



## Full wwPDB EM Validation Report ⓘ

Mar 27, 2025 – 12:39 PM EDT

PDB ID : 9NL5  
EMDB ID : EMD-40921  
Title : E. coli pre-elongation complex without an A-site tRNA with EQ2-EttA in Hydrolytic 1 conformation  
Authors : Singh, S.; Hunt, J.F.  
Deposited on : 2025-03-02  
Resolution : 3.00 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev117  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.41.4

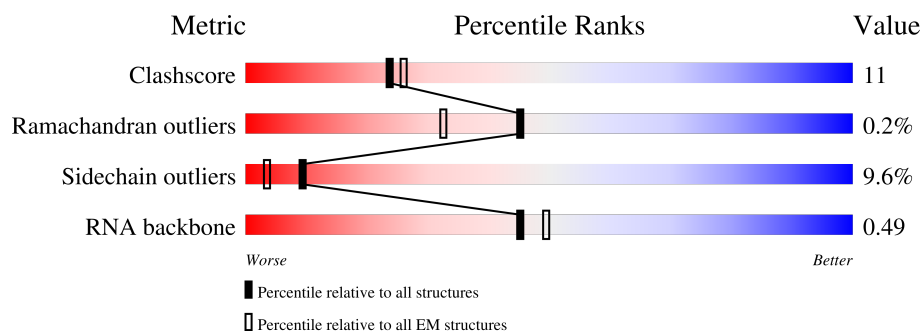
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.00 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.





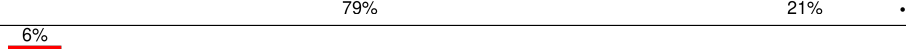
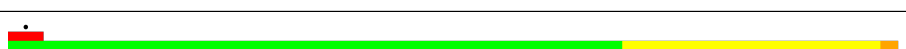



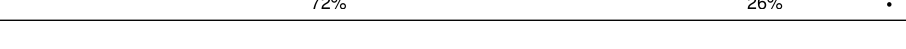



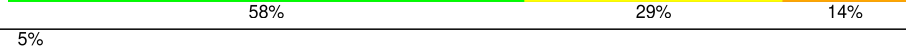

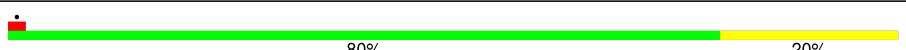


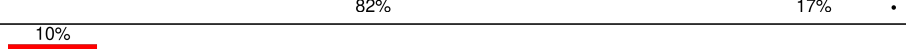







Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	1	220	
2	13	142	
3	14	122	
4	15	143	
5	16	136	
6	17	120	
7	18	116	



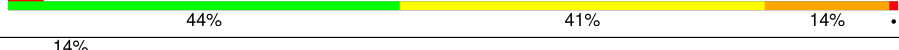
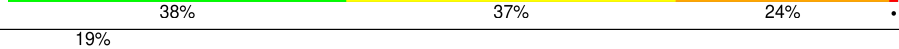
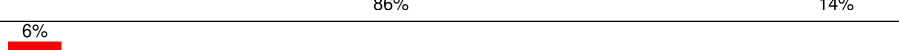
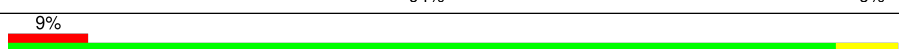
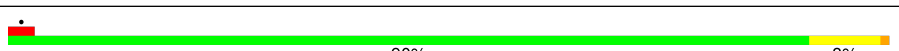
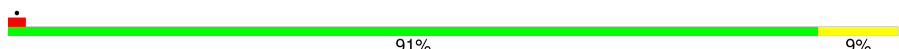

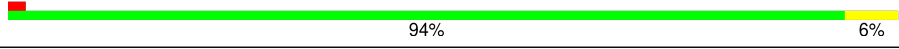

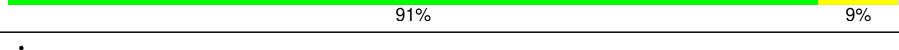
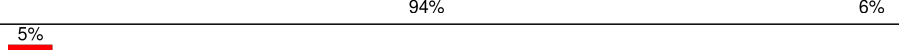

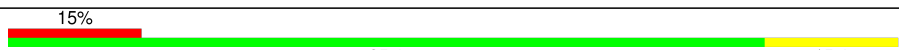



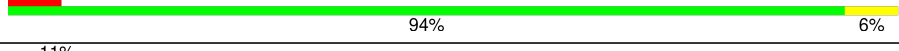

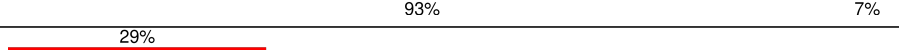
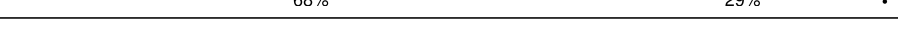


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Mol	Chain	Length	Quality of chain
8	19	114	
9	2	271	
10	20	117	
11	21	103	
12	22	110	
13	23	93	
14	24	102	
15	25	94	
16	27	85	
17	28	77	
18	29	63	
19	3	209	
20	30	58	
21	31	66	
22	32	56	
23	33	50	
24	34	46	
25	35	64	
26	36	38	
27	4	201	
28	5	177	
29	6	176	
30	9	149	
31	E	551	
32	M	9	

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Mol	Chain	Length	Quality of chain
33	R1	2903	
34	R2	119	
35	R3	1531	
36	T	76	
37	sb	218	
38	sc	206	
39	sd	205	
40	se	157	
41	sf	100	
42	sg	151	
43	sh	129	
44	si	127	
45	sj	98	
46	sk	116	
47	sl	123	
48	sm	112	
49	sn	100	
50	so	88	
51	sp	82	
52	sq	80	
53	sr	65	
54	ss	79	
55	st	85	
56	su	65	

## 2 Entry composition [i](#)

There are 60 unique types of molecules in this entry. The entry contains 149888 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Large ribosomal subunit protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	220	Total	C	N	O	S	0	0
			1353	804	270	277	2		

- Molecule 2 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	13	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 3 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	14	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 4 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	15	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 5 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	16	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 6 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	17	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 7 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	18	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 8 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	19	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 9 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	2	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 10 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	20	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 11 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	21	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 12 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	22	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 13 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	23	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 14 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	24	102	Total	C	N	O		
			779	492	146	141	0	0

- Molecule 15 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	25	94	Total	C	N	O	S		
			753	479	137	134	3	0	0

- Molecule 16 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	27	85	Total	C	N	O	S		
			642	396	130	114	2	0	0

- Molecule 17 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	28	77	Total	C	N	O	S		
			625	388	129	106	2	0	0

- Molecule 18 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	29	63	Total	C	N	O	S		
			509	313	99	95	2	0	0

- Molecule 19 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	3	209	Total	C	N	O	S		
			1565	979	288	294	4	0	0

- Molecule 20 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	30	58	Total	C	N	O	S		
			449	281	87	79	2	0	0

- Molecule 21 is a protein called Large ribosomal subunit protein bL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	31	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 22 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	32	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 23 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	33	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 24 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	34	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 25 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	35	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 26 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	36	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 27 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	4	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 28 is a protein called 50S ribosomal protein L5.



Mol	Chain	Residues	Atoms					AltConf	Trace
28	5	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 29 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	6	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 30 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	9	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 31 is a protein called EttA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	E	551	Total	C	N	O	S	0	0
			4352	2740	773	828	11		

- Molecule 32 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	M	9	Total	C	N	O	P	0	0
			193	87	37	60	9		

- Molecule 33 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	R1	2903	Total	C	N	O	P	0	0
			62318	27801	11467	20148	2902		

- Molecule 34 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	R2	119	Total	C	N	O	P	0	0
			2546	1135	466	827	118		

- Molecule 35 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	R3	1531	Total	C	N	O	P	0	0
			32850	14652	6028	10640	1530		

- Molecule 36 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	T	76	Total	C	N	O	P	0	0
			1621	724	295	527	75		

- Molecule 37 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	sb	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 38 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	sc	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 39 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	sd	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 40 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	se	157	Total	C	N	O	S	0	0
			1156	719	218	213	6		

- Molecule 41 is a protein called 30S ribosomal protein S6, non-modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	sf	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 42 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	sg	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 43 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	sh	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 44 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	si	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 45 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	sj	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 46 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	sk	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 47 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	sl	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 48 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	sm	112	Total	C	N	O	S	0	0
			867	537	173	154	3		

- Molecule 49 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	sn	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 50 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	so	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 51 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	sp	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 52 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	sq	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 53 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	sr	65	Total	C	N	O	S	0	0
			529	336	97	95	1		

- Molecule 54 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	ss	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 55 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	st	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 56 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	su	65	Total	C	N	O	S	0	0
			544	335	117	91	1		

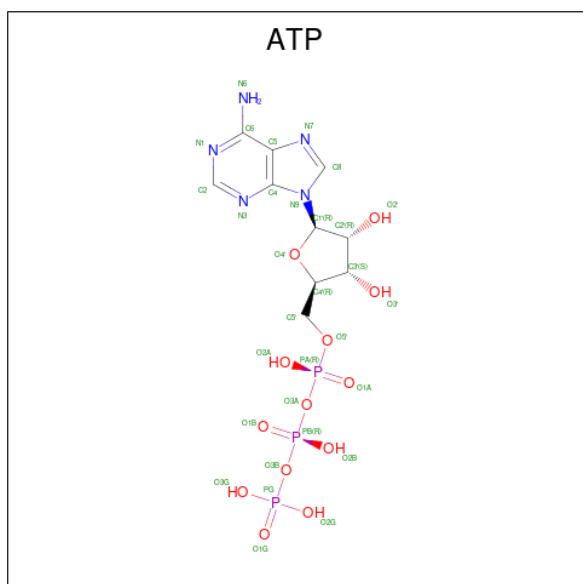
- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	32	1	Total	Mg	0
			1	1	
57	33	1	Total	Mg	0
			1	1	
57	R1	83	Total	Mg	0
			83	83	
57	R2	1	Total	Mg	0
			1	1	
57	R3	38	Total	Mg	0
			38	38	
57	sn	1	Total	Mg	0
			1	1	

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
58	36	1	Total	Zn	0
			1	1	

- Molecule 59 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



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

- Molecule 60 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
60	E	2	Total	Na	0
			2	2	

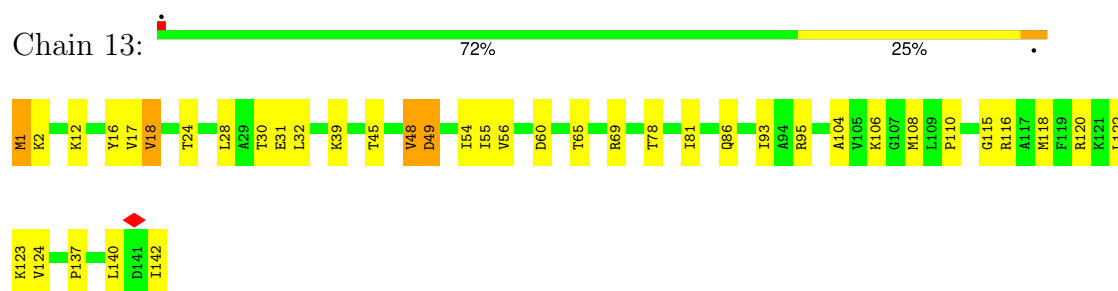
### 3 Residue-property plots

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

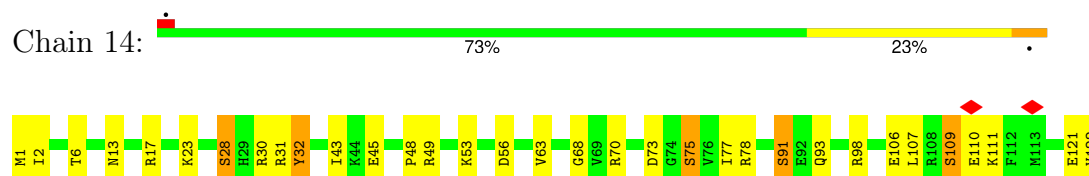
- Molecule 1: Large ribosomal subunit protein uL1



- Molecule 2: Large ribosomal subunit protein uL13



- Molecule 3: 50S ribosomal protein L14



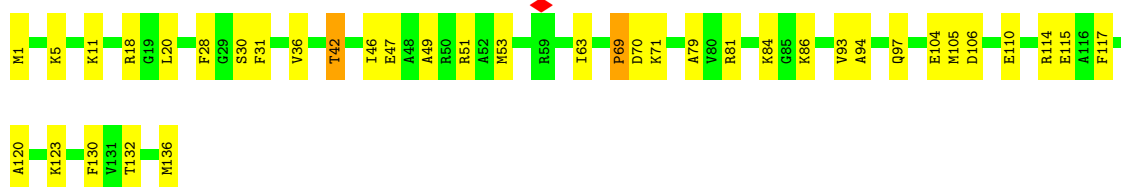
- Molecule 4: 50S ribosomal protein L15

Chain 15: 



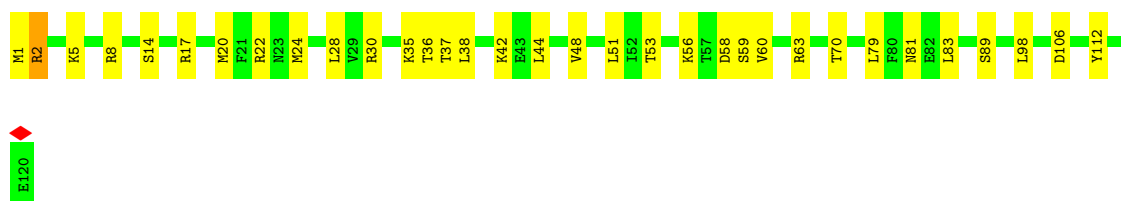
- Molecule 5: 50S ribosomal protein L16

Chain 16: 



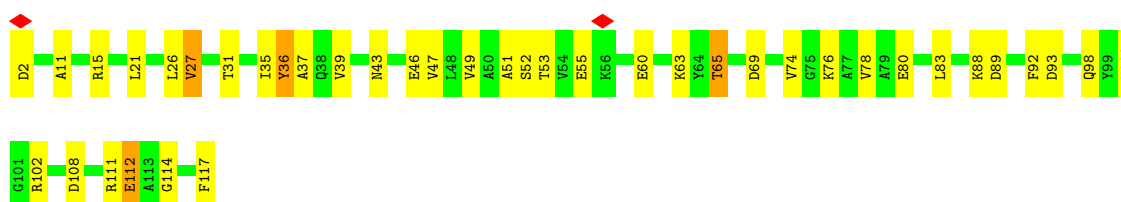
- Molecule 6: Large ribosomal subunit protein bL17

Chain 17: 



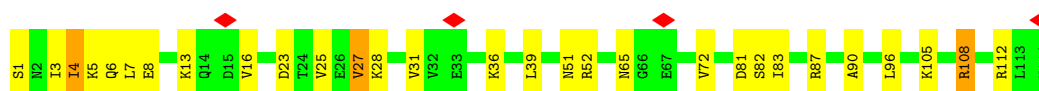
- Molecule 7: Large ribosomal subunit protein uL18

Chain 18: 



- Molecule 8: 50S ribosomal protein L19

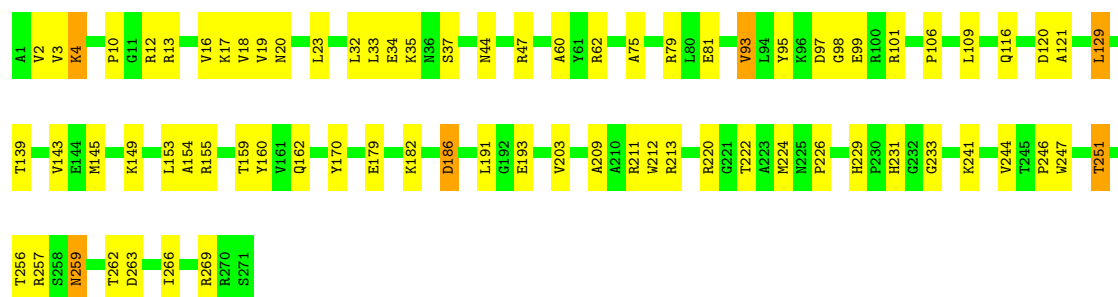
Chain 19: 




- Molecule 9: 50S ribosomal protein L2

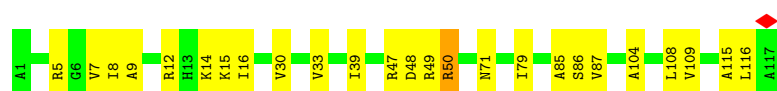


Chain 2:  72% 26% .



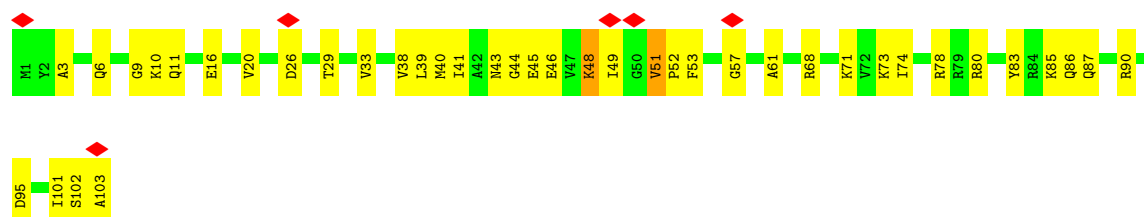
- Molecule 10: Large ribosomal subunit protein bL20

Chain 20:  79% 21% .



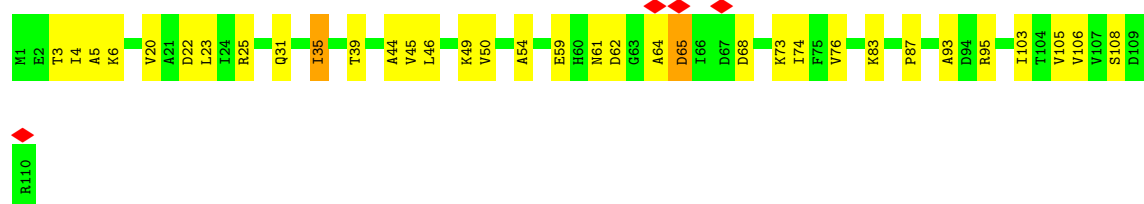
- Molecule 11: Large ribosomal subunit protein bL21

Chain 21:  6% 61% 37% .



- Molecule 12: Large ribosomal subunit protein uL22

Chain 22:  69% 29% .

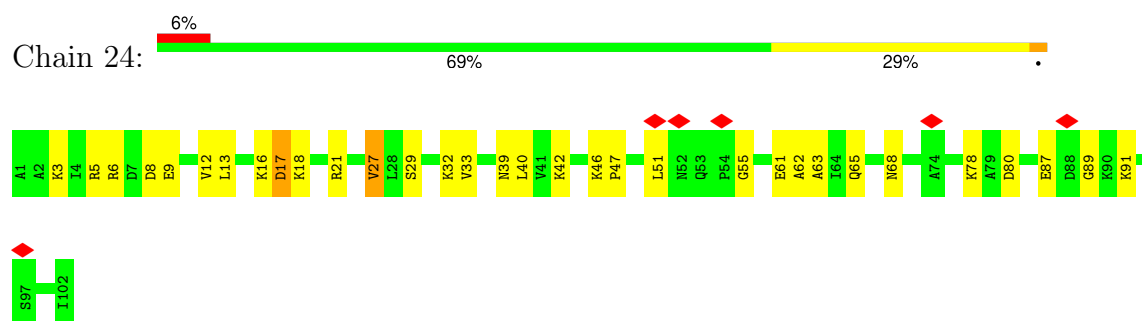


- Molecule 13: Large ribosomal subunit protein uL23

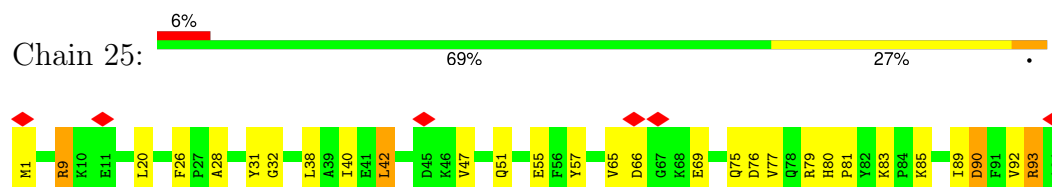
Chain 23:  72% 27% .



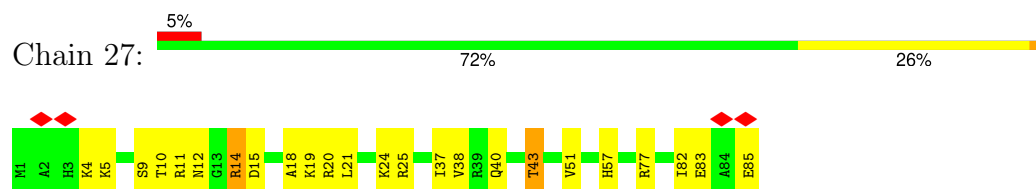
- Molecule 14: Large ribosomal subunit protein uL24



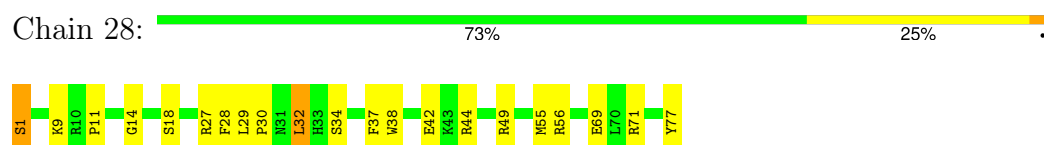
- Molecule 15: Large ribosomal subunit protein bL25



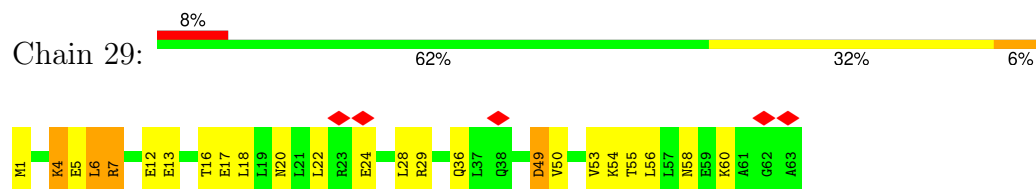
- Molecule 16: Large ribosomal subunit protein bL27



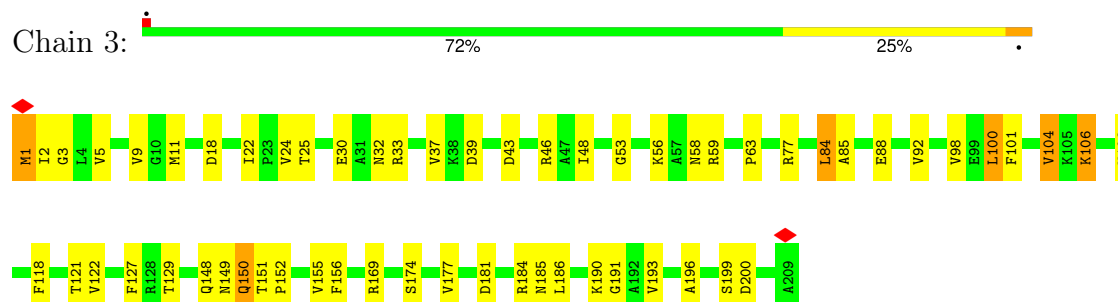
- Molecule 17: 50S ribosomal protein L28



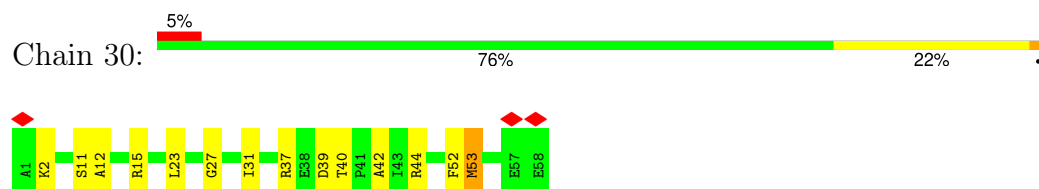
- Molecule 18: Large ribosomal subunit protein uL29



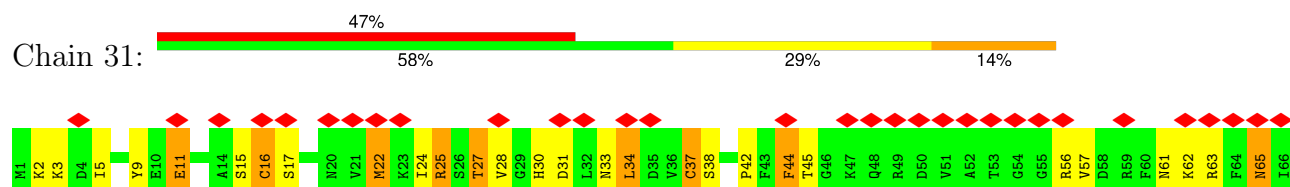
- Molecule 19: 50S ribosomal protein L3



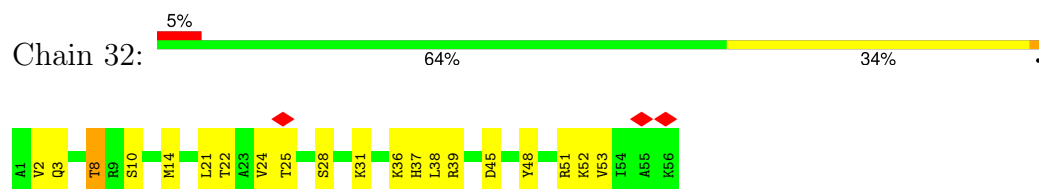
- Molecule 20: 50S ribosomal protein L30



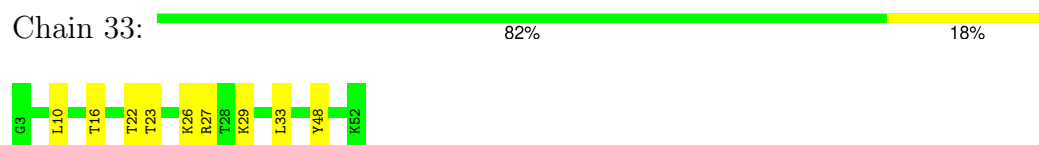
- Molecule 21: Large ribosomal subunit protein bL31



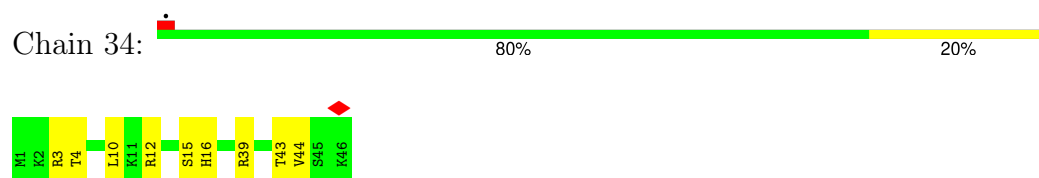
- Molecule 22: 50S ribosomal protein L32



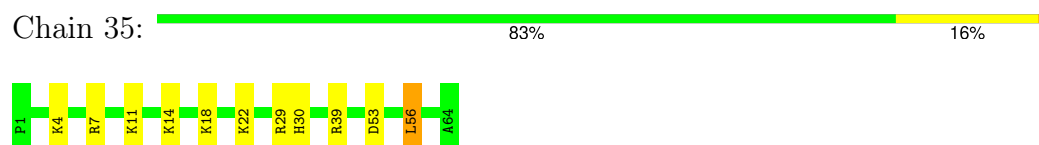
- Molecule 23: Large ribosomal subunit protein bL33



- Molecule 24: 50S ribosomal protein L34

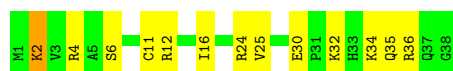


- Molecule 25: Large ribosomal subunit protein bL35

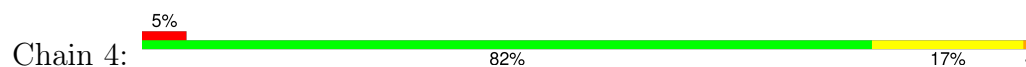


- Molecule 26: 50S ribosomal protein L36

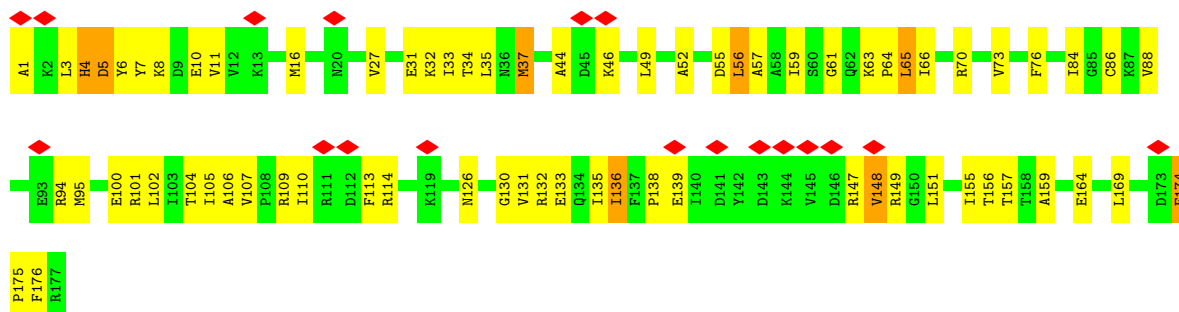




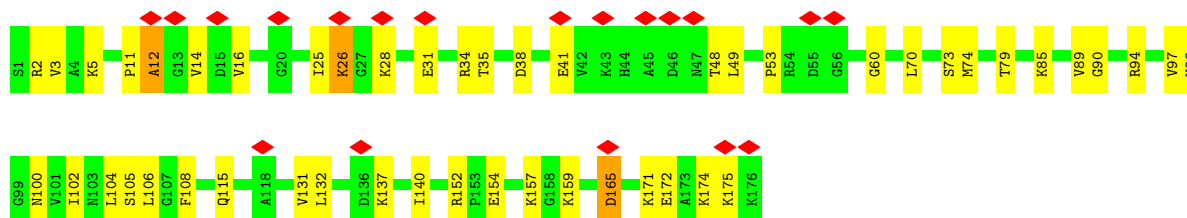
- Molecule 27: Large ribosomal subunit protein uL4



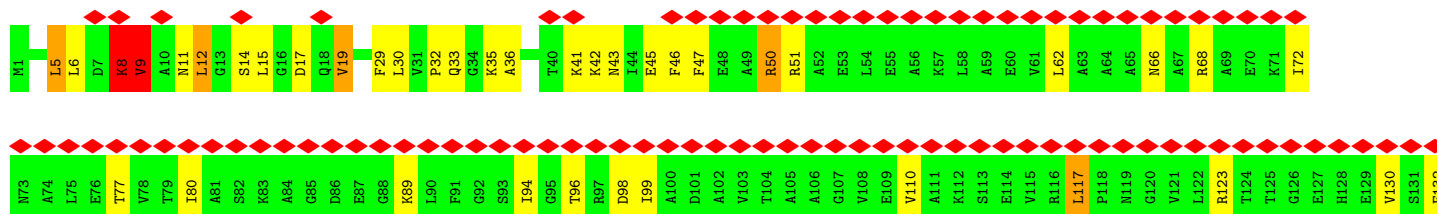
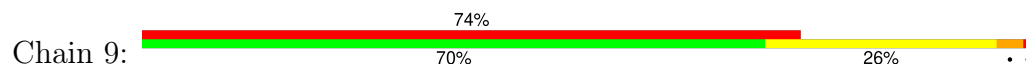
- Molecule 28: 50S ribosomal protein L5

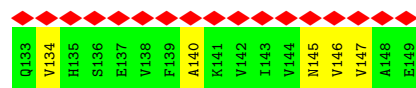


- Molecule 29: Large ribosomal subunit protein uL6

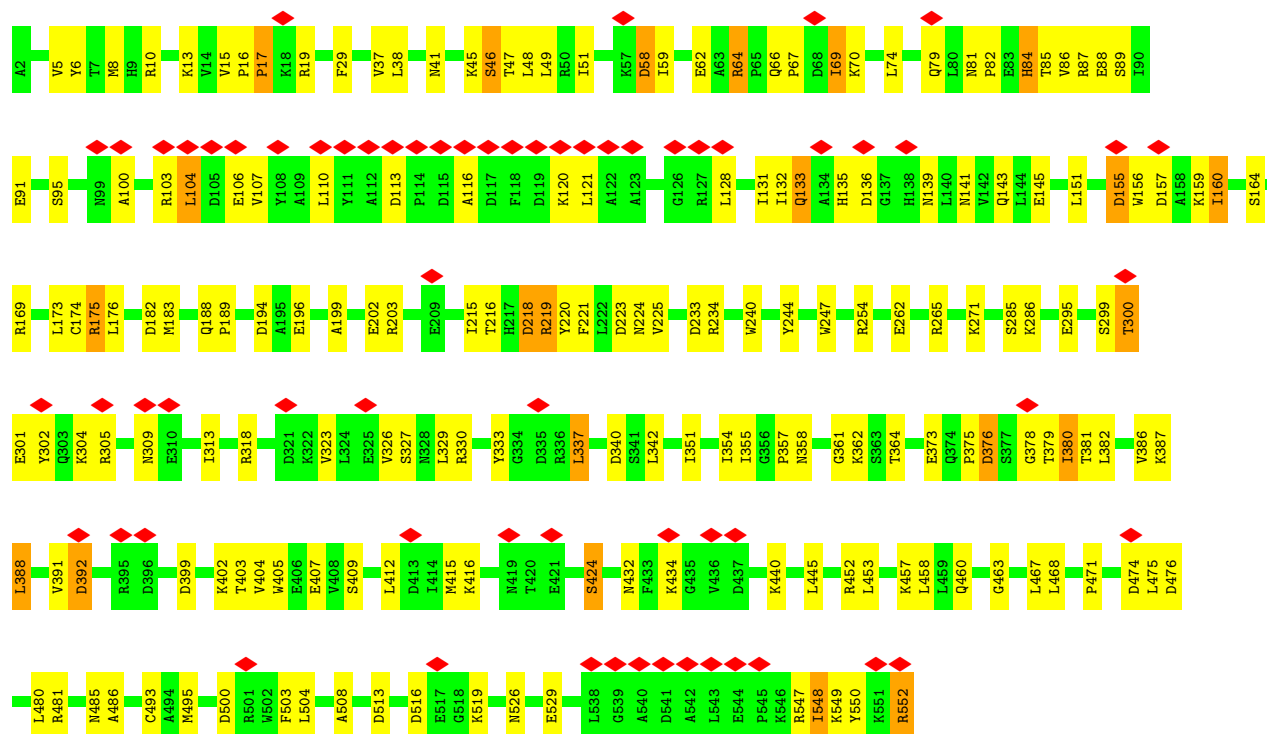


- Molecule 30: Large ribosomal subunit protein bL9

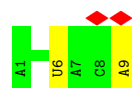
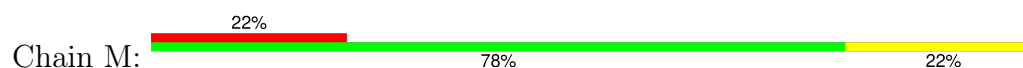




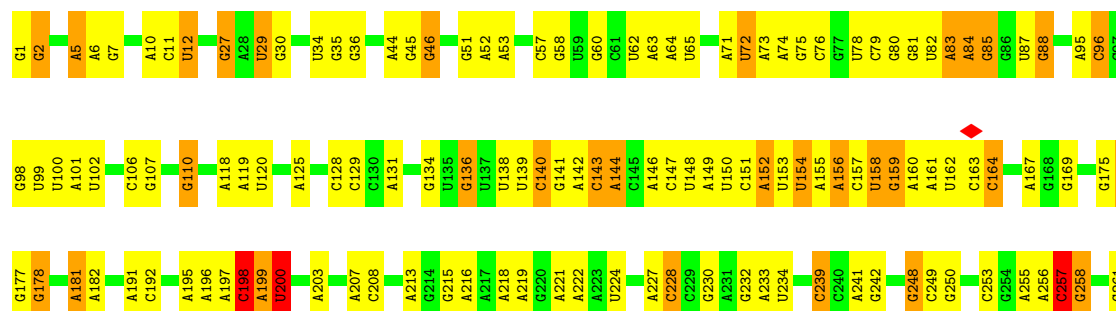
• Molecule 31: EttA



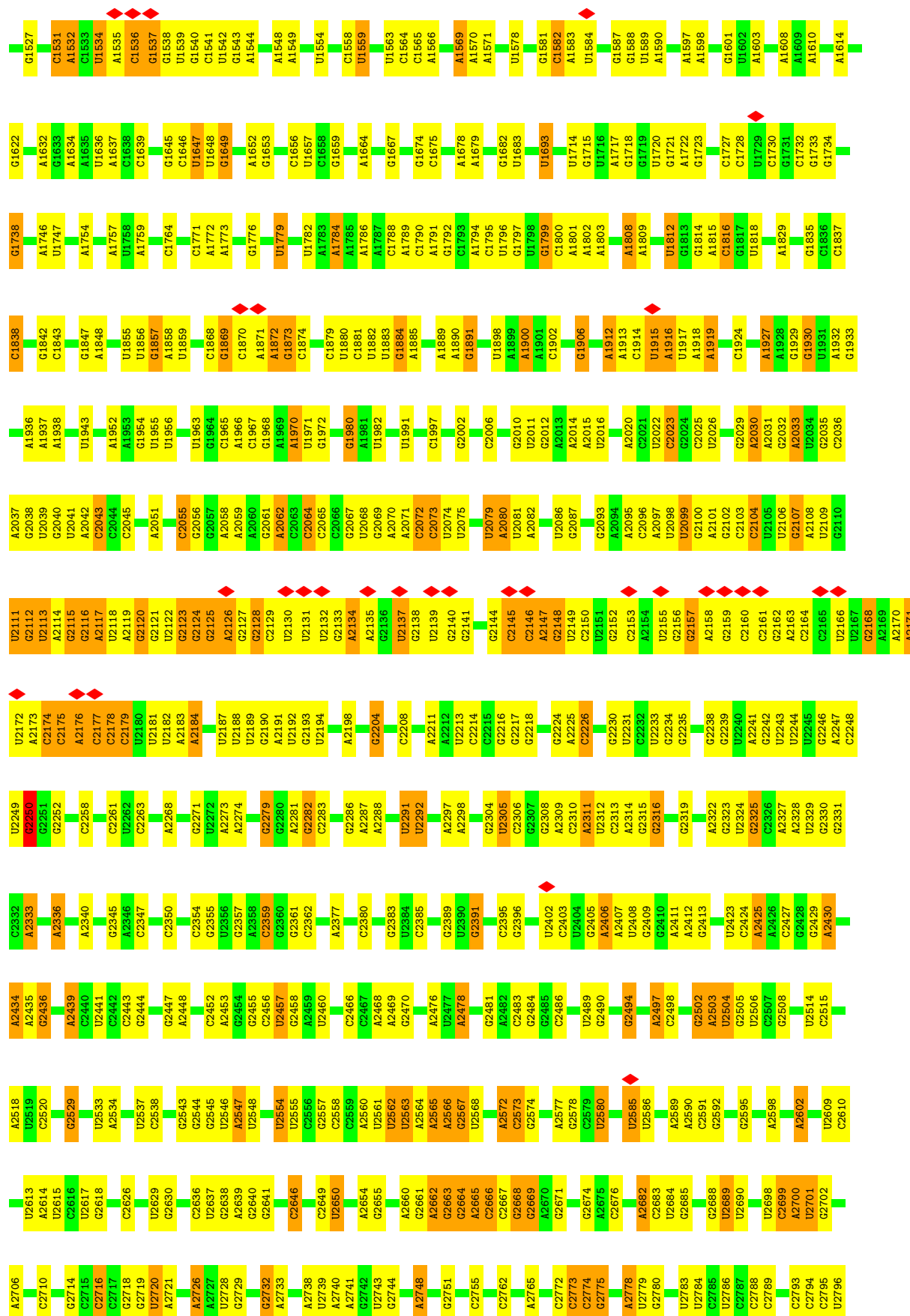
• Molecule 32: mRNA



• Molecule 33: 23S ribosomal RNA

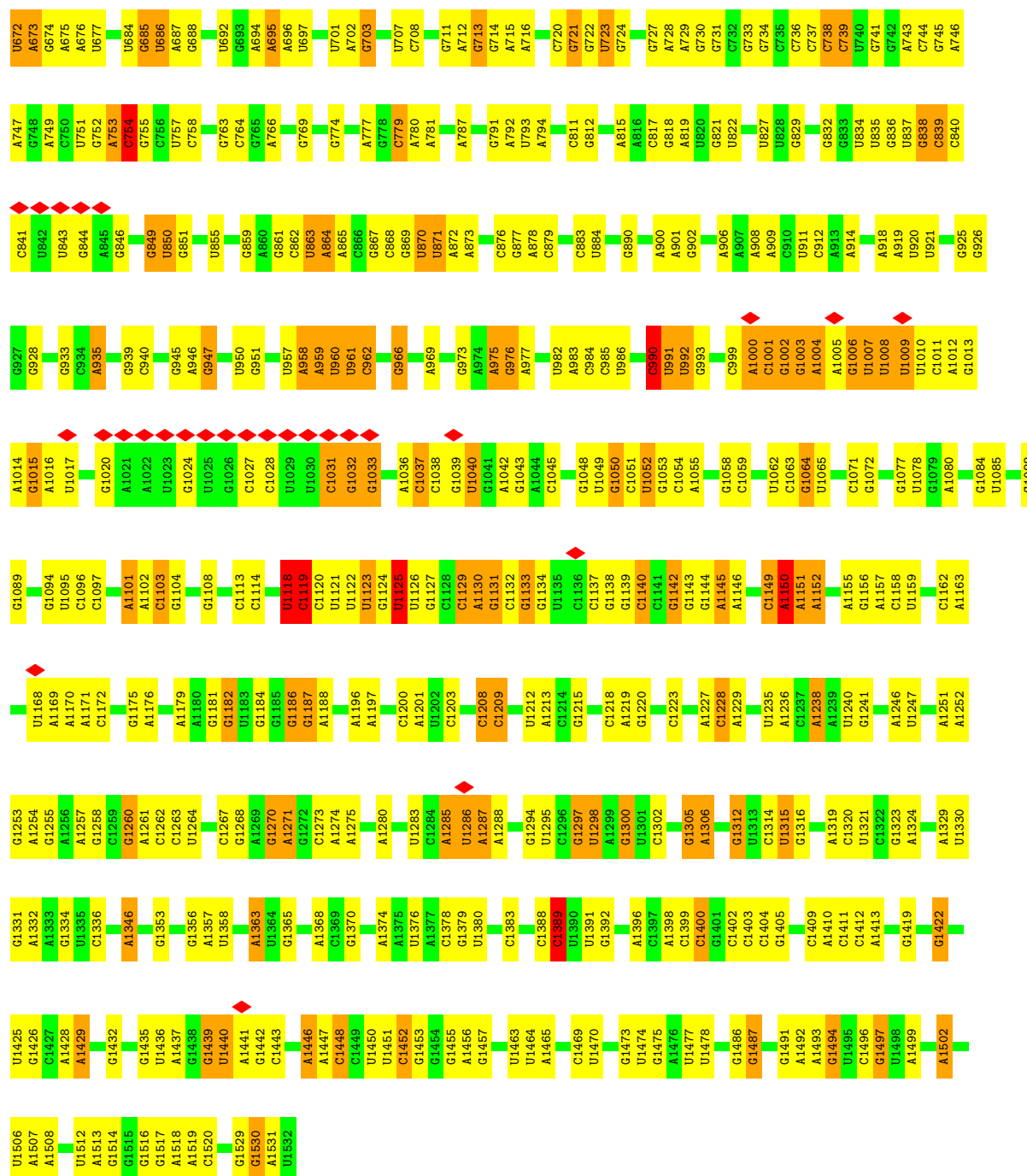




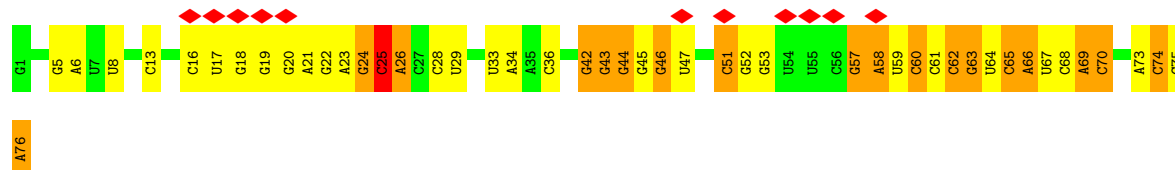




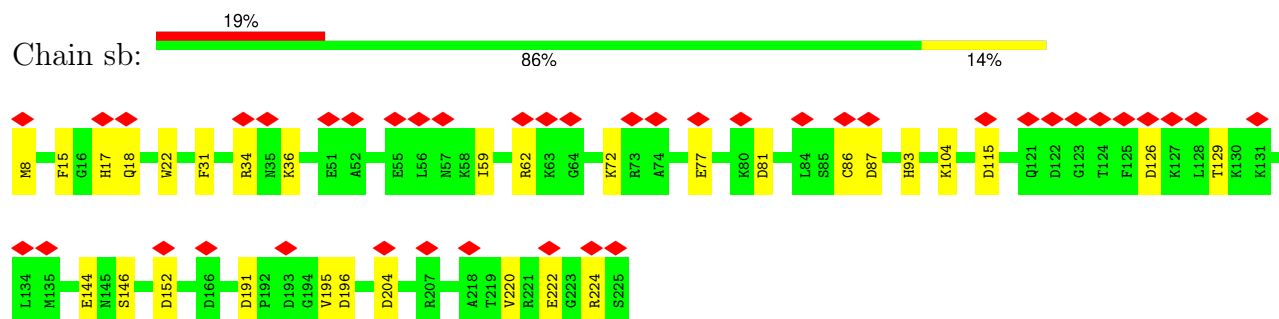




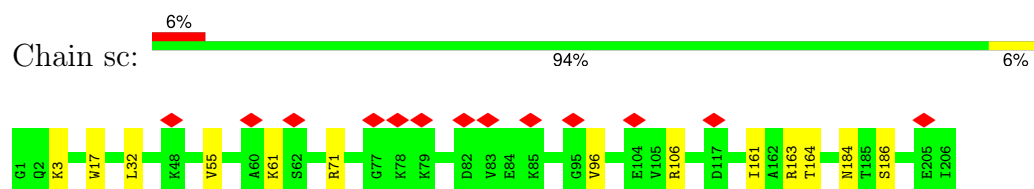
• Molecule 36: tRNA



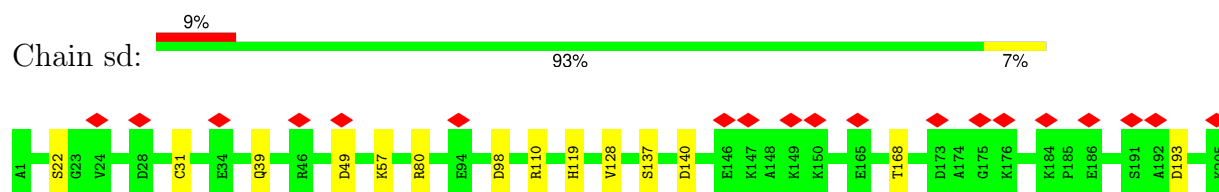
- Molecule 37: Small ribosomal subunit protein uS2



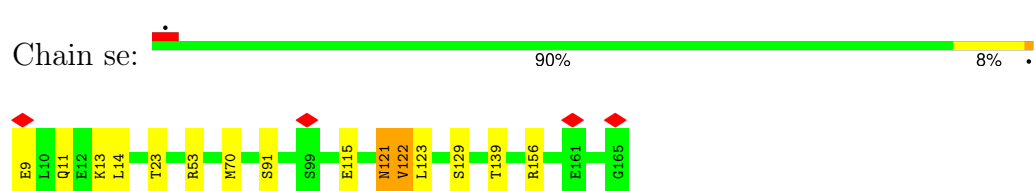
- Molecule 38: Small ribosomal subunit protein uS3



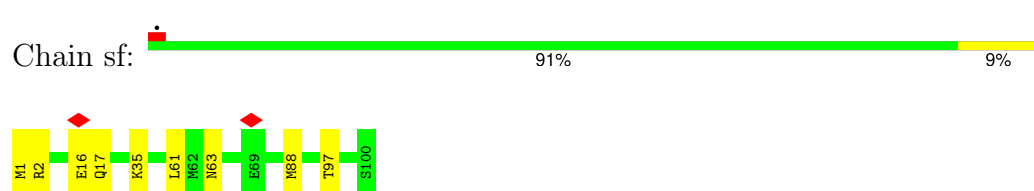
- Molecule 39: 30S ribosomal protein S4



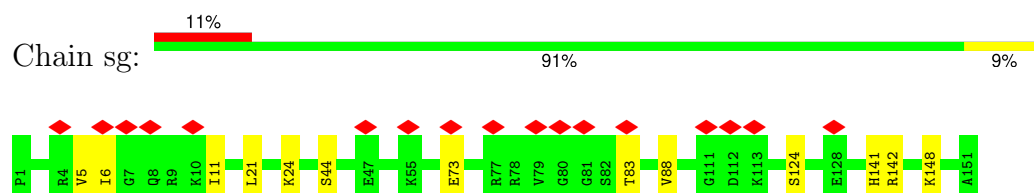
- Molecule 40: Small ribosomal subunit protein uS5



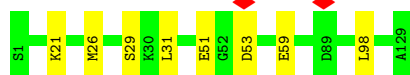
- Molecule 41: 30S ribosomal protein S6, non-modified isoform



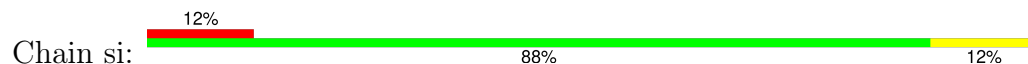
- Molecule 42: 30S ribosomal protein S7



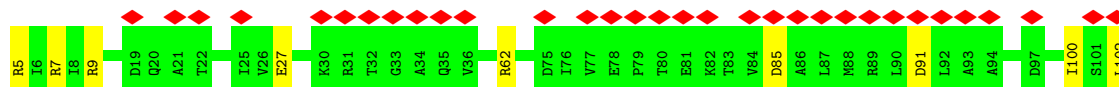
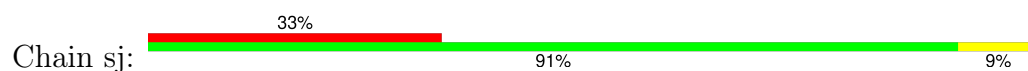
- Molecule 43: 30S ribosomal protein S8



- Molecule 44: Small ribosomal subunit protein uS9



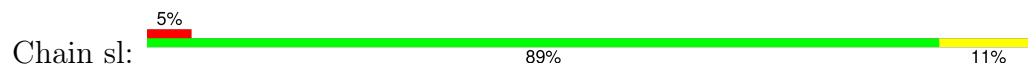
- Molecule 45: 30S ribosomal protein S10



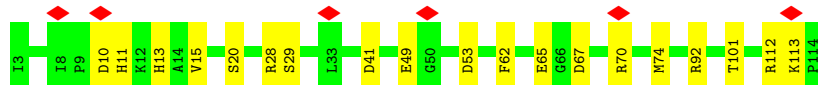
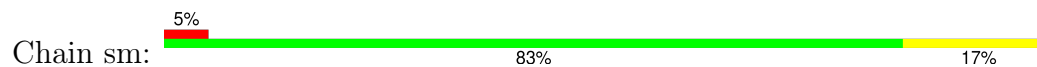
- Molecule 46: Small ribosomal subunit protein uS11



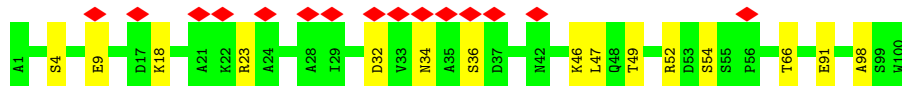
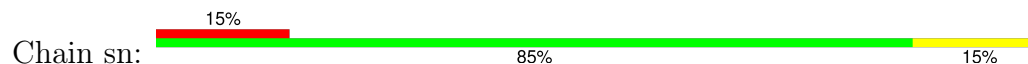
- Molecule 47: Small ribosomal subunit protein uS12



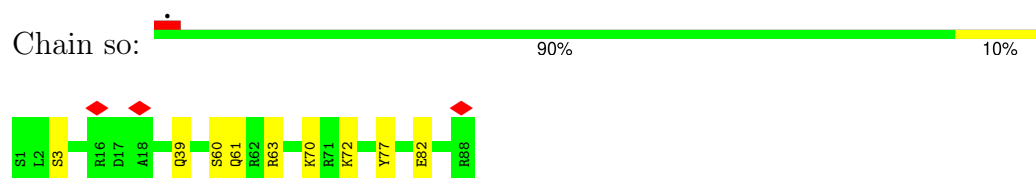
- Molecule 48: Small ribosomal subunit protein uS13



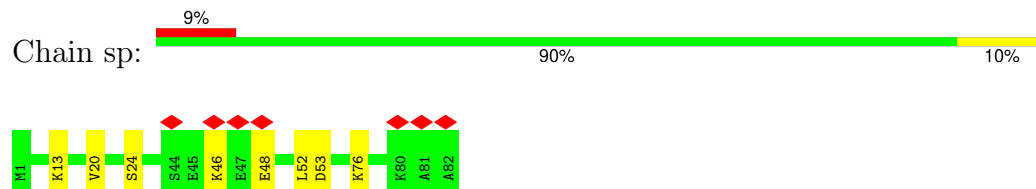
- Molecule 49: Small ribosomal subunit protein uS14



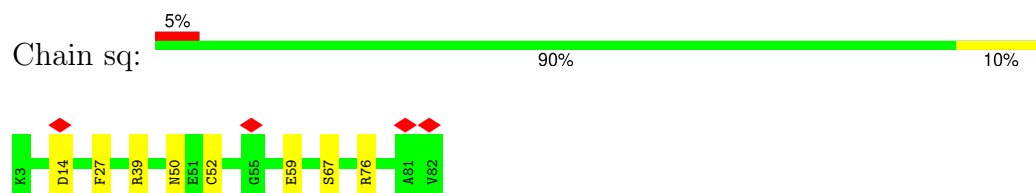
- Molecule 50: Small ribosomal subunit protein uS15



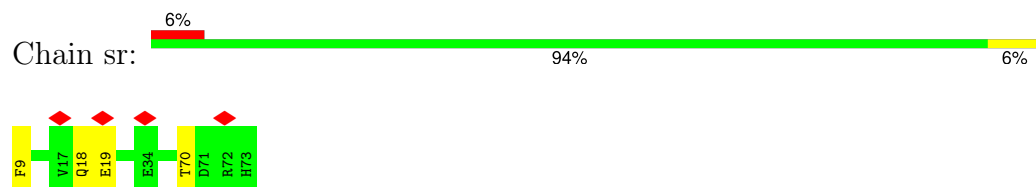
- Molecule 51: Small ribosomal subunit protein bS16



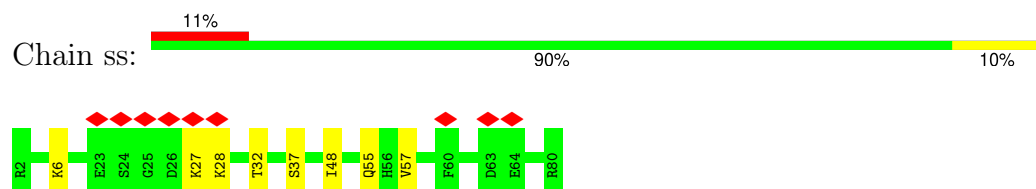
- Molecule 52: Small ribosomal subunit protein uS17



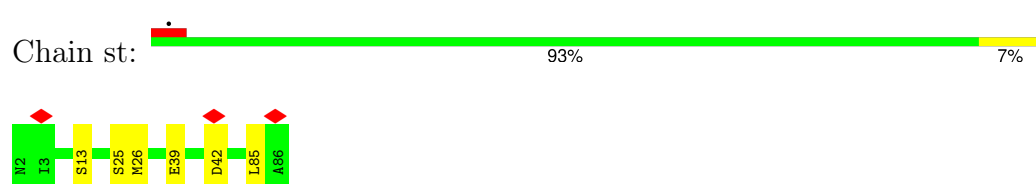
- Molecule 53: 30S ribosomal protein S18



- Molecule 54: 30S ribosomal protein S19

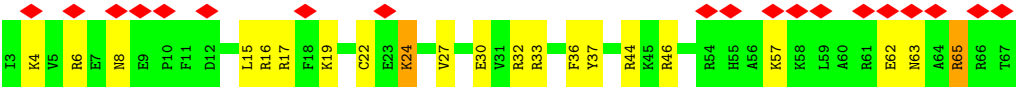


- Molecule 55: 30S ribosomal protein S20



- Molecule 56: Small ribosomal subunit protein bS21





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	86261	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	48	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	4.969	Depositor
Minimum map value	-2.374	Depositor
Average map value	0.024	Depositor
Map value standard deviation	0.204	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	335.04, 335.04, 335.04	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.047, 1.047, 1.047	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	1	0.26	0/1361	0.51	0/1796
2	13	0.38	0/1152	0.54	0/1551
3	14	0.39	0/947	0.62	0/1268
4	15	0.37	0/1054	0.59	0/1403
5	16	0.39	0/1093	0.57	0/1460
6	17	0.37	0/973	0.60	0/1301
7	18	0.31	0/902	0.57	0/1209
8	19	0.38	0/929	0.59	0/1242
9	2	0.43	0/2121	0.59	0/2852
10	20	0.43	0/960	0.53	0/1278
11	21	0.37	0/829	0.59	0/1107
12	22	0.34	0/864	0.56	0/1156
13	23	0.34	0/744	0.58	0/994
14	24	0.36	0/787	0.57	0/1051
15	25	0.33	0/766	0.50	0/1025
16	27	0.38	0/650	0.55	0/858
17	28	0.41	0/635	0.59	0/848
18	29	0.27	0/510	0.53	0/677
19	3	0.39	0/1586	0.57	0/2134
20	30	0.34	0/453	0.58	0/605
21	31	0.28	0/531	0.63	0/709
22	32	0.38	0/450	0.58	0/599
23	33	0.38	0/416	0.53	0/554
24	34	0.39	0/380	0.67	0/498
25	35	0.37	0/513	0.55	0/676
26	36	0.36	0/303	0.60	0/397
27	4	0.36	0/1571	0.54	0/2113
28	5	0.31	0/1434	0.56	0/1926
29	6	0.31	0/1343	0.57	1/1816 (0.1%)
30	9	0.29	0/1122	0.56	0/1515
31	E	0.31	0/4433	0.53	0/5983
32	M	0.43	0/216	0.72	0/334

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	R1	0.79	1/69797 (0.0%)	0.85	41/108890 (0.0%)
34	R2	0.56	0/2847	0.83	0/4440
35	R3	0.65	0/36782	0.88	55/57377 (0.1%)
36	T	0.49	0/1812	0.88	1/2824 (0.0%)
37	sb	0.29	0/1735	0.54	0/2338
38	sc	0.30	0/1651	0.55	0/2225
39	sd	0.31	0/1665	0.56	0/2227
40	se	0.35	0/1169	0.60	0/1573
41	sf	0.34	0/835	0.57	0/1128
42	sg	0.29	0/1195	0.56	0/1602
43	sh	0.34	0/989	0.53	0/1326
44	si	0.34	0/1034	0.74	2/1375 (0.1%)
45	sj	0.31	0/796	0.63	0/1077
46	sk	0.34	0/885	0.58	0/1195
47	sl	0.38	0/969	0.62	0/1300
48	sm	0.28	0/876	0.58	0/1172
49	sn	0.29	0/817	0.56	0/1088
50	so	0.32	0/722	0.58	0/964
51	sp	0.33	0/659	0.60	0/884
52	sq	0.37	0/657	0.63	0/881
53	sr	0.37	0/538	0.59	0/724
54	ss	0.31	0/652	0.55	0/877
55	st	0.29	0/671	0.47	0/888
56	su	0.35	0/550	0.76	0/728
All	All	0.64	1/162331 (0.0%)	0.79	100/242038 (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
13	23	0	1
29	6	0	1
30	9	0	1
31	E	0	1
40	se	0	1
47	sl	0	1
56	su	0	1
All	All	0	7

All (1) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	R1	528	A	N9-C4	-5.24	1.34	1.37

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	si	22	PRO	CA-N-CD	-8.37	99.78	111.50
35	R3	115	G	O5'-P-OP1	-8.10	98.41	105.70
35	R3	5	U	N1-C2-O2	7.87	128.31	122.80
35	R3	1119	C	C2-N1-C1'	7.84	127.42	118.80
35	R3	5	U	N3-C2-O2	-7.78	116.75	122.20
35	R3	470	C	C2-N1-C1'	7.75	127.33	118.80
35	R3	470	C	N1-C2-O2	7.63	123.48	118.90
33	R1	2668	G	O4'-C1'-N9	7.63	114.30	108.20
35	R3	1007	U	C2-N1-C1'	7.44	126.63	117.70
35	R3	4	U	C2-N1-C1'	7.37	126.55	117.70
33	R1	1313	U	C2-N1-C1'	7.30	126.46	117.70
35	R3	4	U	N3-C2-O2	-7.28	117.11	122.20
35	R3	5	U	C2-N1-C1'	7.25	126.41	117.70
33	R1	1109	C	N1-C2-O2	7.10	123.16	118.90
33	R1	1109	C	C2-N1-C1'	7.04	126.54	118.80
33	R1	687	C	N3-C2-O2	-6.86	117.10	121.90
35	R3	120	A	OP1-P-O3'	6.84	120.25	105.20
35	R3	1125	U	C2-N1-C1'	6.78	125.84	117.70
35	R3	4	U	N1-C2-O2	6.71	127.49	122.80
35	R3	402	G	O4'-C1'-N9	6.58	113.46	108.20
35	R3	470	C	N3-C2-O2	-6.41	117.41	121.90
35	R3	439	U	C2-N1-C1'	6.41	125.39	117.70
33	R1	955	U	N3-C2-O2	-6.35	117.75	122.20
33	R1	357	C	N3-C2-O2	-6.29	117.50	121.90
33	R1	512	G	O4'-C1'-N9	6.22	113.18	108.20
35	R3	1007	U	N1-C2-O2	6.21	127.14	122.80
35	R3	439	U	N1-C2-O2	6.20	127.14	122.80
33	R1	528	A	C2-N3-C4	-6.18	107.51	110.60
35	R3	1125	U	C5-C4-O4	-6.13	122.22	125.90
35	R3	552	U	N3-C2-O2	-6.12	117.91	122.20
33	R1	1313	U	N1-C2-O2	6.09	127.06	122.80
35	R3	962	C	C2-N1-C1'	6.04	125.44	118.80
29	6	11	PRO	CA-N-CD	-5.92	103.22	111.50
35	R3	1186	G	O4'-C1'-N9	5.90	112.92	108.20
35	R3	470	C	C6-N1-C2	-5.90	117.94	120.30
33	R1	2573	C	C2-N1-C1'	5.85	125.24	118.80
35	R3	1119	C	C6-N1-C1'	-5.84	113.79	120.80
35	R3	1439	G	O4'-C1'-N9	5.82	112.86	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	R3	1007	U	N3-C2-O2	-5.82	118.12	122.20
33	R1	2073	C	N3-C2-O2	-5.82	117.83	121.90
33	R1	88	G	C4-N9-C1'	5.80	134.04	126.50
33	R1	1313	U	N3-C2-O2	-5.79	118.14	122.20
33	R1	2073	C	C2-N1-C1'	5.74	125.11	118.80
33	R1	687	C	N1-C2-O2	5.71	122.33	118.90
33	R1	2104	C	C2-N1-C1'	5.67	125.04	118.80
35	R3	1389	C	C2-N1-C1'	5.67	125.03	118.80
33	R1	88	G	C8-N9-C1'	-5.66	119.64	127.00
33	R1	2815	C	C2-N1-C1'	5.62	124.98	118.80
35	R3	439	U	N3-C2-O2	-5.62	118.27	122.20
35	R3	114	U	P-O3'-C3'	-5.61	112.97	119.70
33	R1	2250	G	N3-C4-C5	5.60	131.40	128.60
33	R1	198	C	C6-N1-C2	-5.58	118.07	120.30
33	R1	164	C	C2-N1-C1'	5.52	124.88	118.80
33	R1	687	C	C6-N1-C2	-5.51	118.09	120.30
33	R1	164	C	N1-C2-O2	5.50	122.20	118.90
35	R3	288	A	O4'-C1'-N9	5.50	112.60	108.20
35	R3	1150	A	P-O3'-C3'	5.50	126.30	119.70
35	R3	620	C	N1-C2-O2	5.50	122.20	118.90
33	R1	1109	C	C6-N1-C1'	-5.47	114.23	120.80
33	R1	2580	U	N3-C2-O2	-5.47	118.37	122.20
33	R1	1857	G	O4'-C1'-N9	5.47	112.57	108.20
35	R3	552	U	N1-C2-O2	5.46	126.62	122.80
35	R3	1389	C	N3-C2-O2	-5.44	118.09	121.90
33	R1	748	G	O4'-C1'-N9	5.41	112.53	108.20
33	R1	148	U	C2-N1-C1'	5.41	124.19	117.70
35	R3	1389	C	N1-C2-O2	5.41	122.14	118.90
33	R1	1779	U	C5-C6-N1	-5.38	120.01	122.70
33	R1	695	G	O4'-C1'-N9	5.37	112.50	108.20
35	R3	1119	C	C5-C6-N1	5.36	123.68	121.00
33	R1	1005	C	C2-N1-C1'	5.35	124.68	118.80
35	R3	120	A	P-O3'-C3'	5.30	126.06	119.70
35	R3	379	C	N3-C2-O2	-5.29	118.20	121.90
36	T	25	C	O4'-C1'-N1	5.27	112.41	108.20
35	R3	509	A	N7-C8-N9	5.26	116.43	113.80
35	R3	990	C	N1-C2-O2	5.26	122.06	118.90
33	R1	1179	G	N3-C4-N9	5.24	129.14	126.00
35	R3	754	C	C2-N1-C1'	5.23	124.55	118.80
33	R1	257	C	C2-N1-C1'	5.20	124.52	118.80
33	R1	281	C	C2-N1-C1'	5.20	124.52	118.80
35	R3	289	G	O4'-C1'-N9	5.18	112.34	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	R3	1140	C	N1-C2-O2	5.18	122.01	118.90
35	R3	1125	U	N3-C4-O4	5.17	123.02	119.40
33	R1	200	U	N3-C2-O2	-5.16	118.59	122.20
33	R1	2282	G	O4'-C1'-N9	5.14	112.31	108.20
35	R3	1203	C	C2-N1-C1'	5.14	124.45	118.80
35	R3	1125	U	C6-N1-C1'	-5.12	114.03	121.20
35	R3	62	U	C2-N1-C1'	5.12	123.84	117.70
33	R1	281	C	N1-C2-O2	5.11	121.97	118.90
35	R3	231	U	N3-C2-O2	-5.10	118.63	122.20
35	R3	1118	U	C2-N1-C1'	5.10	123.83	117.70
35	R3	990	C	C2-N1-C1'	5.09	124.40	118.80
35	R3	107	G	O4'-C1'-N9	5.08	112.27	108.20
35	R3	470	C	C6-N1-C1'	-5.06	114.72	120.80
33	R1	1179	G	C4-N9-C1'	5.06	133.08	126.50
35	R3	620	C	C2-N1-C1'	5.06	124.36	118.80
33	R1	2457	U	C2-N1-C1'	5.04	123.75	117.70
35	R3	330	C	O4'-C1'-N1	5.04	112.23	108.20
44	si	53	LEU	CA-CB-CG	5.02	126.84	115.30
35	R3	379	C	C6-N1-C2	-5.01	118.30	120.30
33	R1	704	G	O4'-C1'-N9	5.00	112.20	108.20

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	23	37	ASP	Peptide
29	6	12	ALA	Peptide
30	9	8	LYS	Peptide
31	E	16	PRO	Peptide
40	se	121	ASN	Peptide
47	sl	86	VAL	Peptide
56	su	65	ARG	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1353	0	1159	45	0
2	13	1129	0	1162	26	0
3	14	938	0	1012	23	0
4	15	1045	0	1117	33	0
5	16	1074	0	1157	22	0
6	17	960	0	1000	24	0
7	18	892	0	923	21	0
8	19	917	0	965	17	0
9	2	2082	0	2157	51	0
10	20	947	0	1022	20	0
11	21	816	0	839	28	0
12	22	857	0	922	25	0
13	23	738	0	807	18	0
14	24	779	0	834	21	0
15	25	753	0	780	21	0
16	27	642	0	665	18	0
17	28	625	0	655	16	0
18	29	509	0	543	15	0
19	3	1565	0	1616	43	0
20	30	449	0	491	10	0
21	31	522	0	524	19	0
22	32	444	0	461	14	0
23	33	409	0	440	6	0
24	34	377	0	418	7	0
25	35	504	0	574	11	0
26	36	302	0	340	10	0
27	4	1552	0	1619	21	0
28	5	1410	0	1447	53	0
29	6	1323	0	1374	30	0
30	9	1111	0	1148	25	0
31	E	4352	0	4325	115	0
32	M	193	0	98	1	0
33	R1	62318	0	31345	845	0
34	R2	2546	0	1292	42	0
35	R3	32850	0	16533	492	0
36	T	1621	0	825	39	0
37	sb	1704	0	1732	0	0
38	sc	1624	0	1699	0	0
39	sd	1643	0	1710	0	0
40	se	1156	0	1199	0	0
41	sf	817	0	808	0	0
42	sg	1181	0	1240	0	0
43	sh	979	0	1034	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	si	1022	0	1070	0	0
45	sj	786	0	828	0	0
46	sk	869	0	878	0	0
47	sl	955	0	1019	0	0
48	sm	867	0	923	0	0
49	sn	805	0	847	0	0
50	so	714	0	737	0	0
51	sp	649	0	666	0	0
52	sq	648	0	691	0	0
53	sr	529	0	541	0	0
54	ss	637	0	665	0	0
55	st	665	0	714	0	0
56	su	544	0	579	0	0
57	32	1	0	0	0	0
57	33	1	0	0	0	0
57	R1	83	0	0	0	0
57	R2	1	0	0	0	0
57	R3	38	0	0	0	0
57	sn	1	0	0	0	0
58	36	1	0	0	0	0
59	E	62	0	24	6	0
60	E	2	0	0	0	0
All	All	149888	0	102193	2025	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 11.

All (2025) 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)
33:R1:136:G:N1	33:R1:142:A:H2	1.39	1.17
33:R1:136:G:N1	33:R1:142:A:C2	2.11	1.15
33:R1:156:A:C2	33:R1:169:G:N1	2.24	1.06
33:R1:156:A:H2	33:R1:169:G:N1	1.54	1.03
33:R1:2099:U:H3	33:R1:2190:G:H1	1.01	0.96
19:3:5:VAL:H	19:3:32:ASN:HD21	1.14	0.94
33:R1:2848:G:O2'	33:R1:2867:G:N2	1.99	0.93
33:R1:160:A:H8	33:R1:2217:G:H21	1.10	0.93
33:R1:290:U:H3	33:R1:350:G:H1	1.09	0.92
33:R1:1171:G:H1	33:R1:1176:U:H3	1.09	0.90
35:R3:119:A:H2	35:R3:287:U:H3	1.18	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:R1:1847:G:HO2'	33:R1:1848:A:H8	0.97	0.90
33:R1:2073:C:H5	33:R1:2436:G:H1	1.21	0.89
4:15:78:ARG:NH1	33:R1:627:A:OP1	2.07	0.87
33:R1:882:G:H1	33:R1:894:U:H3	1.20	0.87
6:17:2:ARG:HA	6:17:5:LYS:HD3	1.56	0.86
33:R1:2701:U:H5''	33:R1:2702:G:H5''	1.57	0.86
33:R1:805:G:N2	33:R1:829:A:OP1	2.09	0.86
33:R1:414:C:H5	33:R1:2409:G:H1	1.19	0.85
33:R1:1936:A:H2	33:R1:1943:U:H3	1.25	0.85
33:R1:2545:G:H21	33:R1:2565:A:H8	1.22	0.84
33:R1:2324:U:H3'	33:R1:2325:G:H5''	1.60	0.84
35:R3:406:G:H1	35:R3:436:C:H5	1.23	0.84
11:21:51:VAL:HG22	11:21:52:PRO:HD2	1.58	0.83
15:25:32:GLY:HA3	15:25:93:ARG:HB2	1.60	0.83
35:R3:71:A:N6	35:R3:99:C:O2'	2.12	0.82
4:15:30:THR:HG23	33:R1:810:U:H3	1.44	0.82
10:20:5:ARG:NH2	33:R1:585:G:N7	2.29	0.81
35:R3:332:G:O2'	35:R3:333:U:O2	1.98	0.81
3:14:121:GLU:HG2	3:14:122:VAL:HG23	1.62	0.81
1:1:181:ASP:H	1:1:184:LYS:HD2	1.45	0.80
12:22:59:GLU:HA	12:22:64:ALA:HA	1.64	0.79
6:17:17:ARG:NH2	33:R1:2002:G:OP1	2.14	0.79
33:R1:2602:A:H62	36:T:76:A:HO3'	1.26	0.79
16:27:14:ARG:NH1	33:R1:2279:G:N7	2.31	0.79
1:1:47:ASN:ND2	33:R1:2177:C:O2'	2.15	0.79
31:E:87:ARG:HB2	31:E:156:TRP:HB3	1.65	0.79
33:R1:947:A:HO2'	33:R1:984:A:H2	1.28	0.79
35:R3:990:C:H5	35:R3:1215:G:H1	1.28	0.79
6:17:2:ARG:HG2	33:R1:1653:G:H3'	1.65	0.78
19:3:169:ARG:HG2	33:R1:2773:C:H5'	1.66	0.78
1:1:211:LYS:HD3	33:R1:2177:C:H4'	1.65	0.78
33:R1:1045:C:H4'	33:R1:1046:A:H5''	1.63	0.78
33:R1:136:G:O6	33:R1:142:A:N1	2.16	0.78
33:R1:158:U:O2	33:R1:167:A:N6	2.17	0.77
35:R3:673:A:H2'	35:R3:674:G:C8	2.20	0.77
3:14:70:ARG:NH2	33:R1:2683:C:O2	2.18	0.77
24:34:43:THR:OG1	24:34:44:VAL:N	2.17	0.77
30:9:132:PHE:HB2	30:9:140:ALA:HB3	1.68	0.76
25:35:4:LYS:NZ	33:R1:253:C:OP2	2.19	0.76
36:T:53:G:N2	36:T:63:G:N7	2.34	0.76
34:R2:112:G:O2'	34:R2:113:C:O2	2.04	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:R3:999:C:H3'	35:R3:1000:A:H4'	1.67	0.75
21:31:11:GLU:HG2	21:31:25:ARG:HG2	1.67	0.75
35:R3:321:A:H2	35:R3:328:C:HO2'	1.32	0.75
33:R1:962:G:H21	33:R1:2250:G:H1	1.35	0.75
33:R1:2602:A:N6	36:T:76:A:HO3'	1.84	0.75
1:1:51:ASP:HB3	1:1:54:LYS:HG2	1.69	0.74
33:R1:76:C:H5	33:R1:110:G:H1	1.34	0.74
35:R3:962:C:H5	35:R3:973:G:H1	1.32	0.74
9:2:79:ARG:NH1	9:2:81:GLU:OE2	2.21	0.74
8:19:52:ARG:NH2	33:R1:2720:U:OP1	2.21	0.74
31:E:155:ASP:OD1	31:E:155:ASP:N	2.21	0.74
19:3:77:ARG:NH1	19:3:200:ASP:OD1	2.20	0.74
2:13:81:ILE:HD12	33:R1:2514:U:H5''	1.69	0.73
19:3:30:GLU:O	19:3:185:ASN:ND2	2.21	0.73
33:R1:199:A:O2'	33:R1:200:U:O2	2.06	0.73
33:R1:371:A:H2	33:R1:402:A:H62	1.37	0.73
3:14:17:ARG:HB2	3:14:45:GLU:HG2	1.71	0.73
21:31:2:LYS:HB3	21:31:5:ILE:HG12	1.68	0.73
33:R1:475:C:O2	33:R1:479:A:N6	2.21	0.73
22:32:14:MET:HE3	33:R1:2045:C:H5''	1.71	0.72
28:5:104:THR:HG22	28:5:105:ILE:HG23	1.70	0.72
33:R1:197:A:N6	33:R1:2430:A:O2'	2.22	0.72
33:R1:1802:A:H2'	33:R1:1803:A:C8	2.23	0.72
33:R1:1450:G:N2	33:R1:1452:G:O6	2.17	0.72
33:R1:1558:C:H4'	33:R1:1559:U:H5''	1.70	0.72
33:R1:2249:U:H3'	33:R1:2250:G:H5''	1.71	0.72
17:28:11:PRO:HB3	17:28:29:LEU:HD23	1.72	0.72
35:R3:456:A:H62	35:R3:476:U:H3	1.38	0.72
33:R1:2062:A:N6	33:R1:2503:A:N7	2.38	0.71
19:3:59:ARG:NH2	33:R1:2831:G:OP2	2.23	0.71
33:R1:704:G:O2'	33:R1:726:G:N2	2.20	0.71
28:5:147:ARG:HG2	28:5:148:VAL:H	1.56	0.71
33:R1:156:A:H2	33:R1:169:G:H1	0.80	0.71
3:14:109:SER:O	3:14:111:LYS:N	2.24	0.71
33:R1:695:G:H5''	33:R1:1380:G:H4'	1.71	0.71
35:R3:687:A:N6	35:R3:703:G:O2'	2.24	0.71
35:R3:1031:C:OP1	35:R3:1032:G:N2	2.24	0.70
35:R3:1118:U:H1'	35:R3:1179:A:C4	2.25	0.70
28:5:33:ILE:HG12	28:5:95:MET:HG2	1.72	0.70
35:R3:108:G:H5'	35:R3:109:A:H5''	1.73	0.70
31:E:309:ASN:OD1	31:E:485:ASN:ND2	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:R1:1326:U:HO2'	33:R1:2010:G:HO2'	1.37	0.70
35:R3:427:U:H5''	35:R3:428:G:H2'	1.72	0.70
35:R3:1363:A:O2'	35:R3:1365:G:N7	2.24	0.70
1:1:194:VAL:HG12	1:1:198:LYS:HE3	1.73	0.70
34:R2:5:U:H2'	34:R2:6:G:H8	1.56	0.70
35:R3:57:G:H1	35:R3:355:C:H5	1.38	0.70
33:R1:134:G:H1	33:R1:144:A:H2	1.38	0.70
17:28:18:SER:OG	33:R1:2080:A:O5'	2.09	0.70
33:R1:156:A:N1	33:R1:169:G:O6	2.25	0.70
35:R3:343:U:O2'	35:R3:346:G:O6	2.09	0.70
33:R1:2602:A:N6	36:T:76:A:O3'	2.20	0.69
33:R1:2682:A:H61	33:R1:2728:U:H1'	1.57	0.69
3:14:28:SER:OG	33:R1:2566:A:N1	2.24	0.69
34:R2:1:U:H2'	34:R2:2:G:H8	1.57	0.69
6:17:2:ARG:NE	6:17:2:ARG:O	2.25	0.69
28:5:3:LEU:HD22	28:5:100:GLU:HB2	1.73	0.69
33:R1:415:A:H62	33:R1:2408:U:H3	1.39	0.69
1:1:6:LYS:N	33:R1:2130:U:OP1	2.25	0.69
29:6:34:ARG:HH12	29:6:70:LEU:HD22	1.56	0.69
33:R1:2144:G:N3	33:R1:2148:G:N2	2.41	0.69
2:13:17:VAL:HG23	2:13:137:PRO:HB2	1.74	0.69
2:13:81:ILE:HG22	19:3:156:PHE:HB3	1.74	0.68
13:23:89:GLU:N	13:23:89:GLU:OE2	2.26	0.68
31:E:41:ASN:ND2	31:E:476:ASP:OD1	2.26	0.68
33:R1:2315:G:HO2'	33:R1:2316:G:H8	1.41	0.68
35:R3:1011:C:H2'	35:R3:1012:A:C8	2.29	0.68
6:17:53:THR:HA	6:17:56:LYS:HD2	1.74	0.68
33:R1:1906:G:N2	33:R1:1924:C:O2	2.18	0.68
30:9:29:PHE:O	30:9:33:GLN:HB2	1.93	0.68
21:31:28:VAL:HG22	28:5:139:GLU:HG3	1.76	0.68
33:R1:1417:C:O2'	33:R1:1587:G:O2'	2.10	0.68
12:22:83:LYS:HB3	12:22:95:ARG:HE	1.57	0.68
15:25:55:GLU:N	15:25:55:GLU:OE2	2.26	0.68
18:29:5:GLU:HB3	18:29:56:LEU:HD22	1.74	0.68
34:R2:5:U:H2'	34:R2:6:G:C8	2.29	0.68
35:R3:1356:G:H2'	35:R3:1357:A:C8	2.28	0.68
33:R1:413:C:O2'	33:R1:414:C:O2	2.09	0.68
18:29:13:GLU:OE2	18:29:60:LYS:NZ	2.27	0.68
28:5:70:ARG:NH1	33:R1:2298:A:OP1	2.27	0.68
33:R1:848:C:H2'	33:R1:849:A:H8	1.58	0.68
33:R1:1179:G:H5''	33:R1:1180:U:H6	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:27:15:ASP:OD1	33:R1:2263:C:N4	2.27	0.68
35:R3:1447:A:H5''	35:R3:1448:C:H5	1.58	0.68
9:2:47:ARG:HD3	33:R1:778:G:H5''	1.77	0.67
33:R1:136:G:C2	33:R1:142:A:H2	2.09	0.67
33:R1:358:U:H2'	33:R1:359:G:H8	1.57	0.67
33:R1:1918:A:O2'	33:R1:1919:A:N7	2.27	0.67
3:14:43:ILE:HD12	3:14:56:ASP:HB2	1.76	0.67
33:R1:45:G:H5''	33:R1:46:G:H5'	1.75	0.67
35:R3:407:U:H3	35:R3:435:A:H62	1.42	0.67
16:27:40:GLN:NE2	16:27:57:HIS:O	2.26	0.67
33:R1:136:G:C6	33:R1:142:A:N1	2.62	0.67
33:R1:1858:A:N6	33:R1:1884:G:O2'	2.28	0.67
22:32:45:ASP:OD1	22:32:52:LYS:NZ	2.28	0.67
23:33:27:ARG:HH21	31:E:17:PRO:HG2	1.59	0.67
1:1:184:LYS:O	1:1:188:ASN:ND2	2.27	0.67
33:R1:2848:G:HO2'	33:R1:2867:G:H22	1.38	0.67
10:20:49:ARG:NH1	33:R1:993:G:OP1	2.26	0.67
7:18:46:GLU:N	7:18:46:GLU:OE2	2.25	0.67
33:R1:880:G:H1	33:R1:895:U:H3	1.41	0.67
33:R1:1171:G:O6	33:R1:1176:U:O4	2.13	0.67
31:E:203:ARG:HG2	31:E:547:ARG:HG2	1.75	0.67
26:36:32:LYS:HD3	33:R1:2478:A:H5'	1.76	0.67
33:R1:1779:U:H5	33:R1:1784:A:N7	1.92	0.67
33:R1:695:G:O2'	33:R1:696:G:O5'	2.13	0.66
11:21:10:LYS:NZ	33:R1:994:C:O2	2.27	0.66
33:R1:1912:A:HO2'	35:R3:1494:G:HO2'	1.43	0.66
29:6:2:ARG:HA	29:6:5:LYS:HE3	1.76	0.66
10:20:5:ARG:HD2	33:R1:1250:G:H5''	1.77	0.66
19:3:56:LYS:HE3	33:R1:2830:C:H5''	1.76	0.66
33:R1:879:G:H1	33:R1:898:C:H42	1.44	0.66
13:23:30:ILE:HG12	13:23:87:LEU:HD11	1.78	0.66
19:3:25:THR:OG1	19:3:191:GLY:O	2.13	0.66
28:5:59:ILE:O	28:5:101:ARG:NH2	2.22	0.66
35:R3:114:U:H1'	35:R3:353:A:H1'	1.77	0.66
17:28:71:ARG:NH1	17:28:77:TYR:OH	2.27	0.66
35:R3:946:A:H2'	35:R3:947:G:C8	2.30	0.66
33:R1:1597:A:H5''	33:R1:1598:A:H5'	1.77	0.66
33:R1:2328:A:H2'	33:R1:2329:U:C6	2.31	0.66
19:3:46:ARG:NH1	19:3:85:ALA:O	2.27	0.65
9:2:220:ARG:NH1	33:R1:1789:A:OP2	2.30	0.65
12:22:49:LYS:NZ	33:R1:491:G:O6	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:R1:1172:C:O2'	33:R1:1174:U:O4'	2.14	0.65
33:R1:195:A:H61	33:R1:198:C:H3'	1.60	0.65
25:35:14:LYS:HB2	25:35:22:LYS:HE2	1.77	0.65
33:R1:388:G:N2	33:R1:390:U:O2'	2.30	0.65
21:31:63:ARG:NH2	35:R3:1312:G:OP2	2.29	0.65
28:5:130:GLY:HA3	33:R1:2305:U:H5''	1.79	0.65
36:T:58:A:O2'	36:T:60:C:OP2	2.14	0.65
3:14:23:LYS:NZ	33:R1:2561:U:O2	2.30	0.65
3:14:63:VAL:HG12	3:14:107:LEU:HD11	1.79	0.65
33:R1:1054:A:H2'	33:R1:1055:G:H8	1.62	0.65
35:R3:338:A:H3'	35:R3:339:C:H5''	1.79	0.65
5:16:20:LEU:HD13	15:25:81:PRO:HG2	1.79	0.65
28:5:44:ALA:HB1	31:E:416:LYS:HB2	1.79	0.65
35:R3:664:G:H22	35:R3:741:G:H1	1.45	0.65
9:2:60:ALA:O	9:2:62:ARG:NH1	2.29	0.65
19:3:148:GLN:HB2	19:3:152:PRO:HG2	1.78	0.65
33:R1:131:A:H61	33:R1:147:C:H42	1.45	0.65
33:R1:2774:C:O2'	33:R1:2775:G:O5'	2.15	0.65
31:E:133:GLN:O	31:E:133:GLN:NE2	2.26	0.64
27:4:45:ALA:HB2	27:4:89:PRO:HD3	1.77	0.64
20:30:11:SER:HB2	33:R1:988:A:H5''	1.80	0.64
35:R3:402:G:H5''	35:R3:621:A:H1'	1.79	0.64
6:17:22:ARG:HG3	6:17:70:THR:HA	1.78	0.64
9:2:257:ARG:NH1	9:2:263:ASP:OD1	2.30	0.64
1:1:7:ARG:H	1:1:7:ARG:HD3	1.62	0.64
33:R1:157:C:H2'	33:R1:158:U:H5'	1.79	0.64
33:R1:356:G:H2'	33:R1:357:C:C6	2.33	0.64
8:19:105:LYS:HG2	35:R3:1432:G:H5''	1.79	0.64
33:R1:412:A:H2'	33:R1:413:C:H5'	1.80	0.64
33:R1:2774:C:O2'	33:R1:2775:G:H8	1.80	0.64
35:R3:115:G:H8	35:R3:115:G:OP1	1.79	0.64
5:16:84:LYS:NZ	33:R1:2250:G:OP1	2.28	0.64
35:R3:946:A:H2'	35:R3:947:G:H8	1.61	0.64
35:R3:1014:A:N1	35:R3:1218:C:O2'	2.31	0.64
35:R3:82:G:H1'	35:R3:88:U:H3	1.63	0.64
35:R3:744:C:H2'	35:R3:745:G:C8	2.33	0.64
35:R3:131:A:HO2'	35:R3:262:A:H8	1.46	0.64
35:R3:157:U:H3	35:R3:164:G:H1	1.46	0.64
21:31:37:CYS:SG	21:31:38:SER:N	2.71	0.63
33:R1:856:G:H2'	33:R1:857:G:C8	2.32	0.63
35:R3:1151:A:H2'	35:R3:1152:A:C8	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:43:ASP:OD2	33:R1:2123:G:N2	2.31	0.63
35:R3:70:U:H1'	35:R3:71:A:H2	1.62	0.63
30:9:14:SER:N	30:9:17:ASP:OD2	2.31	0.63
33:R1:2162:G:H4'	33:R1:2171:A:H2'	1.81	0.63
35:R3:321:A:H62	35:R3:332:G:H1	1.46	0.63
35:R3:369:G:HO2'	35:R3:370:C:H6	1.44	0.63
33:R1:1869:G:H22	33:R1:1872:A:H5''	1.63	0.63
33:R1:2562:U:H2'	33:R1:2563:U:H5'	1.80	0.63
33:R1:2668:G:O2'	33:R1:2669:G:O5'	2.12	0.63
10:20:49:ARG:NH2	11:21:73:LYS:O	2.31	0.63
31:E:233:ASP:OD2	31:E:254:ARG:NH2	2.32	0.63
31:E:357:PRO:O	31:E:362:LYS:NZ	2.31	0.63
33:R1:219:A:N3	33:R1:234:U:O2'	2.29	0.63
33:R1:134:G:N1	33:R1:144:A:C2	2.57	0.62
4:15:127:VAL:HG21	4:15:142:ILE:HD13	1.82	0.62
12:22:5:ALA:O	33:R1:494:G:O2'	2.14	0.62
31:E:457:LYS:O	31:E:460:GLN:NE2	2.32	0.62
33:R1:1779:U:OP2	33:R1:1784:A:N6	2.26	0.62
35:R3:58:C:O2'	35:R3:388:G:N2	2.29	0.62
33:R1:2144:G:N2	33:R1:2146:C:O2	2.32	0.62
28:5:169:LEU:HD12	28:5:174:PHE:CD1	2.34	0.62
33:R1:721:A:H2'	33:R1:722:A:C8	2.35	0.62
33:R1:2668:G:O2'	33:R1:2669:G:O4'	2.17	0.62
4:15:74:THR:HG23	4:15:107:PHE:HB2	1.81	0.62
35:R3:477:C:H2'	35:R3:478:A:C8	2.34	0.62
31:E:375:PRO:HG2	31:E:378:GLY:HA2	1.81	0.62
28:5:61:GLY:O	28:5:94:ARG:NH2	2.33	0.62
33:R1:281:C:H41	33:R1:359:G:H22	1.47	0.62
33:R1:2140:G:H2'	33:R1:2141:G:C8	2.34	0.62
9:2:259:ASN:OD1	9:2:262:THR:OG1	2.11	0.62
14:24:68:ASN:ND2	33:R1:329:G:OP2	2.33	0.62
17:28:42:GLU:OE1	17:28:44:ARG:NE	2.27	0.62
35:R3:1452:C:O2'	35:R3:1453:G:N2	2.33	0.62
3:14:78:ARG:NH2	33:R1:2685:G:OP1	2.33	0.61
33:R1:136:G:H1	33:R1:142:A:H2	0.67	0.61
35:R3:1412:C:H2'	35:R3:1413:A:C8	2.34	0.61
35:R3:738:C:HO2'	35:R3:739:C:H6	1.46	0.61
35:R3:1004:A:H2'	35:R3:1005:A:H5''	1.81	0.61
33:R1:2029:G:N1	33:R1:2033:A:OP2	2.30	0.61
8:19:23:ASP:OD1	8:19:112:ARG:NH2	2.34	0.61
33:R1:827:U:O2'	33:R1:2068:U:N3	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:R3:928:G:H1	35:R3:1389:C:H5	1.47	0.61
11:21:16:GLU:OE1	11:21:101:ILE:N	2.33	0.61
33:R1:151:C:H2'	33:R1:152:A:C8	2.35	0.61
33:R1:1108:U:O2	33:R1:1109:C:N4	2.33	0.61
35:R3:57:G:N2	35:R3:388:G:O6	2.32	0.61
1:1:195:ALA:HA	1:1:198:LYS:HD2	1.83	0.61
31:E:404:VAL:HG13	31:E:453:LEU:HD12	1.83	0.61
5:16:110:GLU:OE2	5:16:114:ARG:NH2	2.34	0.61
31:E:169:ARG:NH2	31:E:188:GLN:O	2.34	0.61
33:R1:411:G:OP2	33:R1:2406:A:O2'	2.19	0.61
3:14:106:GLU:N	3:14:106:GLU:OE2	2.28	0.61
31:E:116:ALA:HB1	31:E:120:LYS:HD2	1.83	0.61
26:36:34:LYS:NZ	33:R1:2743:U:OP1	2.29	0.61
27:4:97:ASN:HB2	27:4:100:MET:HG3	1.83	0.61
31:E:388:LEU:HD21	31:E:467:LEU:HD13	1.83	0.61
33:R1:1103:A:H3'	33:R1:1104:C:H5''	1.82	0.61
8:19:90:ALA:HB2	8:19:112:ARG:HA	1.83	0.61
33:R1:388:G:O2'	33:R1:390:U:OP2	2.17	0.61
33:R1:414:C:OP1	33:R1:1879:C:O2'	2.19	0.61
33:R1:1171:G:N1	33:R1:1176:U:N3	2.27	0.61
33:R1:1721:G:N2	33:R1:1738:G:O2'	2.17	0.61
33:R1:1847:G:H21	33:R1:1848:A:H62	1.49	0.61
35:R3:373:A:O2'	35:R3:451:A:N7	2.34	0.61
20:30:40:THR:HG22	20:30:42:ALA:H	1.66	0.60
16:27:19:LYS:NZ	33:R1:2261:C:OP1	2.30	0.60
28:5:33:ILE:HD12	28:5:155:ILE:HG12	1.82	0.60
31:E:391:VAL:HA	31:E:458:LEU:HD23	1.82	0.60
33:R1:2176:A:H2'	33:R1:2177:C:C4	2.37	0.60
33:R1:639:U:H2'	33:R1:640:C:C6	2.36	0.60
33:R1:1179:G:H5'	33:R1:1180:U:H5''	1.83	0.60
35:R3:309:A:O2'	35:R3:607:A:N1	2.33	0.60
4:15:29:LYS:O	4:15:30:THR:OG1	2.19	0.60
31:E:552:ARG:NH2	33:R1:2168:G:O6	2.35	0.60
5:16:53:MET:HG3	5:16:120:ALA:HB2	1.83	0.60
31:E:327:SER:O	31:E:379:THR:OG1	2.20	0.60
33:R1:962:G:N2	33:R1:2250:G:H1	2.00	0.60
27:4:163:ASN:ND2	33:R1:320:A:N3	2.49	0.60
31:E:194:ASP:OD1	31:E:358:ASN:ND2	2.35	0.60
33:R1:2174:C:H2'	33:R1:2175:C:C6	2.37	0.60
6:17:42:LYS:NZ	33:R1:2817:U:OP1	2.34	0.60
15:25:65:VAL:HG23	15:25:66:ASP:H	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:E:107:VAL:HG22	31:E:121:LEU:HD12	1.83	0.60
33:R1:1204:A:H4'	33:R1:1205:A:H5''	1.83	0.60
35:R3:17:U:H2'	35:R3:18:C:C6	2.36	0.60
35:R3:1013:G:N1	35:R3:1016:A:OP2	2.35	0.60
1:1:202:THR:OG1	1:1:203:GLN:NE2	2.34	0.60
9:2:233:GLY:HA3	33:R1:2598:A:H5''	1.81	0.60
31:E:405:TRP:O	31:E:409:SER:OG	2.17	0.60
33:R1:324:A:OP2	33:R1:1205:A:N6	2.34	0.60
35:R3:1129:C:H1'	35:R3:1130:A:H2	1.67	0.60
9:2:139:THR:OG1	9:2:162:GLN:OE1	2.20	0.60
33:R1:577:G:O2'	33:R1:1254:A:OP1	2.18	0.60
33:R1:1900:A:H1'	33:R1:1970:A:H2'	1.82	0.60
33:R1:221:A:N1	33:R1:265:A:O2'	2.35	0.60
33:R1:2134:A:N7	33:R1:2156:G:N2	2.50	0.60
35:R3:976:G:OP2	35:R3:1358:U:O2'	2.19	0.60
35:R3:1005:A:H2'	35:R3:1006:G:C5	2.36	0.60
35:R3:1356:G:H2'	35:R3:1357:A:H8	1.66	0.60
35:R3:677:U:H3	35:R3:713:G:H22	1.50	0.59
33:R1:993:G:H2'	33:R1:994:C:H5''	1.83	0.59
32:M:6:U:H3	36:T:34:A:H62	1.49	0.59
33:R1:84:A:N1	33:R1:98:G:O2'	2.26	0.59
33:R1:153:U:H2'	33:R1:154:U:O4'	2.02	0.59
33:R1:1051:G:H22	33:R1:1110:G:H1	1.48	0.59
35:R3:744:C:H2'	35:R3:745:G:H8	1.67	0.59
6:17:8:ARG:NH1	33:R1:1652:A:OP1	2.31	0.59
22:32:48:TYR:OH	33:R1:2883:A:OP1	2.16	0.59
33:R1:156:A:N1	33:R1:169:G:C6	2.71	0.59
36:T:23:A:H2'	36:T:24:G:C8	2.38	0.59
33:R1:2124:G:O2'	33:R1:2125:G:O4'	2.20	0.59
8:19:105:LYS:HE3	35:R3:1432:G:H3'	1.85	0.59
33:R1:2591:C:H2'	33:R1:2592:G:C8	2.37	0.59
2:13:18:VAL:HG12	2:13:140:LEU:HB3	1.84	0.59
31:E:405:TRP:NE1	31:E:424:SER:OG	2.35	0.59
33:R1:1038:G:H2'	33:R1:1039:A:C8	2.38	0.59
33:R1:1149:G:H2'	33:R1:1150:C:C6	2.37	0.59
2:13:65:THR:OG1	33:R1:1141:U:OP2	2.19	0.59
4:15:4:ASN:OD1	33:R1:1203:U:O2'	2.21	0.59
8:19:6:GLN:HG2	19:3:184:ARG:HH12	1.68	0.59
17:28:69:GLU:N	17:28:69:GLU:OE2	2.36	0.59
18:29:4:LYS:HG3	18:29:7:ARG:HH12	1.67	0.59
36:T:23:A:H2'	36:T:24:G:H8	1.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:3:196:ALA:O	19:3:199:SER:OG	2.17	0.58
31:E:49:LEU:HD13	31:E:215:ILE:HD11	1.85	0.58
33:R1:134:G:H22	33:R1:144:A:H2	1.51	0.58
33:R1:689:A:H8	33:R1:779:U:HO2'	1.50	0.58
33:R1:1176:U:O2'	33:R1:1178:C:N4	2.36	0.58
33:R1:1720:U:H2'	33:R1:1721:G:O4'	2.02	0.58
35:R3:451:A:H1'	35:R3:452:A:C2	2.38	0.58
35:R3:1014:A:C2	35:R3:1015:G:H1'	2.37	0.58
21:31:44:PHE:HD1	21:31:45:THR:HG23	1.68	0.58
33:R1:500:G:N1	33:R1:503:A:OP2	2.31	0.58
35:R3:1150:A:O2'	35:R3:1151:A:O5'	2.20	0.58
15:25:69:GLU:OE1	15:25:69:GLU:N	2.34	0.58
31:E:196:GLU:OE2	31:E:196:GLU:N	2.35	0.58
31:E:354:ILE:HD11	31:E:495:MET:HE2	1.85	0.58
33:R1:161:A:H61	33:R1:2218:G:H4'	1.68	0.58
33:R1:590:A:H62	33:R1:667:U:H3	1.51	0.58
35:R3:235:C:H2'	35:R3:236:A:C8	2.38	0.58
17:28:56:ARG:NH2	33:R1:400:G:N7	2.50	0.58
33:R1:1432:G:H2'	33:R1:1433:A:C8	2.39	0.58
33:R1:1912:A:O2'	35:R3:1494:G:O2'	2.15	0.58
35:R3:492:C:H5'	35:R3:493:A:OP2	2.03	0.58
2:13:30:THR:HG21	33:R1:1005:C:O2'	2.03	0.58
33:R1:319:G:H1	33:R1:323:C:H5	1.49	0.58
35:R3:441:A:H61	35:R3:493:A:H61	1.51	0.58
35:R3:1011:C:H2'	35:R3:1012:A:H8	1.66	0.58
5:16:81:ARG:HH21	16:27:5:LYS:HG3	1.67	0.58
31:E:351:ILE:HG22	31:E:508:ALA:HA	1.85	0.58
33:R1:878:A:H3'	33:R1:879:G:H8	1.67	0.58
34:R2:29:A:H2'	34:R2:30:C:C6	2.39	0.58
35:R3:115:G:O2'	35:R3:289:G:H5'	2.03	0.58
18:29:54:LYS:HD3	33:R1:72:U:H5'	1.85	0.58
9:2:209:ALA:HA	9:2:212:TRP:CE2	2.39	0.58
9:2:35:LYS:NZ	9:2:37:SER:OG	2.37	0.57
33:R1:2123:G:H2'	33:R1:2124:G:C5	2.39	0.57
35:R3:473:U:H2'	35:R3:474:G:C8	2.38	0.57
35:R3:1005:A:H5'	35:R3:1006:G:N7	2.19	0.57
36:T:75:C:H3'	36:T:76:A:H5''	1.85	0.57
35:R3:685:G:H2'	35:R3:686:U:C6	2.39	0.57
35:R3:1323:G:H2'	35:R3:1324:A:C8	2.39	0.57
36:T:43:G:H2'	36:T:44:G:C8	2.39	0.57
8:19:105:LYS:O	8:19:108:ARG:NH1	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:2:226:PRO:HD3	9:2:233:GLY:H	1.68	0.57
22:32:39:ARG:NH1	33:R1:2885:G:N7	2.49	0.57
33:R1:1090:A:H2'	33:R1:1091:G:C8	2.38	0.57
33:R1:2243:U:H2'	33:R1:2244:U:C6	2.39	0.57
9:2:4:LYS:HD3	9:2:16:VAL:HG22	1.86	0.57
31:E:361:GLY:N	59:E:602:ATP:O1B	2.31	0.57
19:3:1:MET:HG3	19:3:100:LEU:HD11	1.85	0.57
33:R1:1386:C:H2'	33:R1:1387:A:C8	2.40	0.57
35:R3:672:U:H2'	35:R3:673:A:C8	2.40	0.57
29:6:174:LYS:HD3	33:R1:2529:G:H4'	1.87	0.57
33:R1:64:A:H2'	33:R1:65:U:C6	2.40	0.57
33:R1:881:G:H2'	33:R1:882:G:C8	2.39	0.57
33:R1:2123:G:H2'	33:R1:2124:G:C8	2.40	0.57
33:R1:2124:G:H2'	33:R1:2125:G:C8	2.39	0.57
35:R3:992:U:O2'	35:R3:1043:G:O6	2.14	0.57
25:35:4:LYS:HD3	33:R1:242:G:N7	2.20	0.57
33:R1:156:A:H2	33:R1:169:G:C2	2.19	0.57
33:R1:593:U:H2'	33:R1:594:U:C6	2.40	0.57
1:1:56:ASP:N	1:1:56:ASP:OD1	2.33	0.57
1:1:207:VAL:HG22	1:1:209:ILE:H	1.69	0.57
5:16:31:PHE:HD1	5:16:132:THR:HG22	1.69	0.57
8:19:6:GLN:OE1	19:3:184:ARG:NH2	2.38	0.57
31:E:262:GLU:OE1	31:E:265:ARG:NH2	2.38	0.57
31:E:318:ARG:NH2	35:R3:1300:G:OP2	2.37	0.57
33:R1:265:A:N1	33:R1:427:U:O2'	2.34	0.57
33:R1:890:C:H3'	33:R1:891:G:H4'	1.85	0.57
33:R1:1028:A:H2'	33:R1:1029:A:C8	2.40	0.57
35:R3:106:C:H2'	35:R3:107:G:H5'	1.86	0.57
35:R3:838:G:O2'	35:R3:839:C:O5'	2.23	0.57
7:18:37:ALA:HB3	7:18:78:VAL:HG21	1.87	0.57
22:32:8:THR:HG23	33:R1:2020:A:H5'	1.87	0.57
35:R3:1130:A:O2'	35:R3:1131:G:H8	1.87	0.57
26:36:2:LYS:NZ	33:R1:2478:A:OP2	2.30	0.57
33:R1:1327:A:N6	33:R1:1647:U:O2	2.37	0.57
33:R1:1353:A:H2'	33:R1:1354:A:C8	2.39	0.57
33:R1:2638:G:H1'	33:R1:2778:A:H61	1.69	0.57
14:24:6:ARG:NH2	33:R1:84:A:O2'	2.37	0.56
21:31:34:LEU:HD12	28:5:109:ARG:HH12	1.70	0.56
33:R1:279:A:N6	33:R1:361:G:H1'	2.19	0.56
33:R1:2140:G:H2'	33:R1:2141:G:H8	1.70	0.56
35:R3:206:C:C5	35:R3:207:C:H1'	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:R1:895:U:H4'	33:R1:896:A:H2	1.70	0.56
34:R2:2:G:O6	34:R2:119:A:N6	2.38	0.56
1:1:7:ARG:NH2	1:1:218:MET:SD	2.78	0.56
9:2:231:HIS:HA	9:2:241:LYS:HE3	1.87	0.56
29:6:108:PHE:O	33:R1:2666:C:N4	2.39	0.56
33:R1:2183:A:H2'	33:R1:2184:A:C8	2.40	0.56
34:R2:32:U:H2'	34:R2:33:G:H8	1.71	0.56
35:R3:587:G:N2	35:R3:754:C:OP2	2.35	0.56
1:1:65:LEU:HD21	1:1:68:GLY:HA2	1.87	0.56
19:3:5:VAL:N	19:3:32:ASN:HD21	1.94	0.56
19:3:155:VAL:HG21	33:R1:2618:G:H21	1.69	0.56
33:R1:947:A:O2'	33:R1:984:A:H2	1.89	0.56
35:R3:1071:C:H2'	35:R3:1072:G:H8	1.71	0.56
33:R1:729:G:H5''	33:R1:730:A:H5''	1.88	0.56
33:R1:2291:U:H2'	33:R1:2292:U:C6	2.41	0.56
34:R2:64:G:O2'	34:R2:65:U:OP1	2.22	0.56
35:R3:381:C:H2'	35:R3:382:A:O4'	2.06	0.56
35:R3:727:G:N2	35:R3:730:G:OP2	2.35	0.56
35:R3:1031:C:H4'	35:R3:1033:G:N3	2.21	0.56
35:R3:1124:G:N2	35:R3:1125:U:O4	2.32	0.56
33:R1:657:U:H2'	33:R1:658:U:C6	2.41	0.56
33:R1:2430:A:H2'	33:R1:2430:A:N3	2.20	0.56
4:15:75:ALA:HB2	4:15:105:ILE:HD12	1.86	0.56
17:28:27:ARG:NH2	33:R1:1365:A:OP1	2.33	0.56
29:6:53:PRO:HB3	29:6:60:GLY:HA3	1.88	0.56
9:2:241:LYS:O	33:R1:1902:C:H4'	2.06	0.56
33:R1:645:C:H2'	33:R1:647:G:N7	2.20	0.56
33:R1:2638:G:H1'	33:R1:2778:A:N6	2.21	0.56
1:1:58:ASN:HD22	1:1:165:ASN:HD22	1.54	0.56
6:17:24:MET:HG2	33:R1:1277:G:O2'	2.06	0.56
21:31:5:ILE:HD12	28:5:63:LYS:HD3	1.88	0.56
35:R3:1010:U:H2'	35:R3:1011:C:C6	2.41	0.56
19:3:48:ILE:HG23	19:3:84:LEU:HD21	1.88	0.56
23:33:10:LEU:HB3	23:33:48:TYR:HB3	1.85	0.56
33:R1:458:G:O2'	33:R1:469:G:O6	2.23	0.56
33:R1:948:C:O2	33:R1:984:A:O2'	2.19	0.56
34:R2:7:G:H1	34:R2:113:C:H5	1.53	0.56
35:R3:518:C:O2'	35:R3:530:G:N2	2.39	0.56
35:R3:855:U:OP2	35:R3:871:U:N3	2.32	0.56
35:R3:1507:A:H2'	35:R3:1508:A:C8	2.41	0.56
21:31:42:PRO:O	28:5:114:ARG:NH2	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:E:151:LEU:HD11	31:E:550:TYR:OH	2.06	0.55
35:R3:524:G:H2'	35:R3:525:C:C6	2.41	0.55
35:R3:1270:G:H2'	35:R3:1271:A:C8	2.41	0.55
9:2:34:GLU:OE1	33:R1:1816:C:N4	2.29	0.55
33:R1:742:A:H2'	33:R1:743:A:C8	2.40	0.55
33:R1:1170:C:O2'	33:R1:1171:G:H8	1.90	0.55
35:R3:1122:U:HO2'	35:R3:1123:U:H6	1.52	0.55
29:6:85:LYS:HG2	29:6:131:VAL:HG22	1.89	0.55
35:R3:112:G:H22	35:R3:315:A:H2	1.53	0.55
35:R3:441:A:H61	35:R3:493:A:N6	2.04	0.55
28:5:57:ALA:HB2	28:5:64:PRO:HD3	1.86	0.55
33:R1:1443:U:H2'	33:R1:1444:G:H8	1.70	0.55
35:R3:80:A:N6	35:R3:89:U:O4	2.40	0.55
35:R3:1124:G:HO2'	35:R3:1145:A:N6	2.04	0.55
18:29:36:GLN:OE1	18:29:36:GLN:N	2.39	0.55
31:E:376:ASP:OD1	31:E:376:ASP:N	2.37	0.55
33:R1:160:A:OP2	33:R1:161:A:O2'	2.20	0.55
33:R1:882:G:N2	33:R1:894:U:O2	2.36	0.55
33:R1:2646:C:OP2	33:R1:2732:G:O2'	2.25	0.55
4:15:110:VAL:HB	4:15:127:VAL:HG12	1.88	0.55
19:3:181:ASP:OD2	19:3:184:ARG:HD2	2.06	0.55
33:R1:1064:C:H3'	33:R1:1065:U:H3'	1.88	0.55
34:R2:7:G:H22	34:R2:113:C:H5	1.53	0.55
35:R3:1127:G:H1	35:R3:1145:A:H61	1.54	0.55
35:R3:1238:A:H2	35:R3:1241:G:N3	2.05	0.55
35:R3:1297:G:H4'	35:R3:1298:U:O5'	2.07	0.55
10:20:50:ARG:NH2	33:R1:993:G:OP2	2.38	0.55
31:E:46:SER:OG	59:E:601:ATP:O2B	2.25	0.55
35:R3:1252:A:H61	35:R3:1285:A:H62	1.54	0.55
9:2:143:VAL:HB	9:2:153:LEU:HB2	1.89	0.55
19:3:151:THR:OG1	33:R1:2032:G:N2	2.40	0.55
33:R1:1223:G:N2	33:R1:1226:A:OP2	2.32	0.55
33:R1:1428:C:C5	33:R1:1569:A:H5''	2.41	0.55
33:R1:2291:U:H5'	33:R1:2380:C:H1'	1.88	0.55
9:2:106:PRO:HD2	9:2:109:LEU:HD22	1.89	0.55
14:24:87:GLU:O	14:24:89:GLY:N	2.39	0.55
22:32:2:VAL:HG13	33:R1:2015:A:C6	2.42	0.55
22:32:37:HIS:ND1	22:32:38:LEU:O	2.40	0.55
33:R1:181:A:H1'	33:R1:435:C:H5'	1.88	0.55
35:R3:126:G:OP1	35:R3:605:U:O2'	2.13	0.55
35:R3:769:G:H4'	35:R3:1513:A:H4'	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:R3:1273:C:H2'	35:R3:1274:A:O4'	2.07	0.55
5:16:5:LYS:HG2	33:R1:871:U:OP1	2.06	0.55
28:5:105:ILE:O	28:5:109:ARG:NH2	2.40	0.55
33:R1:1639:C:H4'	33:R1:2700:A:OP1	2.07	0.55
36:T:45:G:O2'	36:T:46:G:H5'	2.05	0.55
2:13:116:ARG:NH2	33:R1:528:A:OP2	2.34	0.54
31:E:66:GLN:NE2	31:E:67:PRO:HD2	2.23	0.54
31:E:100:ALA:O	31:E:104:LEU:HD23	2.06	0.54
35:R3:1071:C:H2'	35:R3:1072:G:C8	2.42	0.54
9:2:75:ALA:HB1	9:2:93:VAL:HG13	1.89	0.54
13:23:64:LYS:HA	13:23:79:ASP:HB2	1.89	0.54
20:30:27:GLY:HA3	20:30:37:ARG:HH21	1.72	0.54
21:31:31:ASP:N	21:31:31:ASP:OD1	2.37	0.54
34:R2:13:G:H8	34:R2:69:G:H21	1.52	0.54
35:R3:696:A:H2'	35:R3:697:U:H6	1.72	0.54
35:R3:990:C:O2'	35:R3:991:U:H5''	2.07	0.54
35:R3:1218:C:H2'	35:R3:1219:A:C8	2.43	0.54
2:13:122:LEU:HG	2:13:124:VAL:HG23	1.90	0.54
28:5:106:ALA:HB1	28:5:136:ILE:HD12	1.89	0.54
33:R1:257:C:H3'	33:R1:258:G:H8	1.73	0.54
34:R2:32:U:H2'	34:R2:33:G:C8	2.42	0.54
35:R3:1002:G:N7	35:R3:1038:C:N4	2.54	0.54
35:R3:1477:U:H2'	35:R3:1478:U:C6	2.41	0.54
36:T:68:C:HO2'	36:T:69:A:H8	1.54	0.54
33:R1:2313:C:H2'	33:R1:2314:A:H8	1.72	0.54
35:R3:330:C:O2'	35:R3:331:G:H5'	2.07	0.54
35:R3:555:U:H2'	35:R3:556:C:C6	2.42	0.54
1:1:221:GLY:N	33:R1:2175:C:O2'	2.36	0.54
19:3:33:ARG:NH2	19:3:53:GLY:O	2.39	0.54
28:5:56:LEU:HD13	28:5:88:VAL:HG23	1.88	0.54
31:E:85:THR:H	31:E:88:GLU:HB2	1.71	0.54
33:R1:1019:U:H3	33:R1:1142:A:H62	1.56	0.54
35:R3:1010:U:H2'	35:R3:1011:C:H6	1.71	0.54
35:R3:1052:U:O2'	35:R3:1055:A:OP2	2.18	0.54
35:R3:1144:G:N2	35:R3:1146:A:H62	2.05	0.54
35:R3:1346:A:N1	35:R3:1374:A:H5''	2.22	0.54
24:34:10:LEU:HD23	33:R1:770:G:H5''	1.90	0.54
33:R1:639:U:H2'	33:R1:640:C:H6	1.72	0.54
35:R3:1077:G:N2	35:R3:1080:A:OP2	2.36	0.54
35:R3:1530:G:H2'	35:R3:1531:A:C8	2.42	0.54
4:15:123:ARG:NH1	4:15:143:GLU:OE2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:6:70:LEU:O	29:6:74:MET:HG3	2.08	0.54
31:E:13:LYS:NZ	31:E:58:ASP:OD1	2.39	0.54
33:R1:1171:G:H2'	33:R1:1172:C:O4'	2.06	0.54
19:3:1:MET:HG2	19:3:2:ILE:N	2.21	0.54
30:9:50:ARG:HH11	30:9:51:ARG:HA	1.73	0.54
35:R3:751:U:H2'	35:R3:752:G:O4'	2.07	0.54
1:1:215:SER:HB2	1:1:221:GLY:HA2	1.89	0.54
2:13:16:TYR:HB3	2:13:140:LEU:HB2	1.90	0.54
4:15:76:GLU:HG2	33:R1:636:G:H1	1.72	0.54
6:17:28:LEU:HD23	6:17:48:VAL:HG11	1.90	0.54
13:23:6:ARG:HH22	13:23:37:ASP:HB3	1.71	0.54
17:28:9:LYS:NZ	33:R1:397:U:OP2	2.28	0.54
33:R1:387:U:H4'	33:R1:388:G:H5'	1.90	0.54
33:R1:2899:A:H2'	33:R1:2900:A:C8	2.43	0.54
26:36:30:GLU:OE2	26:36:32:LYS:HB2	2.07	0.54
28:5:7:TYR:HA	28:5:11:VAL:HG23	1.89	0.54
30:9:5:LEU:HD12	30:9:17:ASP:H	1.73	0.54
33:R1:2130:U:H1'	33:R1:2159:G:H22	1.73	0.54
34:R2:48:U:H2'	34:R2:49:C:C6	2.42	0.54
35:R3:745:G:H2'	35:R3:746:A:C8	2.43	0.54
31:E:128:LEU:O	31:E:131:ILE:HG22	2.09	0.53
35:R3:908:A:H2'	35:R3:909:A:C8	2.43	0.53
35:R3:958:A:O2'	35:R3:959:A:O5'	2.21	0.53
2:13:60:ASP:OD1	2:13:60:ASP:N	2.41	0.53
11:21:102:SER:OG	11:21:103:ALA:N	2.40	0.53
33:R1:849:A:H2'	33:R1:850:U:H6	1.74	0.53
33:R1:1028:A:N3	33:R1:2486:C:O2'	2.34	0.53
33:R1:1178:C:C5	33:R1:1179:G:H1'	2.43	0.53
33:R1:2064:C:H2'	33:R1:2065:C:C6	2.43	0.53
35:R3:1062:U:H2'	35:R3:1063:C:C6	2.44	0.53
35:R3:1513:A:H2'	35:R3:1514:G:C8	2.43	0.53
33:R1:1410:G:H2'	33:R1:1411:U:C6	2.43	0.53
34:R2:39:A:N1	34:R2:44:G:N1	2.57	0.53
35:R3:990:C:HO2'	35:R3:991:U:H6	1.56	0.53
36:T:28:C:H2'	36:T:29:U:H6	1.73	0.53
14:24:51:LEU:H	14:24:51:LEU:HD12	1.73	0.53
31:E:326:VAL:HG12	31:E:380:ILE:HG13	1.90	0.53
33:R1:279:A:H61	33:R1:361:G:H1'	1.73	0.53
35:R3:356:A:N3	35:R3:368:U:O2'	2.36	0.53
35:R3:975:A:H8	35:R3:1357:A:HO2'	1.57	0.53
35:R3:1270:G:O2'	35:R3:1271:A:OP1	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:T:25:C:O2'	36:T:26:A:H8	1.91	0.53
33:R1:644:A:H2'	33:R1:645:C:O4'	2.09	0.53
33:R1:1213:A:H62	33:R1:1236:G:H1'	1.72	0.53
33:R1:1645:G:H5''	33:R1:1646:C:H5'	1.90	0.53
33:R1:1794:A:H2'	33:R1:1795:C:C6	2.44	0.53
33:R1:1796:U:H2'	33:R1:1797:G:H8	1.74	0.53
35:R3:613:C:H2'	35:R3:614:C:C6	2.44	0.53
9:2:179:GLU:OE2	33:R1:1799:G:O2'	2.16	0.53
16:27:37:ILE:HG22	16:27:38:VAL:HG23	1.90	0.53
27:4:145:ASP:HB3	27:4:184:ASP:HB2	1.90	0.53
33:R1:1542:U:H2'	33:R1:1543:G:O4'	2.08	0.53
33:R1:2023:C:H5'	33:R1:2617:U:H4'	1.90	0.53
33:R1:2115:G:H1'	33:R1:2117:A:H62	1.72	0.53
35:R3:147:G:H2'	35:R3:148:G:C8	2.43	0.53
12:22:65:ASP:OD1	12:22:68:ASP:HB2	2.09	0.53
13:23:9:LYS:O	13:23:12:ARG:NH1	2.42	0.53
29:6:97:VAL:HG22	29:6:102:ILE:HD13	1.91	0.53
31:E:169:ARG:HH22	31:E:189:PRO:HA	1.73	0.53
33:R1:1837:C:O2'	33:R1:1927:A:N3	2.40	0.53
33:R1:2139:U:O2	33:R1:2152:G:O6	2.27	0.53
4:15:108:ALA:HB3	4:15:125:LEU:HD22	1.90	0.53
4:15:109:LYS:HG3	4:15:126:ARG:O	2.09	0.53
10:20:87:VAL:HG22	11:21:49:ILE:HG23	1.90	0.53
27:4:48:THR:HG22	27:4:86:ALA:HB3	1.90	0.53
33:R1:828:U:H2'	33:R1:829:A:C8	2.44	0.53
33:R1:2637:U:H2'	33:R1:2638:G:O4'	2.09	0.53
35:R3:1013:G:C2	35:R3:1015:G:H5''	2.42	0.53
5:16:47:GLU:OE2	5:16:51:ARG:NH1	2.41	0.53
9:2:160:TYR:HB3	9:2:193:GLU:HG3	1.90	0.53
33:R1:282:A:N6	33:R1:283:G:O6	2.42	0.53
33:R1:2097:A:H2'	33:R1:2098:U:C6	2.44	0.53
35:R3:106:C:C2'	35:R3:107:G:H5'	2.39	0.53
12:22:23:LEU:HB3	12:22:35:ILE:HD11	1.91	0.53
12:22:83:LYS:HB3	12:22:95:ARG:NE	2.23	0.53
31:E:333:TYR:OH	31:E:373:GLU:OE2	2.26	0.53
33:R1:813:U:H2'	33:R1:814:C:C6	2.44	0.53
33:R1:1889:A:H2'	33:R1:1890:A:C8	2.44	0.53
35:R3:376:G:OP1	35:R3:376:G:H4'	2.09	0.53
35:R3:393:A:C2'	35:R3:394:G:H5'	2.39	0.53
8:19:51:ASN:O	33:R1:2845:U:H5''	2.09	0.52
27:4:44:ARG:HH22	33:R1:1248:G:P	2.32	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:E:85:THR:HA	31:E:159:LYS:HA	1.90	0.52
33:R1:2111:U:H2'	33:R1:2145:C:O2	2.09	0.52
1:1:161:VAL:HG11	1:1:173:THR:HG23	1.91	0.52
9:2:246:PRO:HG2	9:2:247:TRP:CZ3	2.44	0.52
28:5:65:LEU:HD13	34:R2:42:C:C5	2.45	0.52
31:E:337:LEU:HD11	31:E:340:ASP:HB2	1.89	0.52
33:R1:347:A:H2'	33:R1:348:A:C8	2.44	0.52
33:R1:1434:A:H2'	33:R1:1435:G:C8	2.44	0.52
33:R1:1494:A:H2'	33:R1:1495:A:C8	2.45	0.52
33:R1:2638:G:HO2'	33:R1:2639:A:H8	1.57	0.52
35:R3:235:C:H2'	35:R3:236:A:H8	1.73	0.52
35:R3:859:G:OP2	35:R3:869:G:N1	2.34	0.52
6:17:98:LEU:HD22	22:32:53:VAL:HG21	1.91	0.52
11:21:39:LEU:O	11:21:49:ILE:HB	2.09	0.52
17:28:1:SER:OG	33:R1:1366:A:OP1	2.20	0.52
22:32:3:GLN:NE2	33:R1:2016:U:O2	2.42	0.52
31:E:362:LYS:N	59:E:602:ATP:O1B	2.39	0.52
33:R1:150:U:H3	33:R1:175:G:H1	1.56	0.52
35:R3:78:A:H61	35:R3:80:A:H62	1.56	0.52
35:R3:113:G:N2	35:R3:353:A:H8	2.07	0.52
36:T:43:G:H2'	36:T:44:G:H8	1.74	0.52
4:15:30:THR:HG23	33:R1:810:U:N3	2.19	0.52
12:22:35:ILE:O	12:22:39:THR:HG23	2.09	0.52
31:E:89:SER:O	31:E:175:ARG:NH1	2.35	0.52
33:R1:2137:U:H2'	33:R1:2138:G:C8	2.44	0.52
35:R3:113:G:H21	35:R3:353:A:H8	1.56	0.52
35:R3:612:C:H2'	35:R3:613:C:H6	1.74	0.52
35:R3:939:G:H2'	35:R3:940:C:C6	2.45	0.52
14:24:42:LYS:O	33:R1:480:A:O2'	2.28	0.52
15:25:42:LEU:HD13	15:25:47:VAL:HG21	1.92	0.52
31:E:37:VAL:HG12	31:E:45:LYS:HG2	1.92	0.52
31:E:79:GLN:OE1	31:E:79:GLN:N	2.39	0.52
31:E:299:SER:OG	31:E:300:THR:N	2.43	0.52
33:R1:1213:A:N6	33:R1:1236:G:H1'	2.23	0.52
33:R1:1883:U:H2'	33:R1:1884:G:O4'	2.09	0.52
34:R2:40:U:N3	34:R2:44:G:OP2	2.39	0.52
7:18:88:LYS:HE3	7:18:89:ASP:OD1	2.10	0.52
20:30:23:LEU:HD11	20:30:53:MET:SD	2.49	0.52
33:R1:157:C:C2'	33:R1:158:U:H5'	2.38	0.52
33:R1:1548:A:H2'	33:R1:1549:A:C8	2.44	0.52
33:R1:2116:G:N2	33:R1:2162:G:OP1	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:R3:64:G:OP1	35:R3:382:A:N6	2.39	0.52
4:15:41:ARG:NH2	33:R1:807:U:OP2	2.43	0.52
4:15:85:VAL:HG11	4:15:90:VAL:HG22	1.91	0.52
9:2:75:ALA:HB2	9:2:95:TYR:CD1	2.45	0.52
33:R1:2006:C:O2'	33:R1:2823:A:N3	2.42	0.52
33:R1:2514:U:H2'	33:R1:2515:C:C6	2.44	0.52
33:R1:2899:A:H2'	33:R1:2900:A:H8	1.75	0.52
35:R3:1124:G:O2'	35:R3:1145:A:N6	2.43	0.52
35:R3:1187:G:H2'	35:R3:1188:A:C8	2.45	0.52
5:16:30:SER:OG	5:16:106:ASP:OD1	2.28	0.52
29:6:12:ALA:O	29:6:14:VAL:N	2.42	0.52
33:R1:287:G:H2'	33:R1:288:U:C6	2.44	0.52
33:R1:1808:A:H3'	33:R1:1809:A:C8	2.45	0.52
33:R1:2051:A:H5'	33:R1:2578:G:O4'	2.10	0.52
35:R3:508:U:H1'	35:R3:509:A:H2	1.74	0.52
35:R3:958:A:H8	35:R3:985:C:HO2'	1.56	0.52
6:17:20:MET:O	6:17:24:MET:HG3	2.09	0.52
6:17:24:MET:HE2	6:17:44:LEU:HD22	1.91	0.52
7:18:36:TYR:OH	34:R2:28:C:OP1	2.25	0.52
35:R3:1314:C:H2'	35:R3:1315:U:C6	2.45	0.52
35:R3:1516:G:H2'	35:R3:1518:A:OP2	2.09	0.52
10:20:48:ASP:OD1	33:R1:534:U:O2'	2.26	0.52
16:27:43:THR:H	33:R1:2331:G:H4'	1.75	0.52
33:R1:1028:A:N6	33:R1:1125:G:H2'	2.25	0.52
33:R1:2329:U:H2'	33:R1:2330:G:C8	2.45	0.52
35:R3:611:C:H5'	35:R3:612:C:OP2	2.10	0.52
35:R3:961:U:OP2	35:R3:1223:C:O2'	2.23	0.52
9:2:203:VAL:HG13	33:R1:1792:G:H5'	1.91	0.51
16:27:83:GLU:O	16:27:85:GLU:N	2.44	0.51
33:R1:12:U:O2	33:R1:2626:C:H4'	2.10	0.51
33:R1:882:G:O6	33:R1:894:U:O4	2.27	0.51
33:R1:1441:G:H2'	33:R1:1442:U:C6	2.44	0.51
33:R1:1540:G:H2'	33:R1:1541:C:C6	2.46	0.51
33:R1:2233:U:H2'	33:R1:2234:G:C8	2.45	0.51
35:R3:404:G:O2'	35:R3:498:A:N1	2.35	0.51
36:T:28:C:H2'	36:T:29:U:C6	2.44	0.51
9:2:12:ARG:HD2	33:R1:728:G:H4'	1.91	0.51
20:30:12:ALA:HA	20:30:15:ARG:HG3	1.92	0.51
33:R1:1108:U:H2'	33:R1:1109:C:N3	2.25	0.51
33:R1:1410:G:H2'	33:R1:1411:U:H6	1.74	0.51
33:R1:1733:G:H2'	33:R1:1734:G:H8	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:R1:2700:A:H2'	33:R1:2701:U:H6	1.76	0.51
35:R3:79:G:H2'	35:R3:81:A:C4	2.46	0.51
1:1:8:MET:O	1:1:12:ARG:HG2	2.11	0.51
9:2:32:LEU:HD11	9:2:101:ARG:HA	1.93	0.51
14:24:3:LYS:NZ	33:R1:337:C:OP2	2.40	0.51
33:R1:1386:C:H2'	33:R1:1387:A:H8	1.74	0.51
33:R1:1405:U:H2'	33:R1:1406:U:C6	2.45	0.51
33:R1:1563:U:H2'	33:R1:1564:C:C6	2.45	0.51
33:R1:2011:U:H2'	33:R1:2012:G:O4'	2.10	0.51
2:13:120:ARG:HD3	33:R1:2780:G:OP2	2.11	0.51
29:6:100:ASN:N	29:6:100:ASN:OD1	2.44	0.51
33:R1:514:A:N3	33:R1:581:C:O2'	2.36	0.51
33:R1:581:C:H2'	33:R1:582:A:C8	2.46	0.51
33:R1:2155:U:H2'	33:R1:2156:G:O4'	2.11	0.51
33:R1:2654:A:N1	33:R1:2665:A:H5''	2.25	0.51
35:R3:6:G:H4'	35:R3:298:A:H4'	1.92	0.51
1:1:16:ASP:O	1:1:21:TYR:OH	2.25	0.51
12:22:73:LYS:HB2	12:22:106:VAL:HB	1.91	0.51
33:R1:1052:C:N4	33:R1:1107:G:O6	2.43	0.51
33:R1:1443:U:H2'	33:R1:1444:G:C8	2.45	0.51
33:R1:2146:C:O2'	33:R1:2147:A:O5'	2.27	0.51
8:19:83:ILE:O	8:19:83:ILE:HG22	2.11	0.51
29:6:165:ASP:OD1	29:6:165:ASP:N	2.37	0.51
33:R1:2025:C:H2'	33:R1:2026:U:C6	2.45	0.51
35:R3:580:C:H2'	35:R3:581:G:O4'	2.11	0.51
35:R3:587:G:H22	35:R3:754:C:P	2.33	0.51
1:1:46:VAL:HG23	1:1:212:VAL:HG22	1.92	0.51
13:23:8:LEU:HD22	18:29:22:LEU:HA	1.92	0.51
24:34:39:ARG:NH2	33:R1:468:G:N7	2.56	0.51
35:R3:375:U:H2'	35:R3:376:G:O4'	2.10	0.51
33:R1:1209:U:O2'	33:R1:1237:A:N1	2.37	0.51
33:R1:2086:U:H2'	33:R1:2087:G:C8	2.46	0.51
33:R1:2328:A:H2'	33:R1:2329:U:H6	1.75	0.51
35:R3:463:U:H2'	35:R3:464:U:C6	2.46	0.51
35:R3:867:G:O2'	35:R3:873:A:N1	2.35	0.51
33:R1:1:G:H2'	33:R1:2:G:H8	1.74	0.51
33:R1:2123:G:H2'	33:R1:2124:G:C4	2.46	0.51
33:R1:2273:A:H2'	33:R1:2274:A:C8	2.45	0.51
35:R3:321:A:C2'	35:R3:322:C:H5'	2.41	0.51
27:4:170:ARG:NH2	27:4:176:ASP:OD2	2.44	0.51
33:R1:1179:G:H5''	33:R1:1180:U:C6	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:R1:1884:G:HO2'	33:R1:1885:A:H8	1.58	0.51
33:R1:2178:C:H2'	33:R1:2179:C:C6	2.45	0.51
33:R1:2788:C:H2'	33:R1:2789:C:C6	2.46	0.51
34:R2:7:G:H1	34:R2:113:C:H41	1.58	0.51
35:R3:223:A:H2'	35:R3:224:U:C6	2.45	0.51
35:R3:256:U:H3	35:R3:270:A:N6	2.08	0.51
35:R3:460:A:H2'	35:R3:461:A:C8	2.46	0.51
35:R3:908:A:H2'	35:R3:909:A:H8	1.76	0.51
1:1:50:ILE:HB	1:1:57:GLN:HB3	1.93	0.50
31:E:399:ASP:N	31:E:407:GLU:OE2	2.42	0.50
33:R1:177:G:H3'	33:R1:178:G:H8	1.76	0.50
33:R1:580:U:H2'	33:R1:581:C:C6	2.45	0.50
33:R1:632:A:H2'	33:R1:633:A:C8	2.46	0.50
33:R1:1000:A:H2'	33:R1:1001:A:C8	2.47	0.50
33:R1:2661:G:O2'	33:R1:2662:A:O5'	2.29	0.50
35:R3:560:A:H5''	35:R3:561:U:H3'	1.94	0.50
35:R3:723:U:H2'	35:R3:855:U:H4'	1.93	0.50
4:15:57:LEU:HD22	25:35:53:ASP:HB3	1.94	0.50
4:15:79:LEU:HD13	4:15:116:VAL:HG12	1.93	0.50
11:21:43:ASN:OD1	11:21:44:GLY:N	2.43	0.50
11:21:49:ILE:HG13	11:21:53:PHE:N	2.25	0.50
19:3:149:ASN:HB3	33:R1:2572:A:OP2	2.11	0.50
28:5:131:VAL:HG23	28:5:133:GLU:H	1.76	0.50
31:E:13:LYS:HD2	31:E:59:ILE:HG22	1.93	0.50
33:R1:241:A:N1	33:R1:255:A:H5''	2.27	0.50
33:R1:859:G:H4'	33:R1:860:U:O5'	2.11	0.50
33:R1:1531:C:H2'	33:R1:1532:A:C8	2.47	0.50
33:R1:2101:A:H2'	33:R1:2102:G:H8	1.77	0.50
33:R1:2639:A:N6	33:R1:2775:G:O2'	2.44	0.50
35:R3:239:U:H5''	35:R3:240:G:OP2	2.10	0.50
35:R3:337:G:H2'	35:R3:338:A:C8	2.47	0.50
35:R3:462:G:N2	35:R3:471:U:O2	2.43	0.50
35:R3:862:C:H2'	35:R3:863:U:H5'	1.93	0.50
35:R3:928:G:H22	35:R3:1389:C:H5	1.60	0.50
35:R3:1142:G:C8	35:R3:1143:G:C8	2.99	0.50
36:T:33:U:H5	36:T:36:C:OP2	1.94	0.50
28:5:1:ALA:HB3	28:5:4:HIS:HB2	1.93	0.50
31:E:330:ARG:NH1	31:E:340:ASP:OD2	2.44	0.50
33:R1:368:A:H2'	33:R1:369:U:H1'	1.93	0.50
33:R1:675:A:N3	33:R1:2443:C:O2'	2.38	0.50
33:R1:848:C:H2'	33:R1:849:A:C8	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:R3:519:C:H2'	35:R3:520:A:O4'	2.12	0.50
36:T:51:C:H2'	36:T:52:G:C2	2.46	0.50
1:1:51:ASP:N	1:1:57:GLN:OE1	2.38	0.50
7:18:35:ILE:HG23	7:18:74:VAL:HG11	1.94	0.50
33:R1:833:A:H2'	33:R1:834:G:C8	2.45	0.50
33:R1:1020:A:N1	33:R1:1141:U:O2'	2.33	0.50
35:R3:438:U:O2'	35:R3:439:U:O5'	2.23	0.50
35:R3:1132:C:H2'	35:R3:1133:G:C8	2.47	0.50
19:3:58:ASN:OD1	19:3:59:ARG:N	2.45	0.50
21:31:22:MET:N	21:31:22:MET:SD	2.84	0.50
31:E:218:ASP:OD1	31:E:221:PHE:HB3	2.11	0.50
33:R1:84:A:N7	33:R1:101:A:H2	2.09	0.50
33:R1:191:A:H2'	33:R1:192:C:C6	2.47	0.50
33:R1:195:A:N6	33:R1:198:C:H3'	2.25	0.50
33:R1:1790:C:H2'	33:R1:1791:A:C5	2.47	0.50
33:R1:2126:A:C2	33:R1:2127:G:H1'	2.47	0.50
35:R3:59:A:H5''	35:R3:387:U:H5''	1.92	0.50
35:R3:131:A:N1	35:R3:231:U:H5	2.10	0.50
35:R3:662:U:H2'	35:R3:663:A:C8	2.46	0.50
35:R3:714:G:H2'	35:R3:715:A:C8	2.46	0.50
35:R3:753:A:H4'	35:R3:754:C:O5'	2.11	0.50
9:2:224:MET:HG2	33:R1:782:A:C2	2.47	0.50
11:21:80:ARG:NH1	33:R1:572:A:OP2	2.26	0.50
22:32:24:VAL:O	22:32:25:THR:HG22	2.11	0.50
29:6:104:LEU:HB3	29:6:106:LEU:HD13	1.93	0.50
33:R1:357:C:H2'	33:R1:358:U:C2	2.47	0.50
33:R1:1847:G:N2	33:R1:1848:A:H62	2.10	0.50
31:E:234:ARG:NH1	31:E:302:TYR:O	2.45	0.50
33:R1:851:C:H2'	33:R1:852:U:C6	2.47	0.50
33:R1:2847:U:H2'	33:R1:2848:G:O4'	2.11	0.50
36:T:68:C:O2'	36:T:69:A:H8	1.94	0.50
7:18:63:LYS:HE3	34:R2:51:G:OP1	2.12	0.50
9:2:120:ASP:OD1	9:2:120:ASP:N	2.39	0.50
14:24:87:GLU:O	14:24:87:GLU:OE1	2.30	0.50
27:4:136:GLN:OE1	27:4:136:GLN:HA	2.11	0.50
31:E:69:ILE:HG13	31:E:69:ILE:O	2.12	0.50
33:R1:879:G:H22	33:R1:898:C:H42	1.59	0.50
36:T:63:G:C2	36:T:64:U:H1'	2.47	0.50
36:T:66:A:H2'	36:T:67:U:C6	2.47	0.50
2:13:45:THR:HB	2:13:48:VAL:HG13	1.92	0.50
19:3:101:PHE:HA	19:3:104:VAL:HG13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:6:100:ASN:ND2	29:6:115:GLN:OE1	2.44	0.50
33:R1:99:U:H5''	33:R1:100:U:H5'	1.93	0.50
33:R1:1292:G:H2'	33:R1:1293:C:C6	2.47	0.50
33:R1:1496:A:H2'	33:R1:1498:C:C5	2.46	0.50
33:R1:2901:C:H2'	33:R1:2902:C:C6	2.46	0.50
35:R3:696:A:H2'	35:R3:697:U:C6	2.47	0.50
5:16:63:ILE:HG12	5:16:105:MET:HG3	1.94	0.49
10:20:104:ALA:HA	11:21:46:GLU:HG3	1.94	0.49
28:5:110:ILE:HB	28:5:113:PHE:HB2	1.93	0.49
33:R1:1236:G:O2'	33:R1:1237:A:O5'	2.29	0.49
33:R1:1484:U:H2'	33:R1:1485:U:H6	1.77	0.49
33:R1:2230:G:H2'	33:R1:2231:U:C6	2.46	0.49
35:R3:363:A:H2'	35:R3:364:A:C8	2.47	0.49
1:1:27:ILE:HD12	1:1:30:LEU:HD22	1.93	0.49
16:27:77:ARG:NH1	33:R1:2333:A:OP1	2.25	0.49
33:R1:1219:U:H2'	33:R1:1220:G:C8	2.48	0.49
35:R3:181:A:H61	35:R3:194:C:H2'	1.77	0.49
20:30:11:SER:OG	20:30:12:ALA:N	2.46	0.49
33:R1:849:A:H2'	33:R1:850:U:C6	2.47	0.49
33:R1:1198:U:H2'	33:R1:1199:U:C6	2.48	0.49
35:R3:142:G:O2'	35:R3:196:A:N1	2.37	0.49
35:R3:200:G:H2'	35:R3:201:G:H8	1.78	0.49
35:R3:216:U:H2'	35:R3:217:C:H6	1.77	0.49
35:R3:344:A:H5''	35:R3:345:C:H5	1.77	0.49
35:R3:738:C:O2'	35:R3:739:C:H6	1.95	0.49
28:5:35:LEU:HB3	28:5:56:LEU:HD21	1.95	0.49
31:E:399:ASP:OD2	31:E:402:LYS:NZ	2.46	0.49
31:E:415:MET:HE1	31:E:460:GLN:HB2	1.94	0.49
31:E:468:LEU:HB3	31:E:471:PRO:HG3	1.93	0.49
33:R1:1183:U:H2'	33:R1:1184:U:C6	2.46	0.49
33:R1:2176:A:H2'	33:R1:2177:C:C5	2.47	0.49
35:R3:516:U:O2'	35:R3:519:C:H5	1.96	0.49
35:R3:890:G:O2'	35:R3:906:A:N6	2.45	0.49
1:1:21:TYR:HE2	1:1:29:LEU:HD22	1.76	0.49
5:16:49:ALA:HB1	5:16:120:ALA:HB1	1.93	0.49
33:R1:52:A:H2'	33:R1:53:A:C8	2.48	0.49
33:R1:1171:G:O6	33:R1:1176:U:C4	2.66	0.49
34:R2:34:A:C6	34:R2:44:G:C8	3.01	0.49
34:R2:39:A:C6	34:R2:44:G:N1	2.79	0.49
35:R3:74:A:H2'	35:R3:75:G:O4'	2.11	0.49
4:15:21:ARG:HA	33:R1:811:U:H2'	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:20:8:ILE:HG13	10:20:9:ALA:N	2.28	0.49
13:23:48:GLN:HG3	13:23:55:VAL:HG23	1.93	0.49
33:R1:1814:G:OP2	33:R1:1815:A:O2'	2.21	0.49
35:R3:672:U:H2'	35:R3:673:A:H8	1.76	0.49
35:R3:1306:A:OP2	35:R3:1306:A:H8	1.94	0.49
35:R3:1410:A:H2'	35:R3:1411:C:C6	2.47	0.49
9:2:99:GLU:OE2	9:2:101:ARG:NE	2.46	0.49
9:2:149:LYS:HD3	33:R1:2204:G:H4'	1.94	0.49
11:21:48:LYS:HD3	11:21:49:ILE:H	1.77	0.49
17:28:37:PHE:HZ	17:28:55:MET:HG2	1.78	0.49
19:3:39:ASP:OD1	19:3:39:ASP:N	2.37	0.49
26:36:25:VAL:HB	26:36:35:GLN:HB2	1.94	0.49
33:R1:305:C:H2'	33:R1:306:U:C6	2.48	0.49
33:R1:2291:U:OP1	33:R1:2380:C:O2'	2.29	0.49
33:R1:2439:A:N6	33:R1:2585:U:O2'	2.46	0.49
33:R1:2689:U:OP1	33:R1:2719:G:N1	2.34	0.49
35:R3:1120:C:H2'	35:R3:1121:U:C6	2.47	0.49
35:R3:1439:G:HO2'	35:R3:1440:U:H6	1.58	0.49
5:16:79:ALA:HA	33:R1:2494:G:O2'	2.12	0.49
9:2:170:TYR:HB3	9:2:182:LYS:HD2	1.93	0.49
15:25:26:PHE:HE2	15:25:89:ILE:HG13	1.77	0.49
33:R1:813:U:H2'	33:R1:814:C:H6	1.77	0.49
33:R1:878:A:H3'	33:R1:879:G:C8	2.47	0.49
33:R1:1536:C:H4'	33:R1:1537:G:C4	2.47	0.49
33:R1:2168:G:N3	33:R1:2168:G:H2'	2.28	0.49
33:R1:2700:A:H2'	33:R1:2701:U:C6	2.47	0.49
35:R3:211:G:O2'	35:R3:212:G:OP2	2.30	0.49
35:R3:779:C:H2'	35:R3:780:A:O4'	2.13	0.49
35:R3:1037:C:H2'	35:R3:1038:C:C5	2.47	0.49
2:13:110:PRO:O	2:13:115:GLY:HA3	2.13	0.49
3:14:73:ASP:OD1	3:14:75:SER:OG	2.31	0.49
15:25:51:GLN:OE1	15:25:57:TYR:OH	2.31	0.49
35:R3:232:G:H21	35:R3:263:A:H8	1.60	0.49
35:R3:324:G:N1	35:R3:327:A:OP2	2.42	0.49
35:R3:470:C:O2'	35:R3:471:U:H5''	2.13	0.49
35:R3:1391:U:H2'	35:R3:1392:G:C8	2.48	0.49
2:13:95:ARG:NH2	33:R1:2640:G:OP1	2.46	0.49
22:32:2:VAL:HG11	33:R1:2016:U:H1'	1.95	0.49
28:5:32:LYS:HG3	28:5:156:THR:HB	1.94	0.49
31:E:221:PHE:O	31:E:225:VAL:HG22	2.13	0.49
33:R1:832:U:H2'	33:R1:833:A:C8	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:R1:1857:G:H22	33:R1:1884:G:H2'	1.78	0.49
33:R1:2064:C:H2'	33:R1:2065:C:H6	1.77	0.49
33:R1:2846:G:H2'	33:R1:2847:U:C6	2.48	0.49
33:R1:2898:U:H2'	33:R1:2899:A:H8	1.78	0.49
35:R3:3:A:N3	35:R3:613:C:O2'	2.43	0.49
35:R3:1012:A:C6	35:R3:1013:G:C6	3.01	0.49
6:17:106:ASP:OD1	6:17:106:ASP:N	2.44	0.48
33:R1:274:C:H5	33:R1:363:G:H22	1.61	0.48
33:R1:980:A:N7	33:R1:1136:G:H5'	2.27	0.48
33:R1:1048:A:N6	33:R1:1111:A:H1'	2.28	0.48
33:R1:1416:G:H2'	33:R1:1417:C:C6	2.48	0.48
33:R1:1746:A:H2'	33:R1:1747:U:C6	2.48	0.48
35:R3:634:C:H2'	35:R3:635:A:H8	1.77	0.48
3:14:32:TYR:OH	33:R1:2726:A:H5'	2.12	0.48
7:18:31:THR:O	7:18:102:ARG:NH2	2.38	0.48
7:18:39:VAL:N	7:18:49:VAL:O	2.32	0.48
9:2:224:MET:SD	9:2:229:HIS:HB2	2.53	0.48
29:6:157:LYS:HB2	29:6:159:LYS:HG3	1.94	0.48
33:R1:412:A:C2'	33:R1:413:C:H5'	2.43	0.48
35:R3:836:G:H1	35:R3:850:U:H5	1.61	0.48
26:36:30:GLU:HG3	26:36:32:LYS:H	1.78	0.48
33:R1:1074:G:N1	33:R1:1075:C:H1'	2.29	0.48
33:R1:1469:A:H2'	33:R1:1470:A:C8	2.48	0.48
33:R1:2174:C:O2'	33:R1:2175:C:OP1	2.28	0.48
33:R1:2191:A:H2'	33:R1:2192:U:C6	2.48	0.48
35:R3:1048:G:O2'	35:R3:1050:G:OP1	2.32	0.48
36:T:65:C:H2'	36:T:66:A:H8	1.78	0.48
33:R1:1152:C:H2'	33:R1:1153:C:H6	1.78	0.48
33:R1:1534:U:O2'	33:R1:1537:G:O6	2.30	0.48
33:R1:1636:U:H2'	33:R1:1637:A:C8	2.48	0.48
33:R1:2116:G:H22	33:R1:2162:G:P	2.36	0.48
33:R1:2783:U:H2'	33:R1:2784:U:C6	2.48	0.48
35:R3:20:U:H2'	35:R3:21:G:O4'	2.13	0.48
35:R3:396:C:H5'	35:R3:397:A:OP2	2.13	0.48
35:R3:674:G:H2'	35:R3:675:A:H8	1.78	0.48
5:16:18:ARG:HG2	34:R2:90:C:H5'	1.95	0.48
9:2:44:ASN:N	33:R1:1812:U:O2'	2.41	0.48
19:3:25:THR:HG21	19:3:193:VAL:HG22	1.95	0.48
21:31:11:GLU:N	21:31:25:ARG:HE	2.11	0.48
31:E:329:LEU:HD23	31:E:342:LEU:HD23	1.96	0.48
33:R1:645:C:H2'	33:R1:647:G:C8	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:R1:1796:U:H2'	33:R1:1797:G:C8	2.48	0.48
33:R1:2590:A:H2'	33:R1:2591:C:H6	1.78	0.48
35:R3:73:C:H2'	35:R3:74:A:C8	2.48	0.48
35:R3:499:A:H61	35:R3:547:A:H5''	1.78	0.48
35:R3:736:C:H2'	35:R3:737:C:H6	1.78	0.48
35:R3:737:C:C2'	35:R3:738:C:H5'	2.43	0.48
35:R3:950:U:H2'	35:R3:951:G:C8	2.48	0.48
35:R3:1388:C:H2'	35:R3:1389:C:O2	2.13	0.48
6:17:1:MET:O	6:17:2:ARG:HG3	2.13	0.48
7:18:102:ARG:HG3	34:R2:49:C:OP1	2.13	0.48
9:2:10:PRO:O	33:R1:729:G:N2	2.47	0.48
16:27:25:ARG:NH2	33:R1:2355:G:OP1	2.40	0.48
25:35:56:LEU:HD11	33:R1:834:G:H5'	1.96	0.48
27:4:117:ARG:NH2	27:4:183:PHE:O	2.45	0.48
31:E:196:GLU:H	31:E:196:GLU:CD	2.13	0.48
31:E:476:ASP:O	31:E:480:LEU:HB2	2.13	0.48
33:R1:499:U:H2'	33:R1:500:G:O4'	2.13	0.48
33:R1:2014:A:H2'	33:R1:2015:A:C8	2.48	0.48
35:R3:415:A:C4	35:R3:416:G:C8	3.01	0.48
9:2:139:THR:HG23	9:2:160:TYR:HB2	1.94	0.48
15:25:80:HIS:ND1	15:25:83:LYS:HB2	2.28	0.48
33:R1:1056:G:H4'	33:R1:1057:A:C8	2.48	0.48
33:R1:1433:A:H2'	33:R1:1434:A:O4'	2.14	0.48
33:R1:1484:U:H2'	33:R1:1485:U:C6	2.48	0.48
33:R1:2246:G:H2'	33:R1:2247:A:C8	2.48	0.48
33:R1:2803:G:H2'	33:R1:2804:U:H6	1.78	0.48
35:R3:195:A:H2'	35:R3:196:A:C8	2.49	0.48
35:R3:266:G:N2	35:R3:269:C:OP2	2.46	0.48
6:17:48:VAL:HA	6:17:51:LEU:HD12	1.96	0.48
15:25:51:GLN:OE1	15:25:79:ARG:NH2	2.47	0.48
29:6:26:LYS:HD3	29:6:31:GLU:HB2	1.96	0.48
33:R1:586:A:N1	33:R1:809:G:O2'	2.38	0.48
33:R1:740:C:H5'	33:R1:1784:A:H3'	1.95	0.48
33:R1:1070:A:N6	33:R1:1096:A:N3	2.61	0.48
33:R1:2099:U:O4	33:R1:2190:G:O6	2.30	0.48
35:R3:862:C:N4	35:R3:863:U:O4	2.46	0.48
35:R3:1130:A:O2'	35:R3:1131:G:O5'	2.31	0.48
36:T:42:G:H3'	36:T:43:G:H5''	1.94	0.48
17:28:28:PHE:HB3	33:R1:396:G:H1'	1.96	0.48
18:29:20:ASN:HB3	18:29:50:VAL:HG22	1.95	0.48
23:33:22:THR:OG1	23:33:23:THR:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:5:10:GLU:HG3	28:5:11:VAL:N	2.28	0.48
33:R1:500:G:H2'	33:R1:502:A:H2	1.78	0.48
33:R1:979:A:H5'	33:R1:980:A:H5''	1.96	0.48
33:R1:1278:C:H2'	33:R1:1279:G:H8	1.79	0.48
33:R1:2898:U:H2'	33:R1:2899:A:C8	2.48	0.48
35:R3:559:A:H4'	35:R3:560:A:H3'	1.95	0.48
35:R3:632:U:H5''	35:R3:633:G:C8	2.49	0.48
35:R3:862:C:C2'	35:R3:863:U:H5'	2.44	0.48
35:R3:1270:G:H2'	35:R3:1271:A:H8	1.79	0.48
3:14:70:ARG:HG2	3:14:70:ARG:HH11	1.78	0.48
7:18:11:ALA:O	7:18:15:ARG:HB2	2.14	0.48
9:2:99:GLU:OE1	33:R1:1491:G:O2'	2.29	0.48
33:R1:1327:A:H2'	33:R1:1328:A:O4'	2.14	0.48
33:R1:1361:G:H2'	33:R1:1362:C:C6	2.48	0.48
10:20:50:ARG:HH22	33:R1:993:G:P	2.37	0.47
13:23:11:LEU:HD22	13:23:32:LEU:HD13	1.96	0.47
19:3:22:ILE:HG23	19:3:190:LYS:HG3	1.95	0.47
30:9:11:ASN:HD22	33:R1:2095:A:H5'	1.78	0.47
31:E:74:LEU:HB2	31:E:176:LEU:HD22	1.95	0.47
31:E:432:ASN:HB3	31:E:452:ARG:NH1	2.29	0.47
33:R1:5:A:H2'	33:R1:6:A:C8	2.49	0.47
33:R1:143:C:H3'	33:R1:144:A:H8	1.79	0.47
33:R1:228:C:N4	33:R1:2407:A:N3	2.61	0.47
33:R1:248:G:H5'	33:R1:250:G:N7	2.29	0.47
33:R1:1394:U:H2'	33:R1:1395:A:O4'	2.14	0.47
33:R1:1416:G:H2'	33:R1:1417:C:H6	1.79	0.47
33:R1:1884:G:H8	33:R1:1884:G:OP2	1.97	0.47
35:R3:49:U:O4	35:R3:365:U:H5	1.97	0.47
35:R3:210:C:O2'	35:R3:211:G:OP2	2.24	0.47
35:R3:321:A:H2	35:R3:328:C:O2'	1.92	0.47
35:R3:635:A:H2'	35:R3:636:U:C6	2.49	0.47
35:R3:737:C:O2'	35:R3:738:C:H5'	2.13	0.47
35:R3:1102:A:O2'	35:R3:1103:C:H5'	2.14	0.47
8:19:1:SER:O	8:19:5:LYS:HG3	2.15	0.47
30:9:6:LEU:O	30:9:15:LEU:HG	2.14	0.47
31:E:64:ARG:NH2	33:R1:1859:U:O2'	2.47	0.47
33:R1:1064:C:H4'	33:R1:1065:U:OP2	2.13	0.47
33:R1:1447:C:O2'	33:R1:1544:A:N3	2.39	0.47
33:R1:2156:G:OP2	33:R1:2157:G:N1	2.47	0.47
34:R2:34:A:C5	34:R2:44:G:C8	3.02	0.47
12:22:46:LEU:O	12:22:50:VAL:HG12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:28:30:PRO:HB2	17:28:32:LEU:HD13	1.96	0.47
19:3:11:MET:HB2	19:3:24:VAL:O	2.13	0.47
28:5:55:ASP:OD1	28:5:149:ARG:NH2	2.42	0.47
29:6:16:VAL:HG22	29:6:25:ILE:HG13	1.96	0.47
30:9:5:LEU:HD21	30:9:19:VAL:HG21	1.95	0.47
31:E:86:VAL:HB	31:E:156:TRP:HA	1.96	0.47
33:R1:1589:U:H2'	33:R1:1590:A:H8	1.79	0.47
33:R1:1727:C:H2'	33:R1:1728:C:H6	1.79	0.47
33:R1:1754:A:N1	33:R1:2716:C:O2'	2.42	0.47
35:R3:73:C:H2'	35:R3:74:A:H8	1.78	0.47
35:R3:1063:C:OP2	35:R3:1064:G:O2'	2.20	0.47
35:R3:1088:G:H2'	35:R3:1089:G:O4'	2.15	0.47
35:R3:1235:U:H2'	35:R3:1236:A:O4'	2.14	0.47
35:R3:1315:U:H2'	35:R3:1316:G:O4'	2.14	0.47
15:25:9:ARG:NH2	34:R2:76:G:OP1	2.46	0.47
27:4:5:LEU:HD21	27:4:12:LEU:HD13	1.96	0.47
33:R1:570:G:H2'	33:R1:2030:A:N7	2.29	0.47
33:R1:1152:C:H2'	33:R1:1153:C:C6	2.48	0.47
33:R1:2071:A:H2'	33:R1:2072:C:C6	2.49	0.47
33:R1:2304:G:H22	33:R1:2312:U:H3	1.62	0.47
33:R1:2391:G:O6	33:R1:2425:A:H8	1.97	0.47
33:R1:2502:G:H5''	33:R1:2503:A:H5''	1.97	0.47
33:R1:2809:A:H2'	33:R1:2810:A:C8	2.50	0.47
35:R3:439:U:O2	35:R3:439:U:H2'	2.14	0.47
5:16:71:LYS:HB3	5:16:93:VAL:O	2.14	0.47
9:2:145:MET:HE2	9:2:153:LEU:HD21	1.97	0.47
33:R1:603:A:N1	33:R1:625:G:O2'	2.40	0.47
33:R1:897:C:H2'	33:R1:898:C:H5	1.80	0.47
33:R1:2124:G:H21	33:R1:2174:C:H41	1.61	0.47
33:R1:2155:U:H3'	33:R1:2156:G:H8	1.79	0.47
33:R1:2233:U:H2'	33:R1:2234:G:H8	1.80	0.47
35:R3:57:G:N1	35:R3:355:C:H5	2.11	0.47
35:R3:332:G:O2'	35:R3:333:U:O5'	2.32	0.47
35:R3:715:A:H2'	35:R3:716:A:C8	2.50	0.47
35:R3:1162:C:H2'	35:R3:1163:A:H8	1.79	0.47
1:1:69:THR:HG23	1:1:71:ARG:H	1.80	0.47
18:29:55:THR:HG21	33:R1:76:C:O2'	2.15	0.47
21:31:3:LYS:HD3	21:31:3:LYS:HA	1.80	0.47
33:R1:95:A:H2'	33:R1:96:C:O4'	2.15	0.47
33:R1:918:A:H5''	34:R2:97:C:O2'	2.15	0.47
33:R1:2038:G:H2'	33:R1:2039:U:O4'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:R3:56:U:H2'	35:R3:57:G:C8	2.50	0.47
35:R3:379:C:H5	35:R3:384:G:H1	1.62	0.47
14:24:6:ARG:HB2	33:R1:85:G:OP2	2.15	0.47
21:31:27:THR:O	21:31:27:THR:OG1	2.28	0.47
28:5:151:LEU:N	33:R1:2305:U:O2	2.48	0.47
29:6:174:LYS:HE3	29:6:175:LYS:HE3	1.97	0.47
33:R1:159:G:H1'	33:R1:2208:C:O2'	2.14	0.47
33:R1:181:A:H2'	33:R1:182:A:C8	2.50	0.47
33:R1:278:A:H8	33:R1:279:A:C8	2.32	0.47
33:R1:349:U:H2'	33:R1:350:G:C8	2.50	0.47
33:R1:1269:A:H2'	33:R1:1270:C:C6	2.50	0.47
33:R1:2315:G:O2'	33:R1:2316:G:H8	1.97	0.47
34:R2:15:A:H3'	34:R2:16:G:H8	1.79	0.47
34:R2:25:U:O2	34:R2:117:G:O2'	2.27	0.47
34:R2:116:G:H2'	34:R2:117:G:H5''	1.96	0.47
35:R3:4:U:H2'	35:R3:4:U:O2	2.13	0.47
35:R3:50:A:O2'	35:R3:360:G:N2	2.48	0.47
35:R3:166:U:H2'	35:R3:167:A:C8	2.50	0.47
35:R3:612:C:H2'	35:R3:613:C:C6	2.49	0.47
35:R3:1008:U:H2'	35:R3:1009:U:C6	2.49	0.47
35:R3:1037:C:H2'	35:R3:1038:C:C4	2.50	0.47
35:R3:1186:G:O2'	35:R3:1187:G:H8	1.96	0.47
36:T:63:G:H2'	36:T:64:U:O4'	2.15	0.47
11:21:74:ILE:HB	11:21:87:GLN:HB3	1.97	0.47
19:3:150:GLN:HB3	33:R1:2572:A:N7	2.29	0.47
28:5:65:LEU:HB2	34:R2:42:C:C6	2.50	0.47
30:9:96:THR:HG23	30:9:117:LEU:HD11	1.97	0.47
31:E:548:ILE:O	31:E:549:LYS:HB2	2.14	0.47
33:R1:419:U:H2'	33:R1:420:C:C6	2.50	0.47
33:R1:839:U:H2'	33:R1:840:C:C6	2.50	0.47
33:R1:1570:A:H2'	33:R1:1571:A:C8	2.49	0.47
33:R1:1727:C:H2'	33:R1:1728:C:C6	2.50	0.47
33:R1:2081:U:H2'	33:R1:2082:A:H8	1.80	0.47
4:15:85:VAL:HG13	4:15:86:GLU:N	2.30	0.47
7:18:76:LYS:O	7:18:80:GLU:HG2	2.14	0.47
13:23:33:LYS:HG2	13:23:80:TRP:CE3	2.50	0.47
27:4:176:ASP:OD2	27:4:179:SER:OG	2.30	0.47
28:5:56:LEU:HD12	28:5:86:CYS:SG	2.54	0.47
31:E:219:ARG:HB2	31:E:244:TYR:CG	2.50	0.47
31:E:234:ARG:HE	31:E:304:LYS:HG3	1.80	0.47
31:E:240:TRP:CD1	31:E:247:TRP:HB2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:R1:1:G:H2'	33:R1:2:G:C8	2.50	0.47
33:R1:1071:G:O2'	33:R1:1088:A:O3'	2.33	0.47
33:R1:1187:G:N2	33:R1:1188:U:O4	2.47	0.47
35:R3:1181:G:O2'	35:R3:1182:G:N7	2.44	0.47
35:R3:1253:G:H2'	35:R3:1254:A:H8	1.80	0.47
36:T:25:C:C2	36:T:26:A:C8	3.03	0.47
2:13:55:ILE:HA	2:13:123:LYS:HB2	1.97	0.47
13:23:64:LYS:NZ	33:R1:1601:G:OP1	2.48	0.47
28:5:102:LEU:HD12	28:5:106:ALA:HB3	1.96	0.47
33:R1:232:G:H8	33:R1:232:G:OP2	1.98	0.47
33:R1:1682:G:H2'	33:R1:1683:U:C6	2.50	0.47
35:R3:37:U:H4'	35:R3:501:C:OP1	2.15	0.47
35:R3:707:U:H2'	35:R3:708:C:C6	2.49	0.47
35:R3:1251:A:H2'	35:R3:1252:A:C8	2.50	0.47
35:R3:1439:G:O2'	35:R3:1440:U:H6	1.97	0.47
15:25:38:LEU:HB3	15:25:40:ILE:HD13	1.95	0.46
31:E:313:ILE:HG13	31:E:486:ALA:HB1	1.96	0.46
33:R1:933:A:H5''	33:R1:934:U:OP2	2.14	0.46
33:R1:1954:G:O2'	33:R1:1956:U:O4	2.17	0.46
33:R1:2055:C:H2'	33:R1:2504:U:H4'	1.96	0.46
33:R1:2176:A:H2'	33:R1:2177:C:C2	2.50	0.46
33:R1:2455:G:H2'	33:R1:2456:C:C6	2.49	0.46
35:R3:464:U:N3	35:R3:467:U:OP1	2.40	0.46
35:R3:497:G:H2'	35:R3:498:A:C8	2.49	0.46
7:18:53:THR:HB	7:18:65:THR:HB	1.97	0.46
20:30:39:ASP:OD2	20:30:44:ARG:NH2	2.47	0.46
31:E:85:THR:N	31:E:88:GLU:HB2	2.31	0.46
31:E:128:LEU:O	31:E:132:ILE:HG12	2.15	0.46
33:R1:827:U:O2'	33:R1:2068:U:C2	2.69	0.46
33:R1:2834:G:H1'	33:R1:2883:A:N6	2.30	0.46
35:R3:58:C:C2'	35:R3:388:G:H22	2.27	0.46
35:R3:79:G:O2'	35:R3:80:A:N7	2.48	0.46
35:R3:516:U:H5	35:R3:533:A:N7	2.14	0.46
35:R3:686:U:O4	35:R3:703:G:H2'	2.14	0.46
35:R3:1149:C:O2'	35:R3:1150:A:H5'	2.15	0.46
17:28:38:TRP:CD1	30:9:32:PRO:HA	2.50	0.46
28:5:135:ILE:HD12	28:5:136:ILE:N	2.30	0.46
31:E:382:LEU:HD22	31:E:386:VAL:HG11	1.96	0.46
33:R1:1275:A:N1	33:R1:1295:C:O2'	2.42	0.46
35:R3:984:C:H2'	35:R3:985:C:H6	1.80	0.46
6:17:35:LYS:HB2	6:17:112:TYR:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:18:27:VAL:HA	7:18:93:ASP:HB3	1.97	0.46
14:24:32:LYS:HB3	14:24:63:ALA:HB1	1.97	0.46
30:9:30:LEU:HB3	30:9:36:ALA:HB3	1.96	0.46
31:E:110:LEU:HD22	31:E:121:LEU:HD21	1.97	0.46
33:R1:160:A:H8	33:R1:2217:G:N2	1.94	0.46
33:R1:358:U:H2'	33:R1:359:G:C8	2.43	0.46
33:R1:528:A:C2	33:R1:2043:C:H4'	2.50	0.46
33:R1:2074:U:H2'	33:R1:2075:U:C6	2.50	0.46
33:R1:2100:G:H2'	33:R1:2101:A:H8	1.79	0.46
33:R1:2101:A:H2'	33:R1:2102:G:C8	2.50	0.46
35:R3:466:A:O2'	35:R3:467:U:H5''	2.16	0.46
3:14:109:SER:O	3:14:109:SER:OG	2.29	0.46
20:30:11:SER:CB	33:R1:988:A:H5''	2.43	0.46
28:5:109:ARG:HH21	28:5:138:PRO:HD3	1.81	0.46
33:R1:134:G:C6	33:R1:144:A:N1	2.83	0.46
33:R1:832:U:H2'	33:R1:833:A:H8	1.80	0.46
33:R1:2774:C:O2'	33:R1:2775:G:C8	2.59	0.46
34:R2:110:C:H2'	34:R2:111:U:O4'	2.16	0.46
35:R3:189:A:H2'	35:R3:190:A:C8	2.51	0.46
35:R3:674:G:H2'	35:R3:675:A:C8	2.50	0.46
35:R3:821:G:H2'	35:R3:822:U:C6	2.50	0.46
35:R3:1130:A:HO2'	35:R3:1131:G:C5'	2.27	0.46
36:T:73:A:H5'	36:T:74:C:O5'	2.16	0.46
11:21:68:ARG:HB2	11:21:90:ARG:HH21	1.79	0.46
27:4:200:LEU:HD23	27:4:200:LEU:HA	1.82	0.46
31:E:516:ASP:O	31:E:519:LYS:HG2	2.16	0.46
33:R1:931:U:H5''	33:R1:932:U:OP2	2.15	0.46
33:R1:1486:U:H2'	33:R1:1487:U:C6	2.50	0.46
33:R1:2107:G:C4	33:R1:2108:A:C8	3.04	0.46
33:R1:2134:A:C4	33:R1:2157:G:H4'	2.50	0.46
35:R3:335:C:H2'	35:R3:336:A:C8	2.51	0.46
35:R3:464:U:H3	35:R3:467:U:P	2.38	0.46
35:R3:1305:G:H4'	35:R3:1306:A:O5'	2.15	0.46
35:R3:1435:G:H2'	35:R3:1436:U:C6	2.50	0.46
9:2:97:ASP:OD2	9:2:98:GLY:N	2.49	0.46
16:27:12:ASN:HA	16:27:14:ARG:NH2	2.30	0.46
29:6:90:GLY:HA2	29:6:159:LYS:HZ2	1.80	0.46
33:R1:290:U:O4	33:R1:350:G:O6	2.33	0.46
33:R1:857:G:H2'	33:R1:858:G:O4'	2.16	0.46
33:R1:1486:U:H2'	33:R1:1487:U:H6	1.80	0.46
34:R2:1:U:H2'	34:R2:2:G:C8	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:R3:466:A:C4	35:R3:468:A:C8	3.03	0.46
35:R3:713:G:H2'	35:R3:714:G:C8	2.51	0.46
35:R3:1118:U:H1'	35:R3:1179:A:C5	2.51	0.46
19:3:37:VAL:HG23	19:3:92:VAL:HG13	1.98	0.46
33:R1:598:U:H2'	33:R1:599:A:H8	1.80	0.46
33:R1:1656:C:H2'	33:R1:1657:U:H6	1.81	0.46
33:R1:2795:C:H2'	33:R1:2796:U:O4'	2.16	0.46
35:R3:1330:U:H2'	35:R3:1331:G:O4'	2.15	0.46
7:18:83:LEU:HD11	7:18:114:GLY:HA3	1.98	0.46
28:5:84:ILE:HD11	33:R1:2311:A:N3	2.31	0.46
28:5:132:ARG:O	28:5:133:GLU:HG3	2.15	0.46
33:R1:1219:U:H2'	33:R1:1220:G:H8	1.81	0.46
33:R1:1224:U:H2'	33:R1:1225:G:C8	2.51	0.46
33:R1:2098:U:H2'	33:R1:2099:U:O4'	2.16	0.46
33:R1:2831:G:N2	33:R1:2884:U:OP2	2.46	0.46
35:R3:35:G:H2'	35:R3:36:C:C6	2.51	0.46
35:R3:1253:G:H2'	35:R3:1254:A:C8	2.50	0.46
10:20:47:ARG:NE	10:20:48:ASP:OD2	2.46	0.46
31:E:6:TYR:HB2	31:E:183:MET:HE1	1.98	0.46
33:R1:1357:C:H2'	33:R1:1358:G:O4'	2.16	0.46
33:R1:1429:G:H2'	33:R1:1430:G:H8	1.81	0.46
33:R1:1564:C:H2'	33:R1:1565:C:C6	2.51	0.46
33:R1:2067:G:H3'	33:R1:2068:U:H4'	1.98	0.46
33:R1:2783:U:H2'	33:R1:2784:U:H6	1.80	0.46
36:T:5:G:H2'	36:T:6:A:H8	1.81	0.46
13:23:38:ALA:HB1	13:23:43:ILE:HD11	1.98	0.45
33:R1:739:A:H1'	33:R1:740:C:H5	1.81	0.45
33:R1:1880:U:H2'	33:R1:1881:C:C6	2.51	0.45
33:R1:2106:U:H2'	33:R1:2107:G:O4'	2.15	0.45
33:R1:2489:U:H2'	33:R1:2490:G:O4'	2.16	0.45
33:R1:2557:G:H2'	33:R1:2558:C:C6	2.51	0.45
35:R3:570:G:H2'	35:R3:571:U:C6	2.51	0.45
35:R3:649:A:H2'	35:R3:650:G:O4'	2.16	0.45
35:R3:911:U:H2'	35:R3:912:C:C6	2.51	0.45
35:R3:1120:C:H2'	35:R3:1121:U:H6	1.80	0.45
35:R3:1447:A:H5''	35:R3:1448:C:C5	2.46	0.45
14:24:5:ARG:N	14:24:8:ASP:OD2	2.41	0.45
29:6:137:LYS:O	29:6:140:ILE:HG13	2.17	0.45
33:R1:207:A:H2'	33:R1:208:C:O4'	2.15	0.45
33:R1:897:C:H2'	33:R1:898:C:C5	2.51	0.45
33:R1:1071:G:H2'	33:R1:1089:A:H2'	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:R1:2649:C:H2'	33:R1:2650:U:H6	1.80	0.45
35:R3:417:G:H1'	35:R3:418:C:H5'	1.98	0.45
35:R3:453:G:O2'	35:R3:454:G:OP1	2.25	0.45
35:R3:1286:U:H2'	35:R3:1287:A:H5'	1.99	0.45
35:R3:1450:U:H2'	35:R3:1452:C:H1'	1.97	0.45
12:22:5:ALA:HB2	12:22:54:ALA:HB2	1.98	0.45
19:3:46:ARG:NH2	19:3:88:GLU:O	2.48	0.45
28:5:139:GLU:OE1	28:5:139:GLU:N	2.48	0.45
31:E:41:ASN:HD21	31:E:475:LEU:HA	1.80	0.45
33:R1:1794:A:H2'	33:R1:1795:C:H6	1.81	0.45
33:R1:2411:A:H2'	33:R1:2412:A:C8	2.51	0.45
35:R3:115:G:P	35:R3:115:G:O4'	2.75	0.45
35:R3:322:C:O2'	35:R3:323:U:OP2	2.30	0.45
35:R3:636:U:H2'	35:R3:637:C:H6	1.80	0.45
35:R3:1323:G:H2'	35:R3:1324:A:H8	1.80	0.45
4:15:84:LYS:HB2	4:15:84:LYS:HE3	1.68	0.45
9:2:2:VAL:HG12	9:2:18:VAL:HG22	1.98	0.45
11:21:49:ILE:HG13	11:21:53:PHE:H	1.81	0.45
30:9:89:LYS:HG3	30:9:123:ARG:HB2	1.98	0.45
33:R1:580:U:H2'	33:R1:581:C:H6	1.81	0.45
33:R1:2103:C:H2'	33:R1:2104:C:O2	2.16	0.45
35:R3:945:G:C2	35:R3:946:A:C8	3.04	0.45
35:R3:1051:C:O2'	35:R3:1052:U:O5'	2.32	0.45
35:R3:1428:A:H2'	35:R3:1429:A:O4'	2.16	0.45
36:T:5:G:H2'	36:T:6:A:C8	2.51	0.45
1:1:60:ARG:HG2	1:1:61:GLY:N	2.31	0.45
9:2:145:MET:CE	9:2:153:LEU:HD21	2.46	0.45
11:21:9:GLY:O	33:R1:996:A:H1'	2.16	0.45
13:23:39:THR:HG22	13:23:42:GLU:HG3	1.98	0.45
16:27:18:ALA:O	16:27:20:ARG:NH1	2.47	0.45
21:31:65:ASN:C	21:31:65:ASN:ND2	2.70	0.45
33:R1:285:G:H2'	33:R1:286:U:C6	2.51	0.45
33:R1:1871:A:H5''	33:R1:1872:A:OP2	2.17	0.45
33:R1:2100:G:H2'	33:R1:2101:A:C8	2.51	0.45
33:R1:2258:C:O2'	33:R1:2427:C:OP2	2.32	0.45
35:R3:315:A:C5	35:R3:330:C:H5'	2.51	0.45
35:R3:985:C:H2'	35:R3:986:U:C6	2.51	0.45
35:R3:1133:G:H1	35:R3:1142:G:N2	2.14	0.45
11:21:51:VAL:HG22	11:21:52:PRO:CD	2.40	0.45
14:24:65:GLN:HG2	33:R1:328:U:H4'	1.98	0.45
27:4:168:ASP:OD2	27:4:170:ARG:NH1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:6:26:LYS:HE2	29:6:31:GLU:HG3	1.98	0.45
29:6:89:VAL:HG22	29:6:159:LYS:HA	1.97	0.45
33:R1:784:G:H5'	33:R1:785:G:OP1	2.16	0.45
33:R1:1181:U:H2'	33:R1:1182:G:C8	2.52	0.45
33:R1:1181:U:H2'	33:R1:1182:G:H8	1.82	0.45
33:R1:1932:A:H2'	33:R1:1933:G:O4'	2.16	0.45
33:R1:2405:G:O2'	33:R1:2411:A:N6	2.47	0.45
35:R3:31:G:O2'	35:R3:48:C:N4	2.50	0.45
35:R3:635:A:H2'	35:R3:636:U:H6	1.81	0.45
35:R3:1144:G:H21	35:R3:1146:A:H62	1.63	0.45
35:R3:1463:U:H2'	35:R3:1464:U:C6	2.51	0.45
5:16:11:LYS:HD3	5:16:86:LYS:HD3	1.98	0.45
9:2:266:ILE:HG21	9:2:269:ARG:HE	1.81	0.45
10:20:85:ALA:HB2	10:20:115:ALA:HB2	1.98	0.45
11:21:33:VAL:HG13	11:21:61:ALA:HB3	1.98	0.45
12:22:93:ALA:HB2	33:R1:1614:A:N1	2.32	0.45
19:3:149:ASN:OD1	19:3:150:GLN:N	2.48	0.45
28:5:113:PHE:HZ	28:5:175:PRO:HB2	1.81	0.45
30:9:80:ILE:HD11	30:9:99:ILE:HA	1.99	0.45
33:R1:1321:A:C4	33:R1:1322:A:C8	3.05	0.45
35:R3:1036:A:H2'	35:R3:1037:C:C2	2.51	0.45
3:14:48:PRO:HB3	35:R3:1422:G:H4'	1.99	0.45
19:3:2:ILE:HG13	19:3:3:GLY:H	1.82	0.45
27:4:95:LYS:O	33:R1:659:G:O2'	2.32	0.45
33:R1:1222:U:H2'	33:R1:1223:G:C8	2.52	0.45
33:R1:1538:G:H8	33:R1:1538:G:OP2	2.00	0.45
33:R1:2247:A:H2'	33:R1:2248:C:H6	1.81	0.45
35:R3:131:A:H2'	35:R3:132:C:C6	2.51	0.45
35:R3:509:A:C8	35:R3:543:U:O2'	2.69	0.45
19:3:122:VAL:HG21	19:3:129:THR:HG22	1.98	0.45
28:5:16:MET:HE2	28:5:16:MET:HA	1.98	0.45
31:E:355:ILE:HG22	31:E:504:LEU:HD13	1.97	0.45
33:R1:1054:A:H2'	33:R1:1055:G:C8	2.47	0.45
33:R1:2537:U:H2'	33:R1:2538:C:C6	2.52	0.45
33:R1:2543:G:H2'	33:R1:2544:G:C8	2.52	0.45
34:R2:32:U:C2	34:R2:51:G:N2	2.85	0.45
35:R3:595:A:H8	35:R3:595:A:OP2	2.00	0.45
35:R3:1287:A:H2'	35:R3:1288:A:C8	2.52	0.45
5:16:117:PHE:HD2	5:16:130:PHE:HD2	1.65	0.45
11:21:41:ILE:HD11	11:21:57:GLY:HA3	1.98	0.45
17:28:30:PRO:HG2	17:28:32:LEU:HD22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:29:4:LYS:H	18:29:4:LYS:HE2	1.81	0.45
28:5:31:GLU:HG3	28:5:32:LYS:HG2	1.97	0.45
31:E:323:VAL:HG11	31:E:493:CYS:SG	2.57	0.45
33:R1:191:A:H2'	33:R1:192:C:H6	1.82	0.45
33:R1:373:U:H2'	33:R1:374:A:H8	1.82	0.45
33:R1:714:U:H1'	33:R1:717:C:H5	1.81	0.45
33:R1:1589:U:H2'	33:R1:1590:A:C8	2.52	0.45
33:R1:2162:G:H2'	33:R1:2163:A:O4'	2.17	0.45
33:R1:2241:A:H2'	33:R1:2242:G:C8	2.52	0.45
33:R1:2497:A:OP2	33:R1:2497:A:H8	2.00	0.45
35:R3:552:U:O4	35:R3:553:A:N6	2.50	0.45
35:R3:607:A:H2'	35:R3:608:A:C8	2.52	0.45
14:24:47:PRO:HB3	14:24:55:GLY:HA3	1.98	0.44
15:25:75:GLN:HB2	15:25:92:VAL:HG22	1.99	0.44
24:34:16:HIS:HB2	24:34:44:VAL:HG21	1.98	0.44
27:4:63:LYS:HE3	33:R1:2444:G:OP2	2.16	0.44
31:E:66:GLN:HE21	31:E:67:PRO:HD2	1.82	0.44
33:R1:634:C:H2'	33:R1:635:C:C6	2.52	0.44
33:R1:2177:C:H5	33:R1:2178:C:C6	2.35	0.44
33:R1:2803:G:H2'	33:R1:2804:U:C6	2.50	0.44
35:R3:390:U:H2'	35:R3:391:G:H8	1.82	0.44
35:R3:1008:U:H2'	35:R3:1009:U:H6	1.82	0.44
36:T:22:G:H2'	36:T:23:A:H8	1.82	0.44
8:19:105:LYS:HA	8:19:108:ARG:HD3	1.99	0.44
12:22:31:GLN:O	12:22:35:ILE:HG23	2.17	0.44
19:3:190:LYS:HE2	33:R1:2729:G:H5'	1.99	0.44
21:31:56:ARG:HD3	21:31:56:ARG:HA	1.78	0.44
27:4:58:LYS:HG3	27:4:71:GLY:HA2	1.97	0.44
28:5:6:TYR:O	28:5:10:GLU:HG2	2.17	0.44
30:9:9:VAL:HG11	30:9:12:LEU:HB3	1.99	0.44
33:R1:141:G:H2'	33:R1:142:A:O4'	2.18	0.44
33:R1:1201:U:H2'	33:R1:1202:G:H8	1.82	0.44
33:R1:1536:C:O2'	33:R1:1537:G:N2	2.50	0.44
33:R1:2102:G:H2'	33:R1:2103:C:C6	2.53	0.44
33:R1:2193:G:H2'	33:R1:2194:U:C6	2.53	0.44
34:R2:104:A:H2'	34:R2:105:G:O4'	2.16	0.44
35:R3:301:G:HO2'	35:R3:302:G:P	2.40	0.44
35:R3:447:G:N1	35:R3:486:U:OP1	2.37	0.44
1:1:185:LEU:O	1:1:189:LEU:HD12	2.17	0.44
9:2:211:ARG:HD2	9:2:211:ARG:HA	1.63	0.44
11:21:6:GLN:HG3	11:21:11:GLN:HG3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:23:8:LEU:O	18:29:29:ARG:NH2	2.50	0.44
15:25:83:LYS:HB3	15:25:85:LYS:HZ3	1.82	0.44
31:E:45:LYS:NZ	59:E:601:ATP:O2G	2.50	0.44
33:R1:780:G:H2'	33:R1:782:A:N7	2.32	0.44
33:R1:1915:U:H4'	33:R1:1916:A:H5'	2.00	0.44
33:R1:2340:A:H5'	34:R2:41:G:H21	1.83	0.44
33:R1:2639:A:H2'	33:R1:2640:G:O4'	2.17	0.44
35:R3:640:A:O2'	35:R3:641:U:OP1	2.34	0.44
35:R3:1496:C:H2'	35:R3:1497:G:O4'	2.18	0.44
9:2:20:ASN:HB3	9:2:23:LEU:HG	1.99	0.44
14:24:27:VAL:HB	14:24:33:VAL:HG12	1.99	0.44
15:25:20:LEU:HD23	15:25:20:LEU:HA	1.80	0.44
29:6:154:GLU:HG2	29:6:157:LYS:H	1.81	0.44
31:E:234:ARG:H	31:E:234:ARG:HG2	1.67	0.44
33:R1:286:U:H3	33:R1:354:A:N6	2.14	0.44
33:R1:286:U:H2'	33:R1:287:G:C8	2.52	0.44
33:R1:851:C:H2'	33:R1:852:U:H6	1.82	0.44
33:R1:1063:G:H2'	33:R1:1063:G:N3	2.32	0.44
33:R1:1771:C:H2'	33:R1:1772:A:C8	2.53	0.44
35:R3:393:A:H2'	35:R3:394:G:H5'	1.98	0.44
3:14:70:ARG:HG2	3:14:70:ARG:NH1	2.33	0.44
18:29:24:GLU:O	18:29:28:LEU:HB2	2.18	0.44
31:E:219:ARG:HG2	31:E:220:TYR:N	2.33	0.44
31:E:548:ILE:HG23	33:R1:2112:G:O2'	2.18	0.44
33:R1:576:U:H2'	33:R1:577:G:C8	2.53	0.44
33:R1:1169:A:H2'	33:R1:1170:C:C6	2.52	0.44
33:R1:1270:C:H5''	33:R1:1271:G:O5'	2.17	0.44
33:R1:2591:C:H2'	33:R1:2592:G:H8	1.77	0.44
35:R3:471:U:H3'	35:R3:472:U:H5''	1.99	0.44
3:14:30:ARG:HD2	33:R1:2674:G:H4'	2.00	0.44
12:22:20:VAL:HG11	12:22:44:ALA:HA	1.98	0.44
14:24:12:VAL:HB	14:24:17:ASP:O	2.18	0.44
31:E:51:ILE:HG12	31:E:59:ILE:HG21	2.00	0.44
33:R1:149:A:N1	33:R1:176:A:N1	2.65	0.44
33:R1:700:G:O2'	33:R1:1632:A:N3	2.38	0.44
34:R2:52:A:HO2'	34:R2:53:A:H8	1.60	0.44
35:R3:160:A:H2'	35:R3:161:A:O4'	2.18	0.44
35:R3:457:G:H1	35:R3:475:C:H42	1.66	0.44
35:R3:500:G:H4'	35:R3:501:C:OP1	2.18	0.44
35:R3:868:C:H2'	35:R3:869:G:O4'	2.18	0.44
4:15:14:LYS:HG3	4:15:15:ALA:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:24:9:GLU:OE1	14:24:9:GLU:HA	2.18	0.44
29:6:34:ARG:NH1	29:6:70:LEU:HD22	2.29	0.44
31:E:82:PRO:HA	31:E:160:ILE:HG22	1.99	0.44
33:R1:1048:A:C5	33:R1:1111:A:H8	2.36	0.44
33:R1:1171:G:C6	33:R1:1176:U:N3	2.83	0.44
33:R1:1527:G:N1	33:R1:1544:A:OP2	2.41	0.44
33:R1:2120:G:H2'	33:R1:2121:G:C8	2.52	0.44
33:R1:2190:G:H2'	33:R1:2191:A:H8	1.81	0.44
35:R3:500:G:H2'	35:R3:501:C:C6	2.52	0.44
35:R3:861:G:H2'	35:R3:862:C:O4'	2.16	0.44
35:R3:1402:C:H2'	35:R3:1403:C:O4'	2.18	0.44
11:21:83:TYR:OH	11:21:85:LYS:HE3	2.18	0.44
12:22:93:ALA:HB2	33:R1:1614:A:C2	2.53	0.44
19:3:106:LYS:HG3	19:3:174:SER:HA	2.00	0.44
33:R1:106:C:H2'	33:R1:107:G:H8	1.82	0.44
33:R1:2137:U:H2'	33:R1:2138:G:H8	1.82	0.44
33:R1:2148:G:H2'	33:R1:2149:U:C5	2.52	0.44
35:R3:592:G:H2'	35:R3:593:U:C6	2.52	0.44
35:R3:639:G:O2'	35:R3:640:A:H5'	2.18	0.44
35:R3:757:U:H2'	35:R3:758:C:O4'	2.17	0.44
35:R3:1042:A:H2'	35:R3:1043:G:C8	2.53	0.44
35:R3:1121:U:H2'	35:R3:1122:U:C6	2.53	0.44
36:T:53:G:C4	36:T:62:C:C2	3.05	0.44
36:T:69:A:H2'	36:T:70:C:O4'	2.18	0.44
4:15:32:GLY:HA2	33:R1:1190:G:H5''	2.00	0.44
4:15:62:PRO:HB2	25:35:29:ARG:HH21	1.83	0.44
11:21:73:LYS:HB3	11:21:73:LYS:HE3	1.70	0.44
23:33:33:LEU:HD12	23:33:33:LEU:HA	1.84	0.44
27:4:176:ASP:HB2	27:4:179:SER:H	1.83	0.44
28:5:109:ARG:HD2	28:5:136:ILE:HA	2.00	0.44
31:E:404:VAL:HG23	31:E:440:LYS:O	2.18	0.44
33:R1:1980:G:O2'	33:R1:1982:U:OP2	2.36	0.44
35:R3:107:G:H5''	35:R3:379:C:OP1	2.18	0.44
35:R3:494:G:O2'	35:R3:496:A:H1'	2.17	0.44
35:R3:883:C:O2'	35:R3:884:U:H5'	2.18	0.44
35:R3:1412:C:H2'	35:R3:1413:A:H8	1.81	0.44
7:18:108:ASP:O	7:18:112:GLU:HG3	2.18	0.43
10:20:108:LEU:HD23	10:20:108:LEU:HA	1.88	0.43
13:23:39:THR:CG2	13:23:42:GLU:HG3	2.48	0.43
15:25:28:ALA:N	15:25:40:ILE:O	2.48	0.43
18:29:49:ASP:O	18:29:53:VAL:HG23	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:6:3:VAL:HG21	33:R1:2748:A:H5'	1.99	0.43
33:R1:64:A:H2'	33:R1:65:U:H6	1.82	0.43
33:R1:1842:G:H2'	33:R1:1843:C:C6	2.52	0.43
33:R1:2129:C:N3	33:R1:2160:C:N4	2.64	0.43
33:R1:2773:C:C2'	33:R1:2774:C:H5'	2.48	0.43
33:R1:2810:A:H2'	33:R1:2811:G:O4'	2.17	0.43
35:R3:110:C:H2'	35:R3:111:G:O4'	2.17	0.43
35:R3:736:C:H2'	35:R3:737:C:C6	2.53	0.43
35:R3:1439:G:O2'	35:R3:1440:U:O4'	2.34	0.43
36:T:57:G:C5	36:T:58:A:H2	2.36	0.43
3:14:2:ILE:HD12	3:14:6:THR:HG21	1.98	0.43
3:14:31:ARG:HH22	33:R1:2676:C:P	2.42	0.43
9:2:121:ALA:HB3	9:2:129:LEU:HD22	2.00	0.43
9:2:155:ARG:HB2	33:R1:1818:U:H2'	1.99	0.43
9:2:244:VAL:HA	9:2:251:THR:H	1.83	0.43
14:24:46:LYS:HB2	14:24:46:LYS:HE3	1.72	0.43
31:E:47:THR:OG1	59:E:601:ATP:O2A	2.32	0.43
33:R1:279:A:H2'	33:R1:280:U:H5'	2.01	0.43
33:R1:608:A:H2'	33:R1:609:A:C8	2.53	0.43
33:R1:723:C:H2'	33:R1:724:U:O4'	2.18	0.43
33:R1:1340:U:C5	33:R1:1603:A:C8	3.07	0.43
33:R1:1873:G:H2'	33:R1:1874:C:C6	2.53	0.43
33:R1:2112:G:H2'	33:R1:2112:G:N3	2.32	0.43
33:R1:2124:G:N2	33:R1:2174:C:H41	2.16	0.43
33:R1:2457:U:H5	33:R1:2494:G:O6	2.01	0.43
35:R3:330:C:O2'	35:R3:331:G:N2	2.27	0.43
35:R3:1150:A:O2'	35:R3:1151:A:P	2.76	0.43
35:R3:1175:G:H2'	35:R3:1176:A:H8	1.82	0.43
35:R3:1186:G:HO2'	35:R3:1187:G:P	2.41	0.43
35:R3:1512:U:H2'	35:R3:1513:A:C8	2.53	0.43
5:16:42:THR:HA	5:16:93:VAL:HA	1.99	0.43
6:17:58:ASP:OD1	6:17:63:ARG:NE	2.37	0.43
7:18:69:ASP:OD2	7:18:69:ASP:N	2.51	0.43
7:18:111:ARG:NE	7:18:117:PHE:OXT	2.52	0.43
9:2:13:ARG:NH2	33:R1:1693:U:O2'	2.51	0.43
33:R1:279:A:C2'	33:R1:280:U:H5'	2.48	0.43
33:R1:1963:U:O5'	33:R1:1963:U:H6	2.02	0.43
33:R1:2146:C:O2'	33:R1:2147:A:H8	2.00	0.43
35:R3:950:U:H2'	35:R3:951:G:H8	1.82	0.43
35:R3:1187:G:H2'	35:R3:1188:A:H8	1.82	0.43
2:13:39:LYS:NZ	33:R1:1007:C:OP1	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:15:73:ILE:HD12	4:15:106:GLU:OE1	2.18	0.43
10:20:116:LEU:HA	10:20:116:LEU:HD23	1.79	0.43
31:E:5:VAL:N	31:E:29:PHE:O	2.26	0.43
33:R1:278:A:C8	33:R1:279:A:C8	3.06	0.43
33:R1:394:C:H2'	33:R1:395:U:O4'	2.19	0.43
33:R1:2244:U:O2	33:R1:2434:A:H2'	2.18	0.43
33:R1:2329:U:H2'	33:R1:2330:G:H8	1.84	0.43
33:R1:2411:A:H2'	33:R1:2412:A:H8	1.84	0.43
33:R1:2533:U:H2'	33:R1:2534:A:O4'	2.18	0.43
33:R1:2812:G:H2'	33:R1:2813:A:C8	2.53	0.43
35:R3:129:A:H2	35:R3:232:G:H22	1.65	0.43
35:R3:216:U:H2'	35:R3:217:C:C6	2.54	0.43
35:R3:368:U:H5'	35:R3:369:G:H5''	2.00	0.43
35:R3:746:A:H2'	35:R3:747:A:C8	2.53	0.43
35:R3:1410:A:H2'	35:R3:1411:C:H6	1.83	0.43
2:13:104:ALA:O	2:13:108:MET:HG3	2.17	0.43
3:14:70:ARG:NH1	33:R1:2684:U:O4'	2.51	0.43
4:15:96:LYS:HE2	4:15:103:ILE:HA	2.01	0.43
6:17:60:VAL:HG21	33:R1:1455:G:H5'	2.00	0.43
12:22:3:THR:O	12:22:3:THR:OG1	2.25	0.43
21:31:16:CYS:SG	21:31:17:SER:N	2.90	0.43
28:5:4:HIS:O	28:5:8:LYS:HG3	2.18	0.43
29:6:16:VAL:HG11	29:6:49:LEU:HD11	2.00	0.43
30:9:42:LYS:HA	30:9:45:GLU:HG3	2.01	0.43
31:E:392:ASP:N	31:E:392:ASP:OD1	2.52	0.43
31:E:526:ASN:OD1	31:E:529:GLU:HG2	2.18	0.43
33:R1:276:U:O2'	33:R1:277:G:OP1	2.32	0.43
33:R1:1427:A:H4'	33:R1:1428:C:O4'	2.19	0.43
33:R1:1891:G:HO2'	33:R1:2235:G:HO2'	1.59	0.43
33:R1:2281:A:O2'	33:R1:2282:G:H5'	2.18	0.43
35:R3:900:A:H2'	35:R3:901:A:C8	2.53	0.43
35:R3:959:A:H5''	35:R3:960:U:OP2	2.18	0.43
35:R3:1003:G:O3'	35:R3:1004:A:H4'	2.18	0.43
35:R3:1246:A:H2'	35:R3:1247:U:C6	2.53	0.43
2:13:24:THR:HG21	33:R1:1141:U:OP1	2.19	0.43
17:28:14:GLY:HA3	17:28:28:PHE:HE1	1.84	0.43
24:34:12:ARG:HG2	24:34:44:VAL:HG11	2.01	0.43
26:36:4:ARG:HB2	33:R1:2466:C:OP1	2.18	0.43
33:R1:27:G:N2	33:R1:512:G:H1'	2.33	0.43
33:R1:57:C:H2'	33:R1:58:G:O4'	2.19	0.43
33:R1:596:U:H2'	33:R1:597:G:H8	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:R1:654:A:H3'	33:R1:654:A:N3	2.33	0.43
33:R1:858:G:N3	33:R1:2268:A:H2'	2.33	0.43
33:R1:1539:U:H2'	33:R1:1540:G:C8	2.54	0.43
33:R1:2327:A:H2'	33:R1:2328:A:C8	2.53	0.43
33:R1:2577:A:H2'	33:R1:2614:A:N6	2.34	0.43
33:R1:2895:G:H2'	33:R1:2896:C:C6	2.54	0.43
35:R3:343:U:O3'	35:R3:344:A:H8	2.02	0.43
35:R3:414:A:C4	35:R3:415:A:C8	3.06	0.43
35:R3:427:U:H3'	35:R3:428:G:H8	1.83	0.43
35:R3:1001:C:O2	35:R3:1040:U:N3	2.51	0.43
26:36:2:LYS:HE2	26:36:32:LYS:O	2.19	0.43
27:4:194:LYS:HE2	27:4:194:LYS:HA	2.01	0.43
28:5:33:ILE:HG12	28:5:95:MET:CG	2.45	0.43
28:5:73:VAL:HG21	28:5:76:PHE:HD2	1.83	0.43
29:6:2:ARG:H	29:6:2:ARG:HG2	1.46	0.43
30:9:62:LEU:HD23	30:9:62:LEU:HA	1.84	0.43
33:R1:609:A:H2'	33:R1:610:C:O4'	2.19	0.43
33:R1:667:U:H2'	33:R1:668:A:O4'	2.19	0.43
33:R1:1064:C:H5''	33:R1:1066:U:OP2	2.18	0.43
33:R1:1292:G:H2'	33:R1:1293:C:H6	1.83	0.43
33:R1:1478:G:H1	33:R1:1513:U:H3	1.67	0.43
33:R1:2128:G:H2'	33:R1:2129:C:H6	1.83	0.43
33:R1:2134:A:N3	33:R1:2157:G:H4'	2.34	0.43
33:R1:2813:A:H2'	33:R1:2814:A:C8	2.54	0.43
35:R3:108:G:H5'	35:R3:109:A:C5'	2.43	0.43
35:R3:686:U:H2'	35:R3:687:A:C8	2.54	0.43
35:R3:945:G:H21	35:R3:1334:G:H4'	1.84	0.43
35:R3:982:U:H4'	35:R3:983:A:O4'	2.19	0.43
5:16:28:PHE:HB2	5:16:104:GLU:OE2	2.18	0.43
9:2:256:THR:OG1	33:R1:1797:G:O2'	2.33	0.43
14:24:13:LEU:O	14:24:18:LYS:HD2	2.19	0.43
15:25:77:VAL:HG23	15:25:89:ILE:HG12	1.99	0.43
31:E:552:ARG:HH12	33:R1:2168:G:H1	1.67	0.43
33:R1:969:G:H2'	33:R1:970:U:C6	2.54	0.43
33:R1:2175:C:N4	33:R1:2176:A:C6	2.86	0.43
35:R3:120:A:H4'	35:R3:121:U:OP1	2.18	0.43
2:13:56:VAL:HB	2:13:124:VAL:HA	2.01	0.43
4:15:43:GLY:N	33:R1:671:C:OP1	2.45	0.43
9:2:186:ASP:OD1	9:2:186:ASP:N	2.52	0.43
31:E:141:ASN:OD1	31:E:141:ASN:N	2.48	0.43
33:R1:704:G:H1'	33:R1:727:A:N6	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:R1:947:A:H2'	33:R1:948:C:C6	2.54	0.43
33:R1:2458:G:O2'	33:R1:2460:U:O4	2.31	0.43
33:R1:2655:G:O2'	33:R1:2664:G:O6	2.31	0.43
33:R1:2794:C:H2'	33:R1:2795:C:C6	2.54	0.43
35:R3:273:U:O2'	35:R3:274:A:H5''	2.18	0.43
35:R3:604:G:H2'	35:R3:605:U:O4'	2.18	0.43
35:R3:1379:G:O2'	35:R3:1380:U:H5'	2.19	0.43
1:1:208:TYR:CE1	1:1:209:ILE:HG12	2.54	0.43
3:14:91:SER:O	3:14:93:GLN:N	2.52	0.43
10:20:86:SER:HB3	11:21:52:PRO:HD3	2.00	0.43
12:22:87:PRO:HB3	33:R1:1614:A:C6	2.54	0.43
16:27:9:SER:OG	16:27:10:THR:N	2.52	0.43
22:32:28:SER:O	22:32:36:LYS:HA	2.19	0.43
33:R1:1170:C:HO2'	33:R1:1171:G:H8	1.67	0.43
33:R1:2589:A:H2'	33:R1:2590:A:C8	2.53	0.43
33:R1:2698:U:O2'	33:R1:2699:C:H5'	2.18	0.43
35:R3:265:G:N2	35:R3:267:C:H5'	2.34	0.43
35:R3:390:U:H2'	35:R3:391:G:C8	2.54	0.43
36:T:66:A:H2'	36:T:67:U:H6	1.83	0.43
8:19:7:LEU:HD11	19:3:186:LEU:HD21	2.01	0.42
20:30:52:PHE:CG	34:R2:83:G:H4'	2.54	0.42
28:5:157:THR:HG23	28:5:159:ALA:H	1.83	0.42
29:6:98:LYS:HG3	29:6:98:LYS:O	2.18	0.42
31:E:103:ARG:NE	31:E:106:GLU:OE1	2.52	0.42
33:R1:274:C:H41	33:R1:363:G:H21	1.67	0.42
33:R1:645:C:O2'	33:R1:646:U:H5'	2.18	0.42
33:R1:783:A:O2'	33:R1:1779:U:O2	2.26	0.42
33:R1:1856:U:H2'	33:R1:1857:G:O4'	2.19	0.42
35:R3:468:A:H2'	35:R3:468:A:N3	2.33	0.42
35:R3:606:G:N2	35:R3:632:U:OP1	2.24	0.42
35:R3:692:U:O2'	35:R3:694:A:N7	2.38	0.42
35:R3:958:A:H8	35:R3:985:C:O2'	2.02	0.42
35:R3:992:U:H1'	35:R3:993:G:N2	2.34	0.42
35:R3:1118:U:H3'	35:R3:1119:C:H6	1.83	0.42
35:R3:1452:C:H4'	35:R3:1453:G:C2	2.54	0.42
1:1:42:VAL:HG22	1:1:176:GLY:H	1.83	0.42
5:16:123:LYS:NZ	33:R1:2483:C:O2	2.49	0.42
19:3:121:THR:HB	19:3:127:PHE:CD2	2.54	0.42
25:35:7:ARG:HD2	25:35:7:ARG:HA	1.79	0.42
30:9:94:ILE:HG22	30:9:98:ASP:OD2	2.19	0.42
33:R1:315:G:H2'	33:R1:316:C:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:R1:1190:G:H2'	33:R1:1191:G:C8	2.54	0.42
33:R1:1239:G:H2'	33:R1:1240:U:O4'	2.17	0.42
33:R1:1678:A:H2'	33:R1:1679:A:O4'	2.19	0.42
33:R1:2070:A:H2'	33:R1:2071:A:O4'	2.19	0.42
33:R1:2567:G:H2'	33:R1:2568:U:C6	2.54	0.42
33:R1:2804:U:H2'	33:R1:2805:C:H6	1.84	0.42
35:R3:553:A:H2'	35:R3:554:A:H8	1.83	0.42
35:R3:966:G:C2	36:T:34:A:H5'	2.54	0.42
10:20:16:ILE:HD13	10:20:16:ILE:HA	1.86	0.42
29:6:108:PHE:HB3	33:R1:2667:C:H1'	2.00	0.42
30:9:66:ASN:HB3	30:9:134:VAL:HG11	2.02	0.42
31:E:38:LEU:HA	31:E:38:LEU:HD23	1.74	0.42
31:E:151:LEU:HD11	31:E:550:TYR:CZ	2.54	0.42
31:E:500:ASP:HB3	31:E:503:PHE:HB3	2.01	0.42
33:R1:1857:G:N2	33:R1:1884:G:H2'	2.33	0.42
33:R1:1906:G:N1	33:R1:1924:C:N3	2.38	0.42
33:R1:2040:G:H2'	33:R1:2041:U:O4'	2.20	0.42
35:R3:312:C:H2'	35:R3:313:A:C8	2.54	0.42
35:R3:634:C:H2'	35:R3:635:A:C8	2.53	0.42
35:R3:676:A:H2'	35:R3:677:U:H6	1.84	0.42
5:16:81:ARG:NH2	16:27:5:LYS:HG3	2.32	0.42
7:18:52:SER:O	7:18:55:GLU:HG3	2.19	0.42
31:E:164:SER:HB2	59:E:602:ATP:O1G	2.19	0.42
33:R1:1050:A:O2'	33:R1:1051:G:P	2.78	0.42
33:R1:1167:C:H2'	33:R1:1168:G:O4'	2.20	0.42
33:R1:1328:A:H2'	33:R1:1330:C:C5	2.53	0.42
33:R1:2224:G:H4'	33:R1:2226:C:C2	2.55	0.42
33:R1:2469:A:N6	33:R1:2481:G:O2'	2.42	0.42
33:R1:2595:G:N2	33:R1:2598:A:OP2	2.35	0.42
33:R1:2804:U:H2'	33:R1:2805:C:C6	2.54	0.42
35:R3:32:A:N1	35:R3:552:U:H5	2.17	0.42
35:R3:62:U:H5	35:R3:105:G:O6	2.02	0.42
35:R3:287:U:H2'	35:R3:288:A:H5'	2.01	0.42
35:R3:401:C:H2'	35:R3:402:G:H5'	2.01	0.42
35:R3:918:A:H2'	35:R3:919:A:C8	2.54	0.42
35:R3:1170:A:H2'	35:R3:1171:A:O4'	2.19	0.42
3:14:68:GLY:HA3	3:14:78:ARG:HA	2.01	0.42
4:15:63:LYS:HG2	25:35:11:LYS:HB3	2.00	0.42
8:19:4:ILE:O	8:19:8:GLU:HG3	2.20	0.42
9:2:3:VAL:HG22	9:2:17:LYS:HB2	2.00	0.42
12:22:74:ILE:HD13	12:22:105:VAL:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:25:28:ALA:HB3	15:25:40:ILE:HG22	2.01	0.42
22:32:8:THR:HB	22:32:10:SER:H	1.83	0.42
24:34:3:ARG:HD3	24:34:3:ARG:HA	1.79	0.42
27:4:131:THR:HG21	33:R1:320:A:H2'	2.01	0.42
33:R1:30:G:O2'	33:R1:1214:A:N3	2.47	0.42
33:R1:44:A:H2'	33:R1:45:G:O4'	2.20	0.42
35:R3:456:A:N6	35:R3:476:U:H3	2.10	0.42
35:R3:553:A:H2'	35:R3:554:A:C8	2.55	0.42
35:R3:957:U:H2'	35:R3:959:A:OP2	2.19	0.42
35:R3:1143:G:H2'	35:R3:1144:G:H8	1.84	0.42
2:13:93:ILE:HD13	2:13:93:ILE:HA	1.89	0.42
7:18:43:ASN:HD22	7:18:46:GLU:CD	2.22	0.42
10:20:14:LYS:HB3	10:20:14:LYS:HE2	1.78	0.42
11:21:51:VAL:HG13	11:21:52:PRO:O	2.20	0.42
15:25:76:ASP:OD1	15:25:77:VAL:N	2.52	0.42
17:28:37:PHE:CZ	17:28:55:MET:HG2	2.54	0.42
31:E:15:VAL:HG23	31:E:19:ARG:HB3	2.01	0.42
31:E:378:GLY:O	31:E:379:THR:OG1	2.38	0.42
33:R1:255:A:HO2'	33:R1:384:A:H8	1.66	0.42
33:R1:528:A:C2	33:R1:2042:A:H2'	2.54	0.42
33:R1:533:G:H2'	33:R1:534:U:C6	2.55	0.42
33:R1:698:C:O2'	33:R1:734:A:N6	2.48	0.42
33:R1:886:A:H3'	33:R1:886:A:N3	2.34	0.42
33:R1:1370:C:H2'	33:R1:1371:G:O4'	2.20	0.42
33:R1:1485:U:H2'	33:R1:1486:U:H6	1.85	0.42
33:R1:2126:A:H2	33:R1:2127:G:H1'	1.83	0.42
33:R1:2545:G:H2'	33:R1:2546:U:O4'	2.19	0.42
33:R1:2896:C:O2'	33:R1:2897:U:O5'	2.36	0.42
35:R3:757:U:O2'	35:R3:879:C:O2	2.36	0.42
35:R3:766:A:OP2	35:R3:812:G:N2	2.52	0.42
13:23:61:LEU:HD12	33:R1:1341:G:H5'	2.01	0.42
30:9:68:ARG:O	30:9:72:ILE:HG13	2.19	0.42
31:E:169:ARG:HB3	31:E:169:ARG:HH11	1.84	0.42
33:R1:955:U:H5	33:R1:962:G:H1	1.68	0.42
33:R1:1086:A:H3'	33:R1:1086:A:N3	2.35	0.42
33:R1:1733:G:H2'	33:R1:1734:G:C8	2.53	0.42
33:R1:2177:C:H3'	33:R1:2178:C:H5''	2.02	0.42
33:R1:2412:A:H2'	33:R1:2413:G:O4'	2.20	0.42
33:R1:2688:G:H1'	33:R1:2721:A:N6	2.34	0.42
33:R1:2740:A:H2'	33:R1:2741:A:C8	2.54	0.42
35:R3:834:U:H2'	35:R3:835:U:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:R3:984:C:H2'	35:R3:985:C:C6	2.55	0.42
35:R3:1058:G:H2'	35:R3:1059:C:O4'	2.19	0.42
35:R3:1149:C:O2'	35:R3:1150:A:OP1	2.30	0.42
35:R3:1316:G:N1	35:R3:1319:A:OP2	2.50	0.42
36:T:67:U:H2'	36:T:68:C:C6	2.54	0.42
1:1:200:LYS:HG2	1:1:201:PRO:HD2	2.02	0.42
3:14:77:ILE:O	3:14:77:ILE:HG22	2.20	0.42
6:17:36:THR:OG1	6:17:37:THR:N	2.53	0.42
26:36:16:ILE:HD13	26:36:25:VAL:HG22	2.02	0.42
27:4:188:MET:HE2	27:4:193:VAL:HG22	2.02	0.42
33:R1:306:U:H2'	33:R1:307:G:O4'	2.19	0.42
33:R1:638:G:H2'	33:R1:639:U:O4'	2.20	0.42
33:R1:668:A:H2'	33:R1:670:A:H62	1.85	0.42
33:R1:1505:A:H2'	33:R1:1506:U:C6	2.55	0.42
33:R1:1838:C:N4	33:R1:1898:U:H2'	2.35	0.42
33:R1:2081:U:H2'	33:R1:2082:A:C8	2.54	0.42
34:R2:66:A:H61	34:R2:107:G:H3'	1.84	0.42
35:R3:402:G:O2'	35:R3:403:C:H6	2.02	0.42
1:1:53:ARG:HB3	1:1:54:LYS:HE2	2.01	0.42
13:23:30:ILE:HG22	13:23:32:LEU:HG	2.01	0.42
31:E:188:GLN:HE22	31:E:474:ASP:HA	1.85	0.42
31:E:327:SER:HB3	31:E:379:THR:HB	2.02	0.42
33:R1:6:A:H2'	33:R1:7:G:O4'	2.20	0.42
33:R1:1263:U:H2'	33:R1:1264:A:C8	2.55	0.42
33:R1:2113:U:H2'	33:R1:2114:A:C8	2.54	0.42
34:R2:32:U:C2	34:R2:33:G:C8	3.08	0.42
35:R3:67:C:H2'	35:R3:68:G:C8	2.54	0.42
35:R3:157:U:O4	35:R3:164:G:O6	2.38	0.42
35:R3:593:U:H2'	35:R3:594:U:C6	2.55	0.42
35:R3:711:G:O2'	35:R3:712:A:H5'	2.20	0.42
35:R3:811:C:O2'	35:R3:901:A:N1	2.52	0.42
1:1:186:LYS:HE3	1:1:190:GLU:HB2	2.00	0.42
1:1:208:TYR:CD1	1:1:209:ILE:HG23	2.54	0.42
4:15:89:VAL:O	4:15:94:THR:HG21	2.19	0.42
7:18:51:ALA:HB3	7:18:78:VAL:HG22	2.02	0.42
11:21:71:LYS:HG3	11:21:90:ARG:HG3	2.01	0.42
12:22:61:ASN:ND2	33:R1:495:G:O2'	2.51	0.42
15:25:90:ASP:N	15:25:90:ASP:OD2	2.52	0.42
19:3:98:VAL:C	19:3:100:LEU:H	2.22	0.42
27:4:147:LEU:HD11	27:4:170:ARG:HD2	2.02	0.42
33:R1:134:G:O6	33:R1:144:A:N1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:R1:709:U:H2'	33:R1:710:U:C6	2.55	0.42
33:R1:1090:A:H61	33:R1:1101:U:H3	1.67	0.42
33:R1:1297:C:OP1	33:R1:2710:C:H4'	2.19	0.42
33:R1:1717:A:H2'	33:R1:1718:G:O4'	2.20	0.42
34:R2:45:A:C4	34:R2:46:A:C8	3.08	0.42
35:R3:246:A:C2	35:R3:282:A:C5	3.08	0.42
35:R3:728:A:H2'	35:R3:729:A:C8	2.54	0.42
35:R3:1219:A:H2'	35:R3:1220:G:C8	2.54	0.42
25:35:18:LYS:HB2	33:R1:651:G:OP1	2.20	0.41
30:9:8:LYS:HB2	30:9:9:VAL:H	1.73	0.41
31:E:387:LYS:HB3	31:E:463:GLY:HA2	2.02	0.41
33:R1:558:U:H2'	33:R1:559:G:H8	1.85	0.41
33:R1:588:U:H2'	33:R1:589:U:C6	2.55	0.41
33:R1:687:C:H5	33:R1:787:C:H5''	1.85	0.41
33:R1:742:A:H2'	33:R1:743:A:H8	1.83	0.41
33:R1:1540:G:H2'	33:R1:1541:C:H6	1.83	0.41
33:R1:2128:G:H1	33:R1:2160:C:N4	2.18	0.41
33:R1:2508:G:H1	33:R1:2580:U:H5	1.67	0.41
33:R1:2636:C:H2'	33:R1:2637:U:C6	2.55	0.41
33:R1:2751:G:H2'	33:R1:2751:G:N3	2.35	0.41
33:R1:2809:A:OP2	33:R1:2890:G:N1	2.26	0.41
35:R3:187:G:C2	35:R3:191:G:C6	3.08	0.41
35:R3:223:A:H2'	35:R3:224:U:H6	1.85	0.41
35:R3:335:C:H2'	35:R3:336:A:H8	1.83	0.41
35:R3:344:A:H5''	35:R3:345:C:C5	2.55	0.41
35:R3:352:C:O2'	35:R3:354:G:OP1	2.31	0.41
35:R3:721:G:H4'	35:R3:722:G:O4'	2.20	0.41
35:R3:1155:A:H2'	35:R3:1156:G:O4'	2.20	0.41
35:R3:1171:A:H2'	35:R3:1172:C:H6	1.84	0.41
1:1:20:GLN:OE1	1:1:20:GLN:N	2.53	0.41
11:21:3:ALA:HA	11:21:40:MET:O	2.20	0.41
24:34:4:THR:HG22	33:R1:687:C:H1'	2.01	0.41
31:E:404:VAL:HG22	31:E:445:LEU:HD11	2.02	0.41
33:R1:286:U:H3	33:R1:354:A:H61	1.66	0.41
33:R1:743:A:O2'	33:R1:1659:G:OP1	2.33	0.41
33:R1:1130:U:C2	33:R1:2025:C:H5''	2.55	0.41
33:R1:1341:G:OP1	33:R1:1397:U:N3	2.47	0.41
33:R1:1842:G:H2'	33:R1:1843:C:H6	1.85	0.41
33:R1:2147:A:C5	33:R1:2148:G:H1'	2.55	0.41
33:R1:2572:A:OP1	33:R1:2574:G:H4'	2.20	0.41
35:R3:100:G:H2'	35:R3:101:A:H8	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:R3:274:A:HO2'	35:R3:275:G:H8	1.64	0.41
35:R3:592:G:H2'	35:R3:593:U:H6	1.86	0.41
35:R3:692:U:H1'	35:R3:695:A:N7	2.35	0.41
35:R3:983:A:H5'	35:R3:984:C:OP2	2.20	0.41
35:R3:999:C:C3'	35:R3:1000:A:H4'	2.45	0.41
35:R3:1101:A:H4'	35:R3:1102:A:O5'	2.19	0.41
35:R3:1122:U:O2'	35:R3:1123:U:H6	2.03	0.41
35:R3:1228:C:H2'	35:R3:1229:A:H8	1.85	0.41
18:29:4:LYS:H	18:29:4:LYS:CE	2.34	0.41
26:36:24:ARG:NH2	26:36:36:ARG:HG3	2.35	0.41
33:R1:159:G:H22	33:R1:2216:G:N2	2.18	0.41
33:R1:439:A:H2'	33:R1:440:C:O4'	2.21	0.41
33:R1:569:U:H2'	33:R1:570:G:O4'	2.20	0.41
33:R1:898:C:H2'	33:R1:899:A:O4'	2.20	0.41
33:R1:1005:C:H1'	33:R1:1012:U:N3	2.35	0.41
35:R3:144:G:H2'	35:R3:145:G:C8	2.55	0.41
35:R3:201:G:H2'	35:R3:202:G:O4'	2.20	0.41
35:R3:325:A:H2'	35:R3:326:G:O4'	2.21	0.41
35:R3:515:G:H3'	35:R3:516:U:O2	2.20	0.41
35:R3:838:G:C6	35:R3:849:G:C6	3.08	0.41
35:R3:1330:U:C4	35:R3:1331:G:C6	3.08	0.41
7:18:92:PHE:HB2	7:18:117:PHE:CD2	2.55	0.41
14:24:91:LYS:NZ	33:R1:83:A:OP1	2.48	0.41
16:27:18:ALA:HB1	33:R1:2271:G:OP1	2.20	0.41
33:R1:1589:U:C2	33:R1:1590:A:C8	3.08	0.41
35:R3:665:A:H1'	35:R3:733:G:H5'	2.02	0.41
35:R3:1063:C:H3'	35:R3:1064:G:H2'	2.02	0.41
35:R3:1102:A:C6	35:R3:1103:C:N4	2.88	0.41
1:1:40:GLU:HG3	1:1:178:VAL:HB	2.03	0.41
1:1:212:VAL:HB	1:1:224:VAL:HG22	2.03	0.41
5:16:42:THR:O	5:16:46:ILE:HG12	2.20	0.41
12:22:4:ILE:HG22	12:22:106:VAL:HG22	2.02	0.41
29:6:171:LYS:HG2	29:6:172:GLU:H	1.85	0.41
33:R1:257:C:H5'	33:R1:258:G:OP2	2.20	0.41
33:R1:1588:G:H2'	33:R1:1589:U:C6	2.56	0.41
33:R1:1916:A:H2'	33:R1:1917:U:O2	2.20	0.41
33:R1:2395:C:H2'	33:R1:2396:G:O4'	2.20	0.41
33:R1:2503:A:N3	33:R1:2503:A:H5'	2.35	0.41
35:R3:105:G:H2'	35:R3:106:C:O4'	2.19	0.41
35:R3:107:G:O2'	35:R3:108:G:OP2	2.32	0.41
35:R3:185:U:H2'	35:R3:186:C:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:R3:590:U:H2'	35:R3:591:U:C6	2.55	0.41
35:R3:827:U:H2'	35:R3:870:U:O4	2.21	0.41
35:R3:925:G:H1'	35:R3:1502:A:C4	2.56	0.41
35:R3:935:A:O2'	35:R3:1383:C:O2	2.38	0.41
36:T:22:G:O2'	36:T:23:A:H5'	2.20	0.41
36:T:44:G:O2'	36:T:45:G:H5'	2.20	0.41
1:1:16:ASP:N	1:1:16:ASP:OD1	2.53	0.41
1:1:21:TYR:N	1:1:21:TYR:HD1	2.19	0.41
2:13:17:VAL:HG22	2:13:55:ILE:HB	2.01	0.41
4:15:14:LYS:HG3	4:15:15:ALA:N	2.35	0.41
5:16:69:PRO:HA	5:16:94:ALA:HB2	2.02	0.41
12:22:25:ARG:HG3	12:22:74:ILE:HG22	2.02	0.41
16:27:11:ARG:O	16:27:14:ARG:NH2	2.53	0.41
18:29:12:GLU:HA	18:29:12:GLU:OE2	2.20	0.41
19:3:46:ARG:HB3	19:3:84:LEU:HD12	2.02	0.41
28:5:159:ALA:HB1	28:5:164:GLU:HB2	2.03	0.41
30:9:43:ASN:HA	30:9:46:PHE:HD2	1.86	0.41
31:E:286:LYS:HD2	31:E:286:LYS:HA	1.90	0.41
33:R1:308:G:H2'	33:R1:309:A:C8	2.56	0.41
33:R1:518:G:H2'	33:R1:519:U:C6	2.56	0.41
33:R1:598:U:H2'	33:R1:599:A:C8	2.55	0.41
33:R1:688:U:C2'	33:R1:689:A:H5'	2.51	0.41
33:R1:881:G:H2'	33:R1:882:G:H8	1.83	0.41
33:R1:1201:U:H2'	33:R1:1202:G:C8	2.56	0.41
33:R1:1429:G:H2'	33:R1:1430:G:C8	2.55	0.41
33:R1:1858:A:H61	33:R1:1884:G:H1'	1.85	0.41
33:R1:1930:G:O2'	33:R1:1968:G:O6	2.30	0.41
33:R1:2099:U:O2	33:R1:2190:G:N2	2.42	0.41
33:R1:2102:G:H1	33:R1:2187:U:H3	1.68	0.41
33:R1:2452:C:H2'	33:R1:2453:A:C8	2.56	0.41
33:R1:2590:A:H2'	33:R1:2591:C:C6	2.56	0.41
35:R3:123:U:H2'	35:R3:124:C:C6	2.55	0.41
35:R3:178:C:H2'	35:R3:179:A:H8	1.85	0.41
35:R3:672:U:HO2'	35:R3:673:A:P	2.43	0.41
35:R3:722:G:H3'	35:R3:722:G:N3	2.36	0.41
35:R3:1425:U:H2'	35:R3:1426:G:H8	1.85	0.41
35:R3:1464:U:H2'	35:R3:1465:A:H8	1.84	0.41
33:R1:980:A:N3	33:R1:2037:A:O2'	2.43	0.41
33:R1:2313:C:H2'	33:R1:2314:A:C8	2.53	0.41
33:R1:2547:A:H2'	33:R1:2548:U:C6	2.55	0.41
35:R3:1320:C:H2'	35:R3:1321:U:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:R3:1399:C:H4'	35:R3:1400:C:H5''	2.02	0.41
35:R3:1446:A:O2'	35:R3:1447:A:O5'	2.31	0.41
1:1:9:ARG:HG2	1:1:12:ARG:NH2	2.36	0.41
6:17:106:ASP:OD2	33:R1:1649:G:O2'	2.29	0.41
10:20:30:VAL:HG12	10:20:33:VAL:H	1.86	0.41
31:E:48:LEU:HA	31:E:51:ILE:HD12	2.02	0.41
33:R1:910:A:H2'	33:R1:911:A:C8	2.56	0.41
33:R1:1171:G:N2	33:R1:1176:U:O2	2.43	0.41
33:R1:2802:G:H2'	33:R1:2803:G:H8	1.85	0.41
33:R1:2895:G:O2'	33:R1:2896:C:H5'	2.21	0.41
35:R3:272:C:N4	35:R3:273:U:O4	2.54	0.41
1:1:190:GLU:O	1:1:194:VAL:HG23	2.21	0.41
2:13:1:MET:CG	2:13:2:LYS:H	2.34	0.41
6:17:24:MET:HB2	6:17:44:LEU:HD13	2.02	0.41
9:2:154:ALA:HA	9:2:159:THR:HG22	2.02	0.41
11:21:78:ARG:HE	11:21:78:ARG:HB2	1.70	0.41
14:24:39:ASN:HB3	14:24:62:ALA:HB3	2.03	0.41
15:25:31:TYR:O	15:25:92:VAL:HA	2.21	0.41
20:30:11:SER:HB2	20:30:31:ILE:HD11	2.02	0.41
23:33:29:LYS:HE2	33:R1:2286:G:H5'	2.03	0.41
23:33:33:LEU:HD21	33:R1:2286:G:C5	2.56	0.41
28:5:37:MET:SD	28:5:52:ALA:HB1	2.60	0.41
28:5:131:VAL:HG22	28:5:151:LEU:H	1.86	0.41
28:5:174:PHE:O	28:5:176:PHE:N	2.53	0.41
30:9:8:LYS:H	30:9:8:LYS:HG3	1.53	0.41
30:9:145:ASN:OD1	30:9:146:VAL:N	2.53	0.41
31:E:136:ASP:HB3	31:E:143:GLN:OE1	2.21	0.41
33:R1:257:C:H3'	33:R1:258:G:C8	2.55	0.41
33:R1:285:G:H2'	33:R1:286:U:H6	1.86	0.41
33:R1:285:G:C6	33:R1:356:G:O6	2.74	0.41
33:R1:357:C:H2'	33:R1:358:U:N1	2.36	0.41
33:R1:370:G:O2'	33:R1:424:G:OP1	2.30	0.41
33:R1:685:A:H5''	33:R1:788:A:H62	1.85	0.41
33:R1:721:A:H2'	33:R1:722:A:H8	1.82	0.41
33:R1:1344:U:O2	33:R1:1385:A:H5'	2.21	0.41
33:R1:1722:A:H2'	33:R1:1723:G:O4'	2.21	0.41
33:R1:1881:C:H2'	33:R1:1882:U:O4'	2.21	0.41
33:R1:2661:G:O2'	33:R1:2662:A:C8	2.63	0.41
33:R1:2663:G:H2'	33:R1:2664:G:O4'	2.21	0.41
33:R1:2846:G:H2'	33:R1:2847:U:H6	1.85	0.41
33:R1:2857:G:N2	33:R1:2860:A:OP2	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:R3:142:G:N3	35:R3:196:A:H2	2.18	0.41
35:R3:298:A:H2'	35:R3:299:G:O4'	2.21	0.41
35:R3:388:G:N2	35:R3:388:G:OP1	2.49	0.41
35:R3:417:G:O2'	35:R3:418:C:H6	2.03	0.41
35:R3:493:A:H5'	35:R3:494:G:OP2	2.21	0.41
35:R3:763:G:H2'	35:R3:764:C:C6	2.55	0.41
35:R3:1171:A:H2'	35:R3:1172:C:C6	2.56	0.41
35:R3:1260:G:H4'	35:R3:1283:U:O2'	2.21	0.41
35:R3:1456:A:H2'	35:R3:1457:G:O4'	2.20	0.41
1:1:192:LEU:HD13	1:1:196:LEU:HD23	2.03	0.41
9:2:33:LEU:HD12	9:2:33:LEU:HA	1.89	0.41
11:21:57:GLY:HA2	11:21:102:SER:C	2.42	0.41
14:24:40:LEU:HD23	14:24:61:GLU:HG3	2.03	0.41
21:31:57:VAL:O	21:31:61:ASN:N	2.47	0.41
30:9:94:ILE:O	30:9:94:ILE:HG13	2.21	0.41
33:R1:500:G:H2'	33:R1:502:A:C2	2.55	0.41
33:R1:1581:G:H2'	33:R1:1582:C:C6	2.56	0.41
35:R3:3:A:H8	35:R3:3:A:OP2	2.04	0.41
35:R3:131:A:O2'	35:R3:262:A:H8	2.02	0.41
35:R3:286:C:H2'	35:R3:287:U:C6	2.57	0.41
35:R3:321:A:H5''	35:R3:328:C:C4	2.56	0.41
35:R3:636:U:H2'	35:R3:637:C:C6	2.56	0.41
35:R3:1329:A:C5	35:R3:1330:U:C5	3.09	0.41
2:13:31:GLU:HG2	2:13:142:ILE:HG13	2.02	0.40
2:13:32:LEU:HD22	2:13:54:ILE:HG21	2.03	0.40
2:13:49:ASP:HB2	2:13:118:MET:HG2	2.02	0.40
4:15:98:ALA:HB3	4:15:100:ILE:HD12	2.03	0.40
6:17:79:LEU:C	6:17:81:ASN:H	2.25	0.40
8:19:3:ILE:HG13	19:3:9:VAL:HG11	2.02	0.40
12:22:74:ILE:CD1	12:22:105:VAL:HG22	2.50	0.40
13:23:34:VAL:HG23	13:23:81:LYS:HB3	2.03	0.40
14:24:87:GLU:C	14:24:89:GLY:H	2.24	0.40
18:29:6:LEU:HA	18:29:56:LEU:HD11	2.03	0.40
19:3:118:PHE:HB2	33:R1:2823:A:OP1	2.22	0.40
31:E:81:ASN:HB3	31:E:84:HIS:CG	2.56	0.40
31:E:412:LEU:HD22	31:E:412:LEU:H	1.86	0.40
33:R1:239:C:HO2'	33:R1:622:G:HO2'	1.68	0.40
33:R1:716:A:H2'	33:R1:717:C:O4'	2.22	0.40
33:R1:2064:C:H5''	36:T:75:C:O2'	2.20	0.40
33:R1:2331:G:O2'	33:R1:2336:A:N1	2.45	0.40
33:R1:2562:U:C2'	33:R1:2563:U:H5'	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:R3:100:G:C4	35:R3:101:A:C8	3.09	0.40
35:R3:294:U:H2'	35:R3:295:C:C6	2.55	0.40
35:R3:640:A:H2'	35:R3:641:U:C2	2.56	0.40
35:R3:652:U:HO2'	35:R3:653:U:H6	1.67	0.40
35:R3:1096:C:H2'	35:R3:1097:C:H6	1.86	0.40
35:R3:1294:G:H2'	35:R3:1295:U:C6	2.56	0.40
35:R3:1469:C:H2'	35:R3:1470:U:O4'	2.21	0.40
10:20:71:ASN:HB3	10:20:109:VAL:HG11	2.02	0.40
12:22:6:LYS:HA	12:22:103:ILE:O	2.22	0.40
13:23:54:GLU:HB2	13:23:88:LYS:HD2	2.02	0.40
16:27:5:LYS:NZ	33:R1:2252:G:N7	2.69	0.40
21:31:15:SER:O	21:31:33:ASN:HA	2.21	0.40
25:35:39:ARG:NE	33:R1:2362:C:OP1	2.52	0.40
28:5:49:LEU:HG	28:5:66:ILE:HD12	2.04	0.40
31:E:136:ASP:OD1	31:E:139:ASN:HB2	2.21	0.40
31:E:194:ASP:OD1	31:E:194:ASP:N	2.52	0.40
33:R1:365:U:H2'	33:R1:366:C:C6	2.56	0.40
33:R1:753:A:H2'	33:R1:754:U:C6	2.56	0.40
33:R1:2667:C:C2'	33:R1:2668:G:H5'	2.52	0.40
35:R3:320:A:C2	35:R3:333:U:H5	2.38	0.40
35:R3:640:A:HO2'	35:R3:641:U:P	2.43	0.40
35:R3:1102:A:C2'	35:R3:1103:C:H5'	2.51	0.40
35:R3:1120:C:C2	35:R3:1121:U:C5	3.08	0.40
35:R3:1486:G:H2'	35:R3:1487:G:O4'	2.21	0.40
1:1:21:TYR:N	1:1:21:TYR:CD1	2.88	0.40
1:1:183:ASP:OD1	1:1:183:ASP:N	2.55	0.40
2:13:78:THR:HB	33:R1:2641:G:H5''	2.03	0.40
4:15:82:LEU:HD13	4:15:120:VAL:HG11	2.03	0.40
8:19:27:VAL:HA	8:19:82:SER:O	2.22	0.40
10:20:79:ILE:HD13	10:20:79:ILE:HA	1.86	0.40
16:27:24:LYS:HA	16:27:24:LYS:HD3	1.95	0.40
33:R1:128:C:H2'	33:R1:129:C:C6	2.55	0.40
33:R1:138:U:O2'	33:R1:140:C:N4	2.55	0.40
33:R1:596:U:H2'	33:R1:597:G:C8	2.56	0.40
33:R1:1231:U:H2'	33:R1:1232:G:H8	1.86	0.40
33:R1:2079:U:H2'	33:R1:2080:A:O4'	2.21	0.40
33:R1:2144:G:H1'	33:R1:2148:G:H21	1.85	0.40
33:R1:2323:G:O2'	33:R1:2324:U:H5'	2.20	0.40
33:R1:2554:U:H2'	33:R1:2555:U:C6	2.57	0.40
34:R2:106:G:H2'	34:R2:107:G:O4'	2.21	0.40
35:R3:362:G:N1	35:R3:365:U:OP2	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:R3:527:G:O2'	35:R3:535:A:N1	2.40	0.40
35:R3:920:U:H2'	35:R3:921:U:C6	2.56	0.40
35:R3:1162:C:H2'	35:R3:1163:A:C8	2.56	0.40
35:R3:1208:C:H5'	35:R3:1209:C:OP2	2.21	0.40
36:T:53:G:N2	36:T:62:C:O2'	2.55	0.40
4:15:42:SER:OG	33:R1:672:C:OP2	2.29	0.40
4:15:79:LEU:HD23	4:15:79:LEU:HA	1.84	0.40
6:17:79:LEU:HD23	6:17:83:LEU:HD12	2.03	0.40
12:22:22:ASP:OD1	12:22:22:ASP:N	2.53	0.40
19:3:63:PRO:O	33:R1:2786:U:O2'	2.35	0.40
25:35:53:ASP:OD1	33:R1:2359:C:O2'	2.29	0.40
29:6:28:LYS:NZ	29:6:79:THR:O	2.29	0.40
31:E:199:ALA:O	31:E:202:GLU:HG2	2.22	0.40
33:R1:81:G:H2'	33:R1:82:U:O4'	2.22	0.40
33:R1:134:G:N1	33:R1:144:A:H2	2.08	0.40
33:R1:979:A:H5'	33:R1:980:A:C5'	2.52	0.40
33:R1:1090:A:N6	33:R1:1101:U:H3	2.20	0.40
33:R1:1536:C:H4'	33:R1:1537:G:C2	2.57	0.40
33:R1:2176:A:H2'	33:R1:2177:C:C6	2.56	0.40
35:R3:18:C:H4'	35:R3:1078:U:O2	2.21	0.40
35:R3:107:G:H2'	35:R3:108:G:H21	1.85	0.40
35:R3:264:C:H2'	35:R3:265:G:O4'	2.21	0.40
35:R3:864:A:H2'	35:R3:865:A:C8	2.56	0.40
35:R3:1263:C:H2'	35:R3:1264:U:C6	2.57	0.40
8:19:28:LYS:HE3	8:19:28:LYS:HB3	1.84	0.40
12:22:23:LEU:HD11	22:32:21:LEU:HB2	2.03	0.40
28:5:5:ASP:OD1	28:5:5:ASP:N	2.53	0.40
28:5:135:ILE:H	28:5:135:ILE:HG13	1.67	0.40
30:9:99:ILE:HD13	30:9:130:VAL:HG11	2.03	0.40
31:E:219:ARG:HB2	31:E:244:TYR:CD2	2.57	0.40
31:E:434:LYS:HE2	31:E:434:LYS:HB3	1.79	0.40
33:R1:29:U:H2'	33:R1:30:G:C8	2.57	0.40
33:R1:438:G:H2'	33:R1:439:A:C8	2.57	0.40
33:R1:446:G:HO2'	33:R1:447:A:P	2.44	0.40
33:R1:1444:G:H2'	33:R1:1445:G:H8	1.87	0.40
33:R1:2107:G:C6	33:R1:2183:A:C6	3.09	0.40
33:R1:2126:A:H2'	33:R1:2127:G:H4'	2.03	0.40
33:R1:2246:G:H2'	33:R1:2247:A:H8	1.85	0.40
34:R2:14:U:OP2	34:R2:70:C:O2'	2.34	0.40
35:R3:49:U:O2'	35:R3:50:A:H2'	2.21	0.40
35:R3:139:A:H2'	35:R3:140:U:C6	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:R3:371:A:H2'	35:R3:372:C:O4'	2.21	0.40
35:R3:463:U:O2'	35:R3:464:U:O4'	2.25	0.40
35:R3:720:C:H2'	35:R3:721:G:C8	2.56	0.40
35:R3:1004:A:C2'	35:R3:1005:A:H5''	2.51	0.40
35:R3:1127:G:H1	35:R3:1145:A:N6	2.18	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	1	218/220 (99%)	197 (90%)	21 (10%)	0	100	100
2	13	140/142 (99%)	134 (96%)	6 (4%)	0	100	100
3	14	120/122 (98%)	112 (93%)	7 (6%)	1 (1%)	16	51
4	15	141/143 (99%)	127 (90%)	14 (10%)	0	100	100
5	16	134/136 (98%)	128 (96%)	5 (4%)	1 (1%)	19	54
6	17	118/120 (98%)	109 (92%)	9 (8%)	0	100	100
7	18	114/116 (98%)	112 (98%)	2 (2%)	0	100	100
8	19	112/114 (98%)	104 (93%)	8 (7%)	0	100	100
9	2	269/271 (99%)	243 (90%)	26 (10%)	0	100	100
10	20	115/117 (98%)	115 (100%)	0	0	100	100
11	21	101/103 (98%)	91 (90%)	9 (9%)	1 (1%)	13	46
12	22	108/110 (98%)	100 (93%)	8 (7%)	0	100	100
13	23	91/93 (98%)	82 (90%)	9 (10%)	0	100	100
14	24	100/102 (98%)	87 (87%)	13 (13%)	0	100	100
15	25	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
16	27	83/85 (98%)	78 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	28	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
18	29	61/63 (97%)	59 (97%)	2 (3%)	0	100	100
19	3	207/209 (99%)	187 (90%)	20 (10%)	0	100	100
20	30	56/58 (97%)	54 (96%)	2 (4%)	0	100	100
21	31	64/66 (97%)	55 (86%)	9 (14%)	0	100	100
22	32	54/56 (96%)	50 (93%)	4 (7%)	0	100	100
23	33	48/50 (96%)	47 (98%)	1 (2%)	0	100	100
24	34	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
25	35	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
26	36	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
27	4	199/201 (99%)	187 (94%)	12 (6%)	0	100	100
28	5	175/177 (99%)	163 (93%)	12 (7%)	0	100	100
29	6	174/176 (99%)	158 (91%)	16 (9%)	0	100	100
30	9	147/149 (99%)	128 (87%)	17 (12%)	2 (1%)	9	37
31	E	549/551 (100%)	508 (92%)	39 (7%)	2 (0%)	30	66
37	sb	216/218 (99%)	188 (87%)	27 (12%)	1 (0%)	25	61
38	sc	204/206 (99%)	190 (93%)	14 (7%)	0	100	100
39	sd	203/205 (99%)	185 (91%)	18 (9%)	0	100	100
40	se	155/157 (99%)	133 (86%)	20 (13%)	2 (1%)	10	39
41	sf	98/100 (98%)	87 (89%)	11 (11%)	0	100	100
42	sg	149/151 (99%)	135 (91%)	13 (9%)	1 (1%)	19	54
43	sh	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
44	si	125/127 (98%)	100 (80%)	24 (19%)	1 (1%)	16	51
45	sj	96/98 (98%)	83 (86%)	12 (12%)	1 (1%)	13	46
46	sk	114/116 (98%)	105 (92%)	9 (8%)	0	100	100
47	sl	121/123 (98%)	95 (78%)	26 (22%)	0	100	100
48	sm	110/112 (98%)	97 (88%)	13 (12%)	0	100	100
49	sn	98/100 (98%)	84 (86%)	13 (13%)	1 (1%)	13	46
50	so	86/88 (98%)	80 (93%)	6 (7%)	0	100	100
51	sp	80/82 (98%)	70 (88%)	10 (12%)	0	100	100
52	sq	78/80 (98%)	64 (82%)	14 (18%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	sr	63/65 (97%)	60 (95%)	3 (5%)	0	100	100
54	ss	77/79 (98%)	71 (92%)	6 (8%)	0	100	100
55	st	83/85 (98%)	81 (98%)	2 (2%)	0	100	100
56	su	63/65 (97%)	46 (73%)	16 (25%)	1 (2%)	8	34
All	All	6353/6455 (98%)	5789 (91%)	549 (9%)	15 (0%)	45	77

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	14	110	GLU
31	E	17	PRO
40	se	122	VAL
42	sg	11	ILE
45	sj	100	ILE
11	21	51	VAL
30	9	8	LYS
44	si	57	VAL
30	9	9	VAL
56	su	24	LYS
31	E	548	ILE
37	sb	18	GLN
40	se	121	ASN
49	sn	98	ALA
5	16	69	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	106/171 (62%)	93 (88%)	13 (12%)	4	18
2	13	116/116 (100%)	107 (92%)	9 (8%)	10	36
3	14	103/103 (100%)	93 (90%)	10 (10%)	6	27
4	15	102/102 (100%)	97 (95%)	5 (5%)	21	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	16	109/109 (100%)	102 (94%)	7 (6%)	14	44
6	17	100/100 (100%)	94 (94%)	6 (6%)	16	47
7	18	86/86 (100%)	75 (87%)	11 (13%)	3	16
8	19	99/99 (100%)	85 (86%)	14 (14%)	3	13
9	2	216/216 (100%)	205 (95%)	11 (5%)	20	53
10	20	89/89 (100%)	84 (94%)	5 (6%)	17	49
11	21	84/84 (100%)	76 (90%)	8 (10%)	7	28
12	22	93/93 (100%)	87 (94%)	6 (6%)	14	43
13	23	80/80 (100%)	78 (98%)	2 (2%)	42	73
14	24	83/83 (100%)	76 (92%)	7 (8%)	9	33
15	25	78/78 (100%)	73 (94%)	5 (6%)	14	44
16	27	63/63 (100%)	57 (90%)	6 (10%)	7	28
17	28	67/67 (100%)	63 (94%)	4 (6%)	16	47
18	29	55/55 (100%)	46 (84%)	9 (16%)	2	9
19	3	164/164 (100%)	154 (94%)	10 (6%)	15	46
20	30	48/48 (100%)	46 (96%)	2 (4%)	25	59
21	31	59/59 (100%)	46 (78%)	13 (22%)	1	4
22	32	47/47 (100%)	43 (92%)	4 (8%)	8	33
23	33	45/45 (100%)	43 (96%)	2 (4%)	24	58
24	34	38/38 (100%)	37 (97%)	1 (3%)	41	72
25	35	51/51 (100%)	49 (96%)	2 (4%)	27	61
26	36	34/34 (100%)	30 (88%)	4 (12%)	4	19
27	4	165/165 (100%)	156 (94%)	9 (6%)	18	50
28	5	148/148 (100%)	135 (91%)	13 (9%)	8	31
29	6	137/137 (100%)	126 (92%)	11 (8%)	10	35
30	9	114/114 (100%)	102 (90%)	12 (10%)	5	23
31	E	460/463 (99%)	414 (90%)	46 (10%)	6	25
37	sb	180/180 (100%)	151 (84%)	29 (16%)	2	10
38	sc	170/170 (100%)	157 (92%)	13 (8%)	11	37
39	sd	172/172 (100%)	158 (92%)	14 (8%)	9	34
40	se	119/119 (100%)	105 (88%)	14 (12%)	4	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	sf	87/87 (100%)	78 (90%)	9 (10%)	6	24
42	sg	124/124 (100%)	112 (90%)	12 (10%)	6	27
43	sh	104/104 (100%)	96 (92%)	8 (8%)	10	37
44	si	105/105 (100%)	93 (89%)	12 (11%)	4	20
45	sj	86/86 (100%)	78 (91%)	8 (9%)	7	29
46	sk	89/89 (100%)	82 (92%)	7 (8%)	10	35
47	sl	103/103 (100%)	91 (88%)	12 (12%)	4	19
48	sm	91/91 (100%)	72 (79%)	19 (21%)	1	4
49	sn	83/83 (100%)	69 (83%)	14 (17%)	1	9
50	so	76/76 (100%)	67 (88%)	9 (12%)	4	19
51	sp	65/65 (100%)	57 (88%)	8 (12%)	4	18
52	sq	74/74 (100%)	66 (89%)	8 (11%)	5	22
53	sr	55/56 (98%)	51 (93%)	4 (7%)	11	39
54	ss	70/70 (100%)	62 (89%)	8 (11%)	4	20
55	st	65/65 (100%)	59 (91%)	6 (9%)	7	29
56	su	55/55 (100%)	34 (62%)	21 (38%)	0	0
All	All	5212/5281 (99%)	4710 (90%)	502 (10%)	9	27

All (502) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	7	ARG
1	1	10	VAL
1	1	14	LYS
1	1	35	THR
1	1	60	ARG
1	1	162	ARG
1	1	163	TYR
1	1	178	VAL
1	1	181	ASP
1	1	183	ASP
1	1	192	LEU
1	1	193	LEU
1	1	224	VAL
2	13	1	MET
2	13	12	LYS

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Mol	Chain	Res	Type
2	13	18	VAL
2	13	28	LEU
2	13	48	VAL
2	13	49	ASP
2	13	69	ARG
2	13	86	GLN
2	13	106	LYS
3	14	1	MET
3	14	13	ASN
3	14	28	SER
3	14	32	TYR
3	14	49	ARG
3	14	53	LYS
3	14	75	SER
3	14	91	SER
3	14	98	ARG
3	14	109	SER
4	15	78	ARG
4	15	92	LEU
4	15	112	LEU
4	15	129	LYS
4	15	132	ARG
5	16	1	MET
5	16	36	VAL
5	16	42	THR
5	16	70	ASP
5	16	97	GLN
5	16	115	GLU
5	16	136	MET
6	17	2	ARG
6	17	14	SER
6	17	30	ARG
6	17	38	LEU
6	17	59	SER
6	17	89	SER
7	18	2	ASP
7	18	21	LEU
7	18	26	LEU
7	18	27	VAL
7	18	36	TYR
7	18	47	VAL
7	18	60	GLU

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Mol	Chain	Res	Type
7	18	65	THR
7	18	98	GLN
7	18	100	HIS
7	18	112	GLU
8	19	4	ILE
8	19	13	LYS
8	19	16	VAL
8	19	25	VAL
8	19	27	VAL
8	19	31	VAL
8	19	36	LYS
8	19	39	LEU
8	19	65	ASN
8	19	72	VAL
8	19	81	ASP
8	19	87	ARG
8	19	96	LEU
8	19	108	ARG
9	2	4	LYS
9	2	19	VAL
9	2	93	VAL
9	2	116	GLN
9	2	129	LEU
9	2	186	ASP
9	2	191	LEU
9	2	213	ARG
9	2	222	THR
9	2	251	THR
9	2	259	ASN
10	20	7	VAL
10	20	12	ARG
10	20	15	LYS
10	20	39	ILE
10	20	50	ARG
11	21	20	VAL
11	21	26	ASP
11	21	29	THR
11	21	38	VAL
11	21	45	GLU
11	21	48	LYS
11	21	86	GLN
11	21	95	ASP

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Mol	Chain	Res	Type
12	22	35	ILE
12	22	45	VAL
12	22	62	ASP
12	22	65	ASP
12	22	76	VAL
12	22	108	SER
13	23	2	ILE
13	23	37	ASP
14	24	16	LYS
14	24	17	ASP
14	24	21	ARG
14	24	27	VAL
14	24	29	SER
14	24	78	LYS
14	24	80	ASP
15	25	1	MET
15	25	9	ARG
15	25	42	LEU
15	25	90	ASP
15	25	93	ARG
16	27	4	LYS
16	27	14	ARG
16	27	21	LEU
16	27	43	THR
16	27	51	VAL
16	27	82	ILE
17	28	1	SER
17	28	32	LEU
17	28	34	SER
17	28	49	ARG
18	29	1	MET
18	29	4	LYS
18	29	6	LEU
18	29	7	ARG
18	29	16	THR
18	29	17	GLU
18	29	18	LEU
18	29	49	ASP
18	29	58	ASN
19	3	1	MET
19	3	18	ASP
19	3	43	ASP

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Mol	Chain	Res	Type
19	3	84	LEU
19	3	100	LEU
19	3	104	VAL
19	3	106	LYS
19	3	109	VAL
19	3	150	GLN
19	3	177	VAL
20	30	2	LYS
20	30	53	MET
21	31	9	TYR
21	31	11	GLU
21	31	16	CYS
21	31	22	MET
21	31	24	ILE
21	31	25	ARG
21	31	27	THR
21	31	30	HIS
21	31	34	LEU
21	31	37	CYS
21	31	44	PHE
21	31	62	LYS
21	31	65	ASN
22	32	8	THR
22	32	22	THR
22	32	31	LYS
22	32	51	ARG
23	33	16	THR
23	33	26	LYS
24	34	15	SER
25	35	30	HIS
25	35	56	LEU
26	36	2	LYS
26	36	6	SER
26	36	11	CYS
26	36	12	ARG
27	4	5	LEU
27	4	44	ARG
27	4	67	ARG
27	4	74	LYS
27	4	75	SER
27	4	105	LEU
27	4	110	SER

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Mol	Chain	Res	Type
27	4	137	LYS
27	4	146	VAL
28	5	4	HIS
28	5	5	ASP
28	5	27	VAL
28	5	34	THR
28	5	37	MET
28	5	46	LYS
28	5	56	LEU
28	5	65	LEU
28	5	107	VAL
28	5	126	ASN
28	5	136	ILE
28	5	148	VAL
28	5	174	PHE
29	6	26	LYS
29	6	35	THR
29	6	38	ASP
29	6	41	GLU
29	6	48	THR
29	6	73	SER
29	6	94	ARG
29	6	105	SER
29	6	132	LEU
29	6	152	ARG
29	6	165	ASP
30	9	5	LEU
30	9	9	VAL
30	9	12	LEU
30	9	19	VAL
30	9	35	LYS
30	9	41	LYS
30	9	47	PHE
30	9	50	ARG
30	9	77	THR
30	9	110	VAL
30	9	117	LEU
30	9	147	VAL
31	E	8	MET
31	E	10	ARG
31	E	46	SER
31	E	58	ASP

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Mol	Chain	Res	Type
31	E	62	GLU
31	E	64	ARG
31	E	69	ILE
31	E	70	LYS
31	E	84	HIS
31	E	91	GLU
31	E	95	SER
31	E	104	LEU
31	E	113	ASP
31	E	133	GLN
31	E	135	HIS
31	E	145	GLU
31	E	155	ASP
31	E	157	ASP
31	E	160	ILE
31	E	173	LEU
31	E	174	CYS
31	E	175	ARG
31	E	182	ASP
31	E	216	THR
31	E	218	ASP
31	E	219	ARG
31	E	223	ASP
31	E	224	ASN
31	E	271	LYS
31	E	285	SER
31	E	295	GLU
31	E	300	THR
31	E	301	GLU
31	E	305	ARG
31	E	337	LEU
31	E	364	THR
31	E	376	ASP
31	E	380	ILE
31	E	381	THR
31	E	388	LEU
31	E	392	ASP
31	E	403	THR
31	E	424	SER
31	E	481	ARG
31	E	513	ASP
31	E	552	ARG

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Mol	Chain	Res	Type
37	sb	8	MET
37	sb	15	PHE
37	sb	17	HIS
37	sb	22	TRP
37	sb	31	PHE
37	sb	34	ARG
37	sb	36	LYS
37	sb	59	ILE
37	sb	62	ARG
37	sb	72	LYS
37	sb	77	GLU
37	sb	81	ASP
37	sb	86	CYS
37	sb	87	ASP
37	sb	93	HIS
37	sb	104	LYS
37	sb	115	ASP
37	sb	126	ASP
37	sb	129	THR
37	sb	144	GLU
37	sb	146	SER
37	sb	152	ASP
37	sb	191	ASP
37	sb	195	VAL
37	sb	196	ASP
37	sb	204	ASP
37	sb	220	VAL
37	sb	222	GLU
37	sb	224	ARG
38	sc	3	LYS
38	sc	17	TRP
38	sc	32	LEU
38	sc	55	VAL
38	sc	61	LYS
38	sc	71	ARG
38	sc	96	VAL
38	sc	106	ARG
38	sc	161	ILE
38	sc	163	ARG
38	sc	164	THR
38	sc	184	ASN
38	sc	186	SER

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Mol	Chain	Res	Type
39	sd	22	SER
39	sd	31	CYS
39	sd	39	GLN
39	sd	49	ASP
39	sd	57	LYS
39	sd	80	ARG
39	sd	98	ASP
39	sd	110	ARG
39	sd	119	HIS
39	sd	128	VAL
39	sd	137	SER
39	sd	140	ASP
39	sd	168	THR
39	sd	193	ASP
40	se	9	GLU
40	se	11	GLN
40	se	13	LYS
40	se	14	LEU
40	se	23	THR
40	se	53	ARG
40	se	70	MET
40	se	91	SER
40	se	115	GLU
40	se	122	VAL
40	se	123	LEU
40	se	129	SER
40	se	139	THR
40	se	156	ARG
41	sf	1	MET
41	sf	2	ARG
41	sf	16	GLU
41	sf	17	GLN
41	sf	35	LYS
41	sf	61	LEU
41	sf	63	ASN
41	sf	88	MET
41	sf	97	THR
42	sg	5	VAL
42	sg	6	ILE
42	sg	21	LEU
42	sg	24	LYS
42	sg	44	SER

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Mol	Chain	Res	Type
42	sg	73	GLU
42	sg	83	THR
42	sg	88	VAL
42	sg	124	SER
42	sg	141	HIS
42	sg	142	ARG
42	sg	148	LYS
43	sh	21	LYS
43	sh	26	MET
43	sh	29	SER
43	sh	31	LEU
43	sh	51	GLU
43	sh	53	ASP
43	sh	59	GLU
43	sh	98	LEU
44	si	11	ARG
44	si	18	VAL
44	si	21	LYS
44	si	26	LYS
44	si	38	PHE
44	si	45	MET
44	si	51	LEU
44	si	55	ASP
44	si	93	LEU
44	si	114	LYS
44	si	115	VAL
44	si	122	ARG
45	sj	5	ARG
45	sj	7	ARG
45	sj	9	ARG
45	sj	27	GLU
45	sj	62	ARG
45	sj	85	ASP
45	sj	91	ASP
45	sj	102	LEU
46	sk	13	LYS
46	sk	52	ARG
46	sk	71	ASP
46	sk	80	ASN
46	sk	94	SER
46	sk	125	LYS
46	sk	126	ARG

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Mol	Chain	Res	Type
47	sl	2	THR
47	sl	3	VAL
47	sl	14	LYS
47	sl	15	VAL
47	sl	34	THR
47	sl	49	ARG
47	sl	53	ARG
47	sl	57	THR
47	sl	58	ASN
47	sl	63	THR
47	sl	111	GLN
47	sl	122	LYS
48	sm	10	ASP
48	sm	11	HIS
48	sm	13	HIS
48	sm	15	VAL
48	sm	20	SER
48	sm	28	ARG
48	sm	29	SER
48	sm	41	ASP
48	sm	49	GLU
48	sm	53	ASP
48	sm	62	PHE
48	sm	65	GLU
48	sm	67	ASP
48	sm	70	ARG
48	sm	74	MET
48	sm	92	ARG
48	sm	101	THR
48	sm	112	ARG
48	sm	113	LYS
49	sn	4	SER
49	sn	9	GLU
49	sn	18	LYS
49	sn	23	ARG
49	sn	32	ASP
49	sn	34	ASN
49	sn	36	SER
49	sn	46	LYS
49	sn	47	LEU
49	sn	49	THR
49	sn	52	ARG

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Mol	Chain	Res	Type
49	sn	54	SER
49	sn	66	THR
49	sn	91	GLU
50	so	3	SER
50	so	39	GLN
50	so	60	SER
50	so	61	GLN
50	so	63	ARG
50	so	70	LYS
50	so	72	LYS
50	so	77	TYR
50	so	82	GLU
51	sp	13	LYS
51	sp	20	VAL
51	sp	24	SER
51	sp	46	LYS
51	sp	48	GLU
51	sp	52	LEU
51	sp	53	ASP
51	sp	76	LYS
52	sq	14	ASP
52	sq	27	PHE
52	sq	39	ARG
52	sq	50	ASN
52	sq	52	CYS
52	sq	59	GLU
52	sq	67	SER
52	sq	76	ARG
53	sr	9	PHE
53	sr	18	GLN
53	sr	19	GLU
53	sr	70	THR
54	ss	6	LYS
54	ss	27	LYS
54	ss	28	LYS
54	ss	32	THR
54	ss	37	SER
54	ss	48	ILE
54	ss	55	GLN
54	ss	57	VAL
55	st	13	SER
55	st	25	SER

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Mol	Chain	Res	Type
55	st	26	MET
55	st	39	GLU
55	st	42	ASP
55	st	85	LEU
56	su	4	LYS
56	su	6	ARG
56	su	8	ASN
56	su	15	LEU
56	su	16	ARG
56	su	17	ARG
56	su	19	LYS
56	su	22	CYS
56	su	24	LYS
56	su	27	VAL
56	su	30	GLU
56	su	32	ARG
56	su	33	ARG
56	su	36	PHE
56	su	37	TYR
56	su	44	ARG
56	su	46	ARG
56	su	57	LYS
56	su	62	GLU
56	su	63	ASN
56	su	65	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	58	ASN
2	13	58	ASN
2	13	128	ASN
19	3	32	ASN
19	3	185	ASN
31	E	41	ASN
31	E	66	GLN
31	E	188	GLN
31	E	309	ASN
31	E	485	ASN
37	sb	17	HIS
40	se	121	ASN
41	sf	11	HIS

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Mol	Chain	Res	Type
43	sh	15	ASN
55	st	2	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
32	M	8/9 (88%)	1 (12%)	0
33	R1	2902/2903 (99%)	688 (23%)	23 (0%)
34	R2	118/119 (99%)	26 (22%)	1 (0%)
35	R3	1528/1531 (99%)	451 (29%)	30 (1%)
36	T	75/76 (98%)	30 (40%)	0
All	All	4631/4638 (99%)	1196 (25%)	54 (1%)

All (1196) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
32	M	9	A
33	R1	2	G
33	R1	5	A
33	R1	10	A
33	R1	11	C
33	R1	12	U
33	R1	27	G
33	R1	29	U
33	R1	34	U
33	R1	35	G
33	R1	36	G
33	R1	46	G
33	R1	51	G
33	R1	60	G
33	R1	62	U
33	R1	63	A
33	R1	71	A
33	R1	72	U
33	R1	73	A
33	R1	74	A
33	R1	75	G
33	R1	78	U
33	R1	79	C
33	R1	80	G
33	R1	83	A

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Mol	Chain	Res	Type
33	R1	84	A
33	R1	85	G
33	R1	87	U
33	R1	88	G
33	R1	96	C
33	R1	102	U
33	R1	110	G
33	R1	118	A
33	R1	119	A
33	R1	120	U
33	R1	125	A
33	R1	136	G
33	R1	139	U
33	R1	140	C
33	R1	143	C
33	R1	144	A
33	R1	146	A
33	R1	152	A
33	R1	154	U
33	R1	155	A
33	R1	156	A
33	R1	158	U
33	R1	159	G
33	R1	162	U
33	R1	163	C
33	R1	164	C
33	R1	176	A
33	R1	178	G
33	R1	181	A
33	R1	196	A
33	R1	199	A
33	R1	200	U
33	R1	203	A
33	R1	213	A
33	R1	215	G
33	R1	216	A
33	R1	218	A
33	R1	222	A
33	R1	224	U
33	R1	227	A
33	R1	228	C
33	R1	230	G

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Mol	Chain	Res	Type
33	R1	233	A
33	R1	239	C
33	R1	248	G
33	R1	249	C
33	R1	256	A
33	R1	257	C
33	R1	258	G
33	R1	261	G
33	R1	265	A
33	R1	266	G
33	R1	272	A
33	R1	274	C
33	R1	275	C
33	R1	276	U
33	R1	277	G
33	R1	280	U
33	R1	281	C
33	R1	282	A
33	R1	285	G
33	R1	286	U
33	R1	304	U
33	R1	311	A
33	R1	326	G
33	R1	329	G
33	R1	330	A
33	R1	345	A
33	R1	348	A
33	R1	352	A
33	R1	353	C
33	R1	354	A
33	R1	355	U
33	R1	359	G
33	R1	361	G
33	R1	365	U
33	R1	369	U
33	R1	371	A
33	R1	372	G
33	R1	373	U
33	R1	380	G
33	R1	383	C
33	R1	386	G
33	R1	387	U

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Mol	Chain	Res	Type
33	R1	388	G
33	R1	389	G
33	R1	395	U
33	R1	396	G
33	R1	399	U
33	R1	401	A
33	R1	404	A
33	R1	405	U
33	R1	406	G
33	R1	407	G
33	R1	411	G
33	R1	412	A
33	R1	413	C
33	R1	414	C
33	R1	424	G
33	R1	428	A
33	R1	443	A
33	R1	447	A
33	R1	452	G
33	R1	454	A
33	R1	456	C
33	R1	477	A
33	R1	478	A
33	R1	480	A
33	R1	481	G
33	R1	489	G
33	R1	490	C
33	R1	491	G
33	R1	503	A
33	R1	504	A
33	R1	505	A
33	R1	506	G
33	R1	509	C
33	R1	527	C
33	R1	528	A
33	R1	529	A
33	R1	530	G
33	R1	531	C
33	R1	532	A
33	R1	533	G
33	R1	534	U
33	R1	541	A

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Mol	Chain	Res	Type
33	R1	543	G
33	R1	545	U
33	R1	546	U
33	R1	547	A
33	R1	548	G
33	R1	549	G
33	R1	550	C
33	R1	554	U
33	R1	555	G
33	R1	563	A
33	R1	571	U
33	R1	573	U
33	R1	575	A
33	R1	580	U
33	R1	581	C
33	R1	591	U
33	R1	601	C
33	R1	603	A
33	R1	614	A
33	R1	615	U
33	R1	622	G
33	R1	627	A
33	R1	637	A
33	R1	645	C
33	R1	646	U
33	R1	647	G
33	R1	653	U
33	R1	654	A
33	R1	655	A
33	R1	668	A
33	R1	685	A
33	R1	686	U
33	R1	688	U
33	R1	689	A
33	R1	696	G
33	R1	704	G
33	R1	705	A
33	R1	711	G
33	R1	712	G
33	R1	713	G
33	R1	717	C
33	R1	730	A

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Mol	Chain	Res	Type
33	R1	738	G
33	R1	740	C
33	R1	746	U
33	R1	747	U
33	R1	762	U
33	R1	775	G
33	R1	776	G
33	R1	782	A
33	R1	784	G
33	R1	785	G
33	R1	789	A
33	R1	791	C
33	R1	792	A
33	R1	805	G
33	R1	806	C
33	R1	812	C
33	R1	819	A
33	R1	827	U
33	R1	829	A
33	R1	830	G
33	R1	831	G
33	R1	845	A
33	R1	846	U
33	R1	847	U
33	R1	856	G
33	R1	858	G
33	R1	859	G
33	R1	860	U
33	R1	869	G
33	R1	870	U
33	R1	871	U
33	R1	872	U
33	R1	875	G
33	R1	877	A
33	R1	878	A
33	R1	882	G
33	R1	886	A
33	R1	887	U
33	R1	888	C
33	R1	889	C
33	R1	891	G
33	R1	892	A

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Mol	Chain	Res	Type
33	R1	896	A
33	R1	897	C
33	R1	898	C
33	R1	901	C
33	R1	902	C
33	R1	904	G
33	R1	907	G
33	R1	910	A
33	R1	914	G
33	R1	915	C
33	R1	931	U
33	R1	932	U
33	R1	933	A
33	R1	941	A
33	R1	946	C
33	R1	958	U
33	R1	961	C
33	R1	971	G
33	R1	973	A
33	R1	974	G
33	R1	975	A
33	R1	979	A
33	R1	980	A
33	R1	983	A
33	R1	988	A
33	R1	989	G
33	R1	994	C
33	R1	995	C
33	R1	996	A
33	R1	999	U
33	R1	1005	C
33	R1	1012	U
33	R1	1013	C
33	R1	1021	A
33	R1	1022	G
33	R1	1026	G
33	R1	1033	U
33	R1	1045	C
33	R1	1046	A
33	R1	1050	A
33	R1	1051	G
33	R1	1052	C

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Mol	Chain	Res	Type
33	R1	1060	U
33	R1	1061	U
33	R1	1062	G
33	R1	1064	C
33	R1	1065	U
33	R1	1066	U
33	R1	1067	A
33	R1	1070	A
33	R1	1071	G
33	R1	1072	C
33	R1	1073	A
33	R1	1075	C
33	R1	1077	A
33	R1	1078	U
33	R1	1079	C
33	R1	1083	U
33	R1	1084	A
33	R1	1085	A
33	R1	1087	G
33	R1	1088	A
33	R1	1094	U
33	R1	1095	A
33	R1	1096	A
33	R1	1103	A
33	R1	1104	C
33	R1	1106	G
33	R1	1109	C
33	R1	1110	G
33	R1	1111	A
33	R1	1112	G
33	R1	1114	C
33	R1	1115	G
33	R1	1116	G
33	R1	1128	G
33	R1	1130	U
33	R1	1132	U
33	R1	1134	A
33	R1	1135	C
33	R1	1141	U
33	R1	1157	G
33	R1	1166	G
33	R1	1171	G

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Mol	Chain	Res	Type
33	R1	1173	U
33	R1	1174	U
33	R1	1175	A
33	R1	1176	U
33	R1	1179	G
33	R1	1180	U
33	R1	1182	G
33	R1	1186	G
33	R1	1195	G
33	R1	1205	A
33	R1	1206	G
33	R1	1213	A
33	R1	1214	A
33	R1	1237	A
33	R1	1238	G
33	R1	1247	A
33	R1	1248	G
33	R1	1250	G
33	R1	1253	A
33	R1	1256	G
33	R1	1271	G
33	R1	1272	A
33	R1	1281	G
33	R1	1287	A
33	R1	1300	G
33	R1	1301	A
33	R1	1311	G
33	R1	1321	A
33	R1	1323	C
33	R1	1329	U
33	R1	1341	G
33	R1	1345	C
33	R1	1352	U
33	R1	1365	A
33	R1	1367	A
33	R1	1368	G
33	R1	1379	U
33	R1	1383	A
33	R1	1386	C
33	R1	1392	A
33	R1	1393	A
33	R1	1395	A

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Mol	Chain	Res	Type
33	R1	1416	G
33	R1	1419	A
33	R1	1428	C
33	R1	1432	G
33	R1	1452	G
33	R1	1453	A
33	R1	1459	G
33	R1	1461	C
33	R1	1481	U
33	R1	1482	G
33	R1	1493	C
33	R1	1494	A
33	R1	1497	U
33	R1	1503	A
33	R1	1509	A
33	R1	1515	A
33	R1	1519	G
33	R1	1523	U
33	R1	1524	G
33	R1	1531	C
33	R1	1532	A
33	R1	1534	U
33	R1	1535	A
33	R1	1536	C
33	R1	1537	G
33	R1	1554	U
33	R1	1559	U
33	R1	1566	A
33	R1	1569	A
33	R1	1578	U
33	R1	1582	C
33	R1	1583	A
33	R1	1584	U
33	R1	1608	A
33	R1	1610	A
33	R1	1622	G
33	R1	1634	A
33	R1	1647	U
33	R1	1648	U
33	R1	1649	G
33	R1	1664	A
33	R1	1667	G

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Mol	Chain	Res	Type
33	R1	1674	G
33	R1	1675	C
33	R1	1693	U
33	R1	1714	U
33	R1	1715	G
33	R1	1730	C
33	R1	1732	C
33	R1	1738	G
33	R1	1757	A
33	R1	1759	A
33	R1	1764	C
33	R1	1773	A
33	R1	1776	G
33	R1	1782	U
33	R1	1784	A
33	R1	1786	A
33	R1	1788	C
33	R1	1799	G
33	R1	1800	C
33	R1	1801	A
33	R1	1808	A
33	R1	1812	U
33	R1	1816	C
33	R1	1829	A
33	R1	1835	G
33	R1	1838	C
33	R1	1855	U
33	R1	1868	C
33	R1	1869	G
33	R1	1870	C
33	R1	1872	A
33	R1	1873	G
33	R1	1884	G
33	R1	1891	G
33	R1	1900	A
33	R1	1906	G
33	R1	1912	A
33	R1	1913	A
33	R1	1914	C
33	R1	1915	U
33	R1	1916	A
33	R1	1919	A

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Mol	Chain	Res	Type
33	R1	1927	A
33	R1	1929	G
33	R1	1930	G
33	R1	1937	A
33	R1	1938	A
33	R1	1952	A
33	R1	1955	U
33	R1	1965	C
33	R1	1966	A
33	R1	1967	C
33	R1	1970	A
33	R1	1971	U
33	R1	1972	G
33	R1	1980	G
33	R1	1991	U
33	R1	1997	C
33	R1	2022	U
33	R1	2023	C
33	R1	2030	A
33	R1	2031	A
33	R1	2033	A
33	R1	2035	G
33	R1	2036	C
33	R1	2043	C
33	R1	2055	C
33	R1	2056	G
33	R1	2058	A
33	R1	2059	A
33	R1	2061	G
33	R1	2062	A
33	R1	2064	C
33	R1	2069	G
33	R1	2072	C
33	R1	2079	U
33	R1	2080	A
33	R1	2093	G
33	R1	2096	C
33	R1	2099	U
33	R1	2107	G
33	R1	2109	U
33	R1	2111	U
33	R1	2112	G

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Mol	Chain	Res	Type
33	R1	2113	U
33	R1	2115	G
33	R1	2116	G
33	R1	2117	A
33	R1	2118	U
33	R1	2119	A
33	R1	2120	G
33	R1	2122	U
33	R1	2123	G
33	R1	2124	G
33	R1	2125	G
33	R1	2126	A
33	R1	2128	G
33	R1	2131	U
33	R1	2132	U
33	R1	2133	G
33	R1	2134	A
33	R1	2135	A
33	R1	2137	U
33	R1	2145	C
33	R1	2146	C
33	R1	2147	A
33	R1	2148	G
33	R1	2150	C
33	R1	2153	C
33	R1	2157	G
33	R1	2158	A
33	R1	2161	C
33	R1	2164	C
33	R1	2166	U
33	R1	2168	G
33	R1	2170	A
33	R1	2171	A
33	R1	2172	U
33	R1	2173	A
33	R1	2174	C
33	R1	2175	C
33	R1	2176	A
33	R1	2177	C
33	R1	2178	C
33	R1	2179	C
33	R1	2181	U

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Mol	Chain	Res	Type
33	R1	2182	U
33	R1	2184	A
33	R1	2188	U
33	R1	2189	U
33	R1	2198	A
33	R1	2204	G
33	R1	2211	A
33	R1	2213	U
33	R1	2214	C
33	R1	2225	A
33	R1	2226	C
33	R1	2238	G
33	R1	2239	G
33	R1	2250	G
33	R1	2279	G
33	R1	2283	C
33	R1	2287	A
33	R1	2288	A
33	R1	2291	U
33	R1	2292	U
33	R1	2297	A
33	R1	2305	U
33	R1	2306	C
33	R1	2308	G
33	R1	2309	A
33	R1	2310	C
33	R1	2311	A
33	R1	2316	G
33	R1	2319	G
33	R1	2322	A
33	R1	2325	G
33	R1	2333	A
33	R1	2336	A
33	R1	2345	G
33	R1	2347	C
33	R1	2350	C
33	R1	2354	C
33	R1	2357	G
33	R1	2359	C
33	R1	2361	G
33	R1	2377	A
33	R1	2383	G

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Mol	Chain	Res	Type
33	R1	2385	C
33	R1	2389	G
33	R1	2391	G
33	R1	2402	U
33	R1	2403	C
33	R1	2406	A
33	R1	2423	U
33	R1	2424	C
33	R1	2425	A
33	R1	2429	G
33	R1	2430	A
33	R1	2434	A
33	R1	2435	A
33	R1	2436	G
33	R1	2439	A
33	R1	2441	U
33	R1	2447	G
33	R1	2448	A
33	R1	2468	A
33	R1	2470	G
33	R1	2476	A
33	R1	2478	A
33	R1	2484	G
33	R1	2494	G
33	R1	2497	A
33	R1	2498	C
33	R1	2502	G
33	R1	2503	A
33	R1	2504	U
33	R1	2505	G
33	R1	2506	U
33	R1	2518	A
33	R1	2520	C
33	R1	2529	G
33	R1	2547	A
33	R1	2554	U
33	R1	2560	A
33	R1	2562	U
33	R1	2563	U
33	R1	2564	A
33	R1	2565	A
33	R1	2566	A

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Mol	Chain	Res	Type
33	R1	2567	G
33	R1	2572	A
33	R1	2573	C
33	R1	2585	U
33	R1	2586	U
33	R1	2602	A
33	R1	2609	U
33	R1	2610	C
33	R1	2613	U
33	R1	2615	U
33	R1	2629	U
33	R1	2630	G
33	R1	2646	C
33	R1	2650	U
33	R1	2660	A
33	R1	2662	A
33	R1	2663	G
33	R1	2664	G
33	R1	2666	C
33	R1	2669	G
33	R1	2671	G
33	R1	2682	A
33	R1	2689	U
33	R1	2690	U
33	R1	2700	A
33	R1	2701	U
33	R1	2706	A
33	R1	2714	G
33	R1	2716	C
33	R1	2718	G
33	R1	2720	U
33	R1	2726	A
33	R1	2732	G
33	R1	2733	A
33	R1	2738	A
33	R1	2739	U
33	R1	2744	G
33	R1	2748	A
33	R1	2755	C
33	R1	2762	C
33	R1	2765	A
33	R1	2772	C

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Mol	Chain	Res	Type
33	R1	2773	C
33	R1	2774	C
33	R1	2775	G
33	R1	2778	A
33	R1	2779	U
33	R1	2793	C
33	R1	2798	U
33	R1	2800	A
33	R1	2808	G
33	R1	2814	A
33	R1	2815	C
33	R1	2816	G
33	R1	2817	U
33	R1	2818	U
33	R1	2820	A
33	R1	2821	A
33	R1	2840	C
33	R1	2847	U
33	R1	2848	G
33	R1	2849	U
33	R1	2859	G
33	R1	2861	U
33	R1	2867	G
33	R1	2873	A
33	R1	2880	C
33	R1	2883	A
33	R1	2887	A
33	R1	2891	U
33	R1	2893	A
33	R1	2896	C
33	R1	2897	U
33	R1	2900	A
33	R1	2902	C
33	R1	2903	U
34	R2	9	G
34	R2	13	G
34	R2	16	G
34	R2	35	C
34	R2	41	G
34	R2	42	C
34	R2	44	G
34	R2	50	A

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Mol	Chain	Res	Type
34	R2	51	G
34	R2	52	A
34	R2	63	C
34	R2	64	G
34	R2	65	U
34	R2	66	A
34	R2	67	G
34	R2	87	U
34	R2	88	C
34	R2	89	U
34	R2	90	C
34	R2	108	A
34	R2	109	A
34	R2	112	G
34	R2	113	C
34	R2	114	C
34	R2	117	G
34	R2	119	A
35	R3	3	A
35	R3	4	U
35	R3	6	G
35	R3	7	A
35	R3	9	G
35	R3	11	G
35	R3	22	G
35	R3	30	U
35	R3	31	G
35	R3	32	A
35	R3	39	G
35	R3	47	C
35	R3	48	C
35	R3	49	U
35	R3	50	A
35	R3	51	A
35	R3	53	A
35	R3	54	C
35	R3	60	A
35	R3	61	G
35	R3	63	C
35	R3	64	G
35	R3	66	A
35	R3	68	G

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Mol	Chain	Res	Type
35	R3	70	U
35	R3	71	A
35	R3	76	G
35	R3	77	A
35	R3	78	A
35	R3	80	A
35	R3	81	A
35	R3	82	G
35	R3	83	C
35	R3	84	U
35	R3	85	U
35	R3	86	G
35	R3	91	U
35	R3	93	U
35	R3	94	G
35	R3	95	C
35	R3	96	U
35	R3	97	G
35	R3	100	G
35	R3	102	G
35	R3	105	G
35	R3	107	G
35	R3	108	G
35	R3	115	G
35	R3	116	A
35	R3	120	A
35	R3	121	U
35	R3	122	G
35	R3	128	G
35	R3	130	A
35	R3	131	A
35	R3	133	U
35	R3	134	G
35	R3	135	C
35	R3	151	A
35	R3	153	C
35	R3	155	A
35	R3	157	U
35	R3	161	A
35	R3	164	G
35	R3	171	A
35	R3	172	A

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Mol	Chain	Res	Type
35	R3	173	U
35	R3	174	A
35	R3	181	A
35	R3	182	A
35	R3	183	C
35	R3	184	G
35	R3	190	A
35	R3	191	G
35	R3	192	A
35	R3	197	A
35	R3	202	G
35	R3	204	G
35	R3	206	C
35	R3	207	C
35	R3	208	U
35	R3	209	U
35	R3	212	G
35	R3	214	C
35	R3	215	C
35	R3	218	U
35	R3	220	G
35	R3	223	A
35	R3	226	G
35	R3	230	G
35	R3	240	G
35	R3	243	A
35	R3	245	U
35	R3	247	G
35	R3	250	A
35	R3	251	G
35	R3	255	G
35	R3	258	G
35	R3	263	A
35	R3	264	C
35	R3	266	G
35	R3	267	C
35	R3	272	C
35	R3	273	U
35	R3	274	A
35	R3	279	A
35	R3	280	C
35	R3	287	U

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Mol	Chain	Res	Type
35	R3	289	G
35	R3	290	C
35	R3	293	G
35	R3	296	U
35	R3	298	A
35	R3	302	G
35	R3	313	A
35	R3	316	C
35	R3	322	C
35	R3	323	U
35	R3	324	G
35	R3	325	A
35	R3	327	A
35	R3	328	C
35	R3	329	A
35	R3	330	C
35	R3	331	G
35	R3	333	U
35	R3	338	A
35	R3	339	C
35	R3	344	A
35	R3	351	G
35	R3	352	C
35	R3	353	A
35	R3	354	G
35	R3	363	A
35	R3	364	A
35	R3	367	U
35	R3	369	G
35	R3	370	C
35	R3	372	C
35	R3	373	A
35	R3	376	G
35	R3	377	G
35	R3	388	G
35	R3	391	G
35	R3	392	C
35	R3	394	G
35	R3	396	C
35	R3	398	U
35	R3	401	C
35	R3	402	G

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Mol	Chain	Res	Type
35	R3	403	C
35	R3	406	G
35	R3	411	A
35	R3	413	G
35	R3	415	A
35	R3	416	G
35	R3	417	G
35	R3	418	C
35	R3	421	U
35	R3	422	C
35	R3	423	G
35	R3	425	G
35	R3	427	U
35	R3	428	G
35	R3	429	U
35	R3	437	U
35	R3	438	U
35	R3	440	C
35	R3	451	A
35	R3	454	G
35	R3	456	A
35	R3	465	A
35	R3	466	A
35	R3	467	U
35	R3	468	A
35	R3	470	C
35	R3	472	U
35	R3	473	U
35	R3	479	U
35	R3	480	U
35	R3	482	A
35	R3	484	G
35	R3	487	A
35	R3	492	C
35	R3	493	A
35	R3	495	A
35	R3	496	A
35	R3	497	G
35	R3	498	A
35	R3	501	C
35	R3	502	A
35	R3	511	C

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Mol	Chain	Res	Type
35	R3	517	G
35	R3	518	C
35	R3	521	G
35	R3	524	G
35	R3	530	G
35	R3	531	U
35	R3	532	A
35	R3	538	G
35	R3	539	A
35	R3	540	G
35	R3	541	G
35	R3	547	A
35	R3	549	C
35	R3	552	U
35	R3	553	A
35	R3	559	A
35	R3	562	U
35	R3	564	C
35	R3	566	G
35	R3	572	A
35	R3	573	A
35	R3	576	C
35	R3	577	G
35	R3	579	A
35	R3	589	U
35	R3	596	A
35	R3	597	G
35	R3	607	A
35	R3	610	U
35	R3	611	C
35	R3	612	C
35	R3	613	C
35	R3	628	G
35	R3	630	A
35	R3	632	U
35	R3	633	G
35	R3	640	A
35	R3	641	U
35	R3	642	A
35	R3	651	C
35	R3	652	U
35	R3	653	U

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Mol	Chain	Res	Type
35	R3	665	A
35	R3	673	A
35	R3	684	U
35	R3	686	U
35	R3	688	G
35	R3	695	A
35	R3	701	U
35	R3	702	A
35	R3	703	G
35	R3	713	G
35	R3	721	G
35	R3	723	U
35	R3	724	G
35	R3	731	G
35	R3	734	G
35	R3	738	C
35	R3	739	C
35	R3	743	A
35	R3	749	A
35	R3	754	C
35	R3	755	G
35	R3	774	G
35	R3	777	A
35	R3	779	C
35	R3	781	A
35	R3	787	A
35	R3	791	G
35	R3	792	A
35	R3	793	U
35	R3	794	A
35	R3	815	A
35	R3	817	C
35	R3	818	G
35	R3	819	A
35	R3	829	G
35	R3	832	G
35	R3	838	G
35	R3	839	C
35	R3	840	C
35	R3	841	C
35	R3	843	U
35	R3	844	G

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Mol	Chain	Res	Type
35	R3	846	G
35	R3	849	G
35	R3	850	U
35	R3	851	G
35	R3	863	U
35	R3	864	A
35	R3	870	U
35	R3	871	U
35	R3	872	A
35	R3	876	C
35	R3	877	G
35	R3	878	A
35	R3	902	G
35	R3	914	A
35	R3	926	G
35	R3	933	G
35	R3	935	A
35	R3	947	G
35	R3	958	A
35	R3	959	A
35	R3	960	U
35	R3	961	U
35	R3	966	G
35	R3	969	A
35	R3	975	A
35	R3	976	G
35	R3	977	A
35	R3	990	C
35	R3	991	U
35	R3	992	U
35	R3	1000	A
35	R3	1001	C
35	R3	1002	G
35	R3	1003	G
35	R3	1004	A
35	R3	1006	G
35	R3	1007	U
35	R3	1008	U
35	R3	1009	U
35	R3	1015	G
35	R3	1017	U
35	R3	1020	G

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Mol	Chain	Res	Type
35	R3	1024	G
35	R3	1027	C
35	R3	1028	C
35	R3	1031	C
35	R3	1032	G
35	R3	1033	G
35	R3	1037	C
35	R3	1039	G
35	R3	1040	U
35	R3	1045	C
35	R3	1049	U
35	R3	1050	G
35	R3	1052	U
35	R3	1053	G
35	R3	1054	C
35	R3	1065	U
35	R3	1084	G
35	R3	1085	U
35	R3	1094	G
35	R3	1095	U
35	R3	1101	A
35	R3	1103	C
35	R3	1104	G
35	R3	1108	G
35	R3	1113	C
35	R3	1114	C
35	R3	1118	U
35	R3	1119	C
35	R3	1123	U
35	R3	1125	U
35	R3	1126	U
35	R3	1129	C
35	R3	1130	A
35	R3	1131	G
35	R3	1133	G
35	R3	1134	G
35	R3	1137	C
35	R3	1138	G
35	R3	1139	G
35	R3	1140	C
35	R3	1142	G
35	R3	1145	A

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Mol	Chain	Res	Type
35	R3	1150	A
35	R3	1151	A
35	R3	1152	A
35	R3	1157	A
35	R3	1158	C
35	R3	1159	U
35	R3	1168	U
35	R3	1169	A
35	R3	1182	G
35	R3	1184	G
35	R3	1187	G
35	R3	1196	A
35	R3	1197	A
35	R3	1200	C
35	R3	1201	A
35	R3	1208	C
35	R3	1209	C
35	R3	1212	U
35	R3	1213	A
35	R3	1227	A
35	R3	1228	C
35	R3	1238	A
35	R3	1240	U
35	R3	1255	G
35	R3	1257	A
35	R3	1258	G
35	R3	1260	G
35	R3	1261	A
35	R3	1262	C
35	R3	1267	C
35	R3	1268	G
35	R3	1271	A
35	R3	1275	A
35	R3	1280	A
35	R3	1285	A
35	R3	1286	U
35	R3	1287	A
35	R3	1297	G
35	R3	1298	U
35	R3	1300	G
35	R3	1302	C
35	R3	1305	G

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Mol	Chain	Res	Type
35	R3	1306	A
35	R3	1312	G
35	R3	1315	U
35	R3	1332	A
35	R3	1336	C
35	R3	1346	A
35	R3	1353	G
35	R3	1363	A
35	R3	1368	A
35	R3	1370	G
35	R3	1376	U
35	R3	1378	C
35	R3	1389	C
35	R3	1396	A
35	R3	1398	A
35	R3	1400	C
35	R3	1404	C
35	R3	1405	G
35	R3	1409	C
35	R3	1419	G
35	R3	1422	G
35	R3	1429	A
35	R3	1437	A
35	R3	1440	U
35	R3	1441	A
35	R3	1442	G
35	R3	1443	C
35	R3	1446	A
35	R3	1448	C
35	R3	1451	U
35	R3	1452	C
35	R3	1455	G
35	R3	1473	G
35	R3	1474	U
35	R3	1475	G
35	R3	1487	G
35	R3	1491	G
35	R3	1492	A
35	R3	1493	A
35	R3	1494	G
35	R3	1497	G
35	R3	1499	A

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Mol	Chain	Res	Type
35	R3	1502	A
35	R3	1506	U
35	R3	1517	G
35	R3	1519	A
35	R3	1520	C
35	R3	1529	G
35	R3	1530	G
36	T	8	U
36	T	13	C
36	T	16	C
36	T	17	U
36	T	18	G
36	T	19	G
36	T	20	G
36	T	21	A
36	T	24	G
36	T	25	C
36	T	26	A
36	T	42	G
36	T	43	G
36	T	44	G
36	T	46	G
36	T	47	U
36	T	51	C
36	T	57	G
36	T	58	A
36	T	59	U
36	T	60	C
36	T	61	C
36	T	62	C
36	T	63	G
36	T	65	C
36	T	66	A
36	T	69	A
36	T	70	C
36	T	74	C
36	T	76	A

All (54) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
33	R1	198	C

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Mol	Chain	Res	Type
33	R1	271	G
33	R1	276	U
33	R1	446	G
33	R1	453	A
33	R1	479	A
33	R1	784	G
33	R1	859	G
33	R1	903	C
33	R1	1020	A
33	R1	1050	A
33	R1	1236	G
33	R1	1915	U
33	R1	2115	G
33	R1	2146	C
33	R1	2174	C
33	R1	2178	C
33	R1	2663	G
33	R1	2665	A
33	R1	2699	C
33	R1	2839	G
33	R1	2846	G
33	R1	2896	C
34	R2	64	G
35	R3	94	G
35	R3	95	C
35	R3	120	A
35	R3	288	A
35	R3	301	G
35	R3	312	C
35	R3	363	A
35	R3	416	G
35	R3	428	G
35	R3	453	G
35	R3	497	G
35	R3	500	G
35	R3	561	U
35	R3	588	G
35	R3	612	C
35	R3	640	A
35	R3	672	U
35	R3	685	G
35	R3	753	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
35	R3	837	U
35	R3	870	U
35	R3	1003	G
35	R3	1064	G
35	R3	1125	U
35	R3	1137	C
35	R3	1149	C
35	R3	1150	A
35	R3	1270	G
35	R3	1297	G
35	R3	1305	G

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 130 ligands modelled in this entry, 128 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
59	ATP	E	601	60	28,33,33	0.79	0	34,52,52	0.68	1 (2%)
59	ATP	E	602	60	28,33,33	0.79	0	34,52,52	0.59	1 (2%)

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
59	ATP	E	601	60	-	2/18/38/38	0/3/3/3
59	ATP	E	602	60	-	6/18/38/38	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	E	602	ATP	C5-C6-N6	2.31	123.83	120.31
59	E	601	ATP	C5-C6-N6	2.25	123.75	120.31

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	E	602	ATP	C5'-O5'-PA-O3A
59	E	602	ATP	O4'-C4'-C5'-O5'
59	E	602	ATP	C3'-C4'-C5'-O5'
59	E	602	ATP	PB-O3A-PA-O5'
59	E	602	ATP	C5'-O5'-PA-O1A
59	E	601	ATP	PB-O3B-PG-O3G
59	E	602	ATP	PB-O3A-PA-O1A
59	E	601	ATP	O4'-C4'-C5'-O5'

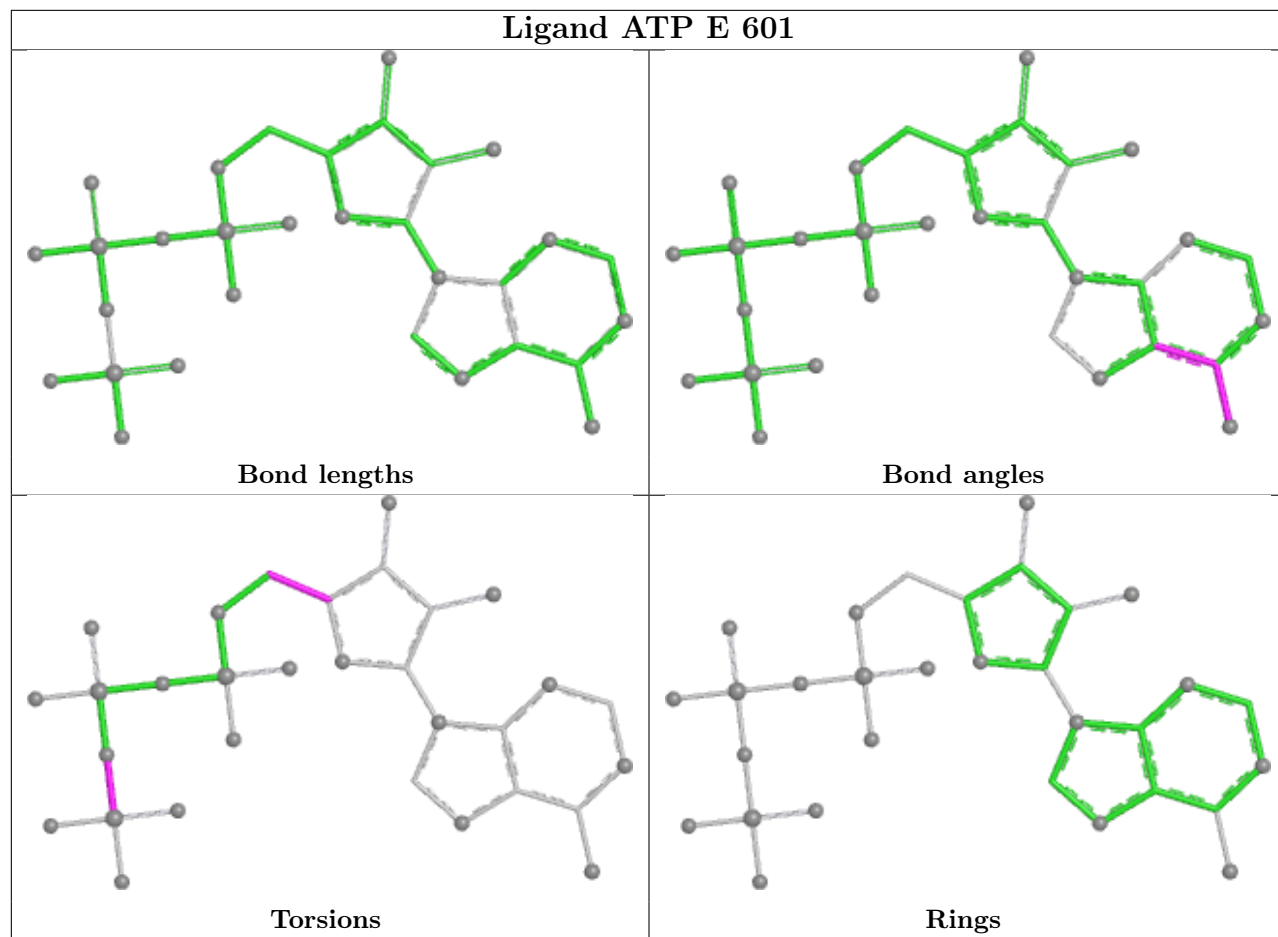
There are no ring outliers.

2 monomers are involved in 6 short contacts:

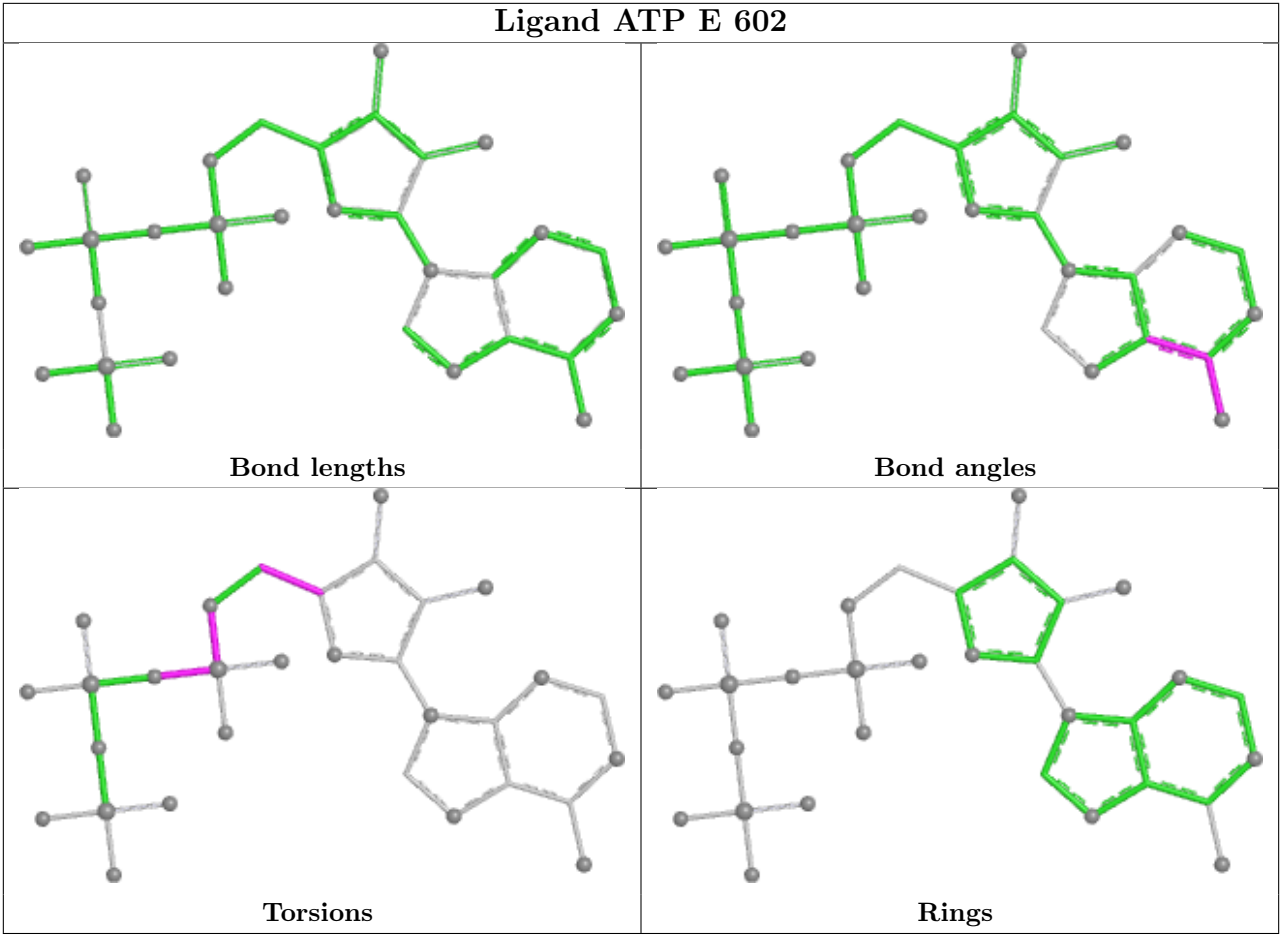
Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	E	601	ATP	3	0
59	E	602	ATP	3	0

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

equivalents in the CSD to analyse the geometry.







5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
35	R3	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	R3	460:A	O3'	461:A	P	5.02
1	R3	210:C	O3'	211:G	P	3.87

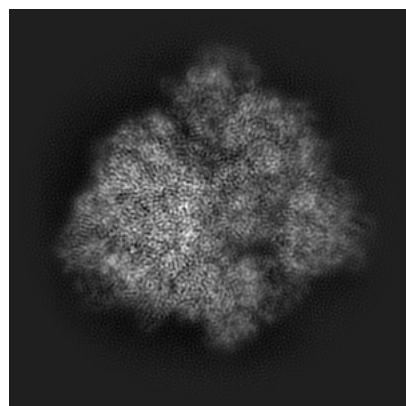
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40921. These allow visual inspection of the internal detail of the map and identification of artifacts.

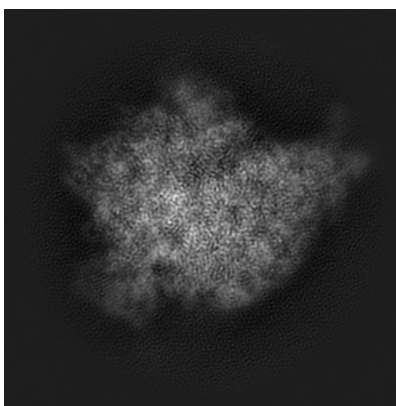
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

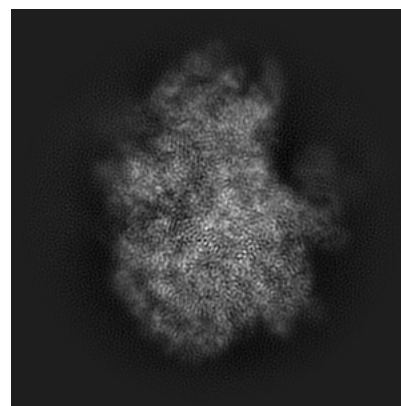
#### 6.1.1 Primary map



X

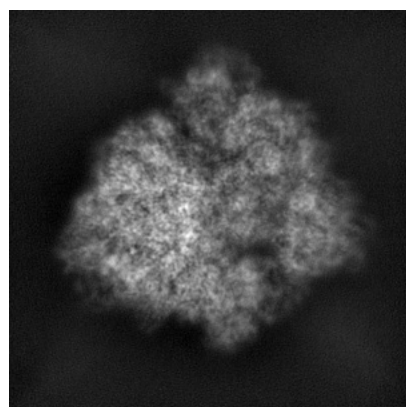


Y

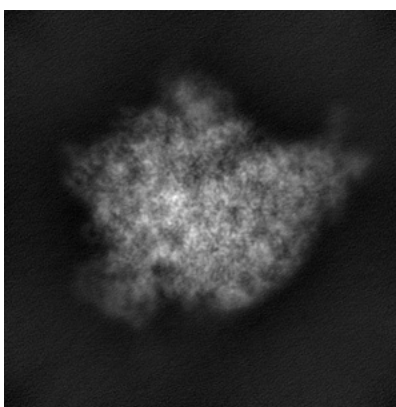


Z

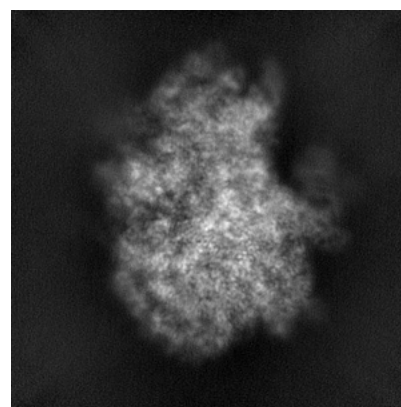
#### 6.1.2 Raw map



X



Y

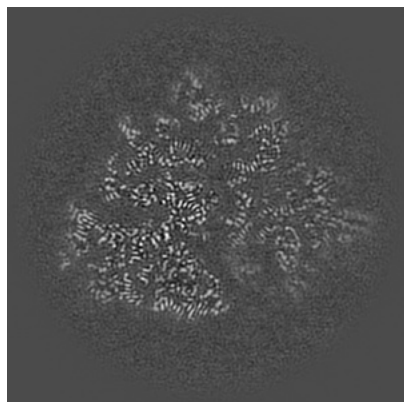


Z

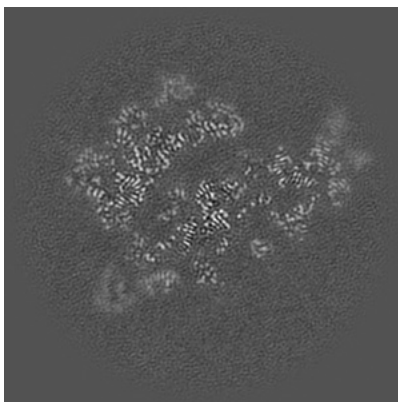
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

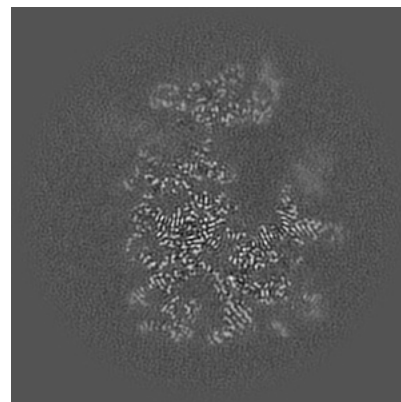
### 6.2.1 Primary map



X Index: 160

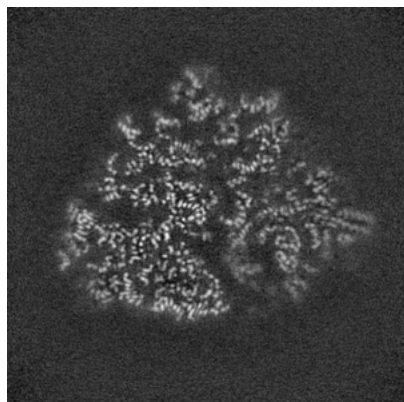


Y Index: 160

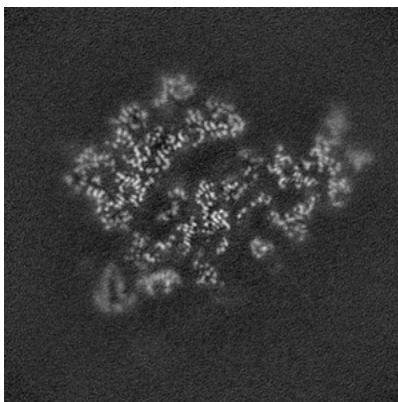


Z Index: 160

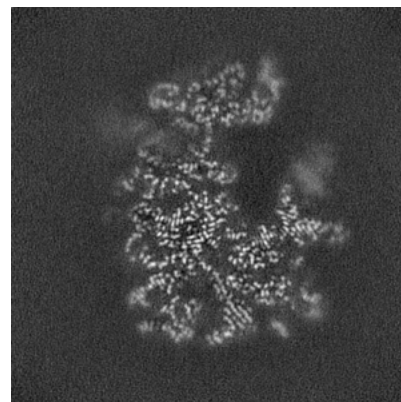
### 6.2.2 Raw map



X Index: 160



Y Index: 160

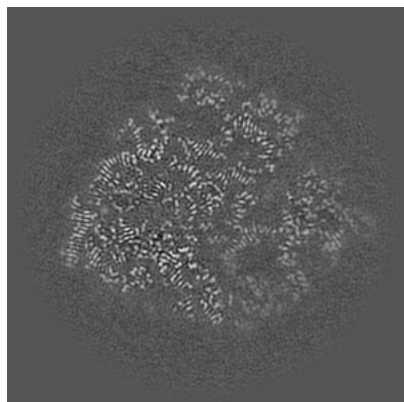


Z Index: 160

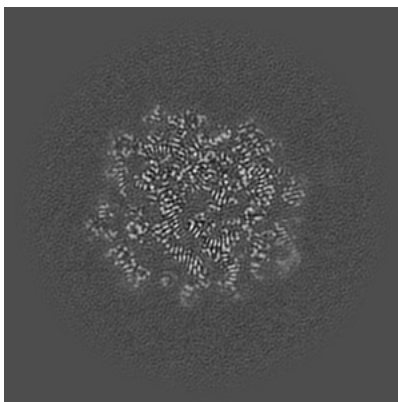
The images above show central slices of the map in three orthogonal directions.

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

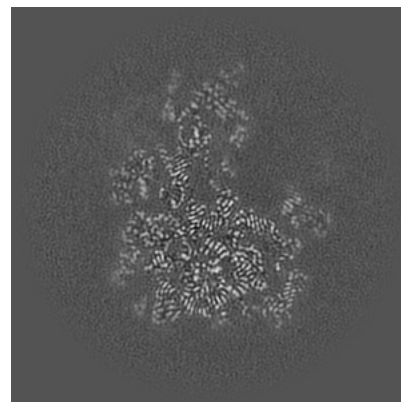
### 6.3.1 Primary map



X Index: 167

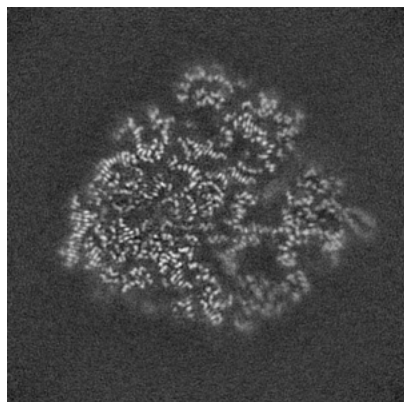


Y Index: 118

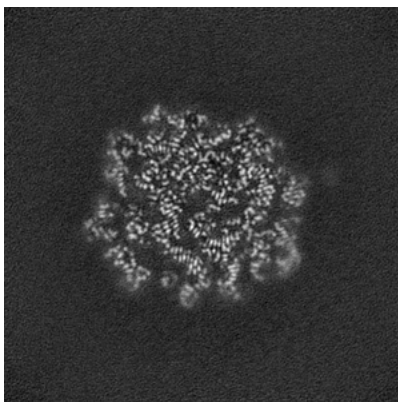


Z Index: 177

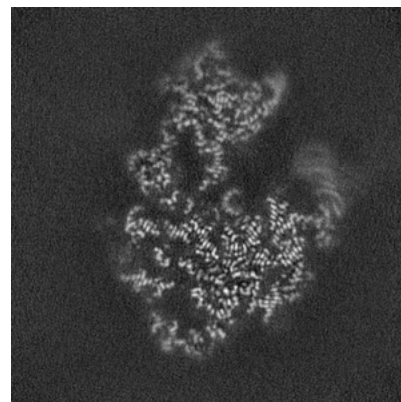
### 6.3.2 Raw map



X Index: 167



Y Index: 118



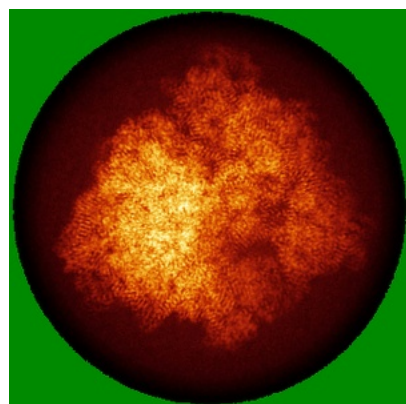
Z Index: 140

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

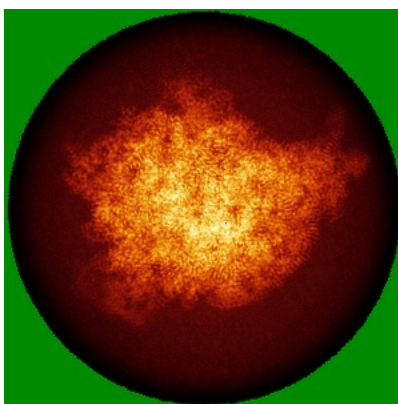


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

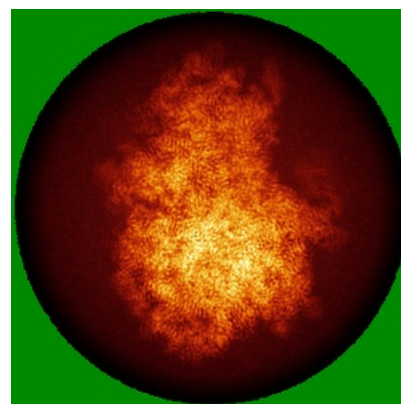
### 6.4.1 Primary map



X

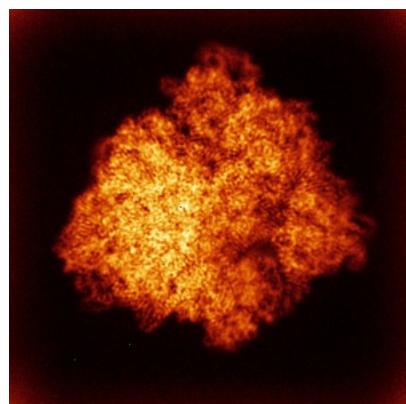


Y

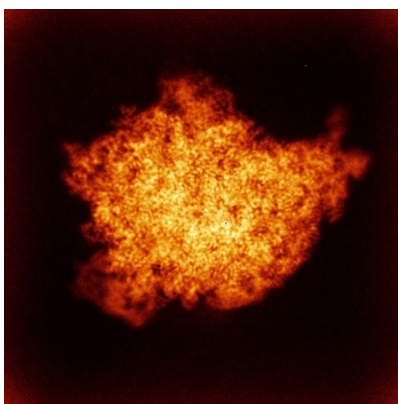


Z

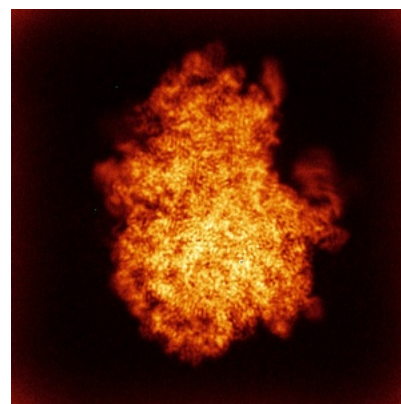
### 6.4.2 Raw map



X



Y

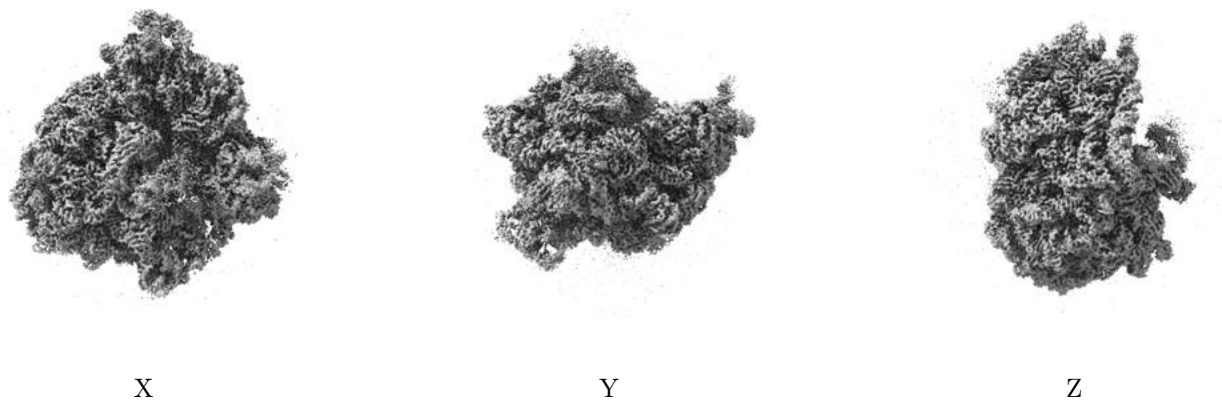


Z

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

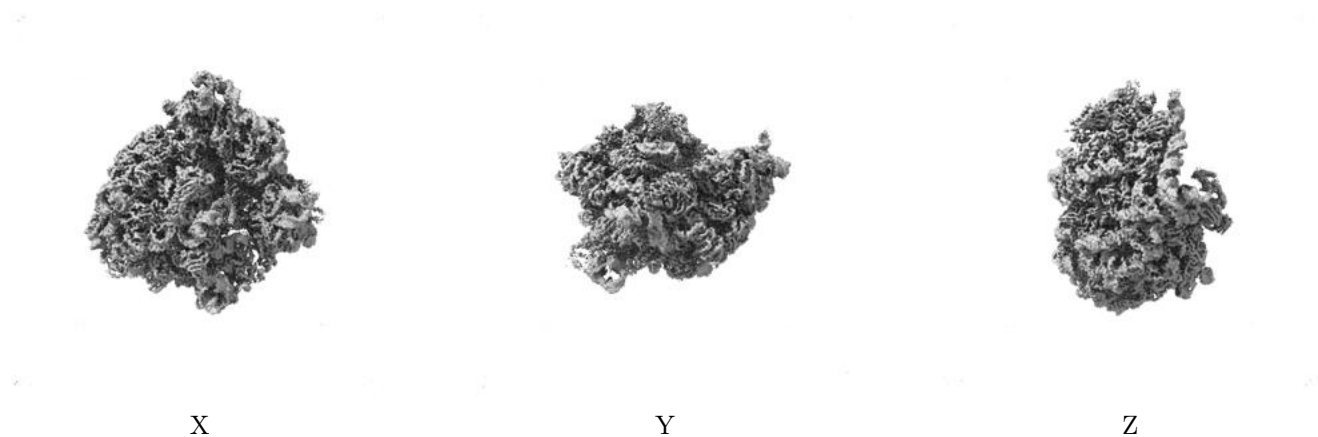
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

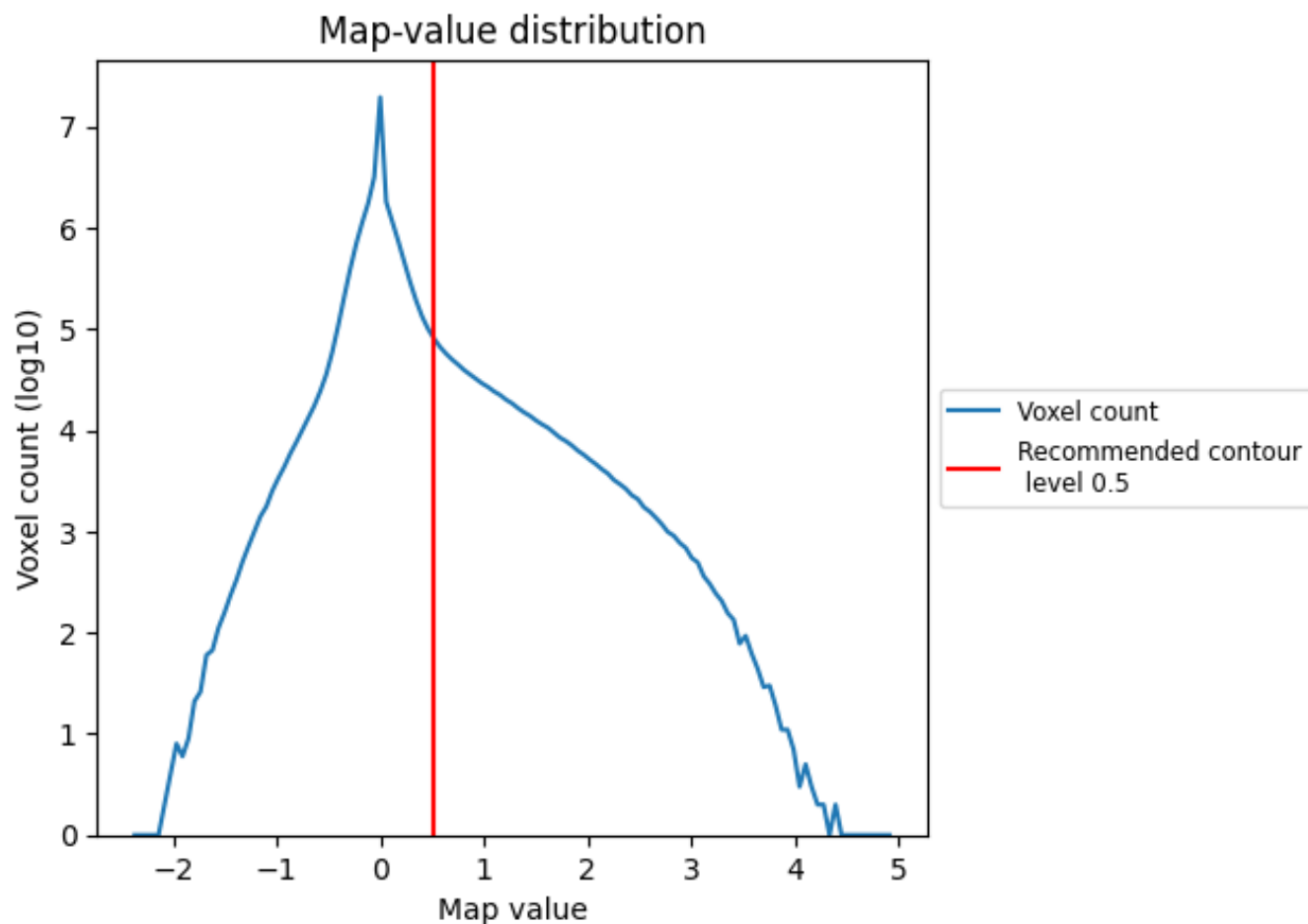
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

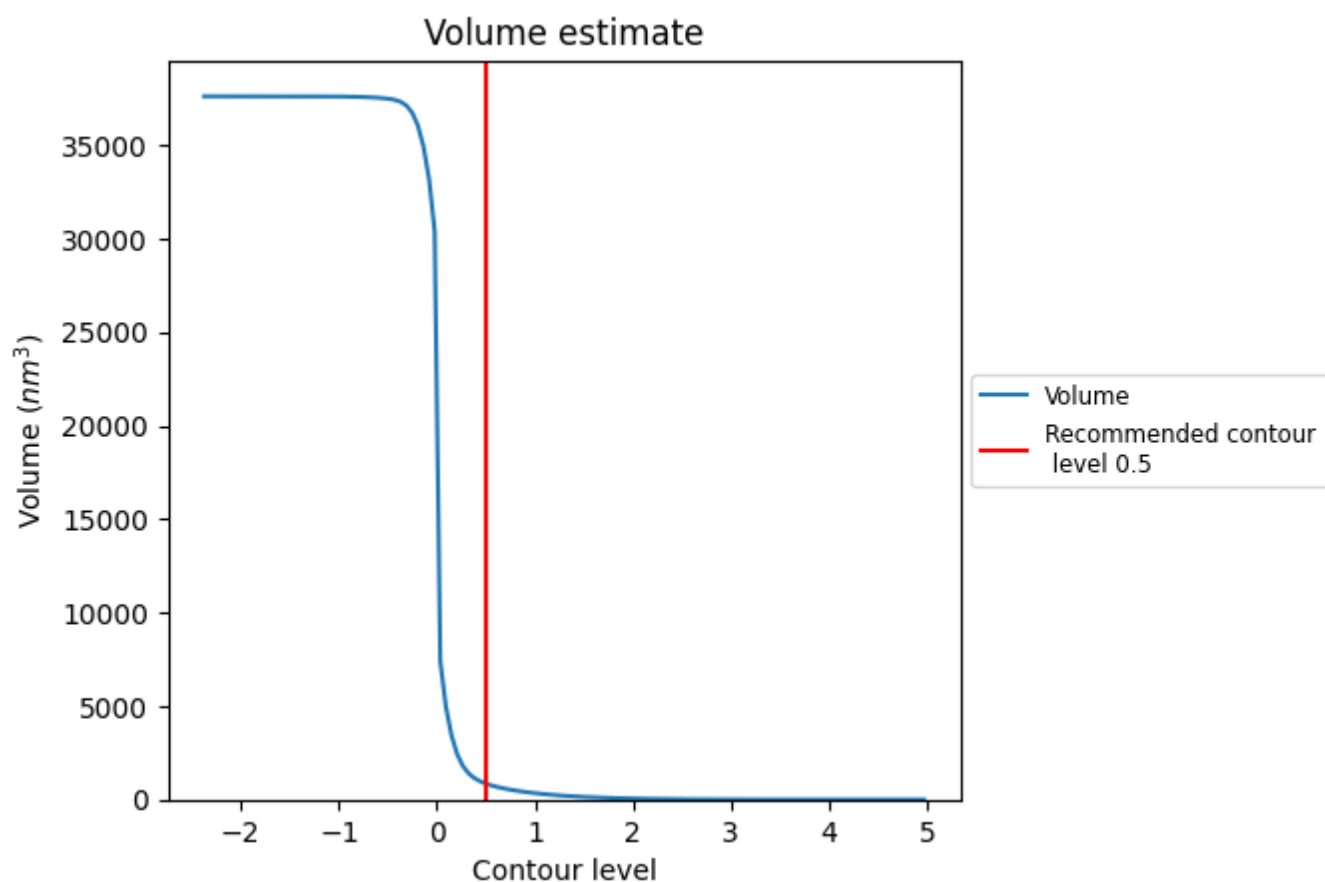
This section contains the results of statistical analysis of the map.

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



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

## 7.2 Volume estimate [i](#)

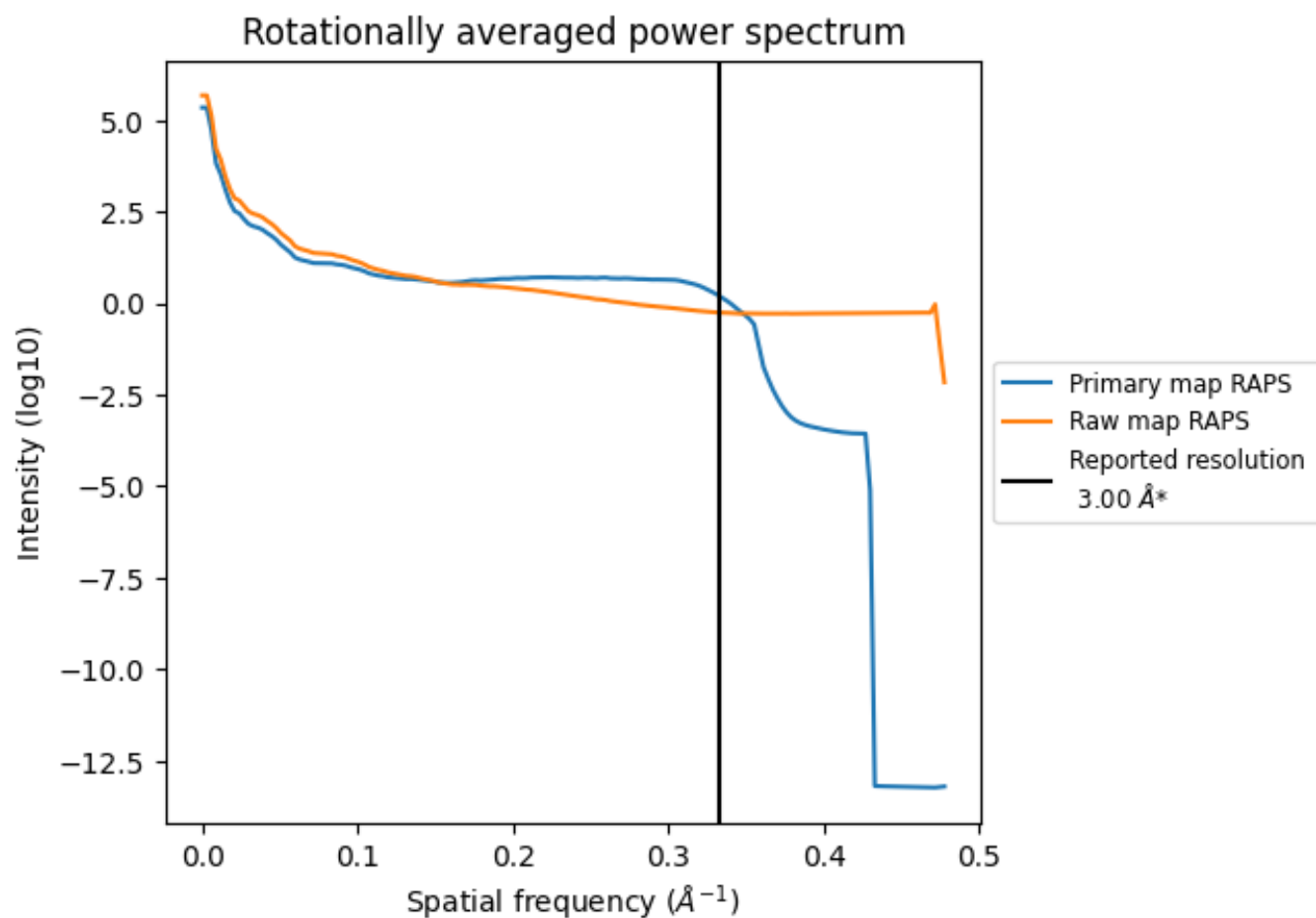


The volume at the recommended contour level is 851 nm<sup>3</sup>; this corresponds to an approximate mass of 768 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.



### 7.3 Rotationally averaged power spectrum ⓘ

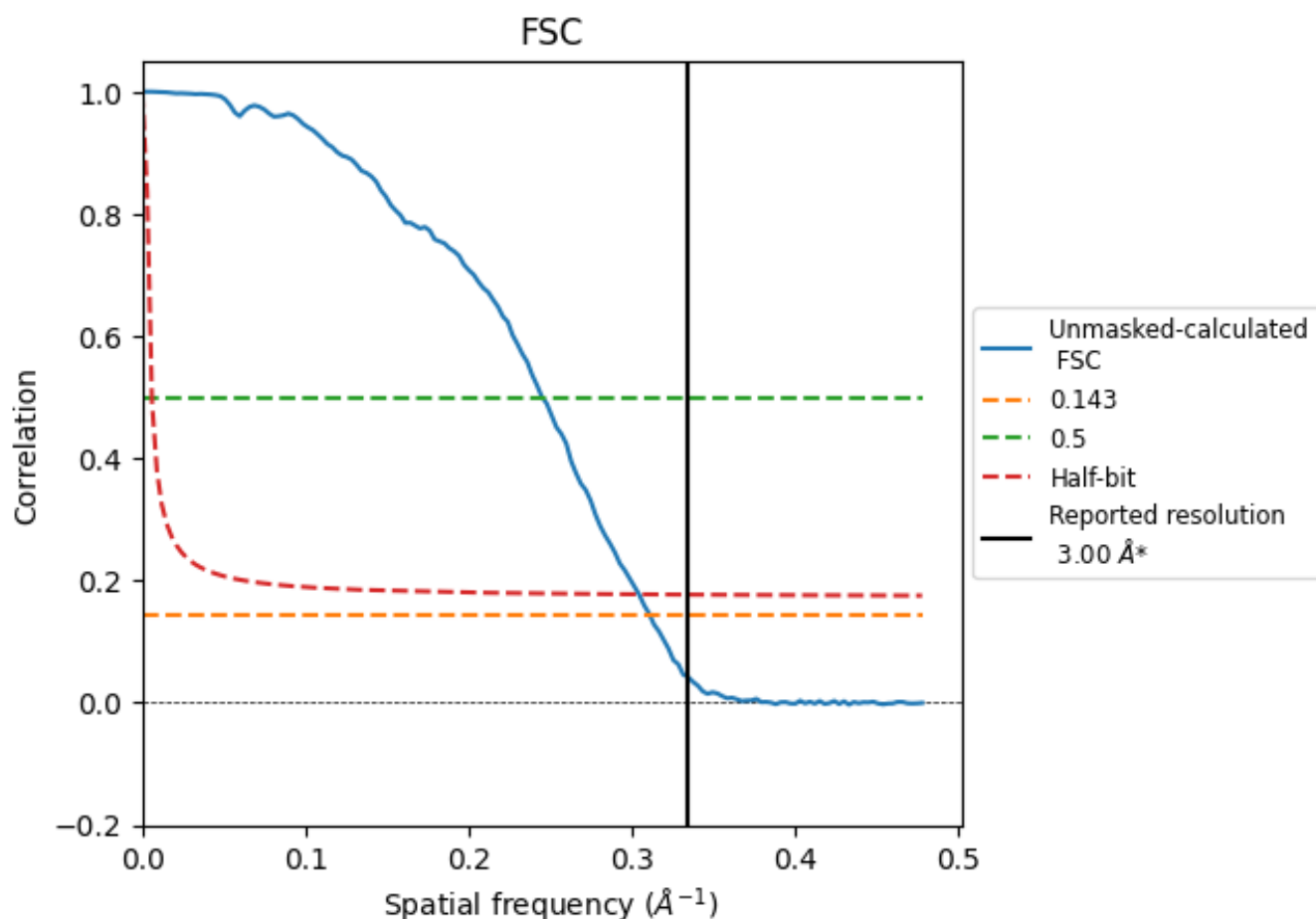


\*Reported resolution corresponds to spatial frequency of 0.333 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.333 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

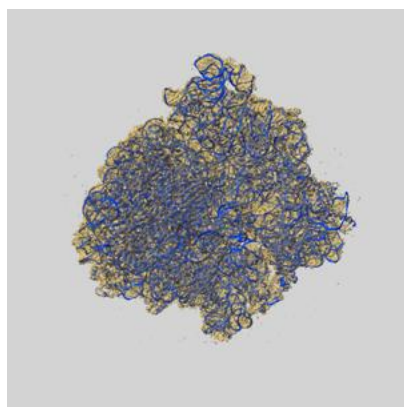
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.22	4.08	3.29

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

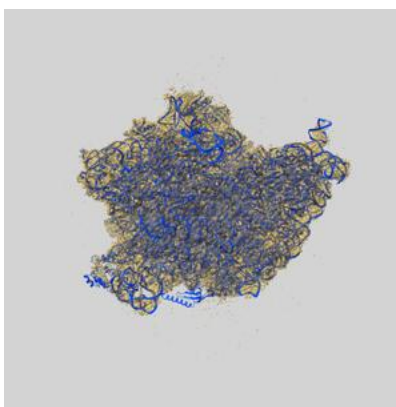
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-40921 and PDB model 9NL5. Per-residue inclusion information can be found in section [3](#) on page [15](#).

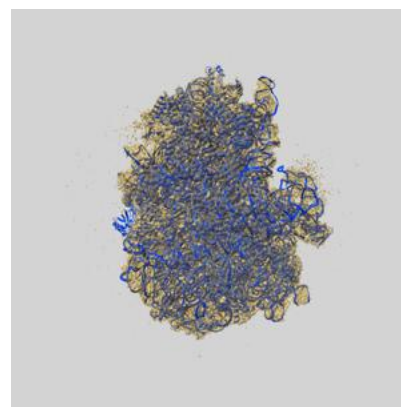
### 9.1 Map-model overlay [i](#)



X



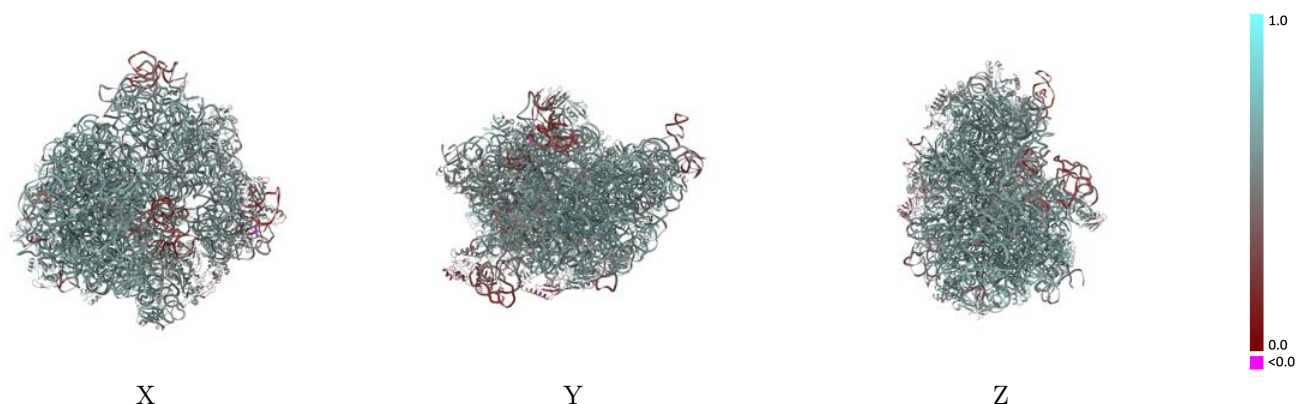
Y



Z

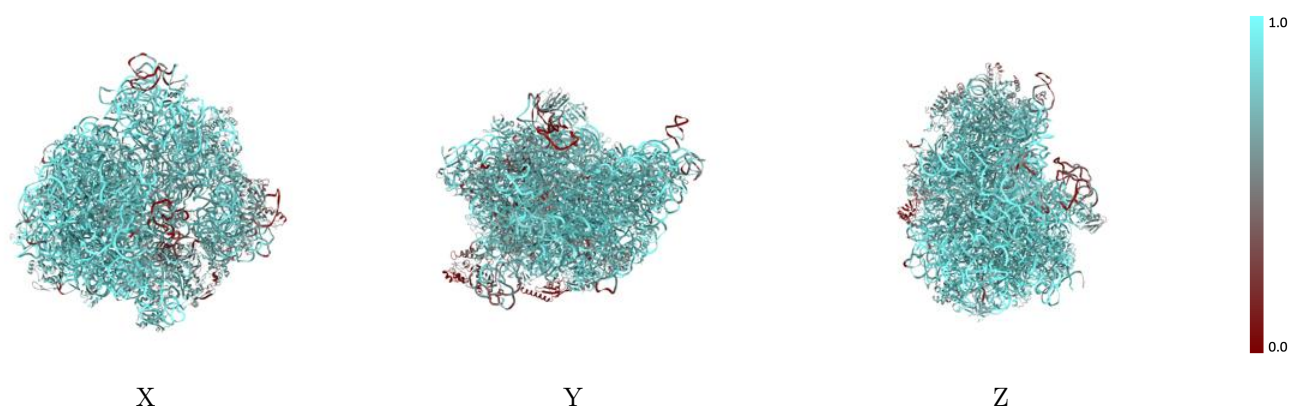
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



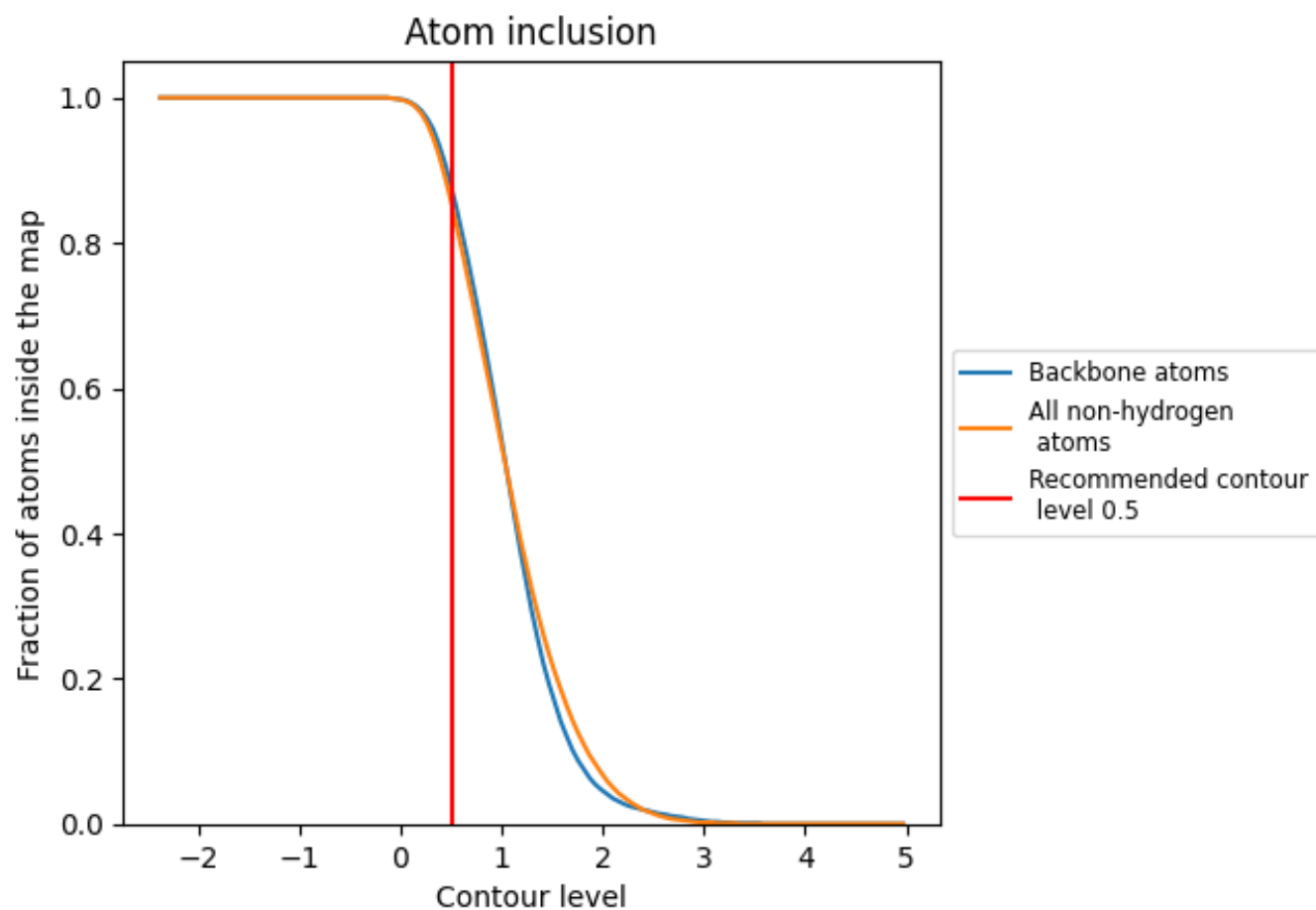
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 86% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8570	 0.5700
1	 0.2330	 0.3310
13	 0.8910	 0.6110
14	 0.8630	 0.6160
15	 0.8640	 0.6030
16	 0.8720	 0.6160
17	 0.9050	 0.6130
18	 0.7680	 0.5680
19	 0.8480	 0.6060
2	 0.9210	 0.6300
20	 0.9140	 0.6250
21	 0.8340	 0.5900
22	 0.8620	 0.6040
23	 0.8260	 0.5960
24	 0.7610	 0.5640
25	 0.7820	 0.5830
27	 0.8770	 0.6120
28	 0.9050	 0.6240
29	 0.7300	 0.5630
3	 0.8970	 0.6180
30	 0.8580	 0.5970
31	 0.3990	 0.4300
32	 0.8600	 0.6030
33	 0.8560	 0.6020
34	 0.9440	 0.6380
35	 0.9180	 0.6330
36	 0.8840	 0.6210
4	 0.7850	 0.5860
5	 0.6740	 0.5170
6	 0.6790	 0.5260
9	 0.2230	 0.3520
E	 0.6950	 0.5450
M	 0.6630	 0.5300
R1	 0.9230	 0.5850
R2	 0.9090	 0.5540



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Chain	Atom inclusion	Q-score
R3	 0.8970	 0.5620
T	 0.7270	 0.4900
sb	 0.6020	 0.4960
sc	 0.7140	 0.5600
sd	 0.7230	 0.5550
se	 0.8020	 0.5720
sf	 0.7840	 0.5590
sg	 0.6870	 0.5360
sh	 0.8220	 0.5980
si	 0.6870	 0.5260
sj	 0.5660	 0.4990
sk	 0.8140	 0.5890
sl	 0.8090	 0.5790
sm	 0.7070	 0.5340
sn	 0.7190	 0.5290
so	 0.8260	 0.5820
sp	 0.7640	 0.5660
sq	 0.7780	 0.5720
sr	 0.8200	 0.5750
ss	 0.6710	 0.5270
st	 0.7880	 0.5620
su	 0.5380	 0.4600