Full wwPDB EM Validation Report ⓘ

Mar 27, 2025 – 02:47 PM EDT

PDB ID	:	9NLE
EMDB ID	:	EMD-29398
Title	:	E. coli initiation complex with EQ2-EttA in Hydrolytic 1 conformation
Authors	:	Singh, S.; Hunt, J.F.
Deposited on	:	2025-03-03
Resolution	:	3.20 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

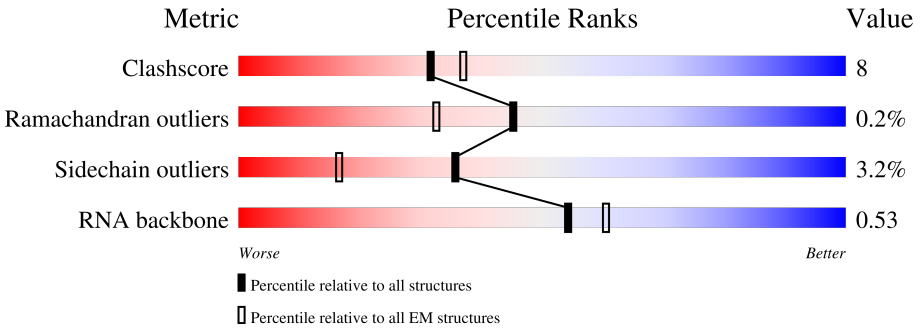
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 3.20 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 >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	220	89% 77% 23%
2	13	142	6% 77% 23%
3	14	122	8% 75% 25%
4	15	143	82% 17%
5	16	136	5% 76% 24%
6	17	120	82% 18%
7	18	116	11% 80% 19%

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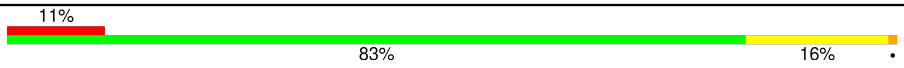
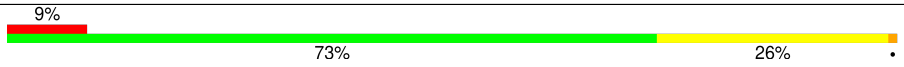
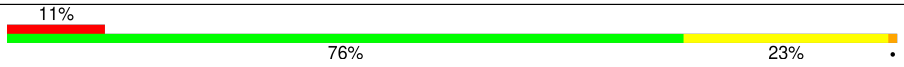
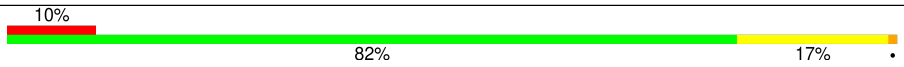
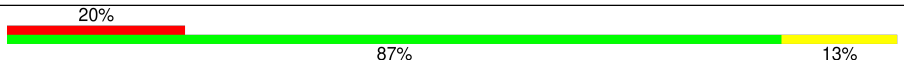
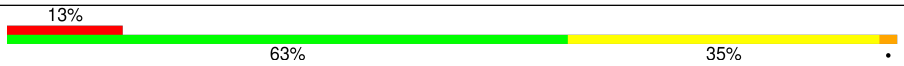
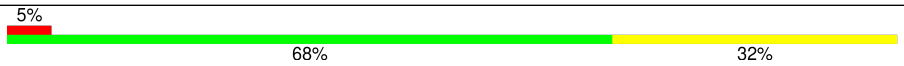
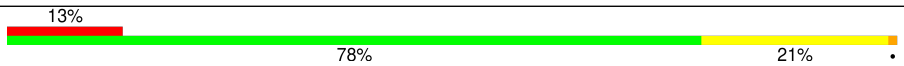
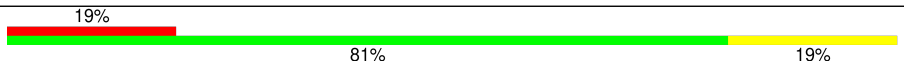
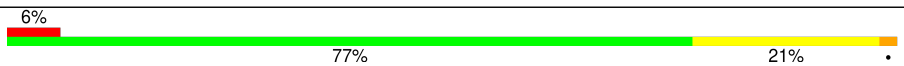
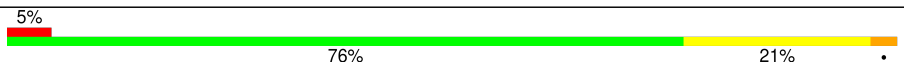
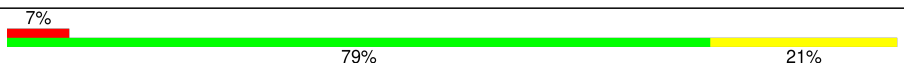
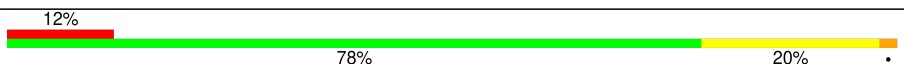
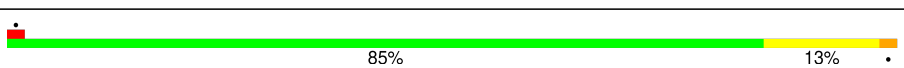
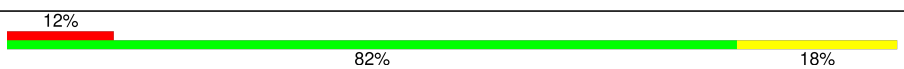
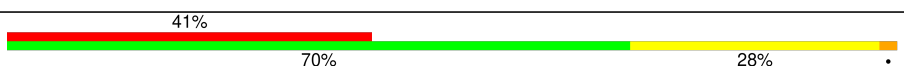
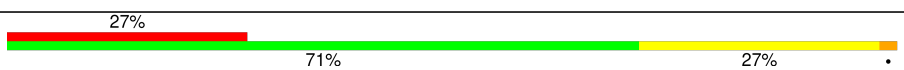
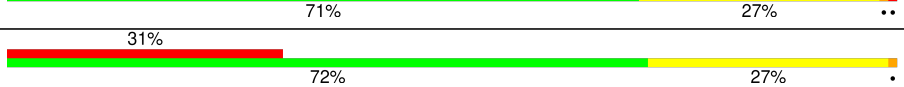
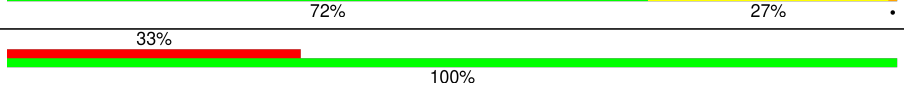
Mol	Chain	Length	Quality of chain
8	19	114	
9	2	271	
10	20	117	
11	21	103	
12	22	110	
13	23	93	
14	24	102	
15	25	94	
16	27	76	
17	28	77	
18	29	63	
19	3	209	
20	30	58	
21	31	66	
22	32	56	
23	33	50	
24	34	46	
25	35	64	
26	36	38	
27	4	201	
28	5	177	
29	6	176	
30	9	149	
31	E	552	
32	M	9	

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Mol	Chain	Length	Quality of chain
33	R1	2903	5% 58% 34% 8%
34	R2	119	5% 53% 40% 7%
35	R3	1531	53% 35% 11%
36	T	77	22% 53% 29% 14%
37	sb	218	27% 96%
38	sc	206	16% 97%
39	sd	205	18% 97%
40	se	157	13% 97%
41	sf	100	23% 92% 7%
42	sg	151	25% 99%
43	sh	129	9% 99%
44	si	127	17% 95% 5%
45	sj	98	42% 93% 7%
46	sk	116	12% 97%
47	sl	123	19% 95% 5%
48	sm	114	29% 97%
49	sn	100	23% 94% 6%
50	so	88	7% 99%
51	sp	82	15% 94% 6%
52	sq	80	18% 98%
53	sr	65	12% 97%
54	ss	79	27% 99%
55	st	85	13% 99%
56	su	70	40% 91% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	H2U	T	20	X	-	-	-
36	4OC	T	32	X	-	-	-
36	MUM	T	54	X	-	-	-
36	PSU	T	55	X	-	-	-
36	4SU	T	8	X	-	-	-

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 150106 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
			Total	C	N	O	S		
1	1	220	1353	804	270	277	2	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	27	76	Total 582	C 360	N 117	O 104	S 1	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	30	58	Total 449	C 281	N 87	O 79	S 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 Energy-dependent translational throttle protein EttA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	E	552	Total	C	N	O	S	0	0
			4360	2745	774	829	12		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	188	GLN	GLU	conflict	UNP P0A9W3
E	341	SER	ASP	conflict	UNP P0A9W3
E	470	GLN	GLU	conflict	UNP P0A9W3

- Molecule 32 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	M	9	Total	C	N	O	P	0	0
			195	88	40	58	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		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R1	1847	G	A	conflict	GB 2019144442

- 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	77	Total	C	N	O	P	S	0	0
			1639	734	294	534	76	1		

- 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 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	sm	114	Total	C	N	O	S	0	0
			883	546	178	156	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
			535	339	100	95	1		

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

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

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

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

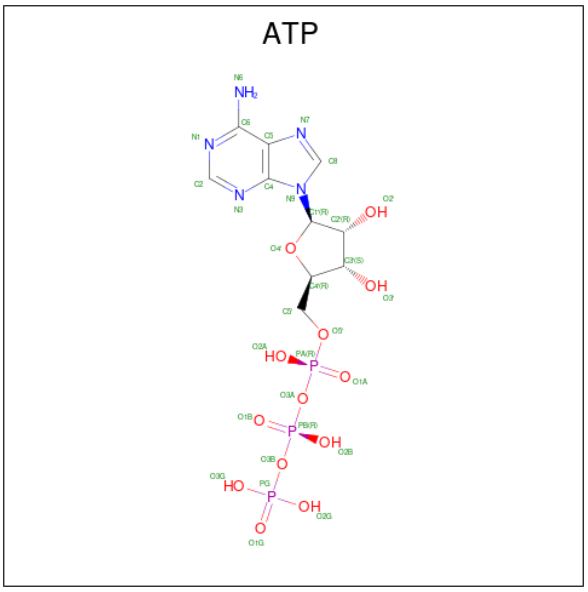
- Molecule 56 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	su	70	Total 590	C 366	N 125	O 98	S 1	0	0

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

Mol	Chain	Residues	Atoms		AltConf
57	15	1	Total 1	Mg 1	0
57	17	1	Total 1	Mg 1	0
57	M	1	Total 1	Mg 1	0
57	R1	204	Total 204	Mg 204	0
57	R3	89	Total 89	Mg 89	0
57	sn	1	Total 1	Mg 1	0
57	sq	1	Total 1	Mg 1	0

- Molecule 58 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

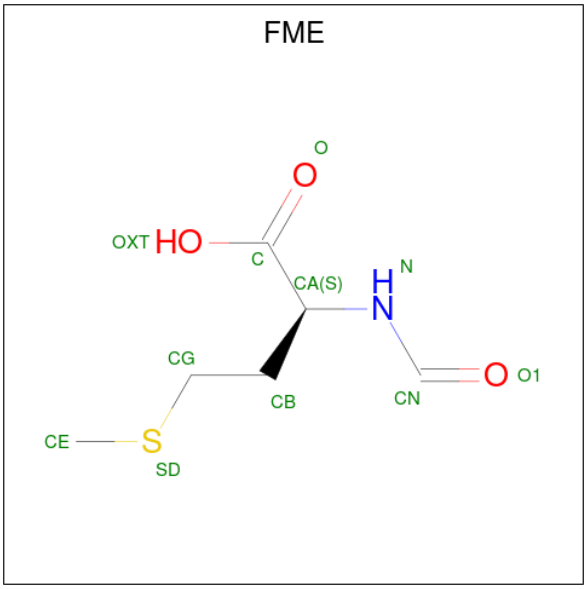


Mol	Chain	Residues	Atoms					AltConf
58	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
58	E	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 59 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 60 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: $C_6H_{11}NO_3S$).



Mol	Chain	Residues	Atoms					AltConf
60	T	1	Total	C	N	O	S	0
			10	6	1	2	1	

3 Residue-property plots (i)

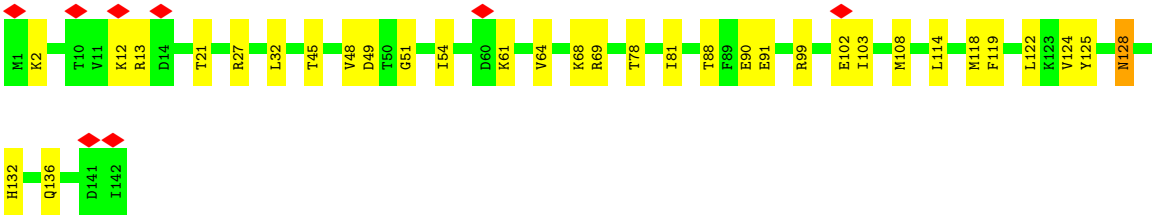
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Large ribosomal subunit protein uL1

Chain 1:

• Molecule 2: Large ribosomal subunit protein uL13

Chain 13:

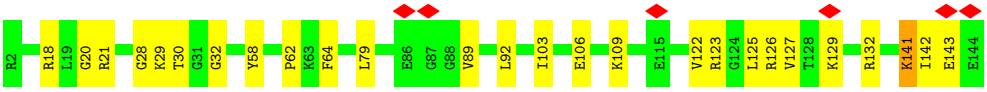


• Molecule 3: 50S ribosomal protein L14

Chain 14:

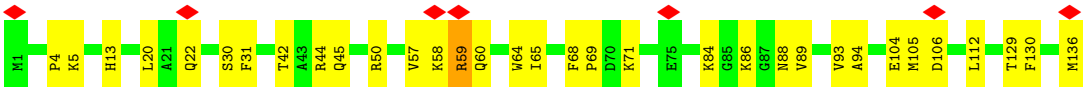
• Molecule 4: 50S ribosomal protein L15

Chain 15:



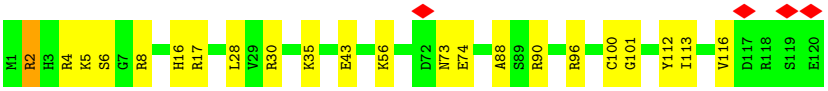
• Molecule 5: 50S ribosomal protein L16

Chain 16:



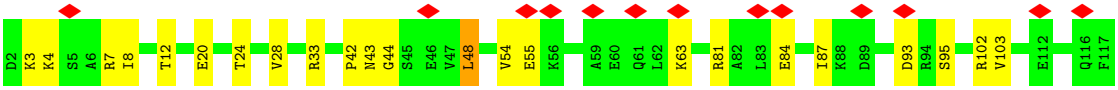
• Molecule 6: Large ribosomal subunit protein bL17

Chain 17:



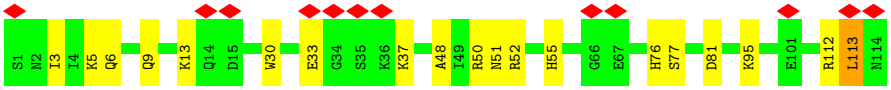
• Molecule 7: Large ribosomal subunit protein uL18

Chain 18:



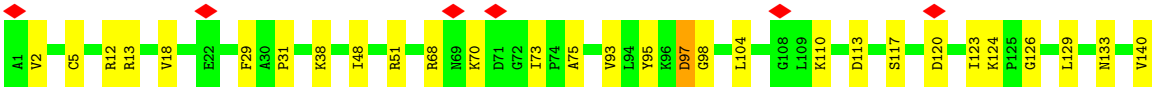
• Molecule 8: 50S ribosomal protein L19

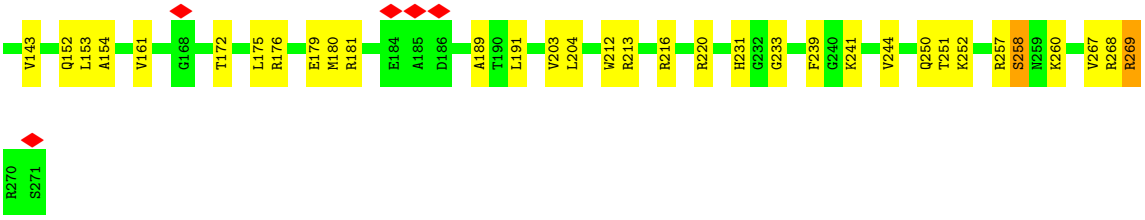
Chain 19:



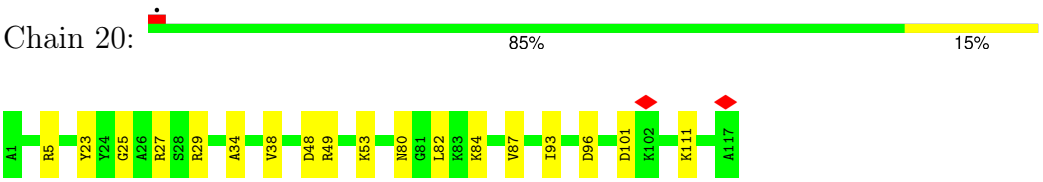
• Molecule 9: 50S ribosomal protein L2

Chain 2:

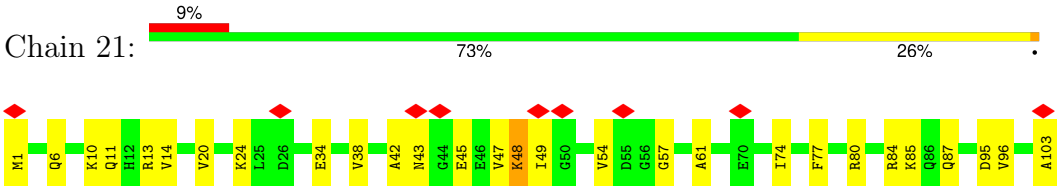




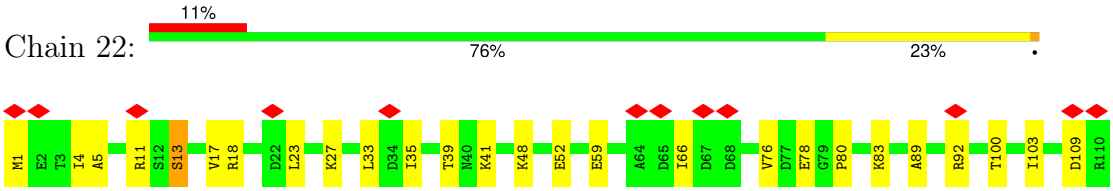
• Molecule 10: Large ribosomal subunit protein bL20



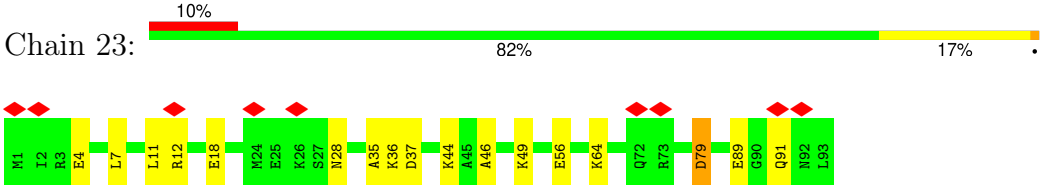
• Molecule 11: Large ribosomal subunit protein bL21



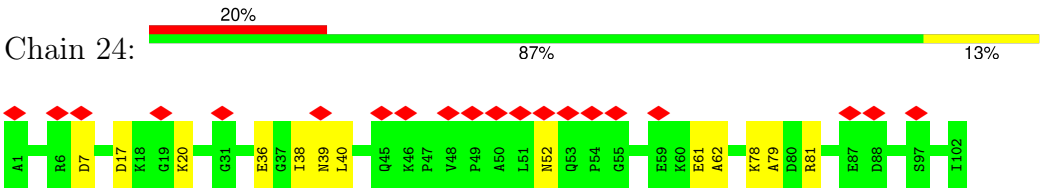
• Molecule 12: Large ribosomal subunit protein uL22



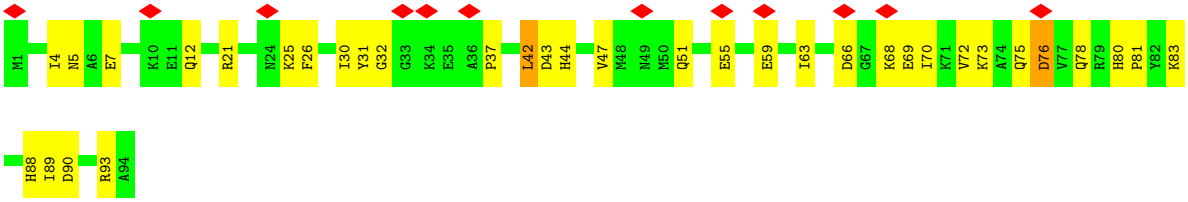
• Molecule 13: Large ribosomal subunit protein uL23



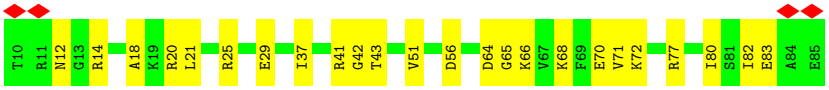
• Molecule 14: Large ribosomal subunit protein uL24



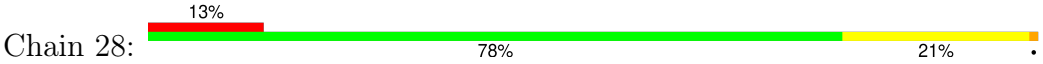
• Molecule 15: Large ribosomal subunit protein bL25

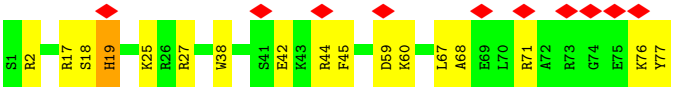


• Molecule 16: Large ribosomal subunit protein bL27

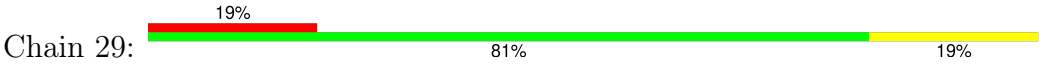


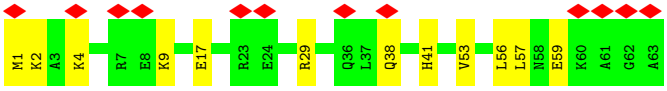
• Molecule 17: 50S ribosomal protein L28



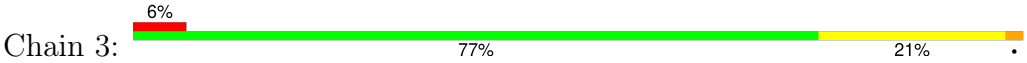


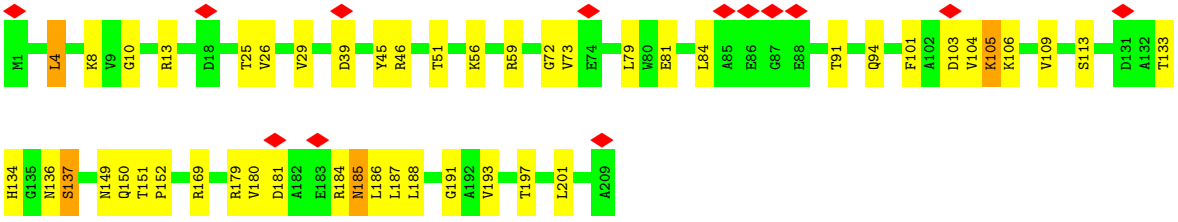
• Molecule 18: Large ribosomal subunit protein uL29



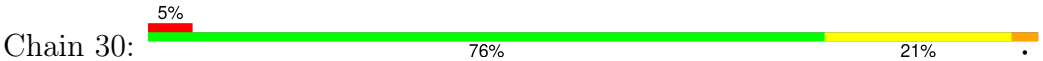


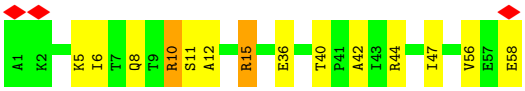
• Molecule 19: 50S ribosomal protein L3





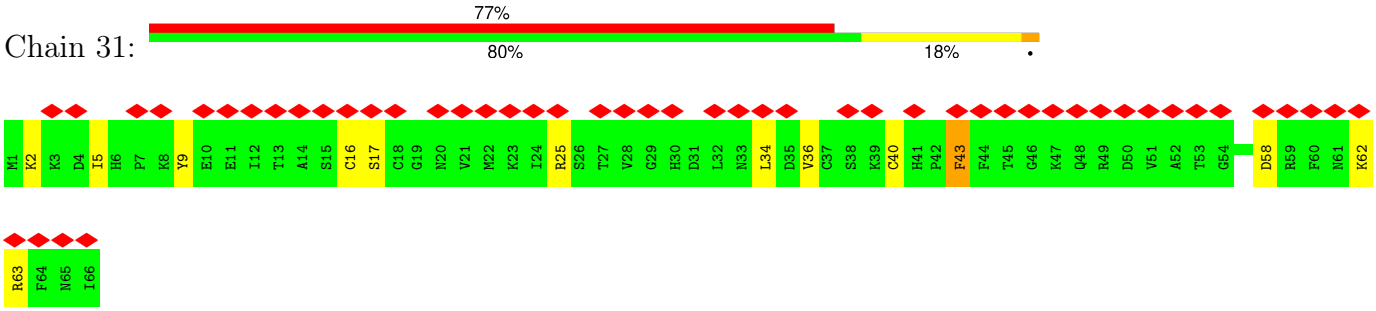
• Molecule 20: 50S ribosomal protein L30





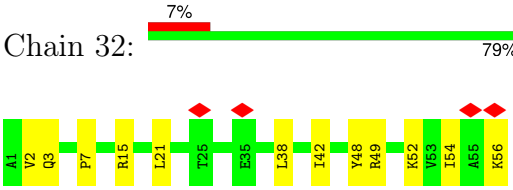
• Molecule 21: Large ribosomal subunit protein bL31

Chain 31:



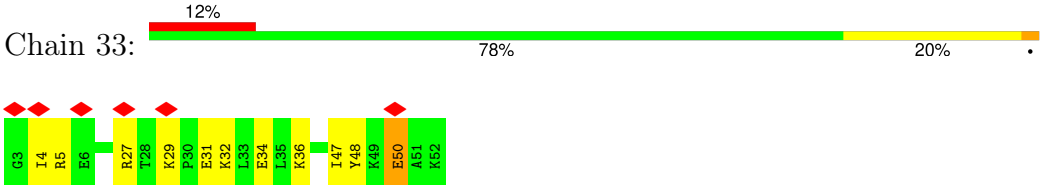
• Molecule 22: 50S ribosomal protein L32

Chain 32:



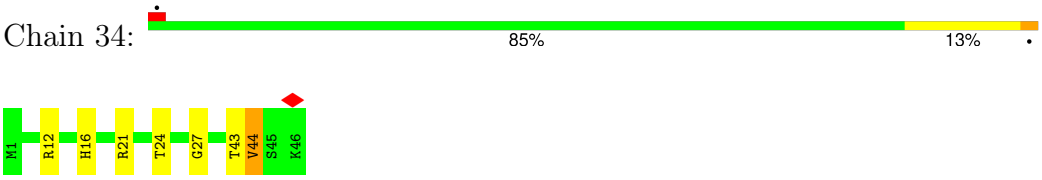
• Molecule 23: Large ribosomal subunit protein bL33

Chain 33:



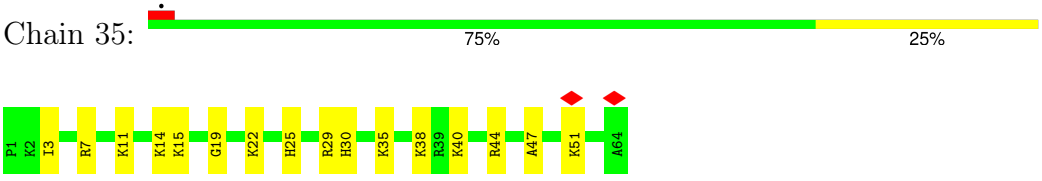
• Molecule 24: 50S ribosomal protein L34

Chain 34:



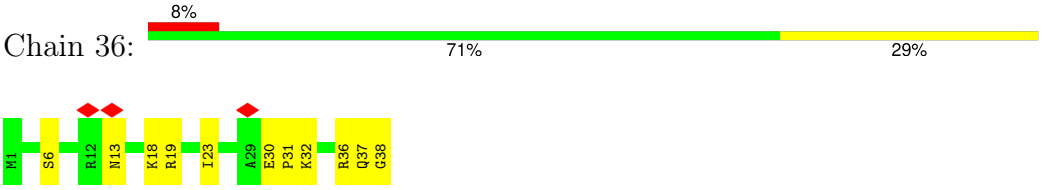
• Molecule 25: Large ribosomal subunit protein bL35

Chain 35:



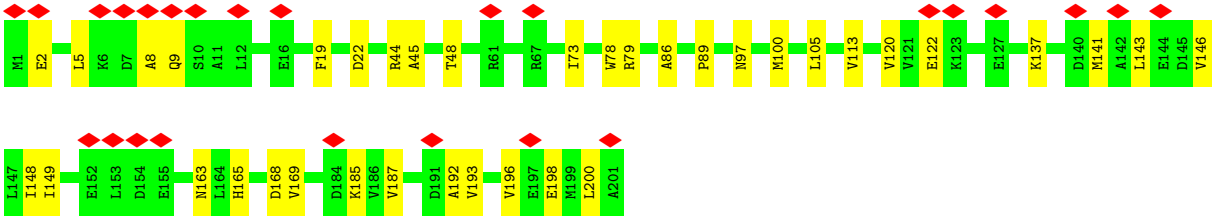
• Molecule 26: 50S ribosomal protein L36

Chain 36:

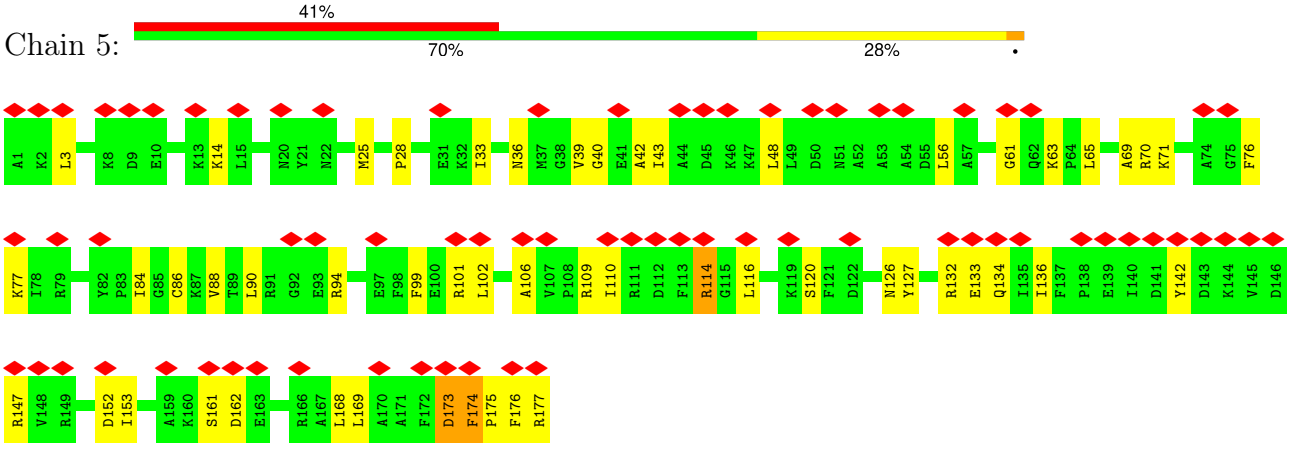


• Molecule 27: Large ribosomal subunit protein uL4

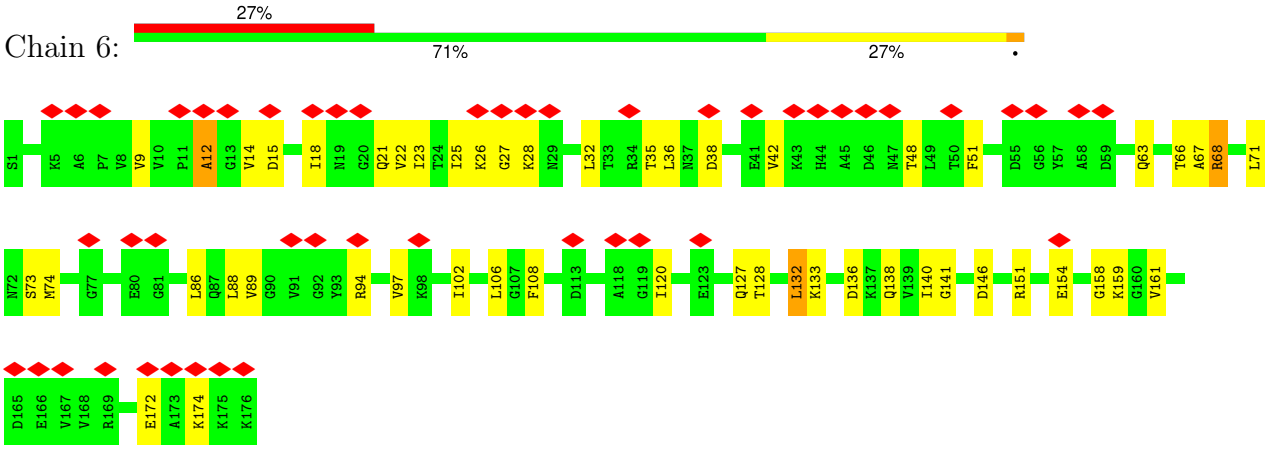
Chain 4:



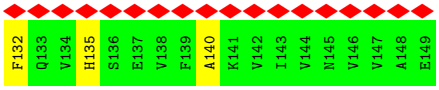
• Molecule 28: 50S ribosomal protein L5



• Molecule 29: Large ribosomal subunit protein uL6

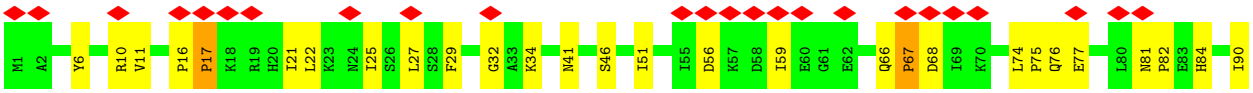


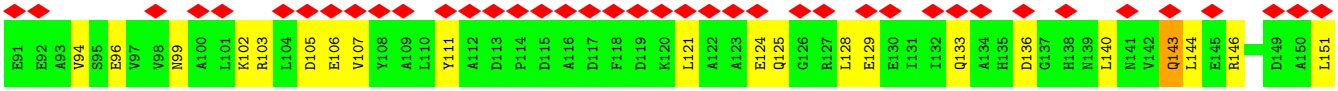
• Molecule 30: Large ribosomal subunit protein bL9

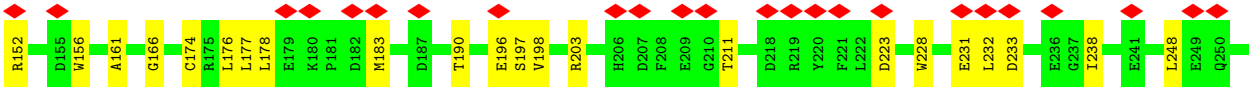


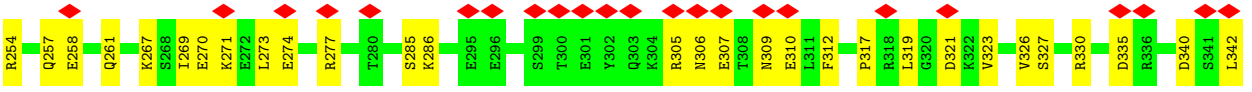
• Molecule 31: Energy-dependent translational throttle protein EttA

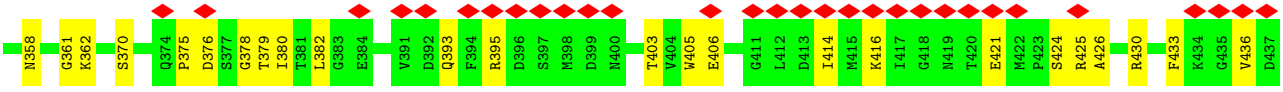
Chain E:

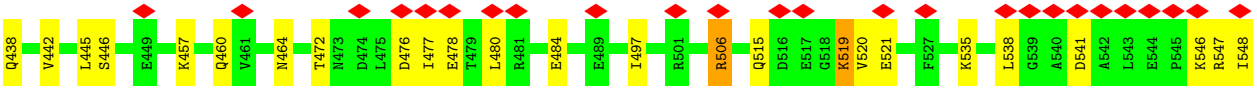


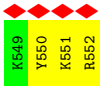






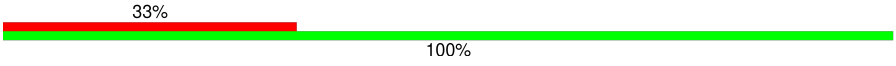






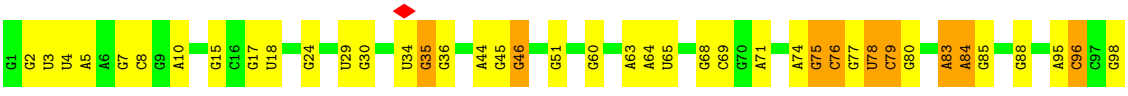
• Molecule 32: mRNA

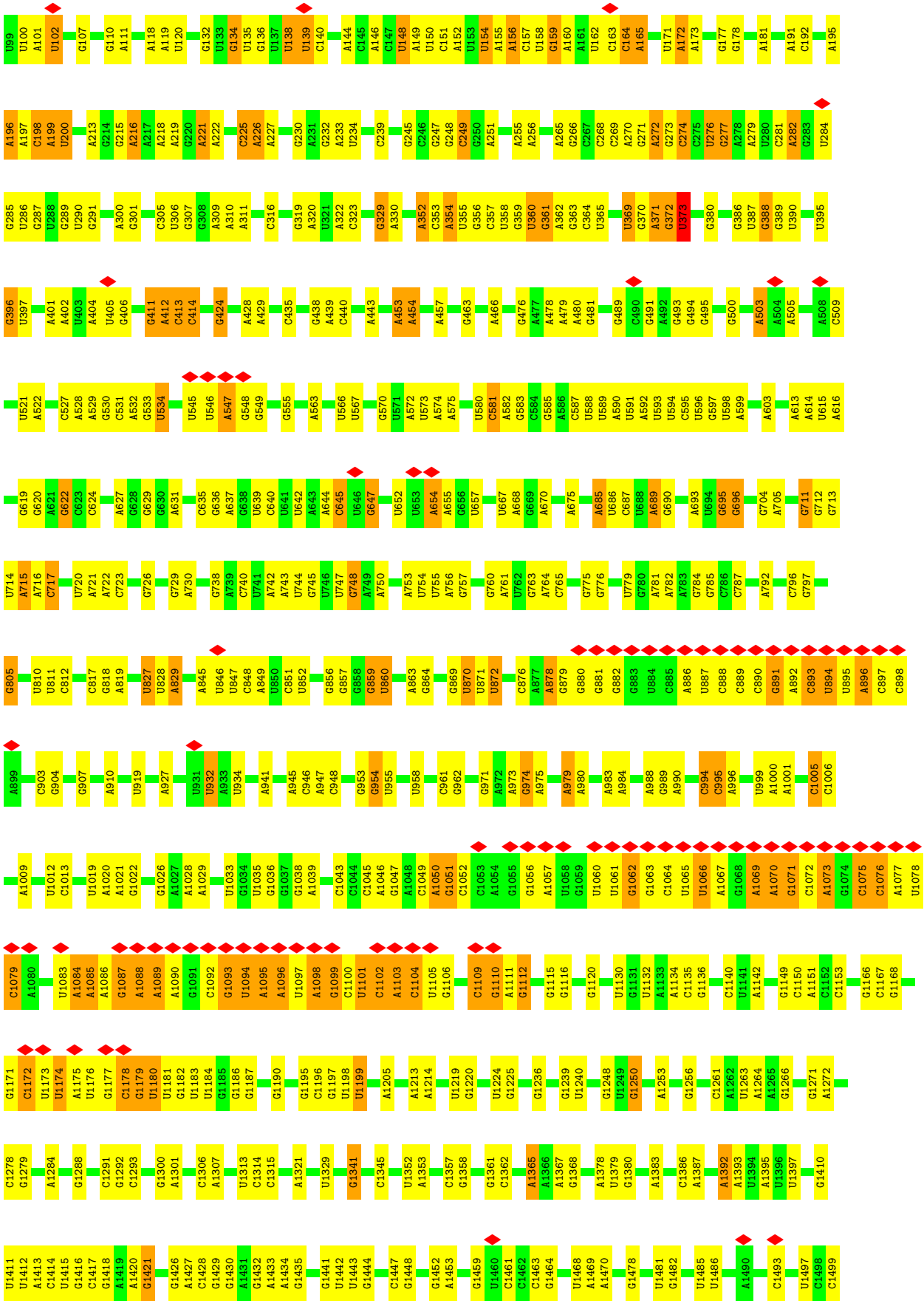
Chain M:

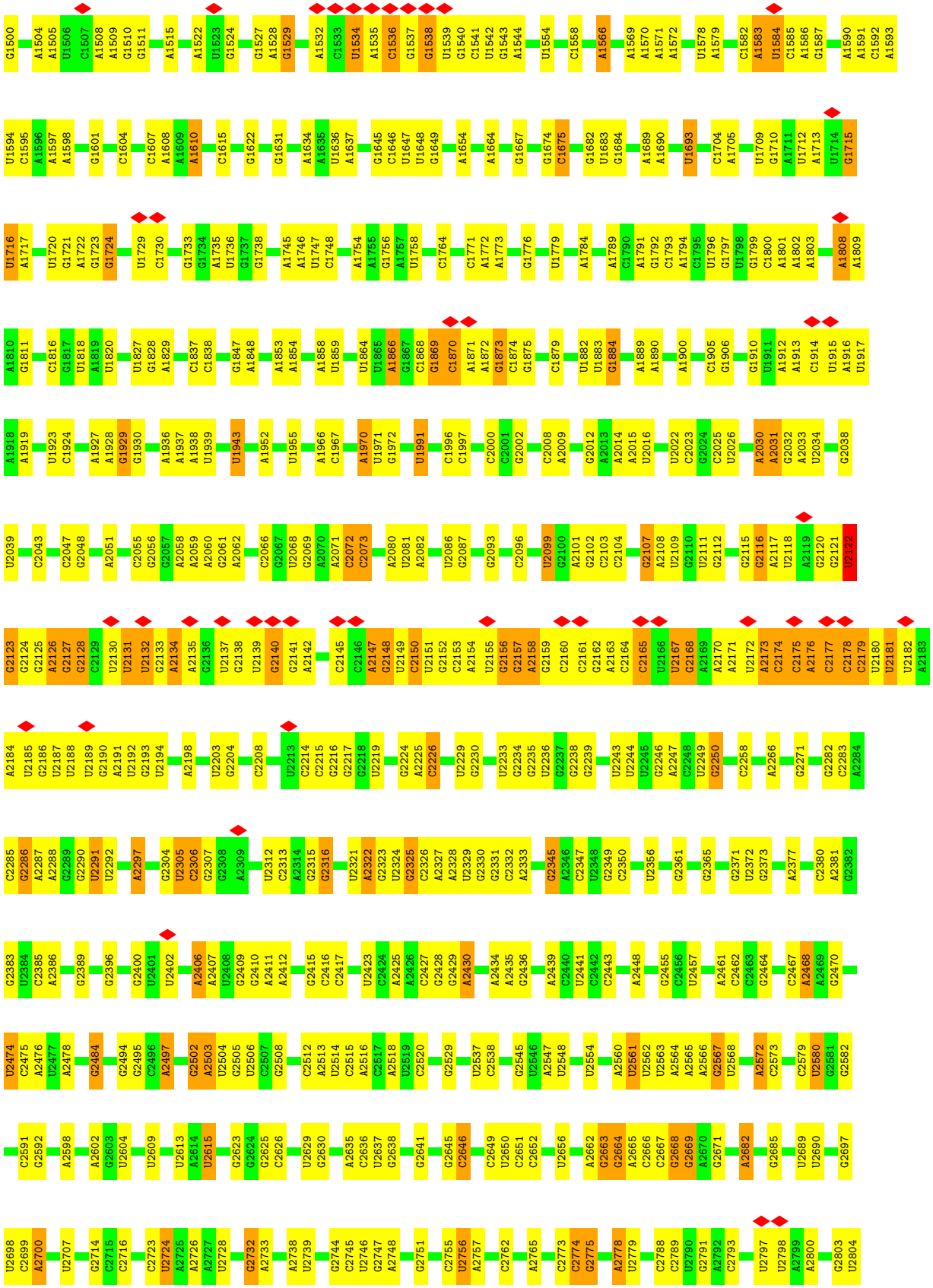


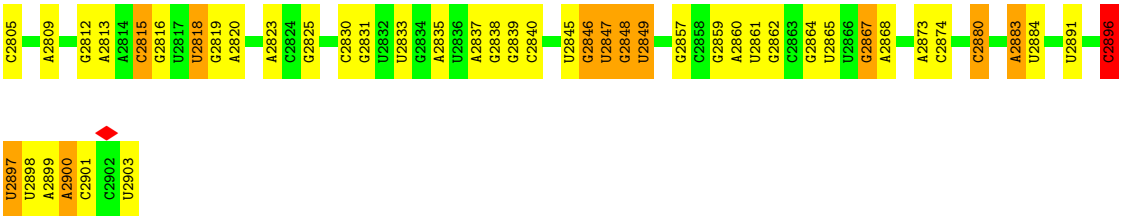
• Molecule 33: 23S ribosomal RNA

Chain R1:



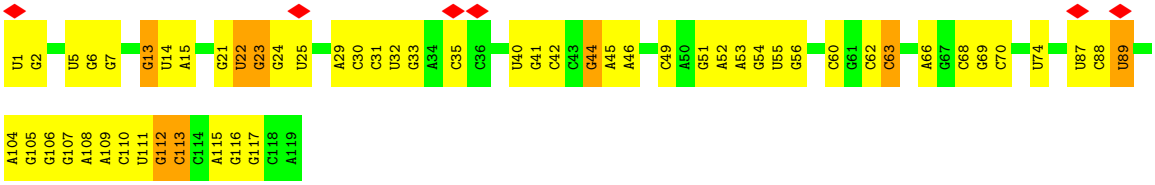






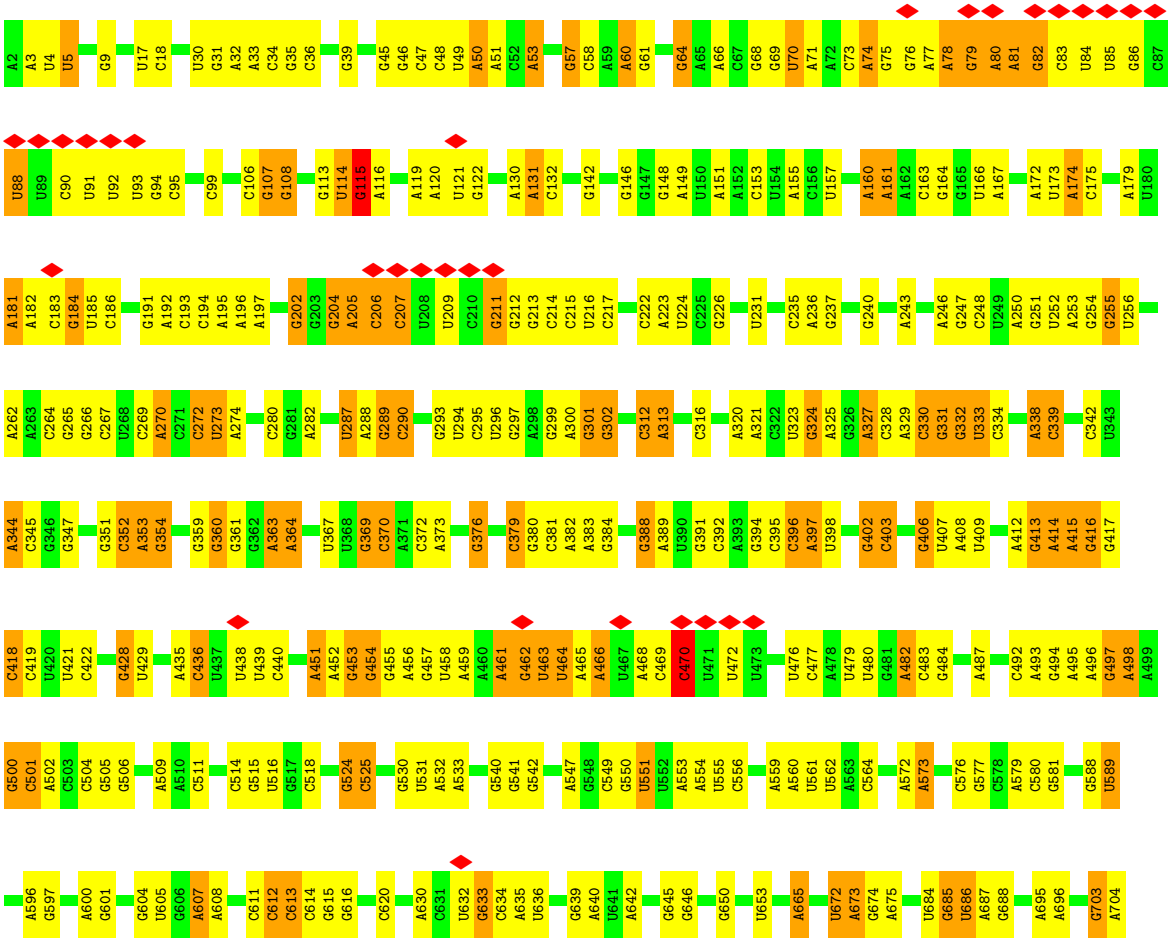
• Molecule 34: 5S ribosomal RNA

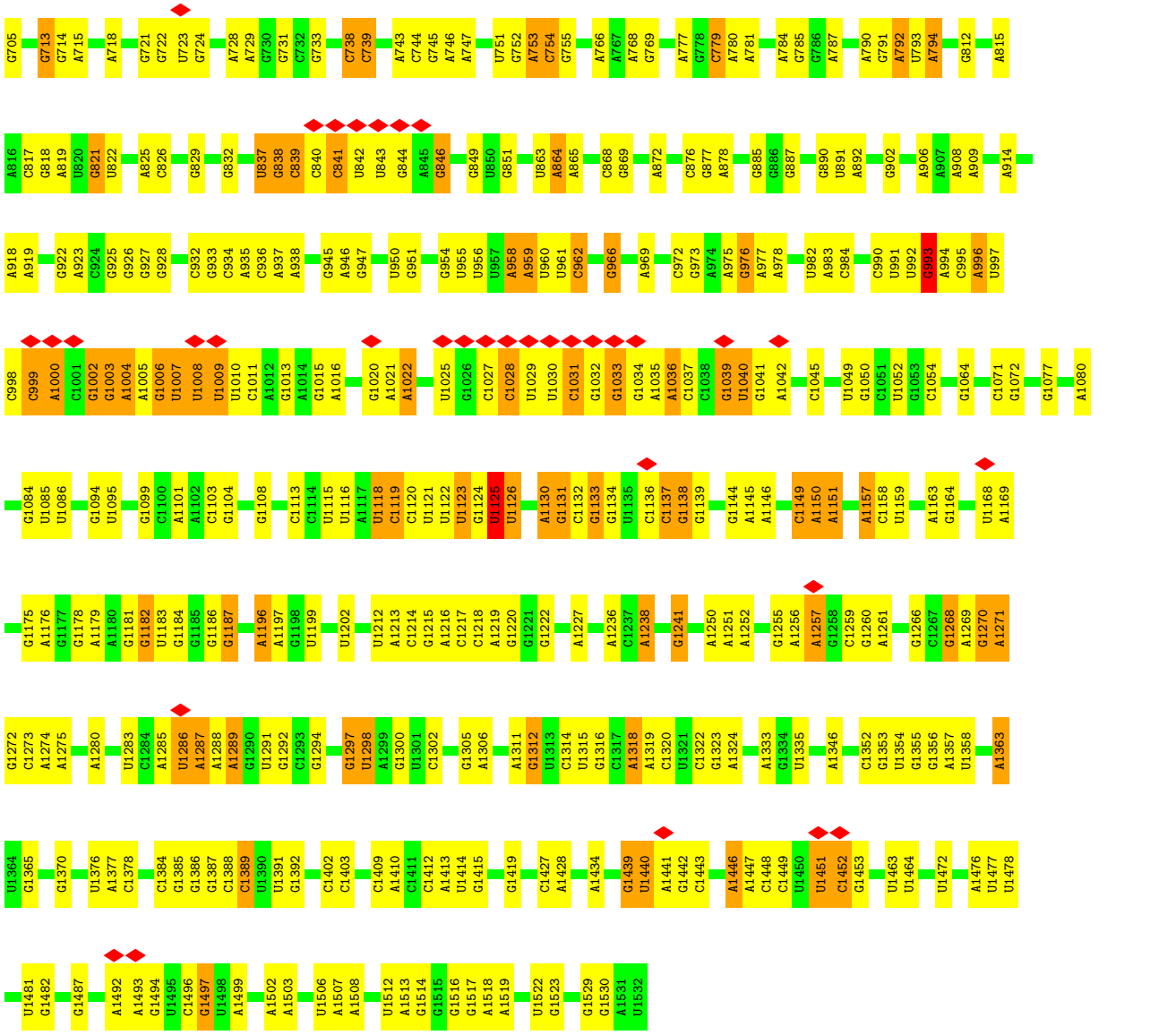
Chain R2:



• Molecule 35: 16S ribosomal RNA

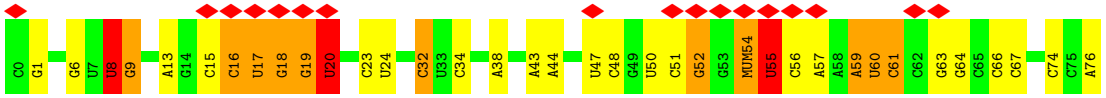
Chain R3:





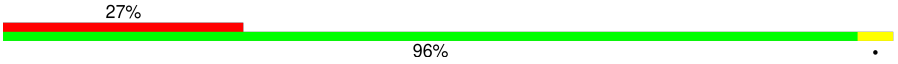
• Molecule 36: tRNA

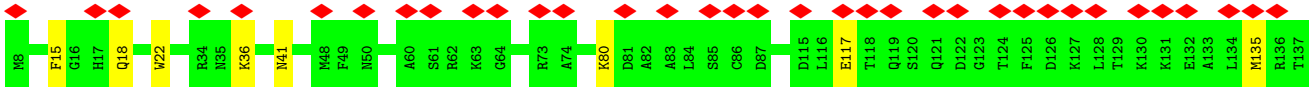
Chain T:

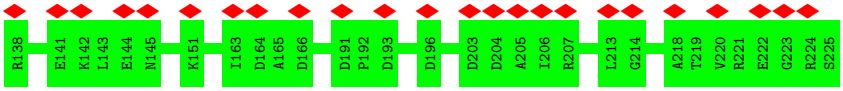


• Molecule 37: Small ribosomal subunit protein uS2

Chain sb:

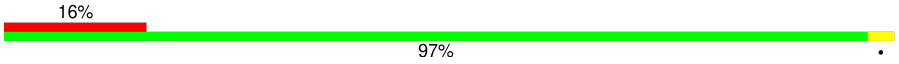


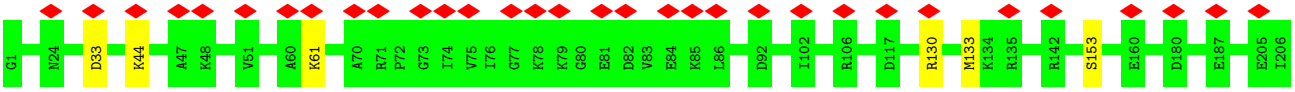




• Molecule 38: Small ribosomal subunit protein uS3

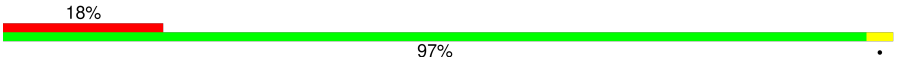
Chain sc:

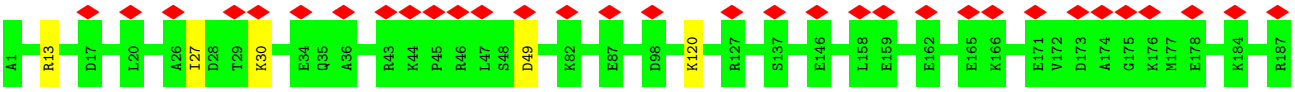


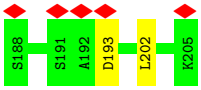


• Molecule 39: 30S ribosomal protein S4

Chain sd:

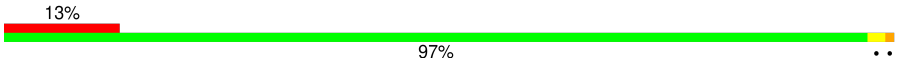


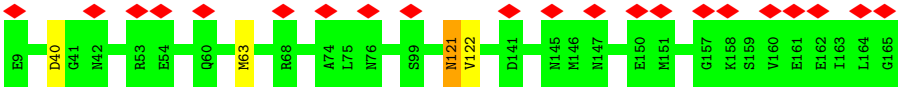




• Molecule 40: Small ribosomal subunit protein uS5

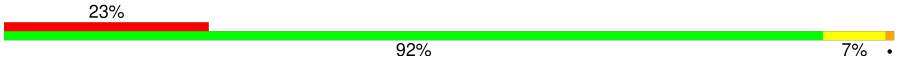
Chain se:





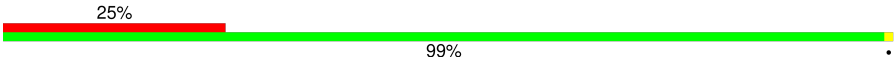
• Molecule 41: 30S ribosomal protein S6, non-modified isoform

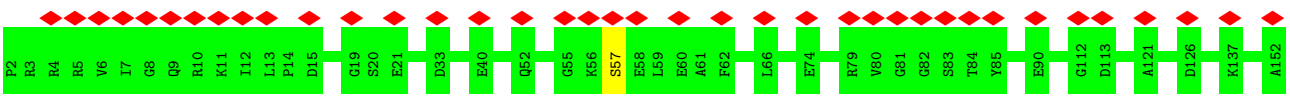
Chain sf:



• Molecule 42: 30S ribosomal protein S7

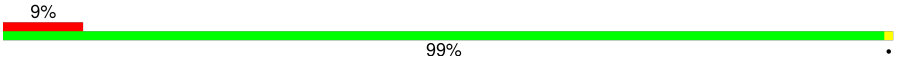
Chain sg:

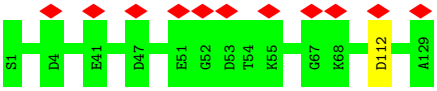




• Molecule 43: 30S ribosomal protein S8

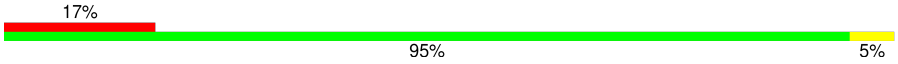
Chain sh:

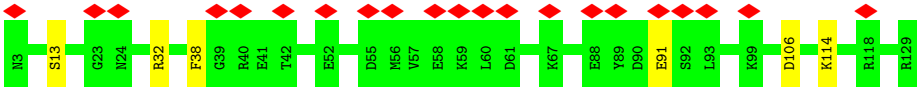




• Molecule 44: Small ribosomal subunit protein uS9

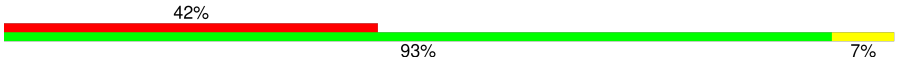
Chain si:

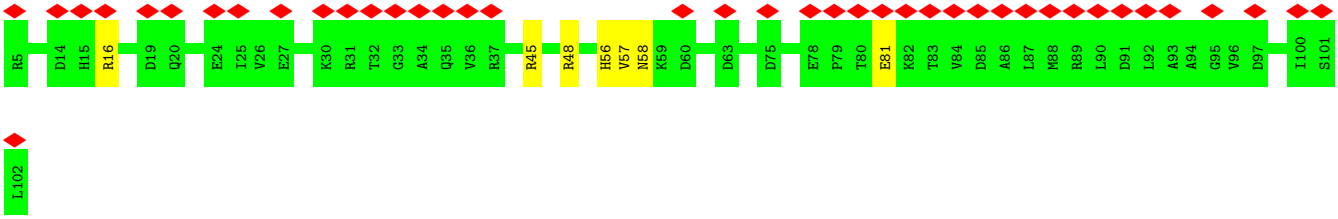




• Molecule 45: 30S ribosomal protein S10

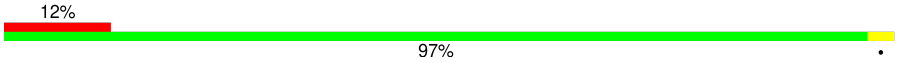
Chain sj:

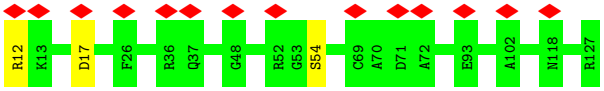




• Molecule 46: Small ribosomal subunit protein uS11

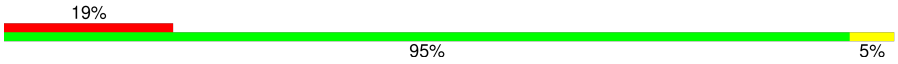
Chain sk:

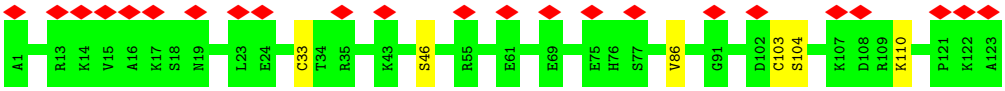




• Molecule 47: Small ribosomal subunit protein uS12

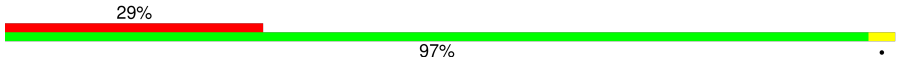
Chain sl:

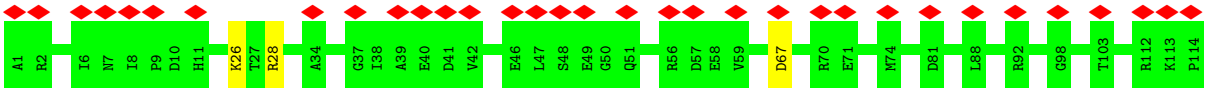




• Molecule 48: 30S ribosomal protein S13

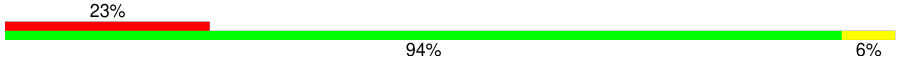
Chain sm:

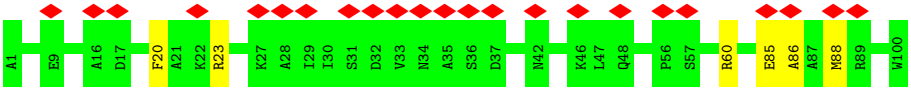




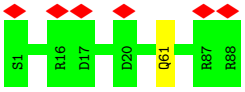
• Molecule 49: Small ribosomal subunit protein uS14

Chain sn:

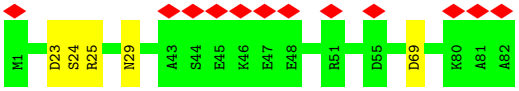




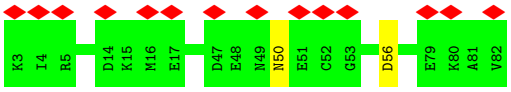
• Molecule 50: Small ribosomal subunit protein uS15



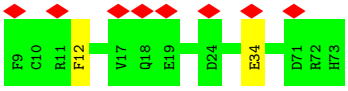
• Molecule 51: Small ribosomal subunit protein bS16



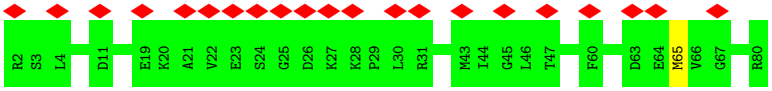
• Molecule 52: Small ribosomal subunit protein uS17



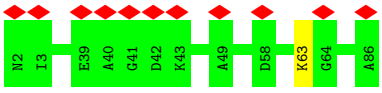
• Molecule 53: 30S ribosomal protein S18



• Molecule 54: 30S ribosomal protein S19

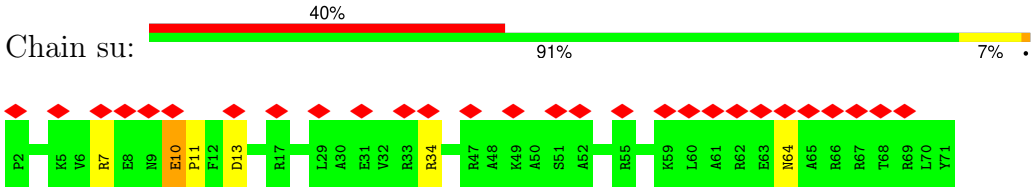


• Molecule 55: 30S ribosomal protein S20



• Molecule 56: Small ribosomal subunit protein bS21

Chain su:


40%
91%
7%
P2
K5
V6
R7
E8
N9
E10
P11
F12
D13
R17
L29
A30
E31
V32
R33
R34
R47
A48
K49
A50
S51
A52
R55
K59
L60
A61
R62
E63
N64
A65
R66
R67
T68
R69
L70
Y71

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	60175	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	64	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.569	Depositor
Minimum map value	-1.287	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.123	Depositor
Recommended contour level	0.45	Depositor
Map size (Å)	380.0, 380.0, 380.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.95, 0.95, 0.95	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MUM, ATP, PSU, 4OC, 4SU, NA, MG, FME, H2U

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	0.24	0/1361	0.54	0/1796
2	13	0.27	0/1152	0.50	0/1551
3	14	0.26	0/947	0.61	0/1268
4	15	0.27	0/1054	0.58	0/1403
5	16	0.27	0/1093	0.58	0/1460
6	17	0.26	0/973	0.58	0/1301
7	18	0.26	0/902	0.56	0/1209
8	19	0.27	0/929	0.57	0/1242
9	2	0.28	0/2121	0.58	0/2852
10	20	0.28	0/960	0.52	0/1278
11	21	0.29	0/829	0.61	0/1107
12	22	0.26	0/864	0.53	0/1156
13	23	0.27	0/744	0.53	0/994
14	24	0.26	0/787	0.51	0/1051
15	25	0.27	0/766	0.52	0/1025
16	27	0.28	0/589	0.56	0/779
17	28	0.25	0/635	0.58	0/848
18	29	0.25	0/510	0.50	0/677
19	3	0.27	0/1586	0.54	0/2134
20	30	0.25	0/453	0.54	0/605
21	31	0.24	0/531	0.49	0/709
22	32	0.26	0/450	0.56	0/599
23	33	0.26	0/416	0.51	0/554
24	34	0.25	0/380	0.63	0/498
25	35	0.26	0/513	0.54	0/676
26	36	0.28	0/303	0.58	0/397
27	4	0.26	0/1571	0.51	0/2113
28	5	0.27	0/1434	0.55	0/1926
29	6	0.27	0/1343	0.55	0/1816
30	9	0.26	0/1122	0.55	0/1515
31	E	0.27	0/4441	0.54	1/5993 (0.0%)
32	M	0.20	0/219	0.69	0/339

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	R1	0.31	0/69797	0.80	24/108890 (0.0%)
34	R2	0.27	0/2847	0.85	3/4440 (0.1%)
35	R3	0.29	0/36782	0.83	24/57377 (0.0%)
36	T	0.26	0/1716	0.81	0/2672
37	sb	0.26	0/1735	0.52	0/2338
38	sc	0.25	0/1651	0.53	0/2225
39	sd	0.25	0/1665	0.56	1/2227 (0.0%)
40	se	0.27	0/1169	0.62	1/1573 (0.1%)
41	sf	0.26	0/835	0.62	1/1128 (0.1%)
42	sg	0.29	0/1195	0.53	0/1602
43	sh	0.27	0/989	0.54	0/1326
44	si	0.26	0/1034	0.63	0/1375
45	sj	0.24	0/796	0.58	0/1077
46	sk	0.28	0/885	0.56	0/1195
47	sl	0.25	0/969	0.61	0/1300
48	sm	0.26	0/892	0.62	0/1193
49	sn	0.26	0/817	0.64	1/1088 (0.1%)
50	so	0.24	0/722	0.52	0/964
51	sp	0.31	0/659	0.64	0/884
52	sq	0.26	0/657	0.57	0/881
53	sr	0.27	0/544	0.56	0/731
54	ss	0.26	0/652	0.54	0/877
55	st	0.24	0/671	0.49	0/888
56	su	0.76	2/598 (0.3%)	0.95	4/792 (0.5%)
All	All	0.30	2/162255 (0.0%)	0.75	60/241914 (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
24	34	0	1
29	6	0	1
30	9	0	1
31	E	0	1
36	T	8	0
39	sd	0	1
40	se	0	1
41	sf	0	2
47	sl	0	1

Continued on next page...

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Mol	Chain	#Chirality outliers	#Planarity outliers
49	sn	0	2
All	All	8	12

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	su	11	PRO	CG-CD	-14.80	1.01	1.50
56	su	11	PRO	N-CD	6.44	1.56	1.47

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	su	11	PRO	N-CD-CG	-12.71	84.14	103.20
56	su	11	PRO	CA-N-CD	-11.42	95.52	111.50
31	E	67	PRO	CA-N-CD	-10.18	97.25	111.50
56	su	11	PRO	CA-CB-CG	-7.70	89.36	104.00
35	R3	5	U	C2-N1-C1'	7.53	126.73	117.70
35	R3	5	U	N1-C2-O2	7.49	128.04	122.80
35	R3	470	C	N1-C2-O2	7.48	123.39	118.90
33	R1	2668	G	O4'-C1'-N9	7.42	114.14	108.20
35	R3	5	U	N3-C2-O2	-7.29	117.10	122.20
40	se	40	ASP	CB-CG-OD1	6.96	124.56	118.30
35	R3	470	C	C2-N1-C1'	6.91	126.41	118.80
33	R1	1314	C	C2-N1-C1'	6.83	126.31	118.80
49	sn	88	MET	CA-CB-CG	6.73	124.74	113.30
33	R1	1313	U	C2-N1-C1'	6.67	125.70	117.70
33	R1	2178	C	N3-C2-O2	-6.60	117.28	121.90
41	sf	54	LEU	CA-CB-CG	6.19	129.54	115.30
33	R1	1005	C	C2-N1-C1'	6.13	125.55	118.80
56	su	10	GLU	C-N-CD	6.12	141.24	128.40
35	R3	1439	G	O4'-C1'-N9	6.04	113.03	108.20
35	R3	962	C	C2-N1-C1'	5.98	125.38	118.80
35	R3	1119	C	C2-N1-C1'	5.88	125.27	118.80
34	R2	113	C	C2-N1-C1'	5.87	125.26	118.80
35	R3	211	G	O4'-C1'-N9	5.76	112.81	108.20
33	R1	2073	C	C2-N1-C1'	5.63	124.99	118.80
35	R3	470	C	N3-C2-O2	-5.59	117.99	121.90
33	R1	2573	C	C2-N1-C1'	5.55	124.91	118.80
33	R1	2122	U	C2-N1-C1'	5.53	124.34	117.70
35	R3	379	C	N1-C2-O2	5.53	122.22	118.90
35	R3	334	C	C2-N1-C1'	5.52	124.87	118.80
35	R3	1335	U	C2-N1-C1'	5.52	124.32	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	R3	115	G	O5'-P-OP1	-5.51	100.74	105.70
33	R1	373	U	C2-N1-C1'	5.50	124.31	117.70
35	R3	1389	C	C2-N1-C1'	5.50	124.85	118.80
33	R1	76	C	C2-N1-C1'	5.48	124.83	118.80
33	R1	76	C	N1-C2-O2	5.47	122.19	118.90
35	R3	436	C	N1-C2-O2	5.47	122.18	118.90
35	R3	1125	U	C2-N1-C1'	5.44	124.23	117.70
35	R3	379	C	C2-N1-C1'	5.42	124.76	118.80
35	R3	436	C	C2-N1-C1'	5.40	124.74	118.80
33	R1	373	U	N1-C2-O2	5.39	126.58	122.80
33	R1	695	G	O4'-C1'-N9	5.37	112.50	108.20
35	R3	402	G	O4'-C1'-N9	5.35	112.48	108.20
33	R1	164	C	N1-C2-O2	5.29	122.07	118.90
33	R1	1314	C	C6-N1-C1'	-5.27	114.48	120.80
33	R1	2580	U	N3-C2-O2	-5.27	118.51	122.20
33	R1	2815	C	C2-N1-C1'	5.24	124.56	118.80
33	R1	1313	U	N1-C2-O2	5.20	126.44	122.80
33	R1	2178	C	N1-C2-O2	5.18	122.01	118.90
39	sd	49	ASP	CB-CG-OD1	5.18	122.96	118.30
33	R1	2573	C	N1-C2-O2	5.17	122.00	118.90
33	R1	76	C	N3-C2-O2	-5.16	118.29	121.90
35	R3	620	C	C2-N1-C1'	5.13	124.44	118.80
35	R3	993	G	C4-N9-C1'	5.13	133.17	126.50
34	R2	60	C	N1-C2-O2	5.12	121.97	118.90
33	R1	2896	C	P-O3'-C3'	5.08	125.80	119.70
33	R1	164	C	C2-N1-C1'	5.07	124.38	118.80
34	R2	25	U	C2-N1-C1'	5.05	123.77	117.70
35	R3	114	U	P-O3'-C3'	-5.04	113.65	119.70
33	R1	687	C	N3-C2-O2	-5.02	118.38	121.90
35	R3	153	C	C2-N1-C1'	5.01	124.31	118.80

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
36	T	8	4SU	C2',C1'
36	T	20	H2U	C2'
36	T	32	4OC	C2'
36	T	54	MUM	C4',C5,C3'
36	T	55	PSU	C4'

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	23	37	ASP	Peptide
24	34	44	VAL	Peptide
29	6	12	ALA	Peptide
30	9	8	LYS	Peptide
31	E	16	PRO	Peptide
39	sd	27	ILE	Peptide
40	se	121	ASN	Peptide
41	sf	53	LYS	Peptide
41	sf	92	THR	Peptide
47	sl	86	VAL	Peptide
49	sn	85	GLU	Peptide
49	sn	86	ALA	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1353	0	1159	35	0
2	13	1129	0	1162	27	0
3	14	938	0	1012	20	0
4	15	1045	0	1117	22	0
5	16	1074	0	1157	21	0
6	17	960	0	1000	12	0
7	18	892	0	923	15	0
8	19	917	0	965	16	0
9	2	2082	0	2157	42	0
10	20	947	0	1022	12	0
11	21	816	0	839	20	0
12	22	857	0	922	18	0
13	23	738	0	807	15	0
14	24	779	0	834	7	0
15	25	753	0	780	21	0
16	27	582	0	599	20	0
17	28	625	0	655	14	0
18	29	509	0	543	8	0
19	3	1565	0	1616	35	0
20	30	449	0	491	10	0
21	31	522	0	524	11	0
22	32	444	0	461	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	33	409	0	440	9	0
24	34	377	0	418	5	0
25	35	504	0	574	11	0
26	36	302	0	343	8	0
27	4	1552	0	1619	25	0
28	5	1410	0	1447	38	0
29	6	1323	0	1374	32	0
30	9	1111	0	1148	29	0
31	E	4360	0	4336	98	0
32	M	195	0	99	0	0
33	R1	62318	0	31345	703	0
34	R2	2546	0	1292	35	0
35	R3	32850	0	16534	357	0
36	T	1639	0	831	28	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	1238	0	0
43	sh	979	0	1034	0	0
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	883	0	944	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	535	0	552	0	0
54	ss	637	0	665	0	0
55	st	665	0	714	0	0
56	su	590	0	629	0	0
57	15	1	0	0	0	0
57	17	1	0	0	0	0
57	M	1	0	0	0	0
57	R1	204	0	0	0	0
57	R3	89	0	0	0	0
57	sn	1	0	0	0	0
57	sq	1	0	0	0	0
58	E	62	0	22	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	E	2	0	0	0	0
60	T	10	0	10	0	0
All	All	150106	0	102237	1638	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 8.

All (1638) 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)
35:R3:1130:A:HO2'	35:R3:1131:G:H8	1.02	0.95
35:R3:359:G:HO2'	35:R3:360:G:H8	0.98	0.95
33:R1:132:G:H1	33:R1:146:A:H62	0.94	0.92
33:R1:2099:U:H3	33:R1:2190:G:H1	0.92	0.89
33:R1:1043:C:O2	33:R1:1112:G:N2	2.05	0.89
33:R1:301:G:N2	33:R1:316:C:O2	2.09	0.86
8:19:3:ILE:HD11	19:3:186:LEU:HD21	1.58	0.85
33:R1:1092:C:N4	33:R1:1093:G:O6	2.10	0.85
33:R1:2073:C:H5	33:R1:2436:G:H1	1.26	0.84
31:E:319:LEU:HD11	31:E:323:VAL:HG22	1.62	0.82
30:9:9:VAL:HG12	30:9:11:ASN:H	1.44	0.80
33:R1:284:U:H3	33:R1:356:G:H1	1.29	0.80
25:35:38:LYS:NZ	33:R1:2365:G:N7	2.30	0.79
35:R3:990:C:H5	35:R3:1215:G:H1	1.31	0.79
33:R1:132:G:H1	33:R1:146:A:N6	1.78	0.79
33:R1:2848:G:O2'	33:R1:2867:G:N2	2.16	0.79
31:E:425:ARG:NH1	36:T:19:G:N7	2.31	0.78
28:5:114:ARG:NE	28:5:114:ARG:O	2.18	0.77
36:T:55:PSU:H2'	36:T:57:A:N7	1.99	0.77
33:R1:1529:G:H1	33:R1:1542:U:H3	1.33	0.76
33:R1:76:C:H5	33:R1:110:G:H1	1.33	0.76
6:17:4:ARG:NH1	33:R1:2874:C:OP1	2.18	0.76
31:E:183:MET:SD	31:E:211:THR:OG1	2.44	0.76
33:R1:805:G:N2	33:R1:829:A:OP1	2.17	0.76
34:R2:112:G:O2'	34:R2:113:C:O2	2.04	0.76
33:R1:414:C:H5	33:R1:2409:G:H1	1.34	0.75
11:21:80:ARG:NH2	33:R1:572:A:OP2	2.19	0.75
33:R1:2304:G:H22	33:R1:2312:U:H3	1.35	0.74
22:32:54:ILE:HG23	22:32:56:LYS:H	1.52	0.74
27:4:44:ARG:NH2	33:R1:1248:G:OP1	2.21	0.74
33:R1:1779:U:OP2	33:R1:1784:A:N6	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:R1:2545:G:H21	33:R1:2565:A:H8	1.34	0.74
21:31:16:CYS:SG	21:31:17:SER:N	2.61	0.74
17:28:59:ASP:OD1	30:9:27:ARG:NH1	2.21	0.74
16:27:68:LYS:NZ	16:27:70:GLU:OE1	2.21	0.73
13:23:11:LEU:O	18:29:29:ARG:NH1	2.20	0.73
23:33:27:ARG:NH2	31:E:436:VAL:O	2.20	0.73
33:R1:1050:A:H2'	33:R1:1051:G:C8	2.23	0.73
35:R3:841:C:O2'	35:R3:846:G:N2	2.21	0.73
5:16:20:LEU:HD13	15:25:81:PRO:HG2	1.68	0.73
33:R1:284:U:O2	33:R1:356:G:N2	2.19	0.73
33:R1:1869:G:H21	33:R1:1872:A:H2'	1.54	0.73
27:4:163:ASN:ND2	33:R1:320:A:N3	2.37	0.73
33:R1:2134:A:N7	33:R1:2156:G:N2	2.37	0.73
5:16:30:SER:OG	5:16:106:ASP:OD1	2.05	0.73
31:E:102:LYS:HG2	31:E:103:ARG:HH21	1.53	0.72
29:6:12:ALA:O	29:6:14:VAL:N	2.22	0.72
9:2:13:ARG:NH2	33:R1:1693:U:O2'	2.23	0.72
27:4:97:ASN:HB2	27:4:100:MET:HG3	1.72	0.72
33:R1:962:G:H21	33:R1:2250:G:H1	1.35	0.72
35:R3:58:C:O2'	35:R3:388:G:N2	2.23	0.72
10:20:48:ASP:OD1	33:R1:534:U:O2'	2.04	0.72
33:R1:1084:A:N3	33:R1:1105:U:O2'	2.22	0.71
15:25:80:HIS:HD2	15:25:83:LYS:HB2	1.55	0.71
33:R1:652:U:OP1	33:R1:654:A:N6	2.23	0.71
35:R3:1144:G:H21	35:R3:1146:A:H62	1.39	0.71
1:1:44:VAL:HB	1:1:175:ILE:HD11	1.73	0.70
31:E:6:TYR:HB3	31:E:29:PHE:HD2	1.57	0.70
35:R3:1004:A:H2'	35:R3:1005:A:H8	1.57	0.70
33:R1:2127:G:H2'	33:R1:2128:G:C8	2.27	0.69
33:R1:2140:G:H2'	33:R1:2141:G:H8	1.57	0.69
33:R1:1433:A:H2'	33:R1:1434:A:C8	2.28	0.69
11:21:77:PHE:HD1	11:21:84:ARG:HG3	1.58	0.69
31:E:317:PRO:O	31:E:464:ASN:ND2	2.24	0.68
33:R1:1063:G:O2'	33:R1:1066:U:OP1	2.11	0.68
33:R1:2102:G:O6	33:R1:2187:U:O2	2.11	0.68
33:R1:2156:G:N7	33:R1:2157:G:N2	2.41	0.68
12:22:59:GLU:HB2	12:22:66:ILE:HD11	1.76	0.68
19:3:4:LEU:HD21	19:3:29:VAL:HG11	1.75	0.68
28:5:70:ARG:HH21	28:5:71:LYS:HD3	1.59	0.68
31:E:103:ARG:HB2	31:E:128:LEU:HD11	1.74	0.68
9:2:257:ARG:NH1	33:R1:1799:G:OP1	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:R1:2682:A:H61	33:R1:2728:U:H1'	1.58	0.68
35:R3:687:A:N6	35:R3:703:G:O2'	2.26	0.68
16:27:77:ARG:NH1	33:R1:2332:C:OP1	2.27	0.68
23:33:36:LYS:HG2	23:33:47:ILE:HG13	1.76	0.68
33:R1:219:A:N3	33:R1:234:U:O2'	2.26	0.68
35:R3:82:G:N3	35:R3:88:U:N3	2.42	0.68
1:1:27:ILE:HD12	1:1:182:ALA:HB1	1.75	0.68
33:R1:1936:A:H2	33:R1:1943:U:H3	1.39	0.68
13:23:4:GLU:OE1	13:23:49:LYS:NZ	2.27	0.68
33:R1:199:A:O2'	33:R1:200:U:O2	2.11	0.67
35:R3:1002:G:H22	35:R3:1039:G:H5"	1.59	0.67
36:T:16:C:OP2	36:T:60:U:O2'	2.09	0.67
5:16:84:LYS:NZ	33:R1:2250:G:OP1	2.28	0.67
17:28:60:LYS:HZ1	33:R1:371:A:H8	1.42	0.67
35:R3:946:A:H2'	35:R3:947:G:C8	2.30	0.67
33:R1:1019:U:OP1	33:R1:1035:U:O2'	2.09	0.67
5:16:86:LYS:NZ	33:R1:955:U:OP1	2.27	0.67
7:18:3:LYS:HE2	34:R2:46:A:H5"	1.76	0.67
33:R1:1417:C:HO2'	33:R1:1587:G:HO2'	1.41	0.67
35:R3:1009:U:H3	35:R3:1020:G:H1	0.72	0.67
34:R2:1:U:H2'	34:R2:2:G:H8	1.59	0.67
35:R3:406:G:H1	35:R3:436:C:H5	1.43	0.67
19:3:181:ASP:HB2	19:3:186:LEU:HB2	1.77	0.66
33:R1:307:G:N1	33:R1:310:A:OP2	2.24	0.66
36:T:59:A:O2'	36:T:60:U:O5'	2.12	0.66
33:R1:848:C:H2'	33:R1:849:A:H8	1.60	0.66
1:1:200:LYS:HD2	1:1:201:PRO:HD2	1.77	0.66
7:18:48:LEU:HD22	7:18:87:ILE:HD11	1.77	0.66
1:1:42:VAL:HG23	1:1:175:ILE:H	1.60	0.66
35:R3:928:G:H1	35:R3:1389:C:H5	1.44	0.66
31:E:478:GLU:N	31:E:478:GLU:OE2	2.26	0.66
31:E:81:ASN:OD1	31:E:84:HIS:ND1	2.28	0.66
35:R3:269:C:H2'	35:R3:270:A:H5"	1.78	0.66
14:24:78:LYS:NZ	14:24:79:ALA:O	2.28	0.66
31:E:146:ARG:HH12	31:E:552:ARG:HB2	1.60	0.66
31:E:362:LYS:HB3	31:E:497:ILE:HD13	1.77	0.66
33:R1:2315:G:HO2'	33:R1:2316:G:H8	1.44	0.66
9:2:5:CYS:SG	9:2:12:ARG:NH1	2.70	0.65
35:R3:380:G:N2	35:R3:383:A:OP2	2.27	0.65
35:R3:1175:G:H2'	35:R3:1176:A:H8	1.59	0.65
29:6:51:PHE:HZ	29:6:71:LEU:HD13	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:R1:948:C:O2	33:R1:984:A:O2'	2.13	0.65
35:R3:962:C:H5	35:R3:973:G:H1	1.43	0.65
35:R3:379:C:H5	35:R3:384:G:H1	1.42	0.65
35:R3:714:G:H2'	35:R3:715:A:C8	2.32	0.65
9:2:97:ASP:OD2	9:2:98:GLY:N	2.30	0.65
9:2:220:ARG:NH1	33:R1:1789:A:OP2	2.29	0.65
35:R3:1002:G:N2	35:R3:1039:G:N3	2.43	0.65
35:R3:1007:U:H2'	35:R3:1008:U:H4'	1.78	0.65
31:E:472:THR:HB	31:E:480:LEU:HD11	1.78	0.65
31:E:327:SER:O	31:E:379:THR:OG1	2.15	0.65
33:R1:1085:A:O2'	33:R1:1104:C:O2	2.15	0.65
35:R3:1004:A:H2'	35:R3:1005:A:C8	2.31	0.65
33:R1:132:G:N2	33:R1:146:A:N7	2.37	0.65
19:3:151:THR:OG1	19:3:152:PRO:HD3	1.97	0.65
31:E:433:PHE:O	31:E:438:GLN:NE2	2.30	0.65
33:R1:274:C:H41	33:R1:363:G:H21	1.44	0.64
33:R1:1019:U:H3	33:R1:1142:A:H62	1.45	0.64
18:29:1:MET:N	33:R1:102:U:O4	2.29	0.64
18:29:1:MET:SD	18:29:4:LYS:NZ	2.65	0.64
33:R1:2121:G:C8	33:R1:2122:U:H5	2.16	0.64
31:E:67:PRO:HD2	31:E:68:ASP:N	2.11	0.64
33:R1:704:G:O2'	33:R1:726:G:N2	2.27	0.64
33:R1:1093:G:O2'	33:R1:1094:U:O4'	2.13	0.64
35:R3:1144:G:N2	35:R3:1146:A:H62	1.95	0.64
35:R3:1522:U:H2'	35:R3:1523:G:H8	1.61	0.64
11:21:10:LYS:NZ	33:R1:994:C:O2	2.29	0.64
29:6:138:GLN:NE2	33:R1:2745:C:O2	2.31	0.64
31:E:103:ARG:NH1	31:E:106:GLU:OE1	2.31	0.64
33:R1:932:U:O2'	33:R1:934:U:O4	2.16	0.64
9:2:216:ARG:NH2	33:R1:781:A:OP1	2.30	0.64
19:3:8:LYS:HB2	19:3:201:LEU:HD11	1.80	0.64
19:3:105:LYS:HG3	19:3:106:LYS:HG2	1.79	0.64
33:R1:1028:A:H2'	33:R1:1029:A:C8	2.33	0.64
33:R1:1043:C:N3	33:R1:1112:G:N1	2.39	0.64
33:R1:2324:U:H3'	33:R1:2325:G:H5"	1.79	0.64
33:R1:1597:A:H5"	33:R1:1598:A:H5'	1.79	0.64
33:R1:1664:A:H61	33:R1:1996:C:H42	1.46	0.64
33:R1:1900:A:H1'	33:R1:1970:A:H2'	1.80	0.64
33:R1:2141:G:H2'	33:R1:2142:A:C8	2.33	0.64
5:16:57:VAL:O	5:16:58:LYS:HG2	1.98	0.63
13:23:44:LYS:NZ	13:23:56:GLU:O	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:27:12:ASN:HA	16:27:14:ARG:HH12	1.61	0.63
17:28:42:GLU:OE1	17:28:44:ARG:NE	2.31	0.63
35:R3:501:C:H2'	35:R3:502:A:C8	2.33	0.63
35:R3:1009:U:O4	35:R3:1020:G:O6	2.17	0.63
26:36:32:LYS:HD3	33:R1:2478:A:H5'	1.80	0.63
29:6:14:VAL:HG22	29:6:27:GLY:HA2	1.81	0.63
33:R1:177:G:H3'	33:R1:178:G:H8	1.63	0.63
33:R1:2175:C:H2'	33:R1:2176:A:H4'	1.79	0.63
35:R3:938:A:N3	35:R3:1376:U:O2'	2.30	0.63
21:31:63:ARG:NH1	35:R3:1312:G:OP2	2.32	0.63
33:R1:1607:C:N4	33:R1:1622:G:OP2	2.28	0.63
36:T:6:G:OP1	36:T:15:C:N4	2.32	0.63
31:E:67:PRO:HD2	31:E:68:ASP:H	1.64	0.63
33:R1:2857:G:N2	33:R1:2860:A:OP2	2.31	0.63
35:R3:501:C:H2'	35:R3:502:A:H8	1.63	0.63
33:R1:195:A:H61	33:R1:198:C:H3'	1.64	0.63
33:R1:1063:G:H1	33:R1:1076:C:HO2'	1.46	0.63
31:E:484:GLU:OE1	31:E:506:ARG:NH1	2.32	0.63
9:2:48:ILE:HD11	9:2:51:ARG:HA	1.81	0.62
33:R1:879:G:H1	33:R1:898:C:H42	1.47	0.62
35:R3:1133:G:H2'	35:R3:1134:G:H8	1.65	0.62
4:15:127:VAL:HG11	4:15:142:ILE:HD13	1.80	0.62
33:R1:1847:G:O2'	33:R1:1848:A:H8	1.81	0.62
33:R1:1057:A:N6	33:R1:1087:G:OP2	2.32	0.62
35:R3:946:A:H2'	35:R3:947:G:H8	1.64	0.62
3:14:63:VAL:HG12	3:14:107:LEU:HD11	1.79	0.62
33:R1:1724:G:O6	33:R1:1736:U:O2	2.17	0.62
33:R1:2162:G:O2'	33:R1:2173:A:N6	2.33	0.62
35:R3:744:C:H2'	35:R3:745:G:H8	1.63	0.62
17:28:2:ARG:NH1	33:R1:1365:A:OP1	2.32	0.62
33:R1:2668:G:O2'	33:R1:2669:G:O5'	2.13	0.62
35:R3:80:A:N6	35:R3:81:A:N3	2.48	0.62
35:R3:1027:C:H2'	35:R3:1028:C:H4'	1.82	0.62
33:R1:2121:G:N2	33:R1:2179:C:O2	2.33	0.62
34:R2:7:G:H1	34:R2:113:C:H5	1.48	0.62
34:R2:14:U:OP2	34:R2:70:C:O2'	2.17	0.62
11:21:45:GLU:HG3	11:21:47:VAL:HG23	1.82	0.61
6:17:2:ARG:HA	6:17:5:LYS:HD3	1.81	0.61
33:R1:45:G:H5"	33:R1:46:G:H5'	1.82	0.61
35:R3:976:G:OP2	35:R3:1358:U:O2'	2.18	0.61
1:1:61:GLY:H	1:1:163:TYR:HB2	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:15:123:ARG:NH1	4:15:143:GLU:OE2	2.33	0.61
33:R1:463:G:N2	33:R1:466:A:OP2	2.32	0.61
31:E:231:GLU:HG2	31:E:238:ILE:HD12	1.82	0.61
4:15:18:ARG:NH2	33:R1:1250:G:N7	2.48	0.61
33:R1:154:U:O4	33:R1:155:A:N6	2.34	0.61
9:2:204:LEU:HD22	9:2:213:ARG:HH21	1.66	0.61
33:R1:2141:G:H2'	33:R1:2142:A:H8	1.66	0.61
12:22:80:PRO:O	12:22:100:THR:OG1	2.17	0.61
15:25:66:ASP:O	15:25:68:LYS:NZ	2.33	0.61
16:27:43:THR:H	33:R1:2331:G:H4'	1.65	0.61
31:E:546:LYS:HD3	31:E:548:ILE:HD11	1.82	0.61
33:R1:1213:A:N6	33:R1:1236:G:H1'	2.15	0.61
33:R1:360:U:O2'	33:R1:361:G:O4'	2.19	0.60
33:R1:2162:G:H4'	33:R1:2173:A:H61	1.66	0.60
35:R3:1316:G:N2	35:R3:1319:A:OP2	2.32	0.60
14:24:39:ASN:HB3	14:24:62:ALA:HB3	1.82	0.60
33:R1:2233:U:H2'	33:R1:2234:G:H8	1.66	0.60
19:3:56:LYS:HE3	33:R1:2830:C:H5"	1.83	0.60
2:13:99:ARG:HG3	2:13:103:ILE:HD11	1.83	0.60
29:6:154:GLU:OE2	29:6:159:LYS:N	2.32	0.60
33:R1:1590:A:H2'	33:R1:1591:A:H8	1.66	0.60
33:R1:2249:U:H3'	33:R1:2250:G:H5"	1.82	0.60
33:R1:2328:A:H2'	33:R1:2329:U:C6	2.37	0.60
33:R1:2898:U:H2'	33:R1:2899:A:C8	2.36	0.60
35:R3:1016:A:HO2'	35:R3:1217:C:HO2'	1.49	0.60
35:R3:1218:C:H2'	35:R3:1219:A:H8	1.64	0.60
21:31:36:VAL:HB	21:31:40:CYS:HB3	1.81	0.60
31:E:375:PRO:HG2	31:E:378:GLY:HA2	1.83	0.60
35:R3:674:G:H2'	35:R3:675:A:H8	1.66	0.60
19:3:59:ARG:NH2	33:R1:2831:G:OP2	2.33	0.60
33:R1:1590:A:H2'	33:R1:1591:A:C8	2.37	0.60
33:R1:2774:C:HO2'	33:R1:2775:G:H8	1.46	0.60
3:14:1:MET:HG3	3:14:67:LYS:HD2	1.84	0.60
19:3:39:ASP:OD1	19:3:39:ASP:N	2.34	0.60
30:9:68:ARG:O	30:9:72:ILE:HG12	2.02	0.60
33:R1:411:G:OP2	33:R1:2406:A:O2'	2.18	0.60
5:16:64:TRP:HB2	5:16:104:GLU:HG2	1.83	0.60
35:R3:131:A:HO2'	35:R3:262:A:H8	1.49	0.60
35:R3:413:G:H21	35:R3:428:G:H1'	1.67	0.60
35:R3:1039:G:O2'	35:R3:1040:U:O4'	2.19	0.60
9:2:143:VAL:HB	9:2:153:LEU:HB2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:E:124:GLU:OE1	31:E:125:GLN:NE2	2.35	0.59
33:R1:2329:U:H2'	33:R1:2330:G:C8	2.37	0.59
35:R3:115:G:H8	35:R3:115:G:OP1	1.84	0.59
35:R3:119:A:H2	35:R3:287:U:H3	1.48	0.59
35:R3:352:C:O2'	35:R3:354:G:OP1	2.14	0.59
16:27:42:GLY:HA2	33:R1:2330:G:H21	1.66	0.59
33:R1:2099:U:O4	33:R1:2190:G:O6	2.20	0.59
2:13:64:VAL:HG22	2:13:68:LYS:HE3	1.85	0.59
33:R1:2117:A:H61	33:R1:2170:A:H61	1.49	0.59
4:15:109:LYS:NZ	33:R1:635:C:OP2	2.35	0.59
33:R1:79:C:H42	33:R1:107:G:H1	1.50	0.59
33:R1:479:A:H4'	33:R1:480:A:H5'	1.84	0.59
33:R1:270:A:N1	33:R1:369:U:O2'	2.35	0.59
33:R1:2184:A:H2'	33:R1:2185:U:C6	2.38	0.59
35:R3:114:U:H1'	35:R3:353:A:H1'	1.84	0.59
21:31:2:LYS:HB3	21:31:5:ILE:HG21	1.84	0.59
35:R3:236:A:H2'	35:R3:237:G:H8	1.68	0.59
29:6:23:ILE:HG12	29:6:71:LEU:HD11	1.84	0.59
33:R1:362:A:H3'	33:R1:363:G:H8	1.66	0.59
33:R1:1109:C:H3'	33:R1:1110:G:H5"	1.84	0.59
33:R1:2774:C:O2'	33:R1:2775:G:O5'	2.21	0.59
3:14:108:ARG:NH1	8:19:33:GLU:OE2	2.36	0.59
13:23:12:ARG:HD3	13:23:35:ALA:HB2	1.85	0.59
28:5:109:ARG:NH2	28:5:142:TYR:OH	2.34	0.59
33:R1:1103:A:OP2	33:R1:1104:C:N4	2.36	0.59
35:R3:634:C:H2'	35:R3:635:A:H8	1.68	0.59
33:R1:1432:G:H2'	33:R1:1433:A:C8	2.38	0.59
33:R1:1682:G:H2'	33:R1:1683:U:C6	2.38	0.59
10:20:5:ARG:NH2	33:R1:585:G:N7	2.50	0.58
33:R1:2134:A:O4'	33:R1:2157:G:O2'	2.21	0.58
6:17:96:ARG:HH21	6:17:116:VAL:HG12	1.67	0.58
33:R1:309:A:N3	33:R1:329:G:O2'	2.34	0.58
33:R1:1469:A:H2'	33:R1:1470:A:C8	2.38	0.58
35:R3:553:A:H2'	35:R3:554:A:C8	2.39	0.58
15:25:7:GLU:N	15:25:7:GLU:OE2	2.36	0.58
33:R1:2123:G:H2'	33:R1:2124:G:C5	2.39	0.58
33:R1:1534:U:O2	33:R1:1537:G:N1	2.26	0.58
35:R3:64:G:OP1	35:R3:382:A:N6	2.37	0.58
35:R3:1118:U:H1'	35:R3:1179:A:C5	2.38	0.58
2:13:102:GLU:HG2	2:13:119:PHE:HZ	1.68	0.58
31:E:457:LYS:O	31:E:460:GLN:NE2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:R1:828:U:H2'	33:R1:829:A:C8	2.38	0.58
28:5:33:ILE:HG23	28:5:90:LEU:HB2	1.85	0.58
29:6:89:VAL:O	29:6:159:LYS:HA	2.03	0.58
23:33:27:ARG:HD2	31:E:17:PRO:HD2	1.86	0.58
35:R3:665:A:H1'	35:R3:733:G:H5'	1.86	0.58
35:R3:838:G:O2'	35:R3:839:C:O5'	2.22	0.58
9:2:176:ARG:HH21	33:R1:1820:U:H5	1.52	0.58
15:25:69:GLU:OE1	15:25:69:GLU:N	2.37	0.58
26:36:23:ILE:HB	26:36:38:GLY:HA3	1.86	0.58
31:E:32:GLY:H	31:E:211:THR:HG22	1.68	0.58
33:R1:2327:A:H2'	33:R1:2328:A:C8	2.39	0.58
33:R1:2508:G:H1	33:R1:2580:U:H5	1.51	0.58
1:1:221:GLY:N	33:R1:2175:C:O2'	2.35	0.58
33:R1:962:G:N2	33:R1:2250:G:H1	2.02	0.58
33:R1:2474:U:H5"	33:R1:2475:C:H5	1.67	0.58
33:R1:3:U:H2'	33:R1:4:U:H6	1.69	0.57
33:R1:695:G:O2'	33:R1:696:G:O5'	2.21	0.57
35:R3:738:C:HO2'	35:R3:739:C:H6	1.51	0.57
7:18:33:ARG:HD3	34:R2:52:A:H62	1.68	0.57
15:25:32:GLY:HA3	15:25:93:ARG:HB2	1.85	0.57
35:R3:993:G:O2'	35:R3:995:C:N4	2.35	0.57
1:1:134:ARG:O	1:1:162:ARG:NH2	2.38	0.57
33:R1:827:U:O2'	33:R1:2068:U:N3	2.37	0.57
33:R1:1912:A:H62	33:R1:1917:U:H5	1.52	0.57
33:R1:2140:G:H2'	33:R1:2141:G:C8	2.39	0.57
35:R3:553:A:H2'	35:R3:554:A:H8	1.70	0.57
19:3:91:THR:HG23	19:3:94:GLN:HB2	1.87	0.57
36:T:51:C:H2'	36:T:52:G:O4'	2.05	0.57
33:R1:721:A:H2'	33:R1:722:A:C8	2.39	0.57
36:T:43:A:H2'	36:T:44:A:H8	1.69	0.57
24:34:12:ARG:HD3	24:34:44:VAL:HG11	1.87	0.57
35:R3:107:G:O2'	35:R3:108:G:H5"	2.04	0.57
35:R3:236:A:H2'	35:R3:237:G:C8	2.38	0.57
33:R1:2774:C:O2'	33:R1:2775:G:H8	1.87	0.57
35:R3:1356:G:H2'	35:R3:1357:A:C8	2.39	0.57
16:27:37:ILE:HD11	16:27:82:ILE:HD11	1.87	0.57
35:R3:1149:C:H2'	35:R3:1150:A:C8	2.40	0.57
35:R3:1218:C:H2'	35:R3:1219:A:C8	2.39	0.57
12:22:11:ARG:NH2	33:R1:1321:A:O2'	2.37	0.57
15:25:30:ILE:HD11	15:25:63:ILE:HD12	1.86	0.57
33:R1:2898:U:H2'	33:R1:2899:A:H8	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:R3:999:C:H2'	35:R3:1000:A:H4'	1.86	0.57
18:29:41:HIS:HD1	33:R1:95:A:HO2'	1.53	0.56
19:3:45:TYR:OH	33:R1:2636:C:O2'	2.20	0.56
23:33:29:LYS:NZ	33:R1:2286:G:OP1	2.38	0.56
33:R1:629:G:N3	33:R1:639:U:O2'	2.37	0.56
33:R1:1095:A:N7	33:R1:1096:A:N6	2.52	0.56
33:R1:1103:A:H5"	33:R1:1104:C:C5	2.40	0.56
34:R2:21:G:H2'	34:R2:22:U:O4'	2.05	0.56
8:19:13:LYS:HD2	8:19:76:HIS:HA	1.87	0.56
33:R1:282:A:N6	33:R1:359:G:O6	2.37	0.56
33:R1:1181:U:H2'	33:R1:1182:G:C8	2.40	0.56
2:13:78:THR:HB	33:R1:2641:G:H5"	1.87	0.56
30:9:12:LEU:HD11	30:9:19:VAL:HG11	1.86	0.56
33:R1:1869:G:N7	33:R1:1870:C:O2'	2.37	0.56
35:R3:324:G:N1	35:R3:327:A:OP2	2.32	0.56
36:T:19:G:N2	36:T:57:A:H1'	2.21	0.56
36:T:55:PSU:HN3	36:T:57:A:H3'	1.70	0.56
17:28:27:ARG:NH2	33:R1:1365:A:OP1	2.33	0.56
33:R1:361:G:O2'	33:R1:362:A:O4'	2.22	0.56
33:R1:2502:G:H5"	33:R1:2503:A:H5"	1.87	0.56
35:R3:359:G:O2'	35:R3:360:G:O5'	2.23	0.56
35:R3:369:G:HO2'	35:R3:370:C:H6	1.53	0.56
35:R3:713:G:H2'	35:R3:714:G:C8	2.39	0.56
35:R3:1409:C:H2'	35:R3:1410:A:H8	1.69	0.56
33:R1:644:A:H2'	33:R1:645:C:O4'	2.06	0.56
2:13:21:THR:HG22	2:13:61:LYS:HB2	1.87	0.56
12:22:78:GLU:O	33:R1:24:G:O2'	2.24	0.56
35:R3:57:G:N2	35:R3:388:G:O6	2.39	0.56
27:4:45:ALA:HB2	27:4:89:PRO:HD3	1.88	0.56
29:6:51:PHE:CZ	29:6:71:LEU:HD13	2.39	0.56
30:9:53:GLU:O	30:9:57:LYS:HG2	2.06	0.56
6:17:17:ARG:NH2	33:R1:2002:G:OP1	2.39	0.56
10:20:80:ASN:ND2	33:R1:1151:A:H4'	2.20	0.56
33:R1:1683:U:H2'	33:R1:1684:G:H8	1.70	0.56
33:R1:1802:A:H2'	33:R1:1803:A:C8	2.40	0.56
35:R3:115:G:O2'	35:R3:289:G:H5'	2.06	0.56
35:R3:396:C:H5'	35:R3:397:A:OP2	2.04	0.56
9:2:231:HIS:HA	9:2:241:LYS:HD2	1.87	0.56
28:5:43:ILE:HG22	31:E:414:ILE:HG12	1.88	0.56
33:R1:2246:G:H2'	33:R1:2247:A:H8	1.70	0.56
1:1:43:ASP:OD2	33:R1:2123:G:O2'	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:20:82:LEU:HD22	10:20:87:VAL:HB	1.88	0.56
33:R1:695:G:H5"	33:R1:1380:G:H4'	1.88	0.56
17:28:67:LEU:HD23	17:28:77:TYR:CZ	2.41	0.55
33:R1:871:U:H2'	33:R1:872:U:C6	2.41	0.55
33:R1:1069:A:N6	33:R1:1073:A:O4'	2.36	0.55
33:R1:1266:G:O2'	33:R1:2012:G:O6	2.22	0.55
33:R1:1582:C:O2'	33:R1:1585:C:N3	2.39	0.55
33:R1:2167:U:H2'	33:R1:2168:G:H5"	1.87	0.55
35:R3:1035:A:N7	35:R3:1036:A:N6	2.54	0.55
6:17:28:LEU:HD11	6:17:113:ILE:HG12	1.88	0.55
9:2:70:LYS:HE2	9:2:73:ILE:HG21	1.87	0.55
19:3:10:GLY:H	19:3:197:THR:HG23	1.71	0.55
33:R1:1771:C:H2'	33:R1:1772:A:C8	2.42	0.55
35:R3:297:G:N2	35:R3:300:A:OP2	2.35	0.55
35:R3:461:A:O2'	35:R3:462:G:OP1	2.23	0.55
35:R3:1439:G:O2'	35:R3:1440:U:O5'	2.22	0.55
9:2:129:LEU:HD12	9:2:133:ASN:HB2	1.89	0.55
29:6:88:LEU:O	29:6:128:THR:OG1	2.25	0.55
33:R1:360:U:O2'	33:R1:361:G:O5'	2.22	0.55
33:R1:1418:G:N2	33:R1:1579:A:N7	2.54	0.55
35:R3:634:C:H2'	35:R3:635:A:C8	2.41	0.55
33:R1:152:A:H61	33:R1:173:A:H61	1.54	0.55
33:R1:2246:G:H2'	33:R1:2247:A:C8	2.41	0.55
4:15:89:VAL:HG23	4:15:123:ARG:HH21	1.71	0.55
7:18:43:ASN:OD1	7:18:44:GLY:N	2.40	0.55
27:4:5:LEU:HD13	27:4:122:GLU:HG2	1.89	0.55
35:R3:1439:G:HO2'	35:R3:1440:U:C5'	2.19	0.55
19:3:45:TYR:HH	33:R1:2636:C:HO2'	1.52	0.55
33:R1:281:C:N4	33:R1:359:G:H1	2.05	0.55
35:R3:1010:U:H2'	35:R3:1011:C:H6	1.72	0.55
29:6:15:ASP:HB2	29:6:26:LYS:HB3	1.89	0.55
31:E:370:SER:O	31:E:370:SER:OG	2.24	0.55
33:R1:1447:C:H2'	33:R1:1448:G:H8	1.72	0.55
35:R3:1120:C:H2'	35:R3:1121:U:C6	2.42	0.55
2:13:99:ARG:O	2:13:103:ILE:HD12	2.06	0.55
2:13:108:MET:O	33:R1:1006:C:O2'	2.23	0.55
3:14:66:LYS:HD2	3:14:81:GLY:H	1.72	0.55
33:R1:1771:C:H2'	33:R1:1772:A:H8	1.72	0.55
35:R3:1036:A:N7	35:R3:1037:C:N4	2.54	0.55
35:R3:1144:G:O6	35:R3:1145:A:N6	2.40	0.55
33:R1:171:U:H2'	33:R1:172:A:C8	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:R3:50:A:O2'	35:R3:360:G:N2	2.40	0.55
35:R3:1013:G:N2	35:R3:1016:A:OP2	2.21	0.55
30:9:117:LEU:HD21	30:9:130:VAL:HG22	1.89	0.54
33:R1:593:U:H2'	33:R1:594:U:C6	2.42	0.54
33:R1:848:C:H2'	33:R1:849:A:C8	2.42	0.54
33:R1:1076:C:H2'	33:R1:1077:A:O4'	2.07	0.54
33:R1:1667:G:O2'	33:R1:1991:U:O4	2.20	0.54
34:R2:31:C:H2'	34:R2:53:A:H61	1.71	0.54
35:R3:1447:A:H5'	35:R3:1448:C:H5	1.72	0.54
15:25:55:GLU:HB3	15:25:59:GLU:HG3	1.87	0.54
33:R1:357:C:H2'	33:R1:358:U:C6	2.42	0.54
35:R3:672:U:O2'	35:R3:673:A:OP1	2.22	0.54
35:R3:744:C:H2'	35:R3:745:G:C8	2.42	0.54
8:19:6:GLN:OE1	19:3:184:ARG:NH1	2.40	0.54
27:4:198:GLU:H	27:4:198:GLU:CD	2.10	0.54
31:E:46:SER:OG	31:E:76:GLN:NE2	2.39	0.54
33:R1:582:A:H2'	33:R1:583:G:H8	1.73	0.54
33:R1:2174:C:H2'	33:R1:2175:C:O4'	2.08	0.54
35:R3:600:A:N6	35:R3:639:G:O6	2.40	0.54
1:1:186:LYS:O	1:1:190:GLU:HG2	2.07	0.54
9:2:2:VAL:HG12	9:2:18:VAL:HG22	1.89	0.54
33:R1:160:A:H2	33:R1:165:A:H61	1.56	0.54
33:R1:371:A:H2	33:R1:402:A:H62	1.56	0.54
33:R1:1306:C:H2'	33:R1:1307:A:H8	1.73	0.54
35:R3:1010:U:H2'	35:R3:1011:C:C6	2.43	0.54
29:6:22:VAL:HG13	29:6:35:THR:HG22	1.90	0.54
33:R1:1219:U:H2'	33:R1:1220:G:C8	2.42	0.54
33:R1:1864:U:OP1	33:R1:2410:G:O2'	2.23	0.54
33:R1:2699:C:O2'	33:R1:2700:A:H8	1.90	0.54
35:R3:413:G:H1'	35:R3:428:G:H21	1.73	0.54
13:23:79:ASP:OD1	13:23:79:ASP:N	2.34	0.54
29:6:9:VAL:HA	29:6:48:THR:HG22	1.89	0.54
13:23:36:LYS:NZ	13:23:79:ASP:O	2.40	0.54
22:32:3:GLN:NE2	33:R1:2016:U:O2	2.41	0.54
33:R1:1469:A:H2'	33:R1:1470:A:H8	1.72	0.54
19:3:109:VAL:HG21	19:3:193:VAL:HG12	1.89	0.54
28:5:161:SER:OG	28:5:162:ASP:N	2.41	0.54
30:9:116:ARG:HB2	30:9:131:SER:HB2	1.88	0.54
33:R1:2233:U:H2'	33:R1:2234:G:C8	2.43	0.54
35:R3:77:A:H2'	35:R3:78:A:H8	1.73	0.54
35:R3:1009:U:H2'	35:R3:1010:U:C6	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:R3:1439:G:O2'	35:R3:1440:U:H6	1.90	0.54
1:1:184:LYS:O	1:1:188:ASN:ND2	2.40	0.54
33:R1:247:G:OP2	33:R1:249:C:N4	2.40	0.54
33:R1:590:A:H62	33:R1:667:U:H3	1.55	0.54
33:R1:2008:C:H2'	33:R1:2009:A:H8	1.74	0.53
35:R3:792:A:H1'	35:R3:794:A:N7	2.24	0.53
35:R3:1409:C:H2'	35:R3:1410:A:C8	2.43	0.53
1:1:51:ASP:O	1:1:57:GLN:NE2	2.41	0.53
3:14:9:ASN:OD1	3:14:18:ARG:NH1	2.40	0.53
31:E:393:GLN:NE2	58:E:602:ATP:O3G	2.35	0.53
30:9:132:PHE:HB2	30:9:140:ALA:HB3	1.90	0.53
33:R1:1683:U:H2'	33:R1:1684:G:C8	2.43	0.53
33:R1:1716:U:H2'	33:R1:1717:A:H8	1.73	0.53
35:R3:1452:C:O2'	35:R3:1453:G:N2	2.41	0.53
33:R1:1664:A:H61	33:R1:1996:C:N4	2.05	0.53
35:R3:296:U:O2'	35:R3:556:C:O2	2.27	0.53
1:1:8:MET:O	1:1:11:ILE:HG13	2.09	0.53
5:16:69:PRO:HA	5:16:94:ALA:HB2	1.91	0.53
12:22:35:ILE:O	12:22:39:THR:HG23	2.08	0.53
33:R1:2812:G:H2'	33:R1:2813:A:C8	2.44	0.53
34:R2:40:U:N3	34:R2:44:G:OP2	2.42	0.53
35:R3:332:G:O2'	35:R3:333:U:O2	2.15	0.53
35:R3:1270:G:H2'	35:R3:1271:A:H8	1.74	0.53
11:21:38:VAL:HG11	11:21:57:GLY:HA3	1.90	0.53
31:E:174:CYS:O	31:E:178:LEU:HD23	2.09	0.53
33:R1:1288:G:OP2	33:R1:1288:G:N2	2.35	0.53
33:R1:1315:C:O2'	33:R1:1392:A:N3	2.37	0.53
9:2:213:ARG:NH1	33:R1:1566:A:H5'	2.23	0.53
13:23:18:GLU:OE1	13:23:18:GLU:N	2.37	0.53
19:3:59:ARG:HH21	33:R1:2830:C:H3'	1.74	0.53
33:R1:1529:G:O6	33:R1:1542:U:O4	2.27	0.53
33:R1:2329:U:H2'	33:R1:2330:G:H8	1.74	0.53
35:R3:289:G:HO2'	35:R3:290:C:H6	1.55	0.53
35:R3:612:C:H2'	35:R3:613:C:H6	1.74	0.53
17:28:60:LYS:NZ	33:R1:371:A:H8	2.06	0.53
33:R1:2243:U:H2'	33:R1:2244:U:C6	2.44	0.53
35:R3:35:G:H2'	35:R3:36:C:C6	2.44	0.53
35:R3:211:G:O2'	35:R3:212:G:O4'	2.26	0.53
12:22:83:LYS:NZ	33:R1:1261:C:OP2	2.38	0.53
24:34:43:THR:OG1	24:34:44:VAL:N	2.40	0.53
33:R1:1426:G:O2'	33:R1:1572:A:N6	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:R1:2224:G:H4'	33:R1:2226:C:C2	2.44	0.53
19:3:169:ARG:HG2	33:R1:2773:C:H5'	1.90	0.52
33:R1:1079:C:N4	33:R1:1088:A:O4'	2.42	0.52
33:R1:2131:U:H1'	33:R1:2158:A:C2	2.44	0.52
33:R1:2637:U:H2'	33:R1:2638:G:O4'	2.10	0.52
35:R3:360:G:H2'	35:R3:361:G:C8	2.43	0.52
35:R3:1270:G:O2'	35:R3:1271:A:OP1	2.27	0.52
1:1:185:LEU:HA	1:1:188:ASN:HD22	1.74	0.52
13:23:18:GLU:CD	13:23:18:GLU:H	2.11	0.52
19:3:133:THR:OG1	19:3:134:HIS:N	2.41	0.52
29:6:38:ASP:OD1	29:6:38:ASP:N	2.36	0.52
33:R1:362:A:H3'	33:R1:363:G:C8	2.43	0.52
33:R1:1386:C:H2'	33:R1:1387:A:C8	2.45	0.52
33:R1:1536:C:O2'	33:R1:1537:G:N2	2.42	0.52
4:15:122:VAL:HG13	4:15:125:LEU:HD12	1.92	0.52
35:R3:106:C:H2'	35:R3:107:G:H5'	1.89	0.52
35:R3:589:U:H3	35:R3:650:G:H1	1.56	0.52
35:R3:1149:C:O2'	35:R3:1150:A:OP1	2.26	0.52
35:R3:1323:G:H2'	35:R3:1324:A:C8	2.44	0.52
10:20:49:ARG:O	10:20:53:LYS:NZ	2.43	0.52
33:R1:151:C:H2'	33:R1:152:A:C8	2.45	0.52
33:R1:2831:G:N2	33:R1:2884:U:OP2	2.41	0.52
7:18:28:VAL:HG11	7:18:103:VAL:HG13	1.90	0.52
19:3:133:THR:OG1	33:R1:1675:C:O2	2.28	0.52
30:9:99:ILE:HG21	30:9:130:VAL:HG11	1.91	0.52
33:R1:2193:G:H2'	33:R1:2194:U:C6	2.45	0.52
28:5:176:PHE:O	28:5:177:ARG:NH1	2.43	0.52
33:R1:160:A:H8	33:R1:2217:G:H21	1.58	0.52
25:35:11:LYS:NZ	33:R1:249:C:O2	2.43	0.52
29:6:108:PHE:O	33:R1:2666:C:N4	2.43	0.52
29:6:120:ILE:HD12	29:6:140:ILE:HG22	1.91	0.52
35:R3:417:G:O2'	35:R3:418:C:H6	1.92	0.52
35:R3:1507:A:H2'	35:R3:1508:A:C8	2.45	0.52
1:1:61:GLY:N	1:1:163:TYR:HB2	2.25	0.52
4:15:32:GLY:HA2	33:R1:1190:G:H5"	1.92	0.52
28:5:56:LEU:HD13	28:5:88:VAL:HG23	1.92	0.52
31:E:426:ALA:O	31:E:430:ARG:HG3	2.09	0.52
33:R1:645:C:H2'	33:R1:647:G:C8	2.45	0.52
33:R1:191:A:H2'	33:R1:192:C:H6	1.75	0.52
33:R1:1071:G:H1'	33:R1:1089:A:C6	2.45	0.52
33:R1:1870:C:OP1	33:R1:1872:A:N6	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:R1:2124:G:H2'	33:R1:2125:G:O4'	2.09	0.52
33:R1:2788:C:O2'	33:R1:2809:A:N3	2.39	0.52
35:R3:790:A:OP1	36:T:38:A:O2'	2.25	0.52
28:5:69:ALA:HB2	28:5:84:ILE:HD12	1.93	0.52
31:E:203:ARG:HG2	31:E:547:ARG:HG2	1.92	0.52
33:R1:890:C:N3	33:R1:891:G:O2'	2.43	0.52
35:R3:407:U:H3	35:R3:435:A:N6	2.08	0.52
35:R3:685:G:H2'	35:R3:686:U:C6	2.45	0.52
35:R3:1178:G:N2	35:R3:1181:G:OP2	2.42	0.52
31:E:541:ASP:OD1	31:E:541:ASP:N	2.41	0.51
33:R1:856:G:H2'	33:R1:857:G:C8	2.44	0.51
25:35:35:LYS:HB2	25:35:40:LYS:HE3	1.93	0.51
28:5:133:GLU:HB2	28:5:136:ILE:HD11	1.91	0.51
33:R1:2121:G:H2'	33:R1:2122:U:C6	2.45	0.51
35:R3:212:G:H2'	35:R3:213:G:H8	1.76	0.51
29:6:63:GLN:HA	29:6:66:THR:HG22	1.92	0.51
31:E:96:GLU:OE1	31:E:96:GLU:N	2.41	0.51
31:E:361:GLY:N	58:E:602:ATP:O2A	2.35	0.51
33:R1:994:C:H5'	33:R1:995:C:OP2	2.11	0.51
34:R2:29:A:H2'	34:R2:30:C:C6	2.45	0.51
35:R3:868:C:H2'	35:R3:869:G:O4'	2.10	0.51
20:30:12:ALA:HA	20:30:15:ARG:HG2	1.91	0.51
33:R1:1062:G:H2'	33:R1:1063:G:C8	2.45	0.51
35:R3:382:A:H2'	35:R3:383:A:C8	2.46	0.51
3:14:4:GLU:OE1	3:14:4:GLU:N	2.44	0.51
21:31:25:ARG:O	28:5:101:ARG:NH1	2.43	0.51
33:R1:619:G:OP2	33:R1:620:G:N2	2.39	0.51
33:R1:1069:A:H5"	33:R1:1073:A:H62	1.76	0.51
35:R3:500:G:O2'	35:R3:501:C:OP1	2.26	0.51
13:23:7:LEU:HD22	13:23:46:ALA:HB2	1.93	0.51
33:R1:598:U:H2'	33:R1:599:A:H8	1.75	0.51
33:R1:1341:G:OP1	33:R1:1397:U:N3	2.42	0.51
35:R3:1271:A:H2'	35:R3:1272:G:C8	2.46	0.51
33:R1:272:A:H2'	33:R1:273:G:H8	1.75	0.51
33:R1:1098:A:H3'	33:R1:1099:G:H8	1.75	0.51
33:R1:1594:U:H2'	33:R1:1595:C:C6	2.45	0.51
33:R1:1631:G:N2	33:R1:1634:A:OP2	2.44	0.51
33:R1:1837:C:O2'	33:R1:1927:A:N3	2.37	0.51
33:R1:2147:A:N6	33:R1:2148:G:N3	2.59	0.51
9:2:68:ARG:NH2	9:2:126:GLY:O	2.42	0.51
16:27:71:VAL:O	16:27:71:VAL:HG12	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:5:134:GLN:NE2	28:5:147:ARG:O	2.39	0.51
29:6:136:ASP:O	29:6:140:ILE:HG23	2.11	0.51
33:R1:2788:C:H2'	33:R1:2789:C:C6	2.45	0.51
35:R3:77:A:H2'	35:R3:78:A:C8	2.46	0.51
35:R3:193:C:H2'	35:R3:194:C:C6	2.46	0.51
5:16:59:ARG:HD2	5:16:60:GLN:HB3	1.92	0.51
15:25:4:ILE:HG21	15:25:42:LEU:HD12	1.91	0.51
28:5:169:LEU:HB3	28:5:174:PHE:HD2	1.74	0.51
33:R1:639:U:H2'	33:R1:640:C:C6	2.45	0.51
33:R1:1447:C:H2'	33:R1:1448:G:C8	2.46	0.51
33:R1:2115:G:O2'	33:R1:2117:A:N7	2.43	0.51
35:R3:166:U:H2'	35:R3:167:A:H8	1.75	0.51
35:R3:1355:G:H2'	35:R3:1356:G:H8	1.76	0.51
1:1:47:ASN:OD1	1:1:170:ILE:HG12	2.11	0.51
17:28:68:ALA:HA	17:28:71:ARG:HH12	1.76	0.51
31:E:99:ASN:O	31:E:103:ARG:HG2	2.11	0.51
33:R1:796:C:H2'	33:R1:797:G:H8	1.76	0.51
33:R1:1086:A:O2'	33:R1:1103:A:N1	2.33	0.51
33:R1:1754:A:N1	33:R1:2716:C:O2'	2.39	0.51
33:R1:2099:U:O2	33:R1:2190:G:N2	2.32	0.51
33:R1:2115:G:N1	33:R1:2165:C:O2	2.42	0.51
35:R3:753:A:H4'	35:R3:754:C:O5'	2.10	0.51
16:27:77:ARG:HH12	33:R1:2332:C:P	2.34	0.50
31:E:405:TRP:NE1	31:E:424:SER:OG	2.44	0.50
33:R1:2547:A:H2'	33:R1:2548:U:C6	2.47	0.50
35:R3:456:A:N6	35:R3:477:C:N3	2.59	0.50
35:R3:1163:A:H2'	35:R3:1164:G:H8	1.77	0.50
18:29:2:LYS:HE2	18:29:56:LEU:HD21	1.92	0.50
33:R1:221:A:H1'	33:R1:233:A:H1'	1.92	0.50
33:R1:2699:C:O2'	33:R1:2700:A:O5'	2.29	0.50
35:R3:1005:A:H2'	35:R3:1006:G:C4	2.46	0.50
35:R3:1287:A:H2	35:R3:1353:G:H1'	1.76	0.50
8:19:5:LYS:NZ	8:19:9:GLN:OE1	2.44	0.50
19:3:149:ASN:HB3	33:R1:2572:A:OP2	2.12	0.50
33:R1:277:G:O2'	33:R1:361:G:N1	2.44	0.50
33:R1:388:G:O2'	33:R1:390:U:OP2	2.21	0.50
33:R1:1239:G:H2'	33:R1:1240:U:O4'	2.11	0.50
33:R1:1704:C:H2'	33:R1:1705:A:C8	2.46	0.50
33:R1:2121:G:H2'	33:R1:2122:U:C5	2.47	0.50
33:R1:2170:A:H2'	33:R1:2171:A:C8	2.46	0.50
33:R1:2474:U:H5"	33:R1:2475:C:C5	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:R3:500:G:H2'	35:R3:501:C:C6	2.47	0.50
35:R3:728:A:H2'	35:R3:729:A:C8	2.46	0.50
11:21:1:MET:N	11:21:42:ALA:O	2.37	0.50
19:3:29:VAL:O	19:3:185:ASN:HB3	2.10	0.50
33:R1:582:A:H2'	33:R1:583:G:C8	2.47	0.50
33:R1:1645:G:H5"	33:R1:1646:C:H5'	1.94	0.50
33:R1:1791:A:N6	33:R1:1828:G:O2'	2.35	0.50
33:R1:2101:A:H2'	33:R1:2102:G:O4'	2.11	0.50
35:R3:950:U:H2'	35:R3:951:G:C8	2.47	0.50
35:R3:1031:C:O3'	35:R3:1033:G:N2	2.45	0.50
1:1:42:VAL:CG2	1:1:175:ILE:H	2.23	0.50
3:14:105:ARG:NH1	8:19:33:GLU:OE2	2.37	0.50
9:2:268:ARG:HG2	9:2:268:ARG:HH11	1.77	0.50
21:31:58:ASP:OD2	21:31:58:ASP:N	2.43	0.50
28:5:147:ARG:HB2	28:5:147:ARG:NH1	2.26	0.50
33:R1:3:U:H2'	33:R1:4:U:C6	2.46	0.50
33:R1:851:C:H2'	33:R1:852:U:C6	2.47	0.50
33:R1:1085:A:OP2	33:R1:1085:A:H8	1.95	0.50
33:R1:1149:G:H2'	33:R1:1150:C:C6	2.47	0.50
33:R1:1278:C:H2'	33:R1:1279:G:H8	1.76	0.50
33:R1:1420:A:O2'	33:R1:1421:G:O5'	2.27	0.50
33:R1:2667:C:H2'	33:R1:2668:G:H5'	1.93	0.50
35:R3:1120:C:H2'	35:R3:1121:U:H6	1.76	0.50
36:T:66:C:H2'	36:T:67:C:C6	2.47	0.50
3:14:26:GLY:HA3	3:14:30:ARG:HH11	1.76	0.50
9:2:244:VAL:HG12	9:2:250:GLN:HA	1.93	0.50
20:30:56:VAL:HG22	20:30:58:GLU:HB2	1.94	0.50
31:E:82:PRO:HB3	31:E:161:ALA:HB2	1.92	0.50
33:R1:2638:G:H1'	33:R1:2778:A:H61	1.76	0.50
35:R3:966:G:N2	36:T:34:C:H5'	2.27	0.50
4:15:58:TYR:OH	33:R1:251:A:OP1	2.24	0.50
11:21:48:LYS:HD2	11:21:49:ILE:N	2.27	0.50
33:R1:358:U:H2'	33:R1:359:G:C8	2.47	0.50
33:R1:476:G:N1	33:R1:479:A:OP2	2.42	0.50
34:R2:111:U:O2'	34:R2:112:G:H5'	2.12	0.50
33:R1:279:A:N6	33:R1:361:G:O4'	2.45	0.50
35:R3:1077:G:N1	35:R3:1080:A:OP2	2.41	0.50
35:R3:1297:G:H4'	35:R3:1298:U:O5'	2.11	0.50
31:E:416:LYS:HA	31:E:421:GLU:HA	1.94	0.50
33:R1:592:A:H2'	33:R1:593:U:C6	2.47	0.50
35:R3:514:C:H2'	35:R3:515:G:H8	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:R3:1125:U:O2'	35:R3:1126:U:OP1	2.24	0.50
35:R3:1352:C:H2'	35:R3:1353:G:C8	2.47	0.50
35:R3:1391:U:H2'	35:R3:1392:G:C8	2.47	0.50
33:R1:276:U:H2'	33:R1:277:G:N3	2.26	0.49
33:R1:580:U:H2'	33:R1:581:C:C6	2.47	0.49
33:R1:721:A:H2'	33:R1:722:A:H8	1.77	0.49
35:R3:1008:U:H2'	35:R3:1009:U:C6	2.47	0.49
35:R3:1130:A:O2'	35:R3:1131:G:O5'	2.30	0.49
35:R3:1363:A:O2'	35:R3:1365:G:N7	2.42	0.49
11:21:1:MET:N	11:21:43:ASN:HA	2.27	0.49
33:R1:1083:U:O2'	33:R1:1084:A:H3'	2.11	0.49
33:R1:1361:G:H2'	33:R1:1362:C:H6	1.77	0.49
35:R3:1009:U:O2	35:R3:1020:G:N2	2.24	0.49
35:R3:1131:G:H2'	35:R3:1132:C:C6	2.47	0.49
35:R3:1137:C:O2	35:R3:1138:G:N2	2.45	0.49
15:25:31:TYR:HA	15:25:93:ARG:HH21	1.77	0.49
31:E:140:LEU:HA	31:E:143:GLN:HG2	1.95	0.49
33:R1:796:C:H2'	33:R1:797:G:C8	2.47	0.49
33:R1:1075:C:H5"	33:R1:1076:C:C6	2.47	0.49
33:R1:1928:A:H2'	33:R1:1929:G:O4'	2.11	0.49
35:R3:1181:G:O2'	35:R3:1182:G:N7	2.34	0.49
33:R1:148:U:H3'	33:R1:149:A:C8	2.47	0.49
33:R1:715:A:H5'	33:R1:716:A:OP2	2.12	0.49
33:R1:1167:C:H2'	33:R1:1168:G:H8	1.78	0.49
33:R1:1410:G:H2'	33:R1:1411:U:C6	2.47	0.49
33:R1:1538:G:H2'	33:R1:1539:U:C6	2.47	0.49
33:R1:1793:C:H2'	33:R1:1794:A:C8	2.48	0.49
35:R3:115:G:OP1	35:R3:115:G:C8	2.66	0.49
35:R3:205:A:H2'	35:R3:207:C:C4	2.47	0.49
35:R3:312:C:H2'	35:R3:313:A:C8	2.47	0.49
19:3:101:PHE:HD1	19:3:104:VAL:HG11	1.76	0.49
19:3:136:ASN:OD1	33:R1:2579:C:O2'	2.30	0.49
22:32:48:TYR:OH	33:R1:2883:A:OP1	2.20	0.49
31:E:176:LEU:HG	31:E:177:LEU:HD12	1.94	0.49
33:R1:2591:C:H2'	33:R1:2592:G:C8	2.47	0.49
33:R1:2897:U:H2'	33:R1:2898:U:C6	2.47	0.49
35:R3:746:A:H2'	35:R3:747:A:C8	2.47	0.49
35:R3:768:A:H4'	35:R3:1523:G:N2	2.27	0.49
31:E:66:GLN:HB3	31:E:67:PRO:HD3	1.94	0.49
31:E:535:LYS:O	31:E:538:LEU:HB2	2.12	0.49
33:R1:172:A:H2'	33:R1:173:A:C8	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:R1:1077:A:H2'	33:R1:1078:U:O4'	2.13	0.49
33:R1:1796:U:H2'	33:R1:1797:G:C8	2.47	0.49
33:R1:2591:C:H2'	33:R1:2592:G:H8	1.77	0.49
33:R1:2896:C:O2'	33:R1:2897:U:O5'	2.19	0.49
35:R3:555:U:H2'	35:R3:556:C:C6	2.48	0.49
33:R1:156:A:H2'	33:R1:157:C:O4'	2.13	0.49
33:R1:239:C:O2'	33:R1:622:G:O2'	2.29	0.49
33:R1:274:C:N4	33:R1:363:G:H21	2.10	0.49
33:R1:1028:A:H2'	33:R1:1029:A:H8	1.77	0.49
33:R1:1109:C:O2'	33:R1:1110:G:OP1	2.30	0.49
34:R2:32:U:H2'	34:R2:33:G:H8	1.78	0.49
35:R3:1005:A:H2'	35:R3:1006:G:C5	2.48	0.49
35:R3:1005:A:N6	35:R3:1025:U:O2'	2.34	0.49
35:R3:1477:U:H2'	35:R3:1478:U:C6	2.48	0.49
1:1:215:SER:HB2	1:1:221:GLY:HA2	1.93	0.49
10:20:111:LYS:HD2	11:21:48:LYS:NZ	2.27	0.49
12:22:4:ILE:HG13	33:R1:495:G:H5"	1.94	0.49
31:E:22:LEU:HB3	31:E:25:ILE:HD12	1.94	0.49
33:R1:319:G:H1	33:R1:323:C:H41	1.59	0.49
33:R1:631:A:N3	33:R1:2415:G:O2'	2.39	0.49
33:R1:1361:G:H2'	33:R1:1362:C:C6	2.48	0.49
33:R1:2151:U:H2'	33:R1:2152:G:H8	1.77	0.49
33:R1:2192:U:H2'	33:R1:2193:G:C8	2.48	0.49
33:R1:2306:C:H5'	33:R1:2307:G:H2'	1.94	0.49
1:1:22:ASP:HB3	1:1:25:GLU:HG2	1.95	0.49
27:4:146:VAL:HG12	27:4:185:LYS:HB2	1.94	0.49
33:R1:1412:U:H2'	33:R1:1413:A:C8	2.47	0.49
33:R1:1722:A:H2'	33:R1:1723:G:O4'	2.13	0.49
35:R3:1412:C:H2'	35:R3:1413:A:C8	2.47	0.49
10:20:25:GLY:O	10:20:29:ARG:NH1	2.46	0.49
31:E:442:VAL:O	31:E:445:LEU:HB2	2.12	0.49
33:R1:1198:U:H2'	33:R1:1199:U:C6	2.48	0.49
33:R1:1434:A:H2'	33:R1:1435:G:C8	2.48	0.49
35:R3:320:A:H2'	35:R3:321:A:O4'	2.12	0.49
1:1:194:VAL:O	1:1:198:LYS:HG2	2.13	0.48
6:17:56:LYS:HD3	6:17:88:ALA:HA	1.94	0.48
14:24:17:ASP:HA	14:24:20:LYS:HD2	1.94	0.48
19:3:137:SER:O	19:3:137:SER:OG	2.31	0.48
25:35:7:ARG:NH2	33:R1:245:G:N7	2.59	0.48
33:R1:742:A:H2'	33:R1:743:A:C8	2.48	0.48
35:R3:73:C:H2'	35:R3:74:A:C8	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:R3:79:G:H5'	35:R3:80:A:H5'	1.95	0.48
36:T:60:U:H5"	36:T:61:C:C5	2.48	0.48
21:31:58:ASP:O	21:31:62:LYS:HG2	2.14	0.48
22:32:49:ARG:NH1	33:R1:2883:A:OP2	2.45	0.48
33:R1:594:U:H2'	33:R1:595:C:C6	2.48	0.48
35:R3:312:C:H2'	35:R3:313:A:H8	1.76	0.48
35:R3:455:G:C2	35:R3:456:A:C6	3.01	0.48
35:R3:1163:A:H2'	35:R3:1164:G:C8	2.49	0.48
35:R3:1285:A:H4'	35:R3:1286:U:H5"	1.95	0.48
1:1:21:TYR:O	1:1:225:ASP:HB2	2.13	0.48
5:16:4:PRO:HG3	5:16:68:PHE:HE2	1.78	0.48
33:R1:2457:U:H5	33:R1:2494:G:H1	1.60	0.48
11:21:85:LYS:NZ	33:R1:1187:G:OP1	2.32	0.48
16:27:12:ASN:OD1	16:27:12:ASN:N	2.38	0.48
33:R1:645:C:H2'	33:R1:647:G:N7	2.28	0.48
33:R1:2291:U:H2'	33:R1:2292:U:C6	2.48	0.48
33:R1:2668:G:O2'	33:R1:2669:G:O4'	2.30	0.48
9:2:153:LEU:HD13	9:2:175:LEU:HD21	1.95	0.48
12:22:48:LYS:O	12:22:52:GLU:HG3	2.14	0.48
13:23:89:GLU:N	13:23:89:GLU:OE1	2.47	0.48
27:4:22:ASP:OD1	27:4:22:ASP:N	2.45	0.48
31:E:121:LEU:O	31:E:125:GLN:HG2	2.14	0.48
33:R1:438:G:H2'	33:R1:439:A:C8	2.49	0.48
33:R1:2031:A:N3	33:R1:2455:G:O2'	2.38	0.48
35:R3:157:U:H3	35:R3:164:G:H1	1.61	0.48
35:R3:1002:G:N2	35:R3:1039:G:H5"	2.25	0.48
35:R3:1186:G:O2'	35:R3:1187:G:H8	1.97	0.48
1:1:87:ALA:O	1:1:92:ALA:N	2.43	0.48
4:15:132:ARG:HG3	4:15:142:ILE:HD12	1.94	0.48
9:2:251:THR:OG1	9:2:252:LYS:N	2.46	0.48
15:25:26:PHE:HE2	15:25:89:ILE:HD12	1.78	0.48
33:R1:1443:U:H2'	33:R1:1444:G:H8	1.78	0.48
33:R1:1796:U:H2'	33:R1:1797:G:H8	1.77	0.48
35:R3:113:G:H2'	35:R3:114:U:C6	2.49	0.48
5:16:42:THR:OG1	5:16:45:GLN:HG3	2.14	0.48
5:16:88:ASN:OD1	5:16:89:VAL:N	2.45	0.48
17:28:38:TRP:HB2	17:28:45:PHE:HE1	1.77	0.48
20:30:40:THR:HG22	20:30:42:ALA:H	1.78	0.48
29:6:97:VAL:HG22	29:6:102:ILE:HG12	1.96	0.48
33:R1:1104:C:H2'	33:R1:1105:U:C6	2.49	0.48
33:R1:2123:G:H2'	33:R1:2124:G:C4	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:R1:2193:G:H2'	33:R1:2194:U:H6	1.78	0.48
35:R3:1008:U:H3	35:R3:1021:A:H61	1.61	0.48
35:R3:1015:G:N2	35:R3:1218:C:O2	2.45	0.48
36:T:18:G:O2'	36:T:19:G:N7	2.46	0.48
33:R1:500:G:N1	33:R1:503:A:OP2	2.47	0.48
33:R1:1716:U:H2'	33:R1:1717:A:C8	2.48	0.48
33:R1:1869:G:N1	33:R1:1872:A:OP2	2.46	0.48
35:R3:235:C:H2'	35:R3:236:A:H8	1.79	0.48
35:R3:272:C:N4	35:R3:273:U:O4	2.47	0.48
35:R3:363:A:O2'	35:R3:364:A:OP1	2.30	0.48
35:R3:950:U:H2'	35:R3:951:G:H8	1.78	0.48
35:R3:1315:U:H2'	35:R3:1316:G:O4'	2.14	0.48
35:R3:1414:U:H2'	35:R3:1415:G:H8	1.79	0.48
15:25:75:GLN:HG3	15:25:76:ASP:OD2	2.14	0.48
22:32:3:GLN:HA	33:R1:2615:U:C2	2.48	0.48
27:4:19:PHE:HD2	27:4:113:VAL:HG21	1.78	0.48
31:E:342:LEU:HD13	31:E:520:VAL:HB	1.95	0.48
33:R1:639:U:H2'	33:R1:640:C:H6	1.78	0.48
33:R1:1808:A:H3'	33:R1:1809:A:C8	2.49	0.48
33:R1:2430:A:H2'	33:R1:2430:A:N3	2.28	0.48
35:R3:1356:G:H2'	35:R3:1357:A:H8	1.79	0.48
36:T:63:G:H2'	36:T:64:G:H8	1.79	0.48
9:2:213:ARG:HH12	33:R1:1566:A:H5'	1.78	0.48
15:25:37:PRO:HG2	34:R2:74:U:H1'	1.94	0.48
33:R1:1050:A:O2'	33:R1:1051:G:O5'	2.28	0.48
33:R1:1720:U:H2'	33:R1:1721:G:O4'	2.13	0.48
35:R3:235:C:H2'	35:R3:236:A:C8	2.49	0.48
2:13:102:GLU:HG2	2:13:119:PHE:CZ	2.49	0.47
8:19:30:TRP:CE3	8:19:37:LYS:HG2	2.49	0.47
12:22:18:ARG:HG3	12:22:76:VAL:HG22	1.95	0.47
33:R1:64:A:H2'	33:R1:65:U:C6	2.49	0.47
35:R3:45:G:H2'	35:R3:46:G:C8	2.49	0.47
35:R3:256:U:H3	35:R3:270:A:H62	1.61	0.47
35:R3:925:G:C2	35:R3:927:G:C8	3.02	0.47
1:1:189:LEU:HD12	1:1:192:LEU:HD11	1.96	0.47
14:24:17:ASP:HB3	14:24:20:LYS:HB2	1.96	0.47
28:5:40:GLY:HA3	33:R1:2307:G:O6	2.15	0.47
3:14:77:ILE:O	3:14:77:ILE:HG22	2.14	0.47
4:15:29:LYS:O	4:15:30:THR:OG1	2.25	0.47
28:5:25:MET:SD	34:R2:54:G:N2	2.87	0.47
9:2:140:VAL:HG11	9:2:189:ALA:HB1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:22:109:ASP:N	12:22:109:ASP:OD1	2.39	0.47
29:6:36:LEU:HD13	29:6:67:ALA:HB1	1.96	0.47
31:E:32:GLY:N	31:E:211:THR:HG22	2.30	0.47
33:R1:1412:U:H2'	33:R1:1413:A:H8	1.80	0.47
33:R1:2142:A:H61	33:R1:2150:C:H42	1.61	0.47
33:R1:2818:U:H2'	33:R1:2819:G:C8	2.50	0.47
35:R3:918:A:H2'	35:R3:919:A:C8	2.50	0.47
35:R3:1219:A:H2'	35:R3:1220:G:C8	2.50	0.47
11:21:14:VAL:HG12	11:21:20:VAL:HG11	1.96	0.47
28:5:61:GLY:O	28:5:94:ARG:NE	2.48	0.47
31:E:267:LYS:O	31:E:270:GLU:HG3	2.14	0.47
31:E:310:GLU:OE1	31:E:310:GLU:N	2.47	0.47
33:R1:947:A:H2'	33:R1:948:C:C6	2.50	0.47
33:R1:1746:A:H2'	33:R1:1747:U:C6	2.49	0.47
33:R1:1952:A:N3	33:R1:2560:A:O2'	2.46	0.47
33:R1:2345:G:N3	33:R1:2381:A:H2'	2.29	0.47
35:R3:174:A:H2'	35:R3:175:C:O4'	2.14	0.47
1:1:58:ASN:ND2	31:E:133:GLN:HB3	2.29	0.47
15:25:70:ILE:HG22	15:25:72:VAL:HG13	1.97	0.47
21:31:43:PHE:CZ	28:5:175:PRO:HA	2.50	0.47
33:R1:352:A:H2'	33:R1:353:C:O4'	2.14	0.47
33:R1:370:G:O2'	33:R1:424:G:OP1	2.28	0.47
34:R2:5:U:H2'	34:R2:6:G:H8	1.80	0.47
34:R2:110:C:H2'	34:R2:111:U:O4'	2.14	0.47
35:R3:363:A:HO2'	35:R3:364:A:P	2.37	0.47
35:R3:1355:G:H2'	35:R3:1356:G:C8	2.50	0.47
1:1:47:ASN:ND2	33:R1:2177:C:O2	2.48	0.47
12:22:5:ALA:O	33:R1:494:G:O2'	2.24	0.47
19:3:81:GLU:OE1	33:R1:2635:A:O2'	2.33	0.47
19:3:149:ASN:OD1	19:3:150:GLN:N	2.34	0.47
22:32:7:PRO:HD2	33:R1:1263:U:O2'	2.15	0.47
30:9:9:VAL:HB	30:9:12:LEU:O	2.14	0.47
33:R1:878:A:H3'	33:R1:879:G:C8	2.49	0.47
33:R1:1183:U:H2'	33:R1:1184:U:C6	2.49	0.47
33:R1:1570:A:H2'	33:R1:1571:A:C8	2.50	0.47
33:R1:2081:U:H2'	33:R1:2082:A:H8	1.78	0.47
35:R3:359:G:C4	35:R3:360:G:C8	3.03	0.47
35:R3:504:C:C2	35:R3:542:G:N2	2.83	0.47
35:R3:1008:U:H1'	35:R3:1022:A:H61	1.79	0.47
35:R3:1122:U:O2'	35:R3:1123:U:H6	1.98	0.47
35:R3:1314:C:H2'	35:R3:1315:U:C6	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:R3:1427:C:H2'	35:R3:1428:A:H8	1.80	0.47
12:22:23:LEU:O	12:22:27:LYS:NZ	2.34	0.47
29:6:32:LEU:HD13	29:6:74:MET:HG2	1.96	0.47
31:E:107:VAL:HG13	31:E:121:LEU:HD11	1.96	0.47
33:R1:593:U:H2'	33:R1:594:U:H6	1.79	0.47
33:R1:2047:C:H2'	33:R1:2048:G:H8	1.78	0.47
33:R1:2180:U:N3	33:R1:2181:U:O4	2.48	0.47
33:R1:2190:G:H2'	33:R1:2191:A:C8	2.50	0.47
34:R2:7:G:H22	34:R2:113:C:H5	1.63	0.47
35:R3:33:A:H2'	35:R3:34:C:C6	2.50	0.47
35:R3:674:G:H2'	35:R3:675:A:C8	2.49	0.47
35:R3:837:U:HO2'	35:R3:838:G:C5'	2.28	0.47
35:R3:1054:C:O2	35:R3:1196:A:N6	2.48	0.47
2:13:114:LEU:O	2:13:118:MET:HG3	2.15	0.47
3:14:23:LYS:HZ2	33:R1:2562:U:H1'	1.80	0.47
15:25:43:ASP:OD1	15:25:44:HIS:N	2.46	0.47
19:3:25:THR:OG1	19:3:191:GLY:O	2.28	0.47
20:30:6:ILE:HG12	20:30:47:ILE:HD11	1.97	0.47
27:4:8:ALA:O	27:4:9:GLN:HG3	2.15	0.47
33:R1:412:A:N7	33:R1:2412:A:H1'	2.30	0.47
33:R1:2328:A:H2'	33:R1:2329:U:H6	1.78	0.47
36:T:43:A:H2'	36:T:44:A:C8	2.47	0.47
7:18:54:VAL:HG12	34:R2:116:G:H4'	1.97	0.47
16:27:72:LYS:HE3	16:27:72:LYS:HB3	1.73	0.47
30:9:90:LEU:HB2	30:9:123:ARG:O	2.15	0.47
31:E:77:GLU:HG2	31:E:77:GLU:O	2.15	0.47
33:R1:880:G:H2'	33:R1:881:G:C4	2.50	0.47
33:R1:2179:C:H5	33:R1:2180:U:C4	2.33	0.47
35:R3:17:U:H2'	35:R3:18:C:C6	2.50	0.47
35:R3:922:G:H2'	35:R3:923:A:C8	2.50	0.47
8:19:5:LYS:O	8:19:9:GLN:HG3	2.15	0.46
9:2:233:GLY:HA3	33:R1:2598:A:H5"	1.97	0.46
9:2:239:PHE:O	9:2:241:LYS:HG2	2.16	0.46
11:21:49:ILE:HG23	11:21:54:VAL:HG23	1.96	0.46
29:6:106:LEU:HD13	29:6:151:ARG:HB2	1.97	0.46
35:R3:205:A:O2'	35:R3:206:C:H5'	2.15	0.46
35:R3:580:C:H2'	35:R3:581:G:O4'	2.14	0.46
9:2:120:ASP:HB3	30:9:91:PHE:CZ	2.51	0.46
33:R1:1049:C:H42	33:R1:2751:G:H1	1.63	0.46
33:R1:1442:U:H2'	33:R1:1443:U:C6	2.50	0.46
33:R1:2071:A:H2'	33:R1:2072:C:C6	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:R3:1118:U:H1'	35:R3:1179:A:C4	2.50	0.46
35:R3:1481:U:H2'	35:R3:1482:G:C8	2.51	0.46
29:6:154:GLU:OE2	29:6:158:GLY:N	2.48	0.46
31:E:307:GLU:OE1	31:E:478:GLU:HG2	2.16	0.46
33:R1:225:C:O2'	33:R1:226:A:OP1	2.33	0.46
33:R1:889:C:H2'	33:R1:890:C:O4'	2.16	0.46
33:R1:1874:C:H2'	33:R1:1875:G:O4'	2.15	0.46
33:R1:2107:G:C4	33:R1:2108:A:C8	3.04	0.46
33:R1:2126:A:H2	33:R1:2173:A:N7	2.12	0.46
33:R1:2537:U:H2'	33:R1:2538:C:H6	1.80	0.46
33:R1:2645:G:OP2	33:R1:2645:G:N2	2.27	0.46
2:13:45:THR:HB	2:13:48:VAL:HG22	1.97	0.46
7:18:20:GLU:OE1	7:18:20:GLU:HA	2.15	0.46
27:4:5:LEU:HA	27:4:120:VAL:HG23	1.98	0.46
28:5:76:PHE:O	28:5:77:LYS:HG2	2.16	0.46
29:6:25:ILE:HG22	29:6:32:LEU:HB2	1.96	0.46
33:R1:138:U:O2'	33:R1:139:U:H5'	2.15	0.46
33:R1:355:U:H2'	33:R1:356:G:C8	2.51	0.46
33:R1:1292:G:H2'	33:R1:1293:C:C6	2.51	0.46
33:R1:2846:G:H2'	33:R1:2847:U:C6	2.50	0.46
35:R3:908:A:H2'	35:R3:909:A:C8	2.50	0.46
35:R3:945:G:C2	35:R3:946:A:C8	3.03	0.46
35:R3:954:G:H2'	35:R3:955:U:C6	2.50	0.46
35:R3:1273:C:H2'	35:R3:1274:A:O4'	2.14	0.46
28:5:42:ALA:HA	28:5:48:LEU:HD12	1.97	0.46
31:E:74:LEU:HB2	31:E:176:LEU:HD22	1.98	0.46
33:R1:196:A:O2'	33:R1:805:G:O6	2.30	0.46
33:R1:272:A:H2'	33:R1:273:G:C8	2.51	0.46
33:R1:827:U:O2'	33:R1:2068:U:C2	2.69	0.46
33:R1:1873:G:H2'	33:R1:1874:C:C6	2.51	0.46
33:R1:2102:G:O6	33:R1:2187:U:C2	2.69	0.46
33:R1:2494:G:C2	33:R1:2495:G:C8	3.04	0.46
33:R1:2803:G:H2'	33:R1:2804:U:C6	2.50	0.46
35:R3:1268:G:H2'	35:R3:1269:A:C8	2.51	0.46
10:20:93:ILE:HD12	11:21:13:ARG:HB2	1.98	0.46
24:34:21:ARG:NH2	33:R1:466:A:H5'	2.31	0.46
33:R1:453:A:O2'	33:R1:454:A:OP1	2.27	0.46
33:R1:588:U:H2'	33:R1:589:U:C6	2.51	0.46
33:R1:675:A:N3	33:R1:2443:C:O2'	2.45	0.46
33:R1:1882:U:H2'	33:R1:1883:U:C6	2.51	0.46
33:R1:2014:A:H2'	33:R1:2015:A:C8	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:R1:2656:U:O2	33:R1:2665:A:N7	2.49	0.46
33:R1:2818:U:H2'	33:R1:2819:G:H8	1.81	0.46
35:R3:645:G:C2	35:R3:646:G:C8	3.03	0.46
2:13:27:ARG:NH1	33:R1:1140:C:O3'	2.49	0.46
5:16:31:PHE:HB3	5:16:130:PHE:CE1	2.51	0.46
8:19:112:ARG:O	8:19:113:LEU:HD12	2.16	0.46
19:3:180:VAL:HG22	19:3:187:LEU:HD12	1.97	0.46
33:R1:642:U:O2'	33:R1:644:A:N7	2.31	0.46
33:R1:859:G:H4'	33:R1:860:U:O5'	2.14	0.46
33:R1:1050:A:H4'	33:R1:1051:G:OP1	2.16	0.46
33:R1:2315:G:O2'	33:R1:2316:G:H8	1.96	0.46
33:R1:2514:U:H2'	33:R1:2515:C:C6	2.50	0.46
33:R1:2900:A:H2'	33:R1:2901:C:O4'	2.15	0.46
35:R3:344:A:H5"	35:R3:345:C:H5	1.81	0.46
35:R3:745:G:H2'	35:R3:746:A:H8	1.80	0.46
35:R3:864:A:H2'	35:R3:865:A:C8	2.50	0.46
35:R3:996:A:H2'	35:R3:997:U:C6	2.51	0.46
1:1:166:ASP:OD1	1:1:167:LYS:N	2.49	0.46
27:4:143:LEU:HD13	27:4:146:VAL:HG11	1.98	0.46
31:E:11:VAL:HG13	31:E:59:ILE:HD12	1.98	0.46
33:R1:2537:U:H2'	33:R1:2538:C:C6	2.51	0.46
35:R3:246:A:C2	35:R3:282:A:C5	3.04	0.46
35:R3:704:A:C4	35:R3:705:G:C8	3.04	0.46
16:27:51:VAL:HG12	16:27:82:ILE:HG13	1.98	0.46
33:R1:881:G:H2'	33:R1:882:G:H8	1.80	0.46
33:R1:1219:U:H2'	33:R1:1220:G:H8	1.81	0.46
33:R1:2663:G:O2'	33:R1:2664:G:OP1	2.32	0.46
35:R3:330:C:O2'	35:R3:331:G:H5'	2.16	0.46
35:R3:1353:G:H2'	35:R3:1354:U:H6	1.81	0.46
35:R3:1496:C:H2'	35:R3:1497:G:O4'	2.16	0.46
3:14:105:ARG:O	3:14:108:ARG:HG3	2.16	0.46
9:2:124:LYS:HE3	9:2:124:LYS:HB2	1.71	0.46
9:2:180:MET:HB2	9:2:267:VAL:HB	1.98	0.46
14:24:40:LEU:HD23	14:24:61:GLU:HG3	1.98	0.46
23:33:5:ARG:NE	33:R1:2285:C:OP2	2.49	0.46
28:5:56:LEU:HD12	28:5:86:CYS:HB2	1.98	0.46
30:9:30:LEU:HB3	30:9:36:ALA:HB3	1.97	0.46
33:R1:289:G:H2'	33:R1:290:U:C6	2.51	0.46
33:R1:305:C:H2'	33:R1:306:U:C6	2.51	0.46
33:R1:1441:G:H2'	33:R1:1442:U:C6	2.50	0.46
35:R3:464:U:C4	35:R3:466:A:H5'	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:13:125:TYR:OH	2:13:132:HIS:NE2	2.36	0.45
3:14:23:LYS:NZ	33:R1:2561:U:O2	2.47	0.45
3:14:73:ASP:OD2	8:19:77:SER:OG	2.20	0.45
19:3:4:LEU:HD22	19:3:101:PHE:HE2	1.81	0.45
27:4:137:LYS:O	27:4:141:MET:HG3	2.15	0.45
28:5:169:LEU:HG	28:5:174:PHE:HE2	1.80	0.45
33:R1:1410:G:H2'	33:R1:1411:U:H6	1.81	0.45
35:R3:550:G:H2'	35:R3:551:U:C6	2.51	0.45
35:R3:779:C:H2'	35:R3:780:A:O4'	2.16	0.45
35:R3:1250:A:H2'	35:R3:1251:A:C8	2.51	0.45
36:T:59:A:O2'	36:T:60:U:O4'	2.32	0.45
9:2:48:ILE:HG22	33:R1:779:U:OP1	2.15	0.45
9:2:154:ALA:HB2	9:2:161:VAL:HG23	1.98	0.45
15:25:26:PHE:CE2	15:25:89:ILE:HD12	2.52	0.45
33:R1:1747:U:H2'	33:R1:1748:C:C6	2.51	0.45
33:R1:1853:A:H2'	33:R1:1854:A:C8	2.51	0.45
35:R3:338:A:H3'	35:R3:339:C:H5"	1.99	0.45
35:R3:612:C:H2'	35:R3:613:C:C6	2.50	0.45
35:R3:1071:C:H2'	35:R3:1072:G:H8	1.80	0.45
35:R3:1291:U:H2'	35:R3:1292:G:H8	1.81	0.45
35:R3:1513:A:H2'	35:R3:1514:G:C8	2.50	0.45
5:16:71:LYS:HB3	5:16:93:VAL:O	2.16	0.45
15:25:78:GLN:HG3	15:25:88:HIS:HB3	1.98	0.45
17:28:18:SER:OG	17:28:19:HIS:N	2.49	0.45
31:E:90:ILE:HD12	31:E:156:TRP:CZ3	2.52	0.45
31:E:152:ARG:NH1	31:E:196:GLU:OE1	2.50	0.45
31:E:152:ARG:NH2	31:E:197:SER:OG	2.49	0.45
33:R1:148:U:H3'	33:R1:149:A:H8	1.81	0.45
33:R1:414:C:OP1	33:R1:1879:C:O2'	2.21	0.45
33:R1:753:A:H2'	33:R1:754:U:H6	1.82	0.45
33:R1:1542:U:H2'	33:R1:1543:G:O4'	2.16	0.45
35:R3:1157:A:N6	35:R3:1178:G:H1'	2.32	0.45
1:1:59:VAL:H	1:1:165:ASN:HD22	1.65	0.45
3:14:71:ARG:HD3	3:14:71:ARG:HA	1.73	0.45
4:15:129:LYS:HE2	33:R1:636:G:OP1	2.16	0.45
16:27:37:ILE:HG21	16:27:80:ILE:HG21	1.99	0.45
28:5:116:LEU:HB3	28:5:127:TYR:OH	2.16	0.45
33:R1:361:G:HO2'	33:R1:362:A:H8	1.63	0.45
33:R1:1912:A:O2'	35:R3:1494:G:O2'	2.16	0.45
35:R3:1412:C:H2'	35:R3:1413:A:H8	1.81	0.45
3:14:91:SER:OG	3:14:93:GLN:OE1	2.26	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:2:75:ALA:HB1	9:2:93:VAL:HG12	1.98	0.45
9:2:75:ALA:HB2	9:2:95:TYR:CD2	2.51	0.45
10:20:34:ALA:O	10:20:38:VAL:HG23	2.17	0.45
15:25:73:LYS:HE2	15:25:73:LYS:HB3	1.68	0.45
19:3:26:VAL:HG22	19:3:188:LEU:HD22	1.98	0.45
33:R1:1532:A:N6	33:R1:1540:G:O6	2.49	0.45
2:13:12:LYS:HA	2:13:12:LYS:HD2	1.82	0.45
5:16:129:THR:OG1	5:16:130:PHE:N	2.49	0.45
13:23:7:LEU:HD13	13:23:46:ALA:HA	1.98	0.45
28:5:39:VAL:HG12	28:5:84:ILE:O	2.16	0.45
30:9:47:PHE:O	30:9:52:ALA:N	2.50	0.45
33:R1:134:G:H2'	33:R1:135:U:C6	2.51	0.45
33:R1:1593:A:H2'	33:R1:1594:U:O4'	2.16	0.45
35:R3:77:A:H8	35:R3:95:C:C2	2.35	0.45
35:R3:195:A:H2'	35:R3:196:A:C8	2.51	0.45
35:R3:1384:C:H2'	35:R3:1385:G:H8	1.81	0.45
31:E:190:THR:O	31:E:190:THR:OG1	2.34	0.45
31:E:254:ARG:O	31:E:258:GLU:HG2	2.17	0.45
33:R1:44:A:H2'	33:R1:45:G:O4'	2.17	0.45
33:R1:1715:G:O2'	33:R1:1716:U:O5'	2.35	0.45
33:R1:2134:A:C4	33:R1:2157:G:H4'	2.51	0.45
33:R1:2651:C:H2'	33:R1:2652:C:C6	2.51	0.45
33:R1:2897:U:H2'	33:R1:2898:U:H6	1.81	0.45
34:R2:6:G:H2'	34:R2:7:G:C8	2.52	0.45
20:30:8:GLN:NE2	20:30:10:ARG:O	2.47	0.45
33:R1:100:U:H4'	33:R1:101:A:O4'	2.17	0.45
33:R1:570:G:H2'	33:R1:2030:A:N7	2.32	0.45
33:R1:722:A:H2'	33:R1:723:C:C6	2.52	0.45
33:R1:2258:C:O2'	33:R1:2427:C:OP2	2.32	0.45
35:R3:148:G:N2	35:R3:175:C:O2	2.50	0.45
35:R3:1002:G:H21	35:R3:1039:G:H2'	1.82	0.45
35:R3:1086:U:H3	35:R3:1099:G:H22	1.65	0.45
6:17:5:LYS:NZ	33:R1:2000:C:OP1	2.50	0.45
9:2:258:SER:O	9:2:258:SER:OG	2.29	0.45
22:32:38:LEU:H	22:32:38:LEU:HD12	1.82	0.45
33:R1:693:A:O2'	33:R1:1353:A:N3	2.49	0.45
33:R1:1923:U:OP1	36:T:24:U:O2'	2.34	0.45
33:R1:2861:U:H2'	33:R1:2862:G:H8	1.81	0.45
35:R3:524:G:H2'	35:R3:525:C:C6	2.52	0.45
35:R3:958:A:O2'	35:R3:959:A:O5'	2.30	0.45
35:R3:1175:G:H2'	35:R3:1176:A:C8	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:R3:1251:A:H2'	35:R3:1252:A:C8	2.51	0.45
18:29:17:GLU:HB2	18:29:53:VAL:HG11	1.99	0.45
21:31:43:PHE:HD1	28:5:114:ARG:HH22	1.64	0.45
31:E:90:ILE:O	31:E:94:VAL:HG22	2.16	0.45
31:E:403:THR:HG23	31:E:406:GLU:H	1.82	0.45
33:R1:1224:U:H2'	33:R1:1225:G:C8	2.51	0.45
33:R1:1591:A:H2'	33:R1:1592:C:C6	2.53	0.45
33:R1:2149:U:O2'	33:R1:2150:C:H6	2.00	0.45
33:R1:2215:C:H2'	33:R1:2216:G:H8	1.81	0.45
33:R1:2235:G:H2'	33:R1:2236:U:C6	2.52	0.45
35:R3:417:G:O2'	35:R3:418:C:H5'	2.17	0.45
35:R3:1287:A:H2'	35:R3:1288:A:C8	2.52	0.45
4:15:20:GLY:HA2	4:15:28:GLY:HA2	2.00	0.44
11:21:34:GLU:OE2	11:21:34:GLU:HA	2.17	0.44
16:27:29:GLU:O	16:27:66:LYS:HA	2.18	0.44
30:9:6:LEU:O	30:9:15:LEU:HD13	2.16	0.44
33:R1:1038:G:H2'	33:R1:1039:A:C8	2.52	0.44
33:R1:1779:U:H5	33:R1:1784:A:N7	2.15	0.44
33:R1:2051:A:OP2	33:R1:2051:A:H8	1.99	0.44
33:R1:2157:G:H2'	33:R1:2158:A:C2	2.52	0.44
33:R1:2512:C:H2'	33:R1:2513:A:O4'	2.17	0.44
33:R1:2646:C:OP2	33:R1:2732:G:O2'	2.35	0.44
36:T:8:4SU:O2'	36:T:9:G:N7	2.50	0.44
20:30:44:ARG:NH2	20:30:58:GLU:OE2	2.50	0.44
22:32:15:ARG:NH2	33:R1:1264:A:OP1	2.38	0.44
31:E:312:PHE:HB2	31:E:430:ARG:HE	1.82	0.44
33:R1:177:G:H3'	33:R1:178:G:C8	2.47	0.44
33:R1:792:A:N3	33:R1:2072:C:O2'	2.44	0.44
33:R1:878:A:H3'	33:R1:879:G:H8	1.82	0.44
33:R1:2747:G:O6	33:R1:2755:C:H5"	2.18	0.44
35:R3:149:A:H1'	35:R3:1446:A:C2	2.52	0.44
36:T:23:C:H2'	36:T:24:U:C6	2.52	0.44
13:23:28:ASN:HD21	13:23:91:GLN:HB3	1.83	0.44
14:24:81:ARG:NH2	33:R1:300:A:O5'	2.50	0.44
15:25:80:HIS:CD2	15:25:83:LYS:HB2	2.43	0.44
25:35:25:HIS:CE1	25:35:47:ALA:HB2	2.52	0.44
31:E:405:TRP:HE1	31:E:424:SER:HG	1.64	0.44
33:R1:895:U:H4'	33:R1:896:A:C2	2.52	0.44
33:R1:2372:U:H2'	33:R1:2373:G:H8	1.82	0.44
35:R3:69:G:H2'	35:R3:70:U:C6	2.53	0.44
35:R3:470:C:O2	35:R3:470:C:H2'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:2:179:GLU:OE2	9:2:269:ARG:NH2	2.42	0.44
16:27:18:ALA:HB1	33:R1:2271:G:OP1	2.16	0.44
28:5:173:ASP:OD1	28:5:173:ASP:N	2.51	0.44
29:6:51:PHE:CE1	29:6:68:ARG:HA	2.52	0.44
31:E:330:ARG:HG2	31:E:376:ASP:HB2	2.00	0.44
33:R1:596:U:H2'	33:R1:597:G:H8	1.83	0.44
33:R1:1463:C:H2'	33:R1:1464:G:C8	2.53	0.44
33:R1:1504:A:H2'	33:R1:1505:A:C8	2.52	0.44
33:R1:2025:C:H2'	33:R1:2026:U:C6	2.53	0.44
33:R1:2121:G:C8	33:R1:2122:U:C5	3.02	0.44
33:R1:2623:G:H4'	33:R1:2825:G:H8	1.82	0.44
35:R3:269:C:C2'	35:R3:270:A:H5"	2.44	0.44
35:R3:492:C:H2'	35:R3:493:A:C4	2.52	0.44
35:R3:559:A:H4'	35:R3:560:A:H3'	1.98	0.44
35:R3:600:A:H2'	35:R3:601:G:H8	1.81	0.44
35:R3:891:U:H2'	35:R3:892:A:H8	1.83	0.44
35:R3:1186:G:HO2'	35:R3:1187:G:P	2.40	0.44
35:R3:1388:C:H2'	35:R3:1389:C:O2	2.17	0.44
8:19:48:ALA:HB1	8:19:95:LYS:HD3	1.99	0.44
22:32:2:VAL:HG13	33:R1:2015:A:C6	2.53	0.44
25:35:14:LYS:HB2	25:35:22:LYS:HE2	2.00	0.44
33:R1:2497:A:OP2	33:R1:2497:A:H8	2.00	0.44
35:R3:412:A:H2'	35:R3:414:A:H4'	1.98	0.44
35:R3:936:C:C2	35:R3:937:A:C8	3.06	0.44
2:13:13:ARG:HG2	2:13:51:GLY:O	2.17	0.44
7:18:81:ARG:O	7:18:84:GLU:HG2	2.17	0.44
8:19:81:ASP:N	8:19:81:ASP:OD1	2.51	0.44
29:6:88:LEU:HG	29:6:161:VAL:HG22	2.00	0.44
30:9:122:LEU:HG	30:9:128:HIS:CG	2.52	0.44
31:E:257:GLN:O	31:E:261:GLN:HG3	2.18	0.44
35:R3:457:G:H2'	35:R3:458:U:O4'	2.18	0.44
6:17:30:ARG:NH2	6:17:74:GLU:OE1	2.51	0.44
6:17:35:LYS:HB2	6:17:112:TYR:CE1	2.53	0.44
12:22:33:LEU:HD22	12:22:48:LYS:HE2	2.00	0.44
23:33:4:ILE:HD11	31:E:17:PRO:HG3	1.99	0.44
31:E:446:SER:HB3	58:E:601:ATP:H3'	1.99	0.44
33:R1:286:U:H2'	33:R1:287:G:C8	2.53	0.44
33:R1:1071:G:P	33:R1:1071:G:H8	2.40	0.44
33:R1:1504:A:H2'	33:R1:1505:A:H8	1.83	0.44
33:R1:1866:A:N6	33:R1:1875:G:O2'	2.51	0.44
35:R3:184:G:H2'	35:R3:185:U:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:R3:555:U:H2'	35:R3:556:C:H6	1.82	0.44
35:R3:825:A:H2'	35:R3:826:C:C6	2.53	0.44
35:R3:978:A:C4	35:R3:1319:A:C2	3.06	0.44
35:R3:1122:U:HO2'	35:R3:1123:U:P	2.39	0.44
35:R3:1272:G:H2'	35:R3:1273:C:C6	2.52	0.44
1:1:42:VAL:HG22	1:1:177:LYS:HA	2.00	0.44
9:2:110:LYS:N	9:2:113:ASP:OD2	2.38	0.44
15:25:47:VAL:O	15:25:51:GLN:N	2.46	0.44
33:R1:1197:G:H2'	33:R1:1198:U:H6	1.81	0.44
33:R1:1213:A:H61	33:R1:1236:G:H1'	1.83	0.44
33:R1:1636:U:H2'	33:R1:1637:A:H8	1.83	0.44
33:R1:2190:G:H2'	33:R1:2191:A:H8	1.83	0.44
27:4:168:ASP:OD1	27:4:169:VAL:N	2.51	0.44
29:6:42:VAL:HG22	29:6:51:PHE:CD2	2.52	0.44
30:9:80:ILE:HD13	30:9:80:ILE:HA	1.85	0.44
31:E:233:ASP:OD2	31:E:254:ARG:NH1	2.26	0.44
33:R1:159:G:H1'	33:R1:2208:C:O2'	2.18	0.44
33:R1:521:U:H2'	33:R1:522:A:H8	1.82	0.44
33:R1:590:A:N6	33:R1:667:U:H3	2.15	0.44
33:R1:720:U:H2'	33:R1:721:A:C8	2.53	0.44
33:R1:1433:A:H2'	33:R1:1434:A:H8	1.78	0.44
33:R1:1746:A:H2'	33:R1:1747:U:H6	1.83	0.44
33:R1:2138:G:C2	33:R1:2154:A:C2	3.06	0.44
34:R2:54:G:H2'	34:R2:55:U:C6	2.53	0.44
35:R3:451:A:H1'	35:R3:452:A:C2	2.53	0.44
35:R3:984:C:N3	35:R3:1222:G:N2	2.66	0.44
35:R3:1384:C:H2'	35:R3:1385:G:C8	2.53	0.44
4:15:64:PHE:HZ	25:35:14:LYS:HG2	1.83	0.43
7:18:7:ARG:NH1	7:18:95:SER:O	2.51	0.43
7:18:102:ARG:HG2	34:R2:49:C:OP1	2.18	0.43
9:2:29:PHE:CD2	9:2:31:PRO:HD2	2.53	0.43
15:25:21:ARG:HA	15:25:25:LYS:O	2.17	0.43
17:28:60:LYS:HD2	33:R1:372:G:C8	2.53	0.43
26:36:6:SER:O	26:36:6:SER:OG	2.31	0.43
27:4:193:VAL:HA	27:4:196:VAL:HG12	1.99	0.43
28:5:28:PRO:HB2	28:5:168:LEU:HD12	2.00	0.43
30:9:5:LEU:HD23	30:9:8:LYS:O	2.18	0.43
30:9:15:LEU:HD12	30:9:47:PHE:HZ	1.82	0.43
31:E:547:ARG:HD2	31:E:547:ARG:HA	1.72	0.43
33:R1:30:G:O2'	33:R1:1214:A:N3	2.43	0.43
33:R1:2126:A:N6	33:R1:2163:A:H5'	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:R1:2304:G:N2	33:R1:2312:U:H3	2.08	0.43
33:R1:2837:A:H2'	33:R1:2838:G:H8	1.83	0.43
35:R3:222:C:H2'	35:R3:223:A:H8	1.83	0.43
35:R3:672:U:HO2'	35:R3:673:A:P	2.41	0.43
36:T:50:U:H2'	36:T:51:C:C6	2.53	0.43
7:18:63:LYS:C	7:18:63:LYS:HD3	2.38	0.43
23:33:31:GLU:OE1	23:33:31:GLU:N	2.49	0.43
31:E:107:VAL:HG21	31:E:125:GLN:NE2	2.32	0.43
33:R1:191:A:H2'	33:R1:192:C:C6	2.53	0.43
33:R1:320:A:H4'	33:R1:322:A:N7	2.34	0.43
33:R1:750:A:OP1	33:R1:1615:C:N4	2.51	0.43
33:R1:1100:C:H2'	33:R1:1101:U:O4'	2.18	0.43
35:R3:413:G:N2	35:R3:428:G:H1'	2.33	0.43
35:R3:463:U:H2'	35:R3:464:U:C6	2.53	0.43
35:R3:743:A:H2'	35:R3:744:C:H6	1.82	0.43
35:R3:1288:A:H2'	35:R3:1289:A:C8	2.54	0.43
36:T:19:G:C2	36:T:57:A:H1'	2.53	0.43
36:T:60:U:H5"	36:T:61:C:H5	1.82	0.43
4:15:109:LYS:HG3	4:15:126:ARG:O	2.19	0.43
10:20:111:LYS:HD2	11:21:48:LYS:HZ2	1.82	0.43
29:6:172:GLU:HG3	29:6:174:LYS:H	1.83	0.43
33:R1:581:C:H2'	33:R1:582:A:C8	2.53	0.43
33:R1:2117:A:N6	33:R1:2170:A:H61	2.15	0.43
35:R3:254:G:H2'	35:R3:255:G:C8	2.53	0.43
35:R3:1150:A:O2'	35:R3:1151:A:O5'	2.27	0.43
35:R3:1319:A:C8	35:R3:1323:G:C5	3.06	0.43
27:4:198:GLU:CD	27:4:198:GLU:N	2.71	0.43
30:9:121:VAL:HG21	30:9:123:ARG:CZ	2.48	0.43
33:R1:624:C:O2'	33:R1:657:U:OP1	2.34	0.43
33:R1:2112:G:H2'	33:R1:2112:G:N3	2.33	0.43
35:R3:264:C:H2'	35:R3:265:G:O4'	2.18	0.43
35:R3:294:U:H2'	35:R3:295:C:C6	2.53	0.43
35:R3:1041:G:H2'	35:R3:1042:A:C8	2.53	0.43
35:R3:1137:C:H1'	35:R3:1138:G:C2	2.53	0.43
23:33:32:LYS:HA	23:33:50:GLU:OE2	2.19	0.43
33:R1:893:C:N4	33:R1:894:U:O2	2.51	0.43
33:R1:895:U:H4'	33:R1:896:A:H2	1.83	0.43
33:R1:1357:C:H2'	33:R1:1358:G:O4'	2.19	0.43
33:R1:1429:G:H2'	33:R1:1430:G:H8	1.83	0.43
33:R1:2149:U:O2'	33:R1:2150:C:O5'	2.32	0.43
35:R3:131:A:H2'	35:R3:132:C:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:3:51:THR:HB	19:3:79:LEU:HD23	1.99	0.43
31:E:273:LEU:O	31:E:277:ARG:HG2	2.18	0.43
33:R1:64:A:H2'	33:R1:65:U:H6	1.83	0.43
33:R1:1009:A:N3	33:R1:1153:C:O2'	2.50	0.43
35:R3:202:G:C2'	35:R3:466:A:H61	2.31	0.43
35:R3:909:A:N3	35:R3:1413:A:O2'	2.43	0.43
35:R3:1463:U:H2'	35:R3:1464:U:C6	2.53	0.43
1:1:215:SER:OG	1:1:216:THR:N	2.52	0.43
3:14:76:VAL:HG12	3:14:78:ARG:H	1.84	0.43
18:29:57:LEU:HD23	18:29:57:LEU:HA	1.82	0.43
27:4:48:THR:HG23	27:4:86:ALA:HB3	2.00	0.43
33:R1:412:A:H2'	33:R1:413:C:H5'	2.00	0.43
33:R1:980:A:N7	33:R1:1136:G:H5'	2.34	0.43
35:R3:35:G:H2'	35:R3:36:C:H6	1.82	0.43
35:R3:252:U:O4	35:R3:253:A:N6	2.51	0.43
35:R3:1071:C:H2'	35:R3:1072:G:C8	2.53	0.43
35:R3:1387:G:H2'	35:R3:1388:C:C6	2.54	0.43
35:R3:1476:A:H2'	35:R3:1477:U:C6	2.54	0.43
36:T:66:C:H2'	36:T:67:C:H6	1.82	0.43
2:13:49:ASP:OD1	2:13:49:ASP:N	2.43	0.43
7:18:4:LYS:O	7:18:8:ILE:HG12	2.19	0.43
33:R1:1278:C:H2'	33:R1:1279:G:C8	2.54	0.43
33:R1:1386:C:H2'	33:R1:1387:A:H8	1.82	0.43
33:R1:1510:G:H2'	33:R1:1511:G:C8	2.54	0.43
33:R1:2122:U:H2'	33:R1:2123:G:H4'	2.01	0.43
33:R1:2864:G:H2'	33:R1:2865:U:C6	2.53	0.43
35:R3:500:G:HO2'	35:R3:501:C:P	2.41	0.43
35:R3:632:U:H5"	35:R3:633:G:C8	2.54	0.43
35:R3:721:G:H4'	35:R3:722:G:O4'	2.19	0.43
35:R3:890:G:O2'	35:R3:906:A:N6	2.52	0.43
35:R3:1512:U:H2'	35:R3:1513:A:C8	2.52	0.43
1:1:7:ARG:O	1:1:11:ILE:HG23	2.18	0.43
2:13:2:LYS:HB3	33:R1:995:C:H42	1.83	0.43
5:16:57:VAL:HG12	5:16:112:LEU:HD21	2.01	0.43
11:21:57:GLY:N	11:21:103:ALA:OXT	2.37	0.43
20:30:5:LYS:NZ	20:30:36:GLU:OE2	2.51	0.43
29:6:140:ILE:HG13	29:6:141:GLY:N	2.34	0.43
33:R1:2322:A:H2'	33:R1:2323:G:C8	2.53	0.43
35:R3:204:G:H21	35:R3:205:A:N6	2.16	0.43
35:R3:407:U:H3	35:R3:435:A:H62	1.65	0.43
35:R3:908:A:H2'	35:R3:909:A:H8	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:R3:982:U:H4'	35:R3:983:A:O4'	2.18	0.43
1:1:6:LYS:HG2	33:R1:2132:U:O4	2.18	0.43
2:13:81:ILE:HD11	33:R1:2514:U:H5'	2.00	0.43
2:13:88:THR:HB	2:13:91:GLU:HG3	2.01	0.43
3:14:106:GLU:N	3:14:106:GLU:OE2	2.52	0.43
3:14:110:GLU:HG2	3:14:110:GLU:O	2.19	0.43
31:E:271:LYS:O	31:E:274:GLU:HG2	2.19	0.43
33:R1:1000:A:H2'	33:R1:1001:A:C8	2.54	0.43
33:R1:1434:A:H2'	33:R1:1435:G:H8	1.83	0.43
35:R3:415:A:C4	35:R3:416:G:C8	3.07	0.43
35:R3:572:A:H5'	35:R3:573:A:OP2	2.19	0.43
35:R3:821:G:H2'	35:R3:822:U:C6	2.54	0.43
35:R3:1259:C:O2'	35:R3:1283:U:O2	2.28	0.43
4:15:79:LEU:HD12	4:15:79:LEU:HA	1.80	0.42
6:17:90:ARG:NH1	33:R1:2880:C:O2'	2.51	0.42
7:18:24:THR:HG22	7:18:42:PRO:HD3	2.01	0.42
30:9:124:THR:HG22	30:9:125:THR:N	2.34	0.42
33:R1:817:C:H2'	33:R1:818:G:O4'	2.19	0.42
33:R1:1093:G:O2'	33:R1:1094:U:O5'	2.37	0.42
33:R1:1827:U:H2'	33:R1:1828:G:O4'	2.19	0.42
33:R1:2461:A:H2'	33:R1:2462:C:C6	2.54	0.42
33:R1:2467:C:H2'	33:R1:2468:A:O4'	2.19	0.42
35:R3:45:G:H2'	35:R3:46:G:H8	1.83	0.42
35:R3:160:A:H2'	35:R3:161:A:C8	2.54	0.42
35:R3:181:A:H61	35:R3:194:C:H2'	1.84	0.42
35:R3:482:A:H2'	35:R3:483:C:O4'	2.19	0.42
35:R3:500:G:H2'	35:R3:501:C:H6	1.82	0.42
35:R3:1323:G:H2'	35:R3:1324:A:H8	1.84	0.42
1:1:177:LYS:O	1:1:179:ASP:N	2.52	0.42
12:22:41:LYS:HD2	22:32:21:LEU:HD11	2.01	0.42
23:33:34:GLU:HA	23:33:48:TYR:O	2.20	0.42
29:6:14:VAL:HG13	29:6:26:LYS:O	2.18	0.42
30:9:116:ARG:HG2	30:9:116:ARG:HH11	1.84	0.42
33:R1:232:G:H8	33:R1:232:G:OP2	2.01	0.42
33:R1:354:A:H2'	33:R1:355:U:O4'	2.18	0.42
33:R1:356:G:H2'	33:R1:357:C:C6	2.54	0.42
33:R1:373:U:O2	33:R1:373:U:H2'	2.19	0.42
33:R1:1057:A:N7	33:R1:1086:A:H2'	2.34	0.42
33:R1:1291:C:C2	33:R1:1292:G:C8	3.07	0.42
33:R1:1713:A:H61	33:R1:1745:A:H61	1.68	0.42
33:R1:2086:U:H2'	33:R1:2087:G:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:R1:2103:C:H2'	33:R1:2104:C:O2	2.19	0.42
33:R1:2410:G:H2'	33:R1:2411:A:O4'	2.19	0.42
35:R3:766:A:OP2	35:R3:812:G:N2	2.52	0.42
2:13:122:LEU:HG	2:13:124:VAL:HG23	2.01	0.42
7:18:8:ILE:O	7:18:12:THR:OG1	2.34	0.42
9:2:70:LYS:O	9:2:117:SER:OG	2.37	0.42
27:4:73:ILE:HD12	27:4:78:TRP:CZ3	2.54	0.42
30:9:103:VAL:HG21	30:9:132:PHE:CZ	2.54	0.42
33:R1:958:U:H2'	34:R2:89:U:H1'	2.00	0.42
33:R1:1292:G:H2'	33:R1:1293:C:H6	1.84	0.42
33:R1:2216:G:H2'	33:R1:2217:G:H8	1.85	0.42
35:R3:745:G:H2'	35:R3:746:A:C8	2.54	0.42
35:R3:751:U:H2'	35:R3:752:G:O4'	2.19	0.42
35:R3:1402:C:H2'	35:R3:1403:C:O4'	2.19	0.42
2:13:125:TYR:HH	2:13:132:HIS:CD2	2.32	0.42
3:14:40:LYS:HD2	3:14:57:VAL:HG13	2.00	0.42
8:19:51:ASN:O	33:R1:2845:U:H5"	2.19	0.42
16:27:41:ARG:HG3	33:R1:2386:A:C2	2.54	0.42
28:5:152:ASP:OD1	28:5:153:ILE:N	2.53	0.42
31:E:25:ILE:HG23	31:E:27:LEU:HG	2.02	0.42
33:R1:500:G:H22	33:R1:503:A:H5'	1.85	0.42
33:R1:1172:C:O2'	33:R1:1174:U:O4'	2.34	0.42
33:R1:1183:U:H2'	33:R1:1184:U:H6	1.84	0.42
33:R1:2215:C:C2	33:R1:2216:G:C8	3.08	0.42
34:R2:32:U:H2'	34:R2:33:G:C8	2.54	0.42
11:21:6:GLN:HB2	11:21:11:GLN:HG2	2.01	0.42
21:31:16:CYS:SG	21:31:36:VAL:HA	2.59	0.42
25:35:3:ILE:HD11	33:R1:592:A:C2	2.54	0.42
26:36:30:GLU:OE2	26:36:31:PRO:HD2	2.18	0.42
29:6:18:ILE:HD13	29:6:18:ILE:HA	1.91	0.42
33:R1:75:G:H22	33:R1:111:A:H2	1.67	0.42
33:R1:149:A:H2'	33:R1:150:U:C6	2.54	0.42
33:R1:871:U:H2'	33:R1:872:U:H6	1.84	0.42
33:R1:1468:U:H2'	33:R1:1522:A:N6	2.34	0.42
33:R1:1604:C:O2'	33:R1:1610:A:N1	2.44	0.42
33:R1:1939:U:OP1	33:R1:2604:U:O2'	2.37	0.42
33:R1:2154:A:H2'	33:R1:2155:U:C5	2.54	0.42
33:R1:2515:C:H2'	33:R1:2516:A:H8	1.85	0.42
33:R1:2846:G:H2'	33:R1:2847:U:H6	1.84	0.42
35:R3:604:G:H2'	35:R3:605:U:O4'	2.20	0.42
35:R3:1266:G:N2	35:R3:1269:A:OP2	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:R3:1427:C:H2'	35:R3:1428:A:C8	2.54	0.42
4:15:62:PRO:HB2	25:35:29:ARG:HH21	1.85	0.42
8:19:13:LYS:O	8:19:13:LYS:HG2	2.20	0.42
9:2:123:ILE:HG23	9:2:191:LEU:HD11	2.00	0.42
27:4:73:ILE:HD12	27:4:73:ILE:HA	1.90	0.42
31:E:107:VAL:HG21	31:E:125:GLN:HE22	1.84	0.42
33:R1:2297:A:N1	33:R1:2321:U:H5	2.16	0.42
35:R3:191:G:C2	35:R3:192:A:C5	3.07	0.42
35:R3:312:C:HO2'	35:R3:313:A:P	2.42	0.42
8:19:55:HIS:HA	19:3:13:ARG:HH21	1.84	0.42
33:R1:215:G:H4'	33:R1:216:A:H4'	2.02	0.42
33:R1:1387:A:H5'	33:R1:1469:A:H1'	2.00	0.42
33:R1:1485:U:H2'	33:R1:1486:U:H6	1.85	0.42
33:R1:1527:G:N1	33:R1:1544:A:OP2	2.50	0.42
33:R1:1709:U:H2'	33:R1:1710:G:H8	1.85	0.42
34:R2:32:U:C2	34:R2:33:G:C8	3.08	0.42
35:R3:613:C:H2'	35:R3:614:C:C6	2.54	0.42
35:R3:1513:A:H2'	35:R3:1514:G:H8	1.84	0.42
1:1:174:THR:HG22	33:R1:2124:G:H5"	2.00	0.42
2:13:69:ARG:O	2:13:90:GLU:HG3	2.20	0.42
8:19:50:ARG:CZ	8:19:52:ARG:HG3	2.50	0.42
9:2:152:GLN:O	33:R1:1818:U:O2'	2.24	0.42
19:3:46:ARG:HG3	19:3:84:LEU:HB2	2.01	0.42
28:5:110:ILE:HD13	28:5:136:ILE:HG12	2.01	0.42
33:R1:364:C:H2'	33:R1:365:U:C6	2.55	0.42
33:R1:685:A:N1	33:R1:787:C:H1'	2.34	0.42
33:R1:1060:U:O4'	33:R1:1062:G:H5'	2.20	0.42
33:R1:2249:U:H3'	33:R1:2250:G:C5'	2.49	0.42
33:R1:2325:G:OP1	33:R1:2325:G:H3'	2.19	0.42
33:R1:2649:C:H2'	33:R1:2650:U:H6	1.83	0.42
34:R2:23:G:O2'	34:R2:24:G:O4'	2.37	0.42
35:R3:254:G:H2'	35:R3:255:G:H8	1.84	0.42
35:R3:321:A:H62	35:R3:332:G:H1	1.68	0.42
35:R3:407:U:H2'	35:R3:408:A:H8	1.85	0.42
5:16:44:ARG:HB3	33:R1:2484:G:OP1	2.20	0.42
12:22:13:SER:O	12:22:17:VAL:HG23	2.19	0.42
16:27:12:ASN:HA	16:27:14:ARG:NH1	2.30	0.42
28:5:102:LEU:HA	28:5:106:ALA:HB3	2.01	0.42
31:E:445:LEU:HD23	31:E:445:LEU:HA	1.79	0.42
33:R1:17:G:H2'	33:R1:18:U:C6	2.55	0.42
33:R1:412:A:H2'	33:R1:412:A:N3	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:R1:1177:G:H2'	33:R1:1178:C:C6	2.53	0.42
33:R1:2849:U:H4'	33:R1:2868:A:C2	2.54	0.42
35:R3:453:G:O2'	35:R3:454:G:OP1	2.35	0.42
35:R3:1481:U:H2'	35:R3:1482:G:H8	1.84	0.42
35:R3:1516:G:H2'	35:R3:1518:A:OP2	2.19	0.42
36:T:16:C:H4'	36:T:17:U:O4'	2.20	0.42
36:T:18:G:H4'	36:T:19:G:OP1	2.19	0.42
10:20:84:LYS:HE3	10:20:84:LYS:HB3	1.79	0.42
12:22:52:GLU:HG3	12:22:52:GLU:H	1.70	0.42
27:4:200:LEU:HA	27:4:200:LEU:HD12	1.91	0.42
31:E:21:ILE:O	31:E:22:LEU:HD23	2.20	0.42
33:R1:1583:A:O2'	33:R1:1584:U:OP2	2.34	0.42
33:R1:2128:G:H1	33:R1:2160:C:H42	1.68	0.42
34:R2:21:G:N2	34:R2:63:C:O2	2.53	0.42
34:R2:66:A:H61	34:R2:107:G:H3'	1.85	0.42
35:R3:402:G:O2'	35:R3:403:C:H6	2.02	0.42
35:R3:505:G:H2'	35:R3:506:G:H8	1.84	0.42
35:R3:1386:G:H2'	35:R3:1387:G:H8	1.85	0.42
4:15:141:LYS:HE3	4:15:141:LYS:HB3	1.95	0.41
12:22:89:ALA:HB2	33:R1:748:G:H5"	2.02	0.41
17:28:17:ARG:HG2	33:R1:380:G:H5"	2.02	0.41
19:3:72:GLY:O	19:3:73:VAL:HG23	2.20	0.41
31:E:326:VAL:HG12	31:E:380:ILE:HG23	2.01	0.41
33:R1:756:A:H2'	33:R1:757:G:O4'	2.19	0.41
33:R1:760:G:H2'	33:R1:761:A:O4'	2.19	0.41
33:R1:1167:C:H2'	33:R1:1168:G:C8	2.54	0.41
33:R1:2282:G:H4'	33:R1:2389:G:O2'	2.19	0.41
35:R3:301:G:O2'	35:R3:302:G:OP1	2.31	0.41
35:R3:769:G:H4'	35:R3:1513:A:H4'	2.01	0.41
35:R3:1005:A:O2'	35:R3:1006:G:O4'	2.34	0.41
16:27:25:ARG:HA	16:27:25:ARG:HD2	1.69	0.41
16:27:65:GLY:HA3	16:27:83:GLU:O	2.20	0.41
26:36:30:GLU:OE1	26:36:32:LYS:HB2	2.19	0.41
27:4:2:GLU:OE1	27:4:2:GLU:N	2.53	0.41
29:6:94:ARG:HG2	29:6:127:GLN:OE1	2.21	0.41
31:E:477:ILE:HG13	31:E:478:GLU:OE2	2.20	0.41
33:R1:35:G:H1'	33:R1:454:A:C4	2.55	0.41
33:R1:83:A:H61	33:R1:101:A:H2'	1.85	0.41
33:R1:581:C:H2'	33:R1:582:A:H8	1.85	0.41
33:R1:711:G:O6	33:R1:720:U:O2	2.38	0.41
33:R1:722:A:H2'	33:R1:723:C:H6	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:R1:744:U:H2'	33:R1:745:G:O4'	2.20	0.41
33:R1:1078:U:N3	33:R1:1089:A:OP1	2.52	0.41
33:R1:1923:U:H2'	33:R1:1924:C:C6	2.55	0.41
33:R1:2008:C:H2'	33:R1:2009:A:C8	2.54	0.41
33:R1:2697:G:H2'	33:R1:2698:U:O4'	2.20	0.41
33:R1:2804:U:H2'	33:R1:2805:C:H6	1.85	0.41
34:R2:30:C:H2'	34:R2:31:C:O4'	2.20	0.41
35:R3:299:G:H2'	35:R3:300:A:C8	2.55	0.41
35:R3:784:A:H2'	35:R3:785:G:C8	2.55	0.41
35:R3:1115:U:H2'	35:R3:1116:U:C6	2.55	0.41
35:R3:1316:G:N2	35:R3:1318:A:H3'	2.35	0.41
2:13:128:ASN:O	2:13:128:ASN:ND2	2.49	0.41
16:27:21:LEU:HD21	16:27:41:ARG:NH2	2.35	0.41
28:5:126:ASN:HD21	33:R1:2315:G:H4'	1.85	0.41
33:R1:755:U:H2'	33:R1:756:A:C8	2.55	0.41
33:R1:1168:G:H1	33:R1:1181:U:H3	1.67	0.41
33:R1:1664:A:N6	33:R1:1996:C:H42	2.15	0.41
33:R1:1858:A:N6	33:R1:1884:G:O2'	2.50	0.41
33:R1:1889:A:H2'	33:R1:1890:A:C8	2.55	0.41
33:R1:1916:A:H2'	33:R1:1917:U:O2	2.20	0.41
35:R3:216:U:H2'	35:R3:217:C:C6	2.56	0.41
4:15:30:THR:HG23	33:R1:810:U:O4	2.20	0.41
13:23:11:LEU:HD13	13:23:11:LEU:HA	1.88	0.41
24:34:16:HIS:HB2	24:34:44:VAL:HG21	2.01	0.41
25:35:44:ARG:NH2	33:R1:2349:G:OP1	2.53	0.41
26:36:19:ARG:NE	33:R1:2756:U:OP2	2.53	0.41
27:4:105:LEU:HD23	27:4:105:LEU:HA	1.92	0.41
28:5:120:SER:O	28:5:120:SER:OG	2.36	0.41
31:E:190:THR:HB	31:E:198:VAL:HG22	2.02	0.41
31:E:548:ILE:HD13	33:R1:2112:G:O2'	2.20	0.41
33:R1:729:G:O2'	33:R1:763:G:H4'	2.19	0.41
33:R1:1179:G:C5'	33:R1:1180:U:H5"	2.51	0.41
33:R1:2148:G:N1	33:R1:2149:U:O4	2.53	0.41
35:R3:60:A:N7	35:R3:108:G:O2'	2.49	0.41
35:R3:394:G:N3	35:R3:394:G:H2'	2.36	0.41
35:R3:821:G:H2'	35:R3:822:U:H6	1.86	0.41
35:R3:936:C:C4	35:R3:937:A:N7	2.88	0.41
2:13:2:LYS:HB3	33:R1:995:C:N4	2.35	0.41
5:16:5:LYS:O	33:R1:870:U:H5'	2.19	0.41
5:16:13:HIS:CG	33:R1:954:G:H5'	2.55	0.41
9:2:203:VAL:HG12	33:R1:1792:G:H5"	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:36:18:LYS:HD2	26:36:23:ILE:HG13	2.03	0.41
27:4:148:ILE:HD13	27:4:187:VAL:CG2	2.51	0.41
31:E:67:PRO:CD	31:E:68:ASP:N	2.81	0.41
31:E:74:LEU:HA	31:E:75:PRO:HD3	1.92	0.41
31:E:125:GLN:O	31:E:129:GLU:HG3	2.20	0.41
31:E:306:ASN:HB3	31:E:307:GLU:H	1.59	0.41
33:R1:1036:G:C6	33:R1:1120:G:C6	3.09	0.41
33:R1:2745:C:H2'	33:R1:2746:U:C6	2.55	0.41
35:R3:131:A:N1	35:R3:231:U:H5	2.19	0.41
35:R3:301:G:HO2'	35:R3:302:G:P	2.43	0.41
35:R3:1002:G:N7	35:R3:1003:G:N2	2.69	0.41
36:T:19:G:H4'	36:T:20:H2U:OP2	2.21	0.41
4:15:21:ARG:NH1	33:R1:587:C:OP2	2.49	0.41
6:17:100:CYS:SG	6:17:101:GLY:N	2.94	0.41
28:5:14:LYS:HE2	28:5:14:LYS:HB2	1.75	0.41
30:9:67:ALA:O	30:9:70:GLU:HG3	2.21	0.41
33:R1:947:A:HO2'	33:R1:984:A:H2	1.67	0.41
33:R1:979:A:H5'	33:R1:980:A:H5"	2.01	0.41
33:R1:1682:G:H2'	33:R1:1683:U:H6	1.83	0.41
33:R1:2142:A:H61	33:R1:2150:C:N4	2.19	0.41
33:R1:2290:G:H2'	33:R1:2291:U:C6	2.56	0.41
35:R3:53:A:N6	35:R3:359:G:O6	2.53	0.41
6:17:8:ARG:HH11	6:17:43:GLU:HG2	1.85	0.41
12:22:76:VAL:HG12	12:22:103:ILE:HG23	2.03	0.41
22:32:42:ILE:HG22	22:32:48:TYR:HB2	2.01	0.41
28:5:65:LEU:HB2	34:R2:42:C:C6	2.56	0.41
31:E:321:ASP:OD1	31:E:321:ASP:N	2.54	0.41
33:R1:68:G:H2'	33:R1:69:C:O4'	2.21	0.41
33:R1:227:A:C2	33:R1:2407:A:H1'	2.56	0.41
33:R1:286:U:H2'	33:R1:287:G:H8	1.86	0.41
33:R1:713:G:H2'	33:R1:714:U:O4'	2.21	0.41
33:R1:1541:C:H2'	33:R1:1542:U:C6	2.56	0.41
33:R1:1704:C:H2'	33:R1:1705:A:H8	1.83	0.41
33:R1:2142:A:N6	33:R1:2150:C:H42	2.19	0.41
33:R1:2291:U:OP1	33:R1:2380:C:O2'	2.39	0.41
35:R3:695:A:H2'	35:R3:696:A:C8	2.55	0.41
35:R3:1311:A:H2'	35:R3:1312:G:O4'	2.20	0.41
35:R3:1376:U:H2'	35:R3:1377:A:C8	2.55	0.41
1:1:67:HIS:NE2	1:1:187:GLU:OE2	2.53	0.41
2:13:13:ARG:NH2	2:13:49:ASP:O	2.49	0.41
2:13:32:LEU:HD22	2:13:54:ILE:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:R1:7:G:H2'	33:R1:8:C:O4'	2.20	0.41
33:R1:79:C:N4	33:R1:107:G:H1	2.18	0.41
33:R1:396:G:C6	33:R1:397:U:C4	3.09	0.41
33:R1:547:A:H3'	33:R1:547:A:N3	2.36	0.41
33:R1:716:A:H2'	33:R1:717:C:O4'	2.20	0.41
33:R1:974:G:H1'	33:R1:975:A:C8	2.55	0.41
33:R1:1341:G:OP2	33:R1:1341:G:H8	2.03	0.41
33:R1:1463:C:H2'	33:R1:1464:G:H8	1.84	0.41
33:R1:1715:G:O2'	33:R1:1716:U:H6	2.03	0.41
33:R1:2108:A:N3	33:R1:2109:U:H1'	2.35	0.41
33:R1:2567:G:H2'	33:R1:2568:U:C6	2.56	0.41
34:R2:104:A:H2'	34:R2:105:G:O4'	2.21	0.41
34:R2:106:G:H2'	34:R2:107:G:O4'	2.21	0.41
35:R3:185:U:H2'	35:R3:186:C:C6	2.55	0.41
35:R3:497:G:H2'	35:R3:498:A:C8	2.56	0.41
3:14:43:ILE:HD12	3:14:56:ASP:HB2	2.03	0.41
4:15:30:THR:HG23	33:R1:810:U:H3	1.85	0.41
20:30:15:ARG:HD3	20:30:15:ARG:HA	1.69	0.41
25:35:15:LYS:HE3	25:35:19:GLY:HA2	2.03	0.41
29:6:86:LEU:HD13	29:6:132:LEU:HD21	2.02	0.41
31:E:41:ASN:ND2	31:E:476:ASP:OD1	2.44	0.41
31:E:269:ILE:HD13	31:E:269:ILE:HA	1.87	0.41
31:E:382:LEU:HD23	31:E:382:LEU:HA	1.89	0.41
33:R1:95:A:H2'	33:R1:96:C:O4'	2.21	0.41
33:R1:197:A:N6	33:R1:2430:A:O2'	2.53	0.41
33:R1:574:A:N6	33:R1:2034:U:OP1	2.54	0.41
33:R1:1869:G:N2	33:R1:1872:A:H2'	2.29	0.41
33:R1:2038:G:H2'	33:R1:2039:U:O4'	2.21	0.41
33:R1:2153:C:H2'	33:R1:2154:A:C8	2.56	0.41
33:R1:2291:U:H5'	33:R1:2380:C:H1'	2.02	0.41
33:R1:2636:C:H2'	33:R1:2637:U:C6	2.56	0.41
35:R3:324:G:H22	35:R3:327:A:H5'	1.85	0.41
35:R3:607:A:H2'	35:R3:608:A:C8	2.56	0.41
35:R3:1036:A:C8	35:R3:1037:C:N4	2.89	0.41
35:R3:1219:A:H2'	35:R3:1220:G:H8	1.85	0.41
35:R3:1451:U:H5'	35:R3:1452:C:C6	2.56	0.41
1:1:58:ASN:HA	1:1:165:ASN:HD22	1.86	0.41
13:23:18:GLU:HG3	33:R1:1392:A:N6	2.34	0.41
13:23:64:LYS:NZ	33:R1:1601:G:OP1	2.53	0.41
27:4:165:HIS:CE1	33:R1:1205:A:C5	3.09	0.41
28:5:3:LEU:HD23	28:5:3:LEU:HA	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:9:66:ASN:HD22	30:9:66:ASN:HA	1.78	0.41
30:9:66:ASN:OD1	30:9:135:HIS:ND1	2.54	0.41
31:E:143:GLN:HG3	31:E:144:LEU:N	2.36	0.41
31:E:166:GLY:HA3	31:E:358:ASN:ND2	2.36	0.41
33:R1:880:G:N2	33:R1:898:C:C4	2.89	0.41
33:R1:1263:U:H2'	33:R1:1264:A:C8	2.56	0.41
33:R1:1499:C:C2	33:R1:1500:G:C8	3.09	0.41
33:R1:1873:G:H2'	33:R1:1874:C:H6	1.85	0.41
33:R1:1889:A:H2'	33:R1:1890:A:H8	1.84	0.41
33:R1:2215:C:H2'	33:R1:2216:G:C8	2.56	0.41
35:R3:191:G:H2'	35:R3:192:A:H8	1.86	0.41
7:18:95:SER:O	7:18:95:SER:OG	2.35	0.40
14:24:38:ILE:HD13	14:24:38:ILE:HA	1.92	0.40
18:29:38:GLN:OE1	18:29:38:GLN:N	2.31	0.40
20:30:11:SER:CB	33:R1:988:A:H5"	2.51	0.40
28:5:36:ASN:ND2	33:R1:2313:C:O4'	2.54	0.40
31:E:51:ILE:HG13	31:E:56:ASP:HB3	2.03	0.40
31:E:67:PRO:CD	31:E:68:ASP:H	2.33	0.40
33:R1:134:G:H2'	33:R1:135:U:H6	1.86	0.40
33:R1:268:C:H2'	33:R1:269:C:H6	1.86	0.40
33:R1:668:A:H2'	33:R1:670:A:H62	1.87	0.40
33:R1:1689:A:H2'	33:R1:1690:A:C8	2.56	0.40
33:R1:1858:A:H2'	33:R1:1859:U:O4'	2.21	0.40
33:R1:2723:C:H2'	33:R1:2724:U:O4'	2.20	0.40
35:R3:115:G:O4'	35:R3:115:G:P	2.79	0.40
5:16:22:GLN:NE2	33:R1:864:G:OP2	2.54	0.40
5:16:42:THR:HA	5:16:93:VAL:HA	2.04	0.40
9:2:104:LEU:HD23	9:2:104:LEU:HA	1.95	0.40
9:2:140:VAL:CG1	9:2:189:ALA:HB1	2.52	0.40
10:20:23:TYR:HB3	10:20:27:ARG:HB3	2.02	0.40
11:21:61:ALA:HB1	11:21:96:VAL:HB	2.03	0.40
16:27:20:ARG:HD2	33:R1:2356:U:O3'	2.20	0.40
17:28:25:LYS:HA	17:28:25:LYS:HD2	1.72	0.40
17:28:76:LYS:HD2	17:28:76:LYS:HA	1.86	0.40
21:31:5:ILE:HD11	28:5:63:LYS:HD3	2.03	0.40
22:32:52:LYS:HD2	22:32:52:LYS:HA	1.95	0.40
24:34:24:THR:HG23	24:34:27:GLY:H	1.86	0.40
26:36:36:ARG:HG2	26:36:37:GLN:H	1.86	0.40
30:9:3:VAL:HG22	30:9:36:ALA:HB1	2.03	0.40
30:9:99:ILE:HD11	30:9:122:LEU:HD22	2.04	0.40
31:E:285:SER:O	31:E:286:LYS:HB3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:R1:29:U:H2'	33:R1:30:G:H8	1.86	0.40
33:R1:77:G:H2'	33:R1:78:U:C6	2.56	0.40
33:R1:594:U:H2'	33:R1:595:C:H6	1.85	0.40
33:R1:1102:C:H2'	33:R1:1103:A:C8	2.57	0.40
33:R1:1196:C:C2	33:R1:1197:G:C8	3.09	0.40
33:R1:2116:G:H1	33:R1:2164:C:H42	1.68	0.40
34:R2:45:A:C4	34:R2:46:A:C8	3.08	0.40
4:15:103:ILE:HD12	4:15:103:ILE:HA	1.97	0.40
11:21:24:LYS:HB3	11:21:24:LYS:HE3	1.84	0.40
19:3:151:THR:HG23	33:R1:2032:G:H21	1.85	0.40
30:9:41:LYS:HA	30:9:41:LYS:HD2	1.83	0.40
31:E:309:ASN:OD1	31:E:309:ASN:N	2.55	0.40
33:R1:84:A:N1	33:R1:98:G:O2'	2.44	0.40
33:R1:281:C:H41	33:R1:359:G:H1	1.70	0.40
33:R1:566:U:H2'	33:R1:567:U:C6	2.57	0.40
33:R1:742:A:H2'	33:R1:743:A:H8	1.86	0.40
33:R1:878:A:H2'	33:R1:879:G:O4'	2.20	0.40
35:R3:1238:A:H2	35:R3:1241:G:N3	2.18	0.40
1:1:11:ILE:HA	1:1:14:LYS:HB3	2.03	0.40
2:13:2:LYS:HD2	33:R1:995:C:N4	2.36	0.40
5:16:50:ARG:HD3	5:16:65:ILE:HD11	2.02	0.40
9:2:172:THR:HA	9:2:181:ARG:O	2.22	0.40
27:4:149:ILE:HG22	27:4:192:ALA:HB1	2.03	0.40
33:R1:439:A:H2'	33:R1:440:C:O4'	2.22	0.40
33:R1:863:A:H2'	33:R1:864:G:H8	1.86	0.40
33:R1:1415:U:O2	33:R1:1587:G:O6	2.39	0.40
33:R1:1528:A:OP2	33:R1:1543:G:N2	2.53	0.40
33:R1:1585:C:H2'	33:R1:1586:A:O4'	2.20	0.40
33:R1:1712:U:OP2	33:R1:1713:A:O2'	2.32	0.40
33:R1:2130:U:H2'	33:R1:2131:U:H6	1.86	0.40
34:R2:13:G:O2'	34:R2:15:A:OP2	2.35	0.40
34:R2:13:G:H8	34:R2:69:G:H21	1.69	0.40
35:R3:383:A:C5	35:R3:384:G:H1'	2.55	0.40
36:T:32:4OC:O5'	36:T:32:4OC:H6	2.22	0.40
2:13:136:GLN:HE21	33:R1:2899:A:H5'	1.85	0.40
4:15:92:LEU:HD11	4:15:106:GLU:O	2.21	0.40
11:21:74:ILE:HB	11:21:87:GLN:HB3	2.04	0.40
20:30:11:SER:OG	20:30:12:ALA:N	2.54	0.40
28:5:132:ARG:HG3	33:R1:2305:U:O2'	2.21	0.40
31:E:515:GLN:HB2	31:E:519:LYS:HB3	2.02	0.40
33:R1:689:A:H2'	33:R1:690:G:O4'	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:R1:1069:A:H5'	33:R1:1070:A:OP1	2.21	0.40
33:R1:2229:U:H2'	33:R1:2230:G:H8	1.86	0.40
33:R1:2416:C:C2	33:R1:2417:C:C5	3.10	0.40
33:R1:2625:G:H2'	33:R1:2626:C:C6	2.56	0.40
34:R2:6:G:H2'	34:R2:7:G:H8	1.86	0.40
35:R3:376:G:H4'	35:R3:376:G:OP1	2.21	0.40
35:R3:635:A:H2'	35:R3:636:U:C6	2.56	0.40
35:R3:1256:A:H4'	35:R3:1257:A:H5'	2.04	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%)	196 (90%)	22 (10%)	0	100	100
2	13	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
3	14	120/122 (98%)	108 (90%)	12 (10%)	0	100	100
4	15	141/143 (99%)	130 (92%)	11 (8%)	0	100	100
5	16	134/136 (98%)	127 (95%)	7 (5%)	0	100	100
6	17	118/120 (98%)	109 (92%)	9 (8%)	0	100	100
7	18	114/116 (98%)	110 (96%)	4 (4%)	0	100	100
8	19	112/114 (98%)	101 (90%)	11 (10%)	0	100	100
9	2	269/271 (99%)	253 (94%)	16 (6%)	0	100	100
10	20	115/117 (98%)	115 (100%)	0	0	100	100
11	21	101/103 (98%)	88 (87%)	13 (13%)	0	100	100
12	22	108/110 (98%)	100 (93%)	8 (7%)	0	100	100
13	23	91/93 (98%)	82 (90%)	9 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	24	100/102 (98%)	87 (87%)	13 (13%)	0	100	100
15	25	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
16	27	74/76 (97%)	69 (93%)	5 (7%)	0	100	100
17	28	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
18	29	61/63 (97%)	60 (98%)	1 (2%)	0	100	100
19	3	207/209 (99%)	195 (94%)	12 (6%)	0	100	100
20	30	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
21	31	64/66 (97%)	55 (86%)	9 (14%)	0	100	100
22	32	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
23	33	48/50 (96%)	48 (100%)	0	0	100	100
24	34	44/46 (96%)	40 (91%)	4 (9%)	0	100	100
25	35	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
26	36	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
27	4	199/201 (99%)	188 (94%)	11 (6%)	0	100	100
28	5	175/177 (99%)	161 (92%)	14 (8%)	0	100	100
29	6	174/176 (99%)	159 (91%)	15 (9%)	0	100	100
30	9	147/149 (99%)	135 (92%)	10 (7%)	2 (1%)	9	40
31	E	550/552 (100%)	508 (92%)	41 (8%)	1 (0%)	44	75
37	sb	216/218 (99%)	194 (90%)	21 (10%)	1 (0%)	25	60
38	sc	204/206 (99%)	197 (97%)	7 (3%)	0	100	100
39	sd	203/205 (99%)	185 (91%)	18 (9%)	0	100	100
40	se	155/157 (99%)	135 (87%)	18 (12%)	2 (1%)	10	41
41	sf	98/100 (98%)	83 (85%)	14 (14%)	1 (1%)	13	47
42	sg	149/151 (99%)	142 (95%)	7 (5%)	0	100	100
43	sh	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
44	si	125/127 (98%)	102 (82%)	22 (18%)	1 (1%)	16	51
45	sj	96/98 (98%)	88 (92%)	7 (7%)	1 (1%)	13	47
46	sk	114/116 (98%)	103 (90%)	11 (10%)	0	100	100
47	sl	121/123 (98%)	92 (76%)	29 (24%)	0	100	100
48	sm	112/114 (98%)	99 (88%)	13 (12%)	0	100	100
49	sn	98/100 (98%)	78 (80%)	20 (20%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
50	so	86/88 (98%)	83 (96%)	3 (4%)	0	100 100
51	sp	80/82 (98%)	71 (89%)	9 (11%)	0	100 100
52	sq	78/80 (98%)	67 (86%)	11 (14%)	0	100 100
53	sr	63/65 (97%)	61 (97%)	2 (3%)	0	100 100
54	ss	77/79 (98%)	71 (92%)	6 (8%)	0	100 100
55	st	83/85 (98%)	82 (99%)	1 (1%)	0	100 100
56	su	68/70 (97%)	64 (94%)	3 (4%)	1 (2%)	8 38
All	All	6352/6454 (98%)	5840 (92%)	502 (8%)	10 (0%)	45 75

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
31	E	17	PRO
30	9	8	LYS
44	si	91	GLU
37	sb	18	GLN
40	se	122	VAL
56	su	10	GLU
40	se	121	ASN
41	sf	92	THR
30	9	9	VAL
45	sj	57	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	1	106/171 (62%)	103 (97%)	3 (3%)	38 68
2	13	116/116 (100%)	115 (99%)	1 (1%)	75 89
3	14	103/103 (100%)	99 (96%)	4 (4%)	27 60
4	15	102/102 (100%)	101 (99%)	1 (1%)	73 87
5	16	109/109 (100%)	106 (97%)	3 (3%)	38 68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	17	100/100 (100%)	96 (96%)	4 (4%)	27 59
7	18	86/86 (100%)	83 (96%)	3 (4%)	31 63
8	19	99/99 (100%)	98 (99%)	1 (1%)	73 87
9	2	216/216 (100%)	210 (97%)	6 (3%)	38 68
10	20	89/89 (100%)	87 (98%)	2 (2%)	47 73
11	21	84/84 (100%)	82 (98%)	2 (2%)	44 71
12	22	93/93 (100%)	90 (97%)	3 (3%)	34 65
13	23	80/80 (100%)	79 (99%)	1 (1%)	65 83
14	24	83/83 (100%)	80 (96%)	3 (4%)	30 62
15	25	78/78 (100%)	73 (94%)	5 (6%)	14 46
16	27	58/58 (100%)	56 (97%)	2 (3%)	32 63
17	28	67/67 (100%)	66 (98%)	1 (2%)	60 81
18	29	55/55 (100%)	53 (96%)	2 (4%)	30 62
19	3	164/164 (100%)	157 (96%)	7 (4%)	25 57
20	30	48/48 (100%)	46 (96%)	2 (4%)	25 58
21	31	59/59 (100%)	56 (95%)	3 (5%)	20 53
22	32	47/47 (100%)	47 (100%)	0	100 100
23	33	45/45 (100%)	44 (98%)	1 (2%)	47 73
24	34	38/38 (100%)	38 (100%)	0	100 100
25	35	51/51 (100%)	49 (96%)	2 (4%)	27 60
26	36	34/34 (100%)	33 (97%)	1 (3%)	37 67
27	4	165/165 (100%)	164 (99%)	1 (1%)	84 92
28	5	148/148 (100%)	144 (97%)	4 (3%)	40 69
29	6	137/137 (100%)	130 (95%)	7 (5%)	20 53
30	9	114/114 (100%)	110 (96%)	4 (4%)	31 63
31	E	461/464 (99%)	441 (96%)	20 (4%)	25 57
37	sb	180/180 (100%)	173 (96%)	7 (4%)	27 60
38	sc	170/170 (100%)	164 (96%)	6 (4%)	31 63
39	sd	172/172 (100%)	167 (97%)	5 (3%)	37 67
40	se	119/119 (100%)	118 (99%)	1 (1%)	79 90
41	sf	87/87 (100%)	82 (94%)	5 (6%)	17 50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
42	sg	124/124 (100%)	123 (99%)	1 (1%)	79 90
43	sh	104/104 (100%)	103 (99%)	1 (1%)	73 87
44	si	105/105 (100%)	100 (95%)	5 (5%)	21 55
45	sj	86/86 (100%)	80 (93%)	6 (7%)	12 42
46	sk	89/89 (100%)	86 (97%)	3 (3%)	32 63
47	sl	103/103 (100%)	98 (95%)	5 (5%)	21 54
48	sm	92/92 (100%)	89 (97%)	3 (3%)	33 64
49	sn	83/83 (100%)	80 (96%)	3 (4%)	30 62
50	so	76/76 (100%)	75 (99%)	1 (1%)	65 83
51	sp	65/65 (100%)	60 (92%)	5 (8%)	10 39
52	sq	74/74 (100%)	72 (97%)	2 (3%)	40 69
53	sr	56/56 (100%)	54 (96%)	2 (4%)	30 62
54	ss	70/70 (100%)	69 (99%)	1 (1%)	62 82
55	st	65/65 (100%)	64 (98%)	1 (2%)	60 81
56	su	60/60 (100%)	56 (93%)	4 (7%)	13 44
All	All	5215/5283 (99%)	5049 (97%)	166 (3%)	36 65

All (166) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	7	ARG
1	1	53	ARG
1	1	60	ARG
2	13	128	ASN
3	14	53	LYS
3	14	58	LEU
3	14	82	ASN
3	14	89	ASN
4	15	141	LYS
5	16	59	ARG
5	16	105	MET
5	16	136	MET
6	17	2	ARG
6	17	6	SER
6	17	16	HIS
6	17	73	ASN
7	18	48	LEU

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Mol	Chain	Res	Type
7	18	55	GLU
7	18	93	ASP
8	19	113	LEU
9	2	38	LYS
9	2	97	ASP
9	2	212	TRP
9	2	258	SER
9	2	260	LYS
9	2	269	ARG
10	20	96	ASP
10	20	101	ASP
11	21	48	LYS
11	21	95	ASP
12	22	1	MET
12	22	13	SER
12	22	92	ARG
13	23	79	ASP
14	24	7	ASP
14	24	36	GLU
14	24	52	ASN
15	25	5	ASN
15	25	12	GLN
15	25	42	LEU
15	25	76	ASP
15	25	90	ASP
16	27	56	ASP
16	27	64	ASP
17	28	19	HIS
18	29	9	LYS
18	29	59	GLU
19	3	4	LEU
19	3	103	ASP
19	3	105	LYS
19	3	113	SER
19	3	137	SER
19	3	179	ARG
19	3	185	ASN
20	30	10	ARG
20	30	15	ARG
21	31	9	TYR
21	31	34	LEU
21	31	43	PHE

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Mol	Chain	Res	Type
23	33	50	GLU
25	35	30	HIS
25	35	51	LYS
26	36	13	ASN
27	4	79	ARG
28	5	99	PHE
28	5	114	ARG
28	5	173	ASP
28	5	174	PHE
29	6	21	GLN
29	6	28	LYS
29	6	68	ARG
29	6	73	SER
29	6	132	LEU
29	6	133	LYS
29	6	146	ASP
30	9	70	GLU
30	9	87	GLU
30	9	112	LYS
30	9	113	SER
31	E	10	ARG
31	E	34	LYS
31	E	105	ASP
31	E	111	TYR
31	E	136	ASP
31	E	143	GLN
31	E	151	LEU
31	E	223	ASP
31	E	228	TRP
31	E	232	LEU
31	E	248	LEU
31	E	305	ARG
31	E	335	ASP
31	E	340	ASP
31	E	395	ARG
31	E	506	ARG
31	E	519	LYS
31	E	521	GLU
31	E	550	TYR
31	E	551	LYS
37	sb	15	PHE
37	sb	22	TRP

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Mol	Chain	Res	Type
37	sb	36	LYS
37	sb	41	ASN
37	sb	80	LYS
37	sb	117	GLU
37	sb	135	MET
38	sc	33	ASP
38	sc	44	LYS
38	sc	61	LYS
38	sc	130	ARG
38	sc	133	MET
38	sc	153	SER
39	sd	13	ARG
39	sd	30	LYS
39	sd	120	LYS
39	sd	193	ASP
39	sd	202	LEU
40	se	63	MET
41	sf	13	ASP
41	sf	72	ASP
41	sf	81	ASN
41	sf	87	SER
41	sf	94	HIS
42	sg	57	SER
43	sh	112	ASP
44	si	13	SER
44	si	32	ARG
44	si	38	PHE
44	si	106	ASP
44	si	114	LYS
45	sj	16	ARG
45	sj	45	ARG
45	sj	48	ARG
45	sj	56	HIS
45	sj	58	ASN
45	sj	81	GLU
46	sk	12	ARG
46	sk	17	ASP
46	sk	54	SER
47	sl	33	CYS
47	sl	46	SER
47	sl	103	CYS
47	sl	104	SER

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Mol	Chain	Res	Type
47	sl	110	LYS
48	sm	26	LYS
48	sm	28	ARG
48	sm	67	ASP
49	sn	20	PHE
49	sn	23	ARG
49	sn	60	ARG
50	so	61	GLN
51	sp	23	ASP
51	sp	24	SER
51	sp	25	ARG
51	sp	29	ASN
51	sp	69	ASP
52	sq	50	ASN
52	sq	56	ASP
53	sr	12	PHE
53	sr	34	GLU
54	ss	65	MET
55	st	63	LYS
56	su	7	ARG
56	su	13	ASP
56	su	34	ARG
56	su	64	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	57	GLN
1	1	58	ASN
1	1	165	ASN
1	1	188	ASN
15	25	80	HIS
21	31	20	ASN
37	sb	18	GLN
37	sb	41	ASN
40	se	81	GLN
46	sk	108	ASN
47	sl	58	ASN
50	so	19	ASN
50	so	34	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
32	M	8/9 (88%)	0	0
33	R1	2902/2903 (99%)	570 (19%)	20 (0%)
34	R2	118/119 (99%)	19 (16%)	0
35	R3	1529/1531 (99%)	399 (26%)	23 (1%)
36	T	74/77 (96%)	19 (25%)	3 (4%)
All	All	4631/4639 (99%)	1007 (21%)	46 (0%)

All (1007) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
33	R1	2	G
33	R1	5	A
33	R1	10	A
33	R1	15	G
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	63	A
33	R1	71	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
33	R1	84	A
33	R1	85	G
33	R1	88	G
33	R1	96	C
33	R1	102	U
33	R1	118	A
33	R1	119	A
33	R1	120	U
33	R1	134	G
33	R1	136	G
33	R1	138	U
33	R1	139	U
33	R1	140	C

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Mol	Chain	Res	Type
33	R1	144	A
33	R1	148	U
33	R1	154	U
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	165	A
33	R1	172	A
33	R1	181	A
33	R1	196	A
33	R1	199	A
33	R1	200	U
33	R1	213	A
33	R1	216	A
33	R1	218	A
33	R1	221	A
33	R1	222	A
33	R1	225	C
33	R1	226	A
33	R1	230	G
33	R1	248	G
33	R1	249	C
33	R1	255	A
33	R1	256	A
33	R1	265	A
33	R1	266	G
33	R1	272	A
33	R1	274	C
33	R1	276	U
33	R1	277	G
33	R1	282	A
33	R1	285	G
33	R1	291	G
33	R1	311	A
33	R1	329	G
33	R1	330	A
33	R1	352	A
33	R1	354	A
33	R1	361	G

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Mol	Chain	Res	Type
33	R1	369	U
33	R1	371	A
33	R1	372	G
33	R1	373	U
33	R1	386	G
33	R1	387	U
33	R1	388	G
33	R1	389	G
33	R1	395	U
33	R1	396	G
33	R1	401	A
33	R1	404	A
33	R1	405	U
33	R1	406	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	429	A
33	R1	435	C
33	R1	443	A
33	R1	454	A
33	R1	457	A
33	R1	478	A
33	R1	481	G
33	R1	489	G
33	R1	491	G
33	R1	493	G
33	R1	503	A
33	R1	505	A
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	545	U

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Mol	Chain	Res	Type
33	R1	546	U
33	R1	547	A
33	R1	548	G
33	R1	549	G
33	R1	555	G
33	R1	563	A
33	R1	573	U
33	R1	575	A
33	R1	581	C
33	R1	591	U
33	R1	603	A
33	R1	613	A
33	R1	614	A
33	R1	615	U
33	R1	616	A
33	R1	622	G
33	R1	627	A
33	R1	637	A
33	R1	645	C
33	R1	647	G
33	R1	654	A
33	R1	655	A
33	R1	685	A
33	R1	686	U
33	R1	689	A
33	R1	696	G
33	R1	705	A
33	R1	711	G
33	R1	712	G
33	R1	715	A
33	R1	717	C
33	R1	730	A
33	R1	738	G
33	R1	740	C
33	R1	747	U
33	R1	748	G
33	R1	764	A
33	R1	765	C
33	R1	775	G
33	R1	776	G
33	R1	782	A
33	R1	784	G

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Mol	Chain	Res	Type
33	R1	785	G
33	R1	805	G
33	R1	811	U
33	R1	812	C
33	R1	819	A
33	R1	827	U
33	R1	829	A
33	R1	845	A
33	R1	846	U
33	R1	847	U
33	R1	860	U
33	R1	869	G
33	R1	870	U
33	R1	872	U
33	R1	876	C
33	R1	878	A
33	R1	886	A
33	R1	887	U
33	R1	888	C
33	R1	891	G
33	R1	892	A
33	R1	893	C
33	R1	894	U
33	R1	896	A
33	R1	897	C
33	R1	904	G
33	R1	907	G
33	R1	910	A
33	R1	919	U
33	R1	927	A
33	R1	932	U
33	R1	941	A
33	R1	945	A
33	R1	946	C
33	R1	953	G
33	R1	954	G
33	R1	961	C
33	R1	971	G
33	R1	973	A
33	R1	974	G
33	R1	979	A
33	R1	983	A

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Mol	Chain	Res	Type
33	R1	989	G
33	R1	990	A
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	1047	G
33	R1	1050	A
33	R1	1051	G
33	R1	1052	C
33	R1	1056	G
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	1069	A
33	R1	1070	A
33	R1	1071	G
33	R1	1072	C
33	R1	1073	A
33	R1	1075	C
33	R1	1076	C
33	R1	1079	C
33	R1	1084	A
33	R1	1085	A
33	R1	1087	G
33	R1	1088	A
33	R1	1089	A
33	R1	1090	A
33	R1	1093	G
33	R1	1094	U

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Mol	Chain	Res	Type
33	R1	1095	A
33	R1	1096	A
33	R1	1097	U
33	R1	1098	A
33	R1	1099	G
33	R1	1101	U
33	R1	1102	C
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	1115	G
33	R1	1116	G
33	R1	1130	U
33	R1	1132	U
33	R1	1134	A
33	R1	1135	C
33	R1	1166	G
33	R1	1171	G
33	R1	1173	U
33	R1	1174	U
33	R1	1175	A
33	R1	1176	U
33	R1	1178	C
33	R1	1179	G
33	R1	1180	U
33	R1	1186	G
33	R1	1195	G
33	R1	1199	U
33	R1	1250	G
33	R1	1253	A
33	R1	1256	G
33	R1	1271	G
33	R1	1272	A
33	R1	1284	A
33	R1	1300	G
33	R1	1301	A
33	R1	1329	U
33	R1	1341	G

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Mol	Chain	Res	Type
33	R1	1345	C
33	R1	1352	U
33	R1	1365	A
33	R1	1367	A
33	R1	1368	G
33	R1	1378	A
33	R1	1379	U
33	R1	1383	A
33	R1	1392	A
33	R1	1393	A
33	R1	1395	A
33	R1	1414	C
33	R1	1416	G
33	R1	1421	G
33	R1	1427	A
33	R1	1428	C
33	R1	1452	G
33	R1	1453	A
33	R1	1459	G
33	R1	1461	C
33	R1	1478	G
33	R1	1481	U
33	R1	1482	G
33	R1	1493	C
33	R1	1497	U
33	R1	1508	A
33	R1	1509	A
33	R1	1515	A
33	R1	1524	G
33	R1	1529	G
33	R1	1534	U
33	R1	1535	A
33	R1	1536	C
33	R1	1538	G
33	R1	1554	U
33	R1	1558	C
33	R1	1566	A
33	R1	1569	A
33	R1	1578	U
33	R1	1583	A
33	R1	1584	U
33	R1	1608	A

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Mol	Chain	Res	Type
33	R1	1610	A
33	R1	1647	U
33	R1	1648	U
33	R1	1649	G
33	R1	1654	A
33	R1	1674	G
33	R1	1675	C
33	R1	1693	U
33	R1	1715	G
33	R1	1716	U
33	R1	1724	G
33	R1	1729	U
33	R1	1730	C
33	R1	1733	G
33	R1	1735	A
33	R1	1738	G
33	R1	1756	G
33	R1	1758	U
33	R1	1764	C
33	R1	1773	A
33	R1	1776	G
33	R1	1800	C
33	R1	1801	A
33	R1	1808	A
33	R1	1811	G
33	R1	1816	C
33	R1	1829	A
33	R1	1838	C
33	R1	1866	A
33	R1	1868	C
33	R1	1869	G
33	R1	1870	C
33	R1	1871	A
33	R1	1873	G
33	R1	1884	G
33	R1	1905	C
33	R1	1906	G
33	R1	1910	G
33	R1	1913	A
33	R1	1914	C
33	R1	1915	U
33	R1	1919	A

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Mol	Chain	Res	Type
33	R1	1929	G
33	R1	1930	G
33	R1	1937	A
33	R1	1938	A
33	R1	1943	U
33	R1	1955	U
33	R1	1966	A
33	R1	1967	C
33	R1	1970	A
33	R1	1971	U
33	R1	1972	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	2043	C
33	R1	2055	C
33	R1	2056	G
33	R1	2058	A
33	R1	2059	A
33	R1	2060	A
33	R1	2061	G
33	R1	2062	A
33	R1	2066	C
33	R1	2069	G
33	R1	2072	C
33	R1	2080	A
33	R1	2093	G
33	R1	2096	C
33	R1	2099	U
33	R1	2107	G
33	R1	2111	U
33	R1	2116	G
33	R1	2118	U
33	R1	2120	G
33	R1	2122	U
33	R1	2123	G
33	R1	2126	A
33	R1	2127	G

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Mol	Chain	Res	Type
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	2139	U
33	R1	2140	G
33	R1	2145	C
33	R1	2147	A
33	R1	2148	G
33	R1	2150	C
33	R1	2156	G
33	R1	2157	G
33	R1	2158	A
33	R1	2159	G
33	R1	2161	C
33	R1	2165	C
33	R1	2167	U
33	R1	2168	G
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	2179	C
33	R1	2181	U
33	R1	2182	U
33	R1	2186	G
33	R1	2188	U
33	R1	2189	U
33	R1	2198	A
33	R1	2203	U
33	R1	2204	G
33	R1	2214	C
33	R1	2219	U
33	R1	2225	A
33	R1	2226	C
33	R1	2238	G
33	R1	2239	G

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Mol	Chain	Res	Type
33	R1	2250	G
33	R1	2266	A
33	R1	2283	C
33	R1	2286	G
33	R1	2287	A
33	R1	2288	A
33	R1	2291	U
33	R1	2297	A
33	R1	2305	U
33	R1	2306	C
33	R1	2316	G
33	R1	2322	A
33	R1	2325	G
33	R1	2326	C
33	R1	2333	A
33	R1	2345	G
33	R1	2347	C
33	R1	2350	C
33	R1	2361	G
33	R1	2371	G
33	R1	2377	A
33	R1	2383	G
33	R1	2385	C
33	R1	2396	G
33	R1	2400	G
33	R1	2402	U
33	R1	2406	A
33	R1	2423	U
33	R1	2425	A
33	R1	2428	G
33	R1	2429	G
33	R1	2430	A
33	R1	2434	A
33	R1	2435	A
33	R1	2439	A
33	R1	2441	U
33	R1	2448	A
33	R1	2464	G
33	R1	2468	A
33	R1	2470	G
33	R1	2474	U
33	R1	2476	A

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Mol	Chain	Res	Type
33	R1	2484	G
33	R1	2497	A
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	2554	U
33	R1	2561	U
33	R1	2563	U
33	R1	2564	A
33	R1	2566	A
33	R1	2567	G
33	R1	2572	A
33	R1	2582	G
33	R1	2602	A
33	R1	2609	U
33	R1	2613	U
33	R1	2615	U
33	R1	2629	U
33	R1	2630	G
33	R1	2646	C
33	R1	2662	A
33	R1	2663	G
33	R1	2664	G
33	R1	2669	G
33	R1	2671	G
33	R1	2682	A
33	R1	2685	G
33	R1	2689	U
33	R1	2690	U
33	R1	2700	A
33	R1	2707	U
33	R1	2714	G
33	R1	2724	U
33	R1	2726	A
33	R1	2732	G
33	R1	2733	A
33	R1	2738	A

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Mol	Chain	Res	Type
33	R1	2739	U
33	R1	2744	G
33	R1	2748	A
33	R1	2757	A
33	R1	2762	C
33	R1	2765	A
33	R1	2774	C
33	R1	2775	G
33	R1	2778	A
33	R1	2779	U
33	R1	2791	G
33	R1	2793	C
33	R1	2797	U
33	R1	2798	U
33	R1	2800	A
33	R1	2815	C
33	R1	2816	G
33	R1	2818	U
33	R1	2820	A
33	R1	2823	A
33	R1	2833	U
33	R1	2835	A
33	R1	2840	C
33	R1	2847	U
33	R1	2848	G
33	R1	2849	U
33	R1	2859	G
33	R1	2867	G
33	R1	2873	A
33	R1	2880	C
33	R1	2883	A
33	R1	2891	U
33	R1	2897	U
33	R1	2900	A
33	R1	2903	U
34	R2	13	G
34	R2	22	U
34	R2	23	G
34	R2	35	C
34	R2	41	G
34	R2	44	G
34	R2	51	G

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Mol	Chain	Res	Type
34	R2	56	G
34	R2	62	C
34	R2	63	C
34	R2	68	C
34	R2	87	U
34	R2	88	C
34	R2	89	U
34	R2	108	A
34	R2	109	A
34	R2	112	G
34	R2	115	A
34	R2	117	G
35	R3	3	A
35	R3	4	U
35	R3	5	U
35	R3	9	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	57	G
35	R3	60	A
35	R3	61	G
35	R3	64	G
35	R3	66	A
35	R3	68	G
35	R3	70	U
35	R3	71	A
35	R3	74	A
35	R3	75	G
35	R3	76	G
35	R3	78	A
35	R3	79	G
35	R3	80	A
35	R3	81	A
35	R3	82	G

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Mol	Chain	Res	Type
35	R3	83	C
35	R3	84	U
35	R3	85	U
35	R3	86	G
35	R3	88	U
35	R3	90	C
35	R3	91	U
35	R3	92	U
35	R3	93	U
35	R3	94	G
35	R3	99	C
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	130	A
35	R3	131	A
35	R3	142	G
35	R3	146	G
35	R3	151	A
35	R3	155	A
35	R3	160	A
35	R3	161	A
35	R3	163	C
35	R3	172	A
35	R3	173	U
35	R3	174	A
35	R3	179	A
35	R3	181	A
35	R3	182	A
35	R3	183	C
35	R3	184	G
35	R3	197	A
35	R3	202	G
35	R3	204	G
35	R3	205	A
35	R3	206	C
35	R3	207	C
35	R3	209	U

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Mol	Chain	Res	Type
35	R3	214	C
35	R3	215	C
35	R3	224	U
35	R3	226	G
35	R3	240	G
35	R3	243	A
35	R3	247	G
35	R3	248	C
35	R3	250	A
35	R3	251	G
35	R3	255	G
35	R3	266	G
35	R3	267	C
35	R3	270	A
35	R3	272	C
35	R3	273	U
35	R3	274	A
35	R3	280	C
35	R3	287	U
35	R3	289	G
35	R3	290	C
35	R3	293	G
35	R3	302	G
35	R3	313	A
35	R3	316	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	332	G
35	R3	333	U
35	R3	338	A
35	R3	339	C
35	R3	342	C
35	R3	344	A
35	R3	347	G
35	R3	351	G
35	R3	352	C

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Mol	Chain	Res	Type
35	R3	353	A
35	R3	354	G
35	R3	360	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	381	C
35	R3	388	G
35	R3	389	A
35	R3	391	G
35	R3	392	C
35	R3	395	C
35	R3	396	C
35	R3	397	A
35	R3	398	U
35	R3	403	C
35	R3	406	G
35	R3	409	U
35	R3	413	G
35	R3	414	A
35	R3	415	A
35	R3	416	G
35	R3	418	C
35	R3	419	C
35	R3	421	U
35	R3	422	C
35	R3	428	G
35	R3	429	U
35	R3	438	U
35	R3	439	U
35	R3	440	C
35	R3	451	A
35	R3	454	G
35	R3	459	A
35	R3	462	G
35	R3	463	U
35	R3	464	U

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Mol	Chain	Res	Type
35	R3	465	A
35	R3	466	A
35	R3	468	A
35	R3	469	C
35	R3	470	C
35	R3	472	U
35	R3	476	U
35	R3	479	U
35	R3	480	U
35	R3	482	A
35	R3	484	G
35	R3	487	A
35	R3	494	G
35	R3	495	A
35	R3	496	A
35	R3	497	G
35	R3	498	A
35	R3	501	C
35	R3	509	A
35	R3	511	C
35	R3	516	U
35	R3	518	C
35	R3	524	G
35	R3	525	C
35	R3	530	G
35	R3	531	U
35	R3	532	A
35	R3	533	A
35	R3	540	G
35	R3	541	G
35	R3	547	A
35	R3	549	C
35	R3	551	U
35	R3	562	U
35	R3	564	C
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

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Mol	Chain	Res	Type
35	R3	607	A
35	R3	611	C
35	R3	613	C
35	R3	615	G
35	R3	616	G
35	R3	630	A
35	R3	633	G
35	R3	640	A
35	R3	642	A
35	R3	653	U
35	R3	665	A
35	R3	673	A
35	R3	684	U
35	R3	686	U
35	R3	688	G
35	R3	703	G
35	R3	713	G
35	R3	718	A
35	R3	723	U
35	R3	724	G
35	R3	731	G
35	R3	738	C
35	R3	739	C
35	R3	754	C
35	R3	755	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	821	G
35	R3	829	G
35	R3	832	G
35	R3	838	G
35	R3	839	C

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Mol	Chain	Res	Type
35	R3	840	C
35	R3	841	C
35	R3	842	U
35	R3	843	U
35	R3	844	G
35	R3	846	G
35	R3	849	G
35	R3	851	G
35	R3	863	U
35	R3	864	A
35	R3	872	A
35	R3	876	C
35	R3	877	G
35	R3	878	A
35	R3	885	G
35	R3	887	G
35	R3	902	G
35	R3	914	A
35	R3	926	G
35	R3	932	C
35	R3	933	G
35	R3	934	C
35	R3	935	A
35	R3	956	U
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	972	C
35	R3	975	A
35	R3	976	G
35	R3	977	A
35	R3	991	U
35	R3	992	U
35	R3	993	G
35	R3	994	A
35	R3	996	A
35	R3	998	C
35	R3	999	C
35	R3	1000	A

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Mol	Chain	Res	Type
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	1022	A
35	R3	1028	C
35	R3	1029	U
35	R3	1030	U
35	R3	1031	C
35	R3	1032	G
35	R3	1033	G
35	R3	1034	G
35	R3	1036	A
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	1064	G
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	1118	U
35	R3	1119	C
35	R3	1123	U
35	R3	1124	G
35	R3	1125	U
35	R3	1126	U
35	R3	1130	A
35	R3	1131	G
35	R3	1133	G
35	R3	1136	C

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Mol	Chain	Res	Type
35	R3	1137	C
35	R3	1138	G
35	R3	1139	G
35	R3	1150	A
35	R3	1151	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	1183	U
35	R3	1184	G
35	R3	1187	G
35	R3	1196	A
35	R3	1197	A
35	R3	1199	U
35	R3	1202	U
35	R3	1212	U
35	R3	1213	A
35	R3	1214	C
35	R3	1216	A
35	R3	1227	A
35	R3	1236	A
35	R3	1238	A
35	R3	1241	G
35	R3	1255	G
35	R3	1257	A
35	R3	1260	G
35	R3	1261	A
35	R3	1268	G
35	R3	1271	A
35	R3	1275	A
35	R3	1280	A
35	R3	1286	U
35	R3	1287	A
35	R3	1289	A
35	R3	1294	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	1318	A
35	R3	1320	C
35	R3	1322	C
35	R3	1333	A
35	R3	1346	A
35	R3	1363	A
35	R3	1370	G
35	R3	1378	C
35	R3	1419	G
35	R3	1434	A
35	R3	1440	U
35	R3	1441	A
35	R3	1442	G
35	R3	1443	C
35	R3	1446	A
35	R3	1449	C
35	R3	1451	U
35	R3	1452	C
35	R3	1472	U
35	R3	1487	G
35	R3	1492	A
35	R3	1493	A
35	R3	1497	G
35	R3	1499	A
35	R3	1502	A
35	R3	1503	A
35	R3	1506	U
35	R3	1517	G
35	R3	1519	A
35	R3	1529	G
35	R3	1530	G
36	T	1	G
36	T	8	4SU
36	T	9	G
36	T	13	A
36	T	16	C
36	T	17	U
36	T	18	G
36	T	19	G
36	T	20	H2U

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Mol	Chain	Res	Type
36	T	47	U
36	T	48	C
36	T	52	G
36	T	55	PSU
36	T	56	C
36	T	59	A
36	T	60	U
36	T	61	C
36	T	74	C
36	T	76	A

All (46) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
33	R1	198	C
33	R1	225	C
33	R1	271	G
33	R1	360	U
33	R1	453	A
33	R1	784	G
33	R1	859	G
33	R1	903	C
33	R1	1020	A
33	R1	1050	A
33	R1	1093	G
33	R1	1172	C
33	R1	1715	G
33	R1	2174	C
33	R1	2178	C
33	R1	2663	G
33	R1	2756	U
33	R1	2839	G
33	R1	2846	G
33	R1	2896	C
35	R3	70	U
35	R3	78	A
35	R3	120	A
35	R3	288	A
35	R3	301	G
35	R3	312	C
35	R3	363	A
35	R3	453	G

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Mol	Chain	Res	Type
35	R3	461	A
35	R3	497	G
35	R3	500	G
35	R3	561	U
35	R3	588	G
35	R3	612	C
35	R3	672	U
35	R3	685	G
35	R3	753	A
35	R3	837	U
35	R3	1125	U
35	R3	1149	C
35	R3	1270	G
35	R3	1297	G
35	R3	1305	G
36	T	8	4SU
36	T	17	U
36	T	55	PSU

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

5 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
36	MUM	T	54	36	18,22,22	3.27	6 (33%)	19,32,32	2.11	5 (26%)
36	PSU	T	55	36	18,21,22	2.30	8 (44%)	21,30,33	1.85	3 (14%)
36	4SU	T	8	36	18,21,22	3.72	7 (38%)	25,30,33	2.41	6 (24%)
36	4OC	T	32	36	20,23,24	2.53	5 (25%)	25,32,35	0.94	1 (4%)
36	H2U	T	20	36	18,21,22	4.50	5 (27%)	19,30,33	4.25	6 (31%)

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
36	MUM	T	54	36	3/3/9/10	4/7/41/41	0/2/2/2
36	PSU	T	55	36	1/1/5/5	3/7/25/26	0/2/2/2
36	4SU	T	8	36	2/2/5/5	2/7/25/26	0/2/2/2
36	4OC	T	32	36	1/1/5/6	1/9/29/30	0/2/2/2
36	H2U	T	20	36	1/1/8/9	6/7/38/39	0/2/2/2

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	T	54	MUM	C6-N1	-11.96	1.32	1.46
36	T	8	4SU	O2-C2	10.81	1.42	1.23
36	T	20	H2U	C2-N1	10.53	1.50	1.35
36	T	20	H2U	O4-C4	10.12	1.43	1.23
36	T	32	4OC	O2-C2	8.92	1.40	1.23
36	T	8	4SU	C4-S4	8.76	1.84	1.68
36	T	20	H2U	O2-C2	7.92	1.37	1.23
36	T	20	H2U	C2-N3	6.93	1.50	1.38
36	T	20	H2U	C4-N3	6.09	1.47	1.37
36	T	55	PSU	C1'-C5	-5.01	1.38	1.50
36	T	32	4OC	C4-N4	4.44	1.45	1.36
36	T	54	MUM	C6-C5	-4.03	1.39	1.51
36	T	8	4SU	C2-N1	-4.01	1.32	1.38
36	T	8	4SU	C4-N3	-3.96	1.33	1.37
36	T	32	4OC	C2-N1	-3.66	1.32	1.40
36	T	55	PSU	C6-C5	3.59	1.39	1.35
36	T	55	PSU	C4-N3	-3.46	1.32	1.38
36	T	55	PSU	C2-N1	-3.42	1.32	1.36
36	T	54	MUM	C2-N3	-3.25	1.32	1.38
36	T	55	PSU	C2-N3	-3.04	1.32	1.37
36	T	8	4SU	C2-N3	-2.73	1.33	1.38
36	T	54	MUM	O2-C2	-2.66	1.18	1.23
36	T	54	MUM	C4-N3	-2.59	1.32	1.37
36	T	55	PSU	O4-C4	-2.56	1.18	1.23
36	T	8	4SU	C5-C4	-2.53	1.39	1.42
36	T	32	4OC	C6-N1	-2.42	1.32	1.38
36	T	55	PSU	C6-N1	-2.37	1.32	1.36
36	T	8	4SU	C6-C5	2.27	1.40	1.35
36	T	54	MUM	O4-C4	-2.25	1.19	1.23
36	T	55	PSU	O2-C2	-2.06	1.19	1.23
36	T	32	4OC	C2-N3	-2.04	1.32	1.36

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	T	20	H2U	O2-C2-N1	-12.74	107.78	123.10
36	T	20	H2U	O4-C4-N3	-7.30	109.04	120.30
36	T	8	4SU	C4-N3-C2	-7.25	120.36	127.31
36	T	20	H2U	O2-C2-N3	-6.81	108.94	121.49
36	T	20	H2U	O4-C4-C5	-6.39	109.11	122.20
36	T	8	4SU	C5-C4-N3	5.48	119.85	114.75
36	T	55	PSU	N1-C2-N3	5.31	120.77	115.17
36	T	8	4SU	N3-C2-N1	5.19	121.65	114.89
36	T	54	MUM	C4-N3-C2	-5.04	120.69	126.83
36	T	54	MUM	N3-C2-N1	4.95	121.62	116.65
36	T	20	H2U	C5-C4-N3	-4.53	111.87	116.69
36	T	20	H2U	N3-C2-N1	-3.97	112.66	116.65
36	T	54	MUM	C5M-C5-C6	3.79	120.79	112.05
36	T	55	PSU	C4-N3-C2	-3.64	121.35	126.37
36	T	8	4SU	C5-C4-S4	-3.62	120.17	124.31
36	T	55	PSU	O2-C2-N1	-3.42	119.26	122.79
36	T	8	4SU	O2-C2-N1	-3.05	118.82	122.80
36	T	54	MUM	C6-C5-C4	2.60	119.00	111.53
36	T	54	MUM	O2-C2-N1	-2.42	120.19	123.10
36	T	8	4SU	C6-C5-C4	-2.34	117.92	119.95
36	T	32	4OC	O2-C2-N3	-2.03	119.12	122.33

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
36	T	20	H2U	C2’
36	T	32	4OC	C2’
36	T	54	MUM	C4’
36	T	54	MUM	C5
36	T	54	MUM	C3’
36	T	55	PSU	C4’
36	T	8	4SU	C2’
36	T	8	4SU	C1’

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	T	20	H2U	O4’-C4’-C5’-O5’
36	T	20	H2U	O4’-C1’-N1-C2
36	T	20	H2U	O4’-C1’-N1-C6
36	T	54	MUM	O4’-C4’-C5’-O5’

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Mol	Chain	Res	Type	Atoms
36	T	54	MUM	C3'-C4'-C5'-O5'
36	T	55	PSU	C4'-C5'-O5'-P
36	T	54	MUM	C4'-C5'-O5'-P
36	T	55	PSU	O4'-C4'-C5'-O5'
36	T	20	H2U	C3'-C4'-C5'-O5'
36	T	55	PSU	C3'-C4'-C5'-O5'
36	T	20	H2U	C2'-C1'-N1-C6
36	T	20	H2U	C4'-C5'-O5'-P
36	T	32	4OC	C3'-C2'-O2'-CM2
36	T	8	4SU	C2'-C1'-N1-C6
36	T	8	4SU	O4'-C1'-N1-C6
36	T	54	MUM	O4'-C1'-N1-C6

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	T	55	PSU	2	0
36	T	8	4SU	1	0
36	T	32	4OC	1	0
36	T	20	H2U	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 303 ligands modelled in this entry, 300 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
60	FME	T	101	36	8,9,10	0.98	0	8,9,11	0.98	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
58	ATP	E	602	59	28,33,33	0.81	0	34,52,52	0.62	1 (2%)
58	ATP	E	601	-	28,33,33	0.70	0	34,52,52	0.88	2 (5%)

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
60	FME	T	101	36	-	1/7/9/11	-
58	ATP	E	602	59	-	2/18/38/38	0/3/3/3
58	ATP	E	601	-	-	9/18/38/38	0/3/3/3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	E	601	ATP	C4'-O4'-C1'	-3.69	106.55	109.92
58	E	602	ATP	C5-C6-N6	2.31	123.83	120.31
58	E	601	ATP	C5-C6-N6	2.29	123.79	120.31

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	E	601	ATP	C5'-O5'-PA-O1A
58	E	601	ATP	C5'-O5'-PA-O2A
58	E	601	ATP	C5'-O5'-PA-O3A
58	E	601	ATP	O4'-C4'-C5'-O5'
58	E	601	ATP	C3'-C4'-C5'-O5'
60	T	101	FME	CB-CG-SD-CE
58	E	601	ATP	PB-O3A-PA-O5'
58	E	601	ATP	PB-O3B-PG-O1G
58	E	602	ATP	PB-O3A-PA-O2A
58	E	602	ATP	C4'-C5'-O5'-PA
58	E	601	ATP	PB-O3B-PG-O2G
58	E	601	ATP	PB-O3B-PG-O3G

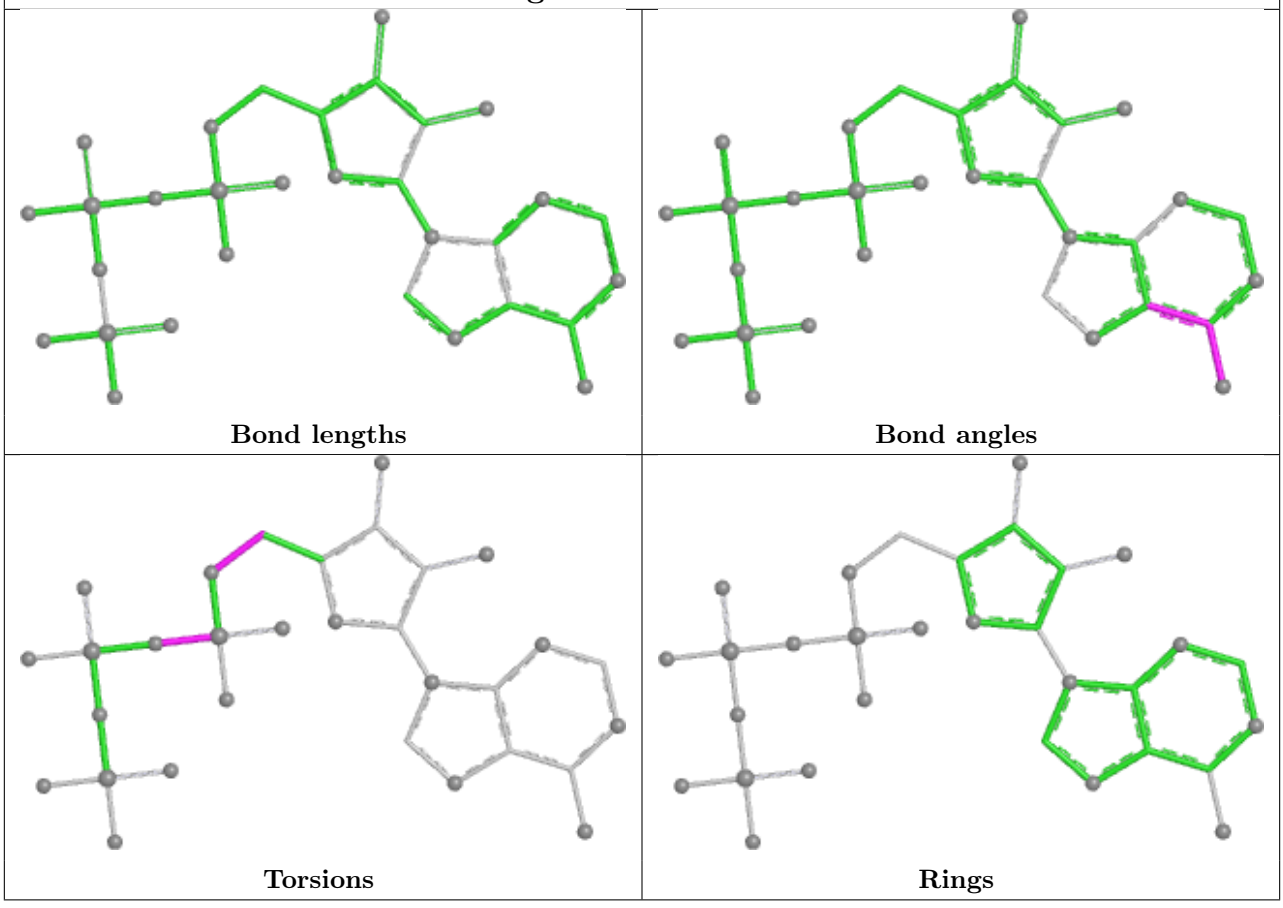
There are no ring outliers.

2 monomers are involved in 3 short contacts:

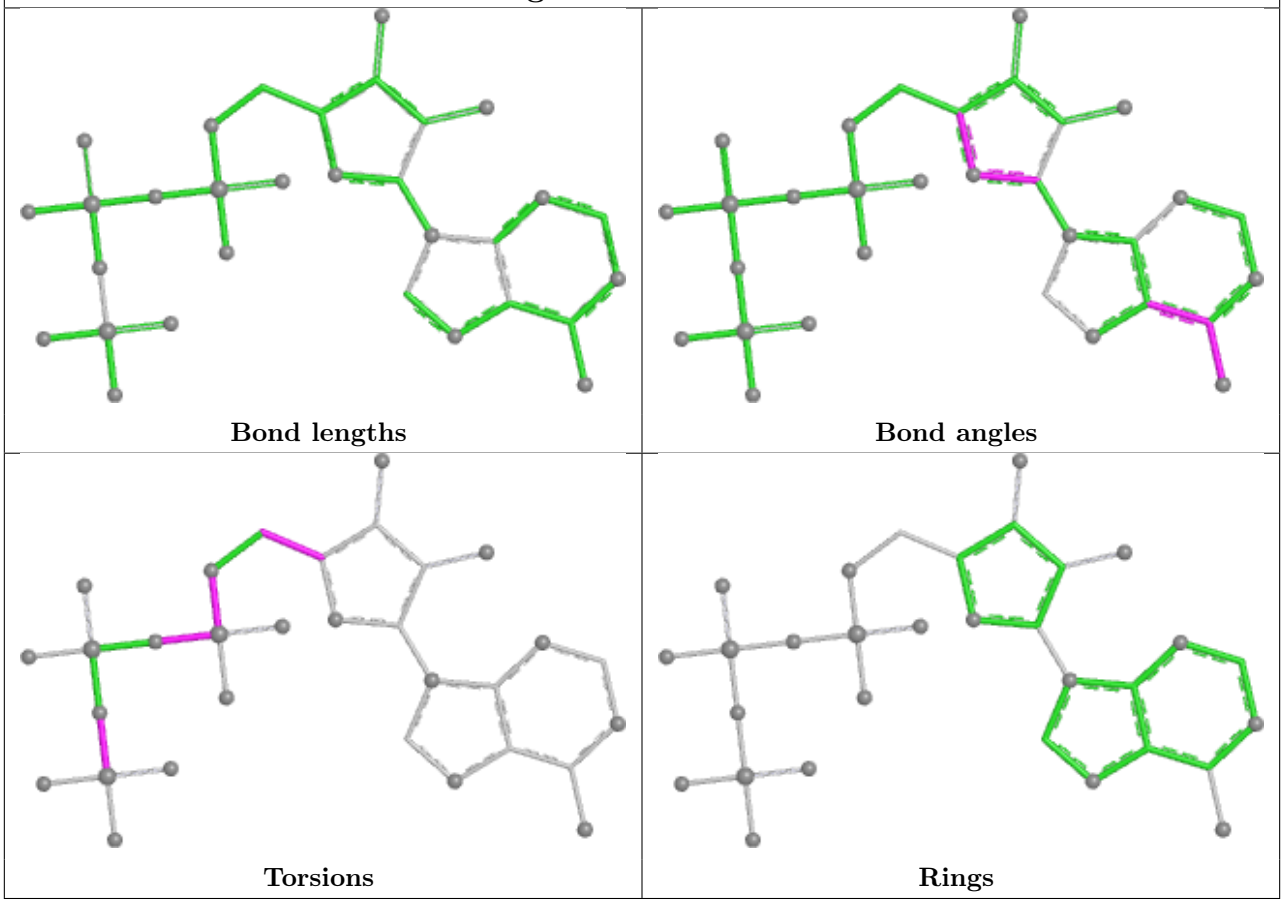
Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	E	602	ATP	2	0
58	E	601	ATP	1	0

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

Ligand ATP E 602



Ligand ATP E 601



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
35	R3	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	R3	210:C	O3'	211:G	P	5.77
1	R3	460:A	O3'	461:A	P	5.31

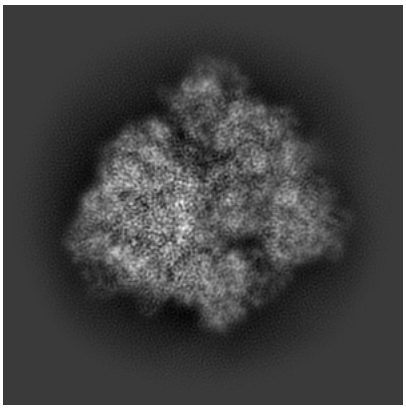
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-29398. These allow visual inspection of the internal detail of the map and identification of artifacts.

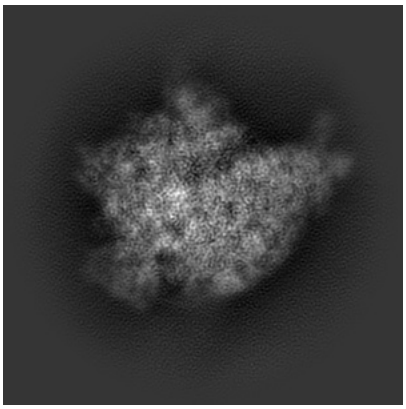
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

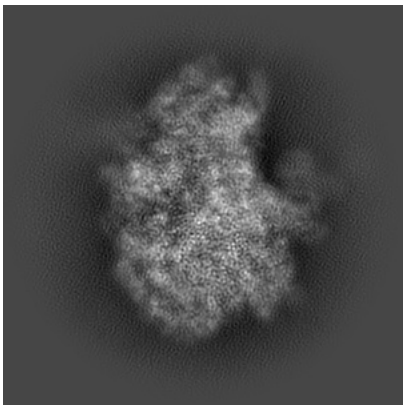
6.1.1 Primary map



X

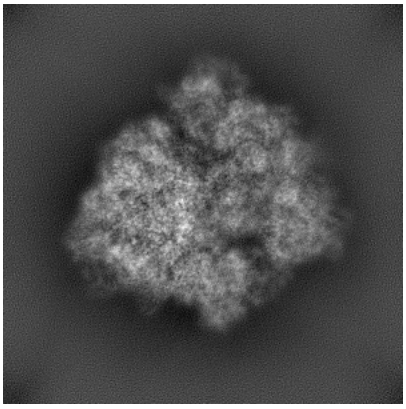


Y

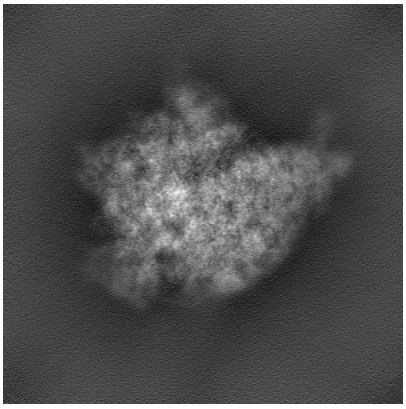


Z

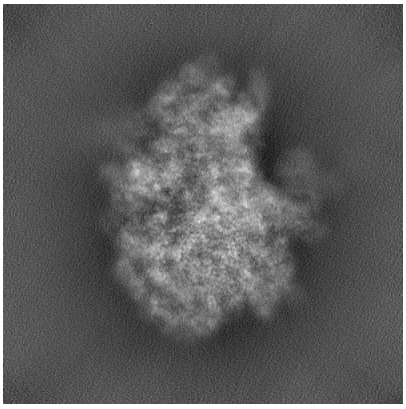
6.1.2 Raw map



X



Y

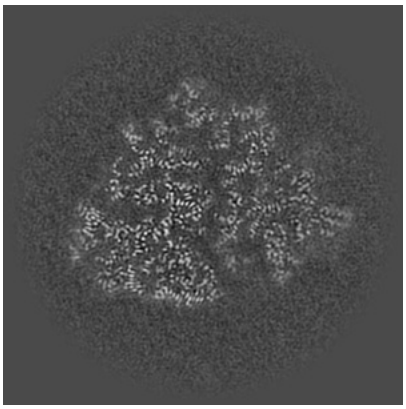


Z

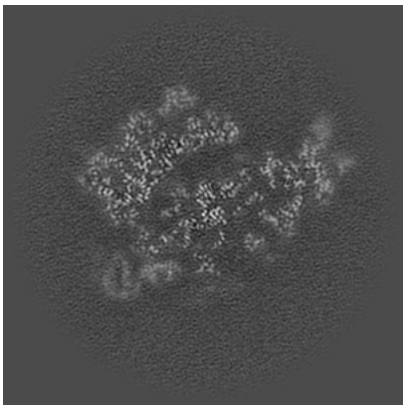
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

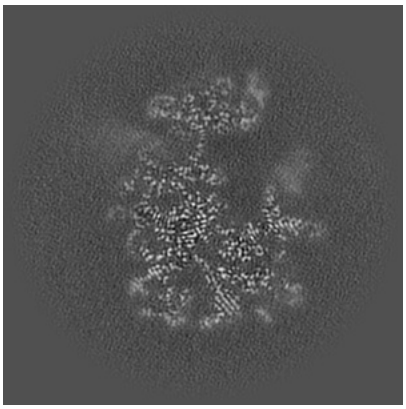
6.2.1 Primary map



X Index: 200

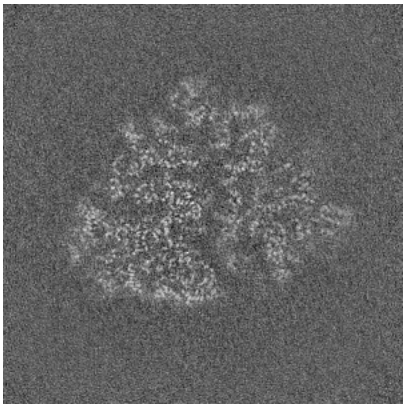


Y Index: 200

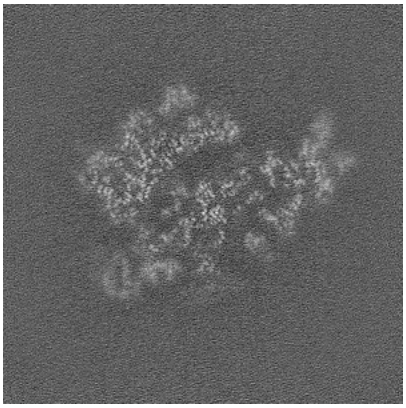


Z Index: 200

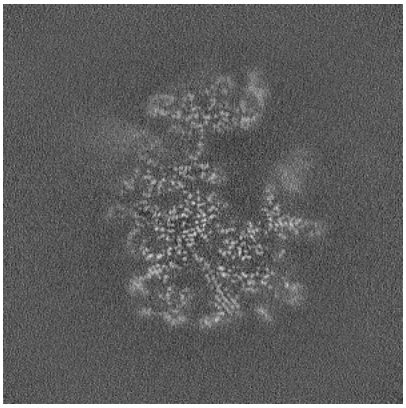
6.2.2 Raw map



X Index: 200



Y Index: 200

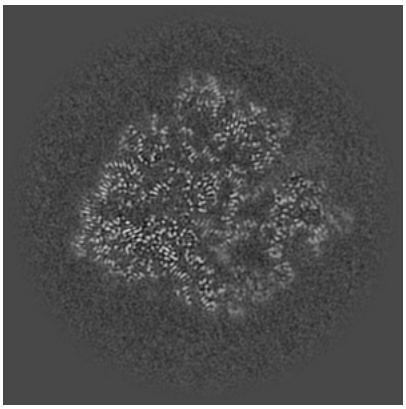


Z Index: 200

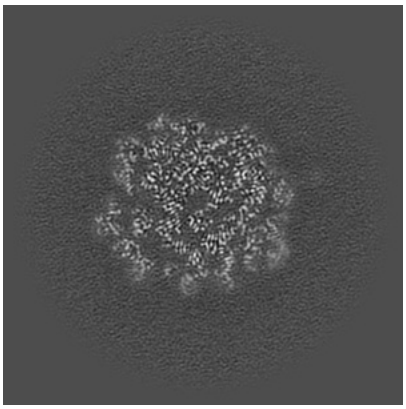
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

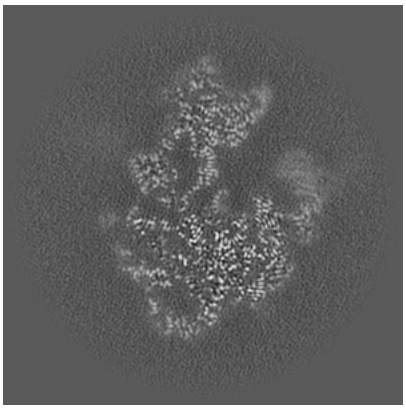
6.3.1 Primary map



X Index: 210

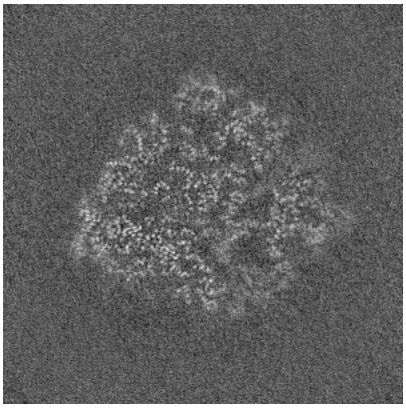


Y Index: 152

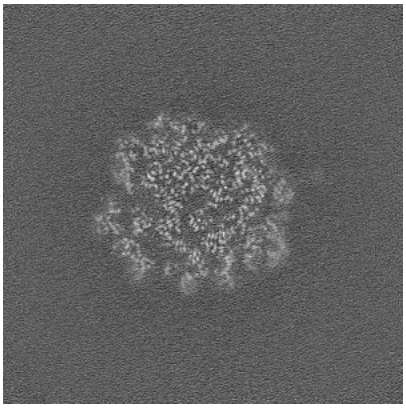


Z Index: 179

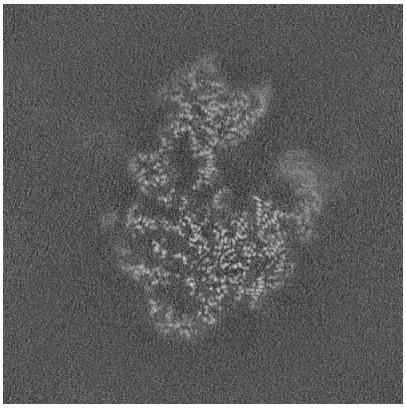
6.3.2 Raw map



X Index: 209



Y Index: 152

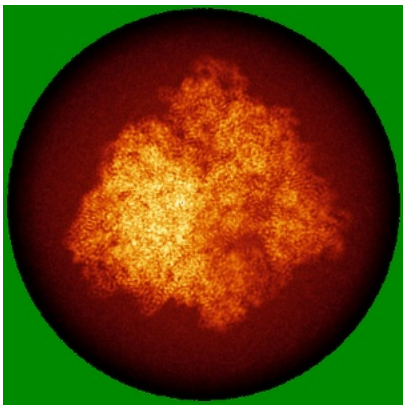


Z Index: 178

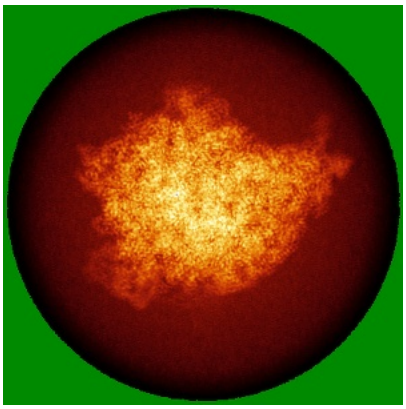
The images above show the largest variance slices of the map in three orthogonal directions.

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

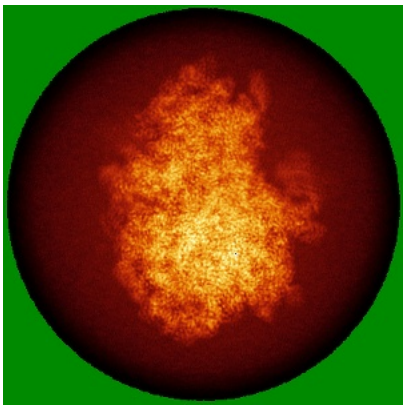
6.4.1 Primary map



X

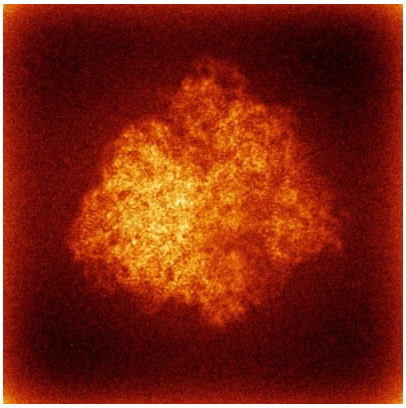


Y

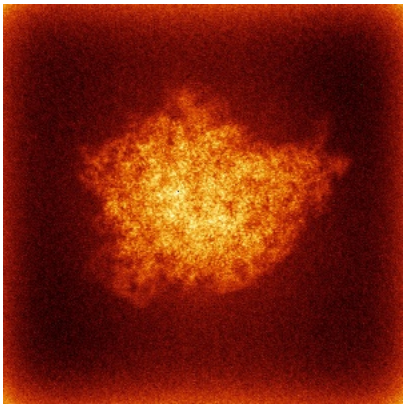


Z

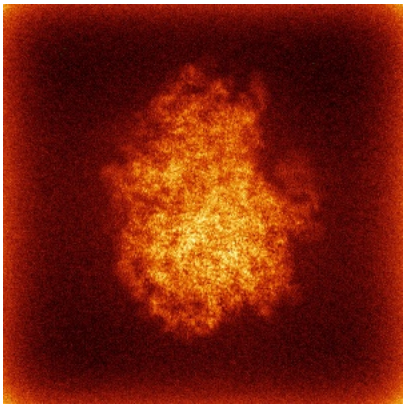
6.4.2 Raw map



X



Y



Z

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

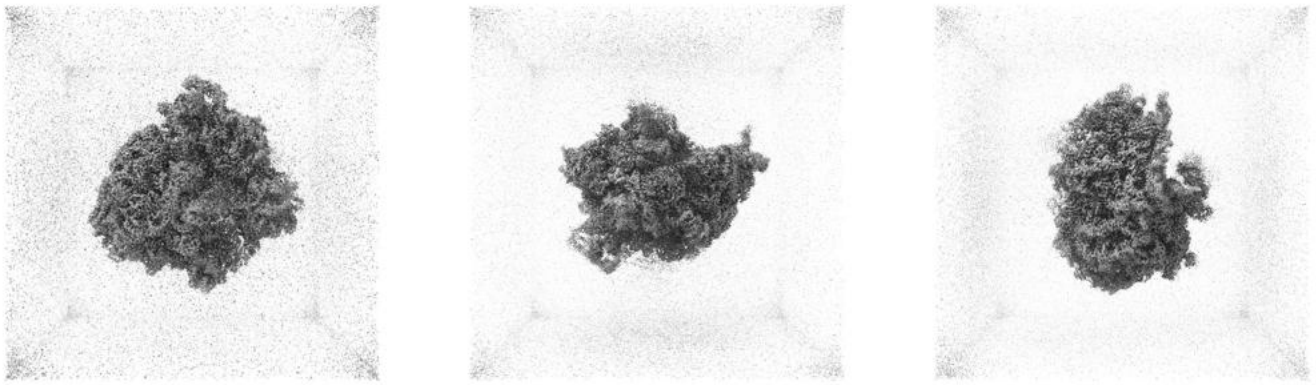
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.45. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

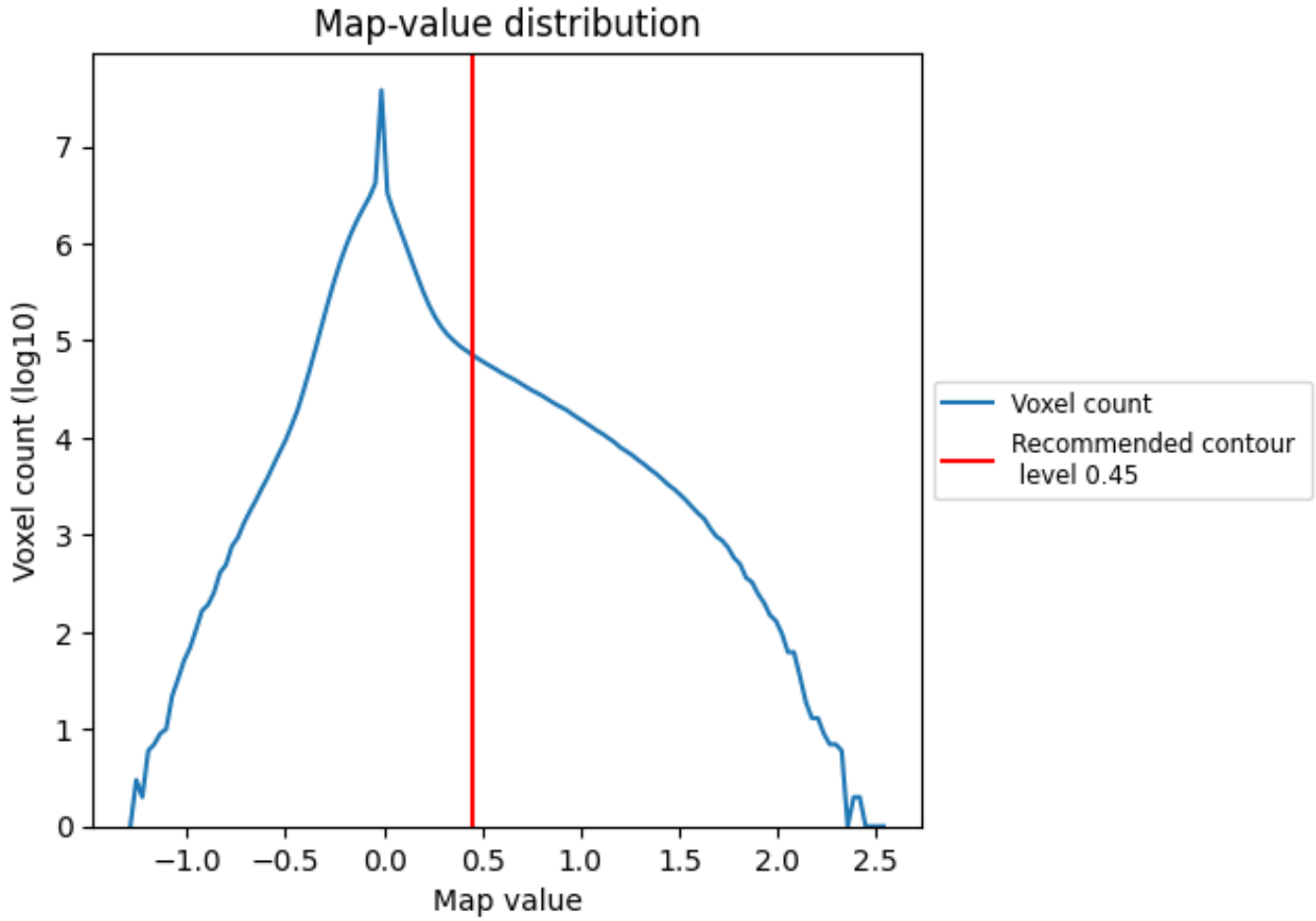
6.6 Mask visualisation (i)

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

7 Map analysis

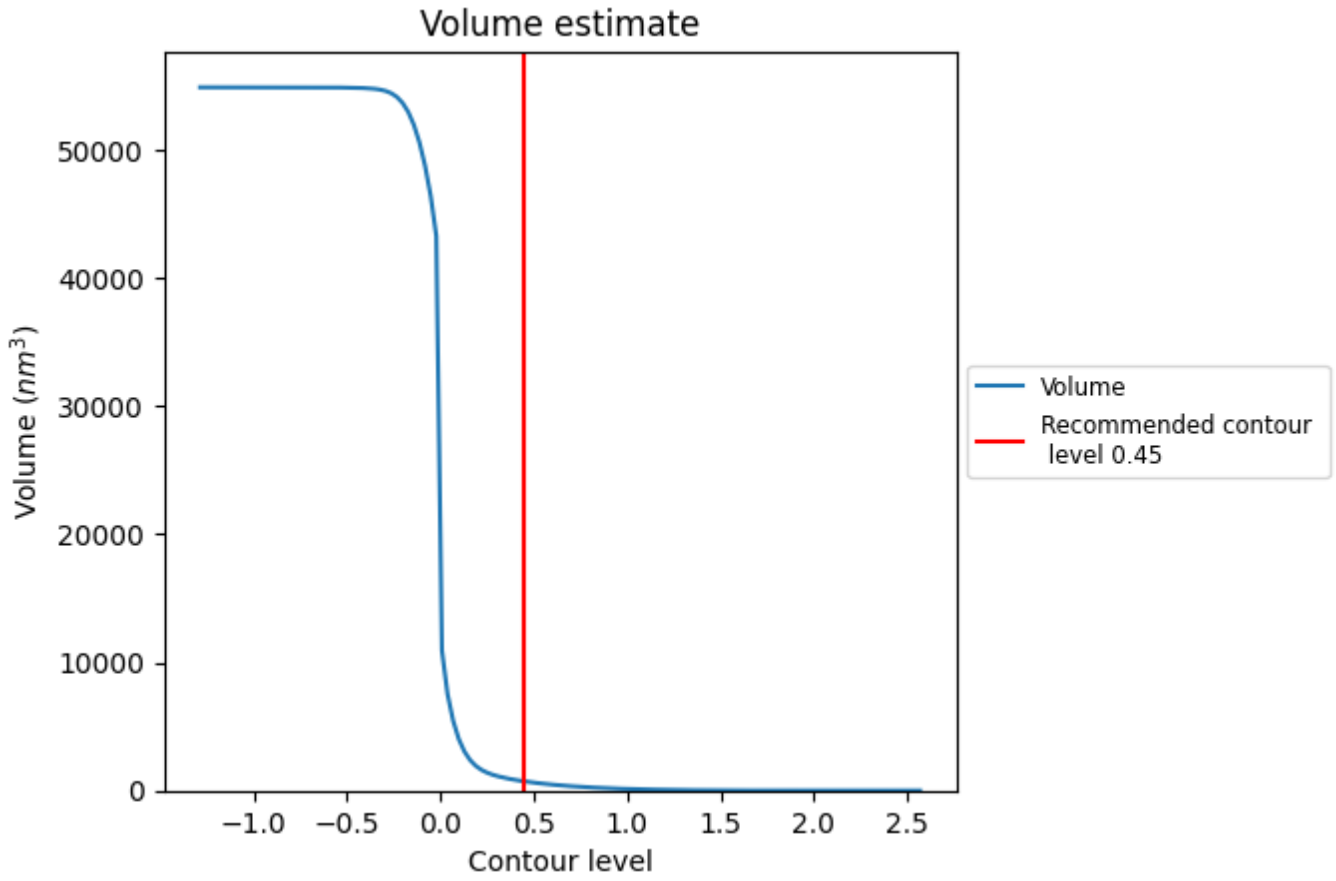
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

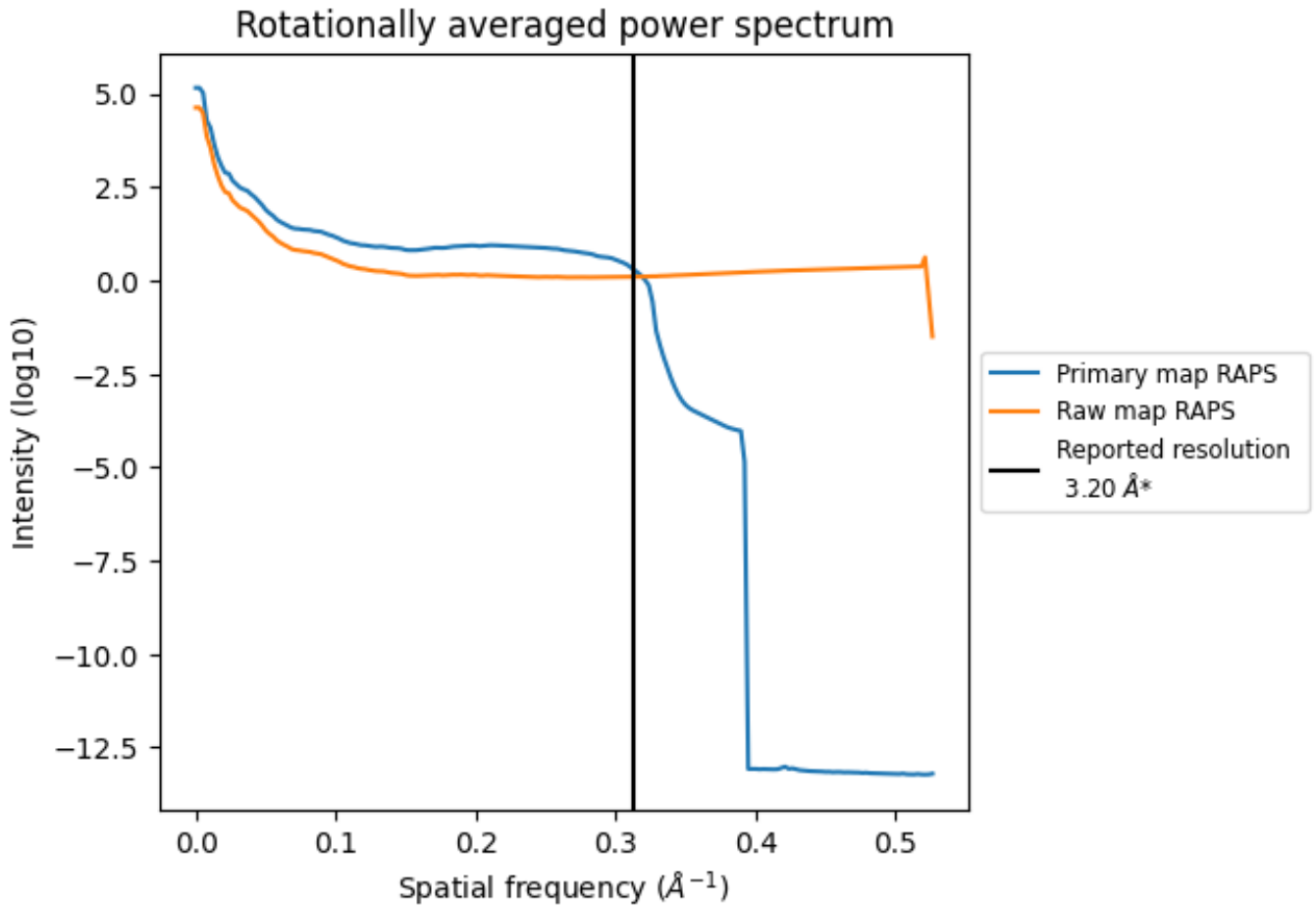
7.2 Volume estimate



The volume at the recommended contour level is 718 nm^3; this corresponds to an approximate mass of 648 kDa.

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

7.3 Rotationally averaged power spectrum (i)

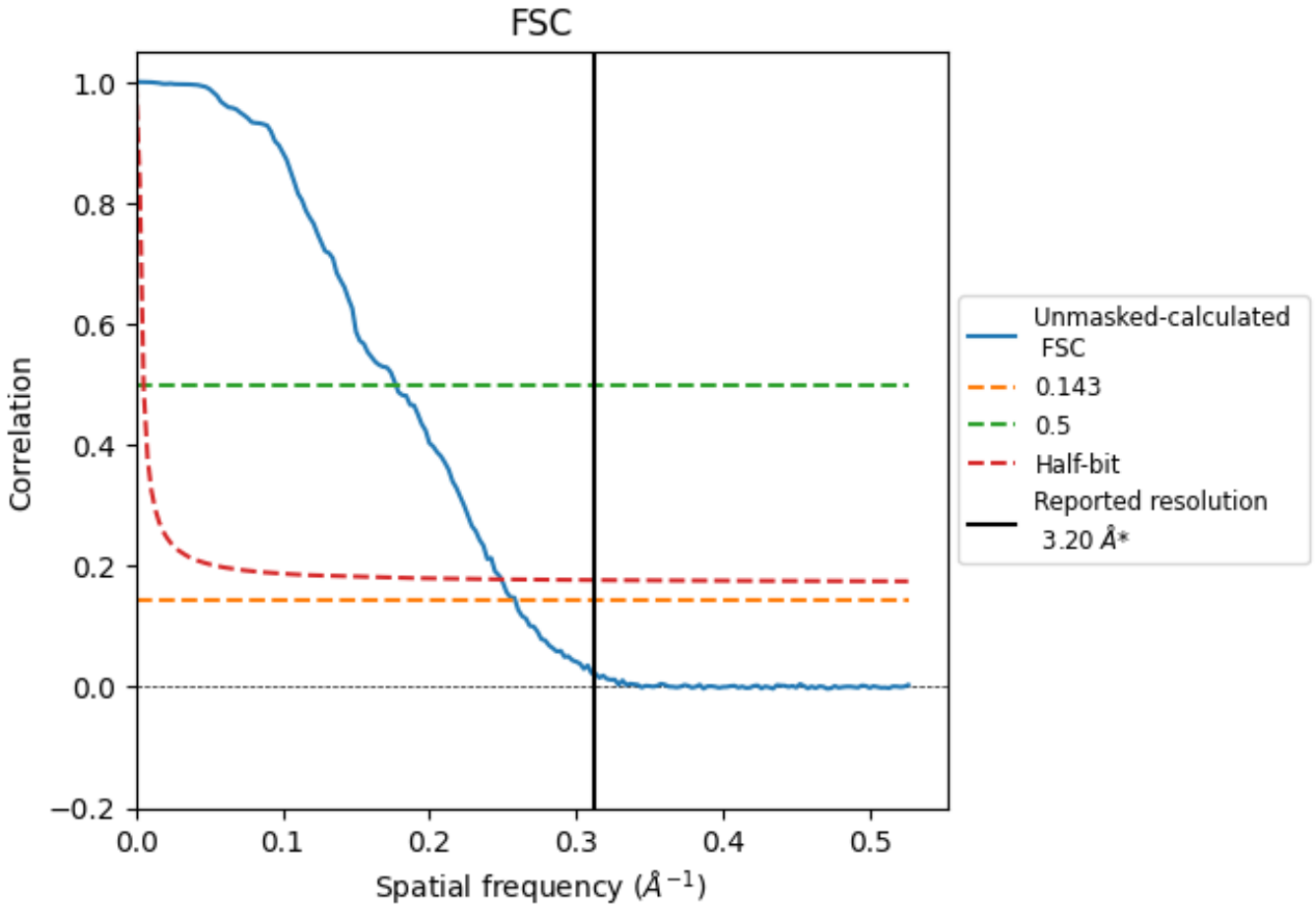


*Reported resolution corresponds to spatial frequency of 0.312 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8.2 Resolution estimates (i)

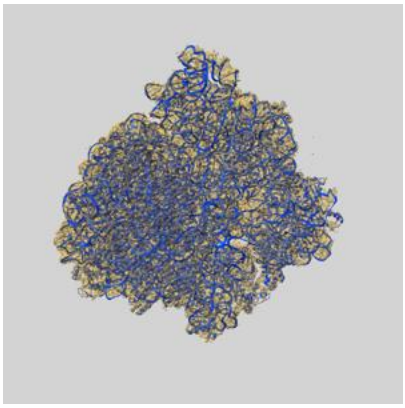
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.87	5.65	4.02

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.87 differs from the reported value 3.2 by more than 10 %

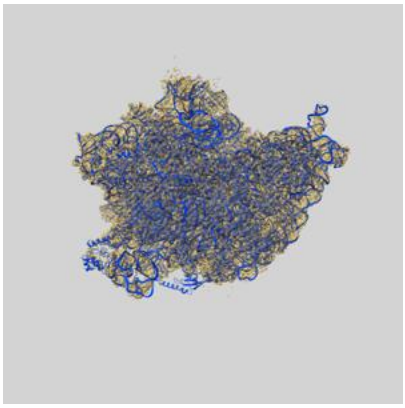
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-29398 and PDB model 9NLE. Per-residue inclusion information can be found in section 3 on page 17.

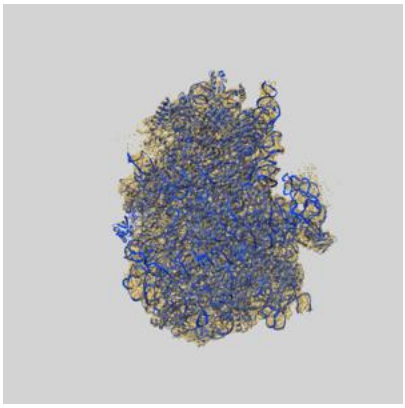
9.1 Map-model overlay



X



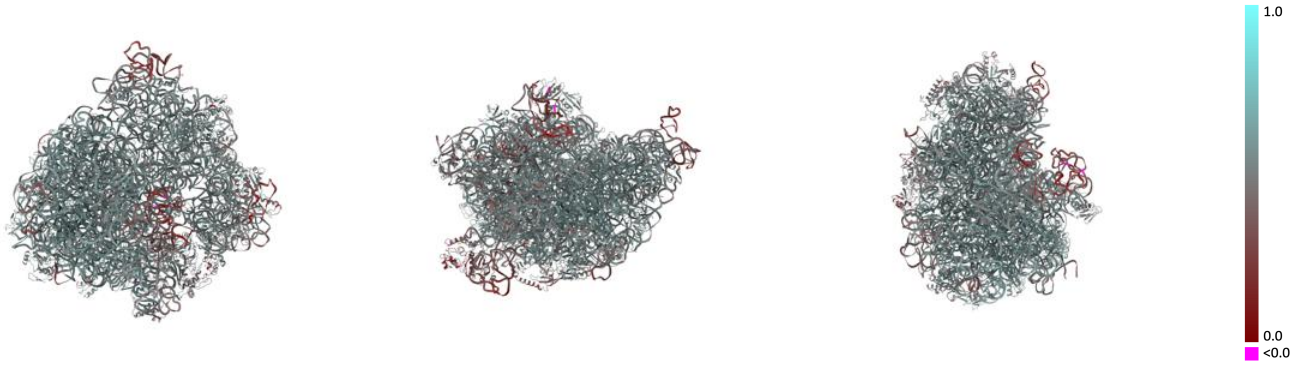
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.45 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.

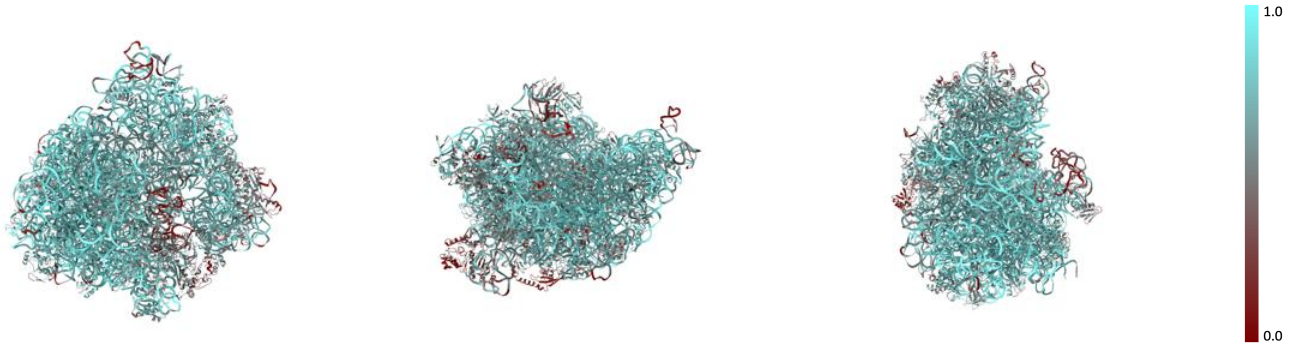
9.2 Q-score mapped to coordinate model



X Y Z

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

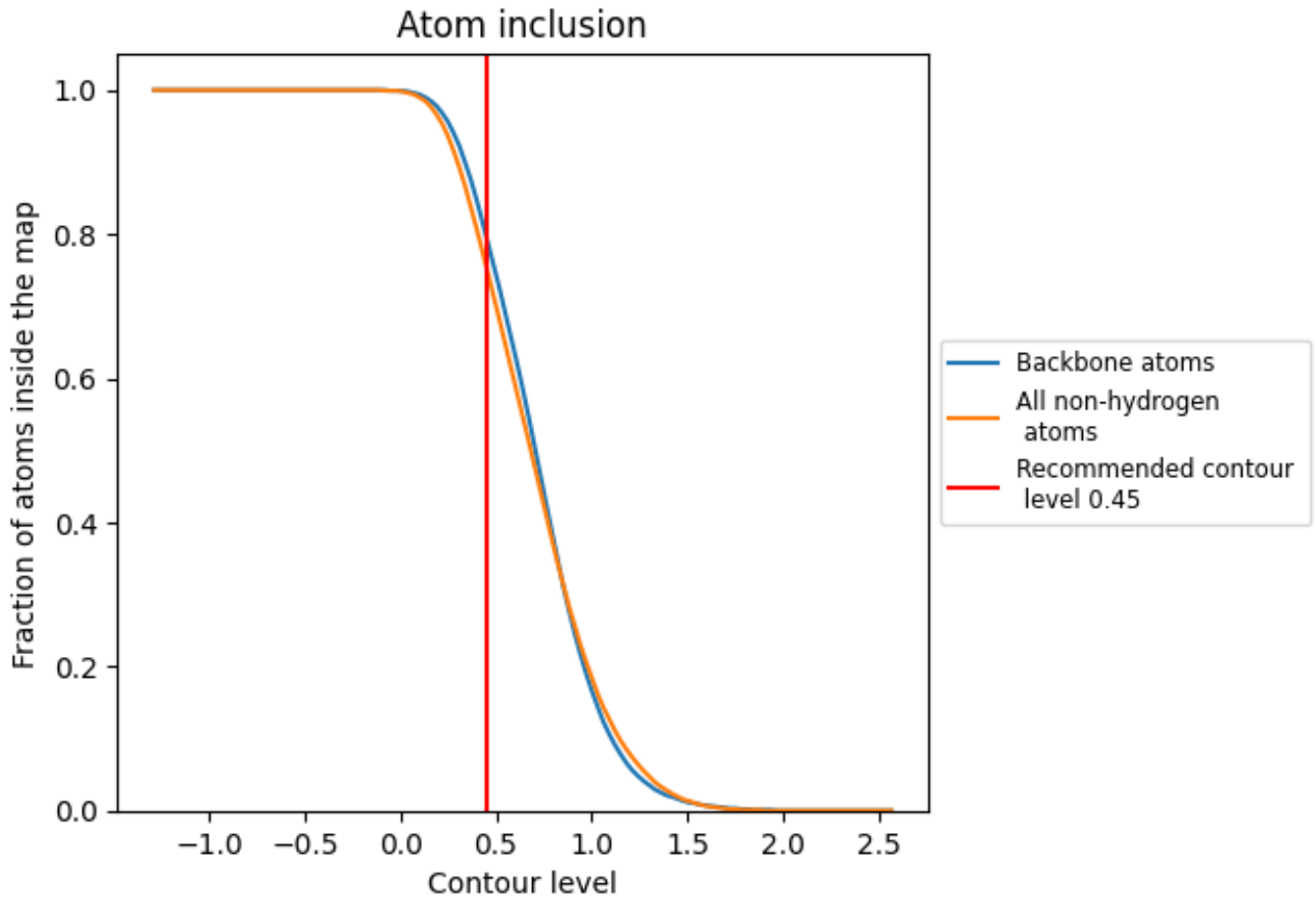
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.45).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 76% 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 (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7550	0.5270
1	0.1410	0.3250
13	0.7490	0.5720
14	0.6870	0.5630
15	0.7460	0.5630
16	0.7000	0.5620
17	0.7800	0.5740
18	0.6580	0.5300
19	0.6820	0.5680
2	0.7370	0.5840
20	0.8010	0.5790
21	0.7190	0.5520
22	0.6930	0.5630
23	0.6450	0.5400
24	0.6190	0.5280
25	0.6650	0.5350
27	0.7350	0.5710
28	0.7140	0.5730
29	0.5940	0.5020
3	0.7350	0.5670
30	0.7190	0.5700
31	0.2290	0.4060
32	0.7220	0.5690
33	0.6630	0.5600
34	0.7720	0.5890
35	0.7760	0.5950
36	0.7190	0.5650
4	0.6700	0.5430
5	0.4620	0.4850
6	0.5400	0.4890
9	0.2010	0.4060
E	0.5150	0.5040
M	0.5920	0.5400
R1	0.8420	0.5360
R2	0.8050	0.4950

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
R3	0.8140	0.5180
T	0.6180	0.4590
sb	0.5300	0.4760
sc	0.5870	0.5330
sd	0.6000	0.5170
se	0.6520	0.5380
sf	0.6070	0.4990
sg	0.5510	0.5170
sh	0.6650	0.5520
si	0.6040	0.5060
sj	0.4780	0.4800
sk	0.6500	0.5510
sl	0.6080	0.5380
sm	0.5600	0.5070
sn	0.5900	0.4860
so	0.6620	0.5510
sp	0.6540	0.5300
sq	0.6080	0.5350
sr	0.6610	0.5360
ss	0.5470	0.4920
st	0.6490	0.5380
su	0.4790	0.5150