44:1:2947:G:C2	2.38	0.59
44:1:2891:U:H2'	44:1:2892:A:H5"	1.85	0.59
1:D:106:ALA:HB2	1:D:166:ALA:HA	1.83	0.58
7:C:34:ILE:HA	7:C:37:THR:HG22	1.85	0.58
21:k:44:LYS:NZ	44:1:1750:A:OP1	2.23	0.58
44:1:955:U:OP2	44:1:1116:G:N2	2.32	0.58
33:S:80:ARG:HB2	33:S:124:LEU:HD11	1.85	0.58
37:W:78:GLY:HA3	37:W:84:GLU:HA	1.85	0.58
40:y:119:PRO:HA	40:y:139:ARG:HD3	1.85	0.58
55:q:51:PRO:HG2	55:q:54:PHE:HB2	1.85	0.58
7:C:20:LEU:HD11	7:C:255:PHE:HD2	1.68	0.58
44:1:2477:G:H1'	44:1:2488:A:C4	2.38	0.58
44:1:3112:G:N2	44:1:3121:U:OP1	2.32	0.58
8:c:9:SER:OG	8:c:10:ILE:N	2.35	0.58
32:r:222:GLU:OE1	48:m:81:THR:OG1	2.18	0.58
36:V:117:PRO:HA	36:V:135:VAL:HG13	1.86	0.58
47:x:293:TYR:HD2	47:x:326:LEU:HD21	1.68	0.58
48:m:422:LYS:NZ	48:m:426:GLU:OE2	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:3:HIS:O	5:B:4:ARG:HG2	2.04	0.58
10:E:49:GLY:O	10:E:163:PHE:N	2.33	0.58
17:H:3:TYR:HE1	46:5:32:LYS:HA	1.69	0.58
17:H:48:VAL:HG23	17:H:49:ASN:H	1.68	0.58
22:L:10:LEU:HD21	44:1:667:C:H1'	1.84	0.58
34:T:13:TYR:HB2	44:1:994:G:H3'	1.84	0.58
44:1:2961:G:OP1	48:m:338:LYS:NZ	2.35	0.58
48:m:111:ASN:OD1	48:m:112:LYS:N	2.35	0.58
3:A:134:VAL:HG12	3:A:151:PRO:HD3	1.86	0.58
6:b:497:ARG:NH2	27:u:123:ASP:OD1	2.31	0.58
6:b:624:ARG:NH1	23:l:41:ARG:O	2.29	0.58
9:d:20:LEU:HD11	9:d:32:ALA:HB2	1.85	0.58
29:P:89:LYS:HA	29:P:92:GLN:HG2	1.85	0.58
37:W:4:SER:HB2	44:1:1209:G:H5'	1.84	0.58
40:y:68:ARG:HH12	40:y:112:ASP:HB3	1.68	0.58
43:K:26:UNK:O	43:K:28:UNK:N	2.37	0.58
44:1:2535:A:H61	44:1:2544:U:H3	1.52	0.58
2:J:32:ARG:NH1	2:J:120:ILE:O	2.37	0.58
16:I:85:TYR:HA	16:I:89:VAL:HG21	1.86	0.58
32:r:30:ARG:HD3	44:1:3120:C:H2'	1.85	0.58
35:U:18:ASP:HA	35:U:62:VAL:HG22	1.85	0.58
39:Y:94:SER:O	52:4:452:THR:OG1	2.20	0.58
44:1:3343:G:O2'	44:1:3362:A:N6	2.36	0.58
46:5:57:PHE:HE1	55:q:61:LEU:HD13	1.69	0.58
1:D:77:ALA:O	1:D:108:ARG:NH1	2.37	0.58
29:P:118:GLN:OE1	44:1:412:G:N2	2.28	0.58
36:V:53:SER:N	36:V:56:ASP:OD2	2.37	0.58
7:C:188:ARG:HB2	7:C:193:LYS:HG3	1.85	0.58
37:W:37:TYR:O	37:W:223:ASN:ND2	2.37	0.58
2:J:49:LYS:HB3	2:J:62:ASN:HA	1.86	0.58
5:B:308:MET:HE2	44:1:3329:U:H5'	1.86	0.58
12:F:33:ARG:NH2	44:1:595:G:OP1	2.35	0.58
22:L:105:ASN:OD1	22:L:108:ILE:HG22	2.03	0.58
24:M:23:ILE:O	24:M:30:GLY:N	2.37	0.58
37:W:41:TRP:HE3	37:W:217:VAL:HG21	1.69	0.58
50:t:139:ARG:NH2	50:t:187:LEU:O	2.37	0.58
50:t:185:ILE:HD11	50:t:228:GLU:HG3	1.85	0.58
50:t:205:GLN:HE22	50:t:240:THR:HG22	1.69	0.58
3:A:230:VAL:HG23	44:1:2424:A:N1	2.19	0.57
9:d:51:LEU:HD11	44:1:1459:C:H4'	1.86	0.57
37:W:74:GLN:NE2	37:W:96:CYS:SG	2.66	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:y:68:ARG:NH2	40:y:112:ASP:O	2.35	0.57
47:x:192:VAL:HG12	47:x:203:THR:HG23	1.84	0.57
1:D:34:LYS:HA	34:T:27:LEU:HD11	1.85	0.57
9:d:19:ARG:NH1	44:1:3324:C:OP1	2.37	0.57
32:r:2:PRO:HB2	32:r:6:TYR:CG	2.39	0.57
44:1:2678:A:N3	46:5:113:ARG:HB2	2.19	0.57
48:m:104:TYR:O	51:n:41:ILE:N	2.32	0.57
50:t:109:PRO:HB3	50:t:138:LEU:HD13	1.85	0.57
52:4:191:MET:HE1	52:4:319:ILE:HB	1.85	0.57
12:F:159:GLN:O	44:1:1362:G:H4'	2.05	0.57
13:f:49:ILE:HD11	13:f:71:VAL:HG22	1.85	0.57
26:N:62:TYR:CD2	26:N:134:LEU:HD13	2.39	0.57
44:1:877:C:HO2'	44:1:880:G:HO2'	1.47	0.57
47:x:203:THR:HB	47:x:213:TRP:HE1	1.69	0.57
5:B:222:LYS:HD3	5:B:331:ASN:HB3	1.86	0.57
26:N:4:TYR:CE2	26:N:5:LYS:HG2	2.39	0.57
44:1:1493:G:OP2	44:1:1493:G:N2	2.34	0.57
7:C:317:PRO:C	7:C:319:LYS:H	2.12	0.57
11:e:96:ILE:HG21	11:e:105:ARG:HG2	1.85	0.57
21:k:69:LEU:HD12	21:k:73:LEU:HD23	1.87	0.57
26:N:127:TYR:OH	44:1:1544:G:OP1	2.21	0.57
45:3:76:C:O2'	45:3:77:A:H8	1.86	0.57
10:E:77:ARG:NH1	44:1:3269:U:OP1	2.37	0.57
26:N:12:ARG:NH1	44:1:297:G:O6	2.35	0.57
26:N:44:ARG:NH1	44:1:269:G:OP2	2.28	0.57
32:r:193:VAL:HG11	32:r:228:LEU:HD11	1.86	0.57
39:Y:4:GLN:HB2	44:1:229:G:H5"	1.85	0.57
43:K:16:UNK:HA	43:K:62:LEU:HA	1.87	0.57
44:1:1306:G:O6	44:1:2366:C:O2'	2.23	0.57
44:1:2876:C:H1'	44:1:2877:G:H5'	1.87	0.57
47:x:470:VAL:HG23	47:x:479:SER:HB3	1.86	0.57
6:b:436:LEU:HD12	27:u:93:MET:HE2	1.86	0.57
6:b:590:LEU:HD13	6:b:599:ARG:HD3	1.85	0.57
21:k:19:ASP:OD2	44:1:1825:G:H5"	2.03	0.57
38:X:49:LYS:HD2	45:3:135:G:H5"	1.85	0.57
44:1:2329:C:O2'	48:m:451:LYS:NZ	2.38	0.57
47:x:468:LEU:HB2	47:x:482:LEU:HB2	1.86	0.57
52:4:42:VAL:HG11	52:4:141:ILE:HG21	1.85	0.57
52:4:163:VAL:HG22	52:4:172:PRO:HG3	1.86	0.57
3:A:48:ILE:HD11	25:p:65:ALA:HB2	1.86	0.57
5:B:21:ARG:NH2	44:1:3309:G:O6	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:85:VAL:HA	5:B:202:THR:HA	1.87	0.57
6:b:86:TYR:O	6:b:149:TYR:OH	2.22	0.57
6:b:177:ASN:HA	6:b:180:LYS:HE2	1.87	0.57
39:Y:92:GLY:HA2	53:o:140:LEU:HD22	1.87	0.57
44:1:2312:A:C8	48:m:337:LYS:HD3	2.39	0.57
44:1:2496:C:H4'	44:1:2497:U:OP1	2.04	0.57
50:t:417:PRO:O	50:t:421:ASN:N	2.36	0.57
3:A:127:ALA:HB2	3:A:134:VAL:HG13	1.86	0.57
6:b:48:ARG:HH12	44:1:2938:G:P	2.27	0.57
6:b:643:LYS:NZ	44:1:2140:U:OP2	2.37	0.57
7:C:140:HIS:H	7:C:180:LYS:HE2	1.68	0.57
10:E:56:LYS:HD2	10:E:98:VAL:HG22	1.86	0.57
44:1:3167:A:H3'	44:1:3168:A:H5"	1.86	0.57
48:m:403:VAL:HG13	48:m:457:PHE:HE2	1.70	0.57
50:t:87:LEU:HD22	50:t:127:LEU:HD11	1.85	0.57
50:t:499:LYS:HE2	50:t:502:ARG:HH12	1.70	0.57
1:D:125:VAL:O	1:D:196:ARG:NH1	2.38	0.56
7:C:35:VAL:HG21	7:C:244:LEU:HD21	1.87	0.56
44:1:1278:A:O2'	44:1:1279:C:O5'	2.22	0.56
50:t:87:LEU:HD23	50:t:91:VAL:HB	1.87	0.56
52:4:27:LYS:NZ	52:4:148:ASP:OD1	2.38	0.56
14:G:158:ASP:HB3	14:G:159:PRO:HD3	1.87	0.56
29:P:8:SER:OG	53:o:85:THR:N	2.39	0.56
30:Q:38:ARG:NH2	44:1:1348:U:OP2	2.38	0.56
44:1:3171:U:H5'	53:o:20:VAL:HG11	1.86	0.56
6:b:1:MET:SD	6:b:2:GLN:N	2.79	0.56
12:F:120:THR:HB	34:T:132:PRO:HB2	1.86	0.56
26:N:72:LYS:NZ	26:N:90:ASN:OD1	2.39	0.56
44:1:2693:C:H1'	44:1:2706:G:H5"	1.88	0.56
44:1:3349:C:H42	44:1:3356:G:H1	1.52	0.56
48:m:47:GLU:HB2	48:m:59:ALA:HB2	1.86	0.56
48:m:260:ASN:OD1	48:m:261:LYS:N	2.35	0.56
33:S:117:ARG:HG3	33:S:118:PHE:CD1	2.41	0.56
5:B:240:ARG:NH2	44:1:874:U:OP1	2.38	0.56
6:b:256:LEU:HD12	6:b:264:ILE:HD13	1.88	0.56
6:b:566:VAL:HG21	52:4:387:VAL:HG21	1.86	0.56
14:G:35:GLY:HA2	44:1:2549:G:C2	2.40	0.56
32:r:66:LYS:HE3	44:1:2838:A:H5"	1.88	0.56
44:1:2446:U:H2'	44:1:2447:A:C8	2.40	0.56
7:C:237:GLN:O	7:C:246:ARG:HD3	2.05	0.56
8:c:17:VAL:HG21	8:c:100:ILE:HD11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:N:4:TYR:CD2	26:N:5:LYS:HG2	2.41	0.56
44:1:2494:A:H2'	44:1:2495:C:O4'	2.05	0.56
1:D:144:VAL:HG13	1:D:173:VAL:HG22	1.88	0.56
26:N:85:THR:OG1	44:1:44:U:OP1	2.20	0.56
44:1:595:G:H1	44:1:609:G:H5"	1.71	0.56
44:1:627:U:H2'	44:1:628:A:C8	2.41	0.56
5:B:108:GLU:O	5:B:109:HIS:ND1	2.39	0.56
18:h:31:LEU:HD12	18:h:34:GLN:HE21	1.71	0.56
44:1:1497:C:O2'	44:1:1602:A:N3	2.36	0.56
44:1:1877:U:H5"	44:1:1878:G:O4'	2.06	0.56
44:1:2400:G:O2'	44:1:2979:U:N3	2.30	0.56
6:b:447:PRO:HD3	27:u:79:VAL:HG11	1.88	0.56
44:1:118:U:O2	44:1:121:A:H5'	2.06	0.56
44:1:2571:U:H1'	44:1:2572:C:H2'	1.88	0.56
2:J:17:LEU:HD13	2:J:129:VAL:HG22	1.87	0.56
6:b:226:ASP:CG	6:b:270:LEU:HD23	2.31	0.56
7:C:349:THR:OG1	44:1:520:U:O4	2.20	0.56
26:N:36:ILE:HG12	26:N:64:VAL:HG23	1.88	0.56
41:Z:9:LYS:NZ	41:Z:83:THR:O	2.29	0.56
6:b:172:ILE:HG22	6:b:180:LYS:HG3	1.87	0.55
20:j:2:GLY:O	20:j:7:SER:OG	2.19	0.55
44:1:371:G:N1	44:1:374:A:OP2	2.36	0.55
44:1:707:U:H5"	44:1:779:G:H1'	1.87	0.55
44:1:2697:A:H61	44:1:2757:U:H3	1.53	0.55
1:D:273:ARG:NH1	49:2:1:G:O2'	2.39	0.55
14:G:143:ILE:C	14:G:145:ASN:H	2.14	0.55
18:h:66:VAL:HG11	38:X:50:ALA:HB1	1.88	0.55
34:T:78:LYS:HE2	34:T:87:LYS:HG3	1.89	0.55
40:y:116:LEU:HD11	40:y:177:LEU:HD21	1.88	0.55
44:1:1567:U:H3	44:1:1571:A:N6	2.04	0.55
44:1:2669:G:H5"	46:5:107:MET:SD	2.46	0.55
47:x:418:VAL:HG21	47:x:459:LEU:HD11	1.87	0.55
3:A:40:TYR:HA	3:A:91:GLY:HA3	1.88	0.55
6:b:175:TYR:CE1	6:b:267:GLN:HA	2.42	0.55
6:b:440:ASN:O	6:b:440:ASN:ND2	2.38	0.55
16:I:87:GLN:OE1	27:u:7:HIS:ND1	2.30	0.55
28:O:83:ALA:O	44:1:1312:C:O2'	2.24	0.55
40:y:74:THR:HB	40:y:98:GLU:HA	1.88	0.55
54:s:177:ASP:OD1	54:s:178:VAL:N	2.38	0.55
6:b:581:VAL:HG11	6:b:587:ASP:HB3	1.87	0.55
12:F:48:ASN:ND2	12:F:182:ASP:OD2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:U:42:LYS:NZ	44:1:1686:U:OP1	2.39	0.55
44:1:1024:G:H1'	44:1:1029:G:H22	1.72	0.55
44:1:2399:A:H2'	44:1:2400:G:C8	2.42	0.55
5:B:59:ASP:HB3	5:B:357:LYS:HD2	1.87	0.55
37:W:158:ILE:HG22	37:W:160:SER:H	1.71	0.55
43:K:149:UNK:O	43:K:153:UNK:N	2.39	0.55
47:x:319:HIS:NE2	47:x:376:THR:OG1	2.31	0.55
47:x:420:ALA:HB2	47:x:450:VAL:HG13	1.89	0.55
52:4:226:ILE:HA	52:4:229:THR:HG22	1.88	0.55
52:4:332:LYS:HG3	52:4:445:TRP:HD1	1.70	0.55
1:D:39:GLN:O	1:D:41:LYS:NZ	2.35	0.55
2:J:55:ARG:NH1	50:t:429:ASP:O	2.40	0.55
8:c:40:LYS:NZ	8:c:93:LEU:O	2.37	0.55
14:G:84:ARG:HH22	45:3:156:U:P	2.28	0.55
33:S:115:ARG:HG2	44:1:1295:G:H4'	1.88	0.55
40:y:62:MET:HE3	40:y:73:PRO:HG3	1.89	0.55
44:1:997:A:H3'	44:1:998:A:H8	1.70	0.55
44:1:1277:C:HO2'	44:1:1278:A:P	2.29	0.55
44:1:2312:A:C4	48:m:337:LYS:HD3	2.42	0.55
50:t:490:ARG:HE	50:t:502:ARG:HA	1.72	0.55
6:b:228:PRO:HG3	6:b:231:GLU:HG2	1.88	0.55
32:r:162:THR:HG21	48:m:223:ASP:OD1	2.07	0.55
35:U:84:LEU:HD21	35:U:93:ILE:HG23	1.88	0.55
37:W:38:ARG:NH2	37:W:224:ASP:OD2	2.40	0.55
44:1:2098:C:H2'	44:1:2099:A:C8	2.41	0.55
44:1:2468:A:O2'	44:1:2478:C:O2	2.24	0.55
6:b:246:LEU:O	6:b:281:LYS:NZ	2.40	0.55
6:b:519:MET:HE3	6:b:524:LEU:HD21	1.89	0.55
17:H:150:SER:OG	17:H:153:ASP:OD2	2.22	0.55
33:S:107:TYR:HB3	33:S:117:ARG:HH22	1.71	0.55
40:y:101:LEU:HB3	40:y:107:VAL:HG21	1.87	0.55
50:t:101:PHE:O	50:t:105:THR:OG1	2.15	0.55
14:G:186:LEU:HB3	14:G:195:SER:HB3	1.89	0.55
44:1:1953:G:O6	44:1:2093:A:N6	2.40	0.55
44:1:2470:C:OP1	54:s:27:ASN:N	2.39	0.55
45:3:80:A:N7	52:4:492:THR:N	2.55	0.55
46:5:82:ARG:O	46:5:84:GLU:N	2.40	0.55
1:D:125:VAL:HG22	1:D:127:GLY:H	1.72	0.54
5:B:279:ASN:ND2	44:1:3098:G:OP1	2.39	0.54
7:C:36:HIS:O	7:C:40:THR:HG23	2.08	0.54
15:g:26:PRO:HD2	44:1:1597:C:H4'	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:h:63:ARG:HG2	38:X:51:VAL:HG21	1.89	0.54
6:b:48:ARG:NH1	44:1:2938:G:OP1	2.36	0.54
7:C:55:LYS:HD2	7:C:59:GLN:HE21	1.70	0.54
29:P:127:ARG:HB3	29:P:139:TYR:O	2.08	0.54
44:1:1816:A:H2'	44:1:1817:G:C8	2.42	0.54
44:1:2423:U:H2'	44:1:2424:A:C8	2.43	0.54
48:m:214:GLU:OE1	48:m:353:TRP:HD1	1.89	0.54
14:G:44:ARG:HH11	44:1:2524:A:H2	1.55	0.54
22:L:58:VAL:HG13	44:1:75:G:H5'	1.88	0.54
3:A:70:ARG:HH21	3:A:72:ARG:NH2	2.05	0.54
8:c:22:LYS:HB2	8:c:94:GLU:HG2	1.90	0.54
44:1:1152:G:OP2	44:1:1152:G:N2	2.30	0.54
44:1:2525:G:O2'	44:1:2526:C:OP2	2.24	0.54
52:4:224:ARG:NH2	52:4:268:VAL:O	2.40	0.54
54:s:31:THR:O	54:s:209:SER:N	2.40	0.54
54:s:86:SER:OG	54:s:89:ASP:OD2	2.26	0.54
14:G:185:ARG:NH2	45:3:155:A:H5'	2.23	0.54
20:j:81:GLY:O	45:3:95:G:O2'	2.21	0.54
44:1:2248:C:O2'	48:m:359:MET:HE2	2.08	0.54
44:1:2892:A:H62	44:1:2909:U:H3	1.56	0.54
47:x:283:CYS:SG	47:x:326:LEU:HB2	2.48	0.54
54:s:32:VAL:HA	54:s:208:SER:HA	1.90	0.54
3:A:183:GLY:HA2	44:1:896:A:H5'	1.89	0.54
26:N:33:LYS:O	26:N:65:ARG:NH2	2.40	0.54
44:1:1062:A:H5"	44:1:1063:G:H5'	1.90	0.54
44:1:2694:A:H1'	44:1:2695:A:C4	2.42	0.54
7:C:67:THR:OG1	44:1:2813:A:OP1	2.26	0.54
16:I:91:ASP:HA	27:u:5:GLN:NE2	2.23	0.54
20:j:45:ARG:NH2	44:1:361:A:O3'	2.40	0.54
38:X:59:SER:HB3	38:X:102:LEU:HG	1.90	0.54
39:Y:70:ILE:HD13	39:Y:82:VAL:HG22	1.90	0.54
44:1:715:A:N1	44:1:781:G:O2'	2.39	0.54
44:1:1219:C:O2'	44:1:1286:A:N1	2.34	0.54
44:1:1252:A:C8	44:1:1253:U:H2'	2.41	0.54
44:1:1895:A:O2'	44:1:3053:G:H4'	2.07	0.54
19:i:43:LEU:HD23	26:N:6:TYR:HE2	1.73	0.54
28:O:49:ARG:NH2	44:1:1193:A:OP1	2.40	0.54
32:r:126:ARG:HB2	44:1:1128:U:H5"	1.90	0.54
40:y:63:THR:HG22	40:y:72:VAL:HG12	1.90	0.54
44:1:1352:A:H4'	44:1:1353:U:H5'	1.90	0.54
54:s:42:ASP:OD1	54:s:45:ARG:N	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:141:ARG:HH21	44:1:1386:A:H5”	1.73	0.54
21:k:2:ALA:N	44:1:1613:A:OP1	2.40	0.54
26:N:174:ILE:HG21	44:1:63:A:H5”	1.90	0.54
41:Z:135:ARG:HH21	44:1:2557:A:H5’	1.73	0.54
46:5:86:LYS:HG3	46:5:87:GLU:H	1.72	0.54
2:J:32:ARG:HB3	2:J:120:ILE:HD12	1.89	0.53
5:B:74:GLU:OE2	5:B:283:TYR:OH	2.25	0.53
6:b:176:PRO:HB2	6:b:178:VAL:HG22	1.90	0.53
29:P:4:TYR:OH	44:1:389:A:OP1	2.23	0.53
31:R:124:TYR:OH	44:1:1721:U:OP2	2.23	0.53
39:Y:74:TYR:OH	45:3:75:G:OP2	2.18	0.53
50:t:471:LYS:HE3	50:t:483:LYS:HE2	1.89	0.53
24:M:77:ARG:NH2	44:1:525:C:OP2	2.40	0.53
44:1:1264:G:H5”	44:1:1265:U:OP1	2.08	0.53
44:1:2830:G:H2’	44:1:2831:G:C8	2.43	0.53
44:1:2865:U:O2’	44:1:2866:U:H2’	2.08	0.53
47:x:185:HIS:NE2	47:x:203:THR:O	2.33	0.53
48:m:353:TRP:HZ3	48:m:355:TYR:HD1	1.54	0.53
14:G:50:VAL:HG12	38:X:30:ALA:HA	1.90	0.53
32:r:146:SER:O	32:r:149:ARG:NH1	2.40	0.53
33:S:117:ARG:NH1	44:1:1322:U:O2’	2.41	0.53
39:Y:43:TYR:HD1	39:Y:126:LEU:HA	1.72	0.53
44:1:675:C:O2’	44:1:679:U:OP1	2.25	0.53
50:t:110:SER:O	50:t:114:GLN:NE2	2.41	0.53
52:4:337:LEU:HB3	52:4:438:GLN:HB2	1.89	0.53
5:B:163:HIS:ND1	5:B:164:THR:O	2.42	0.53
7:C:119:ARG:NH2	44:1:696:C:OP2	2.41	0.53
16:I:85:TYR:OH	27:u:7:HIS:O	2.22	0.53
17:H:62:ARG:NH2	44:1:3115:C:OP1	2.41	0.53
39:Y:86:THR:OG1	39:Y:88:GLU:OE2	2.25	0.53
40:y:107:VAL:HG13	40:y:118:HIS:HB2	1.91	0.53
50:t:361:MET:HE2	50:t:398:ARG:HB3	1.89	0.53
25:p:49:ARG:HB2	25:p:55:TRP:CZ3	2.44	0.53
28:O:37:ARG:NH2	44:1:3183:A:OP1	2.41	0.53
29:P:41:LEU:HD13	29:P:150:VAL:HG11	1.91	0.53
40:y:50:HIS:O	40:y:83:HIS:NE2	2.41	0.53
44:1:528:U:H2’	44:1:529:A:C8	2.43	0.53
54:s:91:LYS:O	54:s:94:ASN:ND2	2.41	0.53
33:S:82:ASP:HB3	33:S:120:SER:HB3	1.88	0.53
33:S:117:ARG:HH11	44:1:1322:U:H4’	1.74	0.53
41:Z:17:ARG:HG3	44:1:1639:C:N4	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:1:655:C:H2'	44:1:656:A:C8	2.44	0.53
48:m:400:ILE:HG13	48:m:428:ILE:HD11	1.90	0.53
14:G:78:PHE:O	14:G:79:GLN:HG3	2.09	0.53
14:G:241:LYS:NZ	44:1:2588:U:OP1	2.42	0.53
21:k:40:GLN:NE2	21:k:55:VAL:HG13	2.23	0.53
26:N:56:LYS:NZ	26:N:145:ASP:OD2	2.38	0.53
44:1:1602:A:OP1	52:4:371:LYS:NZ	2.37	0.53
50:t:399:ASP:OD2	50:t:402:ARG:NH2	2.37	0.53
52:4:247:ILE:HD11	52:4:318:LEU:HB3	1.90	0.53
1:D:85:ARG:HH21	1:D:86:TYR:HE1	1.56	0.53
29:P:60:PHE:HB3	29:P:64:ASN:HB3	1.91	0.53
32:r:165:PRO:HG2	48:m:315:GLN:HE21	1.73	0.53
39:Y:122:LYS:HG2	44:1:185:C:H5"	1.89	0.53
40:y:199:VAL:HG23	40:y:204:ALA:HB2	1.91	0.53
44:1:1009:A:H2	47:x:400:GLY:HA2	1.73	0.53
44:1:1127:G:H21	44:1:1131:G:H21	1.57	0.53
54:s:90:LEU:HD22	54:s:124:LEU:HD11	1.89	0.53
3:A:52:SER:HB3	3:A:191:LEU:HD12	1.91	0.53
6:b:9:PRO:O	6:b:10:THR:OG1	2.26	0.53
24:M:17:VAL:HG11	24:M:74:ARG:HA	1.90	0.53
44:1:577:C:O2'	44:1:579:G:OP1	2.25	0.53
44:1:1816:A:O2'	44:1:1817:G:OP1	2.24	0.53
47:x:239:PRO:HG2	47:x:242:LEU:HD12	1.90	0.53
4:a:100:PRO:HG2	4:a:123:VAL:HG23	1.91	0.53
22:L:58:VAL:O	22:L:70:ARG:N	2.36	0.53
31:R:86:GLU:OE2	31:R:91:SER:OG	2.26	0.53
38:X:108:LEU:HD23	38:X:125:ARG:HD3	1.91	0.53
5:B:216:ASP:OD1	5:B:339:ARG:HB3	2.09	0.52
6:b:249:CYS:H	6:b:339:LEU:HD21	1.74	0.52
7:C:51:ALA:O	45:3:26:U:O2'	2.27	0.52
15:g:106:LYS:NZ	44:1:2550:U:OP1	2.41	0.52
16:I:75:ARG:HA	44:1:2112:U:H3	1.74	0.52
32:r:227:GLU:HA	48:m:117:LEU:HD11	1.89	0.52
33:S:12:ARG:NH2	34:T:139:ARG:HD2	2.24	0.52
45:3:80:A:H62	52:4:492:THR:HA	1.73	0.52
47:x:210:ILE:HG12	47:x:232:ILE:HD13	1.91	0.52
48:m:274:VAL:O	48:m:278:SER:OG	2.20	0.52
52:4:26:ASN:OD1	52:4:27:LYS:N	2.43	0.52
5:B:158:VAL:HG23	5:B:188:ILE:HD12	1.91	0.52
6:b:376:PRO:HB3	40:y:157:GLN:HG2	1.91	0.52
13:f:48:ARG:HH22	44:1:499:G:H5"	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:1:2492:C:OP2	54:s:215:ARG:NH2	2.42	0.52
6:b:256:LEU:HD23	6:b:295:PRO:HB3	1.91	0.52
15:g:20:ILE:HD12	15:g:32:ALA:HB1	1.91	0.52
17:H:49:ASN:O	17:H:51:GLN:N	2.42	0.52
18:h:10:ARG:NH2	45:3:65:A:O3'	2.42	0.52
18:h:34:GLN:HE22	52:4:344:THR:HG23	1.74	0.52
27:u:136:ILE:O	27:u:139:VAL:HG22	2.09	0.52
31:R:134:HIS:CE1	31:R:136:ARG:HG2	2.44	0.52
44:1:339:C:OP1	44:1:1380:G:O2'	2.25	0.52
44:1:831:G:O2'	44:1:1864:A:N3	2.39	0.52
44:1:1525:G:H5'	44:1:1830:G:OP2	2.09	0.52
44:1:2656:A:C6	50:t:471:LYS:HE2	2.45	0.52
52:4:97:ILE:HG21	52:4:127:SER:OG	2.09	0.52
54:s:58:CYS:SG	54:s:152:ARG:HB3	2.50	0.52
6:b:250:VAL:HG11	6:b:278:PHE:CE1	2.45	0.52
6:b:399:ALA:HB1	40:y:32:GLU:HG2	1.91	0.52
11:e:101:SER:HB2	44:1:1389:G:H5"	1.91	0.52
20:j:56:ARG:NH1	44:1:364:G:O6	2.37	0.52
34:T:20:ARG:NH2	49:2:68:C:O3'	2.42	0.52
40:y:99:GLU:OE1	40:y:125:THR:OG1	2.20	0.52
50:t:32:PHE:O	50:t:36:TYR:N	2.29	0.52
50:t:231:ARG:NH2	50:t:232:ARG:HH12	2.07	0.52
50:t:252:ASP:HB3	50:t:255:ILE:HD12	1.91	0.52
6:b:202:LYS:NZ	44:1:1242:G:O6	2.42	0.52
14:G:78:PHE:C	14:G:80:TYR:H	2.18	0.52
36:V:23:MET:HE2	36:V:36:ILE:HG22	1.91	0.52
40:y:158:GLY:HA2	40:y:179:VAL:HB	1.91	0.52
44:1:2452:G:O2'	44:1:2462:A:OP2	2.24	0.52
44:1:2892:A:H8	44:1:3129:A:HO2'	1.54	0.52
47:x:274:MET:HG3	47:x:304:TRP:CD2	2.44	0.52
1:D:55:PHE:CD2	1:D:60:ILE:HD12	2.45	0.52
5:B:366:GLY:HA2	44:1:3086:A:H4'	1.92	0.52
7:C:102:PRO:HD2	44:1:933:A:H61	1.75	0.52
19:i:29:LYS:N	19:i:29:LYS:HD2	2.25	0.52
44:1:1044:U:H1'	46:5:108:ARG:HH12	1.75	0.52
44:1:1899:G:O2'	44:1:2334:U:O4	2.24	0.52
50:t:147:GLU:OE2	50:t:148:GLU:HG2	2.09	0.52
35:U:93:ILE:HD11	35:U:105:LEU:HB3	1.91	0.52
54:s:69:GLY:HA2	54:s:113:SER:HB2	1.91	0.52
54:s:150:ASP:O	54:s:154:THR:HG23	2.09	0.52
6:b:497:ARG:HH21	27:u:126:LEU:HD13	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:55:LYS:HD2	7:C:59:GLN:NE2	2.25	0.52
7:C:188:ARG:HG2	7:C:198:ARG:O	2.09	0.52
22:L:65:TYR:OH	44:1:700:C:OP1	2.25	0.52
26:N:91:GLU:OE2	44:1:276:U:O2'	2.27	0.52
26:N:93:LYS:NZ	44:1:276:U:O2	2.41	0.52
39:Y:56:VAL:HG21	39:Y:104:LEU:HD13	1.91	0.52
44:1:1635:G:N2	44:1:1638:A:OP2	2.33	0.52
45:3:110:C:O2'	45:3:112:U:OP2	2.26	0.52
46:5:91:ARG:O	46:5:95:LEU:HG	2.10	0.52
47:x:141:GLY:O	47:x:169:ARG:NH1	2.43	0.52
48:m:390:VAL:O	48:m:393:VAL:HG12	2.10	0.52
50:t:226:THR:HG23	50:t:244:MET:HE2	1.92	0.52
6:b:92:LYS:HZ2	44:1:2863:G:H22	1.57	0.52
33:S:107:TYR:HB3	33:S:117:ARG:NH2	2.25	0.52
35:U:16:THR:HG22	35:U:64:THR:HG23	1.92	0.52
37:W:96:CYS:HB2	37:W:100:THR:HG21	1.91	0.52
37:W:188:VAL:HG21	37:W:202:ILE:HG13	1.92	0.52
44:1:2393:G:O2'	44:1:2982:A:N6	2.41	0.52
46:5:102:LYS:HE2	46:5:106:ARG:HH21	1.74	0.52
50:t:489:TYR:HA	50:t:492:VAL:HG22	1.91	0.52
1:D:38:THR:HG22	34:T:30:TYR:HB3	1.91	0.52
5:B:250:ALA:HB3	44:1:2880:U:H1'	1.92	0.52
6:b:255:ASP:HB3	6:b:267:GLN:HE22	1.74	0.52
14:G:90:THR:HG23	14:G:214:LEU:HD21	1.91	0.52
22:L:165:SER:O	22:L:167:PHE:N	2.43	0.52
26:N:49:ARG:HH12	44:1:149:U:P	2.33	0.52
31:R:62:ARG:NH2	44:1:3068:U:OP2	2.36	0.52
44:1:1572:U:O2'	44:1:1573:G:OP1	2.22	0.52
6:b:41:ARG:NH1	44:1:2943:G:OP1	2.42	0.51
7:C:3:ARG:HH21	7:C:24:ALA:HA	1.75	0.51
11:e:98:HIS:O	11:e:125:ARG:NH2	2.43	0.51
22:L:63:VAL:HA	22:L:66:ASN:ND2	2.25	0.51
22:L:89:TYR:O	22:L:93:ILE:HG13	2.10	0.51
37:W:31:ARG:NH1	37:W:76:ALA:O	2.43	0.51
48:m:238:ARG:NH2	48:m:257:TYR:OH	2.43	0.51
52:4:30:THR:HA	52:4:33:GLN:HG2	1.91	0.51
6:b:76:PRO:HB3	48:m:167:ASP:HB3	1.93	0.51
6:b:440:ASN:C	6:b:440:ASN:HD22	2.15	0.51
8:c:49:PRO:HG2	8:c:52:ARG:HB3	1.91	0.51
11:e:45:ARG:NH2	44:1:1366:A:O2'	2.42	0.51
21:k:14:LEU:HD22	21:k:45:VAL:HG11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:O:171:LYS:NZ	44:1:3181:C:OP2	2.34	0.51
31:R:21:LYS:HE2	31:R:55:VAL:HA	1.91	0.51
39:Y:106:ILE:HG21	39:Y:109:LEU:HD23	1.90	0.51
44:1:996:A:H2'	44:1:997:A:H8	1.74	0.51
44:1:1309:U:OP2	55:q:9:ARG:N	2.40	0.51
44:1:2929:C:H4'	48:m:198:ALA:HB2	1.92	0.51
50:t:152:SER:O	50:t:156:LEU:HG	2.10	0.51
6:b:90:HIS:NE2	48:m:135:GLU:O	2.36	0.51
7:C:34:ILE:HG21	7:C:120:TYR:CD2	2.44	0.51
44:1:2484:A:H1'	50:t:338:ASP:HB3	1.92	0.51
44:1:2633:U:H1'	44:1:2647:A:H61	1.75	0.51
52:4:164:ASP:OD1	52:4:173:THR:HG22	2.10	0.51
54:s:9:VAL:O	54:s:13:VAL:HG23	2.10	0.51
26:N:42:PRO:HG3	26:N:61:ILE:HG13	1.91	0.51
37:W:73:LEU:HD13	37:W:102:LEU:HD23	1.92	0.51
40:y:117:VAL:HB	40:y:121:ILE:HD12	1.91	0.51
43:K:157:UNK:O	43:K:159:UNK:N	2.44	0.51
3:A:14:SER:OG	44:1:911:C:OP1	2.25	0.51
6:b:647:ARG:NH1	44:1:877:C:O2	2.42	0.51
10:E:68:PRO:HG3	10:E:145:LEU:HD23	1.93	0.51
17:H:72:LYS:NZ	17:H:76:ASP:OD2	2.43	0.51
17:H:137:SER:HB3	17:H:140:VAL:HB	1.91	0.51
38:X:27:ARG:NH2	45:3:150:G:OP1	2.43	0.51
38:X:109:LYS:NZ	38:X:111:ASN:OD1	2.34	0.51
44:1:2099:A:H2'	44:1:2100:A:H5"	1.91	0.51
44:1:2737:C:H2'	44:1:2738:A:C8	2.46	0.51
47:x:403:LYS:HB2	47:x:423:ASP:HB3	1.93	0.51
50:t:252:ASP:OD1	50:t:253:VAL:N	2.43	0.51
50:t:502:ARG:HB2	50:t:507:ALA:HB2	1.93	0.51
53:o:145:GLU:HA	53:o:148:TRP:HD1	1.75	0.51
1:D:44:TYR:CD2	44:1:1084:A:H4'	2.45	0.51
29:P:9:THR:HG22	29:P:10:ASN:H	1.76	0.51
44:1:1566:A:O2'	44:1:1567:U:OP2	2.26	0.51
1:D:179:ARG:HH21	44:1:2746:A:P	2.32	0.51
16:I:86:THR:HG23	16:I:88:GLU:H	1.75	0.51
36:V:40:LYS:HD2	44:1:2931:C:H5"	1.92	0.51
44:1:1009:A:C2	47:x:400:GLY:HA2	2.45	0.51
44:1:2194:G:H1	44:1:2248:C:H5	1.58	0.51
32:r:166:VAL:HG11	48:m:353:TRP:CH2	2.46	0.51
44:1:297:G:OP2	44:1:297:G:N2	2.37	0.51
6:b:530:LYS:O	6:b:534:HIS:N	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:P:56:ARG:NH2	29:P:75:GLU:OE2	2.44	0.51
33:S:117:ARG:HG3	33:S:118:PHE:N	2.26	0.51
39:Y:43:TYR:CD1	39:Y:126:LEU:HA	2.46	0.51
44:1:1622:U:H2'	44:1:1623:G:C8	2.45	0.51
47:x:206:MET:HA	47:x:231:TRP:HB2	1.92	0.51
1:D:146:LEU:HD22	1:D:163:LEU:HB2	1.93	0.51
6:b:482:GLU:HG3	6:b:484:SER:H	1.76	0.51
9:d:10:ARG:HG2	9:d:108:VAL:HG22	1.92	0.51
14:G:91:PHE:CE1	14:G:180:VAL:HG21	2.46	0.51
22:L:76:THR:HB	22:L:79:GLU:H	1.75	0.51
52:4:197:LEU:HD23	52:4:226:ILE:HD11	1.92	0.51
24:M:57:ALA:HB2	33:S:97:VAL:HG21	1.93	0.50
27:u:89:THR:O	27:u:93:MET:HG3	2.12	0.50
32:r:198:LEU:HD11	32:r:224:ASN:HB3	1.91	0.50
40:y:42:LEU:HD13	40:y:46:ILE:HD11	1.93	0.50
41:Z:33:SER:OG	41:Z:35:SER:O	2.28	0.50
44:1:2669:G:H2'	44:1:2670:G:H8	1.76	0.50
45:3:71:A:H2	45:3:82:U:O2	1.95	0.50
52:4:530:LYS:HE3	52:4:573:GLN:HG3	1.93	0.50
5:B:77:THR:OG1	5:B:326:GLY:O	2.27	0.50
7:C:31:ARG:HG3	7:C:120:TYR:OH	2.11	0.50
7:C:140:HIS:CD2	7:C:247:PHE:H	2.29	0.50
27:u:61:LYS:HE2	44:1:3369:G:OP2	2.10	0.50
44:1:3346:U:H3	44:1:3359:A:H61	1.59	0.50
46:5:102:LYS:HE2	46:5:106:ARG:NH2	2.25	0.50
1:D:83:LEU:HB3	1:D:88:ILE:HB	1.93	0.50
11:e:26:HIS:HB2	44:1:655:C:H5"	1.91	0.50
14:G:119:GLY:O	14:G:120:LYS:HG3	2.12	0.50
22:L:27:ASP:HB3	45:3:29:U:H5"	1.92	0.50
24:M:55:ARG:NH1	24:M:76:ALA:O	2.43	0.50
24:M:59:ASN:HB3	24:M:62:GLN:HG3	1.94	0.50
28:O:37:ARG:HH22	44:1:3183:A:P	2.34	0.50
35:U:18:ASP:HB3	35:U:104:ARG:HB3	1.94	0.50
37:W:171:ILE:HD11	37:W:202:ILE:HD12	1.93	0.50
39:Y:53:ASP:O	39:Y:69:LYS:NZ	2.44	0.50
44:1:1348:U:O2	44:1:1349:G:N2	2.44	0.50
50:t:205:GLN:NE2	50:t:240:THR:HG22	2.25	0.50
52:4:506:THR:O	52:4:525:LEU:HB2	2.12	0.50
54:s:150:ASP:O	54:s:154:THR:N	2.43	0.50
16:I:53:HIS:HE1	16:I:123:LEU:HD22	1.76	0.50
33:S:114:HIS:ND1	33:S:116:ALA:HB2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:U:41:ILE:HG12	35:U:71:PHE:HE2	1.77	0.50
40:y:199:VAL:HA	40:y:204:ALA:HA	1.93	0.50
44:1:1721:U:O2'	44:1:1723:A:N7	2.42	0.50
3:A:180:LEU:HD11	25:p:26:VAL:HG21	1.92	0.50
32:r:151:ILE:HD11	32:r:212:LEU:HD13	1.93	0.50
32:r:181:LYS:HA	32:r:196:PRO:HA	1.93	0.50
33:S:89:ASN:ND2	55:q:49:GLY:O	2.44	0.50
37:W:31:ARG:HH11	37:W:85:TYR:HB2	1.75	0.50
48:m:383:LEU:HD21	48:m:454:LEU:HD13	1.93	0.50
1:D:28:THR:OG1	49:2:7:G:OP2	2.28	0.50
5:B:308:MET:HE3	5:B:373:PRO:HA	1.93	0.50
6:b:1:MET:N	6:b:5:TRP:HD1	2.10	0.50
12:F:156:ILE:C	12:F:158:LYS:H	2.19	0.50
17:H:48:VAL:HG11	17:H:54:LYS:HE2	1.92	0.50
23:l:28:ARG:NH1	23:l:36:ARG:O	2.45	0.50
31:R:98:ARG:HD2	31:R:133:LYS:O	2.11	0.50
32:r:205:GLN:HB3	48:m:69:ALA:HB2	1.93	0.50
33:S:81:TYR:CZ	33:S:88:HIS:HB2	2.46	0.50
52:4:28:TYR:HB3	52:4:525:LEU:HD21	1.94	0.50
52:4:275:GLU:OE2	52:4:475:LEU:HB2	2.12	0.50
3:A:180:LEU:HD22	25:p:18:TYR:HB3	1.93	0.50
17:H:73:SER:OG	44:1:3113:A:OP1	2.28	0.50
17:H:90:MET:HG2	17:H:181:VAL:HG12	1.94	0.50
23:l:2:ALA:N	44:1:1493:G:O6	2.45	0.50
29:P:36:ILE:HG22	29:P:114:VAL:HG11	1.93	0.50
34:T:89:LEU:HG	34:T:91:LEU:HD22	1.93	0.50
37:W:34:LEU:HD11	37:W:77:LEU:HD23	1.94	0.50
38:X:105:VAL:HG21	38:X:126:LEU:HD13	1.93	0.50
44:1:370:U:H4'	44:1:404:G:H5'	1.94	0.50
44:1:2747:A:H2'	44:1:2748:A:C8	2.47	0.50
44:1:3116:G:H4'	46:5:26:LYS:HD2	1.94	0.50
6:b:420:TYR:HB2	40:y:86:ASN:C	2.36	0.50
10:E:4:GLN:HG3	11:e:75:LEU:HB2	1.94	0.50
10:E:47:PHE:HZ	44:1:3268:A:H4'	1.77	0.50
17:H:49:ASN:HD22	17:H:49:ASN:C	2.20	0.50
31:R:25:ASP:HB3	31:R:28:GLU:HB2	1.93	0.50
32:r:157:VAL:HG12	32:r:173:ARG:HE	1.77	0.50
37:W:41:TRP:HB2	37:W:103:LEU:HB3	1.94	0.50
41:Z:23:VAL:HG12	41:Z:45:GLY:HA3	1.93	0.50
44:1:628:A:H5'	44:1:1399:A:N1	2.27	0.50
44:1:1313:G:O2'	44:1:1318:A:N1	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:1:3343:G:H21	44:1:3362:A:H2	1.59	0.50
47:x:209:THR:HB	47:x:224:ALA:HB1	1.92	0.50
48:m:287:HIS:HB3	48:m:294:PHE:HB3	1.92	0.50
52:4:108:ILE:O	52:4:111:THR:HG22	2.11	0.50
2:J:142:LYS:NZ	44:1:2703:A:N3	2.59	0.50
5:B:95:THR:HG22	44:1:3243:A:H4'	1.93	0.50
19:i:33:ALA:O	19:i:34:SER:OG	2.29	0.50
29:P:69:ARG:NH2	44:1:2991:A:N3	2.59	0.50
29:P:111:LYS:O	29:P:153:LYS:HG3	2.12	0.50
30:Q:67:ILE:HG23	30:Q:81:VAL:HG21	1.93	0.50
31:R:105:LEU:HD22	31:R:135:LYS:HG3	1.93	0.50
36:V:16:GLY:O	44:1:1897:G:O2'	2.30	0.50
36:V:87:ARG:HH22	36:V:137:VAL:HG21	1.76	0.50
44:1:629:U:H2'	44:1:630:A:C8	2.47	0.50
44:1:1404:G:N2	44:1:1407:A:OP2	2.32	0.50
45:3:9:A:H2'	45:3:10:A:C8	2.47	0.50
47:x:330:THR:HB	47:x:333:ALA:HB3	1.94	0.50
11:e:87:MET:HE3	11:e:88:HIS:CE1	2.47	0.49
26:N:62:TYR:OH	45:3:141:C:O3'	2.29	0.49
27:u:2:ARG:HB3	27:u:4:TYR:CE2	2.47	0.49
34:T:17:ARG:NH2	34:T:21:LYS:O	2.42	0.49
37:W:45:LEU:HD12	37:W:45:LEU:O	2.12	0.49
43:K:147:UNK:O	43:K:149:UNK:N	2.45	0.49
44:1:406:G:H1'	45:3:16:G:N2	2.26	0.49
44:1:1805:C:H2'	44:1:1806:A:C8	2.47	0.49
6:b:98:ILE:HG12	6:b:143:LEU:HD21	1.95	0.49
7:C:120:TYR:HE1	7:C:277:PRO:HB3	1.77	0.49
19:i:33:ALA:HB2	44:1:297:G:O2'	2.12	0.49
36:V:97:ASP:OD1	36:V:97:ASP:N	2.45	0.49
40:y:4:ARG:HG2	40:y:206:THR:HG23	1.94	0.49
43:K:148:UNK:O	43:K:150:UNK:N	2.45	0.49
44:1:691:A:N1	45:3:28:C:O2'	2.41	0.49
44:1:1622:U:H2'	44:1:1623:G:H8	1.77	0.49
49:2:3:U:O2'	49:2:25:G:N3	2.45	0.49
1:D:119:TYR:OH	1:D:139:PRO:O	2.25	0.49
19:i:40:VAL:HG11	26:N:5:LYS:HB3	1.94	0.49
22:L:46:ILE:O	22:L:49:ARG:N	2.43	0.49
28:O:59:ARG:NH1	44:1:1307:G:OP1	2.37	0.49
35:U:37:LEU:O	35:U:41:ILE:HD12	2.13	0.49
36:V:12:ARG:NH1	44:1:3041:U:OP1	2.45	0.49
40:y:6:GLN:NE2	40:y:11:ASN:OD1	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:1:1236:G:N2	44:1:1244:A:OP1	2.45	0.49
54:s:87:VAL:HG12	54:s:116:LEU:HD11	1.93	0.49
6:b:636:SER:HB2	7:C:65:TRP:HB3	1.94	0.49
13:f:60:ARG:HH11	29:P:167:ARG:HB2	1.77	0.49
17:H:180:TYR:HD2	32:r:18:LEU:HD12	1.78	0.49
32:r:7:ILE:O	32:r:11:ILE:HG12	2.12	0.49
39:Y:74:TYR:HD1	45:3:74:U:C4	2.30	0.49
41:Z:18:TYR:HA	41:Z:21:LYS:HD2	1.93	0.49
44:1:1039:U:O2'	44:1:1040:A:O5'	2.30	0.49
44:1:3228:C:H4'	44:1:3229:G:O5'	2.10	0.49
3:A:68:LYS:HD3	3:A:70:ARG:NH1	2.27	0.49
5:B:348:ARG:HG3	44:1:3037:U:H5"	1.94	0.49
17:H:114:VAL:HG11	17:H:165:CYS:SG	2.52	0.49
44:1:546:C:H4'	44:1:547:G:C5	2.47	0.49
44:1:2592:G:H4'	44:1:2594:C:C2	2.47	0.49
44:1:2656:A:OP2	44:1:2694:A:N6	2.41	0.49
44:1:2810:C:OP2	44:1:2955:U:O2'	2.23	0.49
48:m:91:HIS:O	48:m:95:ALA:N	2.34	0.49
48:m:457:PHE:HD1	48:m:464:TRP:CD1	2.30	0.49
49:2:12:U:OP2	49:2:68:C:O2'	2.31	0.49
54:s:35:GLN:HE21	54:s:205:VAL:HB	1.77	0.49
1:D:94:ASN:HB3	49:2:48:U:OP2	2.12	0.49
6:b:630:LEU:HD11	7:C:71:VAL:HG11	1.94	0.49
14:G:189:LEU:HD12	14:G:190:VAL:HG13	1.94	0.49
32:r:164:ARG:HH21	48:m:315:GLN:HE22	1.60	0.49
36:V:7:GLN:NE2	40:y:10:SER:HB2	2.27	0.49
52:4:468:LEU:HB3	52:4:469:PRO:HD3	1.95	0.49
7:C:23:PRO:HD2	7:C:26:PHE:CD2	2.48	0.49
10:E:170:LYS:HB3	10:E:172:HIS:CE1	2.48	0.49
37:W:56:ILE:O	37:W:60:TRP:HD1	1.96	0.49
44:1:2722:U:H2'	44:1:2723:U:C6	2.47	0.49
50:t:93:PHE:HA	50:t:96:GLN:NE2	2.28	0.49
5:B:59:ASP:OD1	5:B:355:SER:OG	2.30	0.49
5:B:95:THR:C	5:B:97:ARG:H	2.21	0.49
16:I:98:LEU:HD23	27:u:70:THR:HG22	1.94	0.49
35:U:19:VAL:C	35:U:22:PRO:HD2	2.38	0.49
40:y:99:GLU:HG3	40:y:101:LEU:H	1.78	0.49
44:1:2653:C:H2'	44:1:2654:C:C6	2.47	0.49
45:3:126:A:O2'	45:3:128:U:OP2	2.23	0.49
50:t:234:ILE:HG22	50:t:235:TRP:CD1	2.48	0.49
52:4:20:LEU:HD12	52:4:25:LEU:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:G:25:PRO:HB2	41:Z:125:GLY:H	1.77	0.49
15:g:31:ARG:NH2	44:1:1598:G:OP2	2.46	0.49
15:g:92:ALA:O	15:g:96:GLU:HG2	2.13	0.49
18:h:86:ARG:HD2	45:3:37:A:OP2	2.12	0.49
31:R:23:TRP:CD1	44:1:1473:G:H5"	2.48	0.49
40:y:41:GLU:HG2	40:y:203:LEU:HD13	1.95	0.49
44:1:3167:A:C6	44:1:3168:A:H1'	2.48	0.49
46:5:87:GLU:OE1	46:5:88:GLU:HB3	2.12	0.49
52:4:193:THR:HG22	52:4:226:ILE:HD12	1.95	0.49
6:b:268:VAL:HG21	6:b:305:LEU:HD13	1.94	0.49
12:F:116:PHE:O	12:F:199:ASN:ND2	2.46	0.49
18:h:75:TYR:O	38:X:46:TYR:HB3	2.13	0.49
40:y:88:LEU:HD12	40:y:92:VAL:HG11	1.94	0.49
44:1:1480:G:O2'	44:1:1871:U:O4	2.29	0.49
44:1:2252:A:H2'	44:1:2253:G:C8	2.47	0.49
45:3:8:C:H2'	45:3:9:A:H8	1.76	0.49
47:x:214:ASP:HB2	47:x:221:LEU:HD21	1.95	0.49
48:m:103:THR:OG1	48:m:278:SER:O	2.20	0.49
50:t:417:PRO:HB3	50:t:458:ALA:HA	1.94	0.49
54:s:195:LYS:HE2	54:s:196:LYS:HG3	1.95	0.49
1:D:31:TYR:HE1	1:D:35:ARG:HH11	1.61	0.48
2:J:15:GLU:OE1	2:J:132:ASN:ND2	2.38	0.48
3:A:9:ARG:NH2	44:1:912:G:OP2	2.46	0.48
5:B:341:SER:O	5:B:343:TYR:N	2.46	0.48
6:b:175:TYR:CE1	6:b:270:LEU:HD12	2.48	0.48
7:C:8:VAL:O	7:C:16:THR:OG1	2.28	0.48
20:j:10:LYS:HB2	44:1:818:C:H5"	1.95	0.48
20:j:25:ARG:NH2	44:1:359:U:O3'	2.41	0.48
44:1:2399:A:H3'	44:1:2400:G:H3'	1.95	0.48
50:t:464:LEU:CD1	50:t:496:MET:HE2	2.43	0.48
52:4:36:GLN:OE1	52:4:531:THR:OG1	2.27	0.48
7:C:4:PRO:HD2	7:C:22:LEU:HD12	1.94	0.48
11:e:87:MET:HE3	11:e:88:HIS:HE1	1.77	0.48
16:I:58:MET:HE1	44:1:1936:A:H4'	1.95	0.48
33:S:26:ARG:HB2	34:T:148:PRO:HB2	1.94	0.48
44:1:1126:G:O6	55:q:32:LYS:NZ	2.46	0.48
44:1:2469:G:HO2'	54:s:26:ARG:HH11	1.59	0.48
48:m:219:ILE:HG21	48:m:245:TYR:HE2	1.78	0.48
50:t:87:LEU:O	50:t:91:VAL:N	2.41	0.48
52:4:507:ILE:HD12	52:4:522:LEU:HD11	1.96	0.48
6:b:182:SER:HG	6:b:322:CYS:HG	1.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:h:31:LEU:HD12	18:h:34:GLN:NE2	2.27	0.48
18:h:99:GLN:HB2	26:N:146:ALA:HB2	1.94	0.48
22:L:180:ARG:O	22:L:184:GLU:HG3	2.13	0.48
31:R:136:ARG:O	31:R:139:VAL:N	2.46	0.48
40:y:118:HIS:CE1	40:y:120:ASP:HB2	2.48	0.48
44:1:3011:A:N1	44:1:3043:C:O2'	2.42	0.48
52:4:179:GLY:HA3	52:4:327:GLU:HG2	1.94	0.48
5:B:123:TYR:CZ	5:B:124:LYS:HG3	2.48	0.48
16:I:6:VAL:O	16:I:10:LYS:HG3	2.13	0.48
19:i:70:ARG:HD2	19:i:84:LYS:HD3	1.95	0.48
22:L:89:TYR:CE2	22:L:93:ILE:HD11	2.49	0.48
33:S:77:VAL:HG12	33:S:126:VAL:HG22	1.95	0.48
33:S:117:ARG:HE	33:S:118:PHE:H	1.60	0.48
44:1:1740:U:H4'	44:1:1741:A:H5"	1.94	0.48
44:1:1765:U:N3	44:1:1766:G:O2'	2.44	0.48
50:t:112:LEU:HD11	50:t:131:ILE:HG13	1.95	0.48
2:J:19:LEU:HD23	2:J:125:MET:HE1	1.94	0.48
6:b:188:THR:OG1	6:b:208:HIS:O	2.28	0.48
15:g:6:THR:HG22	44:1:1486:G:H21	1.78	0.48
28:O:74:ARG:NH1	44:1:3008:A:OP2	2.46	0.48
34:T:13:TYR:H	44:1:994:G:H3'	1.78	0.48
44:1:1223:A:H61	46:5:30:ARG:HH22	1.61	0.48
46:5:38:ASN:CG	46:5:39:LYS:H	2.20	0.48
50:t:404:MET:HE1	50:t:443:ALA:HB1	1.95	0.48
52:4:316:VAL:HG13	52:4:508:VAL:HG22	1.96	0.48
54:s:66:CYS:SG	54:s:67:ILE:N	2.86	0.48
15:g:88:ARG:HG2	44:1:2555:G:O2'	2.14	0.48
17:H:23:ARG:HE	17:H:39:LYS:HA	1.77	0.48
18:h:105:ARG:O	18:h:109:ILE:HG13	2.13	0.48
23:l:43:ASN:HD22	23:l:46:ARG:CZ	2.26	0.48
30:Q:147:ARG:HA	44:1:786:A:H5'	1.94	0.48
35:U:77:LYS:O	35:U:81:LYS:HG3	2.13	0.48
44:1:1554:U:H4'	44:1:1555:U:OP1	2.14	0.48
47:x:260:ILE:HB	47:x:274:MET:SD	2.54	0.48
52:4:70:SER:OG	52:4:400:PRO:O	2.32	0.48
52:4:97:ILE:HD13	52:4:128:SER:HB3	1.94	0.48
24:M:24:LYS:NZ	24:M:61:GLY:O	2.35	0.48
26:N:68:ARG:NH2	44:1:292:U:OP2	2.43	0.48
36:V:10:LYS:NZ	36:V:56:ASP:OD1	2.44	0.48
41:Z:121:ARG:HE	41:Z:126:LYS:HD2	1.77	0.48
44:1:2585:G:H2'	44:1:2585:G:N3	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:t:128:LYS:O	50:t:132:LEU:HD23	2.14	0.48
52:4:218:ILE:HG13	52:4:222:LEU:HD23	1.95	0.48
6:b:168:ARG:H	6:b:168:ARG:HD3	1.78	0.48
6:b:227:ARG:CG	6:b:228:PRO:HD3	2.44	0.48
15:g:68:THR:HG21	44:1:1644:C:H41	1.79	0.48
25:p:10:ILE:HD13	25:p:30:GLU:HB3	1.95	0.48
26:N:44:ARG:NH2	26:N:120:TRP:O	2.47	0.48
31:R:102:LEU:HD22	31:R:138:LEU:HD13	1.96	0.48
44:1:999:G:H2'	44:1:1001:G:N7	2.29	0.48
44:1:1288:U:H2'	44:1:1289:G:H8	1.79	0.48
44:1:1322:U:H2'	44:1:1323:G:H8	1.79	0.48
44:1:2186:U:O2'	44:1:2313:A:N3	2.45	0.48
49:2:52:G:O2'	49:2:53:U:OP1	2.25	0.48
52:4:98:ASP:O	52:4:499:PRO:HA	2.14	0.48
4:a:75:LEU:HG	4:a:114:GLY:HA2	1.96	0.48
5:B:292:ALA:HB2	5:B:302:LYS:HD3	1.95	0.48
10:E:46:ARG:NH1	44:1:3268:A:H5"	2.29	0.48
10:E:142:ASP:O	10:E:146:ILE:HG12	2.14	0.48
22:L:153:ASP:OD1	22:L:154:VAL:N	2.46	0.48
44:1:1355:A:H4'	44:1:1356:U:O5'	2.12	0.48
44:1:1594:A:H1'	44:1:1615:C:H1'	1.96	0.48
50:t:22:LYS:HG3	50:t:23:ARG:HG3	1.96	0.48
52:4:186:ALA:HB2	52:4:234:TYR:CG	2.49	0.48
54:s:145:TYR:HA	54:s:148:VAL:HG12	1.94	0.48
6:b:172:ILE:HD13	6:b:183:PHE:HD2	1.79	0.48
6:b:298:LEU:HG	6:b:302:ARG:HG3	1.96	0.48
37:W:162:GLU:OE2	37:W:173:THR:OG1	2.24	0.48
39:Y:48:LEU:HD21	39:Y:109:LEU:HD21	1.96	0.48
39:Y:85:VAL:HG11	39:Y:99:LEU:HD11	1.95	0.48
44:1:1044:U:H1'	46:5:108:ARG:NH1	2.29	0.48
44:1:1482:A:H2'	44:1:1482:A:N3	2.29	0.48
44:1:1932:A:N1	48:m:437:ARG:NH2	2.50	0.48
44:1:2949:U:H2'	44:1:2950:G:C8	2.49	0.48
44:1:3294:A:H2'	44:1:3295:A:O4'	2.14	0.48
2:J:164:LYS:NZ	2:J:171:VAL:H	2.12	0.47
12:F:98:LYS:HB3	12:F:99:PRO:HD3	1.96	0.47
18:h:41:LEU:O	18:h:44:ILE:HG22	2.13	0.47
32:r:186:HIS:ND1	32:r:188:GLU:O	2.46	0.47
47:x:327:SER:O	47:x:374:MET:HB2	2.14	0.47
56:Lr:12:ARG:O	56:Lr:16:LYS:HG2	2.13	0.47
15:g:20:ILE:HG23	15:g:32:ALA:HB1	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:H:48:VAL:HG23	17:H:49:ASN:N	2.29	0.47
44:1:996:A:H2'	44:1:997:A:C8	2.48	0.47
44:1:1288:U:H2'	44:1:1289:G:C8	2.49	0.47
44:1:3118:C:H5'	46:5:17:VAL:HB	1.96	0.47
44:1:3233:C:H2'	44:1:3234:A:C8	2.49	0.47
3:A:79:ASN:OD1	3:A:114:SER:OG	2.32	0.47
15:g:74:ARG:NH1	15:g:82:ALA:HB2	2.29	0.47
27:u:78:PRO:HG2	40:y:85:ARG:HB2	1.97	0.47
31:R:82:LYS:O	44:1:1914:G:O2'	2.27	0.47
33:S:96:ASP:CG	33:S:97:VAL:H	2.23	0.47
44:1:2654:C:H4'	44:1:2656:A:C8	2.50	0.47
50:t:427:ILE:HG23	50:t:431:PHE:HD2	1.77	0.47
52:4:48:ASP:O	52:4:52:SER:OG	2.24	0.47
52:4:315:GLU:OE1	52:4:317:TYR:OH	2.32	0.47
5:B:216:ASP:CB	5:B:278:ILE:HA	2.44	0.47
6:b:65:LEU:CD1	44:1:2863:G:H1'	2.43	0.47
24:M:32:LEU:HD11	24:M:94:TRP:CG	2.49	0.47
26:N:126:THR:HG23	26:N:127:TYR:CD2	2.49	0.47
35:U:37:LEU:HD12	35:U:41:ILE:HD11	1.96	0.47
44:1:107:A:O2'	44:1:324:A:N3	2.37	0.47
1:D:55:PHE:HD2	1:D:158:ARG:HH21	1.61	0.47
2:J:24:GLY:HA2	44:1:2680:A:C2	2.49	0.47
2:J:164:LYS:HZ1	2:J:171:VAL:HG12	1.80	0.47
6:b:266:ALA:HA	6:b:269:LYS:HE2	1.95	0.47
18:h:76:GLN:O	18:h:81:ARG:NH2	2.26	0.47
19:i:9:ILE:HD12	22:L:174:ARG:HB3	1.95	0.47
22:L:16:LYS:NZ	26:N:195:ASN:OD1	2.34	0.47
29:P:127:ARG:NH1	44:1:1506:A:OP2	2.47	0.47
32:r:214:VAL:HG12	32:r:216:THR:HG23	1.96	0.47
40:y:15:VAL:HA	40:y:61:ARG:HG2	1.97	0.47
40:y:151:TYR:HE2	40:y:192:VAL:HG22	1.79	0.47
44:1:849:C:H2'	44:1:850:U:C6	2.50	0.47
44:1:1065:A:H5"	44:1:1066:G:OP2	2.15	0.47
44:1:1913:A:N3	44:1:2120:A:H2'	2.29	0.47
1:D:107:ARG:HH12	1:D:110:LEU:HD22	1.80	0.47
6:b:92:LYS:NZ	44:1:2863:G:H22	2.13	0.47
6:b:177:ASN:OD1	6:b:181:SER:OG	2.28	0.47
6:b:330:GLU:O	6:b:334:LYS:HG2	2.14	0.47
7:C:190:GLY:O	7:C:193:LYS:NZ	2.45	0.47
14:G:152:LEU:HD13	14:G:180:VAL:HG11	1.97	0.47
16:I:89:VAL:HG22	16:I:101:PHE:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:N:103:GLU:OE2	26:N:118:SER:OG	2.23	0.47
27:u:73:GLN:HG3	27:u:74:ARG:N	2.27	0.47
39:Y:47:ALA:O	39:Y:122:LYS:NZ	2.48	0.47
42:z:18:ARG:O	42:z:23:GLN:HB2	2.15	0.47
44:1:844:G:H2'	44:1:845:G:H5'	1.97	0.47
44:1:1127:G:N2	44:1:1131:G:H21	2.12	0.47
44:1:2496:C:H1'	44:1:2497:U:C6	2.50	0.47
50:t:176:LEU:HA	50:t:179:ILE:HB	1.96	0.47
52:4:28:TYR:CE1	52:4:316:VAL:HG11	2.49	0.47
54:s:42:ASP:O	54:s:46:ASP:HB2	2.14	0.47
3:A:117:GLU:OE2	3:A:163:ARG:NH2	2.33	0.47
5:B:124:LYS:HG2	44:1:3316:A:C6	2.49	0.47
6:b:417:LYS:HG2	6:b:420:TYR:HE1	1.80	0.47
6:b:456:LEU:HD22	27:u:71:PHE:HE2	1.79	0.47
6:b:529:GLY:O	6:b:532:GLU:HG3	2.15	0.47
14:G:161:GLU:HA	14:G:164:VAL:HG22	1.97	0.47
22:L:16:LYS:HG2	44:1:47:C:H5"	1.96	0.47
30:Q:36:LEU:O	30:Q:40:THR:OG1	2.28	0.47
40:y:15:VAL:HG13	40:y:61:ARG:HG3	1.97	0.47
41:Z:46:ILE:HA	41:Z:70:PRO:HA	1.97	0.47
44:1:411:U:H2'	44:1:412:G:C8	2.50	0.47
44:1:518:G:OP2	44:1:518:G:N2	2.38	0.47
44:1:1176:C:H2'	44:1:1177:G:N2	2.30	0.47
44:1:2150:G:O2'	44:1:2189:U:OP1	2.26	0.47
44:1:2209:U:O5'	50:t:194:ASN:ND2	2.47	0.47
44:1:2357:A:H2'	44:1:2358:A:C8	2.49	0.47
44:1:2493:U:O2'	44:1:2494:A:O4'	2.32	0.47
50:t:464:LEU:HD12	50:t:496:MET:HE2	1.96	0.47
52:4:273:HIS:HA	52:4:276:ALA:HB3	1.96	0.47
1:D:63:GLN:HB3	1:D:65:ILE:HG23	1.96	0.47
15:g:89:ILE:HD11	41:Z:19:ALA:HB1	1.97	0.47
24:M:112:LEU:HD11	24:M:117:ARG:HG3	1.97	0.47
26:N:73:ARG:HG2	26:N:75:VAL:HG13	1.97	0.47
32:r:236:LYS:O	32:r:237:VAL:HG23	2.14	0.47
33:S:71:LYS:HE2	33:S:73:LYS:HD2	1.97	0.47
44:1:345:G:O2'	45:3:25:G:N3	2.46	0.47
44:1:761:A:H2'	44:1:762:U:C6	2.50	0.47
44:1:2660:G:OP1	44:1:2750:U:O2'	2.33	0.47
44:1:3269:U:H4'	44:1:3270:U:O5'	2.14	0.47
48:m:333:ASN:ND2	48:m:339:LYS:HD3	2.30	0.47
52:4:194:VAL:O	52:4:197:LEU:HG	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:ARG:NH2	49:2:6:C:OP2	2.46	0.47
5:B:133:TYR:O	5:B:136:LYS:HG2	2.15	0.47
5:B:151:ILE:O	5:B:155:ALA:HB3	2.15	0.47
7:C:347:THR:O	44:1:520:U:N3	2.48	0.47
14:G:64:ILE:O	14:G:68:ARG:HG2	2.14	0.47
17:H:103:ILE:HD13	17:H:112:ILE:HG13	1.96	0.47
22:L:174:ARG:HH11	44:1:712:G:H5"	1.80	0.47
33:S:112:ALA:O	33:S:115:ARG:NH1	2.48	0.47
44:1:209:A:H4'	44:1:211:A:N7	2.30	0.47
44:1:710:A:H2'	44:1:711:A:C8	2.49	0.47
44:1:955:U:P	44:1:1116:G:H22	2.36	0.47
44:1:967:A:H62	44:1:1115:G:N2	2.07	0.47
44:1:1322:U:H2'	44:1:1323:G:C8	2.50	0.47
45:3:154:C:H2'	45:3:155:A:O4'	2.15	0.47
1:D:119:TYR:CZ	1:D:135:VAL:HG22	2.50	0.47
6:b:329:MET:SD	6:b:332:ARG:NH2	2.87	0.47
22:L:53:LEU:HD22	22:L:94:GLY:HA2	1.97	0.47
26:N:83:LYS:NZ	44:1:46:U:O4	2.47	0.47
32:r:231:VAL:CG1	32:r:235:GLY:HA2	2.45	0.47
33:S:145:THR:HG23	46:5:38:ASN:H	1.78	0.47
44:1:383:G:N2	44:1:386:A:OP2	2.31	0.47
44:1:2631:U:N3	44:1:2632:G:N7	2.62	0.47
50:t:333:ILE:HA	50:t:336:LEU:HD22	1.97	0.47
5:B:92:TYR:HB2	5:B:157:VAL:HB	1.96	0.46
5:B:156:SER:O	5:B:188:ILE:HD11	2.15	0.46
6:b:135:ARG:NH2	44:1:2858:U:O2'	2.49	0.46
28:O:49:ARG:HD3	44:1:1191:U:OP2	2.16	0.46
29:P:169:THR:HG22	44:1:618:C:H5'	1.97	0.46
31:R:62:ARG:HH22	44:1:3067:C:H3'	1.80	0.46
31:R:98:ARG:NH1	31:R:132:PHE:O	2.48	0.46
32:r:196:PRO:HG2	32:r:224:ASN:ND2	2.30	0.46
39:Y:74:TYR:CE2	39:Y:77:LYS:HG3	2.47	0.46
40:y:109:CYS:SG	40:y:116:LEU:HB2	2.55	0.46
44:1:616:G:H2'	44:1:617:G:C8	2.50	0.46
50:t:211:LEU:HD12	50:t:222:ALA:HB2	1.98	0.46
52:4:322:LYS:HE2	52:4:502:ARG:HD3	1.97	0.46
6:b:561:ARG:N	6:b:564:ASP:OD2	2.49	0.46
23:l:9:ILE:O	23:l:13:MET:HG3	2.15	0.46
27:u:4:TYR:HB2	27:u:30:ARG:HD2	1.96	0.46
44:1:1131:G:O2'	44:1:1132:C:O5'	2.33	0.46
52:4:226:ILE:HG22	52:4:549:ILE:HD11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:4:229:THR:HA	52:4:232:ARG:HG2	1.96	0.46
9:d:13:THR:OG1	9:d:72:ARG:NH1	2.37	0.46
12:F:86:VAL:O	12:F:114:GLY:HA2	2.16	0.46
12:F:151:ARG:HD2	12:F:207:LEU:HD23	1.96	0.46
25:p:75:ALA:O	25:p:79:VAL:HG23	2.15	0.46
32:r:236:LYS:O	48:m:86:GLN:HG2	2.15	0.46
34:T:14:MET:HG3	44:1:994:G:H4'	1.97	0.46
44:1:967:A:N6	44:1:1115:G:H21	2.08	0.46
44:1:1031:C:H2'	44:1:1032:C:C6	2.50	0.46
44:1:2252:A:OP1	50:t:173:ALA:N	2.47	0.46
44:1:3213:A:H2'	44:1:3214:U:O4'	2.14	0.46
44:1:3365:U:H2'	44:1:3366:G:C8	2.51	0.46
50:t:392:TYR:HB3	50:t:403:ILE:HD13	1.98	0.46
6:b:596:GLY:HA2	6:b:599:ARG:HB3	1.96	0.46
11:e:40:SER:HB3	44:1:639:G:OP1	2.15	0.46
44:1:998:A:H3'	44:1:999:G:C8	2.50	0.46
44:1:2271:A:H5'	44:1:2272:G:C8	2.50	0.46
44:1:2375:G:H4'	44:1:2376:G:OP1	2.14	0.46
46:5:40:LYS:HD3	46:5:43:SER:H	1.80	0.46
47:x:230:LYS:H	47:x:257:ASP:HB3	1.79	0.46
48:m:379:GLU:H	48:m:379:GLU:CD	2.24	0.46
50:t:93:PHE:HA	50:t:96:GLN:HE21	1.79	0.46
52:4:219:THR:OG1	52:4:220:GLY:N	2.48	0.46
5:B:108:GLU:O	5:B:108:GLU:HG2	2.16	0.46
6:b:221:THR:HG22	6:b:223:GLY:H	1.81	0.46
17:H:151:VAL:O	17:H:155:SER:OG	2.31	0.46
18:h:78:LYS:HA	18:h:81:ARG:HG2	1.97	0.46
29:P:86:LYS:HB2	44:1:2353:G:H5"	1.97	0.46
32:r:147:TRP:CZ2	32:r:170:ARG:HB2	2.50	0.46
36:V:41:GLY:N	44:1:2932:U:OP1	2.41	0.46
40:y:114:VAL:HG11	40:y:177:LEU:HA	1.97	0.46
42:z:40:ASP:OD1	42:z:44:GLN:NE2	2.47	0.46
44:1:2251:G:H1	44:1:2266:U:H3	1.62	0.46
44:1:2535:A:N6	44:1:2544:U:H3	2.14	0.46
52:4:66:LEU:HA	52:4:69:ASP:HB2	1.97	0.46
54:s:207:LYS:HG2	54:s:208:SER:O	2.16	0.46
4:a:132:LYS:O	4:a:136:GLU:HG3	2.16	0.46
7:C:46:LYS:HE2	44:1:692:A:H1'	1.97	0.46
7:C:197:ARG:NE	44:1:1381:A:OP1	2.46	0.46
16:I:25:LEU:O	16:I:119:ASN:ND2	2.48	0.46
16:I:30:SER:HA	16:I:33:LYS:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:P:36:ILE:HD12	29:P:44:ALA:HB1	1.96	0.46
44:1:1951:C:H42	44:1:2095:G:H1	1.64	0.46
44:1:2925:C:H41	48:m:209:LYS:HD2	1.80	0.46
47:x:144:SER:C	47:x:508:LYS:HG2	2.40	0.46
6:b:599:ARG:CZ	52:4:462:ALA:HB1	2.46	0.46
10:E:162:SER:N	44:1:3216:G:OP1	2.49	0.46
11:e:23:ASP:OD2	44:1:425:G:H5'	2.15	0.46
13:f:17:GLN:O	13:f:24:ASN:N	2.41	0.46
25:p:36:ARG:NE	25:p:48:LYS:HD3	2.30	0.46
34:T:89:LEU:HD12	34:T:90:ASN:H	1.80	0.46
35:U:71:PHE:HE1	35:U:76:LEU:HB2	1.80	0.46
44:1:2737:C:H2'	44:1:2738:A:H8	1.80	0.46
48:m:90:GLN:OE1	48:m:93:ARG:HD2	2.16	0.46
50:t:123:LEU:HD11	50:t:127:LEU:HD23	1.98	0.46
52:4:276:ALA:O	52:4:280:SER:N	2.40	0.46
1:D:205:SER:HB3	1:D:236:LEU:HD23	1.97	0.46
4:a:77:LYS:C	4:a:79:TRP:H	2.23	0.46
5:B:13:HIS:HD2	5:B:15:GLY:H	1.59	0.46
6:b:23:ASN:HB2	44:1:2828:G:O6	2.16	0.46
6:b:422:LEU:HD12	6:b:428:LYS:HA	1.97	0.46
18:h:40:SER:HA	45:3:49:G:O2'	2.16	0.46
18:h:94:LYS:HD3	44:1:135:C:C4	2.51	0.46
37:W:196:ASP:OD1	37:W:196:ASP:N	2.48	0.46
44:1:2669:G:H2'	44:1:2670:G:C8	2.50	0.46
44:1:3357:U:H2'	44:1:3358:U:H6	1.80	0.46
47:x:170:ILE:HB	47:x:180:HIS:HB2	1.97	0.46
48:m:234:PRO:HG2	48:m:273:TRP:CD2	2.50	0.46
52:4:110:ASP:OD1	52:4:356:ARG:NH2	2.49	0.46
5:B:106:TRP:HB2	5:B:133:TYR:CE1	2.50	0.46
6:b:598:MET:HE1	45:3:76:C:H4'	1.97	0.46
12:F:206:LYS:HE2	44:1:1334:U:OP1	2.16	0.46
33:S:139:TYR:CD1	33:S:140:VAL:HG23	2.51	0.46
37:W:45:LEU:HB3	37:W:215:VAL:HG23	1.98	0.46
44:1:398:A:N6	53:o:88:THR:OG1	2.49	0.46
44:1:1724:U:H1'	44:1:1725:C:C6	2.50	0.46
44:1:3288:G:O2'	44:1:3289:G:H8	1.98	0.46
52:4:20:LEU:HD23	52:4:20:LEU:H	1.81	0.46
1:D:197:SER:HB3	1:D:202:GLY:HA3	1.98	0.46
5:B:198:HIS:CE1	42:z:41:LEU:HD21	2.51	0.46
6:b:178:VAL:HG23	6:b:179:GLY:H	1.80	0.46
6:b:209:PHE:HE2	6:b:218:ALA:HB2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:169:LEU:HD23	7:C:178:LEU:HD11	1.97	0.46
7:C:362:ASP:N	7:C:362:ASP:OD1	2.48	0.46
10:E:39:VAL:O	10:E:87:THR:OG1	2.26	0.46
20:j:54:LYS:O	20:j:58:THR:HG23	2.15	0.46
26:N:8:GLU:HB2	26:N:50:ARG:HH22	1.80	0.46
26:N:94:TYR:CZ	26:N:96:ARG:HB2	2.51	0.46
33:S:137:ARG:NH1	44:1:1213:G:OP1	2.49	0.46
40:y:84:LEU:HB3	40:y:94:ILE:HD13	1.97	0.46
44:1:563:U:H2'	44:1:564:G:C8	2.51	0.46
44:1:1466:G:N2	44:1:1510:G:H5"	2.30	0.46
44:1:1528:G:O2'	44:1:1588:A:N3	2.41	0.46
47:x:139:ILE:HG22	47:x:171:TRP:HZ3	1.79	0.46
50:t:88:ILE:HA	50:t:91:VAL:HG12	1.97	0.46
3:A:179:LEU:O	3:A:184:ARG:HD2	2.16	0.45
10:E:165:LEU:HD23	13:f:6:ARG:O	2.16	0.45
20:j:68:LYS:NZ	45:3:57:C:OP2	2.48	0.45
36:V:86:ARG:HB2	36:V:92:PHE:CE2	2.50	0.45
37:W:17:LYS:HA	44:1:1279:C:H5"	1.98	0.45
44:1:2467:G:N2	44:1:2489:C:N3	2.64	0.45
44:1:2495:C:H2'	44:1:2496:C:C6	2.51	0.45
48:m:192:ASN:HB3	48:m:194:TRP:CD1	2.51	0.45
52:4:45:LEU:HD22	52:4:59:LEU:HD12	1.98	0.45
54:s:120:VAL:HG11	54:s:135:PRO:HG2	1.98	0.45
31:R:4:LEU:HD11	31:R:29:THR:HG23	1.97	0.45
41:Z:10:VAL:HG11	41:Z:85:TYR:HB2	1.98	0.45
44:1:239:G:O2'	44:1:240:U:OP1	2.31	0.45
44:1:970:A:H2'	44:1:971:G:O4'	2.16	0.45
44:1:2168:A:C6	44:1:2170:U:H1'	2.51	0.45
44:1:2534:G:H2'	44:1:2535:A:C8	2.51	0.45
44:1:2655:U:O5'	44:1:2656:A:H5'	2.16	0.45
44:1:2657:A:O2'	44:1:2658:G:OP2	2.30	0.45
44:1:3357:U:H2'	44:1:3358:U:C6	2.51	0.45
5:B:169:THR:HG22	5:B:171:LEU:H	1.81	0.45
5:B:216:ASP:HB3	5:B:278:ILE:HA	1.97	0.45
5:B:387:LEU:HD21	27:u:108:TYR:CD2	2.51	0.45
11:e:32:TRP:CZ2	11:e:53:PRO:HD2	2.52	0.45
27:u:127:VAL:HG23	27:u:134:LEU:HD21	1.98	0.45
33:S:109:ASP:OD1	33:S:113:ARG:NH1	2.45	0.45
40:y:177:LEU:HB3	40:y:179:VAL:HG22	1.96	0.45
41:Z:87:LEU:HG	41:Z:127:ASN:ND2	2.31	0.45
43:K:114:UNK:O	43:K:118:UNK:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:1:162:G:H1	44:1:259:C:H42	1.63	0.45
44:1:628:A:H5'	44:1:1399:A:C6	2.52	0.45
48:m:356:ILE:N	48:m:364:LEU:O	2.45	0.45
3:A:207:VAL:HG23	3:A:208:ASP:OD1	2.17	0.45
5:B:198:HIS:NE2	42:z:41:LEU:HD21	2.32	0.45
6:b:79:ARG:NH2	48:m:167:ASP:OD2	2.49	0.45
6:b:100:ARG:NH2	44:1:2860:U:O5'	2.50	0.45
6:b:228:PRO:HG2	6:b:230:GLU:H	1.81	0.45
7:C:269:SER:C	7:C:271:LYS:H	2.24	0.45
8:c:47:ASN:HB2	8:c:73:GLY:HA2	1.97	0.45
26:N:73:ARG:HG3	26:N:74:PRO:HD2	1.97	0.45
29:P:8:SER:O	53:o:84:ILE:HA	2.16	0.45
43:K:80:LEU:O	43:K:84:ALA:N	2.46	0.45
44:1:589:A:H1'	44:1:1337:A:H5"	1.97	0.45
44:1:1005:G:H4'	48:m:76:ARG:HD2	1.98	0.45
44:1:1895:A:N6	44:1:2335:G:O2'	2.50	0.45
44:1:2509:U:H2'	44:1:2510:U:O4'	2.16	0.45
47:x:241:HIS:NE2	47:x:288:GLY:O	2.46	0.45
1:D:60:ILE:HB	1:D:80:SER:HB3	1.98	0.45
9:d:57:GLN:OE1	44:1:1474:A:O2'	2.35	0.45
12:F:181:ILE:O	12:F:185:ILE:HG12	2.17	0.45
13:f:90:PRO:HG2	13:f:93:THR:HG23	1.98	0.45
14:G:134:TYR:HB3	14:G:190:VAL:HG11	1.99	0.45
14:G:181:LYS:HG2	45:3:154:C:H5"	1.97	0.45
15:g:81:CYS:HB2	15:g:84:CYS:H	1.81	0.45
16:I:75:ARG:HH11	16:I:76:ARG:NE	2.14	0.45
22:L:35:ARG:NH1	44:1:685:G:OP2	2.48	0.45
26:N:9:GLU:OE2	26:N:13:LYS:NZ	2.50	0.45
26:N:31:ARG:NH1	44:1:2516:U:OP1	2.50	0.45
26:N:108:ARG:NH2	44:1:1547:G:OP1	2.38	0.45
32:r:28:GLU:HA	32:r:31:GLU:HG2	1.98	0.45
44:1:1661:G:H2'	44:1:1662:G:C8	2.51	0.45
44:1:1717:U:H2'	44:1:1718:G:C8	2.52	0.45
44:1:2836:C:H5	44:1:2852:C:H42	1.65	0.45
50:t:250:HIS:CG	50:t:251:GLN:H	2.35	0.45
50:t:442:ALA:O	50:t:446:ASN:ND2	2.50	0.45
55:q:55:PRO:HG2	55:q:56:TYR:CD1	2.51	0.45
3:A:244:GLY:HA3	44:1:2242:A:H5"	1.99	0.45
5:B:108:GLU:HB2	5:B:137:TYR:CE1	2.51	0.45
17:H:49:ASN:O	17:H:49:ASN:ND2	2.41	0.45
32:r:189:LEU:HD21	47:x:299:ARG:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:1:115:A:H2'	44:1:265:A:N3	2.32	0.45
44:1:537:A:H2'	44:1:538:G:O4'	2.16	0.45
44:1:877:C:N4	44:1:878:G:O6	2.50	0.45
44:1:2271:A:H5'	44:1:2272:G:H8	1.81	0.45
44:1:2660:G:H2'	44:1:2661:G:C8	2.51	0.45
49:2:70:U:H2'	49:2:71:G:O4'	2.17	0.45
50:t:256:VAL:HG12	50:t:257:MET:HE2	1.97	0.45
3:A:134:VAL:HG12	3:A:150:LEU:HA	1.98	0.45
6:b:611:ARG:HD2	44:1:402:A:C6	2.52	0.45
7:C:177:ASP:OD1	7:C:180:LYS:HE3	2.17	0.45
7:C:329:PRO:HB3	12:F:41:ARG:NH2	2.31	0.45
9:d:112:ASP:OD1	9:d:112:ASP:N	2.46	0.45
18:h:101:THR:HG22	18:h:103:LYS:H	1.82	0.45
44:1:94:G:H2'	44:1:95:A:C8	2.51	0.45
44:1:1005:G:O6	44:1:1006:A:N6	2.50	0.45
44:1:2193:U:H4'	44:1:2312:A:N1	2.31	0.45
44:1:2660:G:O3'	44:1:2749:G:N2	2.49	0.45
50:t:494:PRO:O	50:t:502:ARG:NE	2.42	0.45
53:o:101:LEU:O	53:o:105:THR:OG1	2.28	0.45
5:B:102:LEU:HD21	5:B:155:ALA:HB2	1.99	0.45
6:b:159:ARG:NH2	32:r:5:ASP:OD2	2.50	0.45
6:b:408:GLY:H	6:b:411:VAL:HG12	1.81	0.45
6:b:573:LEU:HD11	52:4:259:VAL:HA	1.99	0.45
7:C:209:TYR:OH	44:1:689:U:O4	2.32	0.45
8:c:17:VAL:HG11	8:c:92:ILE:HD12	1.99	0.45
13:f:90:PRO:HB3	44:1:430:U:O4'	2.17	0.45
14:G:146:LYS:HE2	14:G:173:MET:HB2	1.98	0.45
23:l:45:ARG:HH22	44:1:1841:A:H1'	1.82	0.45
26:N:28:TRP:O	26:N:32:GLN:HG2	2.17	0.45
26:N:180:PHE:O	26:N:184:LYS:HG3	2.16	0.45
35:U:29:ASP:N	35:U:29:ASP:OD1	2.48	0.45
35:U:97:SER:HB2	35:U:103:TYR:CD1	2.52	0.45
41:Z:70:PRO:HG3	41:Z:115:LYS:HB2	1.98	0.45
44:1:992:A:H3'	44:1:993:G:H8	1.82	0.45
44:1:2443:A:N6	44:1:2504:U:H3	2.14	0.45
44:1:2683:U:H2'	44:1:2684:C:C6	2.52	0.45
50:t:408:ALA:HB1	50:t:450:GLU:HG3	1.99	0.45
50:t:457:LEU:HD23	50:t:457:LEU:H	1.82	0.45
52:4:423:MET:HE3	52:4:427:SER:HB3	1.98	0.45
53:o:37:LYS:HA	53:o:37:LYS:HD3	1.79	0.45
2:J:115:LYS:NZ	2:J:117:ASP:HB2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:54:ARG:NH2	44:1:2176:U:OP1	2.47	0.45
5:B:206:ASP:HB2	42:z:36:LYS:HE2	1.99	0.45
6:b:207:GLY:O	6:b:218:ALA:N	2.42	0.45
6:b:271:PHE:HZ	6:b:315:VAL:HG21	1.82	0.45
12:F:84:VAL:HG12	12:F:138:TYR:CD1	2.51	0.45
14:G:63:LYS:HB3	14:G:63:LYS:HE2	1.77	0.45
14:G:129:PRO:HB3	44:1:121:A:C2	2.52	0.45
27:u:50:LYS:HG3	27:u:55:PHE:CE1	2.52	0.45
30:Q:137:THR:HG22	44:1:729:C:H4'	1.98	0.45
44:1:435:C:H2'	44:1:436:A:C8	2.51	0.45
44:1:2615:G:N2	48:m:57:ARG:HH22	2.13	0.45
48:m:359:MET:HB2	48:m:362:ILE:H	1.80	0.45
2:J:37:LEU:HD22	2:J:69:VAL:HG12	1.98	0.45
6:b:325:GLU:HA	6:b:328:VAL:HG12	1.99	0.45
14:G:33:ASN:CG	14:G:38:GLN:HE21	2.25	0.45
30:Q:131:ALA:HB1	30:Q:135:GLN:H	1.82	0.45
40:y:163:PRO:HA	40:y:183:ALA:HB1	1.99	0.45
41:Z:103:GLN:O	41:Z:105:SER:N	2.49	0.45
43:K:50:THR:HG23	43:K:59:THR:HG21	1.99	0.45
44:1:377:A:H1'	44:1:392:G:N2	2.32	0.45
44:1:1452:A:N3	44:1:2346:C:O2'	2.49	0.45
44:1:1816:A:HO2'	44:1:1817:G:P	2.40	0.45
48:m:24:VAL:HG11	48:m:33:SER:HA	2.00	0.45
2:J:164:LYS:NZ	2:J:171:VAL:HG12	2.32	0.44
5:B:312:VAL:HG12	5:B:313:HIS:ND1	2.32	0.44
7:C:67:THR:HG23	7:C:73:ARG:HH21	1.82	0.44
12:F:84:VAL:HG12	12:F:138:TYR:HD1	1.82	0.44
16:I:75:ARG:HD3	16:I:76:ARG:HE	1.82	0.44
24:M:47:ASP:OD1	24:M:55:ARG:HD2	2.16	0.44
31:R:21:LYS:NZ	44:1:1873:U:OP1	2.34	0.44
33:S:113:ARG:C	33:S:115:ARG:H	2.25	0.44
44:1:677:A:N1	44:1:703:G:O2'	2.43	0.44
44:1:1497:C:H2'	44:1:1498:A:C8	2.52	0.44
44:1:1604:G:H4'	44:1:1835:A:H4'	1.99	0.44
44:1:2252:A:P	50:t:174:LYS:HG2	2.57	0.44
48:m:46:LYS:HA	48:m:46:LYS:HD3	1.75	0.44
48:m:105:GLN:HA	51:n:40:THR:HA	1.99	0.44
3:A:193:ARG:NH1	44:1:2181:C:H5"	2.33	0.44
7:C:141:ARG:NH1	44:1:1385:C:OP1	2.47	0.44
33:S:26:ARG:O	34:T:150:THR:HA	2.17	0.44
44:1:1362:G:H2'	44:1:1363:A:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:1:2270:A:N3	44:1:2272:G:N1	2.65	0.44
44:1:2467:G:H21	44:1:2488:A:N6	2.07	0.44
44:1:3282:U:H2'	44:1:3283:U:C6	2.52	0.44
50:t:155:PRO:HA	50:t:158:VAL:HG12	1.98	0.44
5:B:332:ARG:HH22	44:1:3304:U:P	2.40	0.44
14:G:108:ARG:HA	14:G:111:LYS:HB3	1.99	0.44
17:H:90:MET:HE2	17:H:179:ILE:HG22	1.97	0.44
24:M:70:PHE:CE2	24:M:72:LEU:HD22	2.52	0.44
26:N:164:LEU:HD21	44:1:62:A:H5"	1.99	0.44
27:u:19:ILE:HG21	36:V:94:TYR:HE1	1.83	0.44
34:T:66:ASN:HB3	34:T:73:GLY:HA3	1.98	0.44
38:X:63:ILE:HD13	38:X:86:VAL:HG12	1.98	0.44
40:y:109:CYS:HB3	40:y:149:GLY:HA2	2.00	0.44
42:z:22:PHE:O	42:z:26:VAL:HG23	2.16	0.44
44:1:173:G:H1	44:1:245:U:H3	1.65	0.44
44:1:1192:C:N4	55:q:4:ARG:O	2.27	0.44
44:1:1252:A:H8	44:1:1253:U:H2'	1.82	0.44
44:1:2208:A:H4'	44:1:2209:U:H5'	1.98	0.44
44:1:2312:A:N9	48:m:337:LYS:HD3	2.32	0.44
44:1:2669:G:OP1	46:5:110:ARG:NH2	2.50	0.44
46:5:64:LEU:O	46:5:68:LYS:HG3	2.17	0.44
49:2:11:A:H4'	49:2:13:A:C8	2.52	0.44
49:2:72:A:H2'	49:2:74:C:C5	2.53	0.44
52:4:139:VAL:O	52:4:158:MET:N	2.48	0.44
54:s:68:PHE:C	54:s:116:LEU:HD12	2.41	0.44
4:a:85:ASP:OD1	4:a:86:LYS:HG3	2.18	0.44
5:B:108:GLU:HB2	5:B:137:TYR:CD1	2.52	0.44
6:b:257:SER:OG	6:b:258:GLU:N	2.49	0.44
12:F:222:HIS:HB3	12:F:225:GLN:HG2	1.98	0.44
14:G:186:LEU:HA	14:G:186:LEU:HD23	1.70	0.44
26:N:68:ARG:NH1	26:N:124:ASP:O	2.36	0.44
37:W:92:LEU:HD13	37:W:221:TYR:HB2	2.00	0.44
40:y:11:ASN:CG	40:y:209:ASP:HB2	2.42	0.44
40:y:156:ASN:HB2	40:y:201:ASP:OD2	2.17	0.44
40:y:225:GLN:HB2	40:y:228:GLN:HG3	1.99	0.44
44:1:359:U:H4'	44:1:817:A:N6	2.33	0.44
44:1:1058:U:O2'	44:1:1059:G:OP1	2.28	0.44
48:m:260:ASN:ND2	48:m:327:GLY:HA3	2.33	0.44
48:m:339:LYS:HE2	48:m:339:LYS:HB2	1.75	0.44
52:4:402:VAL:HG23	52:4:403:HIS:ND1	2.33	0.44
2:J:44:THR:HG23	49:2:39:C:H4'	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:b:189:LYS:O	44:1:3027:A:H4'	2.17	0.44
7:C:81:GLY:O	44:1:356:C:O2'	2.18	0.44
7:C:181:VAL:O	7:C:182:LEU:HB3	2.16	0.44
17:H:1:MET:O	17:H:1:MET:HG2	2.17	0.44
17:H:63:LYS:HD2	44:1:3122:A:O2'	2.17	0.44
26:N:64:VAL:HG11	26:N:102:ALA:HB1	1.99	0.44
30:Q:133:LYS:HB2	30:Q:135:GLN:OE1	2.18	0.44
35:U:93:ILE:HG13	35:U:106:ALA:O	2.18	0.44
39:Y:52:ARG:O	39:Y:70:ILE:HB	2.18	0.44
39:Y:109:LEU:HD22	39:Y:115:ARG:NH2	2.32	0.44
44:1:187:A:N3	44:1:208:C:O2'	2.44	0.44
44:1:1126:G:C2	44:1:1127:G:H1'	2.53	0.44
46:5:82:ARG:HG2	46:5:83:ARG:N	2.30	0.44
50:t:181:TYR:HA	50:t:184:LEU:HD12	1.98	0.44
52:4:360:TYR:HB3	52:4:432:CYS:SG	2.56	0.44
54:s:91:LYS:HA	54:s:123:LEU:HD22	2.00	0.44
1:D:140:ARG:NE	44:1:1080:A:OP1	2.44	0.44
3:A:32:LEU:HD13	3:A:163:ARG:HD3	2.00	0.44
5:B:233:TRP:NE1	5:B:266:ARG:O	2.50	0.44
6:b:590:LEU:HB3	6:b:599:ARG:CZ	2.47	0.44
7:C:29:PRO:HD2	7:C:277:PRO:HB2	1.99	0.44
7:C:73:ARG:O	7:C:73:ARG:HG2	2.17	0.44
12:F:231:ASN:CG	12:F:233:GLU:HG2	2.42	0.44
17:H:47:LYS:HD2	24:M:5:SER:HB2	2.00	0.44
19:i:66:GLU:HG2	19:i:70:ARG:NH1	2.32	0.44
32:r:44:GLY:C	32:r:46:LYS:H	2.26	0.44
44:1:498:A:O2'	44:1:3273:A:N1	2.49	0.44
44:1:1066:G:H2'	44:1:1067:U:C6	2.53	0.44
44:1:1121:U:OP1	55:q:24:SER:OG	2.24	0.44
44:1:1562:C:O2'	44:1:1563:C:O5'	2.33	0.44
44:1:1619:A:OP1	56:Lr:11:ARG:NH1	2.50	0.44
50:t:233:GLY:HA2	50:t:236:ASP:OD1	2.18	0.44
52:4:243:ARG:HD2	52:4:256:GLU:OE2	2.18	0.44
5:B:219:ALA:HB2	5:B:336:VAL:HG12	2.00	0.44
6:b:150:LEU:HA	6:b:153:VAL:HG22	1.99	0.44
6:b:294:ARG:O	6:b:296:GLU:N	2.51	0.44
6:b:621:GLU:HG3	23:l:41:ARG:HG2	1.98	0.44
7:C:317:PRO:HD2	12:F:149:TYR:O	2.18	0.44
8:c:57:GLU:O	8:c:61:MET:N	2.35	0.44
10:E:125:GLN:HG3	10:E:127:ASN:H	1.83	0.44
13:f:21:ARG:O	44:1:634:C:H5'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:G:41:GLN:HG3	44:1:2525:G:O6	2.18	0.44
15:g:52:GLN:HB2	44:1:1639:C:OP1	2.18	0.44
16:I:45:GLY:C	16:I:46:LEU:HD23	2.43	0.44
24:M:121:MET:HE1	44:1:3215:A:H5'	1.99	0.44
26:N:144:ARG:NH1	44:1:126:U:OP1	2.50	0.44
32:r:205:GLN:HB2	48:m:67:PRO:HG2	1.99	0.44
40:y:52:THR:OG1	40:y:80:GLU:OE2	2.30	0.44
44:1:29:C:H4'	44:1:62:A:H4'	1.98	0.44
44:1:2251:G:H5"	50:t:172:HIS:CD2	2.53	0.44
49:2:78:U:H2'	49:2:79:A:H8	1.83	0.44
50:t:333:ILE:HG22	50:t:378:HIS:NE2	2.33	0.44
52:4:247:ILE:HG13	52:4:318:LEU:HD22	1.98	0.44
1:D:115:LEU:HD11	1:D:119:TYR:CD2	2.53	0.44
1:D:178:ASN:HA	1:D:183:TRP:CE3	2.53	0.44
6:b:185:ARG:NH2	6:b:189:LYS:HA	2.33	0.44
6:b:479:ASP:OD1	6:b:479:ASP:N	2.50	0.44
11:e:109:LEU:HD23	11:e:119:VAL:HG21	2.00	0.44
17:H:66:ALA:O	44:1:3113:A:O2'	2.33	0.44
23:l:21:ARG:NH1	45:3:52:A:OP1	2.46	0.44
26:N:147:ARG:NH2	44:1:113:C:OP1	2.48	0.44
37:W:86:LYS:HB2	37:W:89:LEU:HD22	1.98	0.44
44:1:1068:C:H2'	44:1:1069:C:C6	2.53	0.44
44:1:1203:A:O2'	44:1:1204:A:H5'	2.18	0.44
44:1:3045:G:H2'	44:1:3046:A:O4'	2.18	0.44
44:1:3159:C:H2'	44:1:3160:U:C6	2.52	0.44
49:2:22:A:H2'	49:2:23:A:C8	2.53	0.44
1:D:234:ASP:OD1	1:D:235:SER:N	2.50	0.44
5:B:339:ARG:HG2	5:B:340:LYS:H	1.83	0.44
6:b:489:ILE:HG13	27:u:127:VAL:HG11	2.00	0.44
10:E:2:SER:N	44:1:1387:G:HO2'	2.16	0.44
11:e:122:PRO:O	11:e:123:LYS:HG2	2.18	0.44
14:G:163:VAL:HG12	14:G:166:LEU:HD12	1.99	0.44
16:I:108:ILE:O	16:I:113:GLY:N	2.49	0.44
21:k:32:ASN:HD21	21:k:35:GLY:HA3	1.82	0.44
32:r:181:LYS:HB2	32:r:194:PHE:CZ	2.53	0.44
39:Y:29:VAL:O	39:Y:32:SER:OG	2.34	0.44
44:1:374:A:H1'	44:1:375:A:H5"	2.00	0.44
44:1:1724:U:H1'	44:1:1725:C:C5	2.52	0.44
48:m:104:TYR:O	51:n:40:THR:OG1	2.23	0.44
5:B:56:ILE:HG21	5:B:356:LEU:HD22	2.00	0.43
6:b:299:ASP:HB2	6:b:302:ARG:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:93:MET:HE2	7:C:93:MET:HB3	1.86	0.43
8:c:30:THR:HG22	8:c:91:SER:HB3	1.99	0.43
10:E:69:PHE:CZ	44:1:3267:A:H2'	2.53	0.43
11:e:79:VAL:O	11:e:83:GLU:HG3	2.18	0.43
12:F:155:LYS:HG2	12:F:203:TRP:CE3	2.53	0.43
18:h:45:LYS:O	18:h:49:LYS:HG2	2.17	0.43
39:Y:88:GLU:HB3	53:o:140:LEU:HD23	1.99	0.43
42:z:26:VAL:HG13	42:z:29:ARG:HH12	1.82	0.43
44:1:129:U:H2'	44:1:130:A:C8	2.52	0.43
44:1:2116:G:OP1	44:1:2118:C:N4	2.50	0.43
44:1:2198:A:H62	44:1:2246:G:N2	2.12	0.43
44:1:2874:G:O2'	44:1:2875:U:O4'	2.33	0.43
49:2:49:G:H1'	49:2:50:U:OP2	2.17	0.43
3:A:128:ARG:HB2	44:1:2177:G:H2'	2.00	0.43
5:B:358:TRP:HB2	27:u:1:MET:HE3	2.00	0.43
6:b:409:ALA:HB1	40:y:31:SER:HB3	1.99	0.43
17:H:37:ASN:OD1	17:H:39:LYS:HG2	2.19	0.43
17:H:92:TYR:HB3	17:H:179:ILE:HG23	2.00	0.43
22:L:42:ARG:O	22:L:46:ILE:HG12	2.18	0.43
44:1:839:C:H4'	44:1:1724:U:H2'	2.01	0.43
46:5:62:LYS:HG2	46:5:66:ASP:OD1	2.17	0.43
47:x:158:ARG:NH1	47:x:172:ASP:OD1	2.51	0.43
47:x:201:ILE:HD11	47:x:215:PRO:HG3	2.00	0.43
47:x:298:ASP:O	47:x:299:ARG:HG2	2.18	0.43
48:m:202:ILE:HG13	48:m:388:VAL:HG13	1.99	0.43
54:s:63:MET:HG2	54:s:108:ASN:ND2	2.33	0.43
1:D:72:ASP:O	49:2:115:G:N2	2.50	0.43
3:A:108:PRO:HB2	25:p:86:LEU:HD22	2.01	0.43
15:g:74:ARG:CZ	15:g:82:ALA:HB2	2.48	0.43
17:H:112:ILE:HG22	17:H:126:VAL:HB	2.01	0.43
20:j:28:HIS:HB3	20:j:31:LYS:HB2	2.00	0.43
20:j:55:ARG:NH2	44:1:353:G:O6	2.51	0.43
27:u:73:GLN:CG	27:u:74:ARG:H	2.29	0.43
27:u:78:PRO:HG3	40:y:81:LEU:HG	2.00	0.43
29:P:3:ARG:HH21	45:3:12:A:P	2.40	0.43
47:x:385:LEU:O	47:x:395:ILE:N	2.40	0.43
48:m:95:ALA:HB1	51:n:36:PHE:CE2	2.53	0.43
52:4:138:LEU:HD13	52:4:180:LYS:HD3	2.01	0.43
54:s:8:GLN:HE22	54:s:9:VAL:HG13	1.83	0.43
14:G:29:SER:OG	14:G:31:PRO:HD3	2.17	0.43
22:L:46:ILE:HD11	22:L:51:LEU:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:L:63:VAL:HA	22:L:66:ASN:HD21	1.83	0.43
22:L:185:LYS:O	22:L:189:GLU:HG2	2.18	0.43
26:N:46:ASP:OD2	26:N:46:ASP:N	2.51	0.43
27:u:101:GLN:O	27:u:104:GLU:HG3	2.18	0.43
36:V:57:MET:SD	36:V:75:PRO:HB3	2.58	0.43
41:Z:121:ARG:HB2	41:Z:131:PHE:CZ	2.54	0.43
6:b:256:LEU:O	6:b:293:ILE:HG21	2.17	0.43
6:b:621:GLU:OE2	23:l:41:ARG:NH1	2.45	0.43
18:h:31:LEU:HD11	52:4:345:GLY:HA3	2.00	0.43
20:j:39:TYR:CD1	20:j:40:PRO:HA	2.54	0.43
21:k:35:GLY:O	21:k:36:LYS:HE2	2.19	0.43
26:N:119:TYR:OH	26:N:131:GLU:OE1	2.34	0.43
27:u:53:LYS:HG3	27:u:57:LYS:HE2	2.00	0.43
31:R:105:LEU:HD23	31:R:138:LEU:HD22	2.00	0.43
32:r:48:LYS:HG2	44:1:1300:G:H4'	2.01	0.43
44:1:621:A:OP2	53:o:40:ARG:HB3	2.19	0.43
44:1:1220:U:H4'	44:1:1221:A:H5'	2.01	0.43
44:1:2115:G:H22	44:1:2120:A:H1'	1.83	0.43
50:t:464:LEU:C	50:t:466:ASP:H	2.26	0.43
52:4:197:LEU:CD2	52:4:226:ILE:HD11	2.49	0.43
1:D:50:ARG:HE	1:D:65:ILE:HD11	1.84	0.43
1:D:54:ARG:NH2	1:D:147:ASP:OD2	2.48	0.43
12:F:155:LYS:HG2	12:F:203:TRP:HE3	1.83	0.43
22:L:58:VAL:N	22:L:70:ARG:O	2.42	0.43
32:r:174:PRO:HA	44:1:2871:G:N7	2.34	0.43
41:Z:50:PRO:HD3	41:Z:68:ILE:HG12	2.01	0.43
44:1:552:G:H2'	44:1:553:U:C6	2.53	0.43
44:1:662:U:H2'	44:1:663:C:C6	2.53	0.43
45:3:122:U:H2'	45:3:123:G:C8	2.54	0.43
48:m:38:PHE:O	48:m:41:MET:HG2	2.18	0.43
50:t:120:HIS:HB2	50:t:160:TYR:OH	2.19	0.43
52:4:101:SER:HB2	52:4:438:GLN:HG2	2.00	0.43
1:D:155:THR:N	1:D:179:ARG:HH11	2.17	0.43
2:J:57:PHE:HB3	44:1:2680:A:C2	2.54	0.43
5:B:341:SER:C	5:B:343:TYR:H	2.27	0.43
6:b:231:GLU:HG2	6:b:231:GLU:O	2.19	0.43
6:b:417:LYS:HD3	6:b:429:ASN:HA	2.00	0.43
7:C:75:PRO:HD3	44:1:805:G:H5"	2.01	0.43
8:c:74:ASN:OD1	8:c:74:ASN:N	2.52	0.43
33:S:71:LYS:NZ	44:1:563:U:OP1	2.43	0.43
33:S:124:LEU:HD22	34:T:154:VAL:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:U:23:THR:HG21	35:U:30:PRO:HD3	2.00	0.43
44:1:1243:G:N2	44:1:1270:A:O2'	2.43	0.43
44:1:2484:A:N7	50:t:337:ARG:HB2	2.34	0.43
46:5:46:LEU:O	46:5:50:LYS:HG2	2.19	0.43
47:x:401:HIS:NE2	47:x:419:SER:OG	2.33	0.43
50:t:212:LEU:HD11	50:t:243:ILE:HG23	2.01	0.43
54:s:33:GLU:HG2	54:s:168:ALA:HA	2.01	0.43
1:D:184:ASP:OD1	1:D:185:PHE:N	2.52	0.43
2:J:99:THR:O	2:J:154:THR:OG1	2.31	0.43
3:A:117:GLU:HG2	3:A:124:GLY:H	1.84	0.43
4:a:66:ALA:HB1	22:L:62:THR:HG21	2.01	0.43
7:C:345:GLU:OE1	7:C:345:GLU:N	2.48	0.43
23:l:31:THR:N	45:3:75:G:OP1	2.39	0.43
33:S:13:ARG:HG3	33:S:14:LEU:N	2.34	0.43
34:T:17:ARG:HB2	34:T:22:HIS:CE1	2.53	0.43
34:T:26:HIS:CE1	34:T:29:THR:HG23	2.53	0.43
44:1:2249:G:H2'	44:1:2250:G:C8	2.54	0.43
44:1:2667:A:O2'	44:1:2691:A:OP1	2.31	0.43
44:1:2884:C:H2'	44:1:2885:C:C6	2.54	0.43
44:1:3317:U:H4'	44:1:3318:G:O5'	2.18	0.43
50:t:172:HIS:HB3	50:t:175:GLU:HB2	2.00	0.43
2:J:55:ARG:NH1	50:t:433:SER:OG	2.50	0.43
3:A:200:ARG:HG3	3:A:202:VAL:HG12	2.00	0.43
5:B:37:ARG:HA	5:B:186:GLY:HA2	1.99	0.43
8:c:22:LYS:HE2	8:c:22:LYS:HB3	1.83	0.43
22:L:76:THR:HG22	22:L:78:ALA:H	1.83	0.43
23:l:3:ALA:HB2	44:1:1836:C:H41	1.83	0.43
26:N:145:ASP:O	26:N:147:ARG:N	2.51	0.43
34:T:68:THR:HG22	34:T:69:LYS:H	1.83	0.43
39:Y:125:LYS:HE3	39:Y:125:LYS:HB3	1.87	0.43
44:1:540:U:H2'	44:1:541:U:C6	2.53	0.43
44:1:647:A:H4'	44:1:2373:A:C2	2.54	0.43
44:1:1448:U:H2'	44:1:1449:A:H8	1.84	0.43
44:1:2667:A:N6	44:1:2687:G:H1'	2.34	0.43
49:2:78:U:H2'	49:2:79:A:C8	2.53	0.43
53:o:99:ARG:HD2	53:o:103:TYR:OH	2.19	0.43
1:D:52:VAL:HA	1:D:147:ASP:HB3	2.01	0.43
5:B:148:LEU:HD13	5:B:196:ARG:HE	1.83	0.43
10:E:40:LEU:HD13	10:E:54:TYR:HB2	2.00	0.43
11:e:11:LYS:C	11:e:13:HIS:H	2.27	0.43
19:i:66:GLU:HG2	19:i:70:ARG:HH11	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:L:165:SER:C	22:L:167:PHE:H	2.27	0.43
24:M:15:VAL:HG23	24:M:35:ILE:HD13	1.99	0.43
31:R:95:TRP:CZ2	31:R:99:LEU:HD22	2.54	0.43
35:U:82:LYS:HD2	44:1:1682:U:O2	2.19	0.43
37:W:83:GLU:O	37:W:83:GLU:HG2	2.19	0.43
41:Z:76:ASN:OD1	41:Z:77:TYR:N	2.51	0.43
44:1:1107:C:H2'	44:1:1108:U:C6	2.54	0.43
44:1:1381:A:H2'	44:1:1382:G:C8	2.54	0.43
50:t:256:VAL:O	50:t:260:VAL:HG23	2.19	0.43
6:b:224:ILE:HD11	6:b:274:ILE:HD11	2.00	0.42
10:E:75:PRO:HG3	44:1:3268:A:H1'	2.01	0.42
10:E:154:LEU:HD11	24:M:122:VAL:HG21	2.01	0.42
14:G:84:ARG:NH2	45:3:156:U:OP2	2.50	0.42
17:H:57:VAL:HG23	17:H:68:LEU:HD13	2.01	0.42
18:h:86:ARG:O	18:h:90:ARG:HD2	2.18	0.42
31:R:86:GLU:HB2	44:1:833:G:OP1	2.19	0.42
32:r:4:ASN:HB2	32:r:9:ARG:HH12	1.84	0.42
33:S:12:ARG:HB2	33:S:59:VAL:CG2	2.49	0.42
33:S:78:TRP:CE2	33:S:124:LEU:HD12	2.54	0.42
34:T:35:LYS:NZ	44:1:1084:A:OP1	2.46	0.42
38:X:29:SER:OG	38:X:31:THR:HG22	2.19	0.42
38:X:115:ARG:HD2	38:X:121:LYS:HB3	2.01	0.42
38:X:137:ASN:HD22	52:4:417:LYS:HD3	1.84	0.42
40:y:15:VAL:HG12	40:y:58:ILE:HG22	2.00	0.42
40:y:204:ALA:HB3	40:y:224:LEU:HD11	2.01	0.42
44:1:1488:G:H5"	44:1:1838:G:O6	2.19	0.42
44:1:2112:U:O2	44:1:2113:A:N6	2.52	0.42
44:1:2312:A:C5	48:m:337:LYS:HD3	2.54	0.42
46:5:38:ASN:OD1	46:5:39:LYS:N	2.45	0.42
50:t:135:LEU:HD13	50:t:149:LEU:HD21	2.01	0.42
54:s:196:LYS:HD2	54:s:199:GLN:HG2	2.01	0.42
1:D:126:GLU:HA	1:D:196:ARG:NH1	2.35	0.42
2:J:20:ASN:O	2:J:126:ASP:N	2.50	0.42
5:B:186:GLY:O	5:B:190:GLU:HB3	2.19	0.42
6:b:442:TYR:O	27:u:75:ARG:HD3	2.20	0.42
14:G:122:LYS:O	14:G:123:GLN:HG3	2.19	0.42
20:j:12:HIS:O	44:1:1490:A:O2'	2.34	0.42
22:L:54:LEU:HD22	22:L:119:TYR:CG	2.55	0.42
25:p:4:ARG:HD3	44:1:836:A:P	2.59	0.42
27:u:121:LEU:HA	27:u:124:LYS:HB3	2.00	0.42
32:r:43:THR:HG22	44:1:1299:U:H5"	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:Y:11:ASP:HB3	39:Y:14:LYS:HB2	2.01	0.42
44:1:293:C:H2'	44:1:294:U:O4'	2.19	0.42
44:1:1785:U:H2'	44:1:1786:G:C8	2.54	0.42
44:1:2545:C:H2'	44:1:2546:C:C6	2.54	0.42
44:1:3090:U:H2'	44:1:3091:A:C8	2.54	0.42
54:s:43:PRO:HG2	54:s:44:GLN:OE1	2.19	0.42
56:Lr:10:THR:O	56:Lr:14:LYS:HG2	2.19	0.42
3:A:143:GLU:O	3:A:145:LYS:HG2	2.19	0.42
3:A:152:SER:OG	44:1:2157:G:N7	2.49	0.42
6:b:15:ASN:HB3	6:b:144:ARG:HH21	1.85	0.42
21:k:40:GLN:HE21	21:k:55:VAL:HG13	1.83	0.42
26:N:155:VAL:HG12	44:1:58:G:H4'	2.01	0.42
27:u:74:ARG:C	27:u:75:ARG:HD2	2.44	0.42
40:y:7:PHE:O	40:y:8:GLU:C	2.62	0.42
43:K:154:UNK:O	43:K:156:UNK:N	2.52	0.42
44:1:421:G:O6	44:1:2383:C:O2'	2.32	0.42
44:1:829:U:H3	44:1:895:A:H62	1.68	0.42
44:1:2900:A:N3	44:1:3025:C:O2'	2.47	0.42
44:1:3086:A:H3'	44:1:3087:A:H8	1.83	0.42
47:x:205:SER:OG	47:x:206:MET:N	2.52	0.42
47:x:293:TYR:CE2	47:x:301:VAL:HG11	2.54	0.42
50:t:35:GLN:O	50:t:90:LEU:HD11	2.20	0.42
50:t:123:LEU:HD12	50:t:123:LEU:HA	1.91	0.42
54:s:31:THR:HG22	54:s:209:SER:HB2	2.00	0.42
6:b:434:GLU:O	6:b:435:ILE:HD13	2.19	0.42
8:c:50:VAL:HG11	44:1:2552:C:H2'	2.01	0.42
11:e:23:ASP:OD2	44:1:424:G:O2'	2.35	0.42
36:V:11:PHE:HA	44:1:3040:A:H5'	2.01	0.42
39:Y:28:ARG:O	39:Y:49:PRO:HB3	2.19	0.42
44:1:36:C:H4'	44:1:808:A:H2	1.84	0.42
44:1:563:U:H2'	44:1:564:G:H8	1.84	0.42
44:1:643:U:O2	44:1:1116:G:H5"	2.19	0.42
44:1:733:G:N2	44:1:736:A:OP2	2.45	0.42
44:1:949:C:O2'	44:1:971:G:H5"	2.19	0.42
44:1:1571:A:H2'	44:1:1572:U:O4'	2.18	0.42
44:1:2666:C:O2'	44:1:2691:A:N3	2.45	0.42
44:1:3117:C:H2'	44:1:3118:C:O4'	2.19	0.42
48:m:429:GLU:OE2	48:m:433:ARG:NH1	2.52	0.42
50:t:432:VAL:O	50:t:432:VAL:HG12	2.19	0.42
54:s:147:LYS:HE3	54:s:147:LYS:HB3	1.83	0.42
1:D:152:ARG:HD3	49:2:44:C:H4'	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:30:ARG:O	3:A:163:ARG:NH1	2.36	0.42
3:A:104:LEU:HD12	3:A:158:ILE:HD11	2.02	0.42
6:b:29:THR:OG1	6:b:49:LYS:NZ	2.49	0.42
6:b:486:VAL:HA	6:b:489:ILE:HG22	2.00	0.42
6:b:601:LYS:O	6:b:605:MET:HG3	2.18	0.42
10:E:22:ARG:HD3	44:1:608:A:C6	2.54	0.42
12:F:90:LYS:HG2	12:F:91:GLY:H	1.84	0.42
24:M:21:VAL:HG12	24:M:65:LEU:HD23	2.02	0.42
32:r:8:GLU:O	32:r:12:LYS:HD3	2.19	0.42
33:S:45:LEU:HB3	33:S:51:VAL:HG11	2.01	0.42
44:1:3167:A:H3'	44:1:3168:A:C5'	2.47	0.42
54:s:100:ILE:HG21	54:s:124:LEU:HG	2.01	0.42
4:a:77:LYS:C	4:a:79:TRP:N	2.76	0.42
4:a:79:TRP:CE3	4:a:82:ILE:HD12	2.55	0.42
5:B:261:MET:HE2	5:B:261:MET:HB3	1.95	0.42
6:b:573:LEU:HD22	52:4:363:ASP:OD1	2.20	0.42
7:C:23:PRO:HD2	7:C:26:PHE:HD2	1.83	0.42
22:L:76:THR:HG22	22:L:77:LEU:N	2.35	0.42
26:N:72:LYS:HB3	26:N:72:LYS:HE3	1.88	0.42
27:u:4:TYR:O	27:u:13:CYS:N	2.40	0.42
31:R:84:THR:HG22	44:1:1915:A:H5"	2.01	0.42
33:S:80:ARG:NH1	55:q:47:ASP:OD2	2.53	0.42
37:W:132:PRO:HB2	37:W:133:LEU:H	1.64	0.42
38:X:70:GLU:OE2	52:4:428:ASN:ND2	2.52	0.42
44:1:916:G:H5'	44:1:917:A:OP1	2.18	0.42
44:1:937:G:OP2	44:1:938:C:N4	2.51	0.42
44:1:3116:G:C5	46:5:28:PRO:HD3	2.54	0.42
52:4:381:LYS:HA	52:4:384:LYS:HE2	2.00	0.42
5:B:306:THR:HG21	5:B:316:GLU:HA	2.01	0.42
8:c:18:ILE:HD12	8:c:18:ILE:H	1.85	0.42
12:F:102:VAL:HG13	12:F:126:LEU:HG	2.02	0.42
16:I:56:LYS:NZ	44:1:1936:A:H5"	2.34	0.42
16:I:102:LEU:HD23	16:I:102:LEU:HA	1.89	0.42
18:h:24:LEU:HD21	18:h:50:SER:HB2	2.01	0.42
24:M:109:ARG:HH12	44:1:3211:C:P	2.43	0.42
26:N:124:ASP:OD1	44:1:2433:U:O2'	2.35	0.42
31:R:60:LYS:NZ	44:1:1860:G:O2'	2.53	0.42
34:T:102:ARG:O	34:T:106:LEU:HD23	2.19	0.42
40:y:162:HIS:CD2	40:y:164:GLN:HB2	2.53	0.42
44:1:1144:U:O4'	44:1:1160:C:N4	2.52	0.42
44:1:1574:C:H2'	44:1:1575:A:H5'	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:1:2344:U:H2'	44:1:2345:A:C8	2.55	0.42
44:1:2535:A:H3'	44:1:2536:A:C8	2.55	0.42
44:1:2705:A:N3	44:1:2755:C:H1'	2.35	0.42
6:b:168:ARG:HH21	6:b:214:LEU:HB3	1.84	0.42
6:b:224:ILE:HA	6:b:236:GLU:HG2	2.02	0.42
14:G:203:VAL:HG22	14:G:207:ASP:HB2	2.01	0.42
18:h:94:LYS:HD3	44:1:135:C:N3	2.34	0.42
29:P:9:THR:HG22	29:P:10:ASN:N	2.35	0.42
30:Q:100:THR:HG23	30:Q:120:GLU:HB3	2.01	0.42
32:r:147:TRP:CD1	48:m:41:MET:O	2.73	0.42
33:S:12:ARG:HB3	33:S:57:GLU:OE2	2.20	0.42
35:U:82:LYS:HB3	35:U:82:LYS:HE3	1.74	0.42
37:W:196:ASP:OD1	37:W:199:GLN:NE2	2.49	0.42
44:1:915:A:H8	44:1:2136:C:O2'	2.02	0.42
44:1:1002:A:C5'	44:1:1003:A:H5'	2.50	0.42
44:1:2271:A:H2'	48:m:296:LYS:HD3	2.02	0.42
44:1:3237:U:H2'	44:1:3238:G:C8	2.55	0.42
47:x:182:LEU:HD13	47:x:213:TRP:CG	2.55	0.42
47:x:362:LYS:HG2	47:x:363:ILE:HD12	2.02	0.42
48:m:244:GLU:O	48:m:248:LYS:HG2	2.20	0.42
52:4:195:VAL:HG21	52:4:524:ARG:CZ	2.50	0.42
52:4:332:LYS:HG3	52:4:445:TRP:CD1	2.53	0.42
6:b:336:CYS:HA	6:b:339:LEU:HD12	2.02	0.42
12:F:102:VAL:HG21	12:F:129:LEU:HD12	2.02	0.42
13:f:70:LYS:HE2	44:1:585:A:H5"	2.01	0.42
16:I:26:SER:O	16:I:119:ASN:ND2	2.52	0.42
17:H:180:TYR:CD2	32:r:18:LEU:HD12	2.55	0.42
18:h:75:TYR:HB3	38:X:46:TYR:HD1	1.85	0.42
24:M:47:ASP:HB2	24:M:55:ARG:HG3	2.02	0.42
25:p:79:VAL:O	25:p:83:ILE:HG12	2.20	0.42
31:R:59:SER:N	44:1:3068:U:OP1	2.39	0.42
36:V:33:ASN:HD21	36:V:63:LYS:HB2	1.85	0.42
42:z:2:ALA:N	44:1:3015:G:OP2	2.53	0.42
44:1:385:A:H2'	44:1:386:A:C8	2.54	0.42
44:1:745:C:H2'	44:1:746:A:C8	2.55	0.42
47:x:445:ALA:HB1	47:x:464:LYS:HB3	2.02	0.42
47:x:484:GLY:O	47:x:511:ARG:NH1	2.52	0.42
48:m:95:ALA:HB1	51:n:36:PHE:HE2	1.83	0.42
50:t:87:LEU:HD22	50:t:127:LEU:CD1	2.49	0.42
50:t:185:ILE:O	50:t:189:LYS:HG2	2.18	0.42
52:4:237:GLY:O	52:4:324:ALA:N	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:4:475:LEU:HD12	52:4:475:LEU:O	2.19	0.42
1:D:33:ARG:HH11	34:T:27:LEU:HG	1.85	0.42
1:D:175:HIS:HA	44:1:2747:A:H5'	2.01	0.42
2:J:148:VAL:HG12	2:J:153:LYS:HG3	2.02	0.42
5:B:128:LYS:O	44:1:3150:A:H4'	2.20	0.42
6:b:25:THR:HG21	6:b:53:THR:OG1	2.20	0.42
6:b:178:VAL:HG23	6:b:179:GLY:N	2.34	0.42
7:C:159:ILE:HG23	7:C:164:GLU:HG3	2.00	0.42
7:C:343:LYS:HE2	7:C:343:LYS:HB3	1.88	0.42
20:j:27:PHE:HA	20:j:34:CYS:HA	2.02	0.42
22:L:47:ALA:HB3	22:L:48:PRO:HD3	2.02	0.42
28:O:96:LYS:HB2	53:o:12:LEU:HD13	2.01	0.42
32:r:231:VAL:HG12	32:r:235:GLY:HA2	2.02	0.42
33:S:119:ARG:HG3	33:S:120:SER:N	2.35	0.42
44:1:119:U:H4'	44:1:120:G:H3'	2.01	0.42
44:1:2653:C:N3	44:1:2654:C:N4	2.68	0.42
44:1:2695:A:H2'	44:1:2697:A:C8	2.55	0.42
47:x:168:ALA:O	47:x:182:LEU:N	2.45	0.42
47:x:462:CYS:HA	47:x:468:LEU:HD23	2.01	0.42
49:2:52:G:H2'	49:2:53:U:C6	2.55	0.42
56:Lr:14:LYS:HA	56:Lr:14:LYS:HD3	1.71	0.42
4:a:112:ILE:HB	4:a:130:VAL:HG12	2.01	0.41
5:B:61:ASP:HB3	6:b:413:ASN:HD21	1.85	0.41
5:B:236:LYS:NZ	44:1:2880:U:OP1	2.53	0.41
7:C:188:ARG:NH1	7:C:197:ARG:HB3	2.35	0.41
7:C:252:GLU:O	7:C:256:THR:HG23	2.20	0.41
31:R:134:HIS:HE1	31:R:136:ARG:HG2	1.84	0.41
35:U:36:TYR:CD1	35:U:83:TYR:HB2	2.54	0.41
38:X:73:MET:O	38:X:76:VAL:HG22	2.20	0.41
40:y:105:GLY:O	40:y:149:GLY:HA3	2.20	0.41
40:y:142:ILE:HG22	40:y:162:HIS:CE1	2.55	0.41
44:1:594:U:H2'	44:1:609:G:O6	2.20	0.41
44:1:1263:A:H2'	44:1:1263:A:N3	2.35	0.41
44:1:2713:U:C2	50:t:504:LYS:HE3	2.55	0.41
47:x:302:ARG:HG2	47:x:315:ILE:HG12	2.01	0.41
52:4:341:ASP:OD2	52:4:346:LYS:NZ	2.44	0.41
54:s:178:VAL:O	54:s:182:GLN:HG2	2.19	0.41
1:D:129:TYR:CD1	1:D:177:GLU:HB3	2.55	0.41
1:D:183:TRP:CG	1:D:184:ASP:H	2.38	0.41
6:b:211:TYR:OH	6:b:337:GLU:OE2	2.31	0.41
6:b:444:PHE:CD2	27:u:93:MET:HG2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:d:31:ARG:O	9:d:35:GLU:HG2	2.20	0.41
22:L:32:LYS:O	22:L:36:ARG:HG3	2.19	0.41
27:u:23:ARG:NH2	27:u:27:LYS:HD2	2.35	0.41
29:P:26:PHE:HZ	44:1:412:G:H5'	1.86	0.41
34:T:103:GLN:NE2	34:T:104:GLU:HG2	2.35	0.41
36:V:104:ASN:HD21	36:V:108:GLU:HB2	1.84	0.41
44:1:359:U:H4'	44:1:817:A:H62	1.85	0.41
44:1:1544:G:O2'	44:1:2167:A:N3	2.47	0.41
44:1:2536:A:N3	44:1:2537:U:H5	2.18	0.41
47:x:485:HIS:HE2	47:x:503:SER:HG	1.64	0.41
48:m:227:HIS:CE1	48:m:239:CYS:H	2.38	0.41
49:2:105:C:H2'	49:2:106:U:O4'	2.20	0.41
50:t:479:ASN:OD1	50:t:483:LYS:HE3	2.19	0.41
1:D:179:ARG:NH2	44:1:2746:A:OP1	2.47	0.41
3:A:8:GLN:HA	44:1:2163:C:H4'	2.02	0.41
5:B:302:LYS:HB2	5:B:302:LYS:HE2	1.80	0.41
6:b:92:LYS:CE	44:1:2863:G:H22	2.33	0.41
6:b:597:SER:HB2	52:4:459:SER:HA	2.01	0.41
7:C:280:ILE:HG13	7:C:281:ILE:HG23	2.03	0.41
8:c:36:GLN:HA	41:Z:3:LYS:HE2	2.02	0.41
17:H:23:ARG:NE	17:H:39:LYS:HA	2.35	0.41
22:L:179:PHE:O	22:L:183:ARG:HG3	2.21	0.41
37:W:214:LYS:HE2	37:W:234:ASN:O	2.20	0.41
39:Y:101:PRO:HA	39:Y:104:LEU:HD12	2.02	0.41
41:Z:41:ALA:HB2	41:Z:77:TYR:HE1	1.85	0.41
41:Z:95:VAL:HG13	41:Z:96:VAL:HG23	2.03	0.41
44:1:2883:U:H2'	44:1:2884:C:C6	2.55	0.41
44:1:3121:U:H1'	44:1:3122:A:H5"	2.01	0.41
44:1:3170:A:H2'	44:1:3171:U:C6	2.55	0.41
44:1:3176:G:N2	44:1:3213:A:H1'	2.35	0.41
47:x:249:PRO:O	47:x:265:THR:OG1	2.25	0.41
50:t:497:LEU:O	50:t:502:ARG:NH2	2.53	0.41
52:4:45:LEU:HD13	52:4:64:LEU:HD22	2.03	0.41
1:D:266:ALA:HB1	1:D:270:LYS:HE3	2.03	0.41
6:b:77:PHE:CE2	6:b:163:ILE:HD11	2.55	0.41
6:b:175:TYR:CZ	6:b:267:GLN:HA	2.55	0.41
6:b:177:ASN:HD22	6:b:200:THR:HB	1.85	0.41
17:H:16:VAL:HG11	17:H:79:ILE:HG23	2.02	0.41
17:H:21:LYS:O	17:H:22:SER:C	2.62	0.41
25:p:7:LYS:HG2	44:1:1926:C:H3'	2.02	0.41
30:Q:64:VAL:HG22	30:Q:96:PHE:CE1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:r:138:LYS:HB3	32:r:143:ARG:HB3	2.02	0.41
40:y:11:ASN:ND2	40:y:209:ASP:HB2	2.35	0.41
40:y:97:VAL:HG23	40:y:128:LEU:HD23	2.02	0.41
42:z:26:VAL:HG13	42:z:29:ARG:NH1	2.35	0.41
44:1:155:G:H5"	44:1:156:G:H2'	2.02	0.41
44:1:346:C:C2	45:3:25:G:H4'	2.56	0.41
44:1:2496:C:H5"	50:t:196:LYS:HB2	2.02	0.41
44:1:2689:A:N3	44:1:2689:A:H2'	2.35	0.41
44:1:2920:U:H4'	48:m:201:ALA:HB3	2.02	0.41
47:x:338:ALA:HB2	47:x:356:ALA:HB2	2.02	0.41
50:t:490:ARG:O	50:t:494:PRO:HB3	2.21	0.41
52:4:251:LEU:HD21	52:4:261:GLU:CD	2.45	0.41
52:4:322:LYS:HG3	52:4:502:ARG:HD3	2.02	0.41
54:s:43:PRO:HG2	54:s:44:GLN:CD	2.45	0.41
13:f:47:LYS:NZ	13:f:105:SER:HA	2.35	0.41
17:H:90:MET:HB2	17:H:144:ILE:HG23	2.02	0.41
26:N:177:GLY:HA2	44:1:68:C:O3'	2.20	0.41
31:R:62:ARG:NH2	44:1:3067:C:H3'	2.35	0.41
32:r:172:ILE:HG22	32:r:174:PRO:HD3	2.03	0.41
33:S:68:HIS:C	33:S:70:THR:H	2.28	0.41
35:U:20:SER:N	35:U:61:THR:O	2.53	0.41
44:1:533:A:O2'	44:1:535:G:OP2	2.38	0.41
44:1:637:C:H5"	44:1:2377:G:C2	2.55	0.41
44:1:698:U:H2'	44:1:699:A:O4'	2.21	0.41
44:1:1017:C:N4	50:t:357:ASN:HA	2.36	0.41
45:3:142:C:H2'	45:3:143:U:C6	2.56	0.41
46:5:42:THR:HG22	46:5:47:LYS:HD2	2.01	0.41
46:5:87:GLU:OE1	46:5:88:GLU:N	2.53	0.41
48:m:49:ARG:NH1	48:m:55:LEU:HB2	2.35	0.41
48:m:280:GLU:HG2	48:m:281:ARG:HG2	2.03	0.41
50:t:230:TRP:CG	50:t:262:PHE:HZ	2.38	0.41
1:D:39:GLN:NE2	1:D:48:LYS:HB2	2.35	0.41
1:D:197:SER:O	1:D:202:GLY:N	2.27	0.41
3:A:226:SER:HB3	3:A:239:ALA:HA	2.01	0.41
5:B:153:LYS:HD2	5:B:154:TYR:CZ	2.56	0.41
6:b:188:THR:HG21	6:b:207:GLY:HA3	2.03	0.41
6:b:245:HIS:CE1	48:m:164:THR:HG23	2.55	0.41
7:C:193:LYS:HE3	44:1:1419:A:H5"	2.02	0.41
13:f:64:ILE:HG21	44:1:3275:U:C2	2.55	0.41
15:g:89:ILE:CD1	41:Z:19:ALA:HB1	2.50	0.41
38:X:74:LYS:HA	52:4:372:LEU:HD21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:y:28:VAL:HG12	40:y:50:HIS:HB3	2.01	0.41
40:y:197:MET:HE3	40:y:197:MET:HB2	1.85	0.41
44:1:92:G:O5'	44:1:93:C:H5"	2.20	0.41
44:1:1110:U:H2'	44:1:1111:U:C6	2.56	0.41
44:1:1215:U:OP1	55:q:51:PRO:HA	2.20	0.41
44:1:1918:C:H2'	44:1:1919:G:O4'	2.21	0.41
44:1:2541:U:H1'	44:1:2542:U:O4'	2.20	0.41
44:1:2667:A:H2'	44:1:2668:U:O4'	2.20	0.41
45:3:71:A:H62	45:3:87:G:N2	2.17	0.41
46:5:83:ARG:HG3	46:5:84:GLU:N	2.34	0.41
5:B:215:ILE:HD13	5:B:282:ILE:HD11	2.02	0.41
5:B:226:PHE:CE2	5:B:268:GLY:HA2	2.56	0.41
7:C:281:ILE:HD11	30:Q:25:TYR:HD1	1.84	0.41
10:E:51:ARG:O	10:E:72:ASN:ND2	2.54	0.41
16:I:113:GLY:O	16:I:117:GLU:HG2	2.21	0.41
26:N:190:THR:O	26:N:194:GLN:HG2	2.21	0.41
29:P:69:ARG:HD2	44:1:3309:G:H1'	2.01	0.41
29:P:83:TRP:O	44:1:2352:A:H5"	2.20	0.41
30:Q:93:ILE:HG22	44:1:784:A:C6	2.55	0.41
36:V:48:ARG:O	44:1:2917:G:H4'	2.20	0.41
44:1:1034:U:H2'	44:1:1035:G:C8	2.55	0.41
44:1:1064:A:H4'	44:1:1065:A:O5'	2.19	0.41
44:1:1624:G:O2'	44:1:1643:A:N1	2.50	0.41
44:1:2804:A:H5'	48:m:25:LYS:HG3	2.03	0.41
49:2:19:C:H2'	49:2:20:A:H8	1.84	0.41
50:t:176:LEU:O	50:t:179:ILE:N	2.54	0.41
50:t:469:GLU:OE2	50:t:498:LYS:NZ	2.51	0.41
54:s:116:LEU:O	54:s:120:VAL:N	2.46	0.41
2:J:63:GLU:HB3	2:J:65:ILE:HG23	2.02	0.41
2:J:160:VAL:O	2:J:164:LYS:HG2	2.21	0.41
9:d:102:LYS:NZ	44:1:3373:U:OP2	2.33	0.41
22:L:57:VAL:HG12	22:L:112:ASN:OD1	2.20	0.41
32:r:45:TRP:HA	32:r:48:LYS:HB2	2.02	0.41
33:S:125:LYS:HE2	33:S:125:LYS:HB2	1.83	0.41
34:T:26:HIS:CE1	34:T:28:SER:OG	2.73	0.41
34:T:112:ASN:O	34:T:116:ARG:HG3	2.20	0.41
35:U:93:ILE:HG12	35:U:105:LEU:HD12	2.03	0.41
44:1:994:G:O6	44:1:1056:U:H1'	2.21	0.41
44:1:1448:U:H2'	44:1:1449:A:C8	2.56	0.41
44:1:1817:G:H2'	44:1:1818:U:C6	2.56	0.41
44:1:2844:C:H3'	44:1:2845:A:C5'	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:1:2936:A:H2'	44:1:2937:G:C8	2.56	0.41
44:1:3166:C:C2	44:1:3167:A:C8	3.08	0.41
47:x:203:THR:HB	47:x:213:TRP:NE1	2.35	0.41
52:4:182:ASP:HB2	52:4:234:TYR:HB3	2.03	0.41
52:4:221:GLN:O	52:4:225:THR:OG1	2.20	0.41
54:s:176:GLU:HA	54:s:179:LEU:HB3	2.02	0.41
1:D:23:ARG:NH2	44:1:2703:A:OP2	2.38	0.41
1:D:129:TYR:CG	1:D:177:GLU:HB3	2.56	0.41
1:D:140:ARG:O	44:1:1079:A:H4'	2.20	0.41
5:B:115:LYS:HD3	5:B:129:ALA:HB3	2.03	0.41
6:b:227:ARG:CD	6:b:228:PRO:HD3	2.50	0.41
6:b:358:LEU:HD23	6:b:362:HIS:HB2	2.03	0.41
6:b:388:TYR:HB2	6:b:396:ARG:NH2	2.36	0.41
6:b:527:SER:HA	35:U:112:PRO:HA	2.03	0.41
6:b:615:ARG:HD2	29:P:123:PRO:HB2	2.02	0.41
8:c:81:VAL:HG23	8:c:83:LYS:HG2	2.03	0.41
12:F:73:GLY:O	34:T:143:THR:OG1	2.36	0.41
14:G:151:VAL:O	14:G:177:TYR:HA	2.21	0.41
14:G:160:ILE:O	14:G:164:VAL:HG13	2.20	0.41
16:I:40:ASP:HB3	16:I:43:LYS:HB2	2.03	0.41
17:H:1:MET:HE2	17:H:3:TYR:CD1	2.56	0.41
18:h:31:LEU:HD23	18:h:44:ILE:HA	2.03	0.41
24:M:72:LEU:HD12	24:M:76:ALA:HB3	2.03	0.41
24:M:77:ARG:HD2	44:1:562:C:OP2	2.20	0.41
33:S:68:HIS:O	33:S:73:LYS:NZ	2.54	0.41
33:S:77:VAL:HG21	33:S:106:LEU:HD12	2.02	0.41
33:S:138:GLN:OE1	46:5:33:SER:HA	2.21	0.41
34:T:20:ARG:NH1	49:2:69:C:OP1	2.31	0.41
34:T:43:LYS:HA	34:T:43:LYS:HD2	1.71	0.41
38:X:68:THR:HG22	38:X:141:TYR:CD2	2.56	0.41
39:Y:89:LYS:HD2	39:Y:93:ALA:HB3	2.03	0.41
44:1:242:C:H1'	44:1:243:G:H5'	2.02	0.41
44:1:407:A:C2	45:3:17:A:H1'	2.56	0.41
44:1:637:C:H5"	44:1:2377:G:N2	2.36	0.41
44:1:660:A:N1	44:1:941:G:O2'	2.45	0.41
44:1:971:G:H2'	44:1:972:A:C8	2.55	0.41
44:1:1064:A:H5"	44:1:1066:G:C5'	2.51	0.41
44:1:1095:U:H1'	44:1:1096:U:H3'	2.03	0.41
44:1:1643:A:H2'	44:1:1644:C:C2	2.56	0.41
44:1:1935:G:OP1	48:m:441:GLY:N	2.47	0.41
44:1:2208:A:H2	44:1:2236:G:H22	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:1:3192:U:H2'	44:1:3193:C:C6	2.56	0.41
46:5:78:MET:SD	46:5:79:LEU:HD22	2.60	0.41
47:x:500:ARG:HD3	47:x:512:LEU:HD12	2.03	0.41
48:m:48:ILE:HD11	48:m:57:ARG:HB3	2.02	0.41
48:m:215:LEU:HD22	48:m:370:ILE:HD13	2.02	0.41
48:m:274:VAL:HG21	48:m:285:ALA:HB2	2.02	0.41
48:m:379:GLU:HA	48:m:382:ILE:HD12	2.03	0.41
52:4:240:PRO:HG3	52:4:274:GLN:NE2	2.36	0.41
54:s:125:GLY:N	54:s:126:PRO:HD2	2.36	0.41
1:D:19:PRO:HG2	1:D:24:ARG:HG3	2.02	0.41
6:b:150:LEU:HA	6:b:150:LEU:HD23	1.93	0.41
7:C:233:LEU:HD23	7:C:233:LEU:HA	1.96	0.41
10:E:147:ALA:HA	10:E:150:LYS:HD3	2.02	0.41
14:G:91:PHE:HA	14:G:94:PHE:HB2	2.03	0.41
16:I:43:LYS:NZ	16:I:47:GLY:H	2.19	0.41
17:H:49:ASN:C	17:H:51:GLN:H	2.29	0.41
19:i:54:GLU:HB3	19:i:90:MET:CE	2.51	0.41
20:j:11:ARG:HD3	44:1:817:A:O2'	2.21	0.41
29:P:65:SER:OG	44:1:1446:A:H5"	2.21	0.41
32:r:199:ALA:N	32:r:222:GLU:HB3	2.36	0.41
34:T:43:LYS:HD2	34:T:58:GLN:HE22	1.86	0.41
37:W:60:TRP:HB3	37:W:63:SER:HB2	2.02	0.41
44:1:307:A:H2'	44:1:308:A:C8	2.56	0.41
44:1:2877:G:H1'	44:1:2878:G:H5'	2.02	0.41
44:1:3322:A:H2'	44:1:3323:A:C8	2.57	0.41
54:s:32:VAL:HG12	54:s:170:GLY:O	2.21	0.41
3:A:20:THR:HA	3:A:23:ARG:HG3	2.03	0.40
3:A:145:LYS:HE3	3:A:157:VAL:HG12	2.03	0.40
3:A:181:LYS:HB2	44:1:860:G:C5	2.55	0.40
6:b:18:LEU:HD21	6:b:137:ALA:HB1	2.02	0.40
7:C:22:LEU:HD23	7:C:22:LEU:HA	1.94	0.40
10:E:18:LEU:HD12	44:1:591:G:C2	2.57	0.40
12:F:86:VAL:HG21	12:F:127:LEU:HD21	2.03	0.40
24:M:33:ALA:HB2	24:M:53:VAL:HG21	2.04	0.40
24:M:121:MET:HE1	44:1:3215:A:C5'	2.51	0.40
30:Q:64:VAL:HG11	30:Q:113:LYS:HD3	2.03	0.40
39:Y:73:VAL:HG13	39:Y:80:VAL:HG12	2.03	0.40
40:y:145:ASN:HB3	40:y:151:TYR:HD1	1.86	0.40
44:1:807:A:C8	44:1:2812:C:H1'	2.56	0.40
44:1:844:G:C2'	44:1:845:G:H5'	2.52	0.40
44:1:1110:U:H2'	44:1:1111:U:H6	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:1:1582:C:H5”	44:1:1583:A:OP1	2.21	0.40
44:1:2610:G:H2’	44:1:2611:U:O4’	2.21	0.40
44:1:3218:A:H5”	44:1:3219:G:C5	2.56	0.40
48:m:266:PRO:HB2	48:m:268:TRP:CD1	2.55	0.40
48:m:372:PRO:HA	48:m:373:PRO:HD3	1.93	0.40
48:m:467:LEU:HA	48:m:468:PRO:HD3	1.94	0.40
50:t:14:ILE:HD13	50:t:89:GLU:O	2.21	0.40
50:t:231:ARG:NH2	50:t:232:ARG:NH1	2.68	0.40
52:4:28:TYR:CZ	52:4:150:TYR:HB3	2.55	0.40
54:s:194:LEU:HB3	54:s:200:ASN:OD1	2.21	0.40
2:J:55:ARG:HH12	50:t:430:GLU:HA	1.86	0.40
5:B:94:GLU:OE2	5:B:156:SER:OG	2.28	0.40
5:B:193:ASP:O	5:B:197:GLU:HG3	2.20	0.40
6:b:408:GLY:H	6:b:411:VAL:CG1	2.33	0.40
6:b:501:LYS:HD3	9:d:99:ALA:HB1	2.04	0.40
7:C:317:PRO:C	7:C:319:LYS:N	2.79	0.40
12:F:185:ILE:O	12:F:189:ILE:HG22	2.21	0.40
13:f:99:ARG:NH2	44:1:3175:U:O4	2.54	0.40
17:H:105:GLU:HA	17:H:110:LYS:HA	2.03	0.40
23:l:42:ARG:NH2	44:1:1494:U:OP1	2.49	0.40
28:O:126:VAL:O	33:S:154:HIS:NE2	2.43	0.40
29:P:67:ILE:HD12	29:P:82:ARG:CZ	2.51	0.40
31:R:24:LEU:HB3	31:R:32:ILE:HD13	2.03	0.40
44:1:1468:A:N1	44:1:1880:U:O2’	2.39	0.40
44:1:3084:C:H2’	44:1:3085:G:O4’	2.22	0.40
47:x:325:HIS:CG	47:x:326:LEU:H	2.40	0.40
48:m:234:PRO:HG2	48:m:273:TRP:CE2	2.56	0.40
48:m:344:ALA:HB3	48:m:349:GLU:CG	2.49	0.40
49:2:22:A:H2’	49:2:23:A:H8	1.85	0.40
52:4:349:LYS:H	52:4:349:LYS:HG2	1.68	0.40
2:J:109:HIS:CE1	2:J:125:MET:SD	3.15	0.40
5:B:67:PHE:O	5:B:70:ARG:HB2	2.22	0.40
12:F:58:ALA:O	12:F:62:ILE:HD12	2.21	0.40
12:F:159:GLN:NE2	44:1:1361:U:O2	2.51	0.40
13:f:53:TYR:CZ	13:f:65:ARG:HB2	2.57	0.40
14:G:83:ASP:OD1	14:G:86:THR:HG22	2.21	0.40
14:G:94:PHE:HB3	14:G:189:LEU:HD22	2.04	0.40
14:G:239:GLY:O	14:G:243:GLN:N	2.40	0.40
26:N:71:ARG:HG3	26:N:92:LEU:HD12	2.03	0.40
32:r:193:VAL:HG13	32:r:195:LEU:HD23	2.01	0.40
36:V:75:PRO:HG2	36:V:105:PRO:HD3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:X:99:VAL:HG11	38:X:124:VAL:HG11	2.04	0.40
39:Y:25:SER:O	39:Y:28:ARG:HG2	2.21	0.40
40:y:53:ILE:HG12	40:y:59:ILE:HG22	2.04	0.40
44:1:54:C:H2'	44:1:55:G:H8	1.85	0.40
44:1:618:C:H2'	44:1:619:A:O4'	2.21	0.40
44:1:1786:G:H2'	44:1:1787:A:C8	2.56	0.40
46:5:86:LYS:HG3	46:5:87:GLU:N	2.36	0.40
47:x:132:VAL:HG21	47:x:501:VAL:HG23	2.03	0.40
52:4:73:LEU:HD23	52:4:76:LEU:HD12	2.02	0.40
53:o:46:LYS:HB3	53:o:49:GLU:HB2	2.03	0.40
54:s:36:VAL:HG12	54:s:204:LEU:HD13	2.03	0.40
2:J:20:ASN:OD1	2:J:68:HIS:HB3	2.21	0.40
6:b:173:CYS:O	6:b:253:PHE:HB2	2.21	0.40
6:b:209:PHE:CE1	6:b:332:ARG:HD3	2.56	0.40
6:b:440:ASN:ND2	6:b:440:ASN:C	2.78	0.40
6:b:499:ARG:NH2	35:U:88:GLN:HE22	2.18	0.40
6:b:593:VAL:HG23	6:b:599:ARG:HH21	1.87	0.40
6:b:639:ARG:NH1	44:1:2980:U:O4	2.44	0.40
16:I:17:ASP:OD2	16:I:20:LEU:HB2	2.20	0.40
18:h:118:ILE:HB	22:L:138:VAL:HG21	2.03	0.40
24:M:19:ARG:HG2	24:M:65:LEU:HD22	2.02	0.40
26:N:51:LEU:HD22	26:N:117:ASN:ND2	2.36	0.40
32:r:133:MET:HA	32:r:152:THR:OG1	2.21	0.40
32:r:194:PHE:CD2	44:1:2858:U:H5"	2.57	0.40
33:S:131:LYS:HD3	33:S:131:LYS:HA	1.89	0.40
36:V:86:ARG:HB2	36:V:92:PHE:CZ	2.56	0.40
39:Y:60:ARG:HB2	39:Y:103:LYS:HB3	2.04	0.40
40:y:163:PRO:HG3	40:y:185:THR:HG22	2.04	0.40
44:1:242:C:O2'	44:1:243:G:H5'	2.22	0.40
44:1:571:U:H2'	44:1:572:A:C8	2.56	0.40
44:1:734:C:H2'	44:1:735:A:O4'	2.22	0.40
44:1:2770:G:O2'	44:1:2771:U:O4'	2.33	0.40
44:1:2812:C:H2'	44:1:2813:A:C8	2.57	0.40
46:5:73:GLN:HA	46:5:76:ILE:HG12	2.02	0.40
48:m:333:ASN:O	48:m:337:LYS:N	2.55	0.40
5:B:85:VAL:HG23	5:B:201:LYS:C	2.46	0.40
6:b:441:VAL:HG12	27:u:93:MET:HE1	2.03	0.40
6:b:608:MET:HE1	44:1:401:U:C6	2.57	0.40
7:C:358:THR:O	33:S:26:ARG:NE	2.55	0.40
19:i:57:LEU:HD23	19:i:90:MET:HG3	2.02	0.40
29:P:22:LEU:HD12	29:P:146:ILE:HD12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:r:7:ILE:N	44:1:2898:G:H22	2.20	0.40
32:r:195:LEU:CD1	32:r:223:VAL:HG13	2.46	0.40
33:S:124:LEU:HA	34:T:153:PRO:HD2	2.04	0.40
34:T:17:ARG:HB2	34:T:22:HIS:ND1	2.37	0.40
39:Y:52:ARG:NH2	45:3:83:C:H42	2.20	0.40
44:1:195:U:H4'	53:o:103:TYR:HE1	1.87	0.40
44:1:2180:G:H2'	44:1:2181:C:C6	2.57	0.40
44:1:2836:C:H5	44:1:2852:C:N4	2.19	0.40
47:x:129:VAL:HG22	47:x:455:ASP:CG	2.47	0.40
47:x:179:MET:O	47:x:180:HIS:ND1	2.54	0.40
48:m:103:THR:O	48:m:282:PRO:HG3	2.21	0.40
48:m:400:ILE:O	48:m:403:VAL:HB	2.21	0.40
49:2:36:C:H2'	49:2:37:G:C8	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	249/297 (84%)	241 (97%)	8 (3%)	0	100	100
2	J	157/174 (90%)	141 (90%)	16 (10%)	0	100	100
3	A	243/254 (96%)	219 (90%)	24 (10%)	0	100	100
4	a	92/149 (62%)	81 (88%)	11 (12%)	0	100	100
5	B	384/387 (99%)	346 (90%)	38 (10%)	0	100	100
6	b	645/647 (100%)	588 (91%)	57 (9%)	0	100	100
7	C	359/362 (99%)	330 (92%)	29 (8%)	0	100	100
8	c	95/105 (90%)	94 (99%)	1 (1%)	0	100	100
9	d	105/113 (93%)	102 (97%)	3 (3%)	0	100	100
10	E	156/176 (89%)	145 (93%)	11 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	e	125/130 (96%)	120 (96%)	5 (4%)	0	100	100
12	F	220/244 (90%)	205 (93%)	15 (7%)	0	100	100
13	f	104/107 (97%)	99 (95%)	5 (5%)	0	100	100
14	G	228/256 (89%)	210 (92%)	18 (8%)	0	100	100
15	g	110/121 (91%)	106 (96%)	4 (4%)	0	100	100
16	I	129/166 (78%)	120 (93%)	9 (7%)	0	100	100
17	H	186/191 (97%)	171 (92%)	15 (8%)	0	100	100
18	h	117/120 (98%)	113 (97%)	4 (3%)	0	100	100
19	i	94/100 (94%)	88 (94%)	6 (6%)	0	100	100
20	j	83/88 (94%)	82 (99%)	1 (1%)	0	100	100
21	k	75/78 (96%)	68 (91%)	7 (9%)	0	100	100
22	L	185/199 (93%)	171 (92%)	14 (8%)	0	100	100
23	l	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
24	M	135/138 (98%)	127 (94%)	8 (6%)	0	100	100
25	p	89/92 (97%)	84 (94%)	5 (6%)	0	100	100
26	N	201/204 (98%)	192 (96%)	9 (4%)	0	100	100
27	u	147/199 (74%)	136 (92%)	11 (8%)	0	100	100
28	O	195/199 (98%)	191 (98%)	4 (2%)	0	100	100
29	P	181/184 (98%)	169 (93%)	12 (7%)	0	100	100
30	Q	137/186 (74%)	134 (98%)	3 (2%)	0	100	100
31	R	152/189 (80%)	146 (96%)	6 (4%)	0	100	100
32	r	209/261 (80%)	187 (90%)	22 (10%)	0	100	100
33	S	168/172 (98%)	153 (91%)	15 (9%)	0	100	100
34	T	143/160 (89%)	132 (92%)	11 (8%)	0	100	100
35	U	102/121 (84%)	96 (94%)	6 (6%)	0	100	100
36	V	134/137 (98%)	130 (97%)	4 (3%)	0	100	100
37	W	223/236 (94%)	215 (96%)	8 (4%)	0	100	100
38	X	118/142 (83%)	112 (95%)	6 (5%)	0	100	100
39	Y	124/127 (98%)	120 (97%)	4 (3%)	0	100	100
40	y	240/245 (98%)	230 (96%)	10 (4%)	0	100	100
41	Z	133/136 (98%)	122 (92%)	11 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	z	53/106 (50%)	53 (100%)	0	0	100	100
43	K	53/165 (32%)	50 (94%)	3 (6%)	0	100	100
46	5	106/120 (88%)	97 (92%)	8 (8%)	1 (1%)	14	28
47	x	388/515 (75%)	368 (95%)	20 (5%)	0	100	100
48	m	451/486 (93%)	429 (95%)	22 (5%)	0	100	100
50	t	408/767 (53%)	371 (91%)	37 (9%)	0	100	100
51	n	39/334 (12%)	31 (80%)	8 (20%)	0	100	100
52	4	495/593 (84%)	455 (92%)	40 (8%)	0	100	100
53	o	103/175 (59%)	103 (100%)	0	0	100	100
54	s	215/217 (99%)	203 (94%)	12 (6%)	0	100	100
55	q	62/520 (12%)	62 (100%)	0	0	100	100
56	Lr	18/25 (72%)	18 (100%)	0	0	100	100
All	All	9411/11666 (81%)	8802 (94%)	608 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
46	5	83	ARG

5.3.2 Protein sidechains (i)

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	D	211/245 (86%)	211 (100%)	0	100	100
2	J	138/150 (92%)	138 (100%)	0	100	100
3	A	188/196 (96%)	188 (100%)	0	100	100
4	a	77/119 (65%)	77 (100%)	0	100	100
5	B	322/323 (100%)	322 (100%)	0	100	100
6	b	572/573 (100%)	571 (100%)	1 (0%)	87	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	C	288/289 (100%)	288 (100%)	0	100	100
8	c	81/88 (92%)	81 (100%)	0	100	100
9	d	94/97 (97%)	94 (100%)	0	100	100
10	E	138/153 (90%)	138 (100%)	0	100	100
11	e	109/111 (98%)	109 (100%)	0	100	100
12	F	186/205 (91%)	186 (100%)	0	100	100
13	f	90/91 (99%)	90 (100%)	0	100	100
14	G	189/208 (91%)	189 (100%)	0	100	100
15	g	95/103 (92%)	95 (100%)	0	100	100
16	I	116/141 (82%)	115 (99%)	1 (1%)	70	84
17	H	168/171 (98%)	167 (99%)	1 (1%)	78	89
18	h	104/105 (99%)	104 (100%)	0	100	100
19	i	78/82 (95%)	78 (100%)	0	100	100
20	j	69/71 (97%)	69 (100%)	0	100	100
21	k	68/69 (99%)	68 (100%)	0	100	100
22	L	147/159 (92%)	147 (100%)	0	100	100
23	l	45/46 (98%)	45 (100%)	0	100	100
24	M	108/109 (99%)	108 (100%)	0	100	100
25	p	71/72 (99%)	71 (100%)	0	100	100
26	N	175/176 (99%)	175 (100%)	0	100	100
27	u	132/180 (73%)	132 (100%)	0	100	100
28	O	160/162 (99%)	160 (100%)	0	100	100
29	P	144/146 (99%)	144 (100%)	0	100	100
30	Q	113/151 (75%)	113 (100%)	0	100	100
31	R	127/154 (82%)	127 (100%)	0	100	100
32	r	187/229 (82%)	187 (100%)	0	100	100
33	S	154/156 (99%)	154 (100%)	0	100	100
34	T	124/137 (90%)	124 (100%)	0	100	100
35	U	91/107 (85%)	91 (100%)	0	100	100
36	V	104/105 (99%)	104 (100%)	0	100	100
37	W	201/213 (94%)	201 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	X	104/118 (88%)	104 (100%)	0	100	100
39	Y	109/110 (99%)	109 (100%)	0	100	100
40	y	207/211 (98%)	207 (100%)	0	100	100
41	Z	115/116 (99%)	115 (100%)	0	100	100
42	z	48/95 (50%)	48 (100%)	0	100	100
43	K	31/65 (48%)	31 (100%)	0	100	100
46	5	97/106 (92%)	97 (100%)	0	100	100
47	x	340/451 (75%)	340 (100%)	0	100	100
48	m	400/428 (94%)	399 (100%)	1 (0%)	86	93
50	t	367/665 (55%)	367 (100%)	0	100	100
51	n	38/302 (13%)	38 (100%)	0	100	100
52	4	445/520 (86%)	445 (100%)	0	100	100
53	o	99/153 (65%)	99 (100%)	0	100	100
54	s	198/198 (100%)	198 (100%)	0	100	100
55	q	58/445 (13%)	58 (100%)	0	100	100
56	Lr	19/23 (83%)	19 (100%)	0	100	100
All	All	8139/9898 (82%)	8135 (100%)	4 (0%)	100	100

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	b	440	ASN
16	I	114	PRO
17	H	49	ASN
48	m	150	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	32	GLN
1	D	40	HIS
1	D	63	GLN
1	D	111	GLN
1	D	264	GLN
2	J	95	ASN

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Mol	Chain	Res	Type
3	A	38	HIS
3	A	194	ASN
3	A	205	ASN
4	a	65	GLN
5	B	198	HIS
5	B	243	HIS
6	b	23	ASN
6	b	124	GLN
6	b	365	GLN
6	b	413	ASN
6	b	440	ASN
6	b	454	GLN
6	b	509	ASN
7	C	213	ASN
7	C	237	GLN
10	E	61	ASN
12	F	48	ASN
14	G	24	ASN
14	G	38	GLN
14	G	95	ASN
14	G	192	GLN
16	I	53	HIS
16	I	97	ASN
16	I	126	HIS
17	H	9	GLN
17	H	51	GLN
17	H	100	ASN
18	h	34	GLN
18	h	113	GLN
21	k	57	ASN
23	l	33	ASN
24	M	41	GLN
24	M	56	GLN
26	N	95	GLN
28	O	31	GLN
31	R	134	HIS
31	R	141	HIS
32	r	224	ASN
33	S	3	HIS
33	S	49	HIS
33	S	142	GLN
34	T	22	HIS

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Mol	Chain	Res	Type
34	T	103	GLN
35	U	87	ASN
36	V	7	GLN
36	V	132	ASN
40	y	86	ASN
41	Z	78	ASN
42	z	31	GLN
46	5	56	GLN
47	x	289	GLN
47	x	307	ASN
47	x	341	HIS
48	m	86	GLN
50	t	19	ASN
50	t	119	HIS
50	t	165	ASN
50	t	170	ASN
50	t	205	GLN
50	t	357	ASN
50	t	446	ASN
52	4	113	ASN
52	4	385	GLN
52	4	394	HIS
52	4	429	ASN
52	4	555	GLN
53	o	5	ASN
53	o	24	ASN
54	s	181	ASN
54	s	182	GLN
54	s	188	ASN
54	s	199	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
44	1	3104/3396 (91%)	667 (21%)	57 (1%)
45	3	157/158 (99%)	27 (17%)	0
49	2	115/121 (95%)	24 (20%)	2 (1%)
All	All	3376/3675 (91%)	718 (21%)	59 (1%)

All (718) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
44	1	13	A
44	1	14	U
44	1	26	A
44	1	40	A
44	1	43	A
44	1	49	A
44	1	57	A
44	1	59	G
44	1	60	A
44	1	65	A
44	1	66	A
44	1	76	G
44	1	92	G
44	1	94	G
44	1	109	A
44	1	110	G
44	1	111	C
44	1	116	A
44	1	121	A
44	1	122	A
44	1	124	U
44	1	133	U
44	1	135	C
44	1	136	G
44	1	148	G
44	1	156	G
44	1	157	A
44	1	165	A
44	1	166	C
44	1	172	G
44	1	182	U
44	1	187	A
44	1	190	U
44	1	191	U
44	1	206	G
44	1	210	U
44	1	218	G
44	1	219	A
44	1	220	G
44	1	231	G
44	1	240	U
44	1	241	G
44	1	243	G

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Mol	Chain	Res	Type
44	1	249	U
44	1	252	U
44	1	253	A
44	1	269	G
44	1	283	G
44	1	286	U
44	1	295	A
44	1	305	U
44	1	323	A
44	1	329	U
44	1	337	G
44	1	339	C
44	1	350	C
44	1	351	A
44	1	370	U
44	1	375	A
44	1	376	G
44	1	399	A
44	1	401	U
44	1	402	A
44	1	403	C
44	1	421	G
44	1	422	A
44	1	438	A
44	1	440	A
44	1	516	A
44	1	518	G
44	1	520	U
44	1	521	A
44	1	535	G
44	1	541	U
44	1	543	C
44	1	548	G
44	1	551	A
44	1	552	G
44	1	555	U
44	1	557	A
44	1	559	A
44	1	560	G
44	1	578	A
44	1	579	G
44	1	592	A

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Mol	Chain	Res	Type
44	1	597	G
44	1	604	G
44	1	609	G
44	1	611	A
44	1	620	U
44	1	621	A
44	1	622	A
44	1	636	C
44	1	637	C
44	1	638	C
44	1	642	U
44	1	645	A
44	1	647	A
44	1	660	A
44	1	677	A
44	1	681	U
44	1	691	A
44	1	705	A
44	1	709	A
44	1	712	G
44	1	715	A
44	1	716	A
44	1	764	U
44	1	765	C
44	1	766	U
44	1	767	U
44	1	771	A
44	1	776	U
44	1	778	U
44	1	780	A
44	1	781	G
44	1	785	G
44	1	786	A
44	1	801	A
44	1	806	A
44	1	817	A
44	1	830	A
44	1	835	G
44	1	845	G
44	1	849	C
44	1	861	C
44	1	874	U

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Mol	Chain	Res	Type
44	1	875	G
44	1	880	G
44	1	896	A
44	1	907	G
44	1	908	G
44	1	914	A
44	1	916	G
44	1	917	A
44	1	921	A
44	1	923	C
44	1	925	A
44	1	937	G
44	1	944	C
44	1	954	U
44	1	956	U
44	1	959	C
44	1	960	U
44	1	974	G
44	1	979	U
44	1	980	A
44	1	981	U
44	1	983	A
44	1	984	G
44	1	991	G
44	1	993	G
44	1	995	U
44	1	996	A
44	1	999	G
44	1	1000	C
44	1	1001	G
44	1	1002	A
44	1	1003	A
44	1	1004	U
44	1	1007	U
44	1	1008	U
44	1	1010	G
44	1	1015	U
44	1	1016	C
44	1	1017	C
44	1	1019	G
44	1	1021	G
44	1	1022	U

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Mol	Chain	Res	Type
44	1	1024	G
44	1	1025	A
44	1	1026	A
44	1	1027	A
44	1	1028	U
44	1	1029	G
44	1	1030	A
44	1	1035	G
44	1	1036	A
44	1	1039	U
44	1	1040	A
44	1	1044	U
44	1	1056	U
44	1	1057	A
44	1	1059	G
44	1	1060	U
44	1	1064	A
44	1	1065	A
44	1	1066	G
44	1	1072	G
44	1	1081	U
44	1	1082	U
44	1	1093	A
44	1	1095	U
44	1	1096	U
44	1	1097	G
44	1	1098	A
44	1	1103	A
44	1	1104	G
44	1	1116	G
44	1	1117	G
44	1	1124	U
44	1	1127	G
44	1	1132	C
44	1	1134	G
44	1	1145	G
44	1	1153	A
44	1	1159	A
44	1	1160	C
44	1	1178	G
44	1	1179	A
44	1	1180	A

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Mol	Chain	Res	Type
44	1	1181	U
44	1	1186	G
44	1	1192	C
44	1	1193	A
44	1	1196	C
44	1	1198	C
44	1	1202	A
44	1	1203	A
44	1	1204	A
44	1	1205	A
44	1	1217	A
44	1	1220	U
44	1	1221	A
44	1	1236	G
44	1	1241	U
44	1	1242	G
44	1	1243	G
44	1	1244	A
44	1	1245	A
44	1	1246	G
44	1	1253	U
44	1	1258	U
44	1	1262	G
44	1	1263	A
44	1	1264	G
44	1	1265	U
44	1	1269	U
44	1	1272	C
44	1	1278	A
44	1	1279	C
44	1	1285	G
44	1	1287	A
44	1	1303	A
44	1	1304	A
44	1	1305	U
44	1	1306	G
44	1	1307	G
44	1	1308	A
44	1	1309	U
44	1	1313	G
44	1	1330	A
44	1	1332	A

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Mol	Chain	Res	Type
44	1	1351	U
44	1	1352	A
44	1	1354	G
44	1	1355	A
44	1	1356	U
44	1	1357	G
44	1	1386	A
44	1	1392	G
44	1	1399	A
44	1	1400	G
44	1	1419	A
44	1	1421	G
44	1	1431	G
44	1	1434	G
44	1	1437	C
44	1	1446	A
44	1	1455	U
44	1	1475	A
44	1	1481	A
44	1	1482	A
44	1	1483	G
44	1	1487	G
44	1	1488	G
44	1	1507	G
44	1	1508	C
44	1	1536	G
44	1	1555	U
44	1	1556	C
44	1	1557	A
44	1	1560	G
44	1	1562	C
44	1	1563	C
44	1	1565	G
44	1	1566	A
44	1	1567	U
44	1	1568	U
44	1	1569	U
44	1	1570	U
44	1	1571	A
44	1	1572	U
44	1	1573	G
44	1	1575	A

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Mol	Chain	Res	Type
44	1	1576	G
44	1	1583	A
44	1	1590	G
44	1	1593	A
44	1	1605	A
44	1	1607	U
44	1	1618	G
44	1	1629	U
44	1	1633	C
44	1	1639	C
44	1	1642	A
44	1	1643	A
44	1	1658	G
44	1	1683	A
44	1	1717	U
44	1	1718	G
44	1	1724	U
44	1	1725	C
44	1	1741	A
44	1	1742	U
44	1	1750	A
44	1	1751	G
44	1	1759	C
44	1	1761	C
44	1	1762	C
44	1	1763	U
44	1	1766	G
44	1	1770	G
44	1	1775	G
44	1	1780	G
44	1	1797	A
44	1	1814	A
44	1	1815	U
44	1	1816	A
44	1	1817	G
44	1	1819	U
44	1	1820	U
44	1	1821	U
44	1	1839	A
44	1	1841	A
44	1	1842	A
44	1	1846	C

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Mol	Chain	Res	Type
44	1	1849	C
44	1	1866	C
44	1	1879	A
44	1	1880	U
44	1	1893	A
44	1	1906	G
44	1	1926	C
44	1	1952	G
44	1	1954	G
44	1	2100	A
44	1	2102	U
44	1	2107	A
44	1	2112	U
44	1	2114	C
44	1	2115	G
44	1	2121	G
44	1	2122	G
44	1	2126	A
44	1	2131	A
44	1	2140	U
44	1	2144	A
44	1	2149	A
44	1	2158	A
44	1	2169	G
44	1	2170	U
44	1	2201	G
44	1	2205	U
44	1	2206	G
44	1	2208	A
44	1	2210	G
44	1	2223	A
44	1	2244	A
44	1	2249	G
44	1	2268	U
44	1	2270	A
44	1	2271	A
44	1	2272	G
44	1	2273	G
44	1	2274	U
44	1	2276	G
44	1	2313	A
44	1	2314	U

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Mol	Chain	Res	Type
44	1	2315	G
44	1	2316	G
44	1	2317	A
44	1	2334	U
44	1	2335	G
44	1	2336	U
44	1	2364	G
44	1	2369	G
44	1	2371	G
44	1	2373	A
44	1	2374	C
44	1	2375	G
44	1	2376	G
44	1	2377	G
44	1	2385	G
44	1	2388	U
44	1	2393	G
44	1	2399	A
44	1	2400	G
44	1	2401	A
44	1	2402	A
44	1	2403	G
44	1	2411	U
44	1	2418	G
44	1	2437	G
44	1	2440	G
44	1	2442	G
44	1	2448	G
44	1	2450	G
44	1	2451	G
44	1	2452	G
44	1	2453	U
44	1	2454	G
44	1	2458	A
44	1	2459	A
44	1	2460	U
44	1	2462	A
44	1	2467	G
44	1	2468	A
44	1	2469	G
44	1	2470	C
44	1	2473	C

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Mol	Chain	Res	Type
44	1	2474	G
44	1	2479	C
44	1	2480	A
44	1	2484	A
44	1	2487	U
44	1	2490	C
44	1	2493	U
44	1	2494	A
44	1	2496	C
44	1	2497	U
44	1	2498	U
44	1	2501	U
44	1	2502	A
44	1	2505	U
44	1	2508	U
44	1	2511	A
44	1	2514	U
44	1	2515	A
44	1	2522	G
44	1	2523	A
44	1	2524	A
44	1	2525	G
44	1	2526	C
44	1	2532	U
44	1	2533	G
44	1	2535	A
44	1	2536	A
44	1	2537	U
44	1	2538	U
44	1	2539	C
44	1	2540	A
44	1	2541	U
44	1	2542	U
44	1	2543	U
44	1	2544	U
44	1	2546	C
44	1	2549	G
44	1	2552	C
44	1	2555	G
44	1	2560	C
44	1	2561	A
44	1	2569	A

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Mol	Chain	Res	Type
44	1	2571	U
44	1	2572	C
44	1	2573	G
44	1	2585	G
44	1	2587	U
44	1	2593	A
44	1	2594	C
44	1	2606	G
44	1	2607	G
44	1	2614	G
44	1	2626	A
44	1	2630	C
44	1	2631	U
44	1	2634	U
44	1	2646	C
44	1	2647	A
44	1	2651	G
44	1	2652	U
44	1	2654	C
44	1	2655	U
44	1	2657	A
44	1	2658	G
44	1	2673	A
44	1	2674	A
44	1	2676	A
44	1	2677	G
44	1	2689	A
44	1	2691	A
44	1	2694	A
44	1	2697	A
44	1	2704	A
44	1	2706	G
44	1	2714	G
44	1	2718	U
44	1	2720	G
44	1	2727	A
44	1	2728	G
44	1	2729	U
44	1	2737	C
44	1	2753	G
44	1	2755	C
44	1	2756	C

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Mol	Chain	Res	Type
44	1	2762	A
44	1	2763	U
44	1	2771	U
44	1	2772	C
44	1	2773	C
44	1	2777	G
44	1	2778	G
44	1	2791	G
44	1	2792	A
44	1	2802	A
44	1	2803	A
44	1	2810	C
44	1	2814	G
44	1	2822	U
44	1	2823	G
44	1	2824	G
44	1	2826	U
44	1	2834	G
44	1	2837	A
44	1	2838	A
44	1	2842	U
44	1	2844	C
44	1	2845	A
44	1	2846	U
44	1	2847	A
44	1	2857	C
44	1	2858	U
44	1	2859	U
44	1	2861	U
44	1	2863	G
44	1	2865	U
44	1	2867	C
44	1	2868	U
44	1	2869	U
44	1	2870	C
44	1	2873	U
44	1	2874	G
44	1	2875	U
44	1	2876	C
44	1	2877	G
44	1	2878	G
44	1	2879	C

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Mol	Chain	Res	Type
44	1	2887	A
44	1	2889	C
44	1	2892	A
44	1	2898	G
44	1	2899	C
44	1	2911	A
44	1	2921	U
44	1	2922	G
44	1	2923	U
44	1	2924	U
44	1	2926	A
44	1	2927	C
44	1	2928	C
44	1	2935	U
44	1	2936	A
44	1	2941	A
44	1	2943	G
44	1	2944	U
44	1	2953	U
44	1	2954	U
44	1	2971	A
44	1	2972	G
44	1	2978	U
44	1	2979	U
44	1	2981	U
44	1	2982	A
44	1	2983	C
44	1	2990	G
44	1	2992	U
44	1	2997	G
44	1	3012	A
44	1	3022	G
44	1	3024	A
44	1	3030	G
44	1	3033	A
44	1	3042	U
44	1	3048	A
44	1	3049	A
44	1	3059	G
44	1	3078	U
44	1	3079	U
44	1	3080	G

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Mol	Chain	Res	Type
44	1	3086	A
44	1	3087	A
44	1	3092	C
44	1	3104	U
44	1	3119	U
44	1	3121	U
44	1	3122	A
44	1	3128	G
44	1	3129	A
44	1	3130	A
44	1	3131	U
44	1	3142	A
44	1	3143	C
44	1	3153	U
44	1	3154	C
44	1	3155	U
44	1	3156	U
44	1	3157	U
44	1	3163	A
44	1	3165	A
44	1	3168	A
44	1	3170	A
44	1	3173	G
44	1	3174	A
44	1	3176	G
44	1	3179	U
44	1	3181	C
44	1	3187	A
44	1	3196	U
44	1	3198	U
44	1	3207	U
44	1	3217	C
44	1	3218	A
44	1	3219	G
44	1	3229	G
44	1	3243	A
44	1	3245	A
44	1	3247	G
44	1	3253	G
44	1	3256	G
44	1	3259	U
44	1	3260	G

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Mol	Chain	Res	Type
44	1	3263	G
44	1	3270	U
44	1	3276	G
44	1	3279	A
44	1	3281	U
44	1	3282	U
44	1	3283	U
44	1	3284	G
44	1	3287	U
44	1	3289	G
44	1	3294	A
44	1	3295	A
44	1	3304	U
44	1	3313	U
44	1	3316	A
44	1	3318	G
44	1	3319	U
44	1	3320	A
44	1	3329	U
44	1	3330	A
44	1	3341	U
44	1	3342	A
44	1	3345	G
44	1	3350	C
44	1	3352	U
44	1	3353	G
44	1	3354	U
44	1	3355	U
44	1	3356	G
44	1	3359	A
44	1	3360	C
44	1	3369	G
44	1	3375	A
44	1	3378	C
44	1	3386	G
44	1	3396	U
45	3	21	C
45	3	23	U
45	3	34	U
45	3	35	C
45	3	59	A
45	3	62	C

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Mol	Chain	Res	Type
45	3	63	G
45	3	77	A
45	3	80	A
45	3	82	U
45	3	83	C
45	3	84	C
45	3	85	G
45	3	87	G
45	3	90	U
45	3	95	G
45	3	97	A
45	3	104	A
45	3	106	C
45	3	111	A
45	3	113	U
45	3	125	U
45	3	126	A
45	3	138	A
45	3	148	G
45	3	152	G
45	3	155	A
49	2	7	G
49	2	18	C
49	2	22	A
49	2	30	G
49	2	33	U
49	2	34	C
49	2	35	C
49	2	38	U
49	2	50	U
49	2	51	A
49	2	53	U
49	2	54	U
49	2	55	A
49	2	65	G
49	2	73	C
49	2	74	C
49	2	88	G
49	2	99	G
49	2	102	A
49	2	107	C
49	2	108	A

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Mol	Chain	Res	Type
49	2	109	G
49	2	112	G
49	2	121	U

All (59) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
44	1	13	A
44	1	239	G
44	1	282	G
44	1	374	A
44	1	547	G
44	1	636	C
44	1	637	C
44	1	916	G
44	1	994	G
44	1	1000	C
44	1	1002	A
44	1	1003	A
44	1	1058	U
44	1	1059	G
44	1	1064	A
44	1	1097	G
44	1	1103	A
44	1	1131	G
44	1	1268	G
44	1	1307	G
44	1	1331	U
44	1	1355	A
44	1	1554	U
44	1	1562	C
44	1	1566	A
44	1	1567	U
44	1	1572	U
44	1	1816	A
44	1	2101	C
44	1	2111	G
44	1	2209	U
44	1	2373	A
44	1	2375	G
44	1	2402	A
44	1	2451	G

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Mol	Chain	Res	Type
44	1	2452	G
44	1	2496	C
44	1	2501	U
44	1	2525	G
44	1	2537	U
44	1	2541	U
44	1	2542	U
44	1	2586	G
44	1	2625	C
44	1	2651	G
44	1	2822	U
44	1	2857	C
44	1	2866	U
44	1	2923	U
44	1	3078	U
44	1	3121	U
44	1	3169	U
44	1	3218	A
44	1	3228	C
44	1	3269	U
44	1	3282	U
44	1	3317	U
49	2	49	G
49	2	52	G

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
57	GTP	m	501	59,58	33,34,34	0.95	1 (3%)	50,54,54	1.57	8 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	GTP	m	501	59,58	-	3/22/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	m	501	GTP	C2-N3	2.03	1.38	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	m	501	GTP	C5-C4-N3	-4.80	120.75	128.39
57	m	501	GTP	C2-N3-C4	4.58	120.18	112.30
57	m	501	GTP	N9-C4-N3	3.10	132.15	125.95
57	m	501	GTP	C2-N1-C6	-2.84	119.97	125.11
57	m	501	GTP	N9-C8-N7	-2.73	108.33	113.40
57	m	501	GTP	C5-C6-N1	2.50	119.61	113.25
57	m	501	GTP	C8-N7-C5	2.48	108.68	104.26
57	m	501	GTP	O6-C6-C5	-2.44	120.09	126.53

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	m	501	GTP	C5'-O5'-PA-O1A
57	m	501	GTP	O4'-C4'-C5'-O5'
57	m	501	GTP	C3'-C4'-C5'-O5'

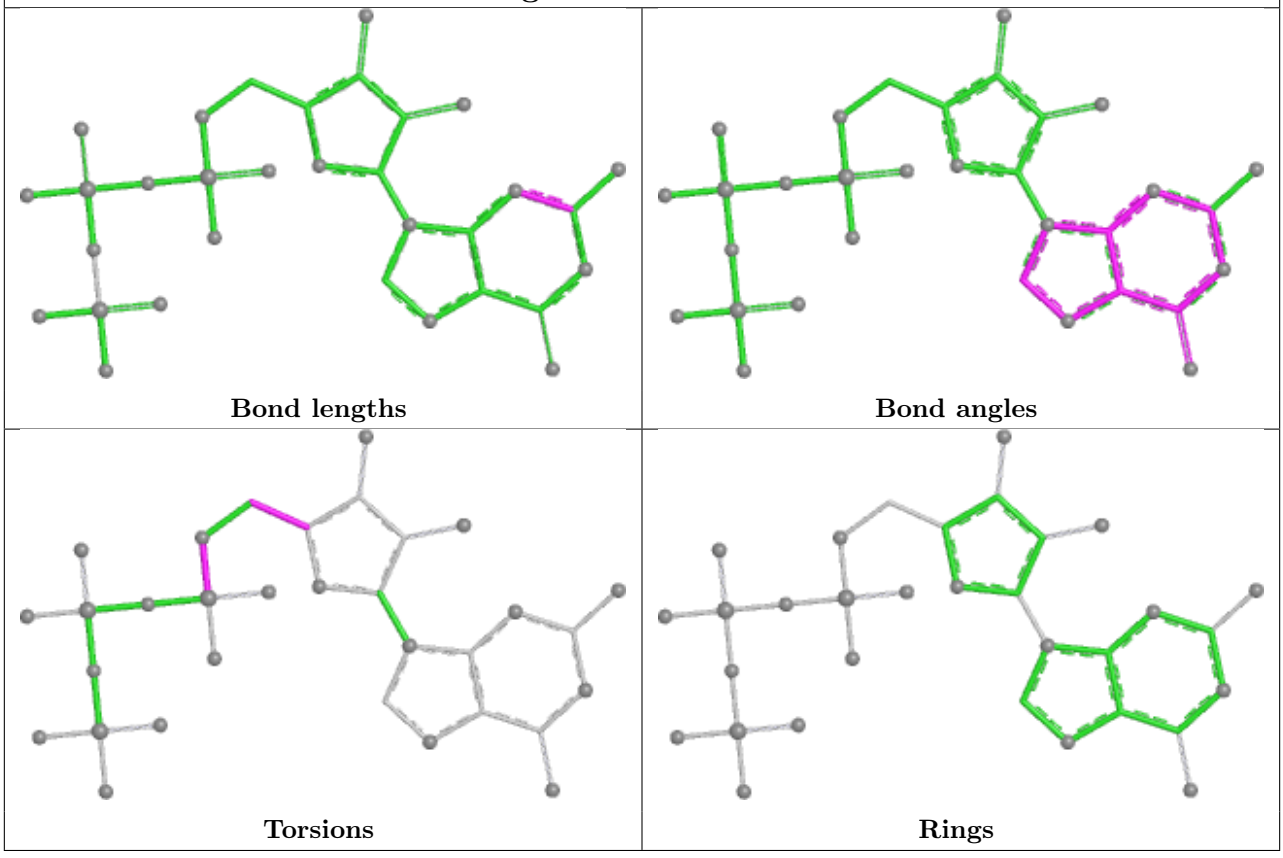
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	m	501	GTP	1	0

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

Ligand GTP m 501



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
46	5	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	114:ASN	C	121:LYS	N	3.15

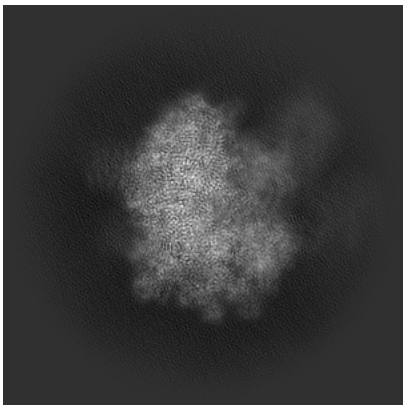
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-73543. These allow visual inspection of the internal detail of the map and identification of artifacts.

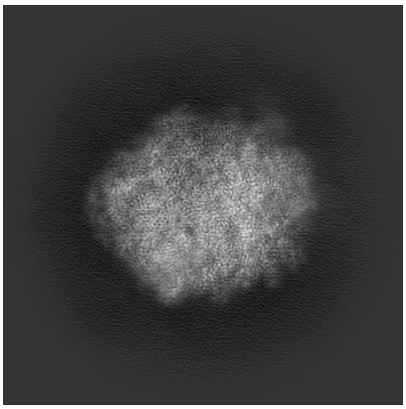
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

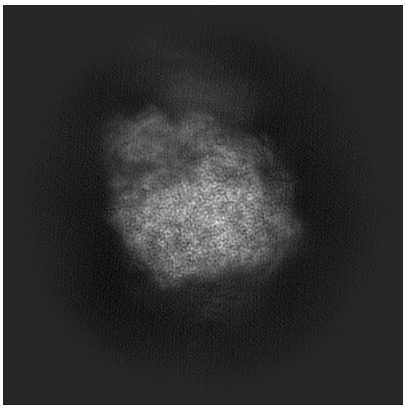
6.1.1 Primary map



X

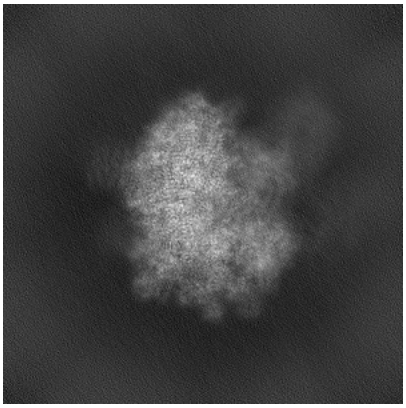


Y

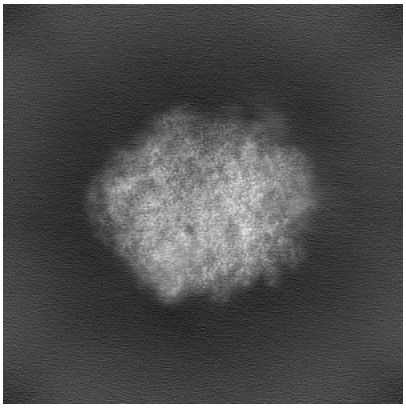


Z

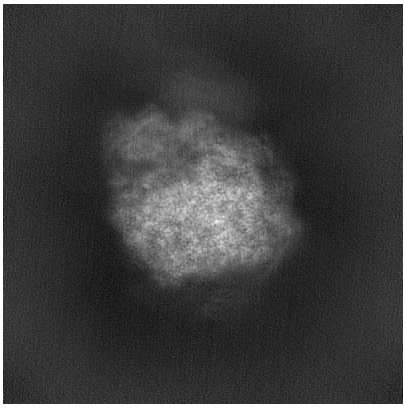
6.1.2 Raw map



X



Y

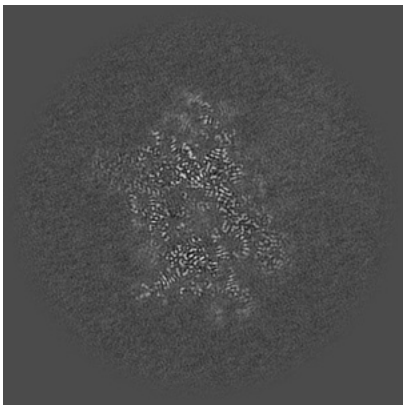


Z

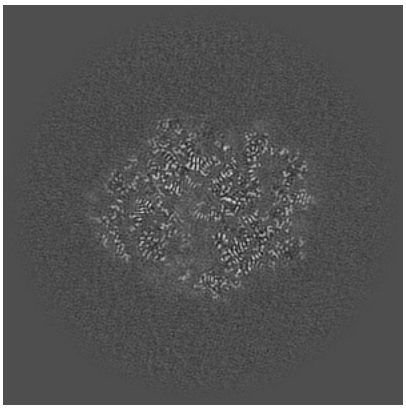
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

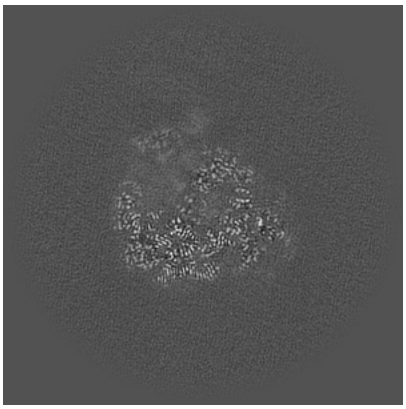
6.2.1 Primary map



X Index: 200

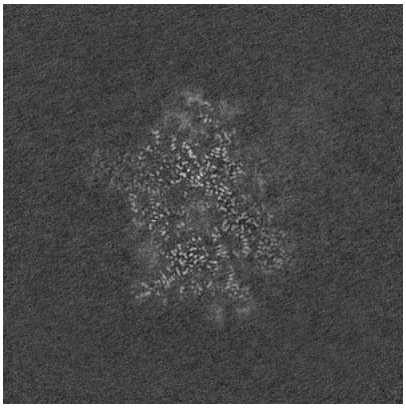


Y Index: 200

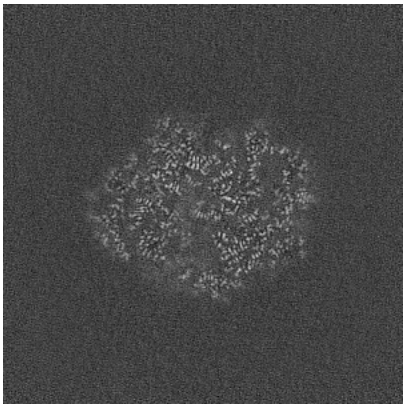


Z Index: 200

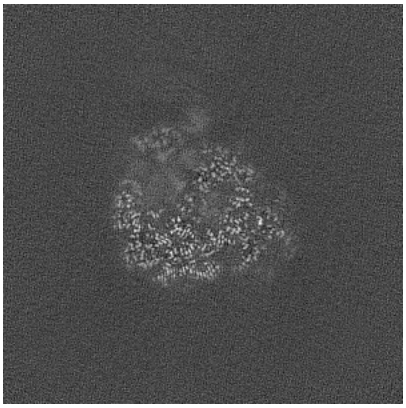
6.2.2 Raw map



X Index: 200



Y Index: 200

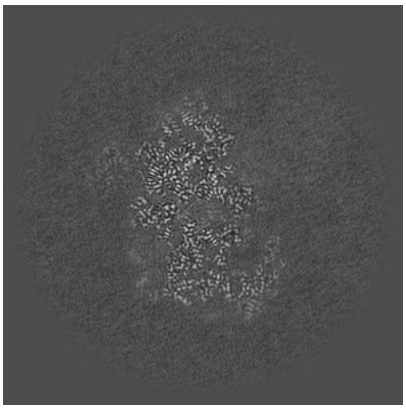


Z Index: 200

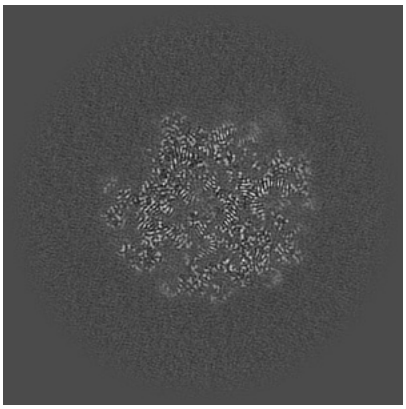
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

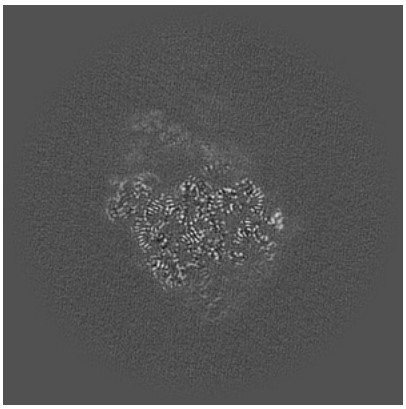
6.3.1 Primary map



X Index: 213

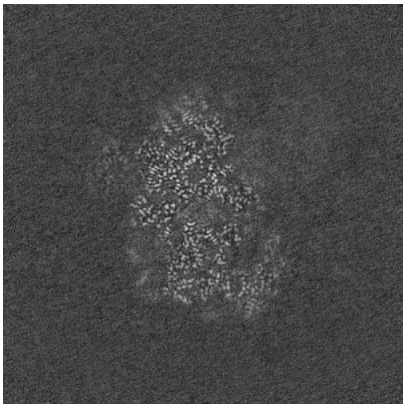


Y Index: 186

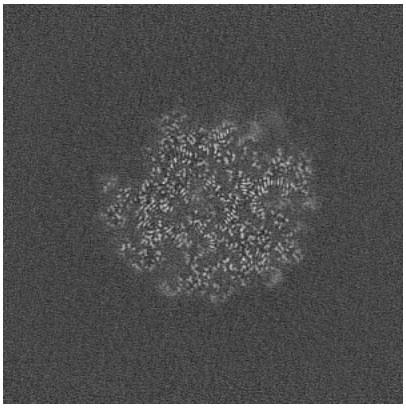


Z Index: 221

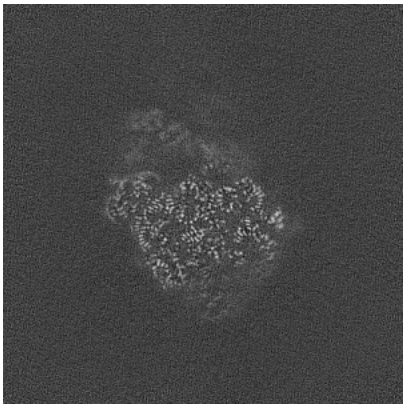
6.3.2 Raw map



X Index: 213



Y Index: 186

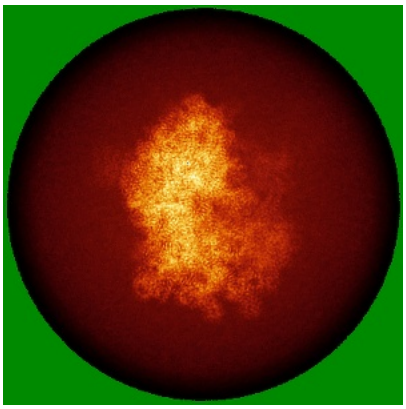


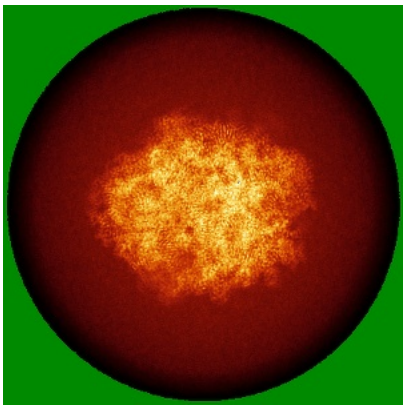
Z Index: 221

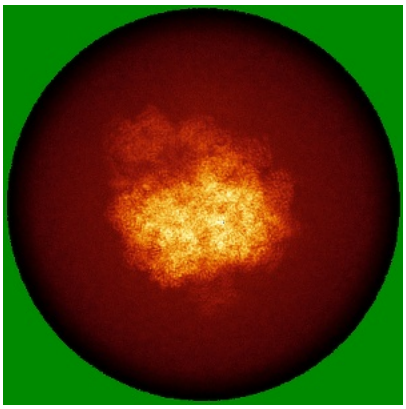
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

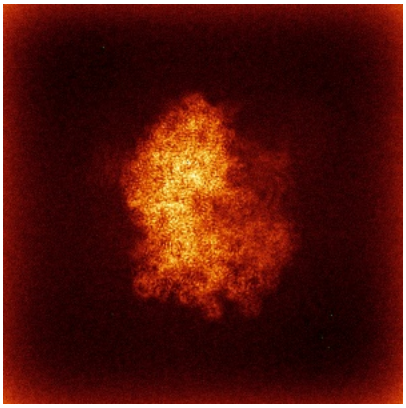
6.4.1 Primary map

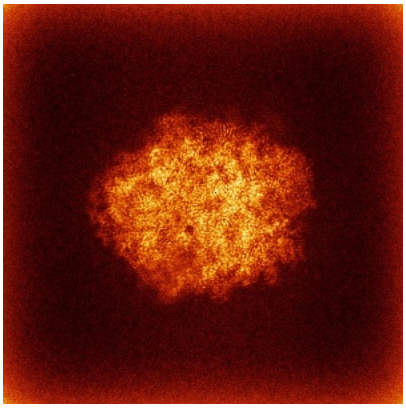

X

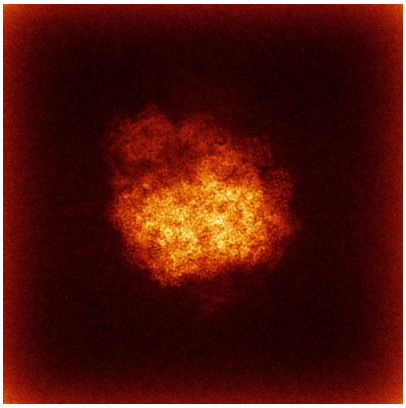

Y


Z

6.4.2 Raw map


X

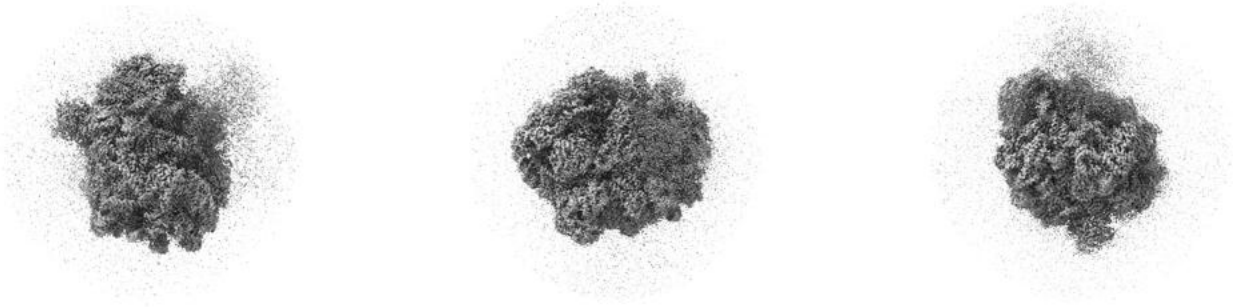

Y


Z

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

6.5 Orthogonal surface views (i)

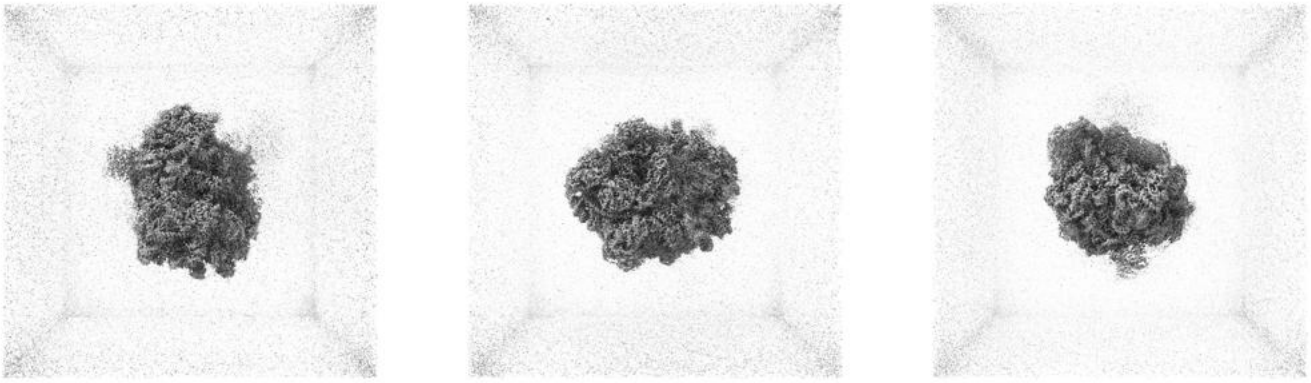
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

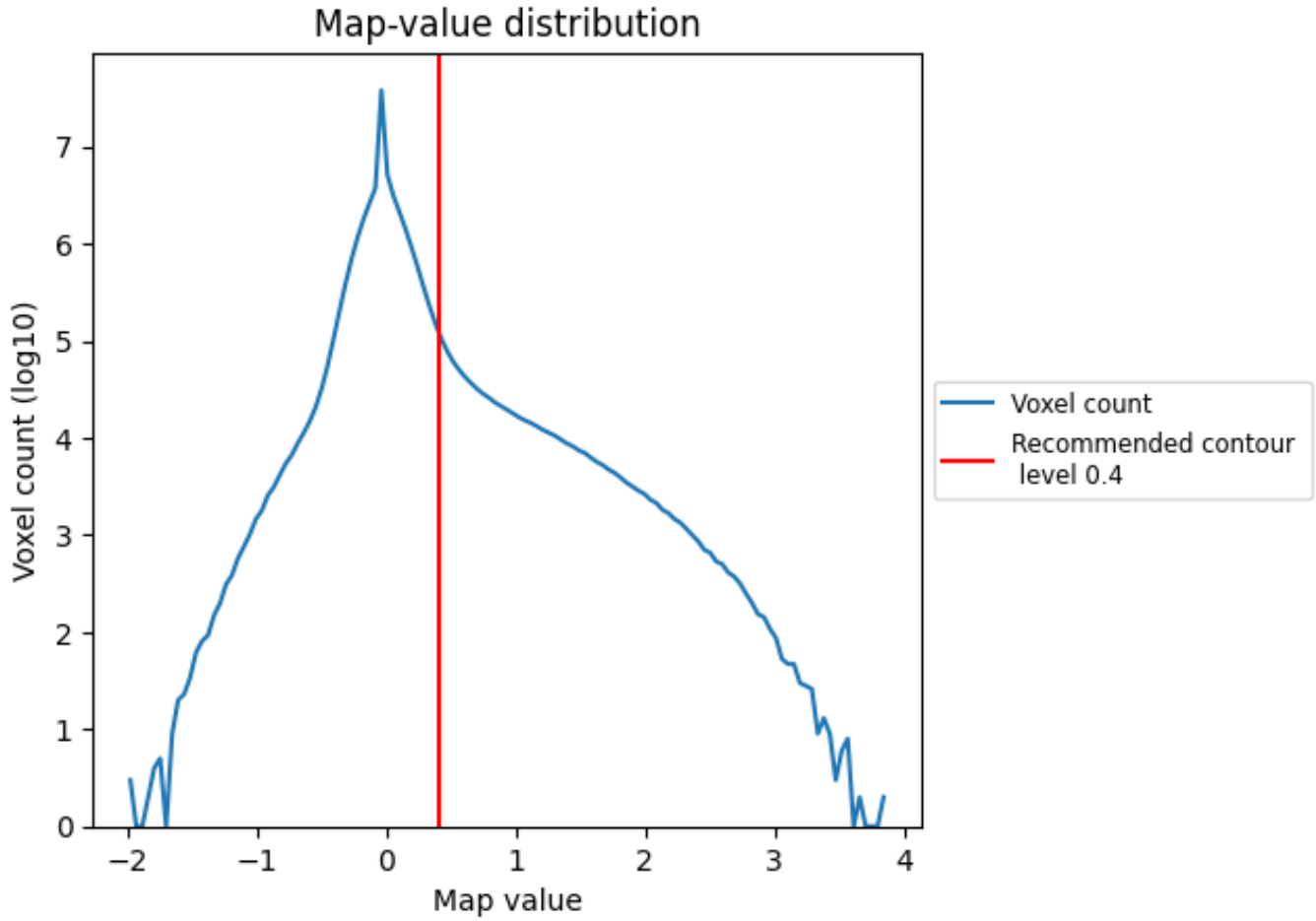
6.6 Mask visualisation (i)

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

7 Map analysis

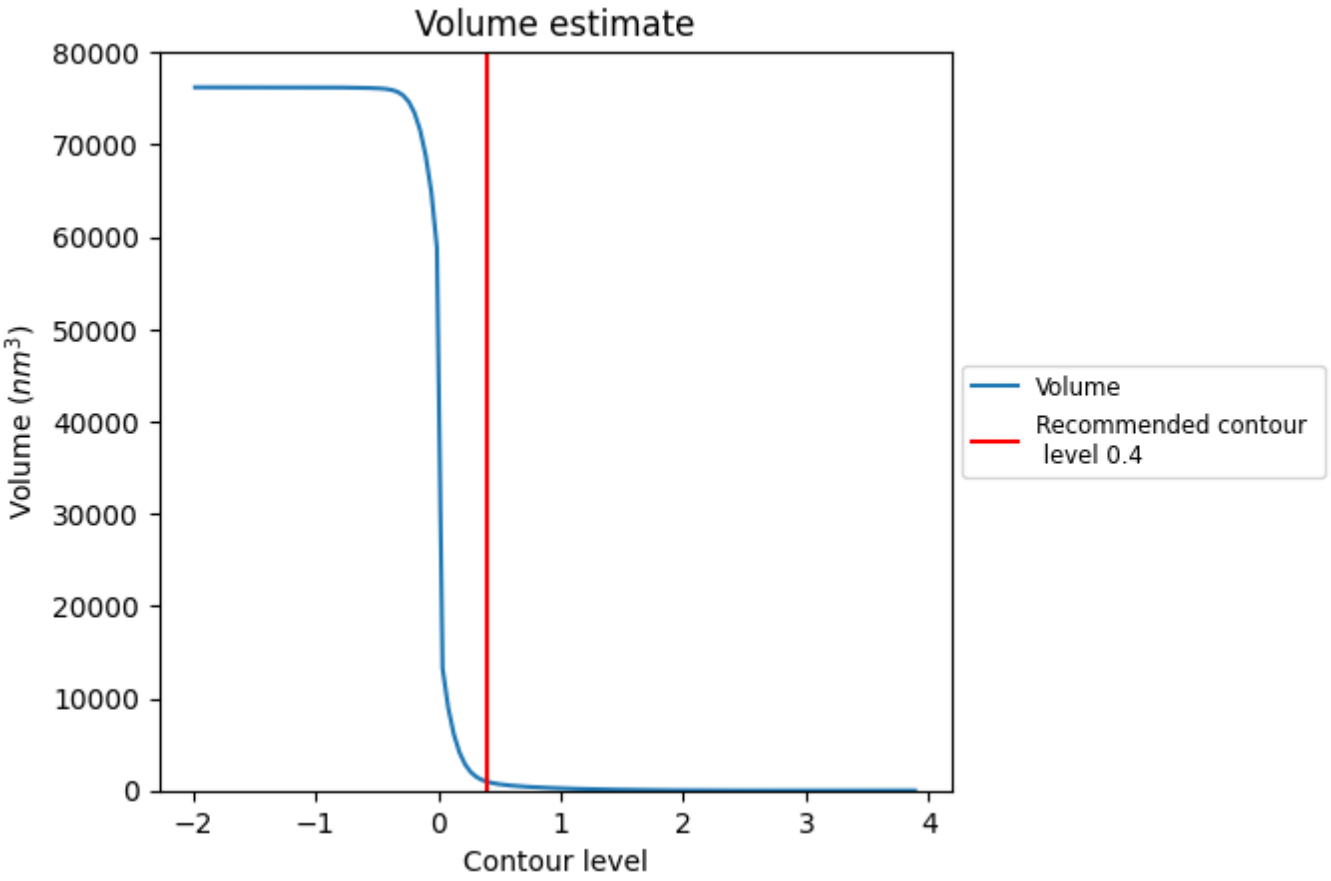
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

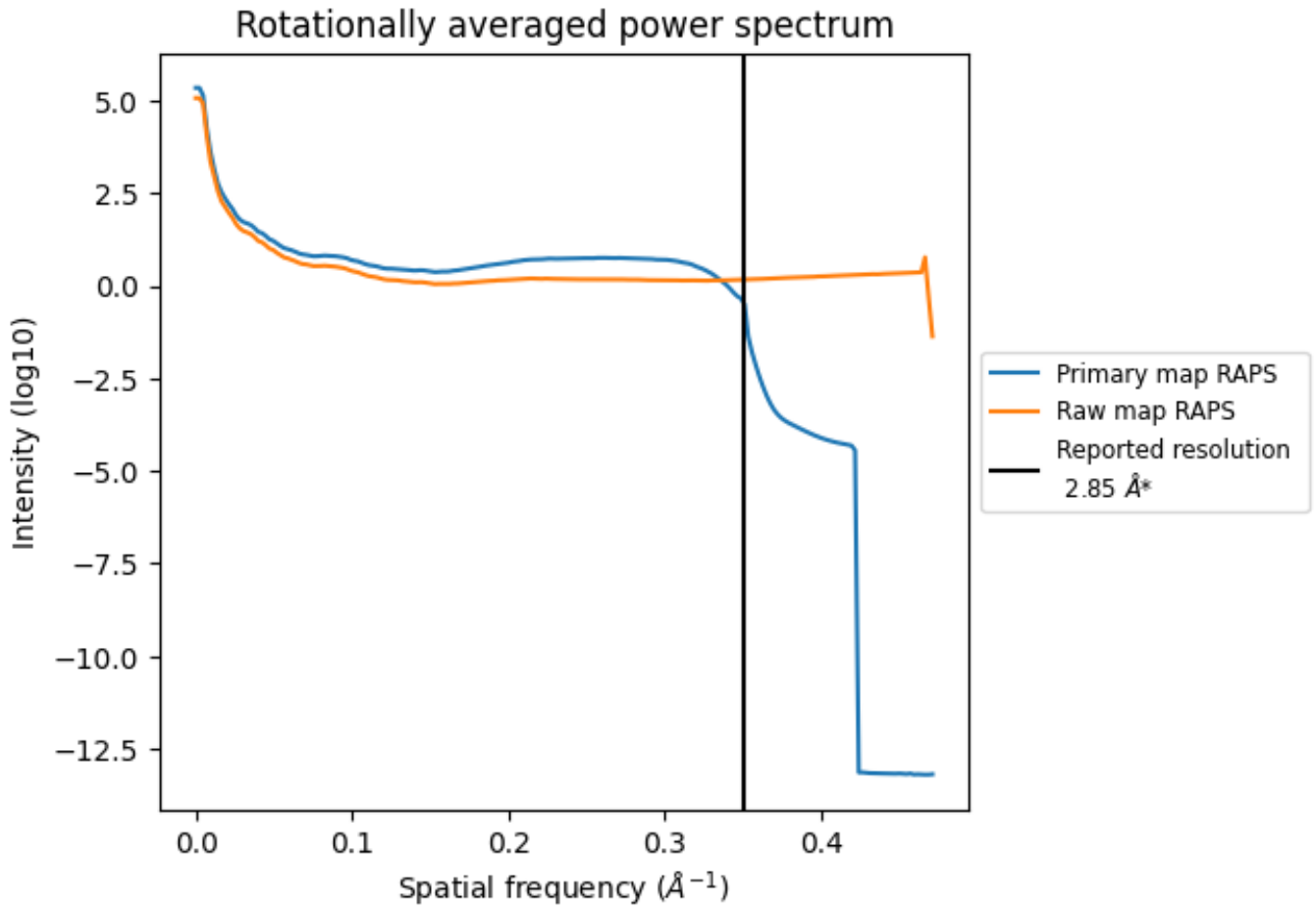
7.2 Volume estimate



The volume at the recommended contour level is 961 nm^3; this corresponds to an approximate mass of 868 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 (i)

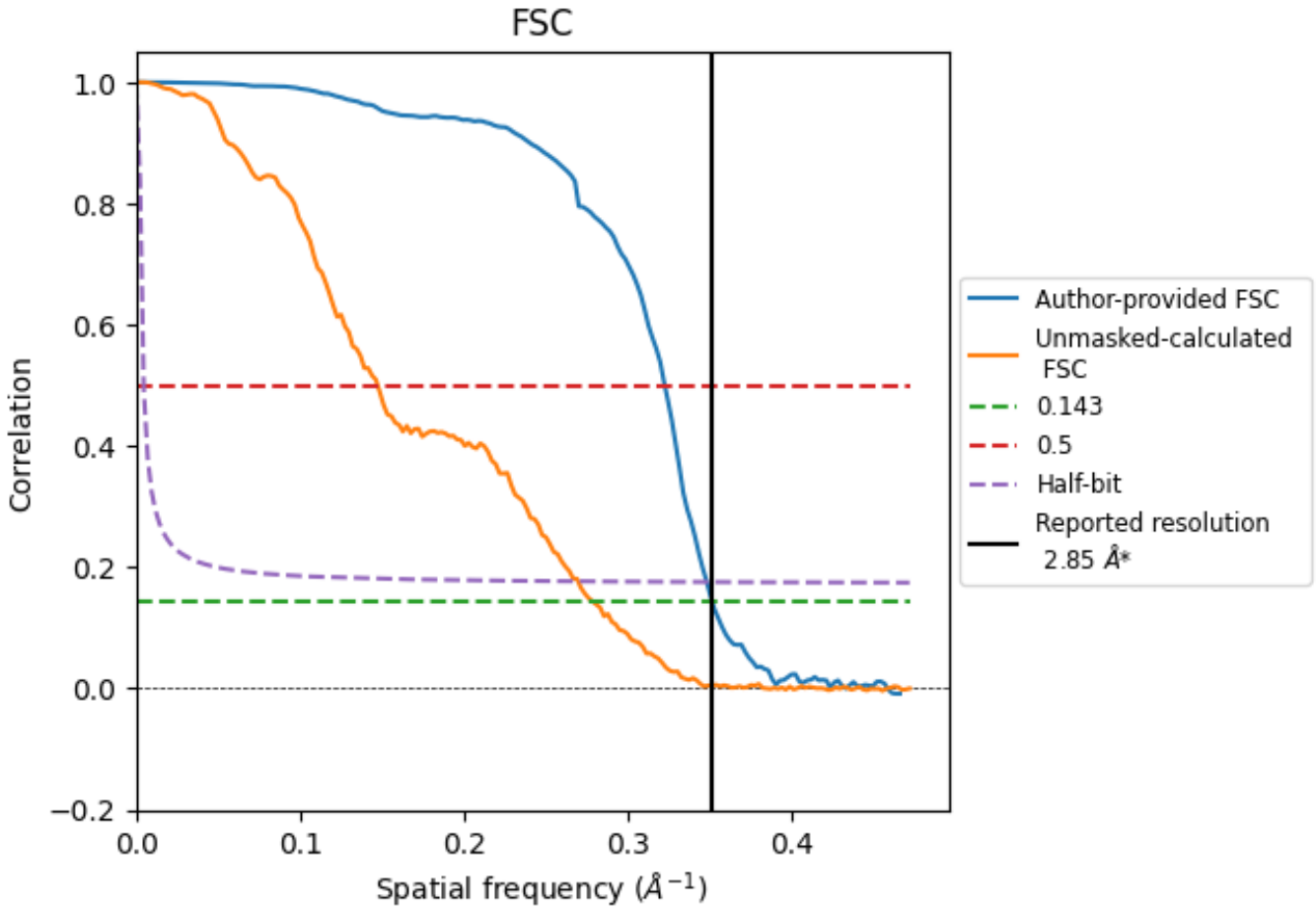


*Reported resolution corresponds to spatial frequency of 0.351 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.351 Å^{-1}

8.2 Resolution estimates (i)

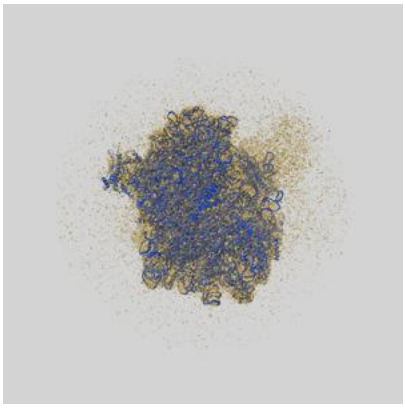
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.85	-	-
Author-provided FSC curve	2.85	3.10	2.87
Unmasked-calculated*	3.59	6.79	3.71

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.59 differs from the reported value 2.85 by more than 10 %

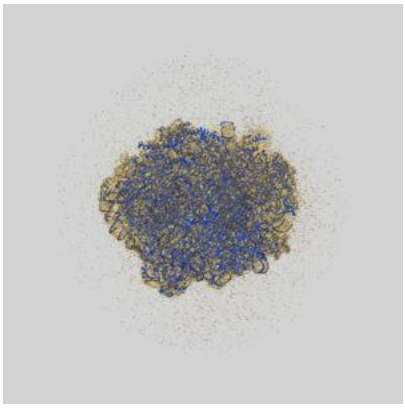
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-73543 and PDB model 9YWB. Per-residue inclusion information can be found in section 3 on page 15.

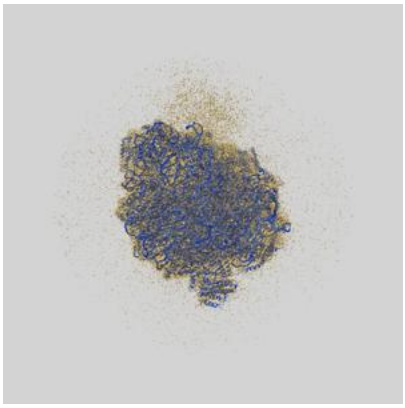
9.1 Map-model overlay



X



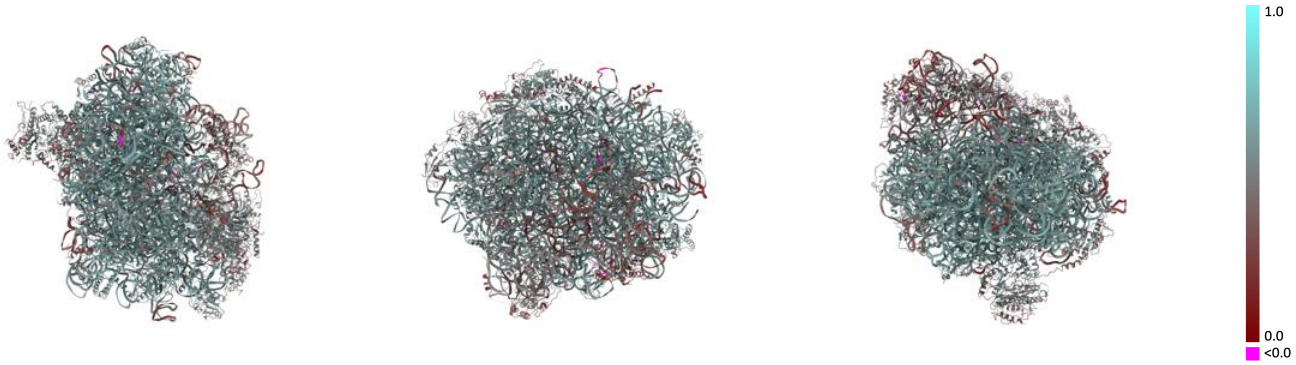
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4 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.

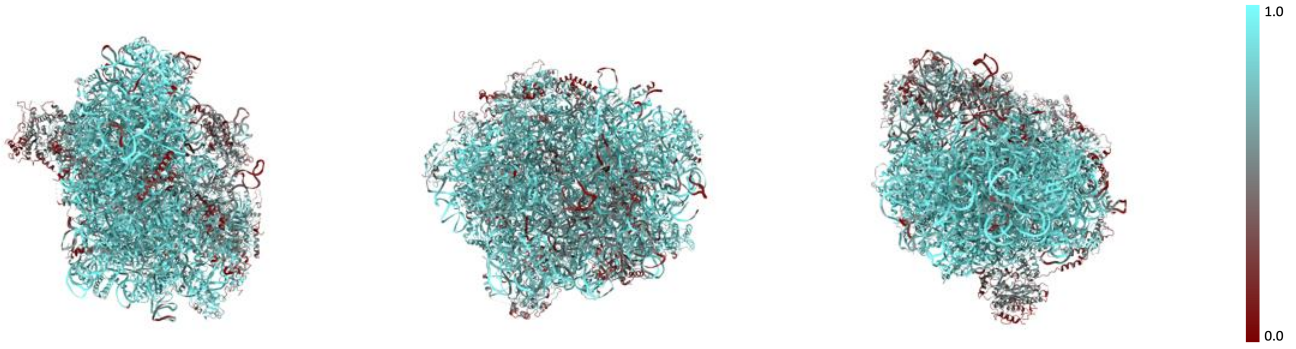
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

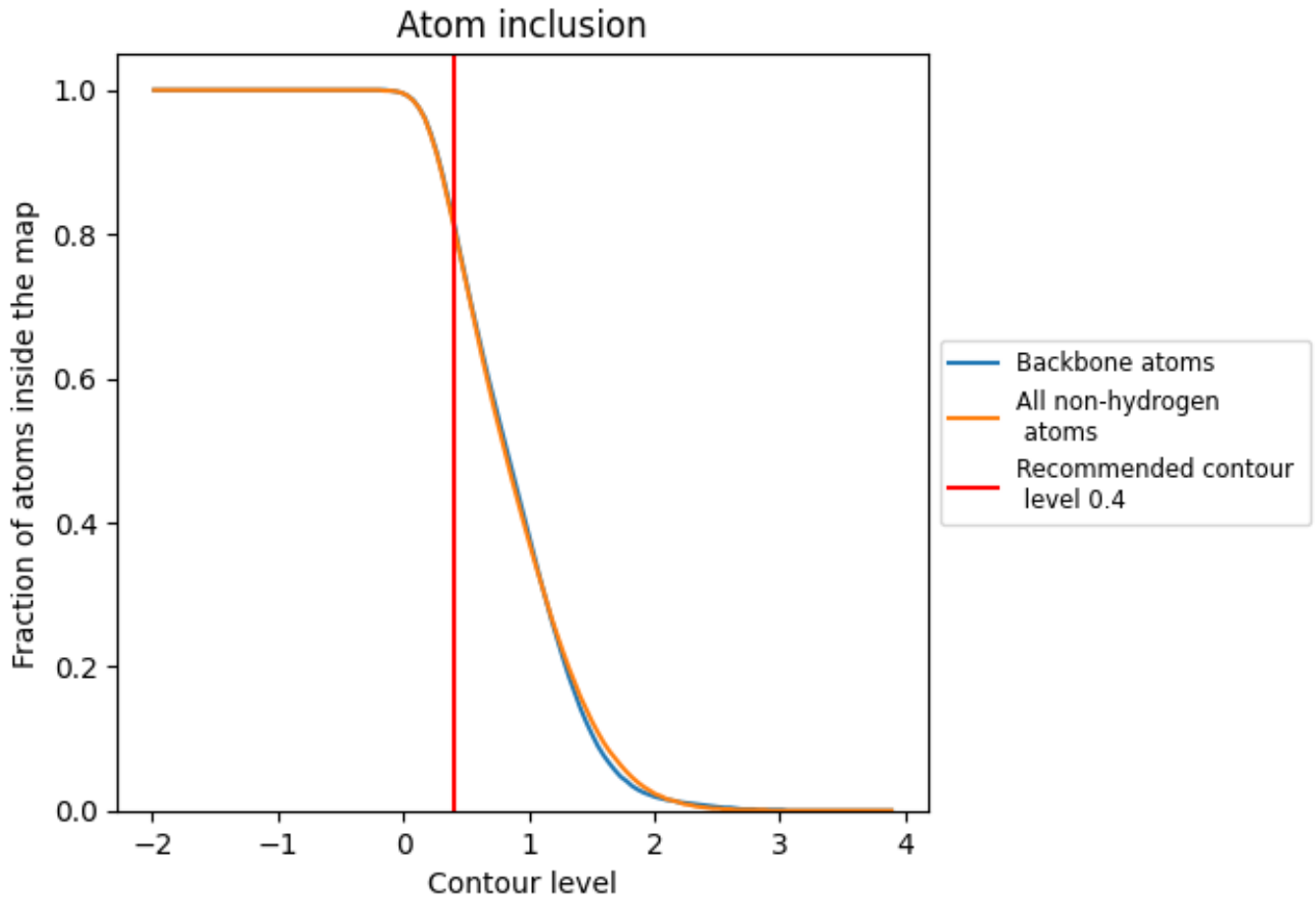
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.4).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8150	0.5420
1	0.8830	0.5560
2	0.8670	0.5010
3	0.9530	0.6030
4	0.4170	0.4550
5	0.6090	0.4540
A	0.9300	0.6080
B	0.9230	0.5950
C	0.8810	0.5840
D	0.5440	0.4100
E	0.8210	0.5560
F	0.8780	0.5780
G	0.8250	0.5480
H	0.8800	0.5760
I	0.3370	0.4470
J	0.6670	0.4760
K	0.5630	0.4120
L	0.8540	0.5650
Lr	0.7870	0.5290
M	0.8930	0.5850
N	0.9150	0.6000
O	0.9450	0.6110
P	0.8550	0.5750
Q	0.8370	0.5700
R	0.8870	0.5810
S	0.8590	0.5530
T	0.5890	0.4370
U	0.7120	0.4700
V	0.9060	0.5900
W	0.7690	0.5260
X	0.9040	0.5870
Y	0.8790	0.5800
Z	0.8710	0.5610
a	0.8680	0.5800
b	0.6090	0.4810



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Chain	Atom inclusion	Q-score
c	0.7920	0.5420
d	0.8510	0.5780
e	0.8870	0.5880
f	0.9440	0.6110
g	0.8740	0.5790
h	0.9000	0.5910
i	0.8280	0.5580
j	0.9600	0.6190
k	0.7480	0.5220
l	0.9540	0.6180
m	0.7160	0.5130
n	0.4800	0.4520
o	0.6030	0.5090
p	0.8700	0.5840
q	0.7550	0.5540
r	0.8690	0.5740
s	0.3160	0.3040
t	0.4820	0.4200
u	0.7500	0.5310
x	0.7520	0.5250
y	0.7870	0.5430
z	0.6200	0.5070