Full wwPDB EM Validation Report

Mar 24, 2025 – 02:35 PM EDT

PDB ID	:	9NJV
EMDB ID	:	EMD-40939
Title	:	E. coli 70S initiation complex (bL33 absent)
Authors	:	Singh, S.; Hunt, J.F.
Deposited on	:	2025-02-28
Resolution	:	3.10 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:

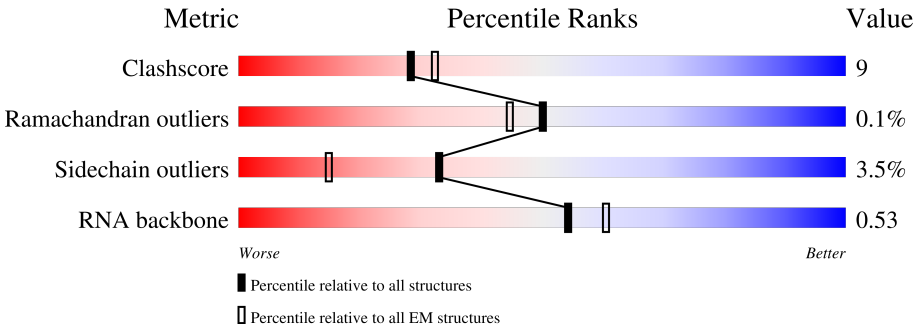
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 3.10 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	13	142	6% 82% 17%
2	14	122	10% 80% 20%
3	15	144	6% 78% 22%
4	16	136	12% 78% 21%
5	17	120	72% 27%
6	18	116	25% 74% 26%
7	19	114	14% 77% 22%

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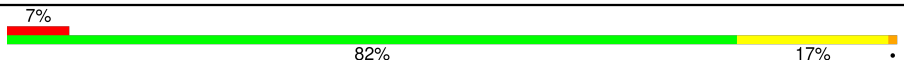
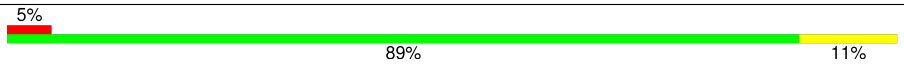
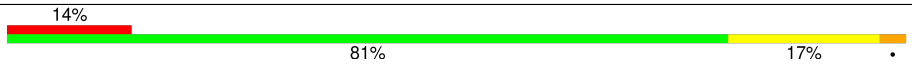
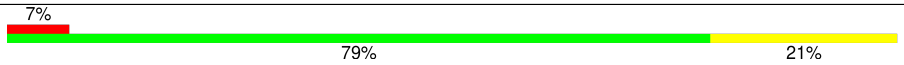
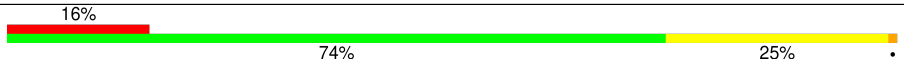
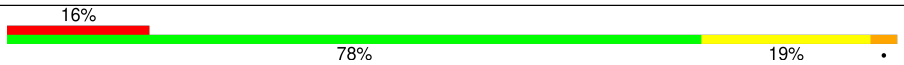
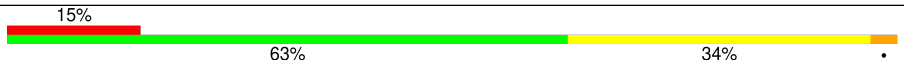
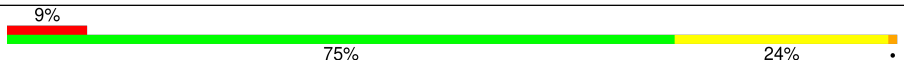
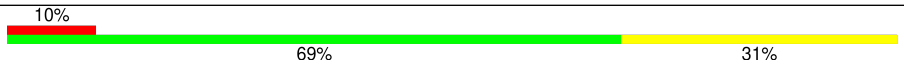
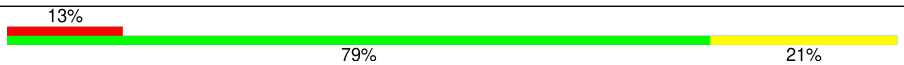
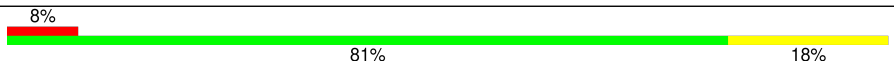
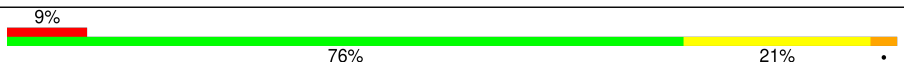
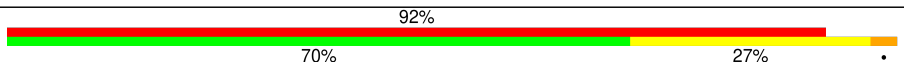
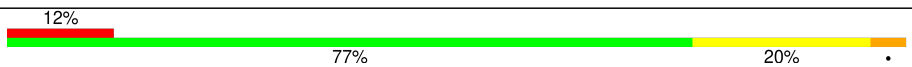
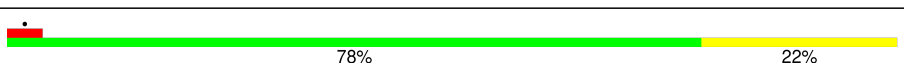
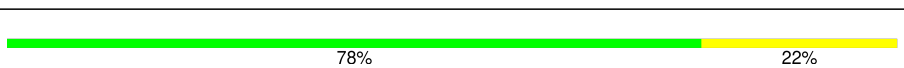
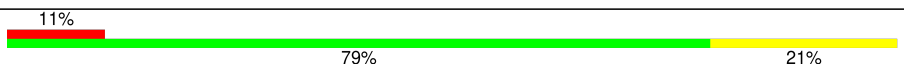
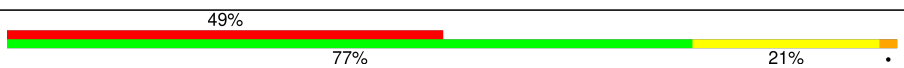
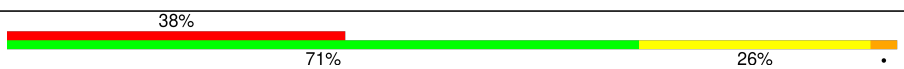
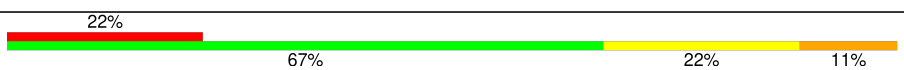
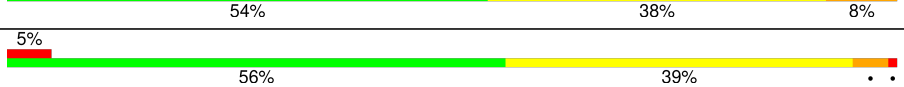
Mol	Chain	Length	Quality of chain
8	2	271	
9	20	117	
10	21	103	
11	22	110	
12	23	93	
13	24	102	
14	25	94	
15	27	76	
16	28	77	
17	29	63	
18	3	209	
19	30	58	
20	31	66	
21	32	56	
22	34	46	
23	35	64	
24	36	38	
25	4	201	
26	5	177	
27	6	176	
28	9	149	
29	M	9	
30	R1	2903	
31	R2	119	
32	R3	1531	

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Mol	Chain	Length	Quality of chain
33	sb	218	60% 94% 6%
34	sc	206	30% 98%
35	sd	205	36% 98%
36	se	157	18% 98%
37	sf	100	37% 98%
38	sg	151	44% 97%
39	sh	129	12% 95% 5%
40	si	127	50% 96%
41	sj	98	62% 96%
42	sk	116	27% 97%
43	sl	123	20% 97%
44	sm	114	44% 96%
45	sn	100	34% 94% 6%
46	so	88	15% 100%
47	sp	82	24% 95% 5%
48	sq	80	30% 99%
49	sr	65	32% 98%
50	ss	79	51% 94% 6%
51	st	85	25% 96%
52	su	65	63% 92% 6%
53	T	77	39% 44% 45% 8%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
53	H2U	T	20	X	-	-	-
53	4OC	T	32	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
53	MUM	T	54	X	-	-	-
53	4SU	T	8	X	-	-	-

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 143736 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 uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	13	142	1129	714	212	199	4	0	0

- Molecule 2 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	14	122	938	587	180	165	6	0	0

- Molecule 3 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	15	144	1053	654	207	190	2	0	0

- Molecule 4 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	16	136	1074	686	205	177	6	0	0

- Molecule 5 is a protein called Large ribosomal subunit protein bL17.

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

- Molecule 6 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	18	116	892	552	178	162	0	0

- Molecule 7 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	19	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 8 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	2	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 9 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	20	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 10 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	21	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 11 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	22	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 12 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	23	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 13 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	24	102	Total	C	N	O	0	0
			779	492	146	141		

- Molecule 14 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	25	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 15 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	27	76	Total	C	N	O	S	0	0
			582	360	117	104	1		

- Molecule 16 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	28	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 17 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	29	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 18 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	3	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 19 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	30	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 20 is a protein called Large ribosomal subunit protein bL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	31	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 21 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	32	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 22 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	34	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 23 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	35	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 24 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	36	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 25 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	4	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 26 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	5	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 27 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	6	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 28 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	9	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 29 is a RNA chain called mRNA.

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

- Molecule 30 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	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 31 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 32 is a RNA chain called 16S ribosomal RNA.

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

- Molecule 33 is a protein called Small ribosomal subunit protein uS2.

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

- Molecule 34 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 35 is a protein called 30S ribosomal protein S4.

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

- Molecule 36 is a protein called Small ribosomal subunit protein uS5.

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

- Molecule 37 is a protein called 30S ribosomal protein S6, non-modified isoform.

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

- Molecule 38 is a protein called 30S ribosomal protein S7.

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

- Molecule 39 is a protein called 30S ribosomal protein S8.

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

- Molecule 40 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 41 is a protein called 30S ribosomal protein S10.

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

- Molecule 42 is a protein called Small ribosomal subunit protein uS11.

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

- Molecule 43 is a protein called Small ribosomal subunit protein uS12.

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

- Molecule 44 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	sm	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 45 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 46 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 47 is a protein called Small ribosomal subunit protein bS16.

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

- Molecule 48 is a protein called Small ribosomal subunit protein uS17.

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

- Molecule 49 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	sr	65	Total	C	N	O	S	0	0
			535	339	100	95	1		

- Molecule 50 is a protein called 30S ribosomal protein S19.

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

- Molecule 51 is a protein called 30S ribosomal protein S20.

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

- Molecule 52 is a protein called Small ribosomal subunit protein bS21.

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

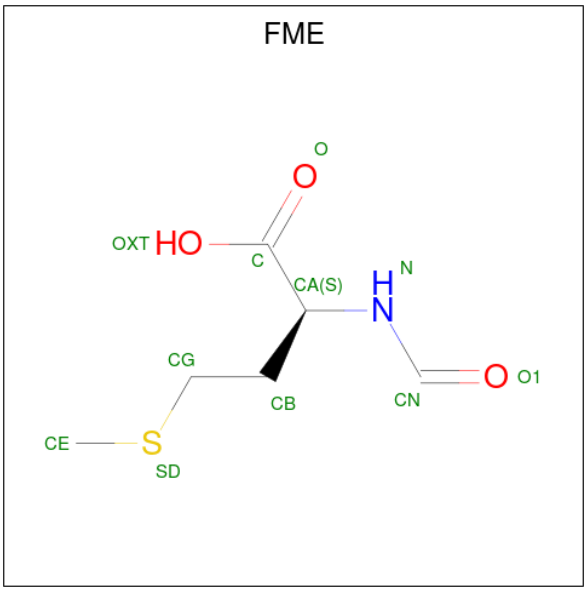
- Molecule 53 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	T	77	Total	C	N	O	P	S	0	0
			1639	734	294	534	76	1		

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
54	R1	111	Total	Mg	0
			111	111	
54	R3	41	Total	Mg	0
			41	41	

- Molecule 55 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: $C_6H_{11}NO_3S$).

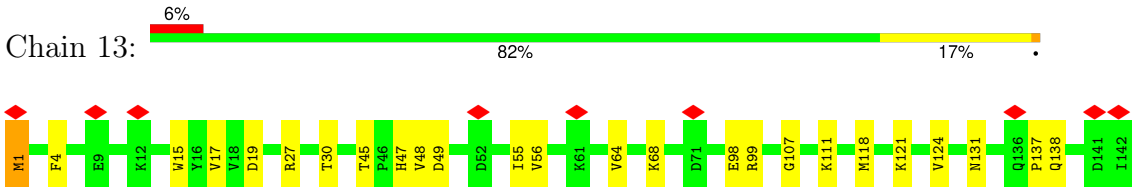


Mol	Chain	Residues	Atoms					AltConf
55	T	1	Total	C	N	O	S	0
			10	6	1	2	1	

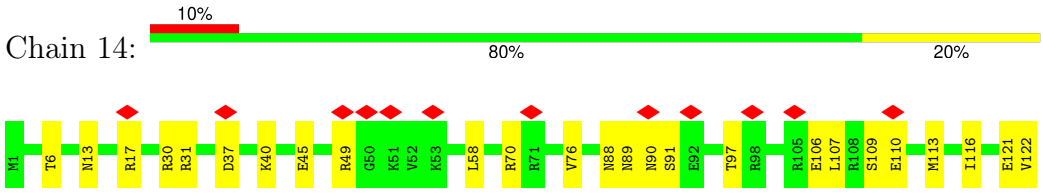
3 Residue-property plots (i)

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.

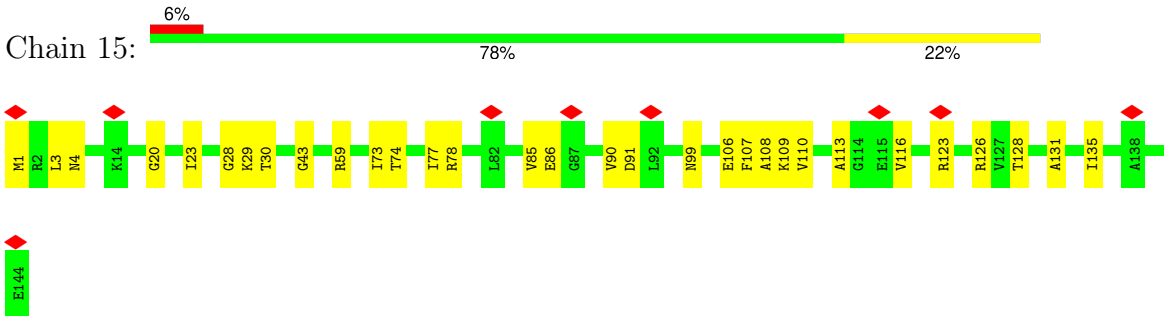
• Molecule 1: Large ribosomal subunit protein uL13



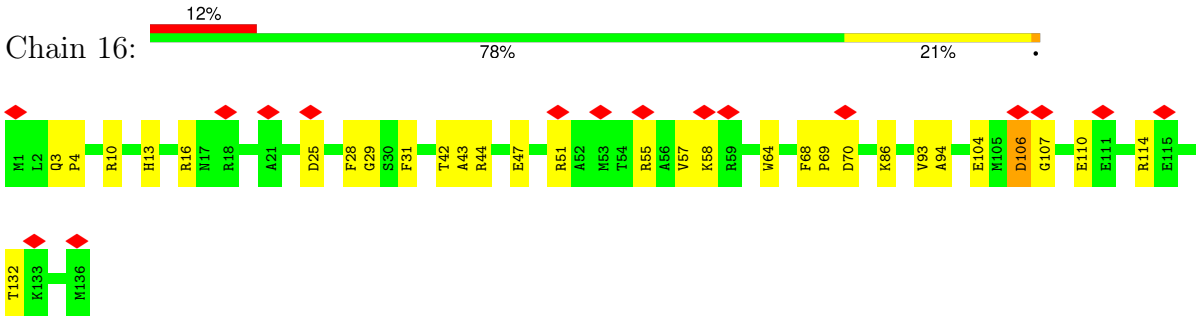
• Molecule 2: 50S ribosomal protein L14



• Molecule 3: Large ribosomal subunit protein uL15

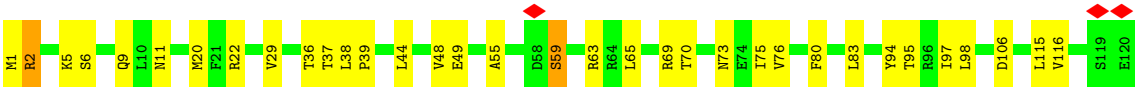


• Molecule 4: 50S ribosomal protein L16



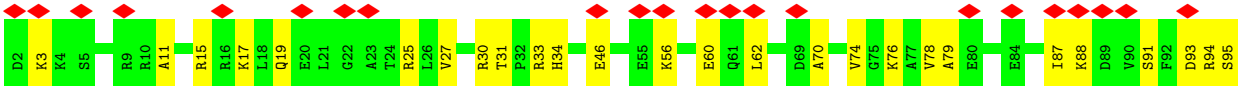
• Molecule 5: Large ribosomal subunit protein bL17

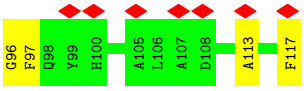
Chain 17:



• Molecule 6: Large ribosomal subunit protein uL18

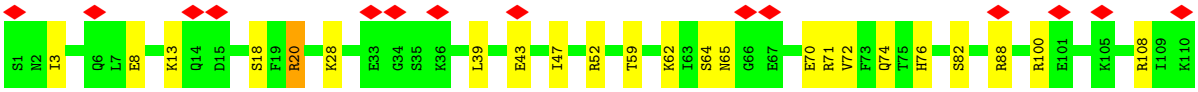
Chain 18:





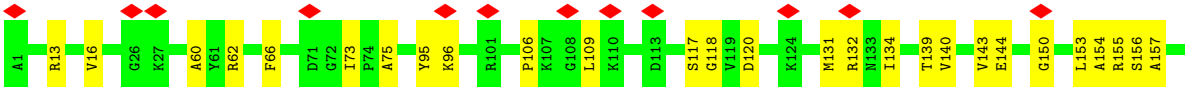
• Molecule 7: 50S ribosomal protein L19

Chain 19:



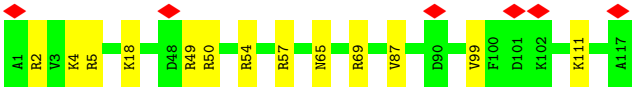
• Molecule 8: 50S ribosomal protein L2

Chain 2:



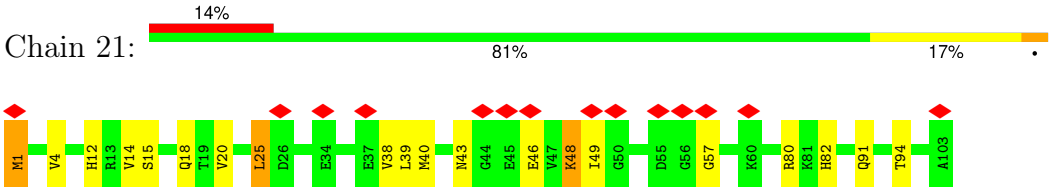
• Molecule 9: Large ribosomal subunit protein bL20

Chain 20:



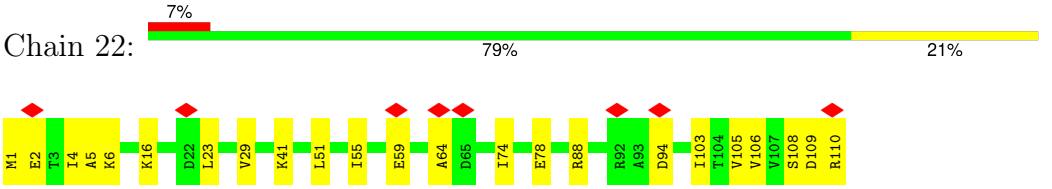
• Molecule 10: Large ribosomal subunit protein bL21

Chain 21:



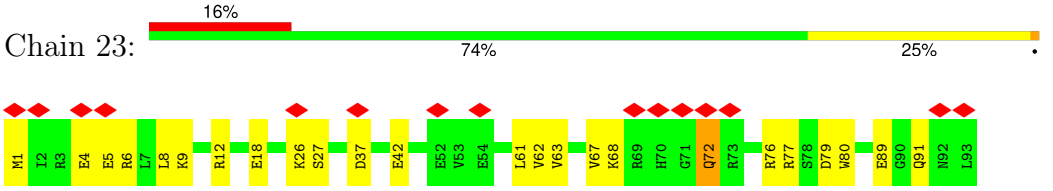
• Molecule 11: Large ribosomal subunit protein uL22

Chain 22:



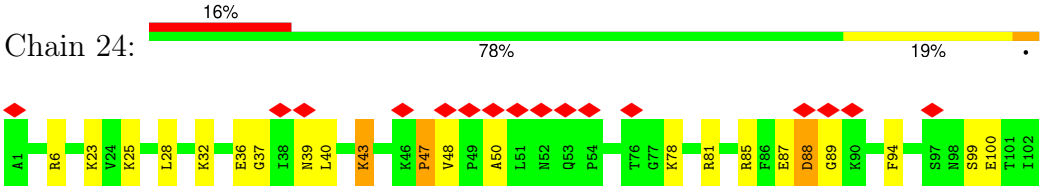
• Molecule 12: Large ribosomal subunit protein uL23

Chain 23:



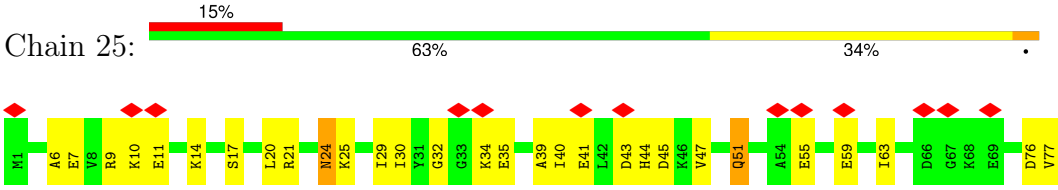
• Molecule 13: Large ribosomal subunit protein uL24

Chain 24:



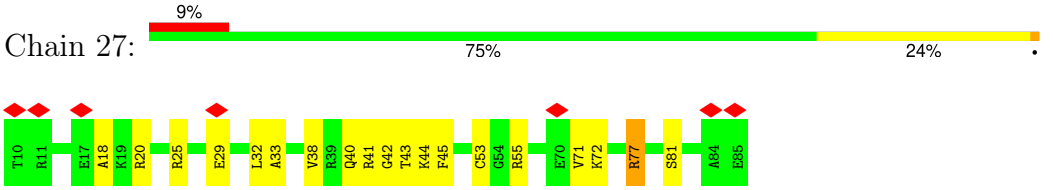
• Molecule 14: Large ribosomal subunit protein bL25

Chain 25:



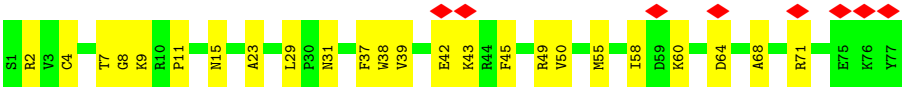
• Molecule 15: Large ribosomal subunit protein bL27

Chain 27:

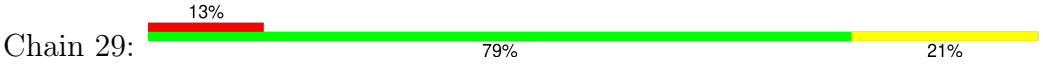


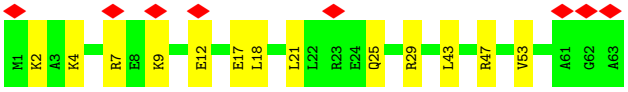
• Molecule 16: 50S ribosomal protein L28

Chain 28:

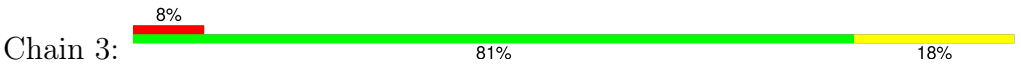


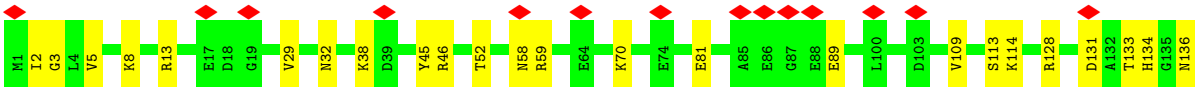
• Molecule 17: Large ribosomal subunit protein uL29

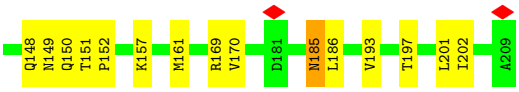




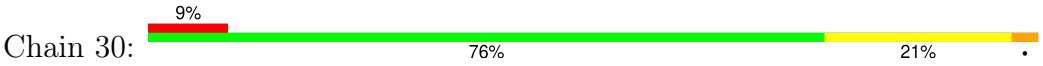
• Molecule 18: 50S ribosomal protein L3

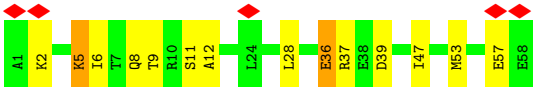




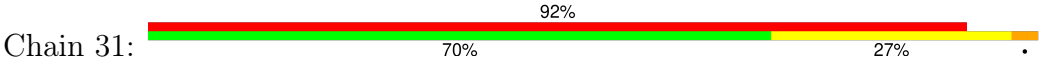


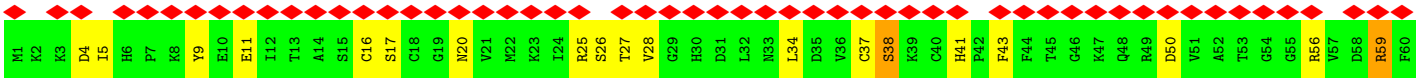
• Molecule 19: 50S ribosomal protein L30

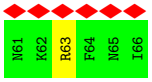




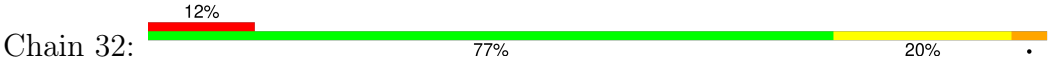
• Molecule 20: Large ribosomal subunit protein bL31

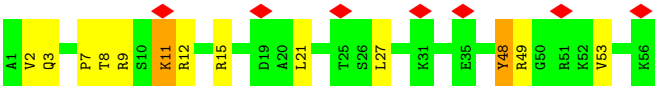






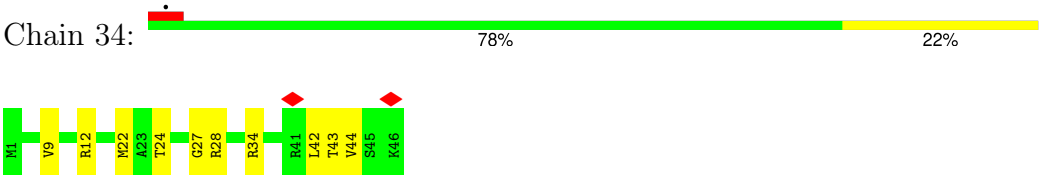
• Molecule 21: 50S ribosomal protein L32





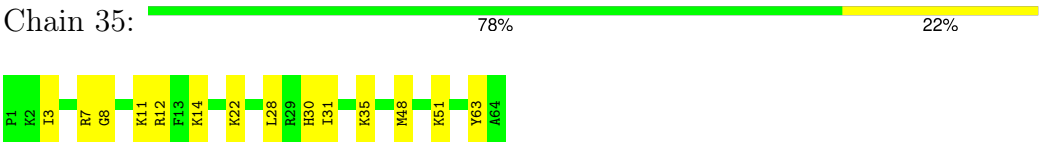
• Molecule 22: 50S ribosomal protein L34

Chain 34:



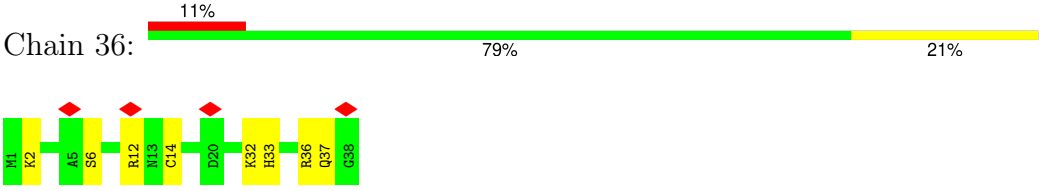
• Molecule 23: Large ribosomal subunit protein bL35

Chain 35:



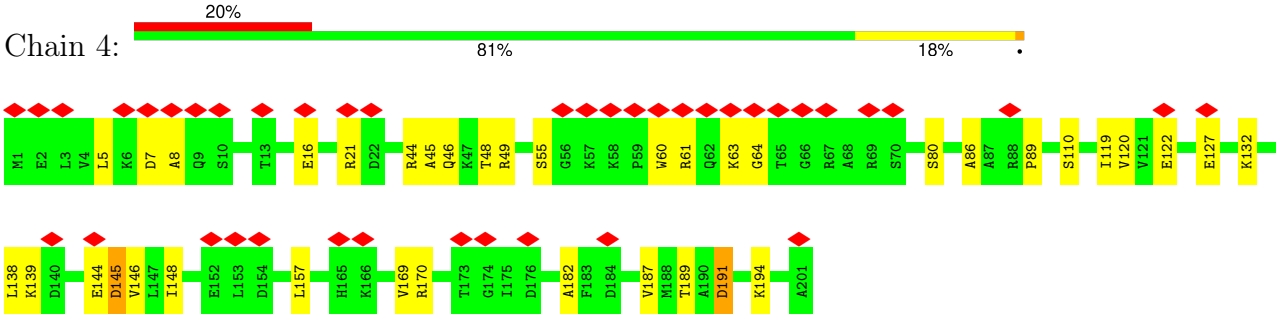
• Molecule 24: 50S ribosomal protein L36

Chain 36:



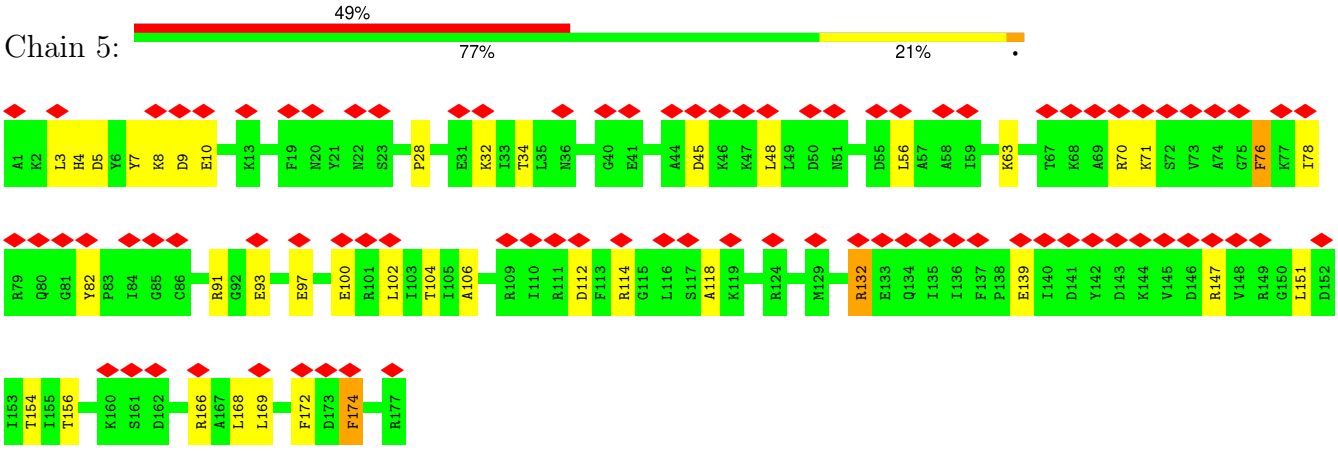
• Molecule 25: Large ribosomal subunit protein uL4

Chain 4:



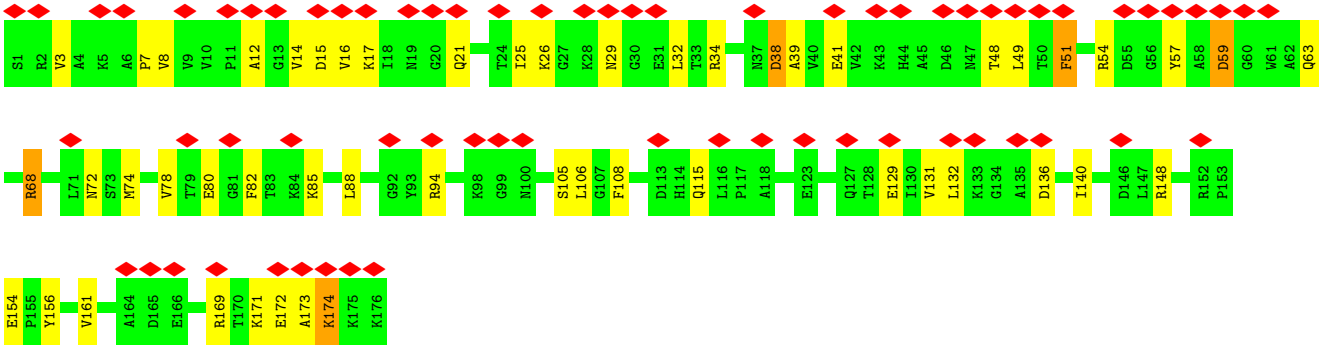
• Molecule 26: 50S ribosomal protein L5

Chain 5:



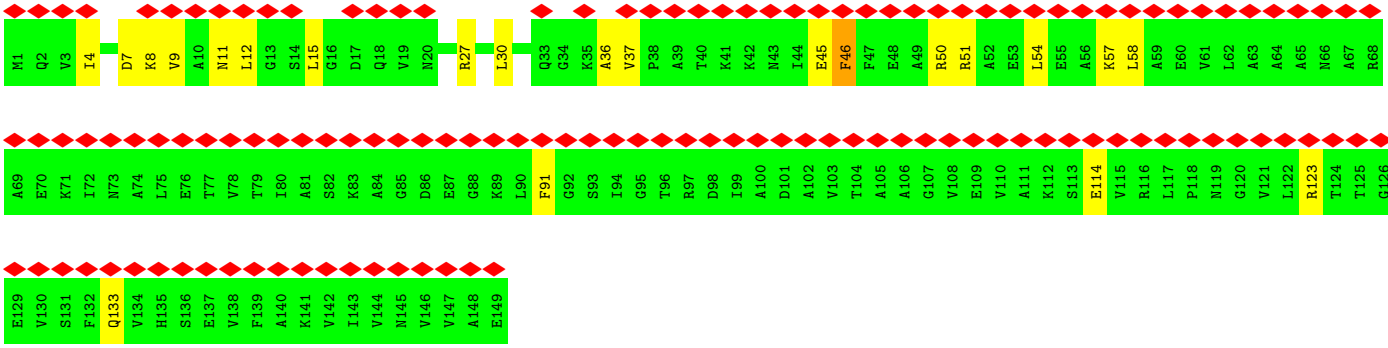
• Molecule 27: Large ribosomal subunit protein uL6

Chain 6:



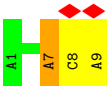
• Molecule 28: Large ribosomal subunit protein bL9

Chain 9:



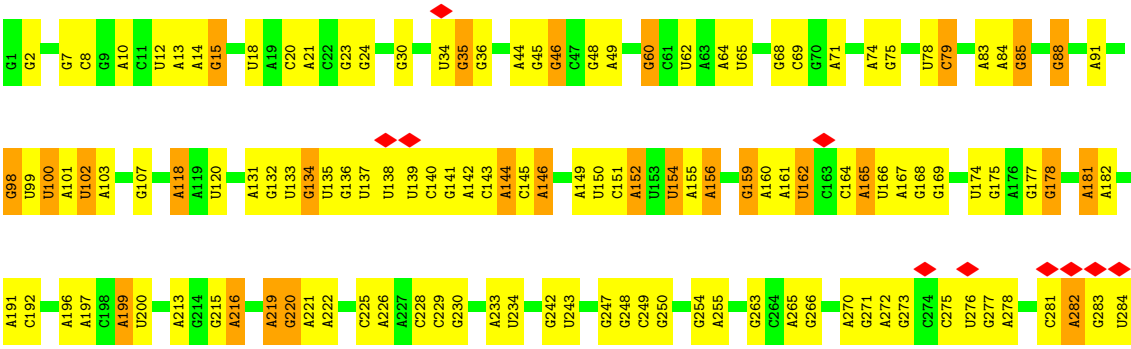
• Molecule 29: mRNA

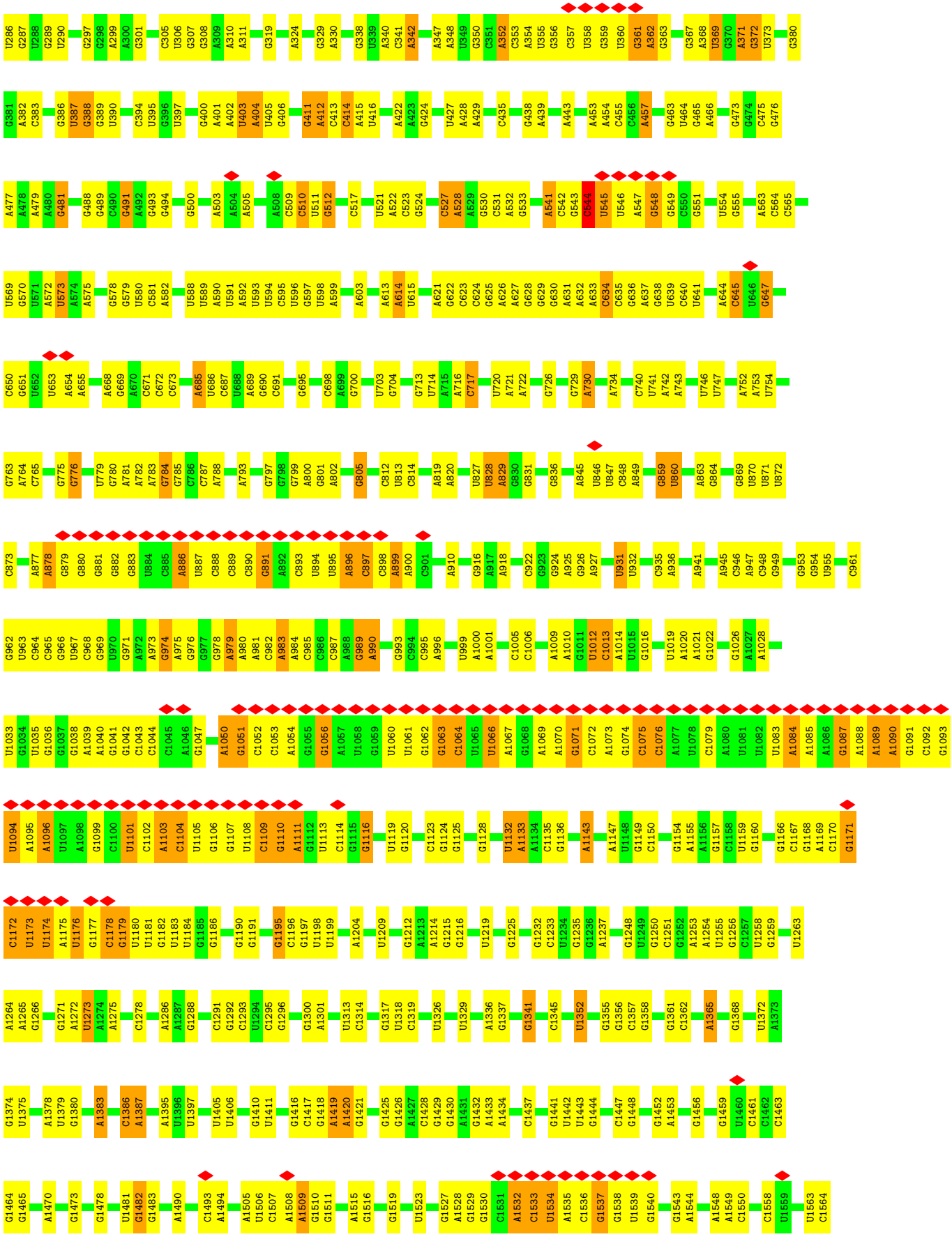
Chain M:

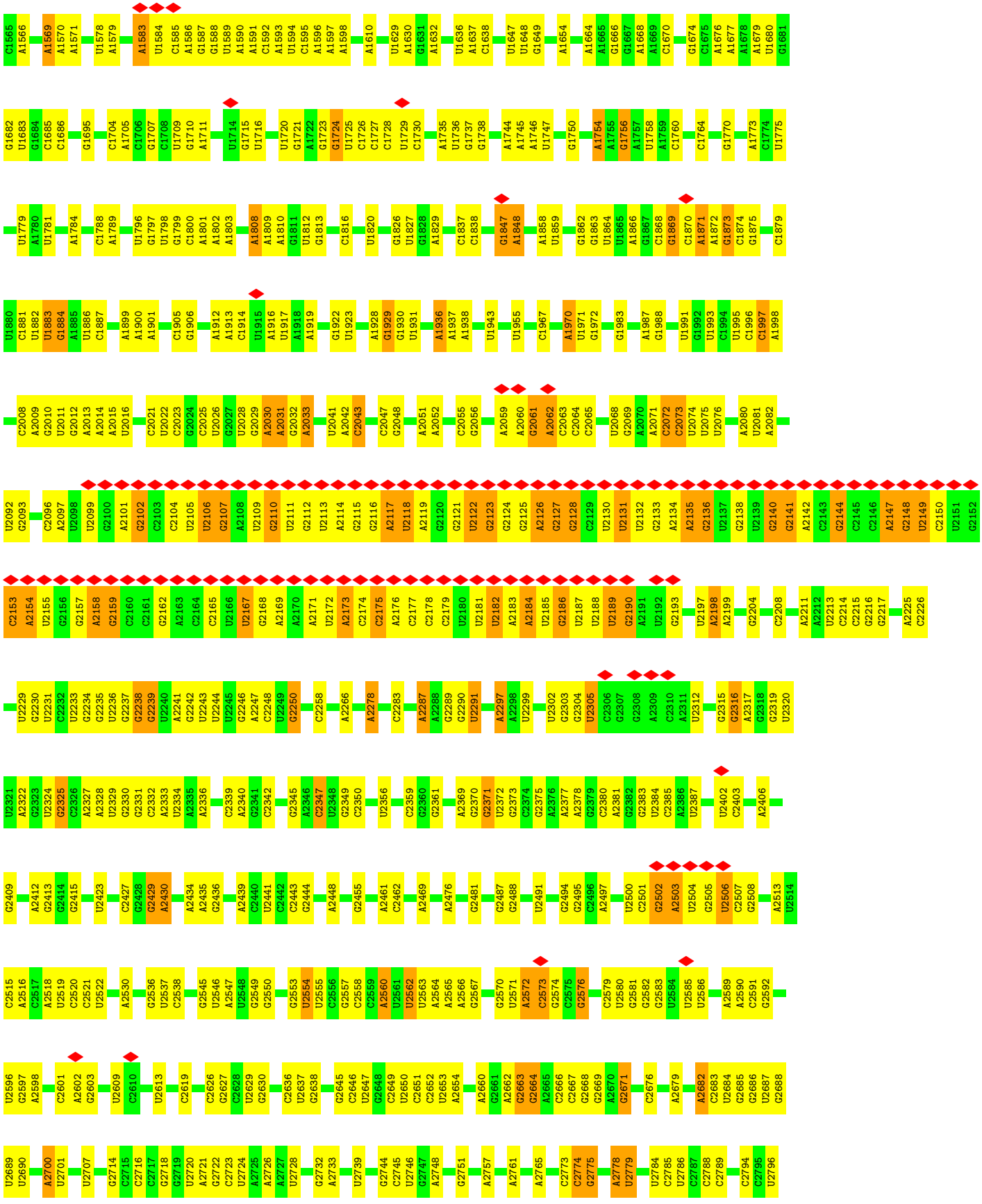


• Molecule 30: 23S ribosomal RNA

Chain R1:

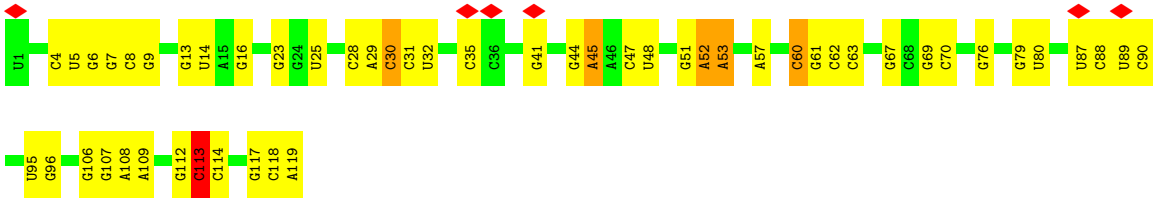






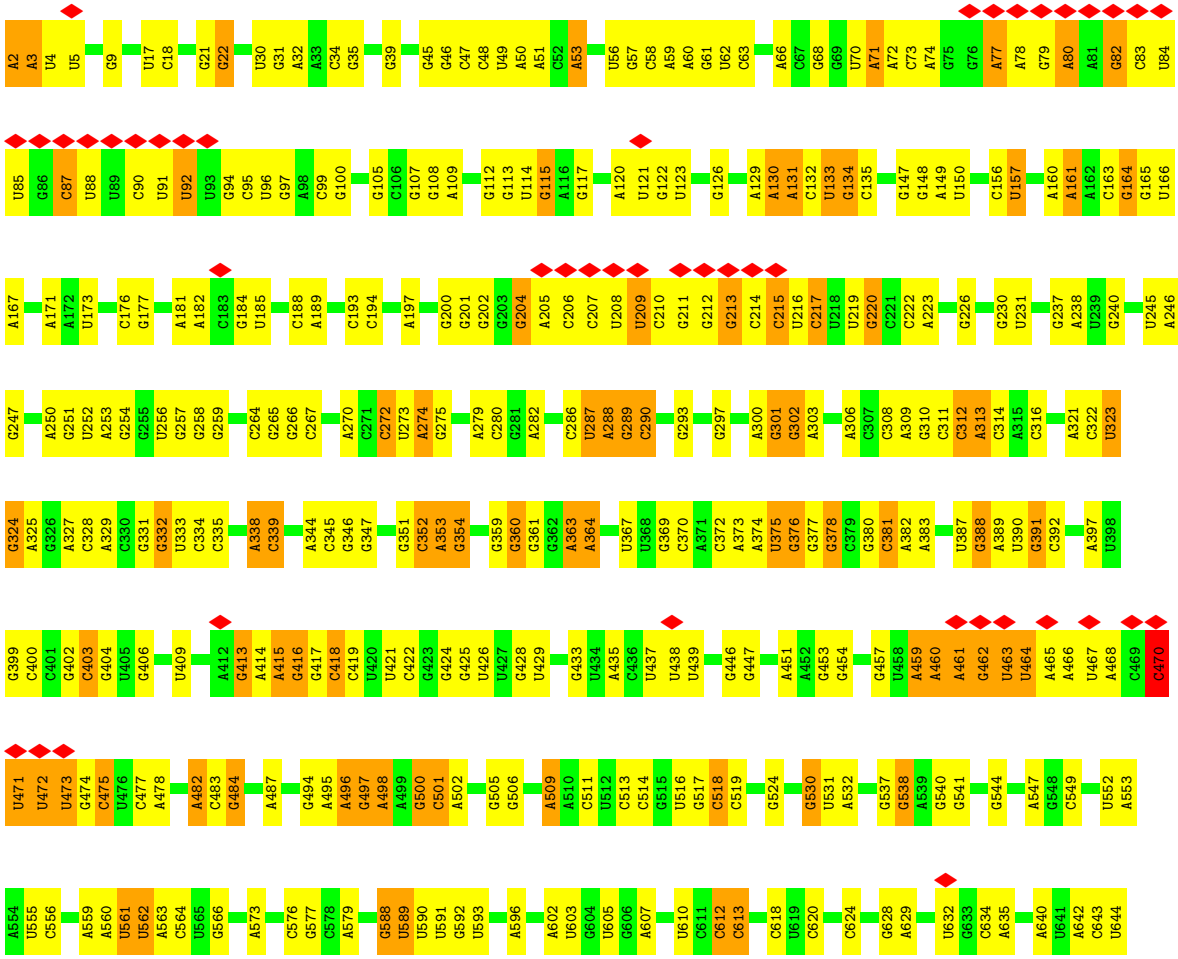
• Molecule 31: 5S ribosomal RNA

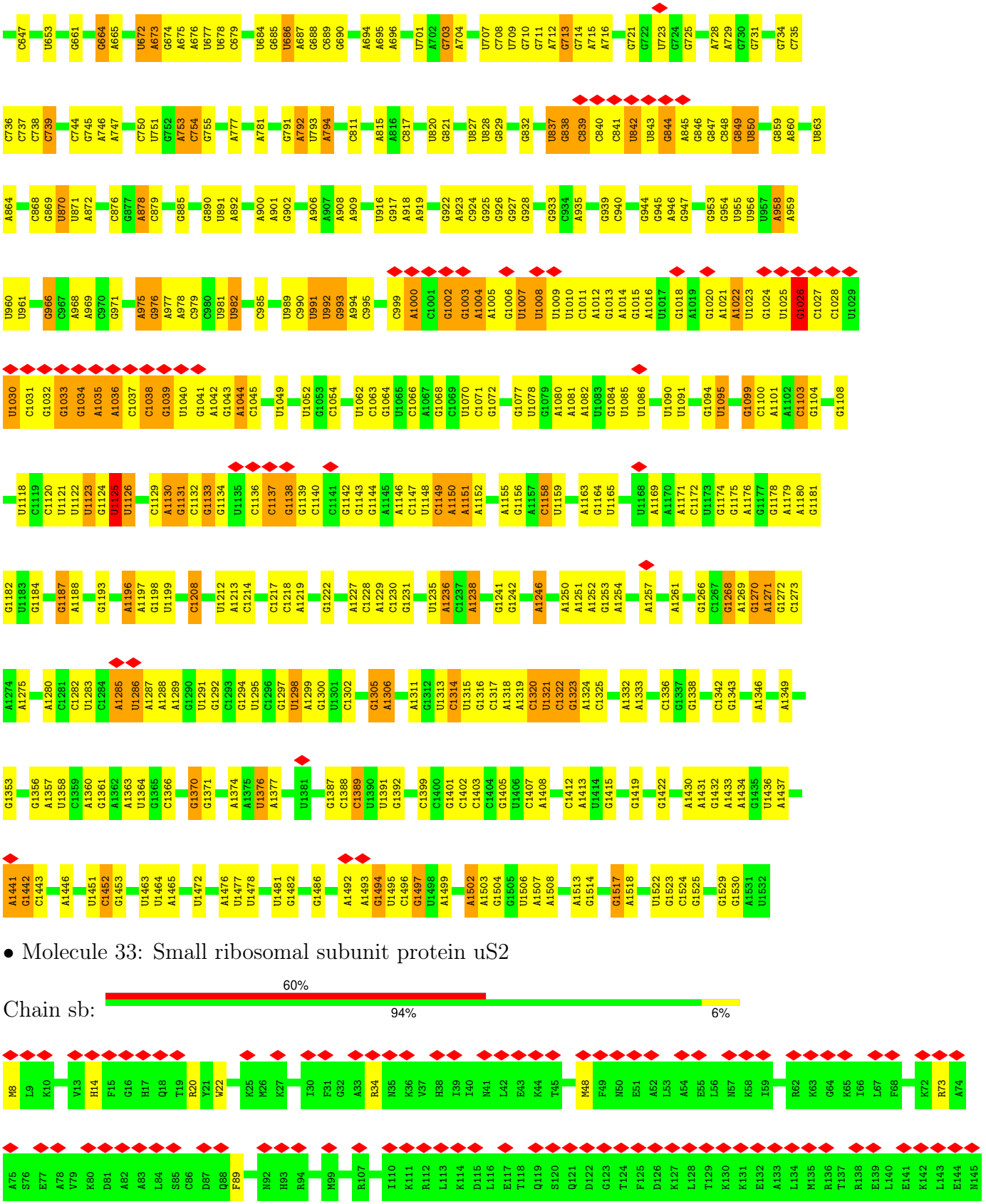
Chain R2:



• Molecule 32: 16S ribosomal RNA

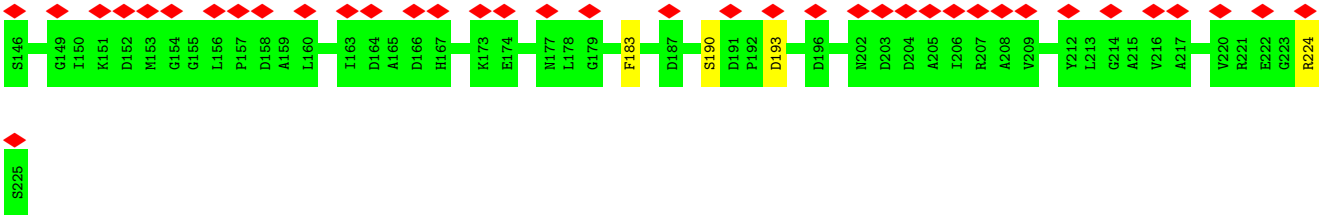
Chain R3:



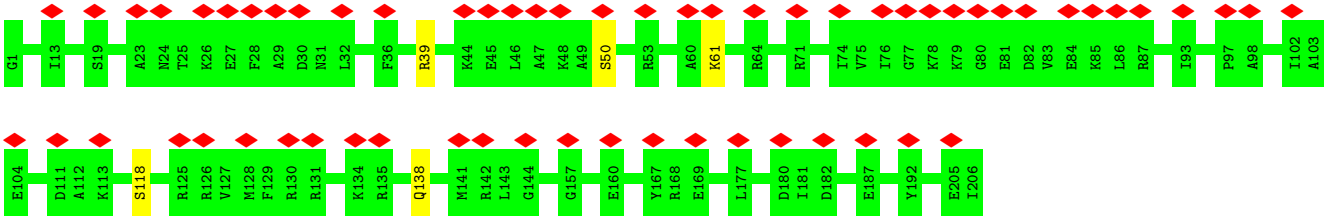


• Molecule 33: Small ribosomal subunit protein uS2

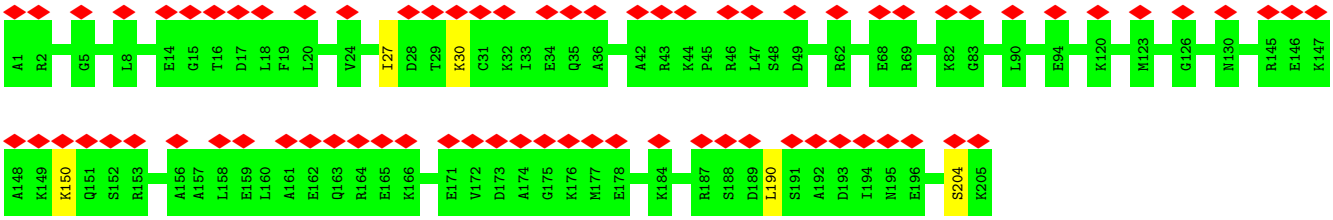
Chain sb:



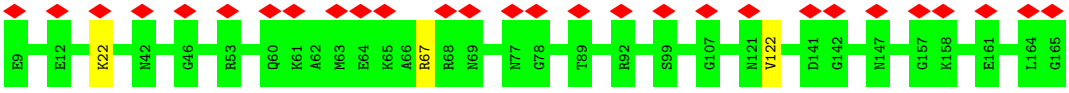
• Molecule 34: Small ribosomal subunit protein uS3



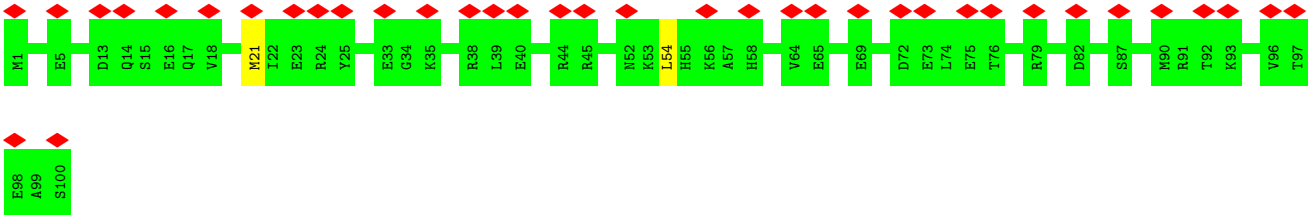
• Molecule 35: 30S ribosomal protein S4



• Molecule 36: Small ribosomal subunit protein uS5

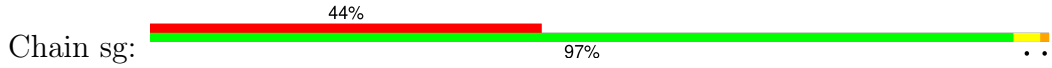


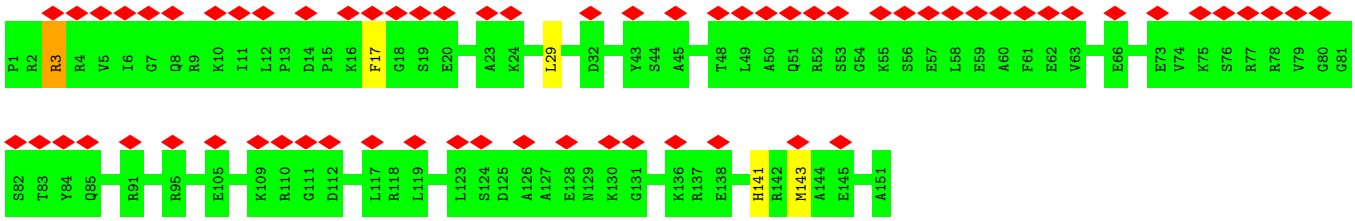
• Molecule 37: 30S ribosomal protein S6, non-modified isoform



• Molecule 38: 30S ribosomal protein S7

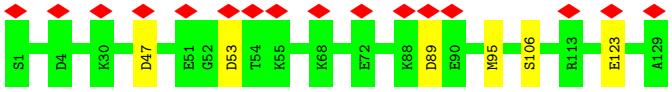
Chain sg:





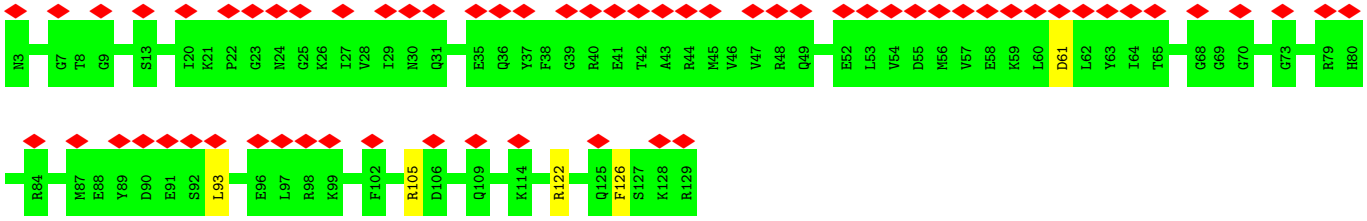
• Molecule 39: 30S ribosomal protein S8

Chain sh:



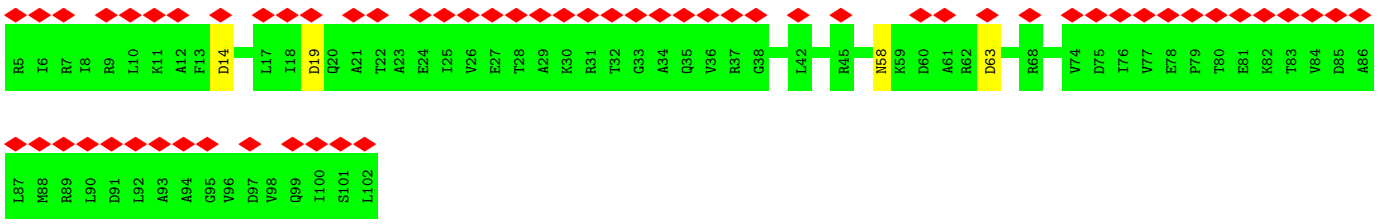
• Molecule 40: Small ribosomal subunit protein uS9

Chain si:



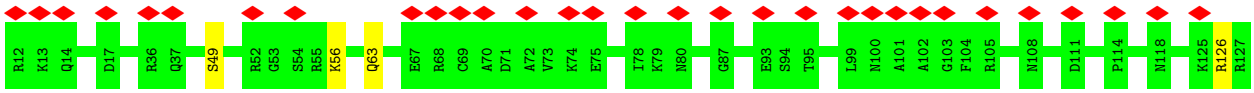
• Molecule 41: 30S ribosomal protein S10

Chain sj:



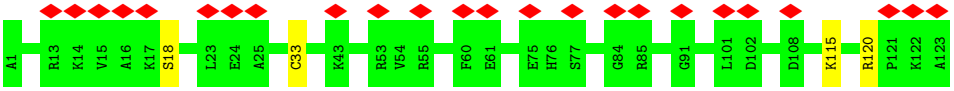
• Molecule 42: Small ribosomal subunit protein uS11

Chain sk:

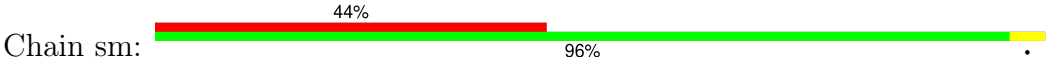


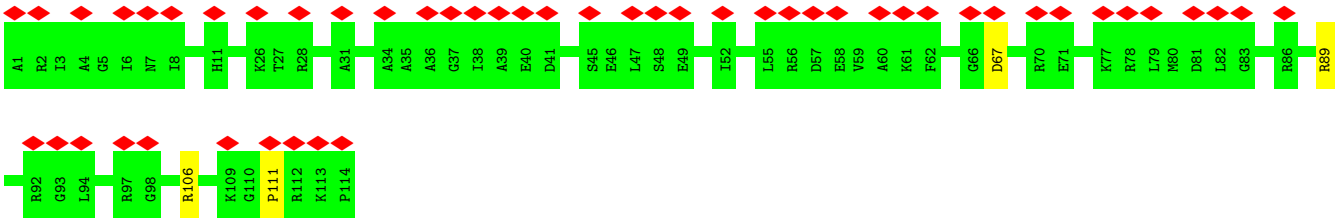
• Molecule 43: Small ribosomal subunit protein uS12

Chain sl:

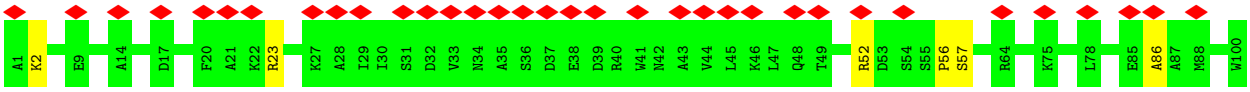


• Molecule 44: 30S ribosomal protein S13

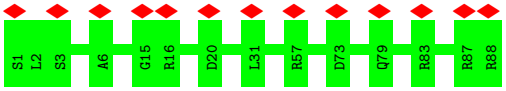




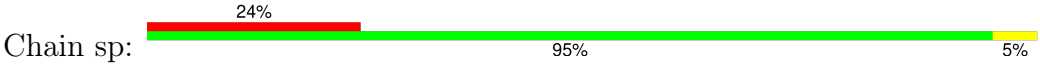
• Molecule 45: Small ribosomal subunit protein uS14

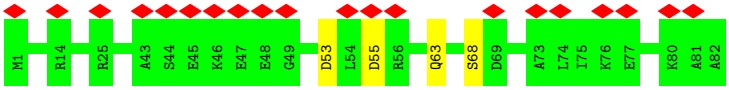


• Molecule 46: Small ribosomal subunit protein uS15

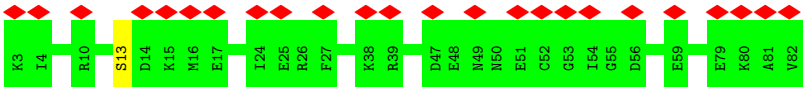


• Molecule 47: Small ribosomal subunit protein bS16

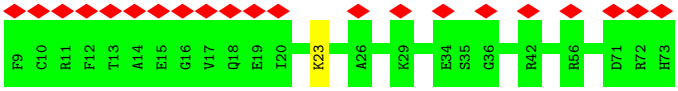




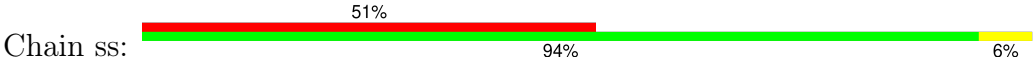
• Molecule 48: Small ribosomal subunit protein uS17

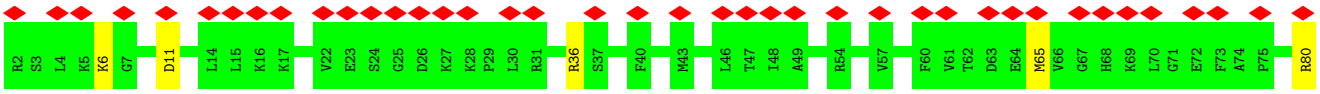


• Molecule 49: 30S ribosomal protein S18

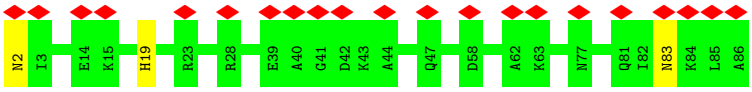


• Molecule 50: 30S ribosomal protein S19

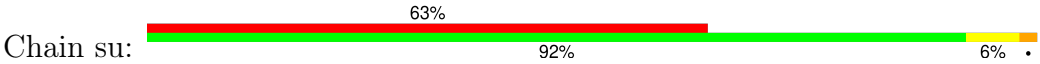


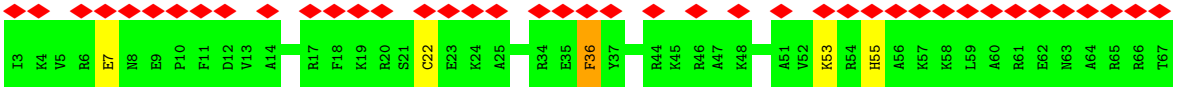


• Molecule 51: 30S ribosomal protein S20

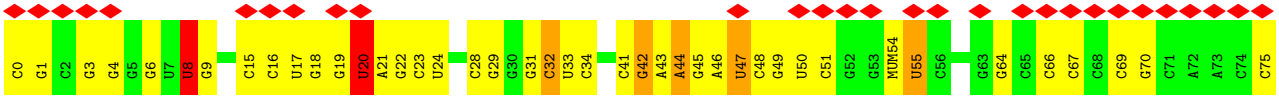


• Molecule 52: Small ribosomal subunit protein bS21





• Molecule 53: tRNA



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	78096	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	2.651	Depositor
Minimum map value	-1.658	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.138	Depositor
Recommended contour level	0.55	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 (i)

5.1 Standard geometry (i)

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

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	13	0.28	0/1152	0.54	1/1551 (0.1%)
2	14	0.28	0/947	0.61	0/1268
3	15	0.27	0/1062	0.57	0/1413
4	16	0.28	0/1093	0.59	0/1460
5	17	0.25	0/973	0.58	0/1301
6	18	0.27	0/902	0.57	0/1209
7	19	0.29	0/929	0.57	0/1242
8	2	0.28	0/2121	0.57	0/2852
9	20	0.28	0/960	0.56	0/1278
10	21	0.27	0/829	0.56	0/1107
11	22	0.26	0/864	0.54	0/1156
12	23	0.29	0/744	0.63	0/994
13	24	0.33	0/787	0.64	1/1051 (0.1%)
14	25	0.26	0/766	0.51	0/1025
15	27	0.27	0/589	0.58	0/779
16	28	0.28	0/635	0.61	0/848
17	29	0.25	0/510	0.53	0/677
18	3	0.27	0/1586	0.56	0/2134
19	30	0.26	0/453	0.56	0/605
20	31	0.24	0/531	0.52	0/709
21	32	0.28	0/450	0.57	0/599
22	34	0.25	0/380	0.64	0/498
23	35	0.26	0/513	0.51	0/676
24	36	0.27	0/303	0.62	0/397
25	4	0.27	0/1571	0.50	0/2113
26	5	0.30	0/1434	0.60	1/1926 (0.1%)
27	6	0.27	0/1343	0.55	1/1816 (0.1%)
28	9	0.26	0/1122	0.55	0/1515
29	M	0.24	0/219	0.70	0/339
30	R1	0.32	0/69794	0.81	18/108878 (0.0%)
31	R2	0.26	0/2847	0.80	3/4440 (0.1%)
32	R3	0.30	0/36782	0.84	20/57377 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	sb	0.25	0/1735	0.52	1/2338 (0.0%)
34	sc	0.25	0/1651	0.54	0/2225
35	sd	0.27	0/1665	0.59	1/2227 (0.0%)
36	se	0.28	0/1169	0.59	0/1573
37	sf	0.27	0/835	0.66	1/1128 (0.1%)
38	sg	0.25	0/1195	0.58	2/1602 (0.1%)
39	sh	0.27	0/989	0.57	1/1326 (0.1%)
40	si	0.26	0/1034	0.64	0/1375
41	sj	0.25	0/796	0.62	1/1077 (0.1%)
42	sk	0.27	0/885	0.57	0/1195
43	sl	0.27	0/969	0.62	0/1300
44	sm	0.25	0/892	0.61	0/1193
45	sn	0.25	0/817	0.60	0/1088
46	so	0.24	0/722	0.53	0/964
47	sp	0.27	0/659	0.63	1/884 (0.1%)
48	sq	0.28	0/657	0.64	0/881
49	sr	0.25	0/544	0.55	0/731
50	ss	0.29	0/652	0.59	0/877
51	st	0.24	0/671	0.52	0/888
52	su	0.28	0/550	0.77	0/728
53	T	0.24	0/1716	0.80	0/2672
All	All	0.30	0/155994	0.76	53/233505 (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
35	sd	0	1
38	sg	0	1
45	sn	0	1
52	su	0	1
53	T	6	0
All	All	6	4

There are no bond length outliers.

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	24	47	PRO	CA-N-CD	-8.64	99.41	111.50
37	sf	54	LEU	CA-CB-CG	7.57	132.70	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	R3	470	C	N1-C2-O2	7.49	123.39	118.90
32	R3	470	C	C2-N1-C1'	7.42	126.96	118.80
32	R3	1208	C	C2-N1-C1'	7.23	126.75	118.80
32	R3	1134	G	N1-C6-O6	-6.95	115.73	119.90
32	R3	1007	U	C2-N1-C1'	6.59	125.61	117.70
30	R1	1313	U	C2-N1-C1'	6.35	125.32	117.70
32	R3	217	C	N3-C2-O2	-6.34	117.46	121.90
33	sb	8	MET	CA-CB-CG	6.10	123.67	113.30
30	R1	510	C	N1-C2-O2	6.09	122.55	118.90
32	R3	1134	G	C5-C6-O6	6.07	132.24	128.60
32	R3	1007	U	N1-C2-O2	6.01	127.01	122.80
30	R1	1533	C	N1-C2-O2	5.88	122.43	118.90
32	R3	470	C	N3-C2-O2	-5.85	117.81	121.90
30	R1	2342	C	N3-C2-O2	-5.83	117.82	121.90
32	R3	1389	C	N1-C2-O2	5.80	122.38	118.90
30	R1	1533	C	N3-C2-O2	-5.79	117.84	121.90
30	R1	544	C	C2-N1-C1'	5.74	125.12	118.80
38	sg	29	LEU	CA-CB-CG	5.68	128.37	115.30
30	R1	2573	C	C2-N1-C1'	5.65	125.01	118.80
32	R3	1007	U	N3-C2-O2	-5.65	118.25	122.20
32	R3	1208	C	C6-N1-C1'	-5.63	114.04	120.80
32	R3	1158	C	C2-N1-C1'	5.58	124.94	118.80
31	R2	60	C	C2-N1-C1'	5.54	124.89	118.80
27	6	38	ASP	CB-CG-OD1	5.50	123.25	118.30
1	13	1	MET	CA-CB-CG	5.49	122.63	113.30
32	R3	1125	U	C2-N1-C1'	5.49	124.28	117.70
32	R3	1140	C	C2-N1-C1'	5.46	124.81	118.80
26	5	45	ASP	CB-CG-OD1	5.41	123.17	118.30
35	sd	190	LEU	CA-CB-CG	5.40	127.73	115.30
30	R1	1314	C	C2-N1-C1'	5.40	124.74	118.80
30	R1	2840	C	C2-N1-C1'	5.36	124.70	118.80
30	R1	2573	C	N1-C2-O2	5.35	122.11	118.90
32	R3	1389	C	N3-C2-O2	-5.29	118.20	121.90
47	sp	53	ASP	CB-CG-OD1	5.28	123.05	118.30
32	R3	1026	G	N9-C1'-C2'	-5.27	106.21	112.00
39	sh	95	MET	CA-CB-CG	5.27	122.25	113.30
30	R1	2073	C	C2-N1-C1'	5.25	124.58	118.80
41	sj	14	ASP	CB-CG-OD1	5.23	123.01	118.30
30	R1	512	G	O4'-C1'-N9	5.23	112.38	108.20
30	R1	2073	C	N3-C2-O2	-5.21	118.26	121.90
30	R1	2858	C	O4'-C1'-N1	-5.20	104.04	108.20
32	R3	470	C	C6-N1-C1'	-5.16	114.61	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	R3	620	C	C2-N1-C1'	5.13	124.44	118.80
31	R2	113	C	N1-C2-O2	5.11	121.97	118.90
38	sg	3	ARG	CA-CB-CG	5.10	124.62	113.40
32	R3	381	C	N1-C2-O2	5.10	121.96	118.90
30	R1	510	C	N3-C2-O2	-5.10	118.33	121.90
30	R1	687	C	N1-C2-O2	5.08	121.95	118.90
30	R1	88	G	C4-N9-C1'	5.04	133.05	126.50
30	R1	2573	C	N3-C2-O2	-5.03	118.38	121.90
31	R2	60	C	N1-C2-O2	5.02	121.91	118.90

All (6) chirality outliers are listed below:

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

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
35	sd	27	ILE	Peptide
38	sg	3	ARG	Peptide
45	sn	86	ALA	Peptide
52	su	7	GLU	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	13	1129	0	1162	15	0
2	14	938	0	1012	17	0
3	15	1053	0	1129	24	0
4	16	1074	0	1157	19	0
5	17	960	0	1000	23	0
6	18	892	0	923	27	0
7	19	917	0	965	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	2	2082	0	2157	36	0
9	20	947	0	1022	15	0
10	21	816	0	839	17	0
11	22	857	0	922	17	0
12	23	738	0	807	19	0
13	24	779	0	834	16	0
14	25	753	0	780	28	0
15	27	582	0	599	21	0
16	28	625	0	655	20	0
17	29	509	0	543	12	0
18	3	1565	0	1616	29	0
19	30	449	0	491	10	0
20	31	522	0	524	15	0
21	32	444	0	461	14	0
22	34	377	0	418	6	0
23	35	504	0	574	8	0
24	36	302	0	343	5	0
25	4	1552	0	1619	25	0
26	5	1410	0	1447	30	0
27	6	1323	0	1374	38	0
28	9	1111	0	1148	18	0
29	M	195	0	99	2	0
30	R1	62318	0	31348	810	0
31	R2	2546	0	1292	33	0
32	R3	32850	0	16534	419	0
33	sb	1704	0	1732	0	0
34	sc	1624	0	1699	0	0
35	sd	1643	0	1710	0	0
36	se	1156	0	1199	0	0
37	sf	817	0	808	0	0
38	sg	1181	0	1240	0	0
39	sh	979	0	1034	0	0
40	si	1022	0	1070	0	0
41	sj	786	0	828	0	0
42	sk	869	0	878	0	0
43	sl	955	0	1019	0	0
44	sm	883	0	944	0	0
45	sn	805	0	847	0	0
46	so	714	0	737	0	0
47	sp	649	0	666	0	0
48	sq	648	0	691	0	0
49	sr	535	0	552	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	ss	637	0	665	0	0
51	st	665	0	714	0	0
52	su	544	0	579	0	0
53	T	1639	0	831	27	0
54	R1	111	0	0	0	0
54	R3	41	0	0	0	0
55	T	10	0	10	0	0
All	All	143736	0	96247	1670	0

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

All (1670) 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)
32:R3:359:G:HO2'	32:R3:360:G:H8	1.04	0.95
30:R1:156:A:H2	30:R1:169:G:H1	1.00	0.94
30:R1:156:A:C2	30:R1:169:G:N1	2.36	0.94
30:R1:2545:G:H21	30:R1:2565:A:H8	1.15	0.92
32:R3:1002:G:H1	32:R3:1038:C:HO2'	0.93	0.92
30:R1:545:U:HO2'	30:R1:548:G:H1	1.18	0.89
28:9:9:VAL:HG12	28:9:11:ASN:H	1.36	0.89
32:R3:1151:A:N6	32:R3:1152:A:N6	2.22	0.87
30:R1:134:G:H1	30:R1:144:A:H2	1.22	0.84
32:R3:457:G:N2	32:R3:475:C:O2	2.10	0.83
32:R3:1026:G:N1	32:R3:1036:A:N6	2.26	0.83
32:R3:1009:U:H3	32:R3:1020:G:H1	1.27	0.82
30:R1:156:A:H2	30:R1:169:G:N1	1.74	0.81
30:R1:848:C:H2'	30:R1:849:A:H8	1.45	0.81
53:T:50:U:H3	53:T:64:G:H1	1.29	0.81
30:R1:880:G:N2	30:R1:897:C:N3	2.27	0.81
32:R3:457:G:N1	32:R3:475:C:N3	2.28	0.80
30:R1:284:U:O2	30:R1:356:G:N2	2.15	0.80
30:R1:1410:G:N2	30:R1:1592:C:O2	2.15	0.79
32:R3:674:G:H2'	32:R3:675:A:H8	1.49	0.78
30:R1:160:A:H8	30:R1:2217:G:H21	1.30	0.78
24:36:2:LYS:NZ	24:36:32:LYS:O	2.17	0.77
53:T:6:G:N2	53:T:66:C:O2	2.15	0.77
53:T:6:G:N1	53:T:66:C:N3	2.32	0.76
32:R3:380:G:N2	32:R3:383:A:OP2	2.19	0.76
30:R1:290:U:H3	30:R1:350:G:H1	1.33	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:R1:2304:G:H22	30:R1:2312:U:H3	1.32	0.75
18:3:151:THR:OG1	30:R1:2032:G:N2	2.20	0.75
30:R1:1056:G:N1	30:R1:1102:C:OP2	2.15	0.75
53:T:3:G:N1	53:T:69:C:N3	2.29	0.75
27:6:148:ARG:HA	27:6:161:VAL:HG21	1.68	0.74
32:R3:592:G:N2	32:R3:647:C:O2	2.16	0.74
30:R1:2073:C:H5	30:R1:2436:G:H1	1.33	0.74
30:R1:2127:G:H2'	30:R1:2128:G:H8	1.52	0.74
27:6:16:VAL:HG12	27:6:25:ILE:HG12	1.70	0.74
32:R3:58:C:O2'	32:R3:388:G:N2	2.21	0.74
4:16:55:ARG:NH1	30:R1:2469:A:O2'	2.20	0.73
9:20:65:ASN:ND2	30:R1:1010:A:OP1	2.22	0.73
25:4:44:ARG:NH2	30:R1:1248:G:OP1	2.18	0.73
30:R1:1779:U:OP2	30:R1:1784:A:N6	2.21	0.73
30:R1:1872:A:O2'	30:R1:1873:G:O4'	2.07	0.73
8:2:270:ARG:NH2	30:R1:1798:U:OP2	2.22	0.73
16:28:60:LYS:NZ	30:R1:371:A:O2'	2.20	0.73
30:R1:1170:C:HO2'	30:R1:1171:G:H8	1.35	0.72
5:17:2:ARG:HA	5:17:5:LYS:HD3	1.70	0.72
9:20:49:ARG:NH1	30:R1:993:G:OP1	2.22	0.72
30:R1:880:G:H2'	30:R1:881:G:H8	1.54	0.72
3:15:91:ASP:HB3	3:15:123:ARG:HB3	1.71	0.72
32:R3:1356:G:H2'	32:R3:1357:A:H8	1.54	0.72
16:28:55:MET:HE3	28:9:27:ARG:HH12	1.54	0.72
30:R1:1063:G:N2	30:R1:1076:C:OP1	2.23	0.72
30:R1:284:U:H3	30:R1:356:G:H1	1.37	0.72
32:R3:1316:G:N2	32:R3:1319:A:OP2	2.23	0.72
4:16:47:GLU:OE1	4:16:51:ARG:NH2	2.23	0.71
8:2:257:ARG:NH1	30:R1:1799:G:OP1	2.23	0.71
30:R1:132:G:H1	30:R1:146:A:H62	1.38	0.71
32:R3:1151:A:C6	32:R3:1152:A:N6	2.58	0.71
53:T:3:G:N2	53:T:69:C:O2	2.15	0.71
8:2:143:VAL:HB	8:2:153:LEU:HB2	1.72	0.71
30:R1:2581:G:OP2	30:R1:2581:G:N2	2.23	0.71
32:R3:673:A:H2'	32:R3:674:G:C8	2.25	0.71
30:R1:134:G:O6	30:R1:144:A:N1	2.23	0.70
32:R3:1151:A:N6	32:R3:1152:A:H62	1.89	0.70
30:R1:1069:A:H1'	30:R1:1096:A:H4'	1.73	0.70
31:R2:112:G:O2'	31:R2:113:C:O2	2.07	0.70
32:R3:1077:G:N2	32:R3:1080:A:OP2	2.23	0.70
30:R1:156:A:N1	30:R1:169:G:O6	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:R1:1862:G:O6	30:R1:1881:C:N4	2.25	0.70
30:R1:277:G:OP2	30:R1:277:G:N2	2.20	0.70
30:R1:2324:U:H3'	30:R1:2325:G:H5"	1.74	0.70
30:R1:2144:G:N3	30:R1:2148:G:N2	2.40	0.69
30:R1:2101:A:H2'	30:R1:2102:G:C8	2.27	0.69
19:30:8:GLN:HB2	19:30:28:LEU:HD23	1.75	0.69
2:14:121:GLU:HG3	2:14:122:VAL:HG23	1.74	0.69
12:23:89:GLU:N	12:23:89:GLU:OE2	2.24	0.69
30:R1:1410:G:N1	30:R1:1592:C:N3	2.37	0.69
30:R1:414:C:H5	30:R1:2409:G:H1	1.42	0.68
10:21:15:SER:H	10:21:18:GLN:HE22	1.40	0.68
30:R1:1597:A:H5"	30:R1:1598:A:H5'	1.76	0.68
4:16:69:PRO:HA	4:16:94:ALA:HB2	1.75	0.67
30:R1:1912:A:O2'	32:R3:1494:G:O2'	2.11	0.67
32:R3:1298:U:O2	32:R3:1299:A:N6	2.28	0.67
30:R1:1288:G:N2	30:R1:1288:G:OP2	2.27	0.67
32:R3:592:G:N1	32:R3:647:C:N3	2.35	0.67
53:T:32:4OC:O2'	53:T:32:4OC:O2	2.13	0.67
7:19:20:ARG:NH2	30:R1:2849:U:O4	2.27	0.67
27:6:3:VAL:HG12	27:6:68:ARG:HD2	1.74	0.67
5:17:37:THR:HG22	5:17:39:PRO:HD2	1.76	0.67
30:R1:1539:U:H2'	30:R1:1540:G:H8	1.60	0.67
27:6:108:PHE:O	30:R1:2666:C:N4	2.22	0.67
18:3:128:ARG:NH2	30:R1:1995:U:OP1	2.28	0.66
32:R3:200:G:H2'	32:R3:201:G:C8	2.30	0.66
32:R3:459:A:N7	32:R3:460:A:N6	2.43	0.66
3:15:20:GLY:HA2	3:15:28:GLY:HA2	1.77	0.66
32:R3:21:G:H2'	32:R3:22:G:C8	2.30	0.66
32:R3:109:A:H62	32:R3:324:G:H21	1.42	0.66
32:R3:634:C:H2'	32:R3:635:A:H8	1.61	0.66
30:R1:154:U:O4	30:R1:155:A:N6	2.28	0.66
30:R1:521:U:H2'	30:R1:522:A:H8	1.59	0.66
30:R1:1216:G:N2	30:R1:1233:C:O2	2.18	0.66
32:R3:115:G:O2'	32:R3:289:G:H5'	1.95	0.66
18:3:38:LYS:NZ	18:3:81:GLU:OE1	2.28	0.66
19:30:36:GLU:O	19:30:37:ARG:NH1	2.28	0.66
30:R1:527:C:N4	30:R1:2779:U:OP2	2.28	0.66
32:R3:297:G:N2	32:R3:300:A:OP2	2.28	0.66
6:18:17:LYS:HE2	6:18:17:LYS:HA	1.77	0.66
32:R3:1034:G:H2'	32:R3:1035:A:C8	2.31	0.66
10:21:4:VAL:HG23	10:21:39:LEU:HB2	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:5:76:PHE:HB3	26:5:78:ILE:HG23	1.78	0.66
12:23:18:GLU:OE2	12:23:18:GLU:N	2.20	0.66
14:25:9:ARG:HG3	14:25:41:GLU:HB2	1.76	0.66
30:R1:976:G:HO2'	30:R1:1155:A:HO2'	1.41	0.66
30:R1:2645:G:OP2	30:R1:2645:G:N2	2.25	0.66
32:R3:811:C:O2'	32:R3:901:A:N1	2.29	0.66
30:R1:2107:G:H1	30:R1:2182:U:H3	1.44	0.66
8:2:216:ARG:NH2	30:R1:781:A:OP1	2.30	0.65
21:32:12:ARG:NH2	30:R1:517:C:OP1	2.29	0.65
26:5:118:ALA:O	26:5:166:ARG:NH1	2.29	0.65
25:4:5:LEU:HD23	25:4:8:ALA:HB3	1.77	0.65
3:15:109:LYS:HE2	3:15:128:THR:HG22	1.78	0.65
30:R1:1019:U:OP1	30:R1:1035:U:O2'	2.13	0.65
30:R1:13:A:O2'	30:R1:15:G:N7	2.28	0.65
30:R1:2339:C:H2'	30:R1:2340:A:H8	1.62	0.65
30:R1:282:A:H2'	30:R1:283:G:C8	2.31	0.65
30:R1:356:G:H2'	30:R1:357:C:C6	2.32	0.65
30:R1:1386:C:H2'	30:R1:1387:A:H8	1.61	0.65
21:32:15:ARG:NH2	30:R1:1264:A:OP1	2.27	0.65
12:23:4:GLU:HG3	17:29:18:LEU:HD11	1.78	0.65
30:R1:1087:G:O6	30:R1:1103:A:N6	2.29	0.65
30:R1:500:G:H22	30:R1:503:A:H5'	1.60	0.64
32:R3:501:C:H2'	32:R3:502:A:H8	1.62	0.64
12:23:67:VAL:HG22	12:23:76:ARG:HG3	1.77	0.64
30:R1:1173:U:O2'	30:R1:1174:U:O3'	2.16	0.64
30:R1:2865:U:OP2	30:R1:2866:U:O2'	2.13	0.64
25:4:119:ILE:HB	25:4:187:VAL:HG12	1.79	0.64
32:R3:58:C:H2'	32:R3:59:A:H8	1.61	0.64
13:24:81:ARG:NH2	30:R1:301:G:OP2	2.31	0.64
18:3:2:ILE:HG13	18:3:3:GLY:H	1.63	0.64
9:20:57:ARG:NH1	30:R1:1154:G:OP2	2.30	0.64
30:R1:358:U:H2'	30:R1:359:G:H8	1.61	0.64
30:R1:2138:G:N2	30:R1:2154:A:N1	2.46	0.64
32:R3:335:C:O2'	32:R3:1433:A:N3	2.27	0.64
30:R1:1882:U:O2'	30:R1:1883:U:O5'	2.13	0.64
32:R3:709:U:H2'	32:R3:710:G:H8	1.62	0.64
1:13:118:MET:HA	1:13:121:LYS:HE3	1.78	0.63
14:25:20:LEU:HD22	14:25:25:LYS:HB2	1.79	0.63
30:R1:79:C:H42	30:R1:107:G:H1	1.46	0.63
16:28:2:ARG:NH1	30:R1:1365:A:OP1	2.32	0.63
30:R1:2096:C:H42	30:R1:2193:G:H22	1.45	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:R3:1016:A:HO2'	32:R3:1217:C:HO2'	1.47	0.63
30:R1:308:G:N2	30:R1:477:A:N7	2.46	0.63
30:R1:569:U:O2'	30:R1:983:A:N1	2.31	0.63
1:13:27:ARG:NH2	30:R1:1143:A:OP1	2.32	0.63
30:R1:30:G:O2'	30:R1:1214:A:N3	2.25	0.63
3:15:1:MET:SD	3:15:1:MET:N	2.66	0.63
13:24:100:GLU:OE1	13:24:100:GLU:N	2.32	0.63
32:R3:1103:C:HO2'	32:R3:1104:G:H8	1.47	0.63
10:21:80:ARG:NH2	30:R1:572:A:OP2	2.32	0.62
30:R1:2291:U:H5'	30:R1:2380:C:H1'	1.80	0.62
32:R3:360:G:H2'	32:R3:361:G:C8	2.33	0.62
32:R3:461:A:H5"	32:R3:463:U:C4	2.34	0.62
18:3:70:LYS:NZ	30:R1:2785:C:O3'	2.32	0.62
26:5:48:LEU:HD11	26:5:147:ARG:HD2	1.80	0.62
30:R1:1176:U:O2'	30:R1:1178:C:N4	2.27	0.62
30:R1:2646:C:OP2	30:R1:2732:G:O2'	2.16	0.62
32:R3:1000:A:H62	32:R3:1003:G:H21	1.46	0.62
7:19:28:LYS:HD2	7:19:39:LEU:HD21	1.82	0.62
4:16:29:GLY:N	4:16:104:GLU:OE2	2.30	0.62
30:R1:453:A:N3	30:R1:457:A:O2'	2.32	0.62
32:R3:413:G:O2'	32:R3:428:G:N2	2.32	0.62
32:R3:672:U:H2'	32:R3:673:A:C8	2.35	0.62
28:9:8:LYS:HA	28:9:15:LEU:H	1.64	0.62
30:R1:414:C:OP1	30:R1:1879:C:O2'	2.15	0.62
32:R3:517:G:N2	32:R3:530:G:OP1	2.30	0.62
32:R3:674:G:H2'	32:R3:675:A:C8	2.34	0.62
32:R3:946:A:H2'	32:R3:947:G:C8	2.33	0.62
11:22:4:ILE:HG22	11:22:106:VAL:HG22	1.81	0.62
30:R1:989:G:OP1	30:R1:1157:G:O2'	2.17	0.62
32:R3:1131:G:O6	32:R3:1144:G:O2'	2.14	0.62
32:R3:946:A:H2'	32:R3:947:G:H8	1.65	0.62
7:19:88:ARG:NH2	7:19:114:ASN:O	2.33	0.61
20:31:11:GLU:HA	20:31:25:ARG:HA	1.80	0.61
32:R3:714:G:H2'	32:R3:715:A:C8	2.35	0.61
23:35:31:ILE:O	23:35:35:LYS:NZ	2.32	0.61
32:R3:77:A:N6	32:R3:91:U:O4	2.33	0.61
5:17:106:ASP:OD2	30:R1:1649:G:O2'	2.16	0.61
32:R3:1356:G:H2'	32:R3:1357:A:C8	2.35	0.61
4:16:86:LYS:NZ	30:R1:955:U:OP1	2.33	0.61
31:R2:14:U:OP2	31:R2:70:C:O2'	2.18	0.61
18:3:46:ARG:NH2	18:3:89:GLU:OE2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:R1:645:C:H2'	30:R1:647:G:C8	2.36	0.61
30:R1:2107:G:N2	30:R1:2182:U:O2	2.32	0.61
32:R3:501:C:H2'	32:R3:502:A:C8	2.36	0.61
3:15:77:ILE:HD11	3:15:108:ALA:HB1	1.81	0.61
4:16:16:ARG:NH1	30:R1:954:G:OP2	2.32	0.61
5:17:49:GLU:OE2	5:17:95:THR:OG1	2.19	0.61
32:R3:1412:C:H2'	32:R3:1413:A:C8	2.36	0.61
53:T:47:U:H4'	53:T:48:C:H5'	1.83	0.61
27:6:49:LEU:HB3	27:6:51:PHE:HE1	1.65	0.61
30:R1:199:A:O2'	30:R1:200:U:O2	2.18	0.61
30:R1:848:C:H2'	30:R1:849:A:C8	2.34	0.61
30:R1:2127:G:H2'	30:R1:2128:G:C8	2.33	0.61
1:13:107:GLY:O	1:13:111:LYS:NZ	2.33	0.61
30:R1:689:A:H8	30:R1:779:U:HO2'	1.47	0.61
30:R1:2857:G:O2'	30:R1:2859:G:O6	2.19	0.61
18:3:109:VAL:HG11	18:3:193:VAL:HB	1.83	0.61
23:35:7:ARG:NH1	30:R1:243:U:OP2	2.34	0.61
30:R1:415:A:O2'	30:R1:1866:A:OP1	2.17	0.61
30:R1:2126:A:N1	30:R1:2162:G:O2'	2.31	0.61
30:R1:151:C:H2'	30:R1:152:A:C8	2.36	0.61
30:R1:1170:C:O2'	30:R1:1171:G:H8	1.84	0.61
30:R1:2162:G:H5"	30:R1:2171:A:C8	2.34	0.61
32:R3:1175:G:H2'	32:R3:1176:A:H8	1.66	0.61
5:17:98:LEU:HD13	21:32:48:TYR:HD1	1.66	0.60
14:25:9:ARG:NH2	31:R2:76:G:OP1	2.34	0.60
26:5:102:LEU:HA	26:5:106:ALA:HB3	1.82	0.60
3:15:106:GLU:N	3:15:106:GLU:OE2	2.34	0.60
27:6:85:LYS:HD2	27:6:131:VAL:HG12	1.83	0.60
30:R1:1538:G:H2'	30:R1:1539:U:C6	2.37	0.60
31:R2:5:U:OP1	31:R2:61:G:O2'	2.17	0.60
8:2:140:VAL:HG23	8:2:191:LEU:HA	1.83	0.60
30:R1:2858:C:O2'	30:R1:2859:G:O5'	2.16	0.60
32:R3:147:G:H2'	32:R3:148:G:C8	2.36	0.60
32:R3:664:G:HO2'	32:R3:725:G:HO2'	1.50	0.60
22:34:9:VAL:HG22	22:34:12:ARG:HH21	1.66	0.60
19:30:5:LYS:HB3	19:30:57:GLU:HB3	1.84	0.60
13:24:25:LYS:HD2	13:24:36:GLU:HB3	1.84	0.60
30:R1:1664:A:H61	30:R1:1996:C:H42	1.48	0.60
8:2:259:ASN:OD1	8:2:262:THR:OG1	2.19	0.60
30:R1:2215:C:H2'	30:R1:2216:G:H8	1.67	0.59
32:R3:1218:C:H2'	32:R3:1219:A:H8	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:27:40:GLN:OE1	15:27:44:LYS:N	2.29	0.59
32:R3:73:C:H2'	32:R3:74:A:C8	2.37	0.59
53:T:31:G:H2'	53:T:32:4OC:H6	1.84	0.59
30:R1:1629:U:O4	30:R1:1630:A:N6	2.34	0.59
30:R1:1109:C:O2	30:R1:1110:G:N2	2.35	0.59
32:R3:82:G:H1'	32:R3:88:U:H3	1.65	0.59
18:3:2:ILE:HG13	18:3:3:GLY:N	2.18	0.59
30:R1:1570:A:H2'	30:R1:1571:A:C8	2.37	0.59
32:R3:1002:G:H21	32:R3:1039:G:H2'	1.68	0.59
3:15:85:VAL:HG13	3:15:86:GLU:H	1.68	0.59
30:R1:277:G:H8	30:R1:361:G:C5	2.20	0.59
6:18:31:THR:HG23	6:18:34:HIS:H	1.66	0.59
12:23:68:LYS:NZ	30:R1:1336:A:OP2	2.25	0.59
18:3:136:ASN:ND2	30:R1:2579:C:O2'	2.36	0.59
30:R1:192:C:O2	30:R1:802:A:O2'	2.19	0.59
30:R1:935:C:H2'	30:R1:936:A:H8	1.66	0.59
5:17:22:ARG:HG3	5:17:70:THR:HA	1.85	0.59
7:19:108:ARG:NH1	32:R3:1463:U:OP1	2.34	0.59
13:24:47:PRO:HD2	13:24:47:PRO:O	2.01	0.59
26:5:132:ARG:NH2	30:R1:2305:U:O2	2.26	0.59
30:R1:263:G:O2'	30:R1:429:A:N3	2.34	0.59
30:R1:285:G:O6	30:R1:355:U:O2	2.20	0.59
30:R1:2047:C:H2'	30:R1:2048:G:H8	1.68	0.59
13:24:48:VAL:HG12	13:24:50:ALA:H	1.66	0.59
18:3:133:THR:HG22	18:3:134:HIS:H	1.66	0.59
27:6:39:ALA:HB3	27:6:63:GLN:HG3	1.82	0.59
32:R3:457:G:O6	32:R3:475:C:N4	2.36	0.59
32:R3:1026:G:C2	32:R3:1036:A:C6	2.91	0.58
30:R1:136:G:H22	30:R1:142:A:H2	1.52	0.58
30:R1:388:G:O2'	30:R1:390:U:OP2	2.19	0.58
32:R3:461:A:O2'	32:R3:462:G:OP1	2.21	0.58
13:24:28:LEU:HD13	13:24:32:LYS:HB2	1.84	0.58
32:R3:1008:U:O2	32:R3:1022:A:N6	2.36	0.58
30:R1:411:G:OP2	30:R1:2406:A:O2'	2.17	0.58
32:R3:322:C:H42	32:R3:332:G:H1	1.50	0.58
32:R3:1178:G:N2	32:R3:1181:G:OP2	2.36	0.58
32:R3:1251:A:H2'	32:R3:1252:A:C8	2.38	0.58
32:R3:958:A:H8	32:R3:985:C:HO2'	1.50	0.58
30:R1:2121:G:O6	30:R1:2175:C:N4	2.37	0.58
32:R3:53:A:N6	32:R3:359:G:O6	2.37	0.58
15:27:29:GLU:OE2	30:R1:922:C:O2'	2.20	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:R1:1443:U:H2'	30:R1:1444:G:H8	1.68	0.58
32:R3:71:A:N6	32:R3:99:C:O2'	2.36	0.58
16:28:39:VAL:HG12	16:28:42:GLU:H	1.69	0.58
30:R1:877:A:O2'	30:R1:900:A:N6	2.36	0.58
6:18:30:ARG:NH2	31:R2:48:U:OP1	2.36	0.58
8:2:60:ALA:O	8:2:62:ARG:NH1	2.37	0.58
30:R1:2372:U:H2'	30:R1:2373:G:H8	1.69	0.58
30:R1:2897:U:H2'	30:R1:2898:U:C6	2.39	0.58
1:13:15:TRP:HB3	1:13:137:PRO:HB3	1.86	0.57
14:25:34:LYS:NZ	14:25:35:GLU:OE2	2.36	0.57
30:R1:1149:G:H2'	30:R1:1150:C:C6	2.39	0.57
30:R1:2071:A:H2'	30:R1:2072:C:C6	2.39	0.57
30:R1:2469:A:N6	30:R1:2481:G:O2'	2.36	0.57
4:16:64:TRP:HE1	30:R1:873:C:H4'	1.69	0.57
30:R1:631:A:N3	30:R1:2415:G:O2'	2.34	0.57
30:R1:2031:A:N3	30:R1:2455:G:O2'	2.31	0.57
30:R1:2184:A:H2'	30:R1:2185:U:C6	2.39	0.57
14:25:20:LEU:HD11	14:25:41:GLU:HG3	1.85	0.57
20:31:28:VAL:HG22	26:5:139:GLU:HG3	1.85	0.57
30:R1:880:G:H2'	30:R1:881:G:C8	2.37	0.57
8:2:220:ARG:NE	30:R1:1827:U:OP2	2.37	0.57
30:R1:2339:C:H2'	30:R1:2340:A:C8	2.39	0.57
32:R3:838:G:O2'	32:R3:839:C:O5'	2.21	0.57
32:R3:1285:A:H4'	32:R3:1286:U:H5"	1.86	0.57
30:R1:340:A:H2'	30:R1:341:C:O4'	2.04	0.57
30:R1:45:G:H5"	30:R1:46:G:H5'	1.85	0.57
32:R3:56:U:H2'	32:R3:57:G:C8	2.40	0.57
32:R3:134:G:H2'	32:R3:135:C:O4'	2.05	0.57
32:R3:413:G:H21	32:R3:428:G:H1'	1.70	0.57
8:2:144:GLU:OE2	8:2:150:GLY:N	2.37	0.57
26:5:132:ARG:HA	26:5:132:ARG:NE	2.19	0.57
30:R1:1668:A:N3	30:R1:1670:C:N4	2.53	0.57
32:R3:359:G:O2'	32:R3:360:G:O5'	2.23	0.57
32:R3:1125:U:O2'	32:R3:1126:U:OP1	2.23	0.57
12:23:8:LEU:HD13	17:29:21:LEU:HB2	1.87	0.57
30:R1:156:A:N1	30:R1:169:G:C6	2.73	0.57
11:22:109:ASP:N	11:22:109:ASP:OD1	2.38	0.57
27:6:173:ALA:O	27:6:174:LYS:HG3	2.05	0.57
30:R1:581:C:H2'	30:R1:582:A:H8	1.70	0.57
30:R1:2347:C:N3	30:R1:2371:G:N2	2.52	0.57
32:R3:1026:G:C6	32:R3:1036:A:N6	2.73	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:2:13:ARG:NH2	30:R1:1695:G:N7	2.52	0.56
28:9:8:LYS:O	28:9:9:VAL:HG23	2.04	0.56
30:R1:2638:G:H1'	30:R1:2778:A:H61	1.70	0.56
2:14:110:GLU:HA	2:14:113:MET:HG2	1.86	0.56
8:2:156:SER:OG	8:2:157:ALA:N	2.38	0.56
11:22:16:LYS:NZ	30:R1:2011:U:OP2	2.34	0.56
15:27:43:THR:HG21	30:R1:2336:A:H61	1.70	0.56
20:31:38:SER:HA	20:31:41:HIS:HD2	1.69	0.56
26:5:132:ARG:NH2	30:R1:2305:U:H1'	2.19	0.56
30:R1:511:U:H4'	30:R1:1235:G:H4'	1.86	0.56
53:T:43:A:H2'	53:T:44:A:C8	2.40	0.56
30:R1:1585:C:H3'	30:R1:1586:A:H8	1.69	0.56
8:2:139:THR:OG1	8:2:162:GLN:OE1	2.23	0.56
30:R1:2316:G:H2'	30:R1:2317:A:H8	1.70	0.56
30:R1:2591:C:H2'	30:R1:2592:G:H8	1.71	0.56
31:R2:7:G:H1	31:R2:113:C:H5	1.53	0.56
32:R3:673:A:H2'	32:R3:674:G:H8	1.71	0.56
30:R1:644:A:H2'	30:R1:645:C:O4'	2.05	0.56
32:R3:133:U:H1'	32:R3:230:G:N2	2.21	0.56
32:R3:474:G:H2'	32:R3:475:C:H5"	1.87	0.56
30:R1:324:A:N6	30:R1:338:G:O2'	2.37	0.56
30:R1:476:G:N1	30:R1:479:A:OP2	2.38	0.56
30:R1:1432:G:H2'	30:R1:1433:A:C8	2.41	0.56
30:R1:1548:A:H2'	30:R1:1549:A:H8	1.71	0.56
32:R3:908:A:H2'	32:R3:909:A:H8	1.70	0.56
3:15:85:VAL:HG11	3:15:90:VAL:HG22	1.88	0.56
30:R1:1178:C:N3	30:R1:1179:G:O2'	2.39	0.56
32:R3:188:C:N4	32:R3:189:A:N1	2.54	0.56
32:R3:322:C:H42	32:R3:332:G:H22	1.52	0.56
2:14:30:ARG:NH2	2:14:37:ASP:OD1	2.38	0.56
30:R1:2848:G:O2'	30:R1:2867:G:N2	2.39	0.56
6:18:15:ARG:NH2	6:18:95:SER:OG	2.36	0.56
30:R1:488:G:N2	30:R1:493:G:O6	2.39	0.56
30:R1:2682:A:H61	30:R1:2728:U:H1'	1.72	0.56
2:14:17:ARG:HB2	2:14:45:GLU:HG2	1.87	0.55
25:4:49:ARG:NH1	30:R1:673:C:OP1	2.38	0.55
30:R1:1047:G:N2	30:R1:1110:G:N3	2.54	0.55
32:R3:115:G:H8	32:R3:115:G:OP1	1.88	0.55
32:R3:114:U:H1'	32:R3:353:A:H1'	1.88	0.55
32:R3:279:A:H5"	32:R3:280:C:H3'	1.87	0.55
32:R3:415:A:H3'	32:R3:416:G:H8	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:18:56:LYS:H	6:18:56:LYS:HD2	1.71	0.55
30:R1:160:A:H5"	30:R1:161:A:H2'	1.89	0.55
30:R1:2101:A:H2'	30:R1:2102:G:H8	1.71	0.55
32:R3:424:G:H2'	32:R3:425:G:H8	1.71	0.55
32:R3:746:A:H2'	32:R3:747:A:C8	2.40	0.55
28:9:7:ASP:OD1	28:9:8:LYS:N	2.40	0.55
30:R1:132:G:H1	30:R1:146:A:N6	2.02	0.55
30:R1:177:G:H5'	30:R1:178:G:C8	2.42	0.55
30:R1:357:C:H2'	30:R1:358:U:C6	2.41	0.55
30:R1:1047:G:H21	30:R1:1110:G:H21	1.53	0.55
32:R3:563:A:O2'	32:R3:566:G:O2'	2.22	0.55
30:R1:219:A:N3	30:R1:234:U:O2'	2.36	0.55
32:R3:313:A:H2'	32:R3:314:C:C6	2.42	0.55
32:R3:923:A:O2'	32:R3:1399:C:OP2	2.25	0.55
19:30:2:LYS:O	19:30:39:ASP:N	2.28	0.55
27:6:80:GLU:OE1	27:6:80:GLU:N	2.40	0.55
30:R1:412:A:N7	30:R1:2412:A:H1'	2.21	0.55
30:R1:1912:A:H62	30:R1:1917:U:H5	1.53	0.55
25:4:44:ARG:HH22	30:R1:1248:G:P	2.30	0.55
30:R1:639:U:H2'	30:R1:640:C:C6	2.41	0.55
32:R3:21:G:H2'	32:R3:22:G:H8	1.72	0.55
14:25:45:ASP:N	14:25:45:ASP:OD1	2.40	0.55
18:3:148:GLN:HB2	18:3:152:PRO:HG2	1.89	0.55
26:5:70:ARG:HG2	26:5:71:LYS:HG3	1.88	0.55
30:R1:145:C:H2'	30:R1:146:A:N3	2.22	0.55
30:R1:2515:C:H2'	30:R1:2516:A:H8	1.72	0.55
14:25:77:VAL:HG22	14:25:89:ILE:HG22	1.87	0.55
27:6:39:ALA:HA	27:6:57:TYR:HD2	1.72	0.55
30:R1:639:U:H2'	30:R1:640:C:H6	1.72	0.55
32:R3:214:C:H3'	32:R3:215:C:C6	2.41	0.55
16:28:11:PRO:HB3	16:28:29:LEU:HD23	1.89	0.55
19:30:9:THR:OG1	19:30:53:MET:O	2.23	0.55
30:R1:1482:G:H2'	30:R1:1483:G:H8	1.72	0.55
32:R3:1012:A:N6	32:R3:1018:G:O6	2.40	0.55
5:17:1:MET:N	30:R1:1654:A:OP2	2.39	0.54
18:3:169:ARG:NH2	30:R1:2773:C:OP1	2.40	0.54
30:R1:305:C:H2'	30:R1:306:U:C6	2.42	0.54
30:R1:465:G:H2'	30:R1:466:A:C8	2.42	0.54
30:R1:1047:G:H21	30:R1:1110:G:N2	2.04	0.54
32:R3:123:U:OP1	32:R3:311:C:O2'	2.19	0.54
2:14:90:ASN:OD1	2:14:91:SER:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:31:56:ARG:HB2	20:31:59:ARG:HH11	1.72	0.54
30:R1:720:U:H2'	30:R1:721:A:H8	1.72	0.54
2:14:31:ARG:NH2	30:R1:2676:C:OP1	2.40	0.54
20:31:50:ASP:HB2	26:5:114:ARG:NH2	2.22	0.54
30:R1:1936:A:H2	30:R1:1943:U:H3	1.55	0.54
30:R1:2246:G:H2'	30:R1:2247:A:H8	1.72	0.54
32:R3:404:G:O2'	32:R3:498:A:N1	2.34	0.54
32:R3:1405:G:H21	32:R3:1518:A:H8	1.54	0.54
30:R1:918:A:N3	31:R2:80:U:O2'	2.39	0.54
30:R1:2243:U:H2'	30:R1:2244:U:C6	2.42	0.54
32:R3:1071:C:H2'	32:R3:1072:G:C8	2.42	0.54
30:R1:270:A:N1	30:R1:369:U:O2'	2.39	0.54
32:R3:1218:C:H2'	32:R3:1219:A:C8	2.42	0.54
8:2:216:ARG:NH1	30:R1:691:C:OP1	2.41	0.54
30:R1:820:A:H4'	30:R1:836:G:H22	1.71	0.54
30:R1:629:G:N3	30:R1:639:U:O2'	2.41	0.54
30:R1:1636:U:O2'	30:R1:1760:C:O2	2.19	0.54
30:R1:2505:G:H2'	30:R1:2576:G:H1	1.73	0.54
4:16:25:ASP:OD1	4:16:25:ASP:N	2.40	0.54
27:6:32:LEU:HD23	27:6:74:MET:HG2	1.89	0.54
30:R1:181:A:H2'	30:R1:182:A:H8	1.73	0.54
30:R1:1273:U:O2'	30:R1:1275:A:OP1	2.23	0.54
30:R1:1326:U:HO2'	30:R1:2010:G:HO2'	1.56	0.54
30:R1:2167:U:C4	30:R1:2169:A:C8	2.96	0.54
30:R1:2215:C:H2'	30:R1:2216:G:C8	2.42	0.54
32:R3:715:A:H2'	32:R3:716:A:C8	2.42	0.54
32:R3:891:U:H2'	32:R3:892:A:H8	1.72	0.54
32:R3:1266:G:N2	32:R3:1269:A:OP2	2.25	0.54
7:19:70:GLU:OE2	7:19:100:ARG:NH1	2.41	0.54
21:32:2:VAL:HG13	30:R1:2015:A:C6	2.43	0.54
30:R1:1169:A:H2'	30:R1:1170:C:C6	2.43	0.54
5:17:73:ASN:HA	5:17:76:VAL:HG12	1.90	0.53
6:18:25:ARG:NH2	31:R2:8:C:O3'	2.41	0.53
8:2:117:SER:OG	8:2:118:GLY:N	2.41	0.53
14:25:11:GLU:OE1	14:25:11:GLU:N	2.41	0.53
20:31:20:ASN:ND2	20:31:37:CYS:SG	2.75	0.53
30:R1:793:A:OP2	30:R1:2071:A:O2'	2.26	0.53
30:R1:1583:A:H4'	30:R1:1584:U:H5	1.72	0.53
32:R3:99:C:HO2'	32:R3:100:G:H8	1.53	0.53
32:R3:924:C:H2'	32:R3:925:G:H8	1.73	0.53
32:R3:1513:A:H2'	32:R3:1514:G:H8	1.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:31:59:ARG:NH2	20:31:63:ARG:HH22	2.07	0.53
21:32:11:LYS:HE2	21:32:11:LYS:HA	1.89	0.53
24:36:36:ARG:HG3	24:36:37:GLN:N	2.22	0.53
25:4:148:ILE:HB	25:4:169:VAL:HG22	1.90	0.53
30:R1:598:U:H2'	30:R1:599:A:H8	1.73	0.53
30:R1:1169:A:H2'	30:R1:1170:C:H6	1.73	0.53
30:R1:1534:U:O2	30:R1:1538:G:N1	2.40	0.53
32:R3:1464:U:H2'	32:R3:1465:A:H8	1.73	0.53
1:13:45:THR:HB	1:13:48:VAL:HG22	1.91	0.53
30:R1:307:G:N1	30:R1:310:A:OP2	2.35	0.53
30:R1:2812:G:H2'	30:R1:2813:A:C8	2.43	0.53
32:R3:1452:C:O2'	32:R3:1453:G:N2	2.41	0.53
30:R1:371:A:H2	30:R1:402:A:H62	1.57	0.53
30:R1:1258:U:H2'	30:R1:1259:G:C8	2.43	0.53
30:R1:1594:U:H2'	30:R1:1595:C:C6	2.44	0.53
32:R3:753:A:H4'	32:R3:754:C:O5'	2.07	0.53
4:16:10:ARG:NH2	30:R1:2278:A:OP1	2.42	0.53
15:27:42:GLY:HA2	30:R1:2330:G:H21	1.73	0.53
30:R1:306:U:H3	30:R1:310:A:H62	1.56	0.53
30:R1:1882:U:H2'	30:R1:1883:U:C5	2.44	0.53
32:R3:237:G:H2'	32:R3:238:A:C8	2.44	0.53
32:R3:253:A:N6	32:R3:274:A:N1	2.57	0.53
4:16:64:TRP:NE1	30:R1:873:C:H4'	2.23	0.53
10:21:91:GLN:NE2	30:R1:993:G:N3	2.56	0.53
17:29:17:GLU:HB2	17:29:53:VAL:HG11	1.91	0.53
18:3:149:ASN:HB3	30:R1:2572:A:OP2	2.06	0.53
32:R3:859:G:H2'	32:R3:860:A:H8	1.73	0.53
32:R3:922:G:H2'	32:R3:923:A:C8	2.44	0.53
32:R3:1026:G:H1	32:R3:1036:A:N6	2.04	0.53
32:R3:1034:G:H2'	32:R3:1035:A:H8	1.72	0.53
6:18:3:LYS:NZ	31:R2:47:C:OP1	2.42	0.53
15:27:40:GLN:NE2	15:27:45:PHE:O	2.41	0.53
30:R1:1038:G:H2'	30:R1:1039:A:H8	1.74	0.53
12:23:18:GLU:H	12:23:18:GLU:CD	2.10	0.53
30:R1:100:U:H4'	30:R1:101:A:O4'	2.08	0.53
32:R3:966:G:N2	53:T:34:C:H5'	2.24	0.53
32:R3:1522:U:H2'	32:R3:1523:G:H8	1.74	0.53
30:R1:704:G:O2'	30:R1:726:G:N2	2.35	0.53
30:R1:2774:C:O2'	30:R1:2775:G:H8	1.92	0.53
32:R3:338:A:H3'	32:R3:339:C:H5"	1.91	0.53
32:R3:736:C:H2'	32:R3:737:C:H6	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:R3:859:G:OP2	32:R3:869:G:N1	2.34	0.53
6:18:94:ARG:NH1	6:18:97:PHE:O	2.42	0.53
26:5:5:ASP:OD1	26:5:5:ASP:N	2.41	0.53
30:R1:135:U:H2'	30:R1:136:G:C8	2.44	0.53
30:R1:1594:U:H2'	30:R1:1595:C:H6	1.74	0.53
30:R1:2071:A:H2'	30:R1:2072:C:H6	1.74	0.53
30:R1:2233:U:H2'	30:R1:2234:G:H8	1.73	0.53
30:R1:2487:G:H2'	30:R1:2488:G:H8	1.74	0.53
32:R3:672:U:H2'	32:R3:673:A:H8	1.74	0.53
32:R3:1026:G:N1	32:R3:1036:A:C6	2.77	0.53
30:R1:463:G:N2	30:R1:466:A:OP2	2.37	0.52
30:R1:1013:C:H2'	30:R1:1014:A:H8	1.73	0.52
30:R1:2812:G:H2'	30:R1:2813:A:H8	1.73	0.52
10:21:14:VAL:HG12	10:21:20:VAL:HG11	1.91	0.52
19:30:6:ILE:HD13	19:30:47:ILE:HD11	1.91	0.52
29:M:7:A:H2'	29:M:8:C:C6	2.45	0.52
30:R1:135:U:H3	30:R1:143:C:H42	1.56	0.52
30:R1:2189:U:H2'	30:R1:2190:G:C8	2.45	0.52
32:R3:505:G:H2'	32:R3:506:G:H8	1.72	0.52
20:31:41:HIS:HB3	20:31:43:PHE:HD1	1.74	0.52
30:R1:197:A:N6	30:R1:2430:A:O2'	2.42	0.52
30:R1:2096:C:N4	30:R1:2193:G:H22	2.07	0.52
32:R3:1235:U:H2'	32:R3:1236:A:O4'	2.08	0.52
5:17:98:LEU:HD12	21:32:53:VAL:HG11	1.91	0.52
15:27:71:VAL:O	15:27:71:VAL:HG12	2.10	0.52
30:R1:18:U:O2'	30:R1:554:U:OP1	2.26	0.52
32:R3:944:G:N1	32:R3:1338:G:OP2	2.37	0.52
32:R3:1513:A:H2'	32:R3:1514:G:C8	2.44	0.52
53:T:32:4OC:HM23	53:T:33:U:H5'	1.91	0.52
25:4:189:THR:HG22	25:4:191:ASP:H	1.75	0.52
30:R1:805:G:N2	30:R1:829:A:OP1	2.42	0.52
6:18:56:LYS:HD2	6:18:56:LYS:N	2.24	0.52
9:20:87:VAL:HG13	10:21:49:ILE:HG13	1.91	0.52
21:32:3:GLN:NE2	30:R1:2016:U:O2	2.35	0.52
30:R1:48:G:N2	30:R1:177:G:OP2	2.41	0.52
30:R1:1447:C:H2'	30:R1:1448:G:H8	1.75	0.52
30:R1:1709:U:H2'	30:R1:1710:G:H8	1.74	0.52
30:R1:2663:G:H2'	30:R1:2664:G:O4'	2.10	0.52
32:R3:560:A:H5"	32:R3:561:U:H3'	1.92	0.52
32:R3:1187:G:H2'	32:R3:1188:A:C8	2.44	0.52
7:19:74:GLN:HB3	18:3:13:ARG:HH22	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:31:26:SER:OG	26:5:139:GLU:OE2	2.28	0.52
30:R1:828:U:H4'	30:R1:831:G:H1	1.75	0.52
30:R1:1254:A:H5"	30:R1:1255:U:H5"	1.92	0.52
53:T:50:U:O4	53:T:64:G:O6	2.28	0.52
22:34:12:ARG:HH11	22:34:44:VAL:HG22	1.75	0.52
26:5:93:GLU:O	26:5:97:GLU:HG2	2.10	0.52
27:6:12:ALA:O	27:6:14:VAL:N	2.39	0.52
30:R1:828:U:H4'	30:R1:831:G:N1	2.24	0.52
30:R1:1357:C:H2'	30:R1:1358:G:O4'	2.10	0.52
32:R3:735:C:H2'	32:R3:736:C:H6	1.75	0.52
32:R3:1013:G:N2	32:R3:1016:A:OP2	2.29	0.52
32:R3:1137:C:O2	32:R3:1138:G:N2	2.42	0.52
8:2:227:VAL:HG22	30:R1:2073:C:H5"	1.91	0.52
12:23:63:VAL:O	12:23:79:ASP:HB2	2.10	0.52
18:3:5:VAL:HG22	18:3:202:ILE:HD13	1.92	0.52
30:R1:644:A:H2	30:R1:2369:A:HO2'	1.57	0.52
30:R1:721:A:H2'	30:R1:722:A:H8	1.75	0.52
30:R1:1104:C:H2'	30:R1:1105:U:O4'	2.10	0.52
32:R3:1036:A:H2'	32:R3:1037:C:C6	2.44	0.52
14:25:10:LYS:HB2	14:25:11:GLU:OE1	2.10	0.52
14:25:17:SER:OG	14:25:21:ARG:NH2	2.31	0.52
30:R1:541:A:H2'	30:R1:542:C:O4'	2.10	0.52
30:R1:947:A:H2'	30:R1:948:C:C6	2.45	0.52
30:R1:625:G:H2'	30:R1:626:A:C8	2.45	0.51
30:R1:2328:A:H2'	30:R1:2329:U:C6	2.45	0.51
16:28:55:MET:HA	16:28:58:ILE:HG22	1.91	0.51
30:R1:1016:G:O6	30:R1:1147:A:N6	2.43	0.51
32:R3:1030:U:O4	32:R3:1033:G:N2	2.40	0.51
5:17:65:LEU:HD22	5:17:69:ARG:HH12	1.76	0.51
13:24:23:LYS:O	13:24:36:GLU:HG3	2.10	0.51
26:5:132:ARG:CZ	30:R1:2305:U:H1'	2.40	0.51
30:R1:49:A:H61	30:R1:177:G:H2'	1.75	0.51
30:R1:358:U:H2'	30:R1:359:G:C8	2.42	0.51
30:R1:1858:A:H61	30:R1:1884:G:H1'	1.74	0.51
3:15:99:ASN:HD21	30:R1:621:A:P	2.33	0.51
18:3:113:SER:OG	18:3:114:LYS:N	2.43	0.51
28:9:27:ARG:NH2	30:R1:2092:U:OP2	2.44	0.51
30:R1:596:U:H2'	30:R1:597:G:H8	1.76	0.51
31:R2:25:U:O2	31:R2:117:G:O2'	2.28	0.51
32:R3:382:A:H2'	32:R3:383:A:C8	2.45	0.51
32:R3:917:G:H2'	32:R3:918:A:C8	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:14:70:ARG:NH1	30:R1:2684:U:O4'	2.44	0.51
3:15:23:ILE:HG12	10:21:82:HIS:CE1	2.46	0.51
20:31:41:HIS:ND1	20:31:43:PHE:HB3	2.26	0.51
32:R3:685:G:N2	32:R3:704:A:OP2	2.43	0.51
32:R3:695:A:H2'	32:R3:696:A:C8	2.45	0.51
17:29:2:LYS:HB3	30:R1:102:U:H3	1.76	0.51
30:R1:690:G:O2'	30:R1:780:G:OP1	2.29	0.51
30:R1:1548:A:H2'	30:R1:1549:A:C8	2.44	0.51
30:R1:1900:A:H1'	30:R1:1970:A:H2'	1.92	0.51
30:R1:2110:G:OP2	30:R1:2118:U:N3	2.40	0.51
30:R1:2246:G:H2'	30:R1:2247:A:C8	2.45	0.51
30:R1:2505:G:O2'	30:R1:2506:U:H5"	2.11	0.51
30:R1:2557:G:H2'	30:R1:2558:C:C6	2.45	0.51
30:R1:2576:G:O2'	30:R1:2579:C:OP2	2.26	0.51
15:27:18:ALA:O	15:27:20:ARG:NH1	2.43	0.51
30:R1:1102:C:H2'	30:R1:1103:A:C8	2.46	0.51
30:R1:1275:A:N1	30:R1:1295:C:O2'	2.41	0.51
32:R3:1002:G:N2	32:R3:1039:G:H2'	2.26	0.51
32:R3:1151:A:H2'	32:R3:1152:A:H8	1.75	0.51
15:27:77:ARG:NH2	30:R1:2332:C:OP1	2.43	0.51
30:R1:1038:G:H2'	30:R1:1039:A:C8	2.46	0.51
32:R3:509:A:C8	32:R3:544:G:H5'	2.46	0.51
32:R3:918:A:H2'	32:R3:919:A:C8	2.46	0.51
31:R2:106:G:H2'	31:R2:107:G:O4'	2.10	0.51
32:R3:359:G:C4	32:R3:360:G:C8	2.99	0.51
32:R3:555:U:H2'	32:R3:556:C:C6	2.46	0.51
32:R3:1405:G:HO2'	32:R3:1518:A:HO2'	1.50	0.51
30:R1:881:G:H2'	30:R1:882:G:C8	2.45	0.51
30:R1:1064:C:OP1	30:R1:1066:U:O2'	2.22	0.51
32:R3:309:A:H2'	32:R3:310:G:H8	1.75	0.51
3:15:59:ARG:HD2	30:R1:250:G:H4'	1.93	0.50
18:3:59:ARG:NH1	30:R1:2831:G:OP2	2.42	0.50
30:R1:282:A:H2'	30:R1:283:G:H8	1.71	0.50
30:R1:387:U:H4'	30:R1:388:G:H5'	1.92	0.50
30:R1:580:U:H2'	30:R1:581:C:H6	1.76	0.50
30:R1:1443:U:H2'	30:R1:1444:G:C8	2.46	0.50
32:R3:1032:G:H21	32:R3:1033:G:H5'	1.76	0.50
32:R3:1129:C:H5	32:R3:1143:G:H1	1.59	0.50
9:20:54:ARG:HD3	30:R1:1155:A:H5"	1.93	0.50
26:5:7:TYR:HB2	26:5:172:PHE:HZ	1.75	0.50
30:R1:1682:G:H2'	30:R1:1683:U:C6	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:R2:95:U:H2'	31:R2:96:G:H8	1.77	0.50
8:2:209:ALA:HA	8:2:212:TRP:NE1	2.26	0.50
32:R3:246:A:C2	32:R3:282:A:C5	3.00	0.50
32:R3:470:C:O2'	32:R3:471:U:H5"	2.12	0.50
32:R3:1338:G:N3	53:T:41:C:O2'	2.44	0.50
15:27:55:ARG:NH2	30:R1:2387:U:OP1	2.45	0.50
26:5:10:GLU:OE1	26:5:10:GLU:N	2.44	0.50
30:R1:598:U:H2'	30:R1:599:A:C8	2.47	0.50
30:R1:859:G:H4'	30:R1:860:U:O5'	2.10	0.50
32:R3:713:G:H2'	32:R3:714:G:C8	2.46	0.50
30:R1:593:U:H2'	30:R1:594:U:C6	2.46	0.50
30:R1:1664:A:H61	30:R1:1996:C:N4	2.09	0.50
32:R3:1270:G:O2'	32:R3:1271:A:OP1	2.25	0.50
10:21:38:VAL:HG11	10:21:57:GLY:HA3	1.94	0.50
12:23:91:GLN:OE1	12:23:91:GLN:N	2.41	0.50
26:5:70:ARG:NH2	30:R1:2299:U:OP2	2.44	0.50
30:R1:581:C:H2'	30:R1:582:A:C8	2.46	0.50
30:R1:1873:G:H2'	30:R1:1874:C:H6	1.76	0.50
32:R3:500:G:O2'	32:R3:501:C:OP1	2.27	0.50
32:R3:1002:G:N2	32:R3:1039:G:N3	2.59	0.50
32:R3:1008:U:H1'	32:R3:1022:A:H61	1.77	0.50
26:5:169:LEU:HD12	26:5:174:PHE:CE1	2.46	0.50
30:R1:878:A:H3'	30:R1:879:G:C8	2.46	0.50
32:R3:82:G:N1	32:R3:87:C:O2'	2.30	0.50
32:R3:1133:G:H22	32:R3:1143:G:H1'	1.77	0.50
32:R3:1319:A:C8	32:R3:1323:G:C6	3.00	0.50
30:R1:306:U:H2'	30:R1:307:G:O4'	2.12	0.50
30:R1:1028:A:N6	30:R1:1125:G:H2'	2.27	0.50
30:R1:1593:A:H2'	30:R1:1594:U:C6	2.46	0.50
30:R1:2025:C:H2'	30:R1:2026:U:C6	2.47	0.50
30:R1:2076:U:OP2	30:R1:2238:G:N2	2.44	0.50
30:R1:2287:A:C8	30:R1:2289:G:C8	2.99	0.50
30:R1:2804:U:H2'	30:R1:2805:C:H6	1.77	0.50
32:R3:939:G:H2'	32:R3:940:C:C6	2.46	0.50
32:R3:1272:G:H2'	32:R3:1273:C:C6	2.47	0.50
32:R3:1305:G:H4'	32:R3:1306:A:O5'	2.12	0.50
12:23:12:ARG:HH11	17:29:29:ARG:HD2	1.77	0.50
15:27:40:GLN:HE22	15:27:45:PHE:H	1.60	0.50
30:R1:721:A:H2'	30:R1:722:A:C8	2.46	0.50
30:R1:2297:A:OP2	30:R1:2297:A:H8	1.95	0.50
30:R1:2857:G:N2	30:R1:2860:A:OP2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:17:38:LEU:HB3	5:17:39:PRO:HD3	1.94	0.49
10:21:25:LEU:HG	10:21:94:THR:HG21	1.93	0.49
30:R1:2241:A:H2'	30:R1:2242:G:C8	2.47	0.49
30:R1:2302:U:H2'	30:R1:2303:G:H8	1.75	0.49
30:R1:2798:U:H4'	30:R1:2799:A:C4	2.47	0.49
25:4:138:LEU:HD13	25:4:146:VAL:HG11	1.94	0.49
30:R1:20:C:H2'	30:R1:21:A:H8	1.76	0.49
30:R1:285:G:C6	30:R1:355:U:O2	2.65	0.49
30:R1:592:A:H2'	30:R1:593:U:C6	2.47	0.49
30:R1:1092:C:H3'	30:R1:1093:G:H8	1.77	0.49
30:R1:1736:U:H2'	30:R1:1737:G:O4'	2.12	0.49
30:R1:2258:C:O2'	30:R1:2427:C:OP2	2.29	0.49
32:R3:750:C:H2'	32:R3:751:U:C6	2.46	0.49
4:16:57:VAL:C	4:16:58:LYS:HG3	2.32	0.49
4:16:110:GLU:OE2	4:16:114:ARG:NH2	2.37	0.49
30:R1:1361:G:H2'	30:R1:1362:C:C6	2.47	0.49
30:R1:2888:C:H2'	30:R1:2889:C:C6	2.47	0.49
32:R3:1000:A:N6	32:R3:1002:G:N7	2.59	0.49
32:R3:1122:U:HO2'	32:R3:1123:U:H6	1.58	0.49
16:28:68:ALA:HA	16:28:71:ARG:HH12	1.77	0.49
23:35:11:LYS:NZ	30:R1:247:G:O6	2.37	0.49
32:R3:1147:C:H2'	32:R3:1148:U:H6	1.76	0.49
3:15:74:THR:HG22	3:15:107:PHE:HB2	1.93	0.49
8:2:132:ARG:HD3	28:9:123:ARG:HH11	1.77	0.49
11:22:23:LEU:HD21	21:32:21:LEU:HB3	1.93	0.49
30:R1:394:C:H2'	30:R1:395:U:O4'	2.13	0.49
32:R3:792:A:H1'	32:R3:794:A:N7	2.28	0.49
12:23:6:ARG:NH2	12:23:42:GLU:OE1	2.44	0.49
30:R1:1386:C:H2'	30:R1:1387:A:C8	2.45	0.49
32:R3:975:A:N1	32:R3:1366:C:O2'	2.39	0.49
27:6:49:LEU:HB3	27:6:51:PHE:CE1	2.47	0.49
30:R1:613:A:H4'	30:R1:614:A:C8	2.48	0.49
30:R1:863:A:H2'	30:R1:864:G:H8	1.77	0.49
30:R1:1044:C:H2'	30:R1:1111:A:H62	1.76	0.49
30:R1:1172:C:O2'	30:R1:1173:U:O5'	2.25	0.49
30:R1:1808:A:H3'	30:R1:1809:A:C8	2.48	0.49
30:R1:594:U:H2'	30:R1:595:C:C6	2.47	0.49
30:R1:720:U:H2'	30:R1:721:A:C8	2.47	0.49
32:R3:1477:U:H2'	32:R3:1478:U:C6	2.47	0.49
14:25:7:GLU:OE1	14:25:7:GLU:N	2.46	0.49
22:34:43:THR:OG1	22:34:44:VAL:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:6:7:PRO:HB3	27:6:48:THR:HG21	1.94	0.49
27:6:25:ILE:HG22	27:6:78:VAL:HG11	1.94	0.49
30:R1:347:A:H2'	30:R1:348:A:C8	2.48	0.49
30:R1:543:G:H2'	30:R1:544:C:C6	2.48	0.49
30:R1:596:U:H2'	30:R1:597:G:C8	2.47	0.49
30:R1:1258:U:H2'	30:R1:1259:G:H8	1.77	0.49
30:R1:2839:G:H2'	30:R1:2840:C:H6	1.77	0.49
32:R3:166:U:H2'	32:R3:167:A:C8	2.48	0.49
32:R3:1370:G:C2	32:R3:1371:G:C8	3.01	0.49
1:13:17:VAL:HG12	1:13:55:ILE:HB	1.95	0.49
2:14:106:GLU:N	2:14:106:GLU:OE2	2.45	0.49
6:18:25:ARG:HH22	31:R2:9:G:P	2.36	0.49
14:25:24:ASN:O	14:25:24:ASN:ND2	2.45	0.49
21:32:8:THR:HG22	21:32:9:ARG:H	1.78	0.49
25:4:55:SER:OG	30:R1:797:G:OP1	2.23	0.49
26:5:3:LEU:HD11	26:5:100:GLU:HB2	1.94	0.49
30:R1:159:G:N3	30:R1:2208:C:O2'	2.45	0.49
30:R1:1505:A:H2'	30:R1:1506:U:C6	2.47	0.49
32:R3:592:G:H2'	32:R3:593:U:C6	2.48	0.49
32:R3:1477:U:H2'	32:R3:1478:U:H6	1.77	0.49
27:6:51:PHE:CE2	27:6:68:ARG:HA	2.48	0.48
27:6:68:ARG:HH12	27:6:72:ASN:HD22	1.59	0.48
30:R1:813:U:H2'	30:R1:814:C:H6	1.78	0.48
30:R1:1589:U:H2'	30:R1:1590:A:H8	1.78	0.48
30:R1:2861:U:H2'	30:R1:2862:G:H8	1.77	0.48
32:R3:204:G:N1	32:R3:215:C:O2	2.46	0.48
32:R3:712:A:H2'	32:R3:713:G:C8	2.48	0.48
30:R1:285:G:O6	30:R1:355:U:C2	2.66	0.48
30:R1:1590:A:H2'	30:R1:1591:A:H8	1.78	0.48
32:R3:272:C:N4	32:R3:273:U:O4	2.46	0.48
32:R3:827:U:H2'	32:R3:870:U:O4	2.13	0.48
32:R3:1524:C:H2'	32:R3:1525:G:C8	2.48	0.48
30:R1:44:A:H2'	30:R1:45:G:O4'	2.14	0.48
30:R1:2667:C:H2'	30:R1:2668:G:H5'	1.94	0.48
31:R2:32:U:C2	31:R2:51:G:N2	2.81	0.48
32:R3:17:U:H2'	32:R3:18:C:C6	2.49	0.48
32:R3:1399:C:O2	32:R3:1502:A:N6	2.45	0.48
19:30:2:LYS:HD2	19:30:2:LYS:HA	1.57	0.48
25:4:5:LEU:HD12	25:4:120:VAL:HG23	1.94	0.48
26:5:28:PRO:HB2	26:5:168:LEU:HD22	1.95	0.48
28:9:54:LEU:O	28:9:58:LEU:HG	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:R1:1042:G:H2'	30:R1:1043:C:C6	2.48	0.48
30:R1:1341:G:OP1	30:R1:1397:U:N3	2.36	0.48
30:R1:1997:C:H2'	30:R1:1998:A:H8	1.78	0.48
32:R3:709:U:H2'	32:R3:710:G:C8	2.45	0.48
32:R3:1004:A:N6	32:R3:1025:U:O2'	2.46	0.48
32:R3:1041:G:O6	32:R3:1042:A:N6	2.46	0.48
32:R3:1319:A:C8	32:R3:1323:G:C5	3.02	0.48
32:R3:1391:U:H2'	32:R3:1392:G:C8	2.49	0.48
32:R3:1441:A:H5'	32:R3:1442:G:OP2	2.14	0.48
3:15:78:ARG:NH2	30:R1:626:A:N3	2.62	0.48
4:16:28:PHE:N	4:16:104:GLU:OE2	2.46	0.48
7:19:3:ILE:HD12	18:3:186:LEU:HD11	1.95	0.48
10:21:46:GLU:N	10:21:46:GLU:OE1	2.46	0.48
13:24:85:ARG:NH1	13:24:87:GLU:OE2	2.47	0.48
15:27:41:ARG:HH21	30:R1:2387:U:C1'	2.26	0.48
25:4:148:ILE:HG21	25:4:157:LEU:HD21	1.95	0.48
30:R1:588:U:H2'	30:R1:589:U:C6	2.49	0.48
30:R1:638:G:H2'	30:R1:639:U:C6	2.49	0.48
30:R1:1050:A:H2'	30:R1:1051:G:O4'	2.14	0.48
30:R1:2134:A:H1'	30:R1:2158:A:H5'	1.95	0.48
30:R1:2230:G:H2'	30:R1:2231:U:C6	2.49	0.48
32:R3:257:G:H2'	32:R3:258:G:H8	1.78	0.48
32:R3:513:C:H2'	32:R3:514:C:C6	2.47	0.48
32:R3:923:A:H2'	32:R3:924:C:C6	2.48	0.48
32:R3:1150:A:O2'	32:R3:1151:A:O4'	2.32	0.48
2:14:6:THR:HG23	30:R1:1666:G:H4'	1.95	0.48
9:20:49:ARG:HH11	30:R1:993:G:H5"	1.79	0.48
13:24:88:ASP:OD1	13:24:89:GLY:N	2.37	0.48
30:R1:285:G:C5	30:R1:286:U:C4	3.01	0.48
30:R1:644:A:H2	30:R1:2369:A:H1'	1.79	0.48
30:R1:2570:G:H2'	30:R1:2571:U:O4'	2.14	0.48
30:R1:2751:G:OP1	30:R1:2751:G:N2	2.45	0.48
30:R1:2774:C:O2'	30:R1:2775:G:O5'	2.29	0.48
31:R2:6:G:H2'	31:R2:7:G:C8	2.47	0.48
32:R3:1179:A:H2'	32:R3:1180:A:O4'	2.13	0.48
25:4:148:ILE:HD13	25:4:187:VAL:CG2	2.43	0.48
30:R1:580:U:H2'	30:R1:581:C:C6	2.48	0.48
30:R1:1682:G:H2'	30:R1:1683:U:H6	1.78	0.48
30:R1:2718:G:O2'	30:R1:2847:U:OP1	2.26	0.48
32:R3:34:C:H2'	32:R3:35:G:H8	1.78	0.48
30:R1:1709:U:H2'	30:R1:1710:G:C8	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:R1:1725:U:H2'	30:R1:1726:C:C6	2.48	0.48
32:R3:301:G:O2'	32:R3:302:G:OP1	2.29	0.48
32:R3:373:A:C2	32:R3:374:A:C8	3.01	0.48
32:R3:505:G:H2'	32:R3:506:G:C8	2.49	0.48
32:R3:1268:G:H2'	32:R3:1269:A:C8	2.49	0.48
24:36:12:ARG:NH1	30:R1:1102:C:O2	2.43	0.48
30:R1:860:U:OP2	30:R1:916:G:N1	2.44	0.48
32:R3:842:U:O2'	32:R3:844:G:OP2	2.32	0.48
32:R3:954:G:H2'	32:R3:955:U:C6	2.49	0.48
32:R3:979:C:H1'	32:R3:1317:C:N4	2.29	0.48
18:3:32:ASN:HD22	18:3:52:THR:HB	1.79	0.48
30:R1:729:G:O2'	30:R1:763:G:H4'	2.13	0.48
30:R1:1286:A:H1'	30:R1:1288:G:OP2	2.13	0.48
30:R1:1720:U:H2'	30:R1:1721:G:O4'	2.14	0.48
30:R1:2834:G:H2'	30:R1:2879:A:H61	1.79	0.48
32:R3:149:A:H2'	32:R3:150:U:C6	2.48	0.48
32:R3:976:G:OP2	32:R3:1358:U:O2'	2.30	0.48
3:15:29:LYS:O	3:15:30:THR:OG1	2.22	0.47
16:28:31:ASN:HB2	30:R1:397:U:H5"	1.95	0.47
27:6:74:MET:O	27:6:78:VAL:HG22	2.14	0.47
30:R1:1405:U:H2'	30:R1:1406:U:C6	2.49	0.47
30:R1:2076:U:H5	30:R1:2596:U:C4	2.32	0.47
30:R1:2487:G:H2'	30:R1:2488:G:C8	2.49	0.47
30:R1:2591:C:H2'	30:R1:2592:G:C8	2.48	0.47
31:R2:23:G:H1	31:R2:60:C:H5	1.61	0.47
32:R3:160:A:H2'	32:R3:161:A:C8	2.48	0.47
32:R3:552:U:H2'	32:R3:553:A:H8	1.79	0.47
32:R3:868:C:H2'	32:R3:869:G:O4'	2.14	0.47
32:R3:1014:A:C2	32:R3:1219:A:H1'	2.49	0.47
23:35:8:GLY:O	23:35:12:ARG:NH1	2.46	0.47
30:R1:742:A:H2'	30:R1:743:A:C8	2.49	0.47
30:R1:813:U:H2'	30:R1:814:C:C6	2.48	0.47
30:R1:1746:A:H2'	30:R1:1747:U:C6	2.48	0.47
30:R1:2008:C:H2'	30:R1:2009:A:H8	1.80	0.47
30:R1:2688:G:N1	30:R1:2720:U:OP2	2.26	0.47
2:14:49:ARG:NH2	32:R3:1422:G:O2'	2.47	0.47
30:R1:685:A:N1	30:R1:787:C:H1'	2.28	0.47
32:R3:213:G:H2'	32:R3:214:C:C2	2.50	0.47
5:17:44:LEU:O	5:17:48:VAL:HG12	2.13	0.47
6:18:79:ALA:HB3	6:18:113:ALA:HB3	1.95	0.47
26:5:91:ARG:NH1	31:R2:45:A:O4'	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:6:88:LEU:HD23	27:6:161:VAL:HG12	1.96	0.47
30:R1:438:G:H2'	30:R1:439:A:H8	1.79	0.47
30:R1:1590:A:H2'	30:R1:1591:A:C8	2.49	0.47
30:R1:1723:G:C2	30:R1:1724:G:H1'	2.49	0.47
30:R1:1871:A:H3'	30:R1:1872:A:H8	1.78	0.47
30:R1:2081:U:H2'	30:R1:2082:A:H8	1.79	0.47
30:R1:2247:A:H2'	30:R1:2248:C:H6	1.79	0.47
30:R1:2720:U:C2	30:R1:2721:A:C8	3.03	0.47
32:R3:916:U:H2'	32:R3:917:G:H8	1.79	0.47
32:R3:1238:A:H2	32:R3:1241:G:N3	2.12	0.47
9:20:5:ARG:NH1	30:R1:1251:C:OP2	2.47	0.47
28:9:46:PHE:HA	28:9:50:ARG:HB2	1.96	0.47
30:R1:2:G:C2	30:R1:2902:C:C2	3.03	0.47
30:R1:1317:G:O6	30:R1:1336:A:N6	2.47	0.47
30:R1:1441:G:H2'	30:R1:1442:U:C6	2.49	0.47
30:R1:2233:U:H2'	30:R1:2234:G:C8	2.49	0.47
31:R2:31:C:H1'	31:R2:53:A:H61	1.80	0.47
32:R3:156:C:H2'	32:R3:157:U:O4'	2.14	0.47
1:13:30:THR:HG21	30:R1:1012:U:O4	2.14	0.47
11:22:29:VAL:HG21	11:22:55:ILE:HD11	1.96	0.47
11:22:88:ARG:HH22	30:R1:2013:A:H2	1.61	0.47
30:R1:2687:U:H2'	30:R1:2688:G:O4'	2.14	0.47
30:R1:2875:C:H2'	30:R1:2876:G:H8	1.80	0.47
32:R3:302:G:H2'	32:R3:303:A:H8	1.79	0.47
32:R3:745:G:H2'	32:R3:746:A:H8	1.80	0.47
32:R3:1315:U:H2'	32:R3:1316:G:O4'	2.15	0.47
8:2:228:ASP:OD1	8:2:228:ASP:N	2.47	0.47
15:27:41:ARG:HD2	15:27:41:ARG:HA	1.67	0.47
20:31:38:SER:HB2	26:5:104:THR:HA	1.97	0.47
27:6:29:ASN:ND2	27:6:80:GLU:O	2.48	0.47
27:6:34:ARG:HB3	27:6:74:MET:HE3	1.96	0.47
30:R1:85:G:C4	30:R1:98:G:N2	2.83	0.47
30:R1:215:G:H4'	30:R1:216:A:H4'	1.97	0.47
30:R1:716:A:H2'	30:R1:717:C:O4'	2.15	0.47
30:R1:974:G:H8	30:R1:990:A:H62	1.63	0.47
30:R1:1101:U:H2'	30:R1:1102:C:C6	2.49	0.47
30:R1:1292:G:H2'	30:R1:1293:C:C6	2.49	0.47
30:R1:1419:A:O4'	30:R1:1579:A:N6	2.47	0.47
30:R1:1437:C:O2'	30:R1:1516:G:O2'	2.30	0.47
30:R1:1796:U:H2'	30:R1:1797:G:C8	2.49	0.47
30:R1:1987:A:H2'	30:R1:1988:G:H8	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:R1:2553:G:C2	30:R1:2583:G:H1'	2.48	0.47
30:R1:2557:G:H2'	30:R1:2558:C:H6	1.80	0.47
6:18:11:ALA:HB2	6:18:96:GLY:N	2.29	0.47
16:28:64:ASP:OD1	16:28:64:ASP:N	2.47	0.47
25:4:45:ALA:HB2	25:4:89:PRO:HD3	1.97	0.47
30:R1:475:C:O2	30:R1:479:A:N6	2.41	0.47
30:R1:1355:G:H2'	30:R1:1356:G:H8	1.78	0.47
30:R1:1464:G:H2'	30:R1:1465:G:C8	2.50	0.47
30:R1:2068:U:H3	30:R1:2430:A:H62	1.61	0.47
32:R3:1222:G:OP2	32:R3:1322:C:N4	2.40	0.47
32:R3:1401:G:O6	32:R3:1504:G:N2	2.48	0.47
8:2:199:HIS:HB3	30:R1:1820:U:O2	2.15	0.47
13:24:37:GLY:HA2	13:24:40:LEU:HD21	1.95	0.47
26:5:56:LEU:HD11	26:5:151:LEU:HD21	1.96	0.47
30:R1:289:G:H2'	30:R1:290:U:C6	2.49	0.47
30:R1:630:G:N2	30:R1:633:A:OP2	2.48	0.47
30:R1:1013:C:H2'	30:R1:1014:A:C8	2.49	0.47
30:R1:1417:C:H2'	30:R1:1418:G:O4'	2.14	0.47
30:R1:1881:C:H2'	30:R1:1882:U:C6	2.50	0.47
30:R1:2105:U:H2'	30:R1:2106:U:O4'	2.15	0.47
30:R1:2861:U:H2'	30:R1:2862:G:C8	2.50	0.47
32:R3:518:C:H4'	32:R3:519:C:O2	2.13	0.47
32:R3:978:A:N7	32:R3:1361:G:N2	2.63	0.47
53:T:0:C:H4'	53:T:1:G:H8	1.79	0.47
8:2:106:PRO:HD2	8:2:109:LEU:HD22	1.97	0.47
8:2:131:MET:HG2	8:2:163:ILE:HD11	1.96	0.47
8:2:269:ARG:HG2	8:2:270:ARG:N	2.30	0.47
13:24:43:LYS:NZ	30:R1:481:G:O5'	2.48	0.47
30:R1:438:G:H2'	30:R1:439:A:C8	2.49	0.47
30:R1:1447:C:H2'	30:R1:1448:G:C8	2.50	0.47
30:R1:1725:U:H3	30:R1:1735:A:H61	1.62	0.47
30:R1:2229:U:H2'	30:R1:2230:G:H8	1.79	0.47
32:R3:978:A:C5	32:R3:1319:A:C2	3.03	0.47
5:17:49:GLU:HB3	30:R1:2840:C:OP1	2.15	0.46
11:22:108:SER:OG	11:22:109:ASP:N	2.48	0.46
27:6:59:ASP:O	27:6:63:GLN:HG2	2.14	0.46
30:R1:242:G:O2'	30:R1:254:G:O6	2.29	0.46
30:R1:271:G:N3	30:R1:367:G:N2	2.63	0.46
30:R1:271:G:C4	30:R1:367:G:N2	2.83	0.46
30:R1:974:G:H1'	30:R1:975:A:C8	2.50	0.46
30:R1:1532:A:H2'	30:R1:1533:C:C6	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:R1:2521:C:C2	30:R1:2545:G:N2	2.82	0.46
31:R2:5:U:H2'	31:R2:6:G:H8	1.79	0.46
32:R3:74:A:C6	32:R3:97:G:C6	3.04	0.46
32:R3:113:G:H2'	32:R3:114:U:C6	2.49	0.46
32:R3:1149:C:H2'	32:R3:1150:A:C8	2.50	0.46
32:R3:1241:G:H2'	32:R3:1242:G:H8	1.80	0.46
3:15:116:VAL:HG11	3:15:135:ILE:HG22	1.97	0.46
5:17:9:GLN:HG2	5:17:11:ASN:H	1.79	0.46
7:19:64:SER:OG	7:19:65:ASN:N	2.48	0.46
12:23:61:LEU:HD12	12:23:62:VAL:N	2.30	0.46
20:31:5:ILE:HD12	26:5:63:LYS:HD3	1.97	0.46
30:R1:1506:U:H2'	30:R1:1507:C:C6	2.49	0.46
32:R3:375:U:H2'	32:R3:376:G:O4'	2.14	0.46
32:R3:847:G:H2'	32:R3:848:C:C6	2.50	0.46
32:R3:1253:G:H2'	32:R3:1254:A:C8	2.50	0.46
2:14:40:LYS:NZ	30:R1:2562:U:OP1	2.31	0.46
3:15:85:VAL:HG13	3:15:86:GLU:N	2.30	0.46
6:18:31:THR:HG21	31:R2:28:C:OP1	2.16	0.46
7:19:47:ILE:HB	7:19:59:THR:HG22	1.98	0.46
8:2:16:VAL:HB	8:2:203:VAL:HG22	1.96	0.46
14:25:14:LYS:NZ	31:R2:79:G:N7	2.63	0.46
14:25:47:VAL:O	14:25:51:GLN:N	2.48	0.46
30:R1:695:G:H5"	30:R1:1380:G:H4'	1.97	0.46
30:R1:1092:C:H3'	30:R1:1093:G:C8	2.50	0.46
30:R1:2430:A:H2'	30:R1:2430:A:N3	2.30	0.46
32:R3:1043:G:H2'	32:R3:1044:A:C8	2.50	0.46
32:R3:1137:C:H1'	32:R3:1138:G:C2	2.51	0.46
53:T:75:C:H5"	53:T:76:A:OP2	2.15	0.46
1:13:138:GLN:OE1	1:13:138:GLN:N	2.45	0.46
7:19:43:GLU:O	7:19:62:LYS:HB2	2.15	0.46
20:31:16:CYS:SG	20:31:17:SER:N	2.88	0.46
30:R1:1266:G:O2'	30:R1:2012:G:O6	2.30	0.46
30:R1:2412:A:H2'	30:R1:2413:G:O4'	2.15	0.46
30:R1:2549:G:C2	30:R1:2560:A:C2	3.04	0.46
31:R2:30:C:H1'	31:R2:57:A:H61	1.80	0.46
32:R3:352:C:O2'	32:R3:354:G:OP1	2.27	0.46
32:R3:1376:U:H2'	32:R3:1377:A:C8	2.50	0.46
4:16:42:THR:OG1	4:16:43:ALA:N	2.49	0.46
12:23:72:GLN:HE21	12:23:72:GLN:C	2.14	0.46
14:25:32:GLY:HA3	14:25:93:ARG:HB2	1.97	0.46
30:R1:1336:A:H2'	30:R1:1337:G:H8	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:R1:1352:U:O2'	30:R1:1570:A:N3	2.42	0.46
30:R1:1509:A:H2'	30:R1:1510:G:C8	2.50	0.46
31:R2:16:G:N2	31:R2:69:G:H1'	2.30	0.46
32:R3:2:A:O2'	32:R3:3:A:OP1	2.30	0.46
32:R3:859:G:H2'	32:R3:860:A:C8	2.51	0.46
32:R3:1011:C:N4	32:R3:1012:A:H62	2.13	0.46
32:R3:1068:G:N1	32:R3:1108:G:H1'	2.30	0.46
3:15:73:ILE:HD12	3:15:106:GLU:OE1	2.16	0.46
8:2:131:MET:HA	8:2:134:ILE:HB	1.96	0.46
11:22:88:ARG:NH1	11:22:94:ASP:OD2	2.48	0.46
18:3:29:VAL:O	18:3:185:ASN:HB3	2.15	0.46
30:R1:523:C:H2'	30:R1:524:G:H8	1.81	0.46
30:R1:1358:G:N1	30:R1:1372:U:OP2	2.36	0.46
30:R1:1802:A:H2'	30:R1:1803:A:C8	2.51	0.46
30:R1:1873:G:H2'	30:R1:1874:C:C6	2.51	0.46
30:R1:2290:G:H2'	30:R1:2291:U:C6	2.50	0.46
32:R3:204:G:N3	32:R3:204:G:H2'	2.31	0.46
32:R3:513:C:H2'	32:R3:514:C:H6	1.80	0.46
32:R3:634:C:H2'	32:R3:635:A:C8	2.45	0.46
32:R3:687:A:N6	32:R3:701:U:O4'	2.49	0.46
32:R3:1005:A:N6	32:R3:1025:U:O2'	2.49	0.46
7:19:52:ARG:NH2	30:R1:2720:U:OP1	2.49	0.46
30:R1:521:U:H2'	30:R1:522:A:C8	2.44	0.46
30:R1:1107:G:H2'	30:R1:1108:U:C6	2.51	0.46
30:R1:1170:C:C2	30:R1:1171:G:C8	3.03	0.46
30:R1:2117:A:H1'	30:R1:2118:U:H5"	1.98	0.46
32:R3:80:A:N1	32:R3:90:C:O2'	2.45	0.46
32:R3:1012:A:H2'	32:R3:1013:G:C8	2.51	0.46
32:R3:1064:G:N3	32:R3:1066:C:N4	2.63	0.46
32:R3:1150:A:O2'	32:R3:1151:A:O5'	2.33	0.46
32:R3:1270:G:H2'	32:R3:1271:A:C8	2.51	0.46
4:16:106:ASP:OD2	4:16:107:GLY:N	2.47	0.46
11:22:51:LEU:HD13	11:22:105:VAL:HG11	1.98	0.46
17:29:9:LYS:HZ1	17:29:12:GLU:HB2	1.80	0.46
20:31:59:ARG:NH2	32:R3:1311:A:OP1	2.48	0.46
30:R1:285:G:C6	30:R1:356:G:C5	3.04	0.46
30:R1:352:A:H2'	30:R1:353:C:O4'	2.15	0.46
30:R1:500:G:N2	30:R1:503:A:H5'	2.29	0.46
30:R1:511:U:O2'	30:R1:1215:G:N2	2.49	0.46
30:R1:1183:U:H2'	30:R1:1184:U:C6	2.51	0.46
30:R1:1232:G:C6	30:R1:1233:C:C4	3.04	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:R1:1744:A:H3'	30:R1:1745:A:H8	1.80	0.46
30:R1:2443:C:H2'	30:R1:2444:G:H8	1.80	0.46
32:R3:126:G:OP1	32:R3:605:U:O2'	2.20	0.46
32:R3:264:C:H2'	32:R3:265:G:O4'	2.16	0.46
32:R3:1405:G:O2'	32:R3:1518:A:O2'	2.16	0.46
8:2:220:ARG:NH1	30:R1:1789:A:OP2	2.49	0.46
12:23:8:LEU:O	17:29:29:ARG:NH2	2.48	0.46
27:6:39:ALA:HA	27:6:57:TYR:CD2	2.50	0.46
30:R1:523:C:H2'	30:R1:524:G:C8	2.50	0.46
30:R1:2136:G:H1	30:R1:2155:U:H3	1.64	0.46
30:R1:2649:C:H2'	30:R1:2650:U:C6	2.51	0.46
31:R2:95:U:H2'	31:R2:96:G:C8	2.51	0.46
14:25:6:ALA:HB1	14:25:40:ILE:HG23	1.98	0.46
15:27:40:GLN:NE2	15:27:45:PHE:H	2.14	0.46
30:R1:669:G:C2	30:R1:801:G:C6	3.04	0.46
30:R1:753:A:H2'	30:R1:754:U:C6	2.51	0.46
32:R3:1103:C:O2'	32:R3:1104:G:H8	1.98	0.46
32:R3:1270:G:H2'	32:R3:1271:A:H8	1.81	0.46
27:6:94:ARG:HB2	27:6:105:SER:HB3	1.97	0.45
30:R1:225:C:H2'	30:R1:226:A:O4'	2.16	0.45
30:R1:890:C:H3'	30:R1:891:G:H4'	1.97	0.45
30:R1:1336:A:H2'	30:R1:1337:G:C8	2.52	0.45
30:R1:2122:U:H5	30:R1:2123:G:C8	2.34	0.45
30:R1:2626:C:H2'	30:R1:2627:G:H8	1.81	0.45
32:R3:222:C:H2'	32:R3:223:A:H8	1.80	0.45
32:R3:1246:A:N6	32:R3:1292:G:O6	2.49	0.45
32:R3:1507:A:H2'	32:R3:1508:A:C8	2.51	0.45
8:2:233:GLY:HA3	30:R1:2598:A:H5"	1.99	0.45
14:25:21:ARG:NH1	14:25:87:GLN:O	2.49	0.45
30:R1:547:A:H5"	30:R1:548:G:N7	2.30	0.45
30:R1:1425:G:H2'	30:R1:1426:G:C8	2.51	0.45
32:R3:555:U:H2'	32:R3:556:C:H6	1.80	0.45
32:R3:588:G:O2'	32:R3:589:U:OP1	2.33	0.45
32:R3:1175:G:H2'	32:R3:1176:A:C8	2.49	0.45
6:18:76:LYS:HE2	6:18:76:LYS:HB2	1.63	0.45
7:19:13:LYS:HD3	7:19:76:HIS:HA	1.98	0.45
14:25:29:ILE:HD12	14:25:39:ALA:HA	1.98	0.45
14:25:80:HIS:ND1	14:25:81:PRO:HD2	2.31	0.45
23:35:14:LYS:HB2	23:35:22:LYS:HE3	1.99	0.45
27:6:15:ASP:OD1	27:6:26:LYS:HB3	2.16	0.45
30:R1:167:A:H2'	30:R1:168:G:O4'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:R1:1113:U:H2'	30:R1:1114:C:C6	2.51	0.45
32:R3:463:U:H2'	32:R3:464:U:C5	2.51	0.45
5:17:59:SER:O	5:17:63:ARG:HG3	2.17	0.45
11:22:5:ALA:O	30:R1:494:G:O2'	2.26	0.45
11:22:74:ILE:HD12	11:22:105:VAL:HG22	1.99	0.45
22:34:12:ARG:HD2	22:34:44:VAL:HG21	1.98	0.45
30:R1:181:A:H2'	30:R1:182:A:C8	2.52	0.45
32:R3:77:A:H5'	32:R3:95:C:H1'	1.98	0.45
32:R3:202:G:O2'	32:R3:468:A:N3	2.38	0.45
32:R3:399:G:H2'	32:R3:400:C:C6	2.51	0.45
32:R3:1010:U:H2'	32:R3:1011:C:C6	2.52	0.45
5:17:29:VAL:HG11	5:17:75:ILE:HG23	1.99	0.45
9:20:18:LYS:NZ	30:R1:1219:U:OP2	2.38	0.45
27:6:148:ARG:HA	27:6:161:VAL:CG2	2.42	0.45
30:R1:286:U:H2'	30:R1:287:G:O4'	2.17	0.45
30:R1:1569:A:H2'	30:R1:1570:A:C8	2.52	0.45
32:R3:17:U:H2'	32:R3:18:C:H6	1.82	0.45
32:R3:592:G:H2'	32:R3:593:U:H6	1.82	0.45
32:R3:978:A:C6	32:R3:1318:A:C6	3.05	0.45
13:24:94:PHE:HB2	13:24:100:GLU:O	2.17	0.45
26:5:32:LYS:HG2	26:5:156:THR:HB	1.98	0.45
30:R1:362:A:H3'	30:R1:363:G:H8	1.82	0.45
30:R1:698:C:O2'	30:R1:734:A:N6	2.44	0.45
30:R1:1263:U:H2'	30:R1:1264:A:C8	2.52	0.45
32:R3:925:G:C2	32:R3:927:G:C8	3.05	0.45
32:R3:1253:G:H2'	32:R3:1254:A:H8	1.82	0.45
32:R3:1271:A:H2'	32:R3:1272:G:C8	2.52	0.45
2:14:13:ASN:HD21	2:14:97:THR:HG23	1.82	0.45
18:3:157:LYS:HE2	18:3:157:LYS:HB2	1.69	0.45
26:5:9:ASP:N	26:5:9:ASP:OD1	2.48	0.45
30:R1:297:G:O6	30:R1:342:A:N6	2.48	0.45
30:R1:2029:G:N1	30:R1:2033:A:OP2	2.48	0.45
30:R1:2082:A:C4	30:R1:2239:G:N2	2.84	0.45
30:R1:2745:C:H2'	30:R1:2746:U:C6	2.52	0.45
32:R3:1388:C:H2'	32:R3:1389:C:O2	2.17	0.45
32:R3:1407:C:H2'	32:R3:1408:A:H8	1.82	0.45
5:17:49:GLU:HG2	5:17:94:TYR:HD2	1.82	0.45
18:3:45:TYR:OH	30:R1:2636:C:O2'	2.18	0.45
27:6:171:LYS:NZ	30:R1:2530:A:N7	2.64	0.45
30:R1:414:C:H1'	30:R1:1864:U:H1'	1.99	0.45
30:R1:1292:G:H2'	30:R1:1293:C:H6	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:R1:1587:G:H2'	30:R1:1588:G:H8	1.81	0.45
30:R1:1886:U:H2'	30:R1:1887:C:C6	2.52	0.45
30:R1:2123:G:N2	30:R1:2175:C:N3	2.65	0.45
30:R1:2328:A:H8	30:R1:2328:A:O5'	2.00	0.45
30:R1:2537:U:H2'	30:R1:2538:C:H6	1.81	0.45
30:R1:2788:C:H2'	30:R1:2789:C:C6	2.52	0.45
32:R3:193:C:H2'	32:R3:194:C:C6	2.52	0.45
32:R3:500:G:HO2'	32:R3:501:C:P	2.38	0.45
32:R3:602:A:H2'	32:R3:603:U:C6	2.52	0.45
32:R3:737:C:H2'	32:R3:738:C:C6	2.52	0.45
32:R3:1090:U:H2'	32:R3:1091:U:C6	2.52	0.45
32:R3:1271:A:H2'	32:R3:1272:G:H8	1.81	0.45
32:R3:1288:A:H2'	32:R3:1289:A:C8	2.52	0.45
32:R3:1316:G:N2	32:R3:1318:A:H3'	2.32	0.45
32:R3:1342:C:H2'	32:R3:1343:G:C8	2.51	0.45
1:13:131:ASN:OD1	1:13:131:ASN:N	2.45	0.45
4:16:42:THR:HA	4:16:93:VAL:HA	1.98	0.45
4:16:64:TRP:CD1	30:R1:873:C:H4'	2.52	0.45
14:25:35:GLU:OE1	14:25:35:GLU:N	2.50	0.45
30:R1:700:G:O2'	30:R1:1632:A:N3	2.40	0.45
30:R1:730:A:OP1	30:R1:1775:U:O2'	2.22	0.45
30:R1:897:C:H5	30:R1:899:A:C8	2.34	0.45
30:R1:981:A:OP2	30:R1:982:C:N4	2.50	0.45
30:R1:1386:C:H1'	30:R1:1470:A:H1'	1.99	0.45
30:R1:1563:U:H2'	30:R1:1564:C:C6	2.52	0.45
30:R1:1709:U:C2	30:R1:1750:G:N2	2.85	0.45
30:R1:1905:C:O2'	30:R1:1929:G:H1'	2.17	0.45
30:R1:2302:U:H2'	30:R1:2303:G:C8	2.52	0.45
30:R1:2834:G:H2'	30:R1:2879:A:N6	2.32	0.45
32:R3:209:U:H5	32:R3:211:G:H8	1.64	0.45
32:R3:390:U:H2'	32:R3:391:G:H8	1.82	0.45
32:R3:628:G:H2'	32:R3:629:A:C8	2.52	0.45
32:R3:728:A:H2'	32:R3:729:A:C8	2.52	0.45
32:R3:1294:G:H2'	32:R3:1295:U:C6	2.52	0.45
32:R3:1430:A:H2'	32:R3:1431:A:O4'	2.16	0.45
3:15:78:ARG:HD2	3:15:113:ALA:HB3	1.99	0.45
8:2:154:ALA:HB2	8:2:161:VAL:HG23	1.99	0.45
12:23:37:ASP:O	12:23:37:ASP:OD1	2.34	0.45
30:R1:361:G:O2'	30:R1:362:A:O4'	2.35	0.45
30:R1:528:A:H2	30:R1:2043:C:H4'	1.81	0.45
30:R1:2241:A:H2'	30:R1:2242:G:H8	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:R1:2589:A:H2'	30:R1:2590:A:H8	1.82	0.45
32:R3:1320:C:H2'	32:R3:1321:U:C6	2.52	0.45
2:14:88:ASN:HB3	2:14:91:SER:O	2.17	0.44
9:20:69:ARG:HH22	30:R1:1012:U:P	2.40	0.44
30:R1:134:G:C6	30:R1:144:A:N1	2.85	0.44
30:R1:155:A:O2'	30:R1:156:A:H8	2.00	0.44
30:R1:638:G:H2'	30:R1:639:U:H6	1.82	0.44
30:R1:644:A:N6	30:R1:2349:G:H1'	2.32	0.44
30:R1:1132:U:H2'	30:R1:1133:A:C8	2.51	0.44
30:R1:1420:A:O2'	30:R1:1421:G:H5'	2.16	0.44
30:R1:2197:U:H1'	30:R1:2198:A:C8	2.53	0.44
30:R1:2866:U:H5'	30:R1:2868:A:H5'	1.98	0.44
30:R1:2896:C:O2'	30:R1:2897:U:O5'	2.28	0.44
53:T:3:G:C6	53:T:70:G:C6	3.05	0.44
6:18:46:GLU:HA	31:R2:113:C:H1'	1.99	0.44
30:R1:645:C:H2'	30:R1:647:G:N7	2.32	0.44
30:R1:689:A:H8	30:R1:779:U:O2'	1.99	0.44
30:R1:813:U:O2'	30:R1:1225:G:H1'	2.17	0.44
30:R1:1047:G:N2	30:R1:1110:G:H2'	2.32	0.44
30:R1:2380:C:H2'	30:R1:2381:A:C8	2.52	0.44
30:R1:2888:C:H2'	30:R1:2889:C:H6	1.83	0.44
32:R3:981:U:H2'	32:R3:982:U:C5	2.52	0.44
6:18:3:LYS:HA	6:18:3:LYS:HD2	1.72	0.44
11:22:41:LYS:HD2	21:32:21:LEU:HD11	1.99	0.44
14:25:43:ASP:OD1	14:25:44:HIS:N	2.51	0.44
30:R1:948:C:H2'	30:R1:949:G:H8	1.81	0.44
30:R1:1159:U:H2'	30:R1:1160:G:H8	1.82	0.44
30:R1:1746:A:H2'	30:R1:1747:U:H6	1.82	0.44
30:R1:1788:C:C2	30:R1:1789:A:C8	3.05	0.44
30:R1:2030:A:H4'	30:R1:2031:A:H8	1.81	0.44
32:R3:115:G:N2	32:R3:117:G:O6	2.46	0.44
32:R3:289:G:HO2'	32:R3:290:C:H6	1.63	0.44
32:R3:302:G:H2'	32:R3:303:A:C8	2.53	0.44
32:R3:472:U:H5"	32:R3:473:U:C5	2.52	0.44
32:R3:678:U:H2'	32:R3:679:C:H6	1.82	0.44
32:R3:738:C:O2'	32:R3:739:C:H6	2.01	0.44
32:R3:1015:G:H1'	32:R3:1218:C:O2'	2.18	0.44
32:R3:1342:C:H2'	32:R3:1343:G:H8	1.83	0.44
5:17:55:ALA:HA	5:17:80:PHE:CE1	2.53	0.44
15:27:40:GLN:HE22	15:27:45:PHE:N	2.15	0.44
18:3:8:LYS:HB2	18:3:201:LEU:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:R1:60:G:C8	30:R1:62:U:H5	2.36	0.44
30:R1:1171:G:H2'	30:R1:1172:C:O4'	2.17	0.44
30:R1:1190:G:H2'	30:R1:1191:G:H8	1.83	0.44
30:R1:1209:U:O2'	30:R1:1237:A:N1	2.46	0.44
30:R1:2148:G:C4	30:R1:2149:U:H5	2.36	0.44
30:R1:2369:A:N6	30:R1:2370:G:O6	2.51	0.44
30:R1:2839:G:H2'	30:R1:2840:C:C6	2.53	0.44
30:R1:2875:C:H2'	30:R1:2876:G:C8	2.53	0.44
32:R3:129:A:H1'	32:R3:130:A:C8	2.53	0.44
32:R3:312:C:H2'	32:R3:313:A:C8	2.53	0.44
32:R3:447:G:O2'	32:R3:487:A:N6	2.50	0.44
32:R3:993:G:O2'	32:R3:995:C:N4	2.48	0.44
32:R3:1314:C:H2'	32:R3:1315:U:C6	2.52	0.44
1:13:98:GLU:OE1	1:13:98:GLU:N	2.47	0.44
30:R1:341:C:H5"	30:R1:342:A:OP2	2.17	0.44
30:R1:629:G:H5"	30:R1:650:C:O2'	2.17	0.44
30:R1:1174:U:O2'	30:R1:1176:U:OP2	2.27	0.44
30:R1:1429:G:H2'	30:R1:1430:G:H8	1.83	0.44
30:R1:1812:U:H2'	30:R1:1813:G:H8	1.83	0.44
30:R1:2329:U:H2'	30:R1:2330:G:C8	2.52	0.44
30:R1:2804:U:H2'	30:R1:2805:C:C6	2.52	0.44
32:R3:990:C:O2'	32:R3:991:U:H5"	2.18	0.44
5:17:97:ILE:O	5:17:98:LEU:HD23	2.18	0.44
9:20:69:ARG:NH2	30:R1:1012:U:OP2	2.50	0.44
27:6:154:GLU:HG3	27:6:156:TYR:H	1.83	0.44
30:R1:191:A:H2'	30:R1:192:C:H6	1.82	0.44
30:R1:367:G:H2'	30:R1:368:A:O4'	2.17	0.44
30:R1:987:C:O2'	30:R1:1000:A:N3	2.43	0.44
32:R3:115:G:OP1	32:R3:115:G:C8	2.70	0.44
32:R3:446:G:H2'	32:R3:447:G:O4'	2.18	0.44
32:R3:1120:C:H2'	32:R3:1121:U:H6	1.82	0.44
32:R3:1405:G:N2	32:R3:1518:A:H8	2.15	0.44
53:T:0:C:H4'	53:T:1:G:C8	2.53	0.44
53:T:49:G:O6	53:T:66:C:N4	2.50	0.44
11:22:78:GLU:O	30:R1:24:G:O2'	2.36	0.44
18:3:8:LYS:HD3	18:3:197:THR:HA	2.00	0.44
29:M:8:C:H2'	29:M:9:A:O4'	2.18	0.44
30:R1:1463:C:H2'	30:R1:1464:G:H8	1.83	0.44
32:R3:166:U:H2'	32:R3:167:A:H8	1.83	0.44
32:R3:477:C:H2'	32:R3:478:A:C8	2.52	0.44
5:17:83:LEU:HD21	5:17:115:LEU:HD13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:27:20:ARG:HD3	30:R1:2356:U:O3'	2.18	0.44
15:27:43:THR:H	30:R1:2331:G:H4'	1.82	0.44
30:R1:742:A:H2'	30:R1:743:A:H8	1.82	0.44
30:R1:1447:C:O2'	30:R1:1544:A:N3	2.48	0.44
30:R1:1527:G:N1	30:R1:1544:A:OP2	2.50	0.44
30:R1:2028:U:H2'	30:R1:2029:G:C8	2.53	0.44
32:R3:1496:C:O2'	32:R3:1517:G:O6	2.35	0.44
12:23:9:LYS:HA	17:29:29:ARG:HH22	1.82	0.44
12:23:77:ARG:HE	12:23:77:ARG:HB2	1.66	0.44
18:3:161:MET:HE1	30:R1:2619:C:O2	2.17	0.44
30:R1:593:U:H2'	30:R1:594:U:H6	1.83	0.44
30:R1:931:U:O2'	30:R1:1168:G:O2'	2.33	0.44
30:R1:1196:C:C2	30:R1:1197:G:C8	3.06	0.44
30:R1:1198:U:H2'	30:R1:1199:U:C6	2.52	0.44
30:R1:1537:G:H3'	30:R1:1537:G:N3	2.33	0.44
30:R1:1837:C:H2'	30:R1:1899:A:H61	1.83	0.44
30:R1:1928:A:H2'	30:R1:1929:G:O4'	2.18	0.44
32:R3:219:U:H2'	32:R3:220:G:O4'	2.18	0.44
32:R3:953:G:C6	32:R3:1229:A:C6	3.06	0.44
32:R3:1054:C:O2	32:R3:1196:A:N6	2.51	0.44
32:R3:1305:G:H1'	32:R3:1306:A:OP2	2.18	0.44
4:16:4:PRO:HG3	4:16:68:PHE:HE2	1.83	0.43
9:20:111:LYS:CE	10:21:48:LYS:HZ2	2.31	0.43
21:32:27:LEU:HD23	21:32:27:LEU:HA	1.86	0.43
28:9:50:ARG:C	28:9:51:ARG:HD3	2.39	0.43
30:R1:372:G:O2'	30:R1:400:G:O6	2.22	0.43
30:R1:594:U:H2'	30:R1:595:C:H6	1.83	0.43
30:R1:1410:G:H2'	30:R1:1411:U:C6	2.52	0.43
30:R1:1510:G:H2'	30:R1:1511:G:H8	1.83	0.43
30:R1:1586:A:H2'	30:R1:1587:G:O4'	2.18	0.43
30:R1:2638:G:H1'	30:R1:2778:A:N6	2.33	0.43
32:R3:82:G:H1'	32:R3:88:U:N3	2.32	0.43
32:R3:108:G:H5'	32:R3:109:A:H5"	2.00	0.43
32:R3:253:A:H2'	32:R3:254:G:H8	1.83	0.43
32:R3:409:U:H3	32:R3:433:G:H1	1.64	0.43
53:T:41:C:H2'	53:T:42:G:O4'	2.17	0.43
14:25:80:HIS:CD2	14:25:83:LYS:HD3	2.53	0.43
30:R1:149:A:H2'	30:R1:150:U:H6	1.82	0.43
30:R1:955:U:H5	30:R1:962:G:H1	1.65	0.43
30:R1:1707:G:C8	30:R1:1756:G:C5	3.06	0.43
30:R1:1723:G:O6	30:R1:1737:G:O2'	2.29	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:R1:2847:U:H2'	30:R1:2848:G:O4'	2.17	0.43
32:R3:676:A:H2'	32:R3:677:U:H6	1.82	0.43
32:R3:1291:U:H2'	32:R3:1292:G:H8	1.83	0.43
1:13:64:VAL:HG22	1:13:68:LYS:HE3	1.98	0.43
10:21:80:ARG:H	30:R1:565:C:P	2.42	0.43
13:24:78:LYS:HB3	13:24:78:LYS:HE3	1.76	0.43
22:34:34:ARG:NH2	22:34:42:LEU:O	2.47	0.43
30:R1:177:G:H3'	30:R1:178:G:H8	1.83	0.43
30:R1:623:C:H2'	30:R1:624:C:C6	2.53	0.43
30:R1:967:U:H2'	30:R1:968:C:C6	2.53	0.43
30:R1:1425:G:O5'	30:R1:1425:G:H8	2.00	0.43
30:R1:2189:U:N3	30:R1:2190:G:O6	2.52	0.43
30:R1:2235:G:H2'	30:R1:2236:U:C6	2.53	0.43
30:R1:2545:G:N2	30:R1:2565:A:H8	1.98	0.43
32:R3:204:G:H1	32:R3:215:C:H1'	1.84	0.43
32:R3:252:U:O4	32:R3:253:A:N6	2.48	0.43
32:R3:256:U:H2'	32:R3:257:G:C8	2.53	0.43
32:R3:711:G:H2'	32:R3:712:A:H8	1.83	0.43
32:R3:1402:C:H2'	32:R3:1403:C:O4'	2.19	0.43
32:R3:1415:G:C6	32:R3:1486:G:C6	3.06	0.43
3:15:3:LEU:HD22	25:4:182:ALA:HB2	2.00	0.43
14:25:17:SER:HG	14:25:21:ARG:HH21	1.60	0.43
16:28:15:ASN:HD22	16:28:23:ALA:HB1	1.83	0.43
24:36:14:CYS:SG	24:36:33:HIS:ND1	2.91	0.43
30:R1:1361:G:H2'	30:R1:1362:C:H6	1.82	0.43
30:R1:2074:U:H2'	30:R1:2075:U:C6	2.53	0.43
32:R3:184:G:H2'	32:R3:185:U:C6	2.53	0.43
32:R3:837:U:H2'	32:R3:838:G:C8	2.53	0.43
32:R3:1436:U:O4	32:R3:1437:A:N6	2.52	0.43
19:30:2:LYS:H	19:30:39:ASP:HB3	1.82	0.43
25:4:132:LYS:HB3	25:4:132:LYS:HE2	1.81	0.43
30:R1:141:G:H2'	30:R1:142:A:C8	2.53	0.43
30:R1:165:A:H2'	30:R1:166:U:C6	2.54	0.43
30:R1:703:U:H2'	30:R1:704:G:O4'	2.18	0.43
30:R1:971:G:O2'	30:R1:983:A:N3	2.45	0.43
30:R1:1091:G:H2'	30:R1:1092:C:C6	2.54	0.43
30:R1:1770:G:C6	30:R1:1983:G:C6	3.06	0.43
30:R1:2838:G:H2'	30:R1:2839:G:H8	1.82	0.43
32:R3:164:G:C2	32:R3:165:G:C8	3.07	0.43
32:R3:230:G:H2'	32:R3:231:U:O4'	2.19	0.43
32:R3:612:C:H2'	32:R3:613:C:H6	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:15:110:VAL:O	3:15:128:THR:HG23	2.18	0.43
9:20:2:ARG:HH12	9:20:4:LYS:HE2	1.83	0.43
30:R1:412:A:H2'	30:R1:412:A:N3	2.34	0.43
30:R1:947:A:C6	30:R1:971:G:C6	3.06	0.43
30:R1:1549:A:H2'	30:R1:1550:C:C6	2.54	0.43
30:R1:1809:A:H2'	30:R1:1810:A:C8	2.54	0.43
30:R1:2183:A:N1	30:R1:2184:A:N6	2.67	0.43
30:R1:2536:G:H2'	30:R1:2537:U:C6	2.53	0.43
31:R2:4:C:H2'	31:R2:5:U:C6	2.54	0.43
32:R3:414:A:C4	32:R3:415:A:C8	3.07	0.43
32:R3:1155:A:H2'	32:R3:1156:G:O4'	2.18	0.43
2:14:70:ARG:NH2	30:R1:2683:C:O2	2.52	0.43
8:2:251:THR:OG1	8:2:252:LYS:N	2.52	0.43
10:21:4:VAL:HG22	10:21:40:MET:HG2	2.00	0.43
16:28:7:THR:OG1	16:28:8:GLY:N	2.52	0.43
17:29:9:LYS:HZ2	17:29:12:GLU:N	2.17	0.43
30:R1:1473:G:C6	30:R1:1519:G:C6	3.07	0.43
30:R1:1664:A:N6	30:R1:1996:C:H42	2.15	0.43
32:R3:890:G:O2'	32:R3:906:A:N6	2.51	0.43
18:3:149:ASN:CG	18:3:150:GLN:H	2.21	0.43
30:R1:1109:C:O2'	30:R1:1110:G:OP1	2.35	0.43
30:R1:1173:U:C5	30:R1:1176:U:H4'	2.54	0.43
30:R1:1463:C:H2'	30:R1:1464:G:C8	2.54	0.43
30:R1:1482:G:H2'	30:R1:1483:G:C8	2.51	0.43
30:R1:1869:G:N2	30:R1:1872:A:N7	2.67	0.43
30:R1:2375:G:N2	30:R1:2378:A:OP2	2.46	0.43
30:R1:2545:G:H2'	30:R1:2546:U:O4'	2.18	0.43
30:R1:2851:A:H2'	30:R1:2852:G:O4'	2.18	0.43
32:R3:918:A:H2'	32:R3:919:A:H8	1.84	0.43
19:30:57:GLU:OE2	19:30:57:GLU:HA	2.19	0.43
27:6:169:ARG:HA	27:6:169:ARG:HE	1.84	0.43
30:R1:488:G:H2'	30:R1:489:G:H2'	2.01	0.43
30:R1:628:G:C6	30:R1:636:G:C2	3.07	0.43
30:R1:871:U:H2'	30:R1:872:U:C6	2.53	0.43
30:R1:1685:C:H2'	30:R1:1686:C:H6	1.84	0.43
30:R1:2236:U:H2'	30:R1:2237:G:O4'	2.19	0.43
30:R1:2461:A:H2'	30:R1:2462:C:C6	2.54	0.43
30:R1:2663:G:HO2'	30:R1:2664:G:P	2.40	0.43
32:R3:184:G:H2'	32:R3:185:U:H6	1.84	0.43
32:R3:837:U:H2'	32:R3:838:G:H8	1.83	0.43
3:15:109:LYS:HG3	3:15:126:ARG:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:28:55:MET:HB3	28:9:27:ARG:HH12	1.83	0.43
21:32:8:THR:HG22	21:32:9:ARG:N	2.34	0.43
28:9:30:LEU:HB3	28:9:36:ALA:HB3	2.00	0.43
30:R1:282:A:C6	30:R1:359:G:C6	3.07	0.43
30:R1:489:G:C6	30:R1:491:G:C2	3.07	0.43
30:R1:2061:G:N2	30:R1:2062:A:N7	2.53	0.43
32:R3:878:A:H2'	32:R3:879:C:H6	1.84	0.43
32:R3:1250:A:N3	32:R3:1370:G:O2'	2.46	0.43
5:17:94:TYR:O	5:17:116:VAL:HG22	2.19	0.42
5:17:97:ILE:C	5:17:98:LEU:HD23	2.40	0.42
9:20:111:LYS:HE3	10:21:48:LYS:HZ2	1.84	0.42
17:29:21:LEU:HA	17:29:25:GLN:HB3	2.00	0.42
25:4:61:ARG:HH12	25:4:64:GLY:HA3	1.85	0.42
28:9:45:GLU:O	28:9:50:ARG:N	2.52	0.42
30:R1:632:A:H2'	30:R1:633:A:C8	2.54	0.42
30:R1:671:C:H2'	30:R1:672:C:C6	2.54	0.42
30:R1:741:U:H2'	30:R1:742:A:H8	1.83	0.42
30:R1:962:G:H21	30:R1:2250:G:H1	1.67	0.42
30:R1:971:G:OP2	30:R1:974:G:N2	2.53	0.42
30:R1:1317:G:C6	30:R1:1336:A:C6	3.07	0.42
30:R1:2041:U:H2'	30:R1:2042:A:H8	1.84	0.42
32:R3:820:U:H4'	32:R3:821:G:OP2	2.19	0.42
32:R3:1130:A:C5	32:R3:1146:A:C6	3.07	0.42
32:R3:1387:G:H2'	32:R3:1388:C:C6	2.53	0.42
32:R3:1495:U:C2	32:R3:1496:C:C5	3.07	0.42
6:18:62:LEU:HD22	6:18:70:ALA:HA	2.01	0.42
8:2:73:ILE:HG22	8:2:95:TYR:HD2	1.83	0.42
10:21:15:SER:N	10:21:18:GLN:HE22	2.13	0.42
14:25:55:GLU:HG2	14:25:59:GLU:OE2	2.19	0.42
18:3:170:VAL:HG21	30:R1:2679:A:H5'	2.01	0.42
30:R1:168:G:H2'	30:R1:169:G:H8	1.84	0.42
30:R1:572:A:H5"	30:R1:573:U:OP2	2.19	0.42
30:R1:926:G:H2'	30:R1:927:A:H8	1.83	0.42
30:R1:978:G:H3'	30:R1:979:A:H5"	2.01	0.42
30:R1:1295:C:C2	30:R1:1296:G:C8	3.07	0.42
30:R1:2130:U:H2'	30:R1:2131:U:C6	2.54	0.42
30:R1:2186:G:H2'	30:R1:2187:U:O4'	2.19	0.42
32:R3:312:C:HO2'	32:R3:313:A:P	2.40	0.42
7:19:112:ARG:O	7:19:113:LEU:HG	2.20	0.42
11:22:88:ARG:HA	11:22:88:ARG:HD2	1.86	0.42
13:24:85:ARG:NH2	13:24:100:GLU:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:25:30:ILE:HD11	14:25:63:ILE:HD12	2.01	0.42
25:4:63:LYS:NZ	30:R1:2444:G:OP2	2.40	0.42
25:4:194:LYS:HB2	25:4:194:LYS:HE3	1.70	0.42
27:6:169:ARG:HA	27:6:169:ARG:NE	2.35	0.42
30:R1:638:G:C6	30:R1:651:G:N1	2.88	0.42
30:R1:2429:G:H5"	30:R1:2430:A:OP2	2.19	0.42
30:R1:2494:G:C2	30:R1:2495:G:C8	3.07	0.42
30:R1:2788:C:O2'	30:R1:2809:A:N3	2.39	0.42
32:R3:417:G:O2'	32:R3:418:C:H5'	2.19	0.42
32:R3:1151:A:H2'	32:R3:1152:A:C8	2.53	0.42
1:13:99:ARG:HE	1:13:99:ARG:HB3	1.71	0.42
14:25:83:LYS:NZ	30:R1:1119:U:OP1	2.52	0.42
17:29:43:LEU:O	17:29:47:ARG:HG3	2.19	0.42
26:5:48:LEU:HD12	26:5:48:LEU:HA	1.83	0.42
30:R1:68:G:H2'	30:R1:69:C:O4'	2.19	0.42
30:R1:285:G:H2'	30:R1:286:U:C6	2.54	0.42
30:R1:1042:G:H2'	30:R1:1043:C:H6	1.83	0.42
30:R1:1071:G:H1'	30:R1:1089:A:N7	2.35	0.42
30:R1:1108:U:H2'	30:R1:1109:C:N3	2.35	0.42
30:R1:1874:C:H2'	30:R1:1875:G:O4'	2.18	0.42
30:R1:2185:U:H2'	30:R1:2186:G:C8	2.54	0.42
30:R1:2650:U:H2'	30:R1:2651:C:H6	1.83	0.42
30:R1:2846:G:H2'	30:R1:2847:U:C6	2.54	0.42
32:R3:286:C:H2'	32:R3:287:U:C6	2.54	0.42
32:R3:588:G:HO2'	32:R3:589:U:P	2.40	0.42
32:R3:589:U:H2'	32:R3:590:U:H6	1.84	0.42
32:R3:1349:A:H1'	32:R3:1374:A:N6	2.34	0.42
6:18:33:ARG:NH2	31:R2:52:A:N7	2.67	0.42
16:28:43:LYS:HE2	16:28:43:LYS:HA	2.01	0.42
30:R1:161:A:H1'	30:R1:162:U:H5"	2.00	0.42
30:R1:579:G:H2'	30:R1:580:U:C6	2.54	0.42
30:R1:1595:C:H2'	30:R1:1596:A:C8	2.55	0.42
30:R1:1726:C:H2'	30:R1:1727:C:C6	2.54	0.42
30:R1:1727:C:H2'	30:R1:1728:C:O4'	2.20	0.42
30:R1:2372:U:H2'	30:R1:2373:G:C8	2.52	0.42
31:R2:4:C:H2'	31:R2:5:U:H6	1.85	0.42
32:R3:301:G:HO2'	32:R3:302:G:P	2.43	0.42
32:R3:537:G:H2'	32:R3:538:G:H8	1.83	0.42
6:18:27:VAL:HA	6:18:93:ASP:HB3	2.00	0.42
15:27:38:VAL:HG12	15:27:40:GLN:HG2	2.01	0.42
27:6:82:PHE:HB2	27:6:140:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:R1:589:U:O2'	30:R1:590:A:H5'	2.19	0.42
30:R1:783:A:H2'	30:R1:784:G:H4'	2.01	0.42
30:R1:1041:G:C2	30:R1:1042:G:N7	2.88	0.42
30:R1:1071:G:H22	30:R1:1090:A:N6	2.18	0.42
30:R1:1528:A:OP2	30:R1:1543:G:N2	2.42	0.42
30:R1:2329:U:H2'	30:R1:2330:G:H8	1.84	0.42
30:R1:2601:C:N4	30:R1:2603:G:O6	2.52	0.42
30:R1:2784:U:H2'	30:R1:2785:C:C6	2.54	0.42
32:R3:91:U:H3'	32:R3:92:U:H5"	2.01	0.42
32:R3:373:A:N3	32:R3:482:A:N6	2.68	0.42
32:R3:908:A:H2'	32:R3:909:A:C8	2.52	0.42
32:R3:1324:A:H2'	32:R3:1325:C:C6	2.55	0.42
6:18:56:LYS:HZ1	31:R2:117:G:P	2.43	0.42
8:2:218:THR:O	30:R1:1789:A:H5"	2.20	0.42
21:32:7:PRO:HD2	30:R1:1263:U:O2'	2.19	0.42
30:R1:347:A:H2'	30:R1:348:A:H8	1.83	0.42
30:R1:924:G:H2'	30:R1:925:A:H8	1.85	0.42
30:R1:2650:U:C2	30:R1:2671:G:N2	2.87	0.42
32:R3:1010:U:H2'	32:R3:1011:C:H6	1.84	0.42
53:T:66:C:H2'	53:T:67:C:C6	2.54	0.42
8:2:73:ILE:HD11	30:R1:1490:A:C4	2.55	0.42
15:27:41:ARG:NH2	30:R1:2387:U:H4'	2.35	0.42
30:R1:64:A:H2'	30:R1:65:U:C6	2.55	0.42
30:R1:160:A:OP2	30:R1:161:A:O2'	2.32	0.42
30:R1:278:A:N6	30:R1:361:G:C8	2.87	0.42
30:R1:285:G:N7	30:R1:356:G:N1	2.68	0.42
30:R1:799:G:C6	30:R1:800:A:C6	3.08	0.42
30:R1:1053:C:N4	30:R1:1054:A:H62	2.17	0.42
30:R1:1063:G:H22	30:R1:1075:C:H2'	1.85	0.42
30:R1:1374:G:H2'	30:R1:1375:U:C6	2.54	0.42
30:R1:2140:G:N2	30:R1:2153:C:H42	2.18	0.42
30:R1:2831:G:H1'	30:R1:2883:A:H2'	2.02	0.42
30:R1:2901:C:H2'	30:R1:2902:C:C5	2.54	0.42
32:R3:45:G:H2'	32:R3:46:G:C8	2.55	0.42
32:R3:176:C:C2	32:R3:177:G:C2	3.07	0.42
32:R3:322:C:HO2'	32:R3:323:U:H6	1.66	0.42
8:2:75:ALA:HB2	8:2:95:TYR:CD2	2.55	0.42
13:24:6:ARG:NH2	30:R1:99:U:O2	2.50	0.42
15:27:32:LEU:HD12	15:27:33:ALA:H	1.84	0.42
16:28:7:THR:OG1	16:28:9:LYS:HG3	2.19	0.42
17:29:4:LYS:HA	17:29:7:ARG:NH1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:35:3:ILE:HD11	30:R1:592:A:C2	2.54	0.42
28:9:9:VAL:HB	28:9:12:LEU:O	2.19	0.42
30:R1:177:G:H5'	30:R1:178:G:N7	2.35	0.42
30:R1:820:A:H4'	30:R1:836:G:N2	2.34	0.42
30:R1:2315:G:O2'	30:R1:2316:G:H8	2.02	0.42
30:R1:2522:U:O2'	30:R1:2647:U:OP1	2.31	0.42
32:R3:288:A:O2'	32:R3:289:G:H3'	2.20	0.42
32:R3:1401:G:H2'	32:R3:1402:C:O4'	2.20	0.42
6:18:56:LYS:HB3	6:18:60:GLU:OE2	2.19	0.42
6:18:94:ARG:HG2	6:18:97:PHE:O	2.20	0.42
10:21:4:VAL:HA	10:21:12:HIS:O	2.19	0.42
23:35:28:LEU:HD12	23:35:28:LEU:HA	1.81	0.42
25:4:127:GLU:OE1	25:4:127:GLU:N	2.41	0.42
30:R1:543:G:C6	30:R1:551:G:C6	3.08	0.42
30:R1:963:U:C2	30:R1:964:C:C5	3.08	0.42
30:R1:1405:U:H2'	30:R1:1406:U:H6	1.85	0.42
30:R1:1637:A:H2'	30:R1:1638:C:C6	2.55	0.42
30:R1:1754:A:N1	30:R1:2716:C:O2'	2.47	0.42
30:R1:1862:G:C2	30:R1:1863:G:C8	3.07	0.42
30:R1:2074:U:O2'	30:R1:2597:G:H1'	2.20	0.42
31:R2:29:A:H2'	31:R2:30:C:O4'	2.20	0.42
32:R3:112:G:H21	32:R3:354:G:H4'	1.85	0.42
32:R3:131:A:H2'	32:R3:132:C:C6	2.55	0.42
32:R3:378:G:OP2	32:R3:378:G:N2	2.53	0.42
32:R3:382:A:H2'	32:R3:383:A:H8	1.84	0.42
10:21:1:MET:SD	10:21:1:MET:N	2.84	0.41
27:6:8:VAL:N	27:6:48:THR:OG1	2.53	0.41
30:R1:570:G:H2'	30:R1:2030:A:N7	2.35	0.41
30:R1:1168:G:N3	30:R1:1168:G:H2'	2.35	0.41
30:R1:2064:C:H2'	30:R1:2065:C:C6	2.55	0.41
32:R3:163:C:H2'	32:R3:164:G:O4'	2.20	0.41
32:R3:924:C:H2'	32:R3:925:G:C8	2.55	0.41
32:R3:1476:A:H2'	32:R3:1477:U:C6	2.55	0.41
9:20:50:ARG:NH1	30:R1:993:G:OP2	2.54	0.41
14:25:76:ASP:OD1	14:25:77:VAL:N	2.49	0.41
16:28:38:TRP:HB2	16:28:45:PHE:HE1	1.85	0.41
30:R1:7:G:H2'	30:R1:8:C:O4'	2.20	0.41
30:R1:1167:C:H2'	30:R1:1168:G:O4'	2.20	0.41
30:R1:1532:A:O2'	30:R1:1533:C:O5'	2.31	0.41
32:R3:999:C:C4	32:R3:1000:A:H1'	2.55	0.41
32:R3:1163:A:H2'	32:R3:1164:G:H8	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:R3:1315:U:O2	32:R3:1360:A:H2	2.03	0.41
4:16:31:PHE:HD1	4:16:132:THR:HG22	1.85	0.41
25:4:48:THR:HG23	25:4:86:ALA:HB3	2.01	0.41
25:4:144:GLU:HG3	25:4:145:ASP:H	1.84	0.41
27:6:172:GLU:HG3	27:6:174:LYS:H	1.85	0.41
30:R1:2554:U:H2'	30:R1:2555:U:C6	2.55	0.41
32:R3:258:G:H2'	32:R3:259:G:H8	1.85	0.41
32:R3:672:U:HO2'	32:R3:673:A:P	2.43	0.41
6:18:56:LYS:H	6:18:56:LYS:CD	2.34	0.41
8:2:120:ASP:HB3	28:9:91:PHE:CE2	2.55	0.41
11:22:29:VAL:HG11	11:22:55:ILE:HD11	2.01	0.41
12:23:5:GLU:H	12:23:5:GLU:HG2	1.66	0.41
16:28:2:ARG:HD2	16:28:29:LEU:HD22	2.03	0.41
21:32:49:ARG:HG3	30:R1:2884:U:C6	2.55	0.41
25:4:7:ASP:OD1	25:4:7:ASP:N	2.45	0.41
25:4:46:GLN:NE2	30:R1:1248:G:N7	2.68	0.41
30:R1:174:U:C2	30:R1:175:G:C8	3.07	0.41
30:R1:415:A:N6	30:R1:2409:G:O6	2.53	0.41
30:R1:966:G:H2'	30:R1:967:U:C6	2.55	0.41
30:R1:1094:U:N3	30:R1:1096:A:H5"	2.35	0.41
30:R1:1318:U:H2'	30:R1:1319:C:C6	2.55	0.41
30:R1:2508:G:H1	30:R1:2580:U:H5	1.69	0.41
32:R3:322:C:N4	32:R3:332:G:H22	2.16	0.41
32:R3:643:C:H2'	32:R3:644:U:H6	1.86	0.41
32:R3:828:U:H3	32:R3:859:G:H1'	1.85	0.41
32:R3:849:G:H3'	32:R3:850:U:O2	2.21	0.41
32:R3:1095:U:OP2	32:R3:1108:G:N1	2.44	0.41
53:T:23:C:H2'	53:T:24:U:H6	1.86	0.41
1:13:4:PHE:CD2	9:20:99:VAL:HG11	2.55	0.41
16:28:60:LYS:NZ	30:R1:371:A:H8	2.18	0.41
22:34:24:THR:HG23	22:34:27:GLY:H	1.84	0.41
25:4:60:TRP:HD1	25:4:61:ARG:O	2.03	0.41
26:5:34:THR:OG1	26:5:154:THR:HB	2.19	0.41
30:R1:64:A:H2'	30:R1:65:U:H6	1.84	0.41
30:R1:871:U:H2'	30:R1:872:U:H6	1.86	0.41
30:R1:948:C:H2'	30:R1:949:G:C8	2.55	0.41
30:R1:1317:G:H2'	30:R1:1318:U:C6	2.56	0.41
30:R1:1509:A:H2'	30:R1:1510:G:H8	1.85	0.41
30:R1:1510:G:H2'	30:R1:1511:G:C8	2.55	0.41
31:R2:61:G:H2'	31:R2:62:C:H6	1.86	0.41
32:R3:1037:C:H2'	32:R3:1038:C:C2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:R3:1062:U:H2'	32:R3:1063:C:C6	2.55	0.41
3:15:131:ALA:O	3:15:135:ILE:HG23	2.20	0.41
8:2:66:PHE:HB3	8:2:150:GLY:O	2.20	0.41
11:22:59:GLU:HA	11:22:64:ALA:HA	2.02	0.41
25:4:139:LYS:HE2	25:4:139:LYS:HB3	1.81	0.41
30:R1:863:A:H2'	30:R1:864:G:C8	2.56	0.41
30:R1:2064:C:H2'	30:R1:2065:C:H6	1.86	0.41
30:R1:2652:C:H2'	30:R1:2653:U:O4'	2.21	0.41
30:R1:2896:C:C2	30:R1:2897:U:C5	3.09	0.41
32:R3:45:G:H2'	32:R3:46:G:H8	1.84	0.41
32:R3:413:G:N2	32:R3:428:G:H1'	2.33	0.41
32:R3:689:C:H2'	32:R3:690:G:C8	2.56	0.41
32:R3:1009:U:C2	32:R3:1021:A:N1	2.89	0.41
6:18:117:PHE:O	30:R1:2377:A:O2'	2.34	0.41
11:22:6:LYS:HA	11:22:103:ILE:O	2.20	0.41
13:24:87:GLU:O	13:24:89:GLY:N	2.53	0.41
27:6:21:GLN:OE1	27:6:38:ASP:HA	2.21	0.41
30:R1:299:A:N3	30:R1:319:G:O2'	2.46	0.41
30:R1:578:G:OP1	30:R1:1255:U:O2'	2.36	0.41
30:R1:634:C:H2'	30:R1:635:C:C6	2.56	0.41
30:R1:639:U:C2	30:R1:640:C:C5	3.08	0.41
30:R1:886:A:N6	30:R1:889:C:H5"	2.35	0.41
30:R1:1858:A:H2'	30:R1:1859:U:O4'	2.21	0.41
30:R1:2324:U:C3'	30:R1:2325:G:H5"	2.45	0.41
30:R1:2497:A:OP2	30:R1:2497:A:H8	2.03	0.41
30:R1:2549:G:C2	30:R1:2550:G:N7	2.89	0.41
30:R1:2686:G:H2'	30:R1:2687:U:C6	2.55	0.41
31:R2:6:G:H2'	31:R2:7:G:H8	1.85	0.41
31:R2:52:A:O2'	31:R2:53:A:C8	2.72	0.41
32:R3:115:G:P	32:R3:115:G:O4'	2.78	0.41
32:R3:360:G:H2'	32:R3:361:G:H8	1.81	0.41
32:R3:402:G:O2'	32:R3:403:C:H6	2.03	0.41
32:R3:496:A:H5'	32:R3:497:G:OP2	2.19	0.41
32:R3:1164:G:H2'	32:R3:1165:U:H6	1.86	0.41
53:T:28:C:H2'	53:T:29:G:H8	1.86	0.41
6:18:87:ILE:HD12	6:18:87:ILE:H	1.85	0.41
6:18:88:LYS:HE2	6:18:88:LYS:HB2	1.72	0.41
18:3:133:THR:HG21	30:R1:1676:A:H1'	2.02	0.41
30:R1:882:G:H2'	30:R1:883:G:O4'	2.21	0.41
30:R1:2014:A:H2'	30:R1:2015:A:C8	2.54	0.41
30:R1:2162:G:O4'	30:R1:2173:A:N6	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:R3:1412:C:H2'	32:R3:1413:A:H8	1.84	0.41
32:R3:1524:C:H2'	32:R3:1525:G:H8	1.85	0.41
53:T:3:G:H2'	53:T:4:G:C8	2.55	0.41
53:T:23:C:H2'	53:T:24:U:C6	2.54	0.41
53:T:44:A:H2'	53:T:45:G:O4'	2.21	0.41
1:13:56:VAL:HB	1:13:124:VAL:HG23	2.03	0.41
2:14:76:VAL:H	7:19:72:VAL:HG22	1.85	0.41
16:28:37:PHE:CZ	16:28:50:VAL:HG21	2.56	0.41
23:35:3:ILE:HD11	30:R1:592:A:H2	1.86	0.41
26:5:132:ARG:NE	26:5:132:ARG:CA	2.82	0.41
27:6:17:LYS:HB3	27:6:17:LYS:HE3	1.71	0.41
30:R1:271:G:C2	30:R1:272:A:C5	3.09	0.41
30:R1:289:G:C2	30:R1:352:A:N1	2.89	0.41
30:R1:382:A:H2'	30:R1:383:C:O4'	2.21	0.41
30:R1:592:A:H2'	30:R1:593:U:H6	1.85	0.41
30:R1:741:U:H2'	30:R1:742:A:C8	2.55	0.41
30:R1:1000:A:H2'	30:R1:1001:A:C8	2.56	0.41
30:R1:1195:G:C2	30:R1:1196:C:C5	3.09	0.41
30:R1:1589:U:H2'	30:R1:1590:A:C8	2.56	0.41
30:R1:1704:C:H2'	30:R1:1705:A:C8	2.56	0.41
30:R1:1710:G:H2'	30:R1:1711:A:C8	2.56	0.41
30:R1:1847:G:HO2'	30:R1:1848:A:P	2.43	0.41
30:R1:2147:A:H2'	30:R1:2148:G:H4'	2.02	0.41
30:R1:2637:U:H2'	30:R1:2638:G:O4'	2.21	0.41
30:R1:2684:U:H2'	30:R1:2685:G:O4'	2.20	0.41
30:R1:2723:C:H2'	30:R1:2724:U:O4'	2.20	0.41
30:R1:2813:A:C4	30:R1:2814:A:C8	3.09	0.41
32:R3:736:C:H2'	32:R3:737:C:C6	2.55	0.41
32:R3:1171:A:H2'	32:R3:1172:C:C6	2.56	0.41
32:R3:1238:A:N3	32:R3:1238:A:H2'	2.35	0.41
32:R3:1323:G:H2'	32:R3:1324:A:C8	2.55	0.41
32:R3:1481:U:H2'	32:R3:1482:G:C8	2.56	0.41
32:R3:1496:C:H2'	32:R3:1497:G:O4'	2.21	0.41
53:T:20:H2U:O4'	53:T:20:H2U:O2	2.39	0.41
53:T:50:U:H2'	53:T:51:C:C6	2.55	0.41
28:9:4:ILE:HD12	28:9:37:VAL:O	2.21	0.41
28:9:114:GLU:OE1	28:9:133:GLN:N	2.53	0.41
30:R1:35:G:H1'	30:R1:454:A:C4	2.56	0.41
30:R1:118:A:N3	30:R1:178:G:H1'	2.36	0.41
30:R1:403:U:H5'	30:R1:404:A:OP1	2.21	0.41
30:R1:962:G:H2'	30:R1:963:U:H6	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:R1:979:A:H5'	30:R1:980:A:H5"	2.03	0.41
30:R1:2051:A:OP2	30:R1:2051:A:H8	2.04	0.41
30:R1:2798:U:H4'	30:R1:2799:A:N3	2.36	0.41
30:R1:2850:A:N7	30:R1:2868:A:O2'	2.47	0.41
32:R3:109:A:H62	32:R3:324:G:N2	2.14	0.41
32:R3:237:G:H2'	32:R3:238:A:H8	1.84	0.41
32:R3:1099:G:H2'	32:R3:1100:C:O4'	2.21	0.41
8:2:220:ARG:HG3	30:R1:1789:A:OP1	2.21	0.40
8:2:228:ASP:OD2	30:R1:780:G:N1	2.53	0.40
20:31:9:TYR:HD1	20:31:27:THR:HB	1.85	0.40
30:R1:132:G:H2'	30:R1:133:U:O2	2.20	0.40
30:R1:283:G:H2'	30:R1:284:U:O4'	2.21	0.40
30:R1:464:U:C4	30:R1:788:A:C5	3.09	0.40
30:R1:965:C:C2	30:R1:966:G:C8	3.09	0.40
30:R1:1679:A:H2'	30:R1:1680:U:H6	1.86	0.40
30:R1:2081:U:H2'	30:R1:2082:A:C8	2.55	0.40
30:R1:2130:U:H2'	30:R1:2131:U:N1	2.36	0.40
30:R1:2141:G:H2'	30:R1:2142:A:O4'	2.21	0.40
32:R3:728:A:H2'	32:R3:729:A:H8	1.86	0.40
32:R3:945:G:C2	32:R3:946:A:C8	3.09	0.40
32:R3:992:U:H1'	32:R3:993:G:N2	2.36	0.40
32:R3:1149:C:O2'	32:R3:1150:A:H5'	2.21	0.40
3:15:4:ASN:O	3:15:4:ASN:ND2	2.54	0.40
6:18:74:VAL:O	6:18:78:VAL:HG12	2.21	0.40
18:3:70:LYS:NZ	30:R1:2786:U:H5'	2.36	0.40
30:R1:20:C:H2'	30:R1:21:A:C8	2.54	0.40
30:R1:220:G:H22	30:R1:427:U:H2'	1.86	0.40
30:R1:564:C:H2'	30:R1:565:C:H6	1.86	0.40
30:R1:640:C:H2'	30:R1:641:U:H6	1.86	0.40
30:R1:895:U:O2'	30:R1:896:A:H5'	2.21	0.40
30:R1:1036:G:C6	30:R1:1120:G:C6	3.09	0.40
30:R1:1040:A:N6	30:R1:1116:G:O6	2.54	0.40
30:R1:2513:A:C6	30:R1:2574:G:C6	3.09	0.40
30:R1:2722:G:H2'	30:R1:2723:C:C6	2.57	0.40
32:R3:107:G:OP1	32:R3:325:A:N6	2.55	0.40
32:R3:308:C:C2	32:R3:309:A:C8	3.09	0.40
32:R3:377:G:N1	32:R3:387:U:C2	2.89	0.40
32:R3:922:G:H2'	32:R3:923:A:H8	1.87	0.40
32:R3:928:G:H1	32:R3:1389:C:H41	1.69	0.40
32:R3:1174:G:C2	32:R3:1175:G:C8	3.10	0.40
32:R3:1230:C:H2'	32:R3:1231:G:H8	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:6:41:GLU:HA	27:6:54:ARG:HH21	1.86	0.40
27:6:63:GLN:HE22	30:R1:2757:A:H2	1.67	0.40
30:R1:141:G:H2'	30:R1:142:A:O4'	2.21	0.40
30:R1:714:U:O2'	30:R1:716:A:N7	2.45	0.40
30:R1:1383:A:H1'	30:R1:1405:U:O2'	2.21	0.40
30:R1:1826:G:H2'	30:R1:1827:U:C6	2.56	0.40
32:R3:591:U:H2'	32:R3:592:G:H8	1.85	0.40
32:R3:612:C:H2'	32:R3:613:C:C6	2.56	0.40
32:R3:686:U:O4	32:R3:703:G:O2'	2.23	0.40
32:R3:735:C:H2'	32:R3:736:C:C6	2.54	0.40
32:R3:1282:C:H2'	32:R3:1283:U:C6	2.56	0.40
2:14:88:ASN:OD1	2:14:89:ASN:N	2.55	0.40
12:23:26:LYS:HB2	12:23:26:LYS:HE2	1.80	0.40
14:25:20:LEU:HD23	14:25:20:LEU:HA	1.81	0.40
16:28:37:PHE:HZ	16:28:50:VAL:HG21	1.86	0.40
24:36:6:SER:O	24:36:6:SER:OG	2.30	0.40
27:6:68:ARG:NH1	27:6:72:ASN:HB2	2.36	0.40
30:R1:776:G:N2	30:R1:2241:A:OP1	2.51	0.40
30:R1:1084:A:H2'	30:R1:1105:U:O2'	2.22	0.40
30:R1:1123:C:H2'	30:R1:1124:G:H8	1.87	0.40
30:R1:1149:G:H2'	30:R1:1150:C:H6	1.84	0.40
30:R1:1922:G:H2'	30:R1:1923:U:C6	2.57	0.40
30:R1:2061:G:H8	30:R1:2501:C:HO2'	1.63	0.40
30:R1:2135:A:O2'	30:R1:2159:G:O2'	2.24	0.40
32:R3:56:U:H2'	32:R3:57:G:H8	1.86	0.40
32:R3:363:A:O2'	32:R3:364:A:P	2.80	0.40
32:R3:483:C:H5"	32:R3:484:G:OP2	2.21	0.40
32:R3:561:U:O2'	32:R3:562:U:OP1	2.38	0.40
32:R3:707:U:H2'	32:R3:708:C:C6	2.57	0.40
1:13:47:HIS:ND1	1:13:48:VAL:HG13	2.37	0.40
2:14:107:LEU:HB2	2:14:116:ILE:HD11	2.04	0.40
3:15:43:GLY:N	30:R1:671:C:OP1	2.49	0.40
5:17:36:THR:HG22	30:R1:1278:C:OP1	2.22	0.40
15:27:25:ARG:HG3	15:27:29:GLU:OE1	2.22	0.40
15:27:55:ARG:NH1	30:R1:2384:U:OP2	2.55	0.40
16:28:55:MET:HB3	28:9:27:ARG:NH1	2.37	0.40
19:30:11:SER:OG	19:30:12:ALA:N	2.55	0.40
26:5:4:HIS:O	26:5:8:LYS:HG3	2.20	0.40
30:R1:544:C:C4	30:R1:545:U:C4	3.09	0.40
30:R1:1291:C:C2	30:R1:1292:G:C8	3.09	0.40
30:R1:2502:G:H5"	30:R1:2503:A:H5"	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:R1:2649:C:H2'	30:R1:2650:U:H6	1.85	0.40
30:R1:2700:A:H2'	30:R1:2701:U:C6	2.56	0.40
32:R3:744:C:H2'	32:R3:745:G:C8	2.57	0.40
32:R3:1081:A:C4	32:R3:1082:A:C8	3.10	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	13	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
2	14	120/122 (98%)	104 (87%)	16 (13%)	0	100	100
3	15	142/144 (99%)	129 (91%)	13 (9%)	0	100	100
4	16	134/136 (98%)	124 (92%)	10 (8%)	0	100	100
5	17	118/120 (98%)	112 (95%)	6 (5%)	0	100	100
6	18	114/116 (98%)	110 (96%)	4 (4%)	0	100	100
7	19	112/114 (98%)	106 (95%)	6 (5%)	0	100	100
8	2	269/271 (99%)	250 (93%)	19 (7%)	0	100	100
9	20	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
10	21	101/103 (98%)	92 (91%)	9 (9%)	0	100	100
11	22	108/110 (98%)	101 (94%)	6 (6%)	1 (1%)	14	45
12	23	91/93 (98%)	81 (89%)	10 (11%)	0	100	100
13	24	100/102 (98%)	89 (89%)	10 (10%)	1 (1%)	13	42
14	25	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
15	27	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
16	28	75/77 (97%)	75 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	29	61/63 (97%)	60 (98%)	1 (2%)	0	100	100
18	3	207/209 (99%)	190 (92%)	17 (8%)	0	100	100
19	30	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
20	31	64/66 (97%)	55 (86%)	9 (14%)	0	100	100
21	32	54/56 (96%)	50 (93%)	4 (7%)	0	100	100
22	34	44/46 (96%)	38 (86%)	6 (14%)	0	100	100
23	35	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
24	36	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
25	4	199/201 (99%)	189 (95%)	10 (5%)	0	100	100
26	5	175/177 (99%)	161 (92%)	14 (8%)	0	100	100
27	6	174/176 (99%)	161 (92%)	13 (8%)	0	100	100
28	9	147/149 (99%)	129 (88%)	18 (12%)	0	100	100
33	sb	216/218 (99%)	198 (92%)	18 (8%)	0	100	100
34	sc	204/206 (99%)	198 (97%)	6 (3%)	0	100	100
35	sd	203/205 (99%)	179 (88%)	24 (12%)	0	100	100
36	se	155/157 (99%)	135 (87%)	19 (12%)	1 (1%)	22	53
37	sf	98/100 (98%)	85 (87%)	13 (13%)	0	100	100
38	sg	149/151 (99%)	141 (95%)	8 (5%)	0	100	100
39	sh	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
40	si	125/127 (98%)	104 (83%)	21 (17%)	0	100	100
41	sj	96/98 (98%)	88 (92%)	8 (8%)	0	100	100
42	sk	114/116 (98%)	104 (91%)	10 (9%)	0	100	100
43	sl	121/123 (98%)	93 (77%)	28 (23%)	0	100	100
44	sm	112/114 (98%)	101 (90%)	11 (10%)	0	100	100
45	sn	98/100 (98%)	82 (84%)	15 (15%)	1 (1%)	13	42
46	so	86/88 (98%)	82 (95%)	4 (5%)	0	100	100
47	sp	80/82 (98%)	70 (88%)	10 (12%)	0	100	100
48	sq	78/80 (98%)	68 (87%)	10 (13%)	0	100	100
49	sr	63/65 (97%)	59 (94%)	4 (6%)	0	100	100
50	ss	77/79 (98%)	68 (88%)	9 (12%)	0	100	100
51	st	83/85 (98%)	81 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
52	su	63/65 (97%)	42 (67%)	19 (30%)	2 (3%)	3 18
All	All	5532/5628 (98%)	5057 (91%)	469 (8%)	6 (0%)	50 79

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	24	88	ASP
36	se	122	VAL
11	22	2	GLU
52	su	22	CYS
52	su	36	PHE
45	sn	2	LYS

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	13	116/116 (100%)	113 (97%)	3 (3%)	41 68
2	14	103/103 (100%)	101 (98%)	2 (2%)	52 75
3	15	103/103 (100%)	103 (100%)	0	100 100
4	16	109/109 (100%)	104 (95%)	5 (5%)	23 52
5	17	100/100 (100%)	96 (96%)	4 (4%)	27 58
6	18	86/86 (100%)	84 (98%)	2 (2%)	45 70
7	19	99/99 (100%)	94 (95%)	5 (5%)	20 49
8	2	216/216 (100%)	211 (98%)	5 (2%)	45 70
9	20	89/89 (100%)	89 (100%)	0	100 100
10	21	84/84 (100%)	80 (95%)	4 (5%)	21 51
11	22	93/93 (100%)	91 (98%)	2 (2%)	47 71
12	23	80/80 (100%)	76 (95%)	4 (5%)	20 50
13	24	83/83 (100%)	80 (96%)	3 (4%)	30 60
14	25	78/78 (100%)	75 (96%)	3 (4%)	28 59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
15	27	58/58 (100%)	54 (93%)	4 (7%)	13 39
16	28	67/67 (100%)	65 (97%)	2 (3%)	36 64
17	29	55/55 (100%)	55 (100%)	0	100 100
18	3	164/164 (100%)	161 (98%)	3 (2%)	54 76
19	30	48/48 (100%)	46 (96%)	2 (4%)	25 56
20	31	59/59 (100%)	55 (93%)	4 (7%)	13 40
21	32	47/47 (100%)	45 (96%)	2 (4%)	25 55
22	34	38/38 (100%)	36 (95%)	2 (5%)	19 48
23	35	51/51 (100%)	47 (92%)	4 (8%)	10 35
24	36	34/34 (100%)	34 (100%)	0	100 100
25	4	165/165 (100%)	157 (95%)	8 (5%)	21 51
26	5	148/148 (100%)	143 (97%)	5 (3%)	32 62
27	6	137/137 (100%)	128 (93%)	9 (7%)	14 41
28	9	114/114 (100%)	112 (98%)	2 (2%)	54 76
33	sb	180/180 (100%)	169 (94%)	11 (6%)	15 43
34	sc	170/170 (100%)	165 (97%)	5 (3%)	37 65
35	sd	172/172 (100%)	169 (98%)	3 (2%)	56 78
36	se	119/119 (100%)	117 (98%)	2 (2%)	56 78
37	sf	87/87 (100%)	86 (99%)	1 (1%)	70 84
38	sg	124/124 (100%)	121 (98%)	3 (2%)	44 70
39	sh	104/104 (100%)	99 (95%)	5 (5%)	21 51
40	si	105/105 (100%)	100 (95%)	5 (5%)	21 51
41	sj	86/86 (100%)	83 (96%)	3 (4%)	31 61
42	sk	89/89 (100%)	85 (96%)	4 (4%)	23 53
43	sl	103/103 (100%)	99 (96%)	4 (4%)	27 58
44	sm	92/92 (100%)	88 (96%)	4 (4%)	25 55
45	sn	83/83 (100%)	79 (95%)	4 (5%)	21 51
46	so	76/76 (100%)	76 (100%)	0	100 100
47	sp	65/65 (100%)	62 (95%)	3 (5%)	23 52
48	sq	74/74 (100%)	73 (99%)	1 (1%)	62 81
49	sr	56/56 (100%)	55 (98%)	1 (2%)	54 76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
50	ss	70/70 (100%)	65 (93%)	5 (7%)	12 39
51	st	65/65 (100%)	62 (95%)	3 (5%)	23 52
52	su	55/55 (100%)	52 (94%)	3 (6%)	18 47
All	All	4599/4599 (100%)	4440 (96%)	159 (4%)	33 61

All (159) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	13	1	MET
1	13	19	ASP
1	13	49	ASP
2	14	58	LEU
2	14	109	SER
4	16	3	GLN
4	16	13	HIS
4	16	44	ARG
4	16	70	ASP
4	16	106	ASP
5	17	2	ARG
5	17	6	SER
5	17	20	MET
5	17	59	SER
6	18	19	GLN
6	18	91	SER
7	19	8	GLU
7	19	18	SER
7	19	20	ARG
7	19	71	ARG
7	19	82	SER
8	2	96	LYS
8	2	155	ARG
8	2	162	GLN
8	2	200	MET
8	2	212	TRP
10	21	1	MET
10	21	25	LEU
10	21	43	ASN
10	21	48	LYS
11	22	1	MET
11	22	110	ARG
12	23	1	MET

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Mol	Chain	Res	Type
12	23	27	SER
12	23	72	GLN
12	23	80	TRP
13	24	39	ASN
13	24	43	LYS
13	24	99	SER
14	25	24	ASN
14	25	51	GLN
14	25	80	HIS
15	27	53	CYS
15	27	72	LYS
15	27	77	ARG
15	27	81	SER
16	28	4	CYS
16	28	49	ARG
18	3	58	ASN
18	3	131	ASP
18	3	185	ASN
19	30	5	LYS
19	30	36	GLU
20	31	4	ASP
20	31	34	LEU
20	31	38	SER
20	31	59	ARG
21	32	11	LYS
21	32	48	TYR
22	34	22	MET
22	34	28	ARG
23	35	30	HIS
23	35	48	MET
23	35	51	LYS
23	35	63	TYR
25	4	16	GLU
25	4	21	ARG
25	4	80	SER
25	4	110	SER
25	4	122	GLU
25	4	145	ASP
25	4	170	ARG
25	4	191	ASP
26	5	76	PHE
26	5	82	TYR

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Mol	Chain	Res	Type
26	5	112	ASP
26	5	132	ARG
26	5	174	PHE
27	6	51	PHE
27	6	59	ASP
27	6	68	ARG
27	6	106	LEU
27	6	115	GLN
27	6	129	GLU
27	6	132	LEU
27	6	136	ASP
27	6	174	LYS
28	9	46	PHE
28	9	57	LYS
33	sb	14	HIS
33	sb	20	ARG
33	sb	22	TRP
33	sb	34	ARG
33	sb	48	MET
33	sb	73	ARG
33	sb	89	PHE
33	sb	183	PHE
33	sb	190	SER
33	sb	193	ASP
33	sb	224	ARG
34	sc	39	ARG
34	sc	50	SER
34	sc	61	LYS
34	sc	118	SER
34	sc	138	GLN
35	sd	30	LYS
35	sd	150	LYS
35	sd	204	SER
36	se	22	LYS
36	se	67	ARG
37	sf	21	MET
38	sg	17	PHE
38	sg	141	HIS
38	sg	143	MET
39	sh	47	ASP
39	sh	53	ASP
39	sh	89	ASP

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Mol	Chain	Res	Type
39	sh	106	SER
39	sh	123	GLU
40	si	61	ASP
40	si	93	LEU
40	si	105	ARG
40	si	122	ARG
40	si	126	PHE
41	sj	19	ASP
41	sj	58	ASN
41	sj	63	ASP
42	sk	49	SER
42	sk	56	LYS
42	sk	63	GLN
42	sk	126	ARG
43	sl	18	SER
43	sl	33	CYS
43	sl	115	LYS
43	sl	120	ARG
44	sm	67	ASP
44	sm	89	ARG
44	sm	106	ARG
44	sm	111	PRO
45	sn	23	ARG
45	sn	52	ARG
45	sn	56	PRO
45	sn	57	SER
47	sp	55	ASP
47	sp	63	GLN
47	sp	68	SER
48	sq	13	SER
49	sr	23	LYS
50	ss	6	LYS
50	ss	11	ASP
50	ss	36	ARG
50	ss	65	MET
50	ss	80	ARG
51	st	2	ASN
51	st	19	HIS
51	st	83	ASN
52	su	36	PHE
52	su	53	LYS
52	su	55	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
13	24	53	GLN
27	6	72	ASN
28	9	66	ASN
36	se	121	ASN
37	sf	11	HIS
37	sf	58	HIS
43	sl	4	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
29	M	8/9 (88%)	1 (12%)	0
30	R1	2900/2903 (99%)	566 (19%)	12 (0%)
31	R2	118/119 (99%)	19 (16%)	1 (0%)
32	R3	1530/1531 (99%)	379 (24%)	24 (1%)
53	T	74/77 (96%)	15 (20%)	2 (2%)
All	All	4630/4639 (99%)	980 (21%)	39 (0%)

All (980) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
29	M	7	A
30	R1	10	A
30	R1	12	U
30	R1	14	A
30	R1	15	G
30	R1	23	G
30	R1	34	U
30	R1	35	G
30	R1	36	G
30	R1	46	G
30	R1	60	G
30	R1	71	A
30	R1	74	A
30	R1	75	G
30	R1	78	U
30	R1	79	C
30	R1	83	A
30	R1	84	A
30	R1	85	G

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Mol	Chain	Res	Type
30	R1	88	G
30	R1	91	A
30	R1	98	G
30	R1	100	U
30	R1	102	U
30	R1	103	A
30	R1	118	A
30	R1	120	U
30	R1	131	A
30	R1	134	G
30	R1	137	U
30	R1	138	U
30	R1	139	U
30	R1	140	C
30	R1	144	A
30	R1	146	A
30	R1	152	A
30	R1	154	U
30	R1	156	A
30	R1	159	G
30	R1	162	U
30	R1	164	C
30	R1	165	A
30	R1	178	G
30	R1	181	A
30	R1	196	A
30	R1	199	A
30	R1	213	A
30	R1	216	A
30	R1	219	A
30	R1	220	G
30	R1	221	A
30	R1	222	A
30	R1	228	C
30	R1	229	C
30	R1	230	G
30	R1	233	A
30	R1	248	G
30	R1	249	C
30	R1	255	A
30	R1	265	A
30	R1	266	G

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Mol	Chain	Res	Type
30	R1	273	G
30	R1	275	C
30	R1	276	U
30	R1	281	C
30	R1	282	A
30	R1	311	A
30	R1	329	G
30	R1	330	A
30	R1	342	A
30	R1	352	A
30	R1	354	A
30	R1	360	U
30	R1	361	G
30	R1	362	A
30	R1	369	U
30	R1	371	A
30	R1	372	G
30	R1	373	U
30	R1	380	G
30	R1	386	G
30	R1	387	U
30	R1	388	G
30	R1	389	G
30	R1	401	A
30	R1	403	U
30	R1	404	A
30	R1	405	U
30	R1	406	G
30	R1	411	G
30	R1	412	A
30	R1	413	C
30	R1	414	C
30	R1	416	U
30	R1	422	A
30	R1	424	G
30	R1	428	A
30	R1	435	C
30	R1	443	A
30	R1	455	C
30	R1	457	A
30	R1	473	G
30	R1	481	G

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Mol	Chain	Res	Type
30	R1	491	G
30	R1	505	A
30	R1	509	C
30	R1	510	C
30	R1	512	G
30	R1	527	C
30	R1	528	A
30	R1	530	G
30	R1	531	C
30	R1	532	A
30	R1	533	G
30	R1	541	A
30	R1	544	C
30	R1	545	U
30	R1	546	U
30	R1	548	G
30	R1	549	G
30	R1	555	G
30	R1	563	A
30	R1	573	U
30	R1	575	A
30	R1	591	U
30	R1	603	A
30	R1	614	A
30	R1	615	U
30	R1	622	G
30	R1	627	A
30	R1	634	C
30	R1	637	A
30	R1	645	C
30	R1	647	G
30	R1	653	U
30	R1	654	A
30	R1	655	A
30	R1	668	A
30	R1	685	A
30	R1	686	U
30	R1	713	G
30	R1	717	C
30	R1	730	A
30	R1	740	C
30	R1	746	U

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Mol	Chain	Res	Type
30	R1	747	U
30	R1	752	A
30	R1	764	A
30	R1	765	C
30	R1	775	G
30	R1	776	G
30	R1	782	A
30	R1	784	G
30	R1	785	G
30	R1	805	G
30	R1	812	C
30	R1	819	A
30	R1	827	U
30	R1	828	U
30	R1	829	A
30	R1	845	A
30	R1	846	U
30	R1	847	U
30	R1	860	U
30	R1	869	G
30	R1	870	U
30	R1	878	A
30	R1	886	A
30	R1	887	U
30	R1	888	C
30	R1	891	G
30	R1	893	C
30	R1	894	U
30	R1	896	A
30	R1	897	C
30	R1	898	C
30	R1	899	A
30	R1	910	A
30	R1	931	U
30	R1	932	U
30	R1	941	A
30	R1	945	A
30	R1	946	C
30	R1	953	G
30	R1	961	C
30	R1	969	G
30	R1	973	A

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Mol	Chain	Res	Type
30	R1	974	G
30	R1	979	A
30	R1	983	A
30	R1	984	A
30	R1	985	C
30	R1	989	G
30	R1	990	A
30	R1	995	C
30	R1	996	A
30	R1	999	U
30	R1	1005	C
30	R1	1006	C
30	R1	1009	A
30	R1	1012	U
30	R1	1013	C
30	R1	1021	A
30	R1	1022	G
30	R1	1026	G
30	R1	1033	U
30	R1	1051	G
30	R1	1052	C
30	R1	1056	G
30	R1	1060	U
30	R1	1061	U
30	R1	1062	G
30	R1	1063	G
30	R1	1064	C
30	R1	1066	U
30	R1	1067	A
30	R1	1070	A
30	R1	1071	G
30	R1	1072	C
30	R1	1073	A
30	R1	1074	G
30	R1	1075	C
30	R1	1076	C
30	R1	1079	C
30	R1	1083	U
30	R1	1084	A
30	R1	1085	A
30	R1	1087	G
30	R1	1088	A

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Mol	Chain	Res	Type
30	R1	1089	A
30	R1	1090	A
30	R1	1094	U
30	R1	1095	A
30	R1	1096	A
30	R1	1099	G
30	R1	1101	U
30	R1	1103	A
30	R1	1104	C
30	R1	1106	G
30	R1	1109	C
30	R1	1110	G
30	R1	1111	A
30	R1	1116	G
30	R1	1128	G
30	R1	1132	U
30	R1	1133	A
30	R1	1135	C
30	R1	1136	G
30	R1	1143	A
30	R1	1166	G
30	R1	1171	G
30	R1	1172	C
30	R1	1173	U
30	R1	1174	U
30	R1	1175	A
30	R1	1176	U
30	R1	1177	G
30	R1	1178	C
30	R1	1179	G
30	R1	1180	U
30	R1	1181	U
30	R1	1182	G
30	R1	1186	G
30	R1	1195	G
30	R1	1204	A
30	R1	1212	G
30	R1	1250	G
30	R1	1253	A
30	R1	1256	G
30	R1	1265	A
30	R1	1271	G

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Mol	Chain	Res	Type
30	R1	1272	A
30	R1	1273	U
30	R1	1300	G
30	R1	1301	A
30	R1	1329	U
30	R1	1341	G
30	R1	1345	C
30	R1	1352	U
30	R1	1365	A
30	R1	1368	G
30	R1	1378	A
30	R1	1379	U
30	R1	1383	A
30	R1	1386	C
30	R1	1387	A
30	R1	1395	A
30	R1	1416	G
30	R1	1419	A
30	R1	1420	A
30	R1	1428	C
30	R1	1434	A
30	R1	1452	G
30	R1	1453	A
30	R1	1456	G
30	R1	1459	G
30	R1	1461	C
30	R1	1478	G
30	R1	1481	U
30	R1	1482	G
30	R1	1493	C
30	R1	1494	A
30	R1	1508	A
30	R1	1509	A
30	R1	1515	A
30	R1	1523	U
30	R1	1529	G
30	R1	1530	G
30	R1	1532	A
30	R1	1534	U
30	R1	1535	A
30	R1	1536	C
30	R1	1537	G

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Mol	Chain	Res	Type
30	R1	1558	C
30	R1	1566	A
30	R1	1569	A
30	R1	1578	U
30	R1	1583	A
30	R1	1610	A
30	R1	1647	U
30	R1	1648	U
30	R1	1674	G
30	R1	1677	A
30	R1	1715	G
30	R1	1716	U
30	R1	1724	G
30	R1	1729	U
30	R1	1730	C
30	R1	1738	G
30	R1	1754	A
30	R1	1756	G
30	R1	1758	U
30	R1	1764	C
30	R1	1773	A
30	R1	1781	U
30	R1	1800	C
30	R1	1801	A
30	R1	1808	A
30	R1	1816	C
30	R1	1829	A
30	R1	1838	C
30	R1	1848	A
30	R1	1868	C
30	R1	1869	G
30	R1	1870	C
30	R1	1871	A
30	R1	1873	G
30	R1	1883	U
30	R1	1884	G
30	R1	1901	A
30	R1	1906	G
30	R1	1913	A
30	R1	1914	C
30	R1	1916	A
30	R1	1919	A

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Mol	Chain	Res	Type
30	R1	1929	G
30	R1	1930	G
30	R1	1931	U
30	R1	1936	A
30	R1	1937	A
30	R1	1938	A
30	R1	1955	U
30	R1	1967	C
30	R1	1970	A
30	R1	1971	U
30	R1	1972	G
30	R1	1991	U
30	R1	1993	U
30	R1	1997	C
30	R1	2021	C
30	R1	2022	U
30	R1	2023	C
30	R1	2030	A
30	R1	2031	A
30	R1	2033	A
30	R1	2043	C
30	R1	2052	A
30	R1	2055	C
30	R1	2056	G
30	R1	2059	A
30	R1	2060	A
30	R1	2061	G
30	R1	2062	A
30	R1	2063	C
30	R1	2069	G
30	R1	2072	C
30	R1	2080	A
30	R1	2093	G
30	R1	2097	A
30	R1	2099	U
30	R1	2102	G
30	R1	2104	C
30	R1	2106	U
30	R1	2107	G
30	R1	2109	U
30	R1	2110	G
30	R1	2111	U

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Mol	Chain	Res	Type
30	R1	2112	G
30	R1	2113	U
30	R1	2114	A
30	R1	2115	G
30	R1	2116	G
30	R1	2117	A
30	R1	2118	U
30	R1	2119	A
30	R1	2122	U
30	R1	2123	G
30	R1	2124	G
30	R1	2125	G
30	R1	2126	A
30	R1	2127	G
30	R1	2128	G
30	R1	2131	U
30	R1	2132	U
30	R1	2133	G
30	R1	2135	A
30	R1	2136	G
30	R1	2140	G
30	R1	2141	G
30	R1	2144	G
30	R1	2147	A
30	R1	2148	G
30	R1	2149	U
30	R1	2150	C
30	R1	2153	C
30	R1	2154	A
30	R1	2157	G
30	R1	2158	A
30	R1	2159	G
30	R1	2165	C
30	R1	2167	U
30	R1	2168	G
30	R1	2172	U
30	R1	2173	A
30	R1	2174	C
30	R1	2175	C
30	R1	2176	A
30	R1	2177	C
30	R1	2178	C

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Mol	Chain	Res	Type
30	R1	2179	C
30	R1	2181	U
30	R1	2182	U
30	R1	2184	A
30	R1	2186	G
30	R1	2188	U
30	R1	2190	G
30	R1	2198	A
30	R1	2199	A
30	R1	2204	G
30	R1	2211	A
30	R1	2213	U
30	R1	2214	C
30	R1	2225	A
30	R1	2226	C
30	R1	2238	G
30	R1	2239	G
30	R1	2250	G
30	R1	2266	A
30	R1	2278	A
30	R1	2283	C
30	R1	2287	A
30	R1	2291	U
30	R1	2297	A
30	R1	2305	U
30	R1	2316	G
30	R1	2319	G
30	R1	2320	U
30	R1	2322	A
30	R1	2325	G
30	R1	2327	A
30	R1	2333	A
30	R1	2334	U
30	R1	2345	G
30	R1	2347	C
30	R1	2350	C
30	R1	2359	C
30	R1	2361	G
30	R1	2371	G
30	R1	2383	G
30	R1	2385	C
30	R1	2402	U

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Mol	Chain	Res	Type
30	R1	2403	C
30	R1	2423	U
30	R1	2429	G
30	R1	2430	A
30	R1	2434	A
30	R1	2435	A
30	R1	2439	A
30	R1	2441	U
30	R1	2448	A
30	R1	2476	A
30	R1	2491	U
30	R1	2500	U
30	R1	2502	G
30	R1	2503	A
30	R1	2504	U
30	R1	2506	U
30	R1	2507	C
30	R1	2518	A
30	R1	2519	U
30	R1	2520	C
30	R1	2547	A
30	R1	2554	U
30	R1	2560	A
30	R1	2562	U
30	R1	2563	U
30	R1	2564	A
30	R1	2566	A
30	R1	2567	G
30	R1	2572	A
30	R1	2573	C
30	R1	2576	G
30	R1	2582	G
30	R1	2585	U
30	R1	2586	U
30	R1	2602	A
30	R1	2609	U
30	R1	2613	U
30	R1	2629	U
30	R1	2630	G
30	R1	2654	A
30	R1	2660	A
30	R1	2662	A

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Mol	Chain	Res	Type
30	R1	2663	G
30	R1	2664	G
30	R1	2669	G
30	R1	2671	G
30	R1	2682	A
30	R1	2689	U
30	R1	2690	U
30	R1	2700	A
30	R1	2707	U
30	R1	2714	G
30	R1	2726	A
30	R1	2733	A
30	R1	2739	U
30	R1	2744	G
30	R1	2748	A
30	R1	2761	A
30	R1	2765	A
30	R1	2774	C
30	R1	2775	G
30	R1	2778	A
30	R1	2779	U
30	R1	2794	C
30	R1	2796	U
30	R1	2797	U
30	R1	2800	A
30	R1	2808	G
30	R1	2815	C
30	R1	2816	G
30	R1	2818	U
30	R1	2820	A
30	R1	2835	A
30	R1	2840	C
30	R1	2849	U
30	R1	2858	C
30	R1	2859	G
30	R1	2861	U
30	R1	2867	G
30	R1	2873	A
30	R1	2879	A
30	R1	2880	C
30	R1	2893	A
30	R1	2897	U

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Mol	Chain	Res	Type
30	R1	2900	A
30	R1	2903	U
31	R2	13	G
31	R2	30	C
31	R2	35	C
31	R2	41	G
31	R2	44	G
31	R2	45	A
31	R2	53	A
31	R2	63	C
31	R2	67	G
31	R2	87	U
31	R2	88	C
31	R2	89	U
31	R2	90	C
31	R2	108	A
31	R2	109	A
31	R2	113	C
31	R2	114	C
31	R2	118	C
31	R2	119	A
32	R3	3	A
32	R3	4	U
32	R3	5	U
32	R3	9	G
32	R3	22	G
32	R3	30	U
32	R3	31	G
32	R3	32	A
32	R3	39	G
32	R3	47	C
32	R3	48	C
32	R3	49	U
32	R3	50	A
32	R3	51	A
32	R3	53	A
32	R3	60	A
32	R3	61	G
32	R3	62	U
32	R3	63	C
32	R3	66	A
32	R3	68	G

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Mol	Chain	Res	Type
32	R3	70	U
32	R3	71	A
32	R3	72	A
32	R3	77	A
32	R3	78	A
32	R3	79	G
32	R3	80	A
32	R3	82	G
32	R3	83	C
32	R3	84	U
32	R3	85	U
32	R3	87	C
32	R3	92	U
32	R3	94	G
32	R3	96	U
32	R3	105	G
32	R3	115	G
32	R3	121	U
32	R3	122	G
32	R3	130	A
32	R3	131	A
32	R3	133	U
32	R3	134	G
32	R3	157	U
32	R3	161	A
32	R3	164	G
32	R3	171	A
32	R3	173	U
32	R3	181	A
32	R3	182	A
32	R3	197	A
32	R3	204	G
32	R3	205	A
32	R3	206	C
32	R3	207	C
32	R3	208	U
32	R3	209	U
32	R3	210	C
32	R3	212	G
32	R3	213	G
32	R3	215	C
32	R3	216	U

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Mol	Chain	Res	Type
32	R3	217	C
32	R3	220	G
32	R3	226	G
32	R3	240	G
32	R3	245	U
32	R3	247	G
32	R3	250	A
32	R3	251	G
32	R3	266	G
32	R3	267	C
32	R3	270	A
32	R3	272	C
32	R3	274	A
32	R3	275	G
32	R3	287	U
32	R3	289	G
32	R3	290	C
32	R3	293	G
32	R3	302	G
32	R3	306	A
32	R3	313	A
32	R3	316	C
32	R3	321	A
32	R3	323	U
32	R3	324	G
32	R3	327	A
32	R3	328	C
32	R3	329	A
32	R3	331	G
32	R3	332	G
32	R3	333	U
32	R3	334	C
32	R3	338	A
32	R3	339	C
32	R3	344	A
32	R3	345	C
32	R3	346	G
32	R3	347	G
32	R3	351	G
32	R3	352	C
32	R3	353	A
32	R3	354	G

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Mol	Chain	Res	Type
32	R3	360	G
32	R3	363	A
32	R3	364	A
32	R3	367	U
32	R3	369	G
32	R3	370	C
32	R3	372	C
32	R3	376	G
32	R3	378	G
32	R3	381	C
32	R3	388	G
32	R3	389	A
32	R3	391	G
32	R3	392	C
32	R3	397	A
32	R3	403	C
32	R3	406	G
32	R3	413	G
32	R3	415	A
32	R3	416	G
32	R3	418	C
32	R3	419	C
32	R3	421	U
32	R3	422	C
32	R3	426	U
32	R3	429	U
32	R3	435	A
32	R3	437	U
32	R3	438	U
32	R3	439	U
32	R3	451	A
32	R3	454	G
32	R3	459	A
32	R3	460	A
32	R3	462	G
32	R3	463	U
32	R3	464	U
32	R3	465	A
32	R3	466	A
32	R3	467	U
32	R3	470	C
32	R3	471	U

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Mol	Chain	Res	Type
32	R3	472	U
32	R3	473	U
32	R3	475	C
32	R3	482	A
32	R3	484	G
32	R3	494	G
32	R3	495	A
32	R3	496	A
32	R3	497	G
32	R3	498	A
32	R3	501	C
32	R3	509	A
32	R3	511	C
32	R3	516	U
32	R3	518	C
32	R3	524	G
32	R3	530	G
32	R3	531	U
32	R3	532	A
32	R3	538	G
32	R3	540	G
32	R3	541	G
32	R3	547	A
32	R3	549	C
32	R3	559	A
32	R3	562	U
32	R3	564	C
32	R3	573	A
32	R3	576	C
32	R3	577	G
32	R3	579	A
32	R3	589	U
32	R3	596	A
32	R3	607	A
32	R3	610	U
32	R3	613	C
32	R3	618	C
32	R3	624	C
32	R3	632	U
32	R3	640	A
32	R3	642	A
32	R3	653	U

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Mol	Chain	Res	Type
32	R3	661	G
32	R3	664	G
32	R3	665	A
32	R3	673	A
32	R3	684	U
32	R3	686	U
32	R3	688	G
32	R3	694	A
32	R3	703	G
32	R3	713	G
32	R3	721	G
32	R3	723	U
32	R3	731	G
32	R3	734	G
32	R3	739	C
32	R3	754	C
32	R3	755	G
32	R3	777	A
32	R3	781	A
32	R3	791	G
32	R3	792	A
32	R3	793	U
32	R3	794	A
32	R3	815	A
32	R3	817	C
32	R3	829	G
32	R3	832	G
32	R3	838	G
32	R3	839	C
32	R3	840	C
32	R3	841	C
32	R3	842	U
32	R3	843	U
32	R3	844	G
32	R3	845	A
32	R3	846	G
32	R3	849	G
32	R3	850	U
32	R3	863	U
32	R3	864	A
32	R3	870	U
32	R3	871	U

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Mol	Chain	Res	Type
32	R3	872	A
32	R3	876	C
32	R3	878	A
32	R3	885	G
32	R3	900	A
32	R3	902	G
32	R3	926	G
32	R3	933	G
32	R3	935	A
32	R3	956	U
32	R3	958	A
32	R3	959	A
32	R3	960	U
32	R3	961	U
32	R3	966	G
32	R3	968	A
32	R3	969	A
32	R3	971	G
32	R3	975	A
32	R3	976	G
32	R3	977	A
32	R3	982	U
32	R3	989	U
32	R3	991	U
32	R3	992	U
32	R3	993	G
32	R3	994	A
32	R3	1000	A
32	R3	1002	G
32	R3	1003	G
32	R3	1004	A
32	R3	1006	G
32	R3	1007	U
32	R3	1008	U
32	R3	1022	A
32	R3	1023	U
32	R3	1024	G
32	R3	1026	G
32	R3	1027	C
32	R3	1028	C
32	R3	1030	U
32	R3	1031	C

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Mol	Chain	Res	Type
32	R3	1033	G
32	R3	1034	G
32	R3	1035	A
32	R3	1036	A
32	R3	1038	C
32	R3	1039	G
32	R3	1040	U
32	R3	1044	A
32	R3	1045	C
32	R3	1049	U
32	R3	1052	U
32	R3	1070	U
32	R3	1078	U
32	R3	1084	G
32	R3	1085	U
32	R3	1086	U
32	R3	1094	G
32	R3	1095	U
32	R3	1099	G
32	R3	1101	A
32	R3	1103	C
32	R3	1118	U
32	R3	1123	U
32	R3	1124	G
32	R3	1125	U
32	R3	1126	U
32	R3	1130	A
32	R3	1131	G
32	R3	1133	G
32	R3	1136	C
32	R3	1137	C
32	R3	1138	G
32	R3	1139	G
32	R3	1142	G
32	R3	1150	A
32	R3	1151	A
32	R3	1158	C
32	R3	1159	U
32	R3	1169	A
32	R3	1182	G
32	R3	1184	G
32	R3	1187	G

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Mol	Chain	Res	Type
32	R3	1193	G
32	R3	1196	A
32	R3	1197	A
32	R3	1198	G
32	R3	1199	U
32	R3	1208	C
32	R3	1212	U
32	R3	1213	A
32	R3	1214	C
32	R3	1227	A
32	R3	1228	C
32	R3	1236	A
32	R3	1238	A
32	R3	1246	A
32	R3	1257	A
32	R3	1261	A
32	R3	1268	G
32	R3	1271	A
32	R3	1275	A
32	R3	1280	A
32	R3	1285	A
32	R3	1286	U
32	R3	1287	A
32	R3	1298	U
32	R3	1300	G
32	R3	1302	C
32	R3	1305	G
32	R3	1306	A
32	R3	1313	U
32	R3	1314	C
32	R3	1320	C
32	R3	1321	U
32	R3	1322	C
32	R3	1323	G
32	R3	1332	A
32	R3	1333	A
32	R3	1336	C
32	R3	1346	A
32	R3	1353	G
32	R3	1363	A
32	R3	1364	U
32	R3	1370	G

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Mol	Chain	Res	Type
32	R3	1376	U
32	R3	1419	G
32	R3	1432	G
32	R3	1434	A
32	R3	1441	A
32	R3	1442	G
32	R3	1443	C
32	R3	1446	A
32	R3	1451	U
32	R3	1452	C
32	R3	1472	U
32	R3	1492	A
32	R3	1493	A
32	R3	1494	G
32	R3	1497	G
32	R3	1499	A
32	R3	1502	A
32	R3	1503	A
32	R3	1506	U
32	R3	1517	G
32	R3	1529	G
32	R3	1530	G
53	T	8	4SU
53	T	9	G
53	T	15	C
53	T	16	C
53	T	17	U
53	T	18	G
53	T	19	G
53	T	21	A
53	T	22	G
53	T	42	G
53	T	44	A
53	T	46	A
53	T	47	U
53	T	55	PSU
53	T	76	A

All (39) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	R1	360	U

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Mol	Chain	Res	Type
30	R1	784	G
30	R1	859	G
30	R1	1020	A
30	R1	1050	A
30	R1	1715	G
30	R1	1847	G
30	R1	2189	U
30	R1	2506	U
30	R1	2663	G
30	R1	2839	G
30	R1	2896	C
31	R2	52	A
32	R3	2	A
32	R3	120	A
32	R3	288	A
32	R3	301	G
32	R3	312	C
32	R3	363	A
32	R3	375	U
32	R3	453	G
32	R3	461	A
32	R3	497	G
32	R3	500	G
32	R3	561	U
32	R3	588	G
32	R3	612	C
32	R3	672	U
32	R3	753	A
32	R3	837	U
32	R3	870	U
32	R3	1125	U
32	R3	1132	C
32	R3	1149	C
32	R3	1270	G
32	R3	1297	G
32	R3	1305	G
53	T	8	4SU
53	T	17	U

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	$\#\|Z\| > 2$
53	4OC	T	32	53	20,23,24	2.47	4 (20%)	25,32,35	1.66	4 (16%)
53	4SU	T	8	53	18,21,22	3.52	7 (38%)	25,30,33	2.31	6 (24%)
53	H2U	T	20	53	18,21,22	4.47	5 (27%)	19,30,33	4.05	6 (31%)
53	PSU	T	55	53	18,21,22	2.15	8 (44%)	21,30,33	2.39	4 (19%)
53	MUM	T	54	53	18,22,22	2.91	5 (27%)	19,32,32	2.16	5 (26%)

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
53	4OC	T	32	53	1/1/5/6	4/9/29/30	0/2/2/2
53	4SU	T	8	53	2/2/5/5	4/7/25/26	0/2/2/2
53	H2U	T	20	53	2/2/8/9	3/7/38/39	0/2/2/2
53	PSU	T	55	53	-	3/7/25/26	0/2/2/2
53	MUM	T	54	53	1/1/9/10	0/7/41/41	0/2/2/2

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	T	20	H2U	O4-C4	10.55	1.44	1.23
53	T	54	MUM	C6-N1	-10.33	1.34	1.46
53	T	8	4SU	O2-C2	9.74	1.40	1.23
53	T	20	H2U	C2-N1	8.90	1.48	1.35
53	T	32	4OC	O2-C2	8.56	1.39	1.23
53	T	20	H2U	O2-C2	8.38	1.37	1.23
53	T	20	H2U	C2-N3	8.15	1.52	1.38
53	T	8	4SU	C4-S4	7.43	1.82	1.68
53	T	20	H2U	C4-N3	5.42	1.46	1.37
53	T	8	4SU	C4-N3	-5.02	1.32	1.37
53	T	32	4OC	C4-N4	4.62	1.45	1.36
53	T	8	4SU	C2-N1	-4.24	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	T	55	PSU	C1'-C5	-4.15	1.40	1.50
53	T	54	MUM	C6-C5	-3.93	1.40	1.51
53	T	55	PSU	C6-C5	3.82	1.39	1.35
53	T	32	4OC	C2-N1	-3.43	1.32	1.40
53	T	55	PSU	C2-N1	-3.32	1.32	1.36
53	T	8	4SU	C2-N3	-3.31	1.32	1.38
53	T	55	PSU	C4-N3	-3.11	1.33	1.38
53	T	8	4SU	C5-C4	-3.11	1.38	1.42
53	T	55	PSU	C2-N3	-3.08	1.32	1.37
53	T	54	MUM	O2-C2	-2.84	1.18	1.23
53	T	54	MUM	C2-N3	-2.50	1.33	1.38
53	T	55	PSU	O4-C4	-2.44	1.18	1.23
53	T	32	4OC	C6-N1	-2.42	1.32	1.38
53	T	8	4SU	C6-N1	-2.33	1.32	1.38
53	T	55	PSU	C6-N1	-2.16	1.32	1.36
53	T	54	MUM	C2-N1	-2.04	1.32	1.35
53	T	55	PSU	O2-C2	-2.02	1.19	1.23

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	T	20	H2U	O2-C2-N1	-11.74	108.98	123.10
53	T	20	H2U	O4-C4-N3	-7.55	108.66	120.30
53	T	55	PSU	N1-C2-N3	7.46	123.03	115.17
53	T	20	H2U	O2-C2-N3	-6.90	108.78	121.49
53	T	8	4SU	C4-N3-C2	-6.71	120.89	127.31
53	T	20	H2U	O4-C4-C5	-6.50	108.89	122.20
53	T	54	MUM	N3-C2-N1	5.14	121.81	116.65
53	T	54	MUM	C4-N3-C2	-5.11	120.60	126.83
53	T	8	4SU	N3-C2-N1	5.08	121.50	114.89
53	T	8	4SU	C5-C4-N3	4.98	119.38	114.75
53	T	55	PSU	C4-N3-C2	-4.37	120.34	126.37
53	T	55	PSU	O2-C2-N1	-4.37	118.28	122.79
53	T	32	4OC	C1'-N1-C2	4.25	127.83	118.44
53	T	54	MUM	C5M-C5-C6	3.74	120.68	112.05
53	T	20	H2U	C5-C4-N3	-3.57	112.89	116.69
53	T	8	4SU	C5-C4-S4	-3.49	120.32	124.31
53	T	20	H2U	N3-C2-N1	-3.44	113.19	116.65
53	T	32	4OC	C1'-N1-C6	-3.40	113.51	120.78
53	T	54	MUM	O2-C2-N1	-3.34	119.09	123.10
53	T	32	4OC	O2-C2-N3	-3.28	117.16	122.33
53	T	55	PSU	C6-N1-C2	-3.18	119.74	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	T	32	4OC	C5-C4-N3	-3.09	117.77	122.60
53	T	8	4SU	O2-C2-N1	-2.99	118.90	122.80
53	T	54	MUM	C6-C5-C4	2.54	118.82	111.53
53	T	8	4SU	C6-C5-C4	-2.30	117.96	119.95

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
53	T	8	4SU	C3'
53	T	8	4SU	C2'
53	T	20	H2U	C1'
53	T	20	H2U	C2'
53	T	32	4OC	C2'
53	T	54	MUM	C5

All (14) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
53	T	32	4OC	3	0
53	T	20	H2U	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 153 ligands modelled in this entry, 152 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
55	FME	T	101	53	8,9,10	0.99	0	8,9,11	0.83	0

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
55	FME	T	101	53	-	1/7/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	T	101	FME	CB-CA-N-CN

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
30	R1	3
32	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	6.02
1	R3	460:A	O3'	461:A	P	5.42
1	R1	2188:U	O3'	2189:U	P	4.22
1	R1	2194:U	O3'	2195:U	P	3.88
1	R1	2097:A	O3'	2098:U	P	3.44

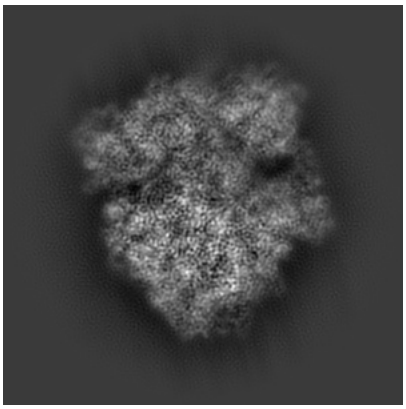
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-40939. These allow visual inspection of the internal detail of the map and identification of artifacts.

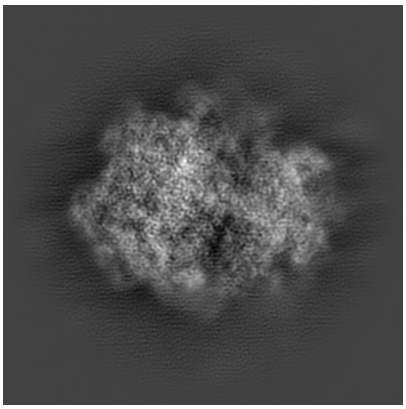
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

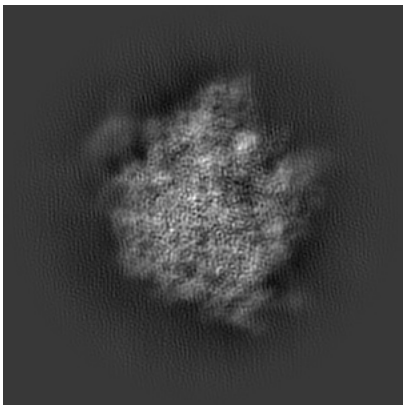
6.1.1 Primary map



X

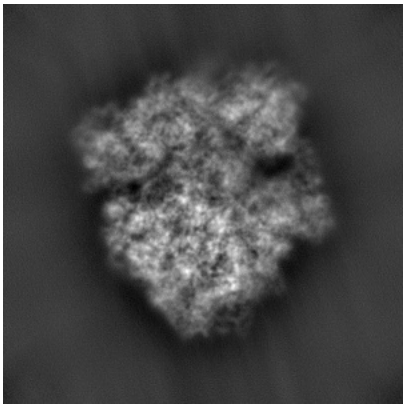


Y

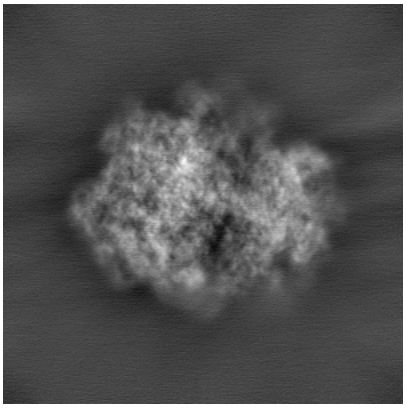


Z

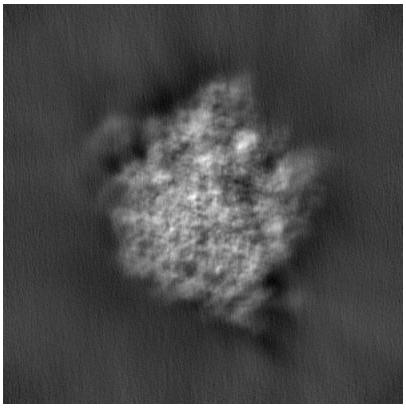
6.1.2 Raw map



X



Y

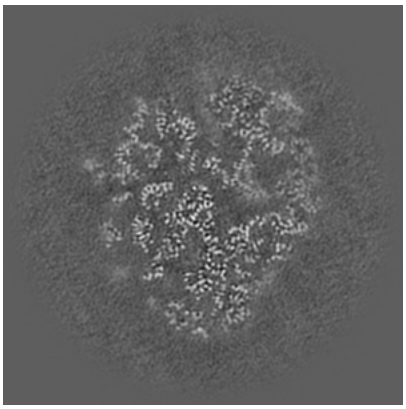


Z

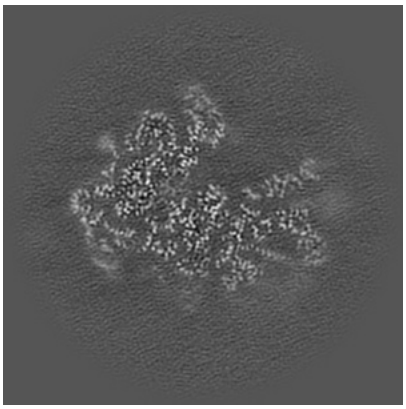
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

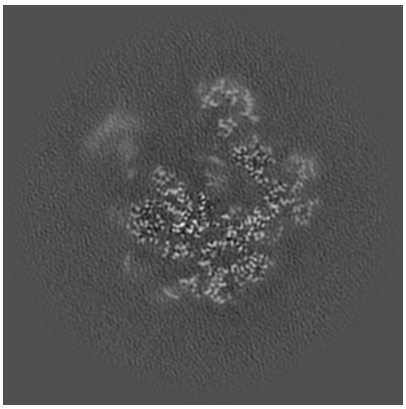
6.2.1 Primary map



X Index: 200

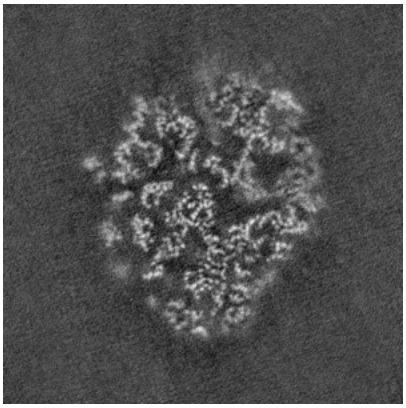


Y Index: 200



Z Index: 200

6.2.2 Raw map



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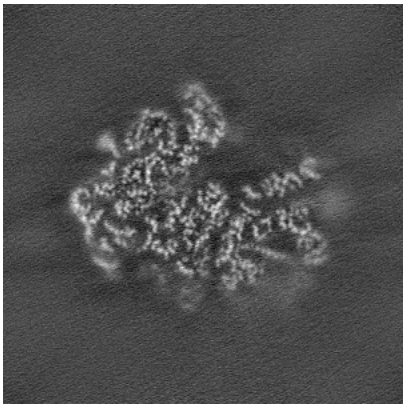
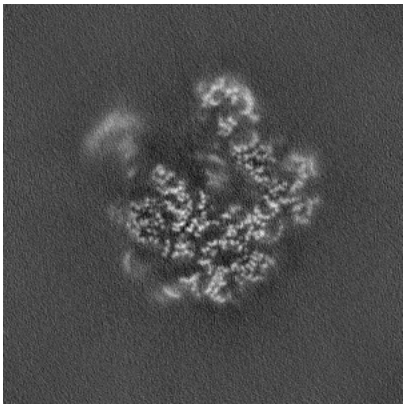


Y Index: 200

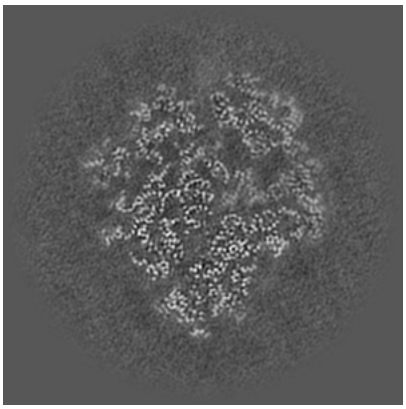


Z Index: 200

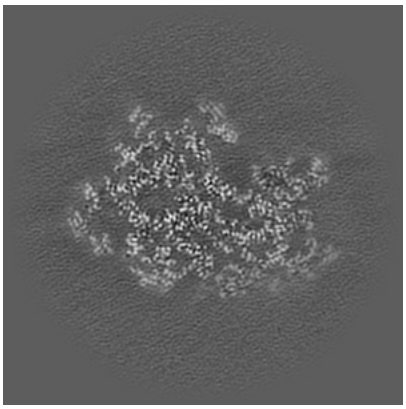
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

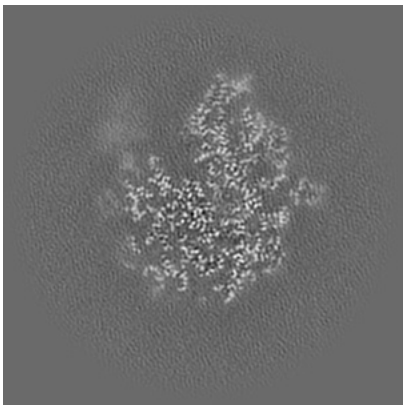
6.3.1 Primary map



X Index: 207

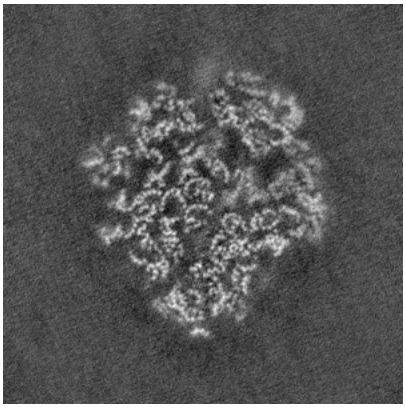


Y Index: 185

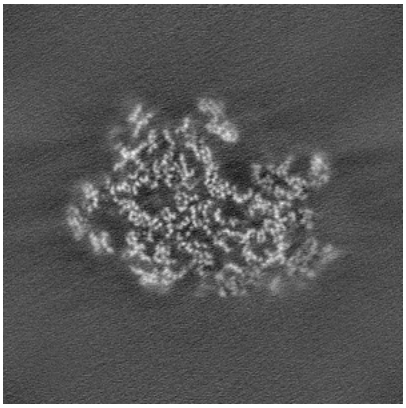


Z Index: 182

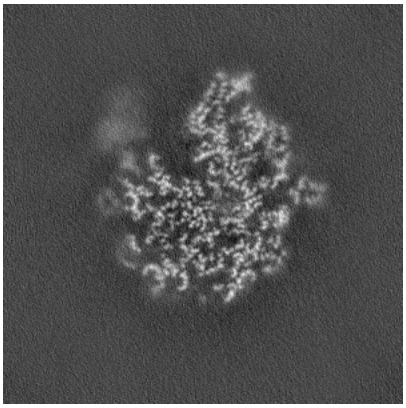
6.3.2 Raw map



X Index: 207



Y Index: 184

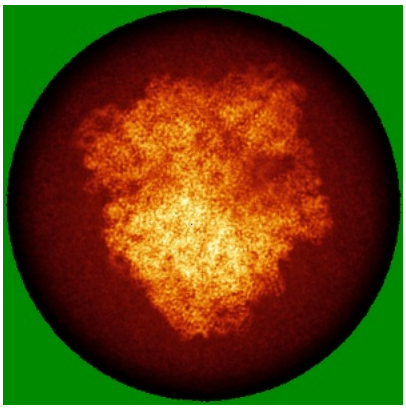


Z Index: 182

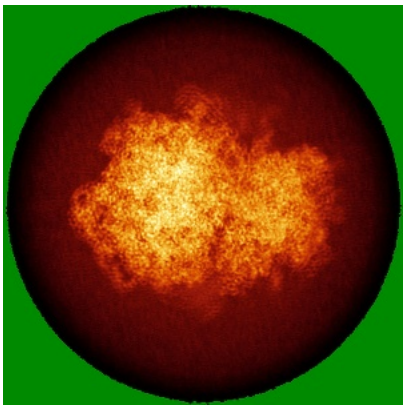
The images above show the largest variance slices of the map in three orthogonal directions.

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

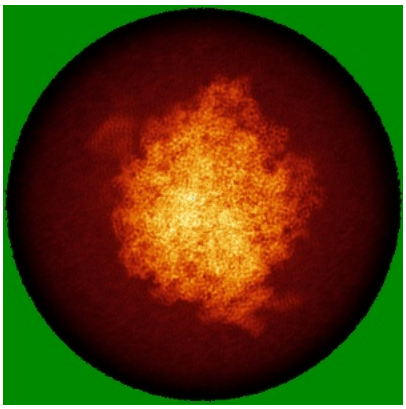
6.4.1 Primary map



X

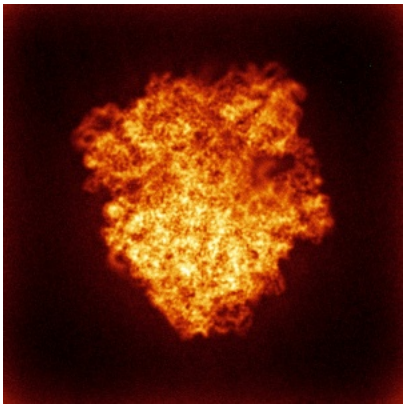


Y

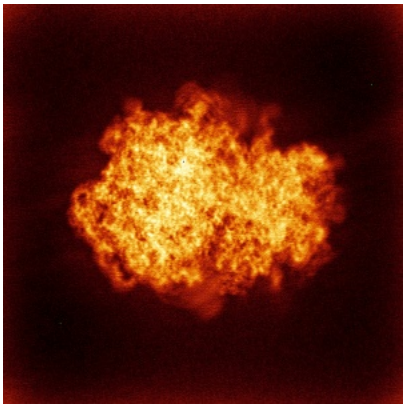


Z

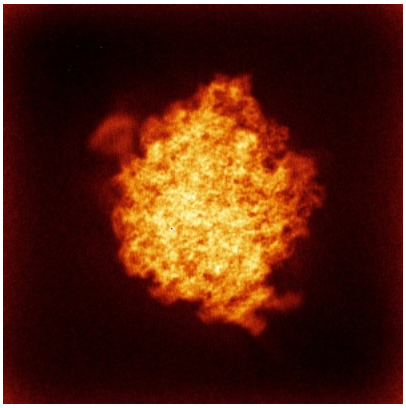
6.4.2 Raw map



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 0.55. 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.

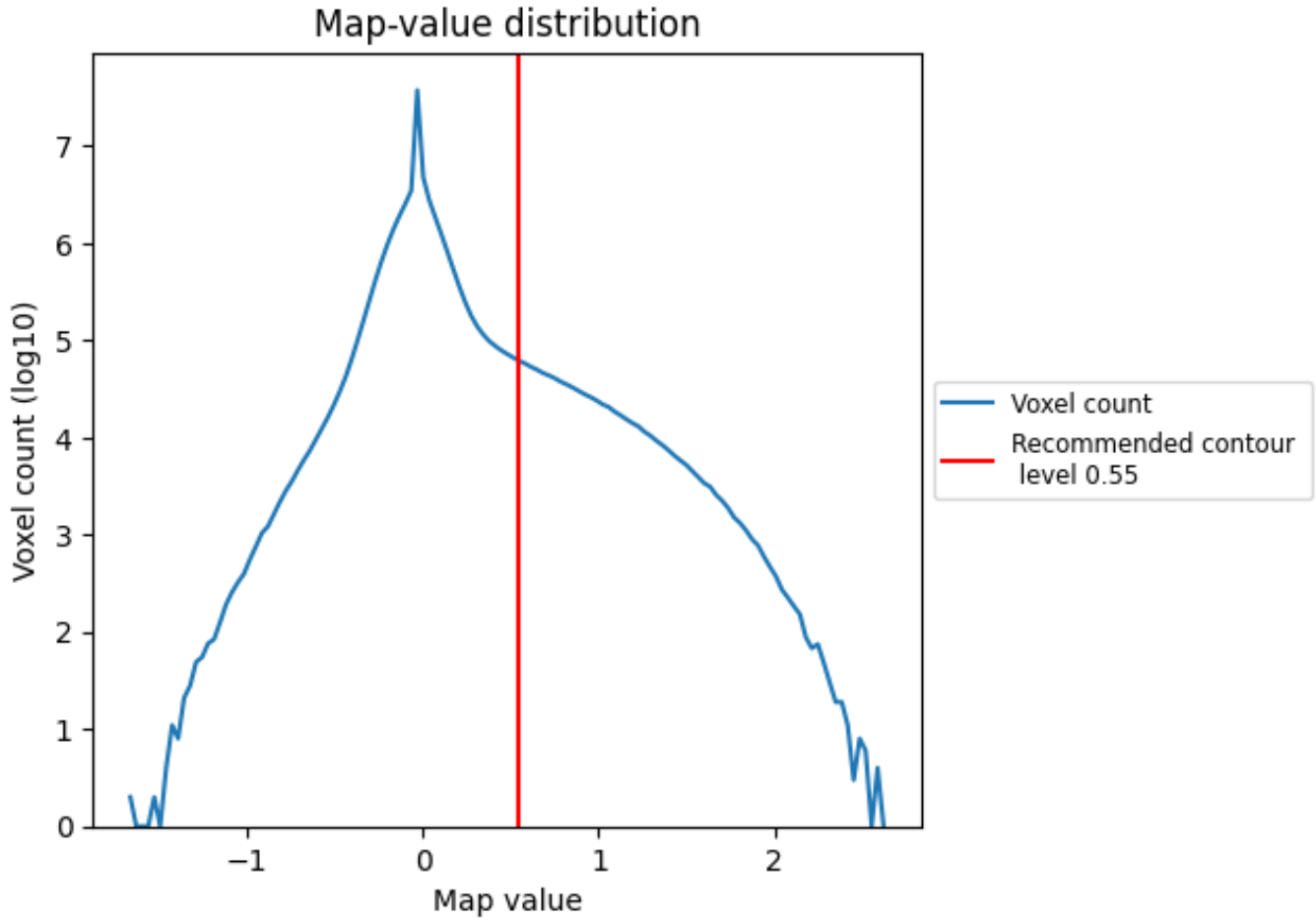
6.6 Mask visualisation (i)

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

7 Map analysis

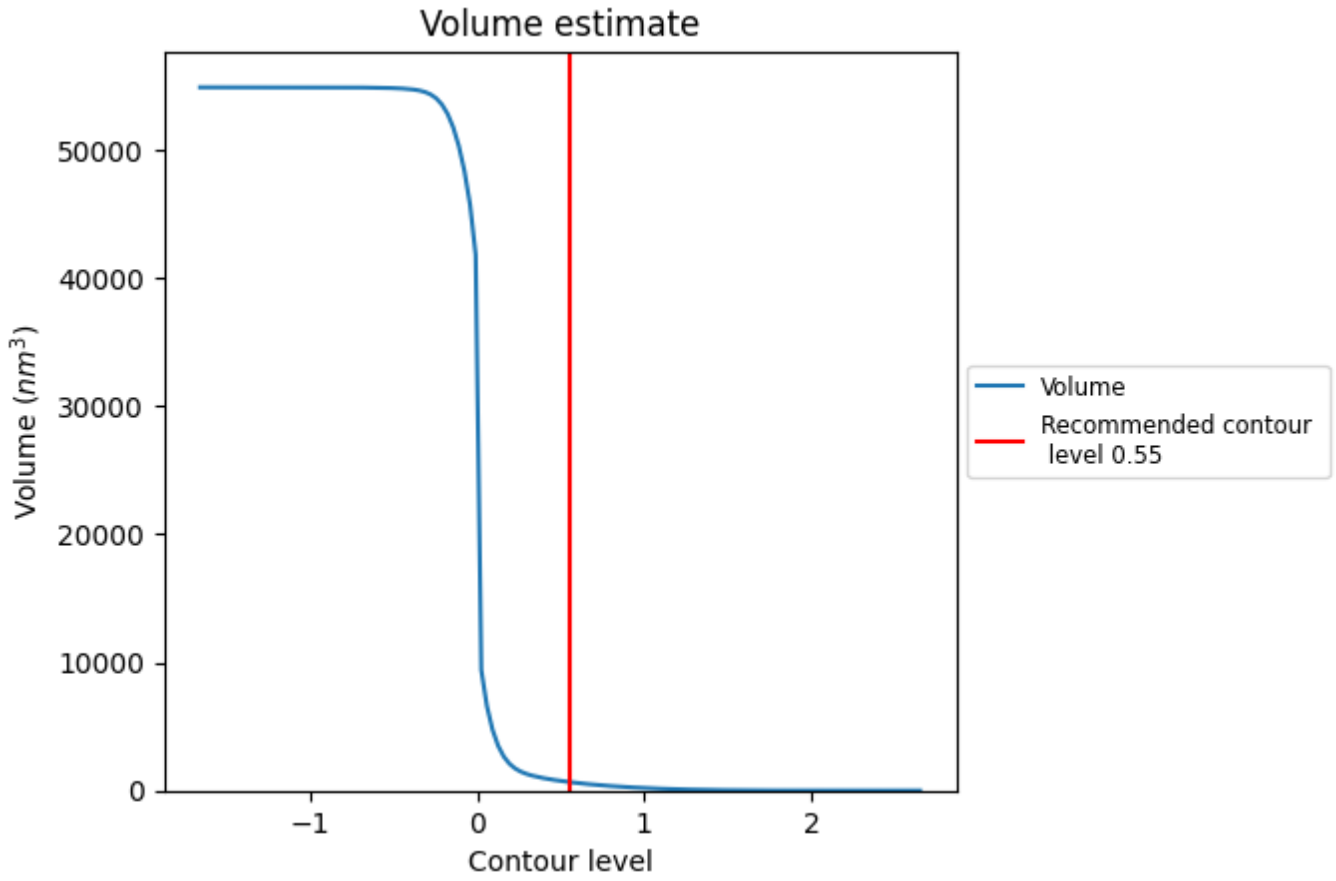
This section contains the results of statistical analysis of the map.

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.

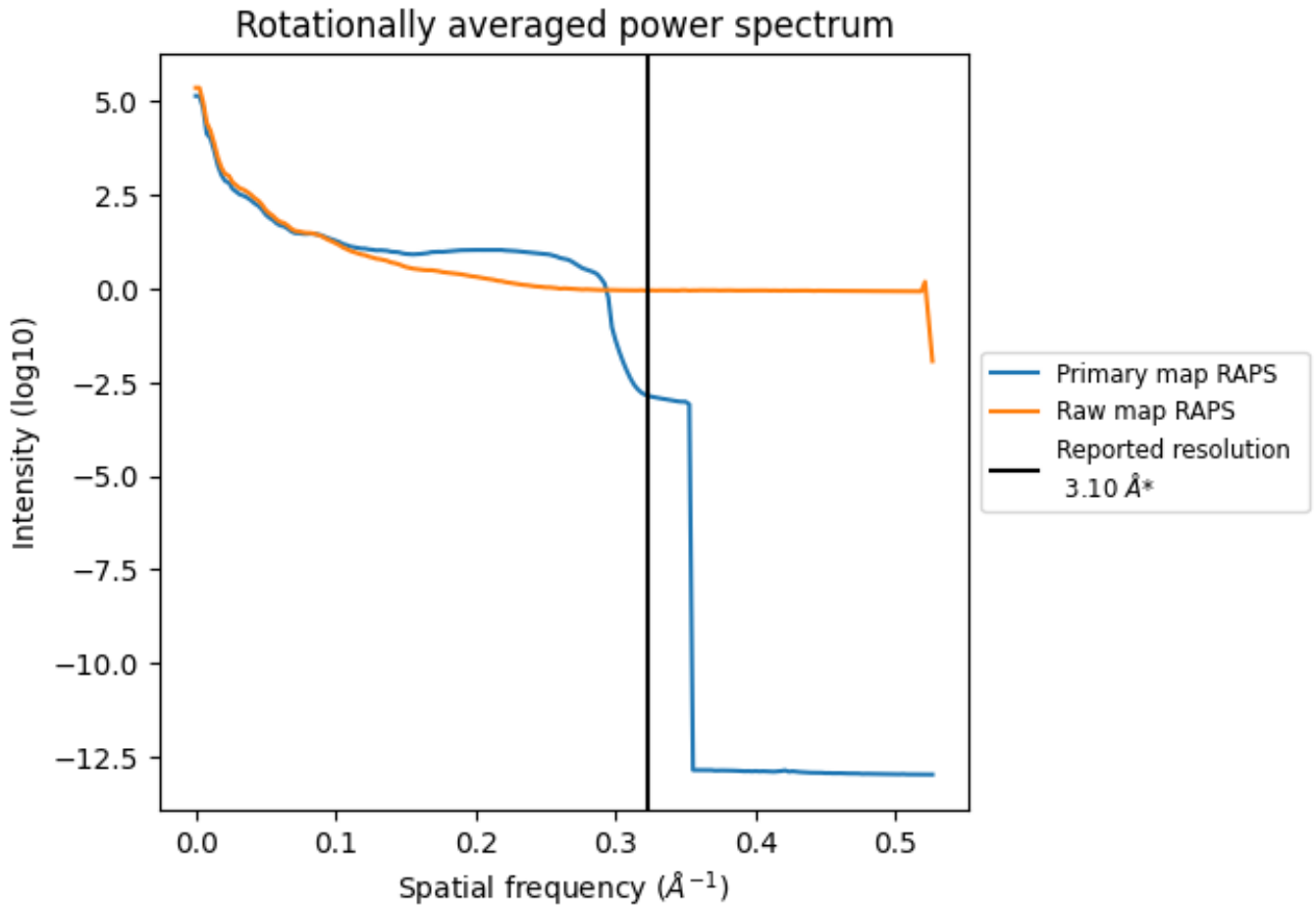
7.2 Volume estimate



The volume at the recommended contour level is 668 nm^3; this corresponds to an approximate mass of 604 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)

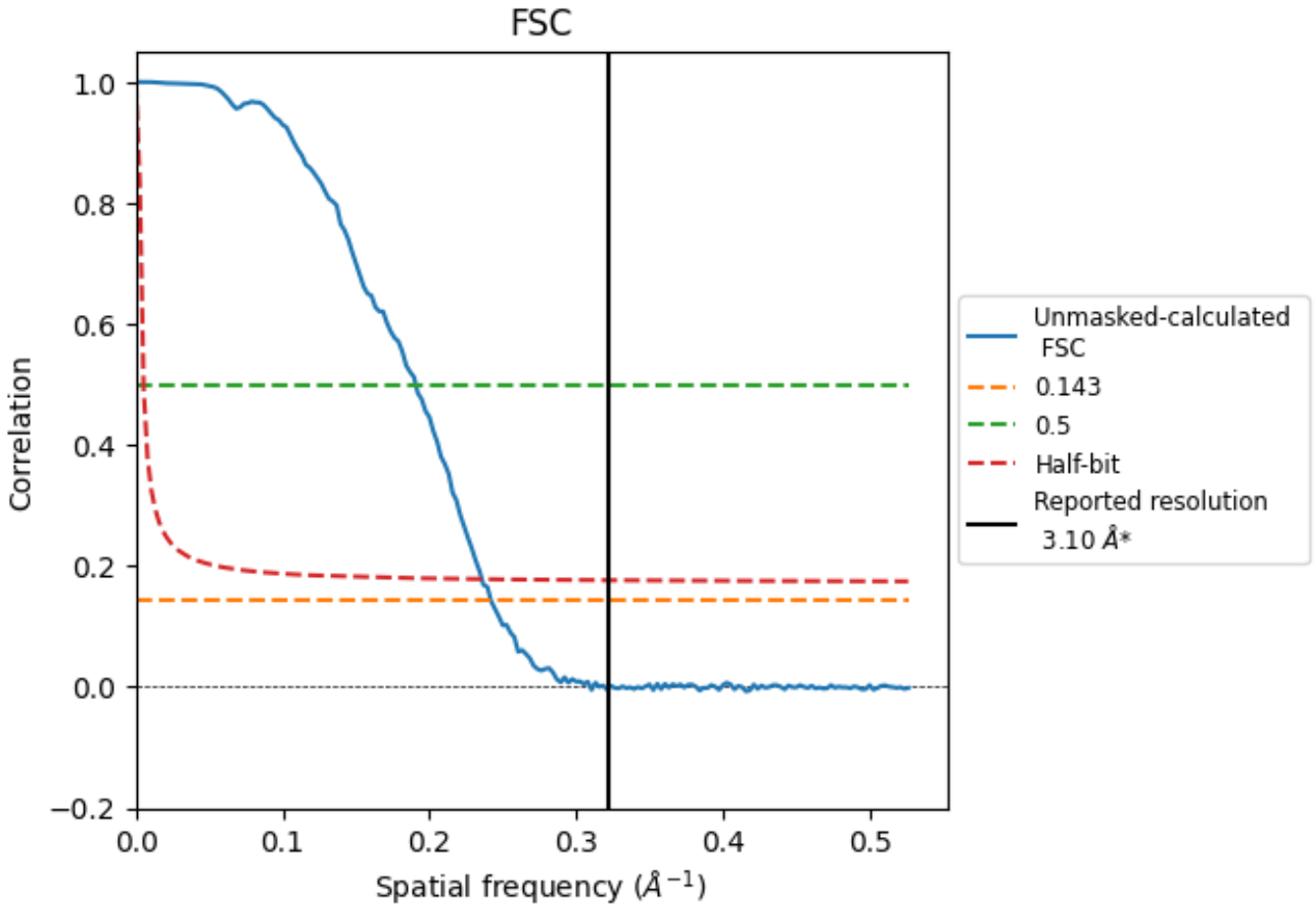


*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

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 0.323 $Å^{-1}$

8.2 Resolution estimates (i)

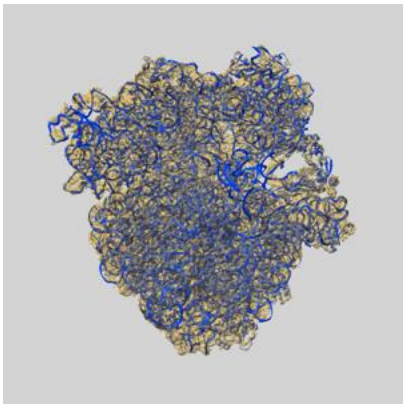
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.13	5.24	4.24

*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 4.13 differs from the reported value 3.1 by more than 10 %

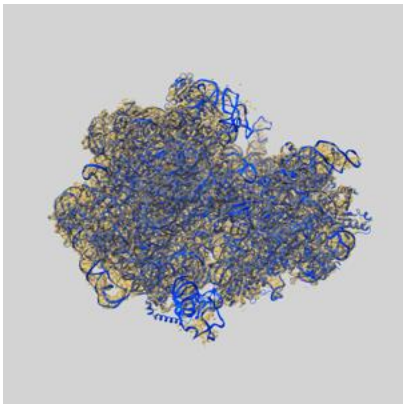
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-40939 and PDB model 9NJV. Per-residue inclusion information can be found in section 3 on page 15.

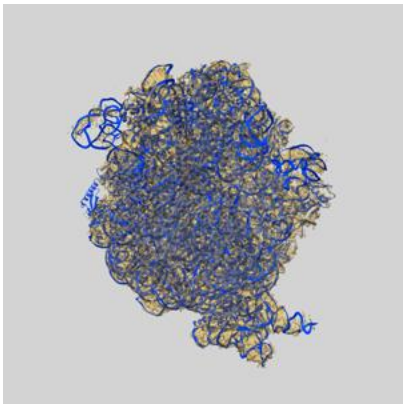
9.1 Map-model overlay



X



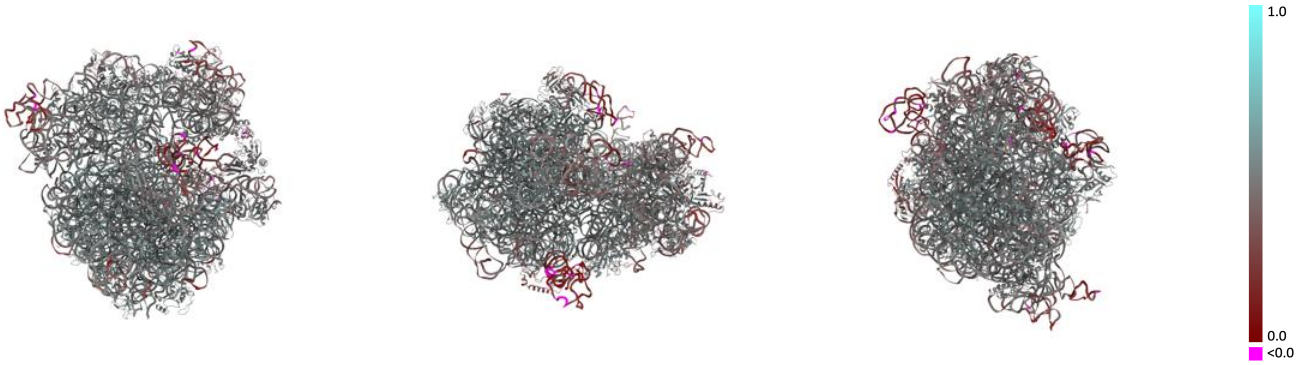
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.55 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.

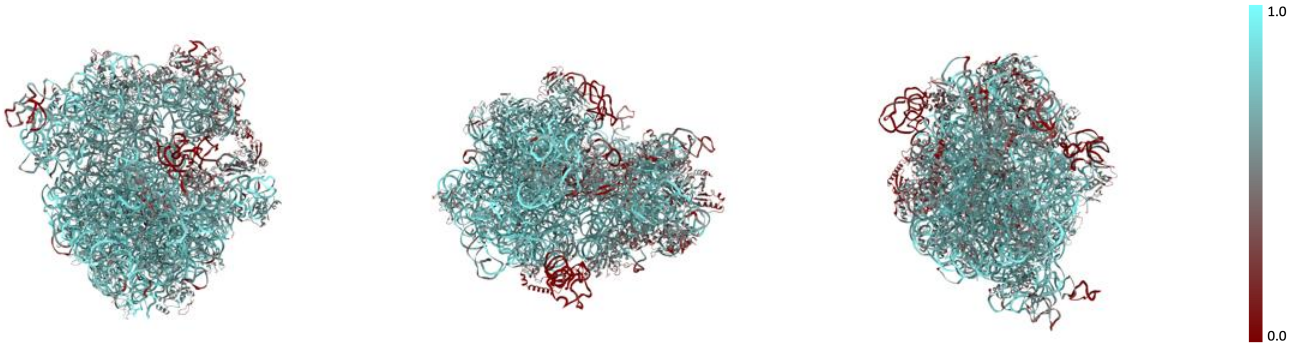
9.2 Q-score mapped to coordinate model



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.

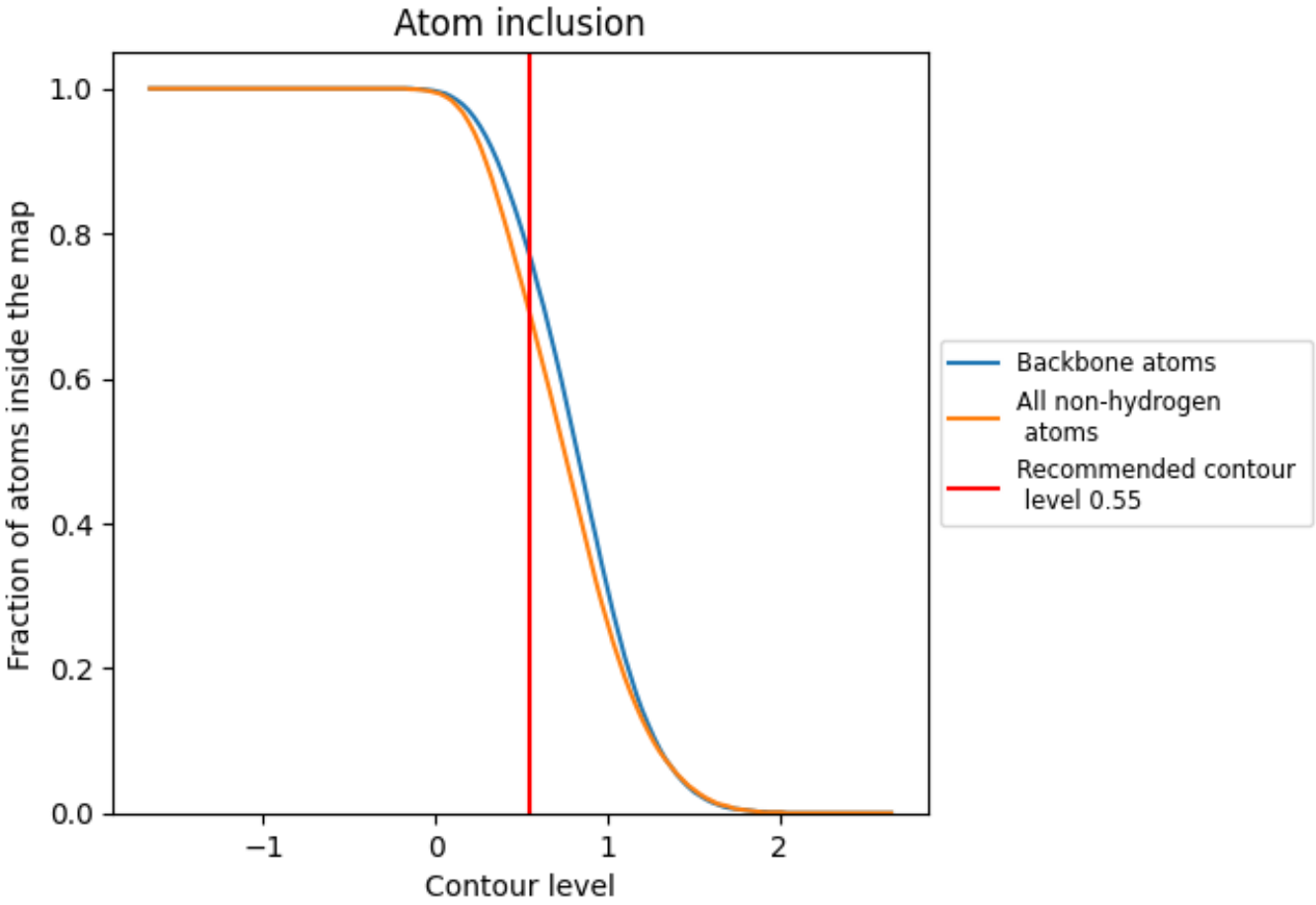
9.3 Atom inclusion mapped to coordinate model



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 (0.55).

9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 69% 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 (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6890	0.4710
13	0.6700	0.5280
14	0.6220	0.5380
15	0.6720	0.5290
16	0.6290	0.5340
17	0.7400	0.5410
18	0.5500	0.4890
19	0.6340	0.5400
2	0.6720	0.5470
20	0.7030	0.5400
21	0.6440	0.5200
22	0.6520	0.5320
23	0.5870	0.5110
24	0.5890	0.5000
25	0.5980	0.4970
27	0.6590	0.5420
28	0.6750	0.5390
29	0.5920	0.4820
3	0.6880	0.5330
30	0.6480	0.5200
31	0.1190	0.3700
32	0.6850	0.5250
34	0.7180	0.5530
35	0.7130	0.5540
36	0.6340	0.5330
4	0.5840	0.5160
5	0.4250	0.4610
6	0.4510	0.4620
9	0.1070	0.3380
M	0.6210	0.4640
R1	0.7670	0.4660
R2	0.7740	0.4510
R3	0.7370	0.4540
T	0.4980	0.4020
sb	0.3430	0.4390

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Chain	Atom inclusion	Q-score
sc	0.5090	0.4890
sd	0.4850	0.4720
se	0.5620	0.5070
sf	0.4820	0.4570
sg	0.4110	0.4560
sh	0.6090	0.5120
si	0.4190	0.4510
sj	0.3180	0.4360
sk	0.5310	0.4940
sl	0.5640	0.5190
sm	0.4350	0.4620
sn	0.4650	0.4700
so	0.5870	0.4990
sp	0.5630	0.4880
sq	0.5330	0.4910
sr	0.4880	0.4860
ss	0.4070	0.4480
st	0.5510	0.4940
su	0.3210	0.3830