Full wwPDB EM Validation Report ⓘ

Mar 24, 2025 – 02:44 PM EDT

PDB ID	:	9NL7
EMDB ID	:	EMD-40928
Title	:	E. coli initiation complex with EQ2-YbiT in Non-hydrolytic 2/PtIM(b) conformation
Authors	:	Singh, S.; Hunt, J.F.
Deposited on	:	2025-03-02
Resolution	:	3.30 Å(reported)

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

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

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

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

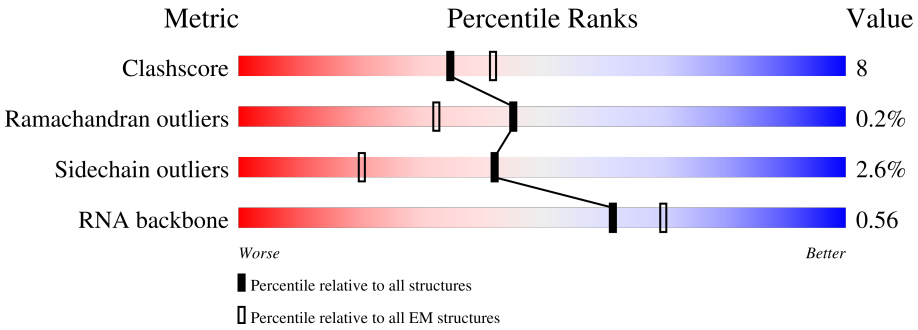
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

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

Mol	Chain	Length	Quality of chain
1	1	220	45% 80% 20%
2	13	142	77% 22%
3	14	122	81% 19%
4	15	144	79% 21%
5	16	136	78% 22%
6	17	120	81% 18%
7	18	116	6% 73% 26%

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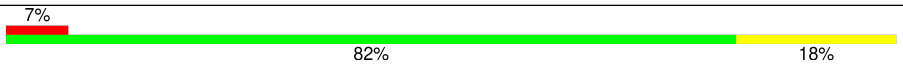
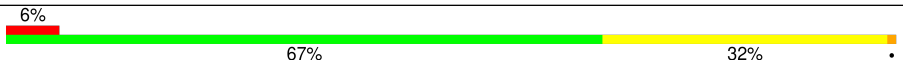
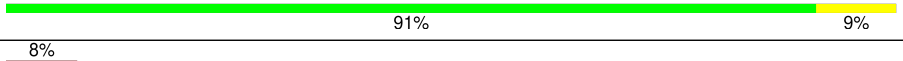
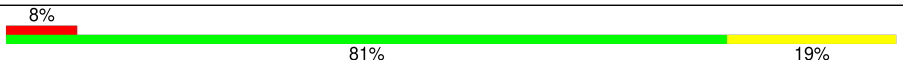
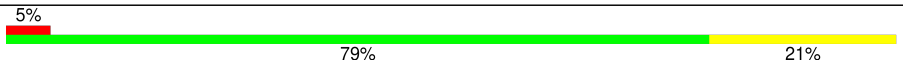
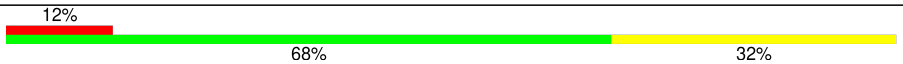
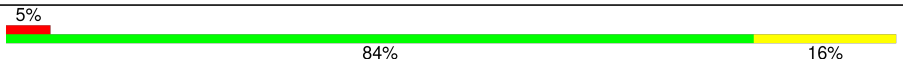
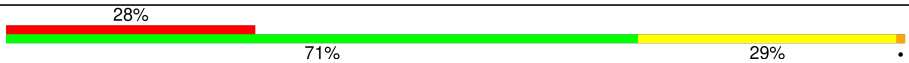
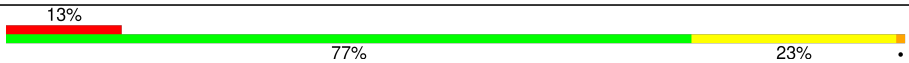
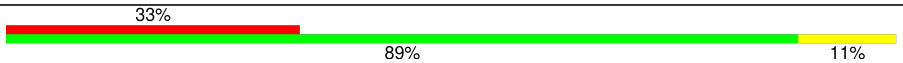
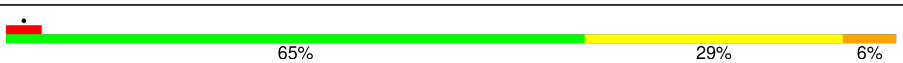
Mol	Chain	Length	Quality of chain
8	19	114	
9	2	271	
10	20	117	
11	21	103	
12	22	110	
13	23	93	
14	24	102	
15	25	94	
16	27	75	
17	28	77	
18	29	63	
19	3	209	
20	30	58	
21	31	66	
22	32	56	
23	33	50	
24	34	46	
25	35	64	
26	36	38	
27	4	201	
28	5	177	
29	6	176	
30	9	149	
31	M	9	
32	R1	2903	

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Mol	Chain	Length	Quality of chain
33	R2	119	64% 33%
34	R3	1539	6% 62% 33% 6%
35	T	77	26% 39% 43% 13% 5%
36	Y	530	28% 58% 40%
37	sb	218	21% 98%
38	sc	206	11% 100%
39	sd	205	10% 96%
40	se	157	97%
41	sf	100	14% 96%
42	sg	151	24% 97%
43	sh	129	98%
44	si	127	21% 94% 6%
45	sj	98	44% 97%
46	sk	116	6% 97%
47	sl	123	8% 97%
48	sm	114	28% 96%
49	sn	100	20% 95% 5%
50	so	88	100%
51	sp	82	7% 98%
52	sq	80	9% 98%
53	sr	65	12% 98%
54	ss	80	28% 98%
55	st	85	94% 6%
56	su	70	19% 100%

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	H2U	T	20	X	-	-	-
35	4OC	T	32	X	-	-	-
35	5MU	T	54	X	-	-	-
35	PSU	T	55	X	-	-	-
35	4SU	T	8	X	-	-	-

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 150079 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

- Molecule 4 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	15	144	1053	654	207	190	2	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 16 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	27	75	Total 575	C 356	N 116	O 102	S 1	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 31 is a RNA chain called mRNA.

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

- Molecule 32 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	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 33 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 34 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	R3	1539	Total	C	N	O	P	0	0
			33012	14725	6052	10697	1538		

- Molecule 35 is a RNA chain called tRNA.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	8	4SU	G	conflict	GB 932857508

- Molecule 36 is a protein called Probable ATP-binding protein YbiT.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Y	530	Total	C	N	O	S	0	0
			4210	2659	718	814	19		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	181	GLN	GLU	conflict	UNP P0A9U3
Y	464	GLN	GLU	conflict	UNP P0A9U3

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 48 is a protein called 30S ribosomal protein S13.

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

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

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

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

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

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

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

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

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

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

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

- Molecule 54 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	ss	80	Total	C	N	O	S	0	0
			645	413	121	108	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
ss	1	MET	-	initiating methionine	UNP P0A7U3

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

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

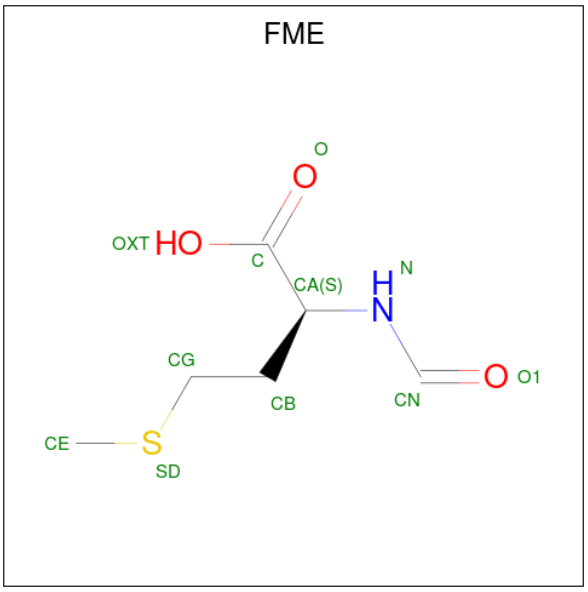
- Molecule 56 is a protein called Small ribosomal subunit protein bS21.

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

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

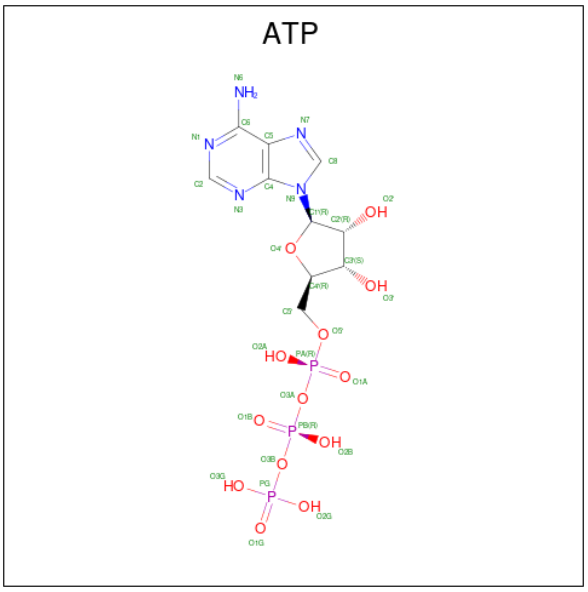
Mol	Chain	Residues	Atoms		AltConf
57	17	1	Total	Mg	0
			1	1	
57	32	1	Total	Mg	0
			1	1	
57	4	1	Total	Mg	0
			1	1	
57	R1	179	Total	Mg	0
			179	179	
57	R3	68	Total	Mg	0
			68	68	

- Molecule 58 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: $C_6H_{11}NO_3S$).



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

- Molecule 59 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

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

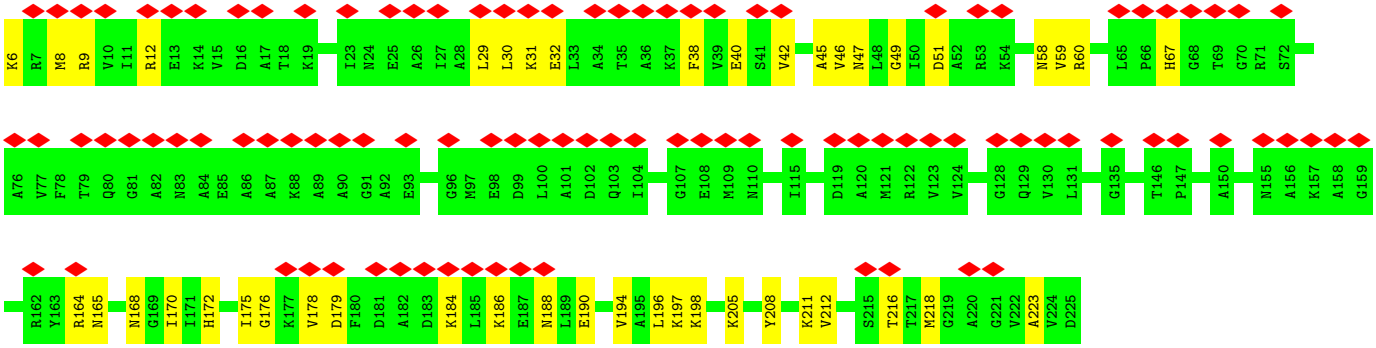
Mol	Chain	Residues	Atoms		AltConf
			Total	Na	
60	Y	2	2	2	0

3 Residue-property plots (i)

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

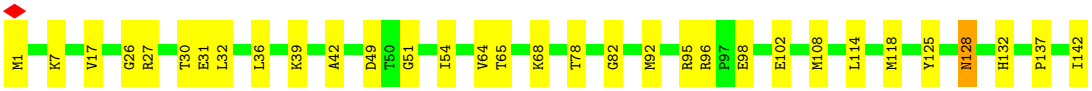
• Molecule 1: Large ribosomal subunit protein uL1

Chain 1:



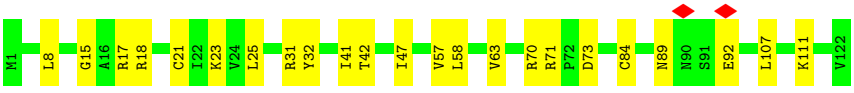
• Molecule 2: Large ribosomal subunit protein uL13

Chain 13:



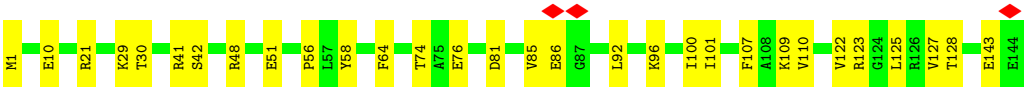
• Molecule 3: 50S ribosomal protein L14

Chain 14:



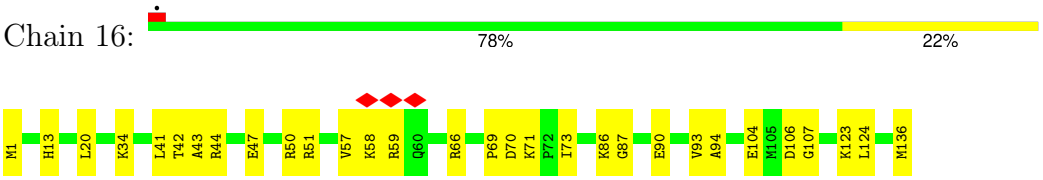
• Molecule 4: Large ribosomal subunit protein uL15

Chain 15:



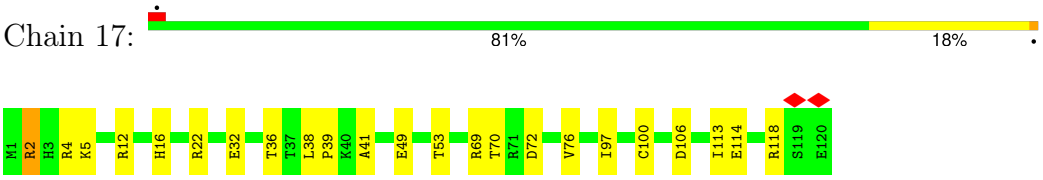
• Molecule 5: 50S ribosomal protein L16

Chain 16:



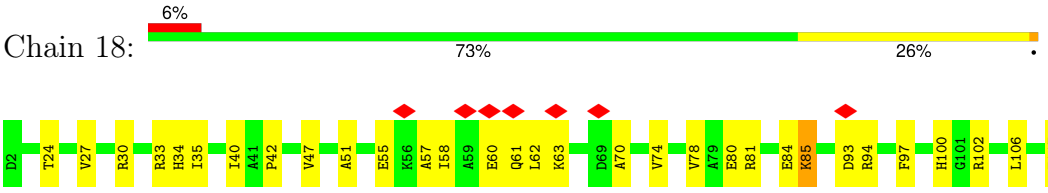
• Molecule 6: Large ribosomal subunit protein bL17

Chain 17:



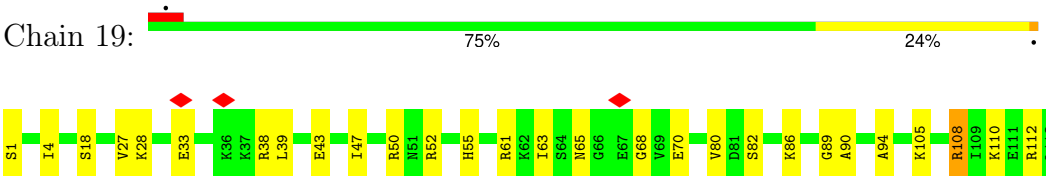
• Molecule 7: Large ribosomal subunit protein uL18

Chain 18:



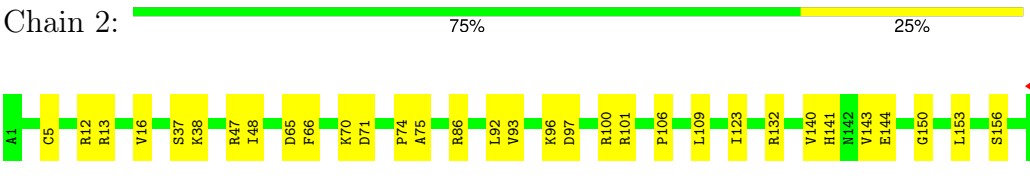
• Molecule 8: 50S ribosomal protein L19

Chain 19:



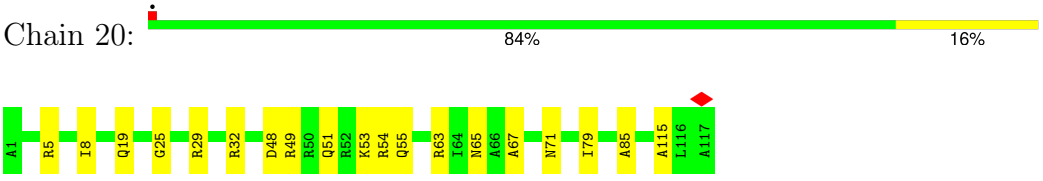
• Molecule 9: 50S ribosomal protein L2

Chain 2:



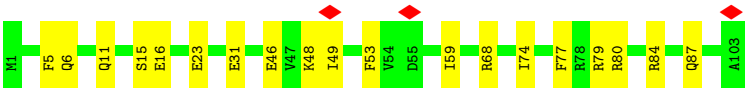
• Molecule 10: Large ribosomal subunit protein bL20

Chain 20:



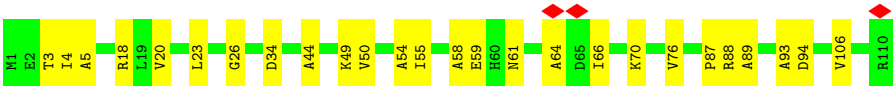
• Molecule 11: Large ribosomal subunit protein bL21

Chain 21:



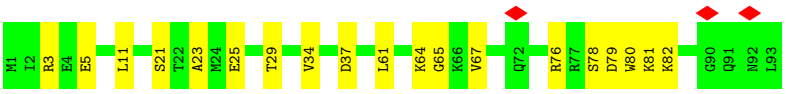
• Molecule 12: Large ribosomal subunit protein uL22

Chain 22:



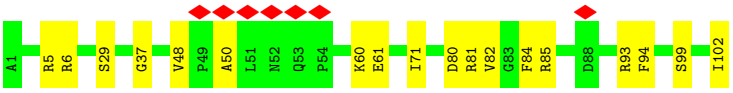
• Molecule 13: Large ribosomal subunit protein uL23

Chain 23:



• Molecule 14: Large ribosomal subunit protein uL24

Chain 24:



• Molecule 15: Large ribosomal subunit protein bL25

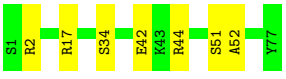
Chain 25:

• Molecule 16: 50S ribosomal protein L27

Chain 27:

• Molecule 17: 50S ribosomal protein L28

Chain 28:

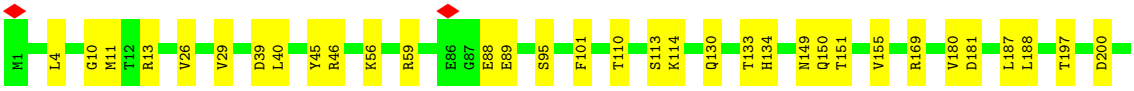


• Molecule 18: Large ribosomal subunit protein uL29

Chain 29:

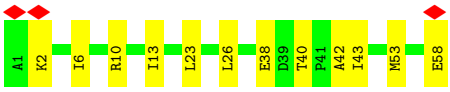
• Molecule 19: 50S ribosomal protein L3

Chain 3:



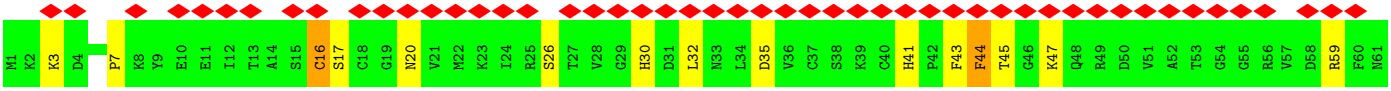
• Molecule 20: 50S ribosomal protein L30

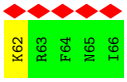
Chain 30:



• Molecule 21: Large ribosomal subunit protein bL31

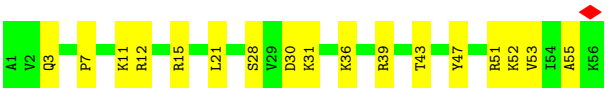
Chain 31:





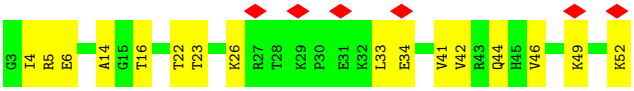
• Molecule 22: 50S ribosomal protein L32

Chain 32:



• Molecule 23: Large ribosomal subunit protein bL33

Chain 33:

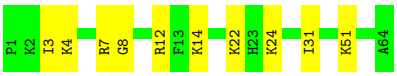


• Molecule 24: 50S ribosomal protein L34

Chain 34:

• Molecule 25: Large ribosomal subunit protein bL35

Chain 35:

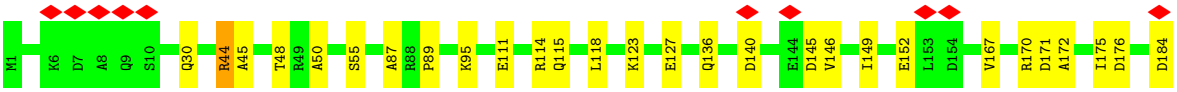


• Molecule 26: 50S ribosomal protein L36

Chain 36:

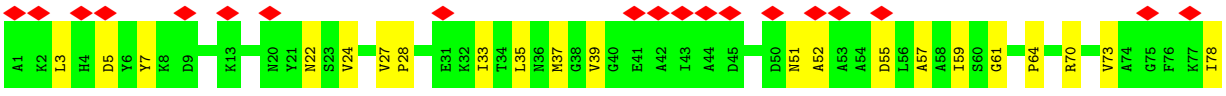
• Molecule 27: Large ribosomal subunit protein uL4

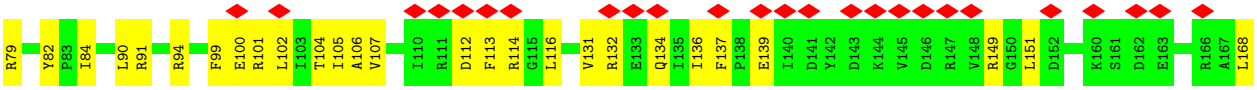
Chain 4:



• Molecule 28: 50S ribosomal protein L5

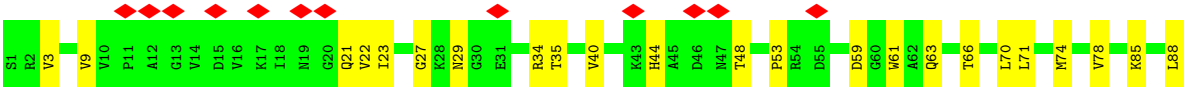
Chain 5:





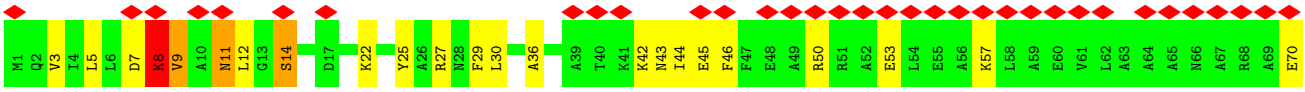
• Molecule 29: Large ribosomal subunit protein uL6

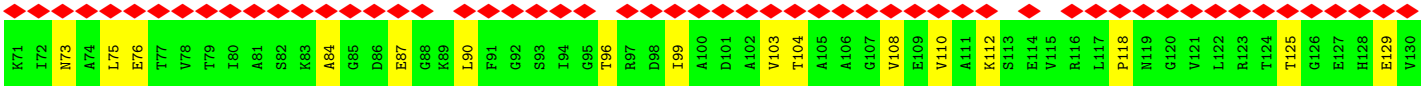
Chain 6:

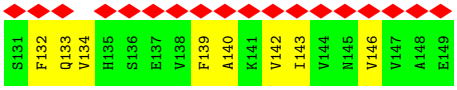


• Molecule 30: Large ribosomal subunit protein bL9

Chain 9:

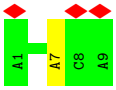






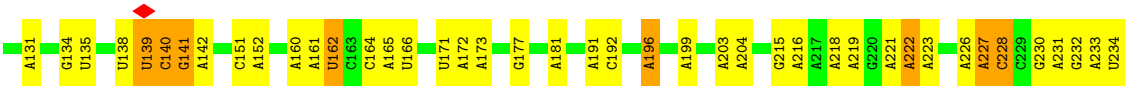
• Molecule 31: mRNA

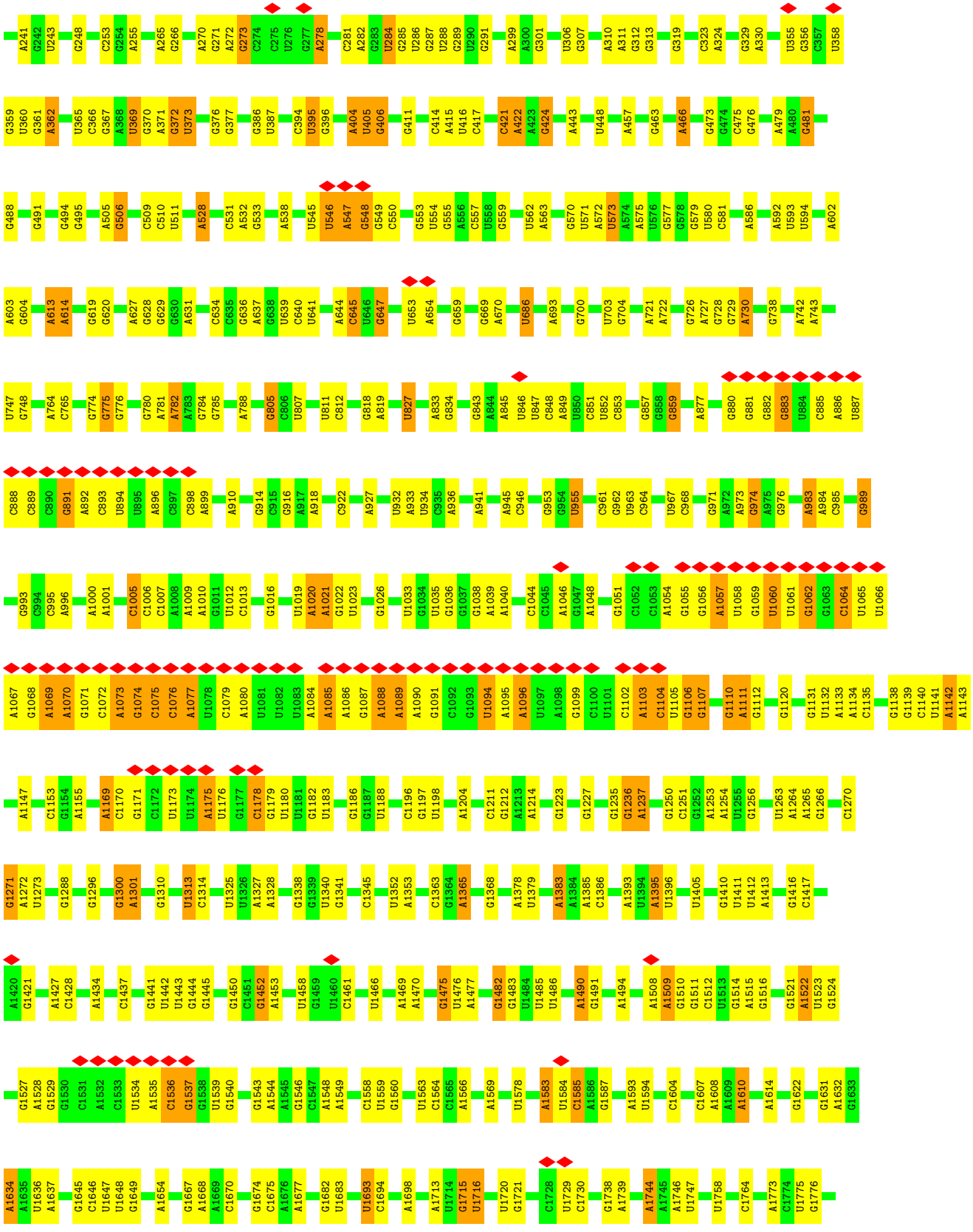
Chain M:

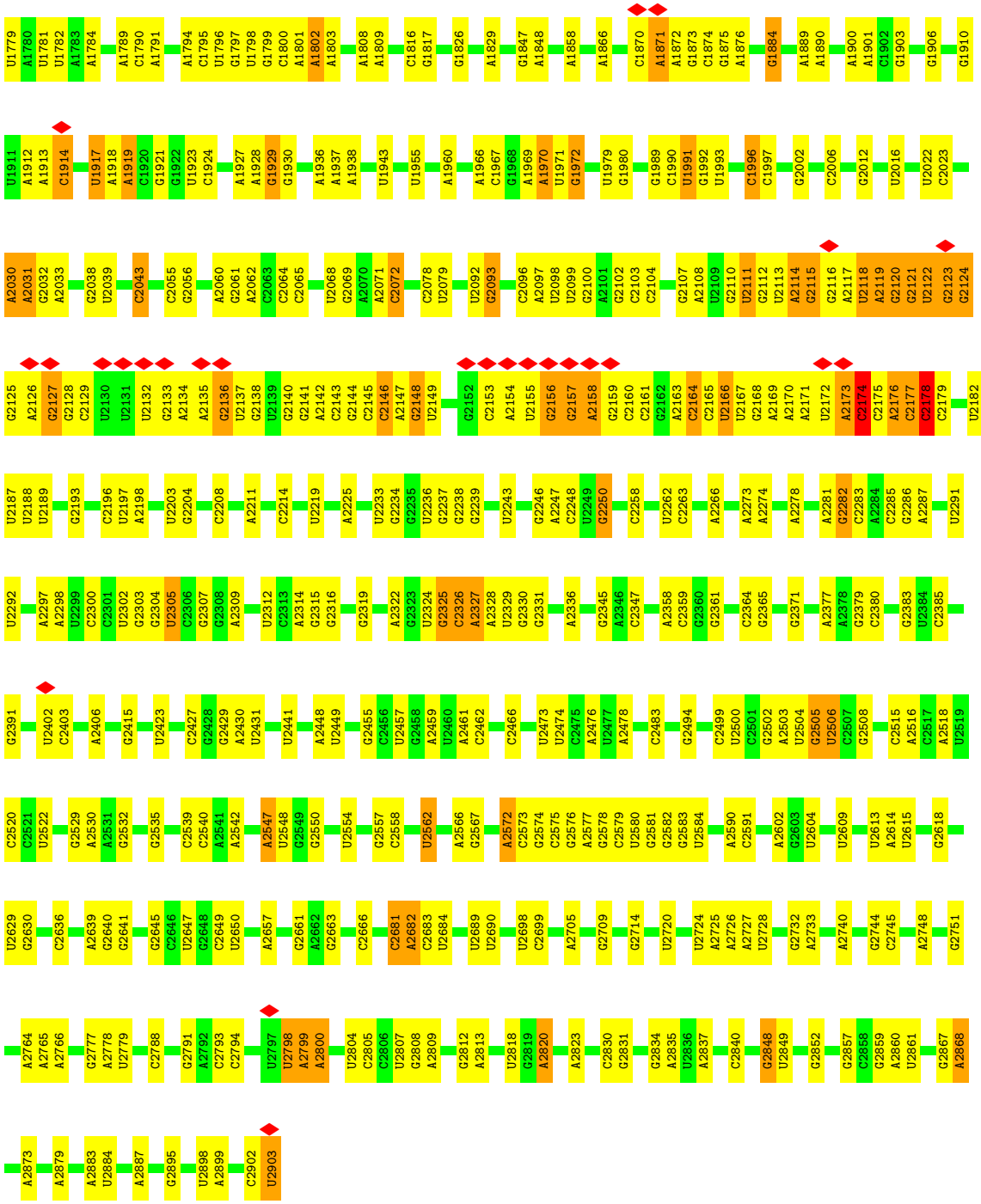


• Molecule 32: 23S ribosomal RNA

Chain R1:

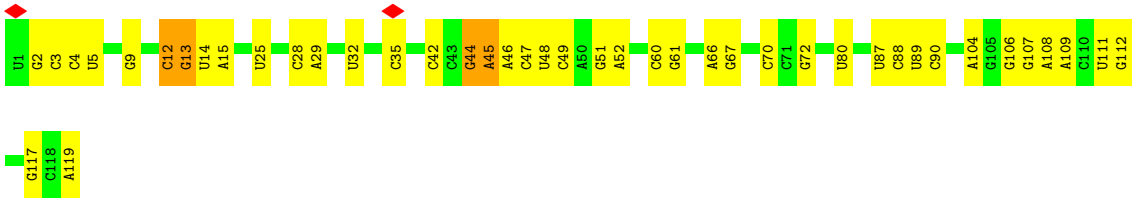



A241 G242 U243 G248 C253 G254 A255 A265 G266 A270 G271 A272 G273 C274 C275 U276 G277 A278 C281 A282 G283 U284 G285 U286 G287 U288 G289 U290 G291 A299 A300 G301 U306 G307 A310 A311 G312 G313 G319 C323 A324 G329 A330 U355 G356 C357 U358
G359 U360 G361 A362 U365 C366 G367 A368 U369 G370 A371 G372 U373 G376 G377 G386 U387 C394 U395 G396 A404 U405 G406 G411 C414 A415 U416 C417 C421 A422 A423 G424 A443 U448 A457 G463 A466 G473 G474 C475 G476 A479 A480 G481
G488 G491 G494 G495 A505 G506 C509 C510 U511 A528 C531 A532 G533 A538 U545 U546 A547 G548 G549 C550 G553 U554 G555 A556 C557 U558 C559 U562 A563 G570 U571 A572 U573 A574 A575 U576 G577 G578 G579 U580 C581 A586 A592 U593 U594 A602
A603 G604 A613 A614 G619 G620 A627 G628 G629 G630 A631 C634 C635 C636 A637 G638 U639 C640 U641 A644 C645 U646 G647 U653 A654 G659 G669 A670 U686 A693 G700 U703 G704 A721 A722 G726 A727 G728 G729 A730 G738 A742 A743
U747 G748 A764 C765 G774 G775 G776 G780 A781 A782 A783 G784 G785 A788 G805 C806 U807 U811 C812 G818 A819 U827 A833 G834 G843 A844 A845 U846 U847 C848 A849 U850 C851 U852 C853 G857 G858 G859 A877 G880 G881 G882 G883 U884 C885 A886 U887
C888 C889 C890 G891 A892 C893 U894 U895 A896 C897 C898 A899 A910 G914 C915 G916 A917 A918 C922 A927 U932 A933 U934 C935 A936 A941 A945 C946 G953 G954 U955 C961 G962 U963 C964 U967 C968 G971 A972 A973 G974 A975 G976 A983 A984 C985 G989
G993 C994 C995 A996 A1000 A1001 C1005 C1006 C1007 A1008 A1009 A1010 G1011 U1012 C1013 G1016 U1019 A1020 A1021 G1022 U1023 G1026 U1033 G1034 U1035 G1036 G1037 G1038 A1039 A1040 C1044 C1045 A1046 G1047 A1048 G1051 C1052 C1053 A1054 G1055 G1056 A1057 U1058 G1059 U1060 U1061 G1062 G1063 C1064 U1065 U1066
A1067 G1068 A1069 A1070 G1071 C1072 A1073 G1074 C1075 C1076 A1077 U1078 C1079 A1080 U1081 U1082 U1083 A1084 A1085 A1086 G1087 A1088 A1089 A1090 G1091 C1092 G1093 U1094 A1095 A1096 U1097 A1098 G1099 C1100 U1101 C1102 A1103 C1104 U1105 G1106 G1107 G1110 A1111 G1112 G1120 G1131 U1132 A1133 A1134 C1135 G1138 G1139 C1140 U1141 A1142 A1143
A1147 C1153 G1154 A1155 A1169 C1170 G1171 C1172 U1173 U1174 A1175 U1176 G1177 C1178 G1179 U1180 U1181 G1182 U1183 G1186 G1187 U1188 C1196 G1197 U1198 A1204 C1211 G1212 A1213 A1214 G1223 G1227 G1235 G1236 A1237 G1250 C1251 G1252 A1253 A1254 U1255 G1256 U1263 A1264 A1265 G1266 C1270
G1271 A1272 U1273 G1288 G1296 G1300 A1301 G1310 U1313 C1314 U1325 U1326 A1327 A1328 G1338 G1339 U1340 G1341 C1345 U1352 A1353 C1363 G1364 A1365 G1368 A1378 U1379 A1383 A1384 A1385 C1386 A1393 U1394 A1395 U1396 U1405 G1410 U1411 U1412 A1413 G1416 C1417
A1420 G1421 A1427 C1428 A1434 C1437 G1441 U1442 U1443 G1444 G1445 G1450 C1451 G1452 A1453 U1458 G1459 U1460 C1461 U1466 A1469 A1470 G1475 U1476 A1477 G1482 G1483 U1484 U1485 U1486 A1490 G1491 A1494 A1508 A1509 G1510 G1511 C1512 U1513 G1514 A1515 G1516 G1521 A1522 U1523 G1524
G1527 A1528 G1529 G1530 C1531 A1532 C1533 U1534 A1535 C1536 G1537 G1538 U1539 G1540 G1543 A1544 A1545 G1546 C1547 A1548 A1549 C1558 U1559 G1560 U1563 C1564 C1565 A1566 A1569 U1578 A1583 U1584 C1585 A1586 G1587 A1593 U1594 C1604 C1607 A1608 A1609 A1610 A1614 G1622 G1631 A1632 G1633
A1634 A1635 U1636 A1637 G1645 C1646 U1647 U1648 G1649 A1654 G1667 A1668 A1669 C1670 G1674 C1675 A1676 A1677 G1682 U1683 U1693 C1694 A1698 A1713 U1714 G1715 U1716 U1720 G1721 C1728 U1729 C1730 G1738 A1739 A1744 A1745 A1746 U1747 U1758 C1764 A1773 C1774 U1775 G1776



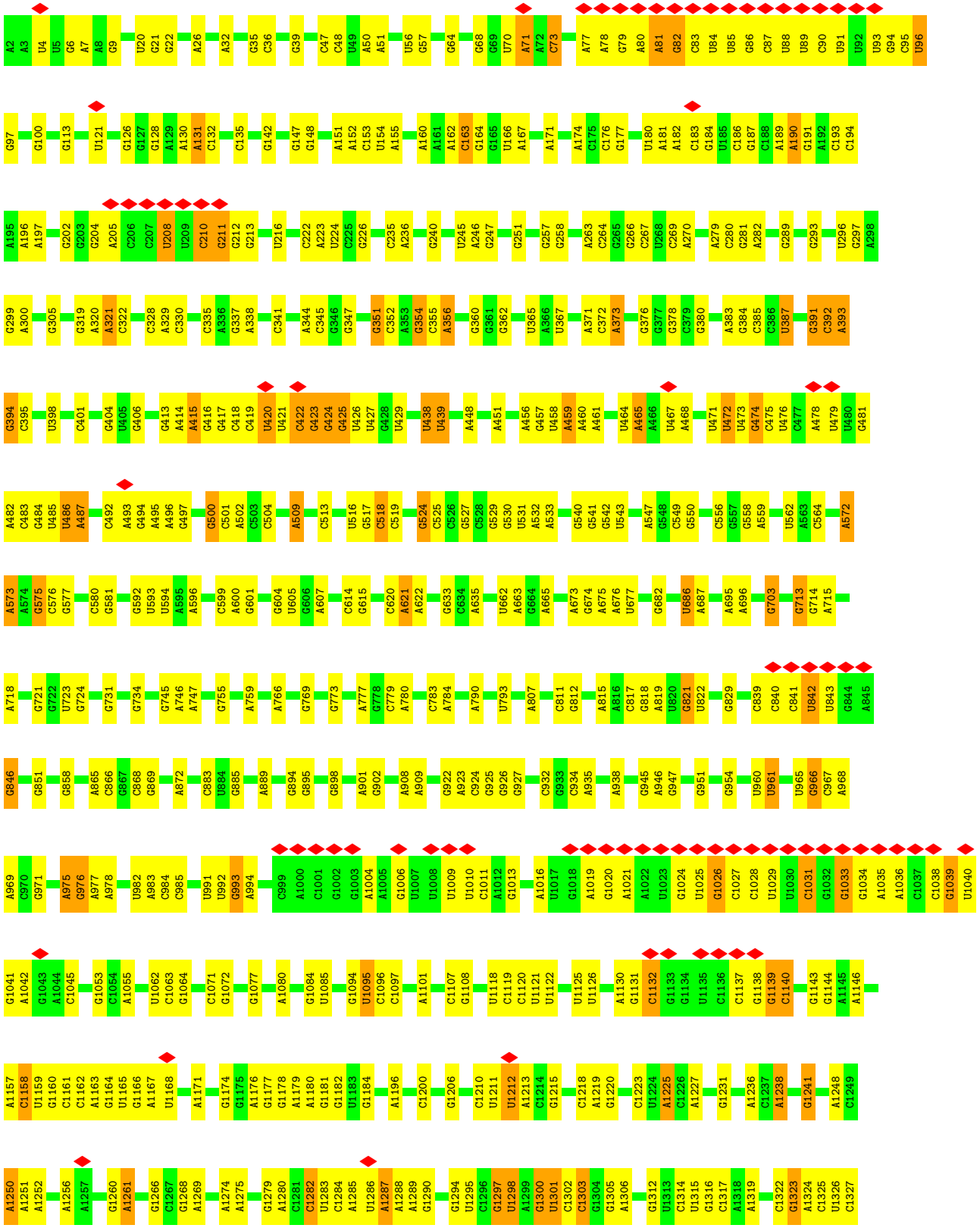
• Molecule 33: 5S ribosomal RNA

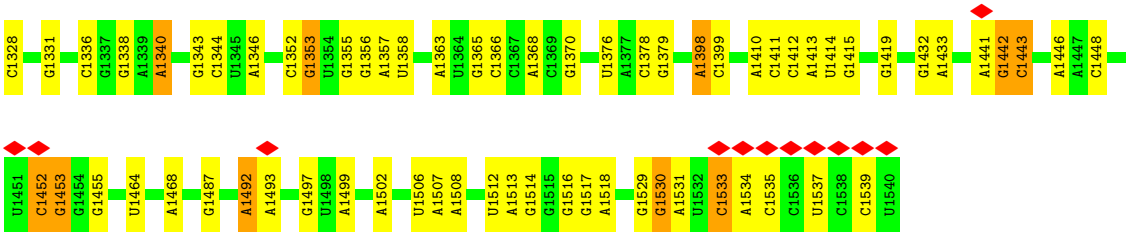
Chain R2:



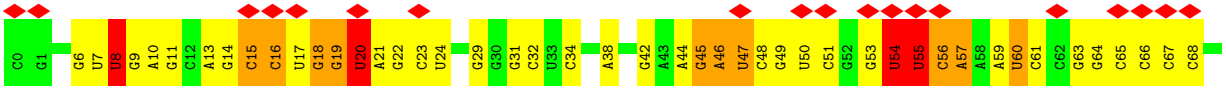
• Molecule 34: 16S ribosomal RNA

Chain R3:

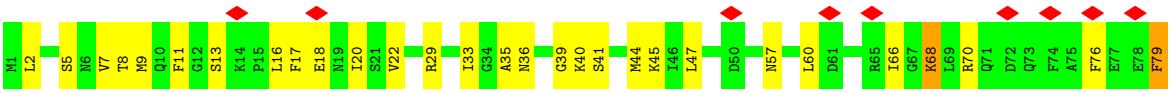


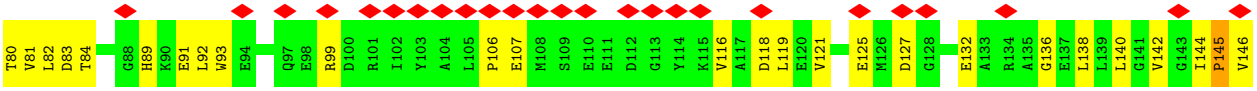


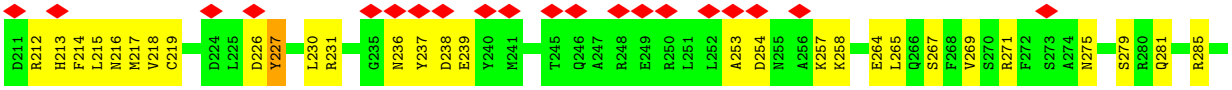
• Molecule 35: tRNA

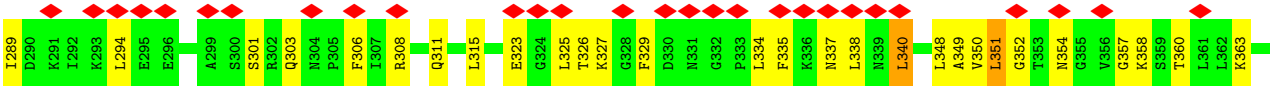


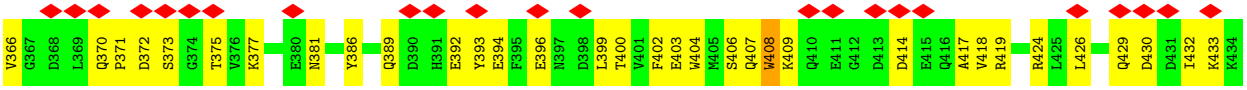
• Molecule 36: Probable ATP-binding protein YbiT

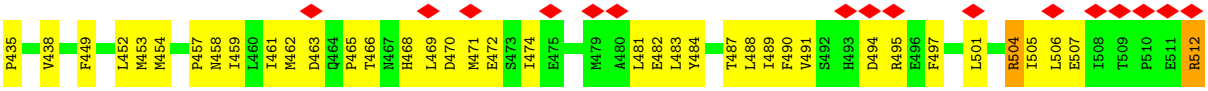


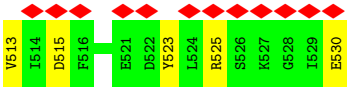






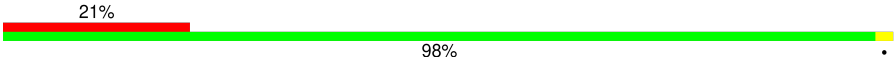


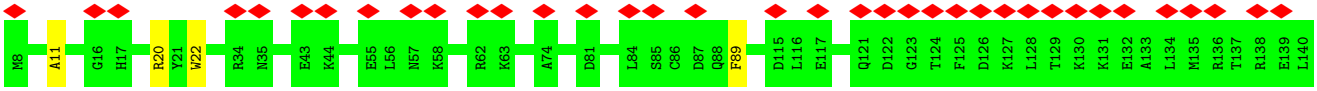


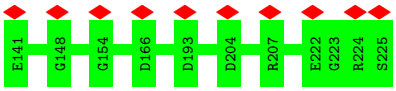


• Molecule 37: Small ribosomal subunit protein uS2

Chain sb:

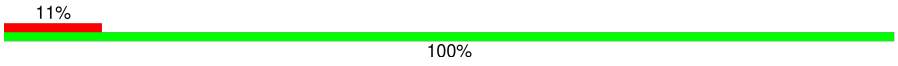


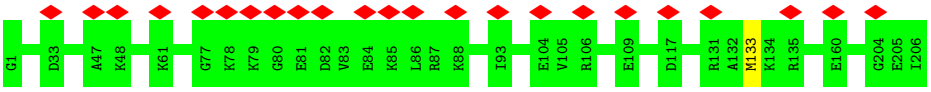




• Molecule 38: Small ribosomal subunit protein uS3

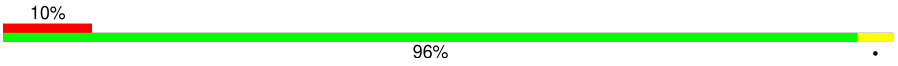
Chain sc:

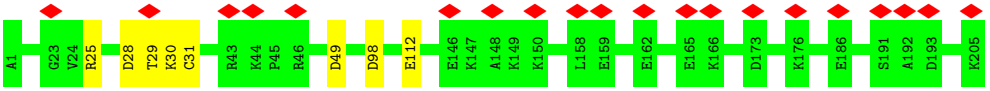




• Molecule 39: 30S ribosomal protein S4

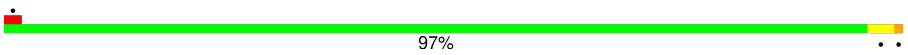
Chain sd:

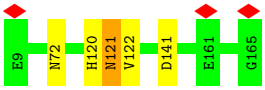




• Molecule 40: Small ribosomal subunit protein uS5

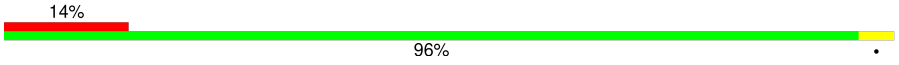
Chain se:

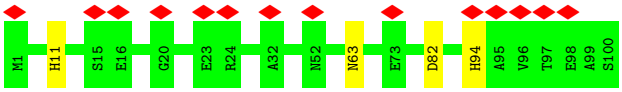




• Molecule 41: 30S ribosomal protein S6, non-modified isoform

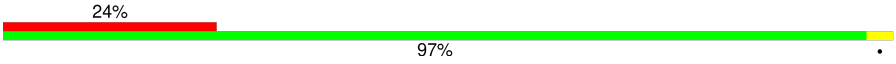
Chain sf:

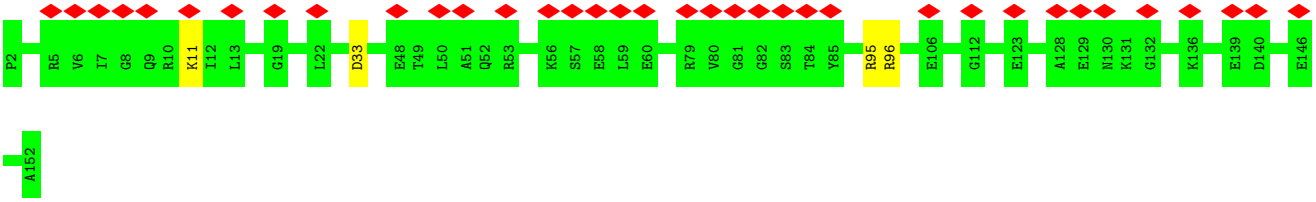




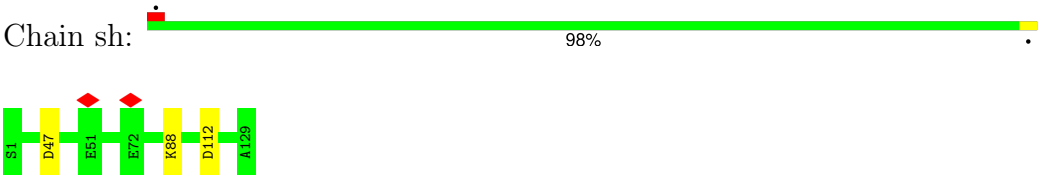
• Molecule 42: 30S ribosomal protein S7

Chain sg:

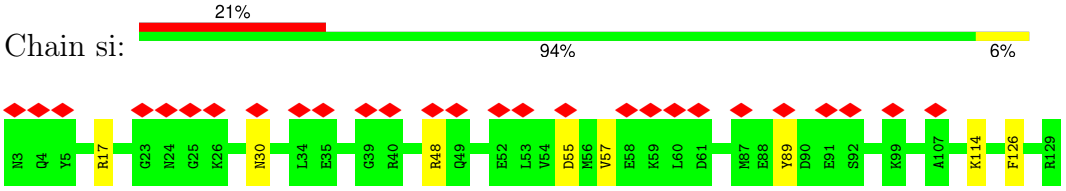




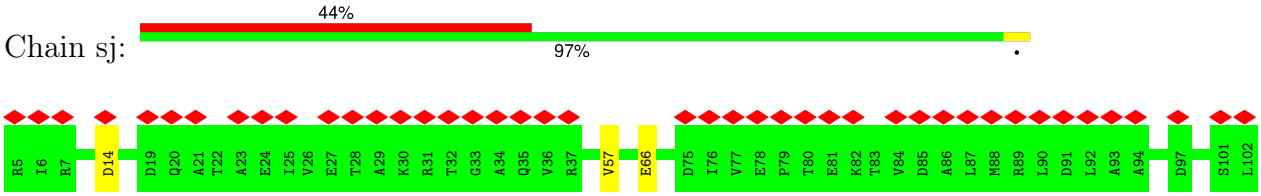
• Molecule 43: 30S ribosomal protein S8



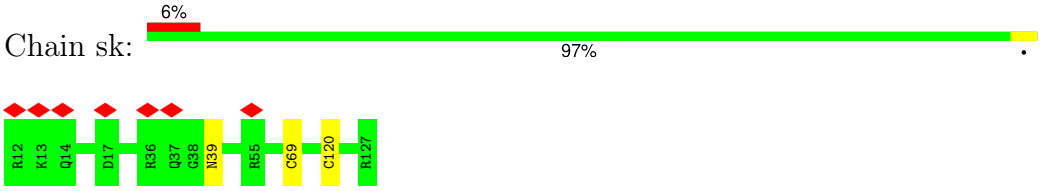
• Molecule 44: Small ribosomal subunit protein uS9



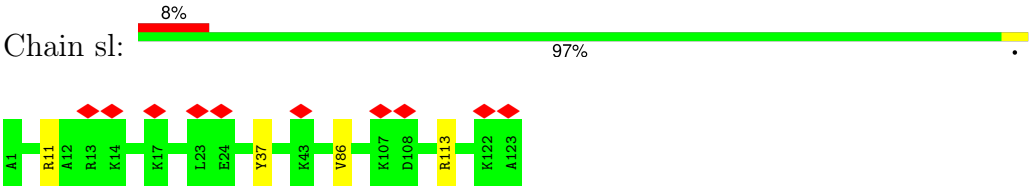
• Molecule 45: 30S ribosomal protein S10



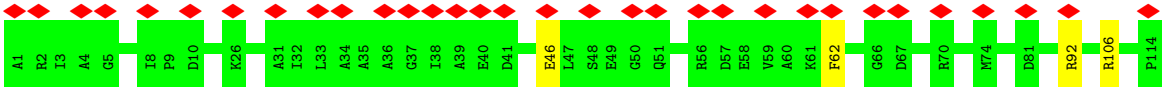
• Molecule 46: Small ribosomal subunit protein uS11



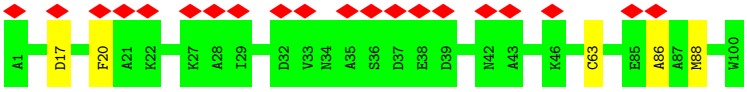
• Molecule 47: Small ribosomal subunit protein uS12



• Molecule 48: 30S ribosomal protein S13

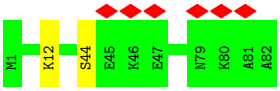


• Molecule 49: Small ribosomal subunit protein uS14

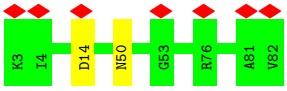


• Molecule 50: Small ribosomal subunit protein uS15

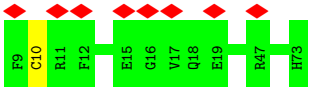
• Molecule 51: Small ribosomal subunit protein bS16



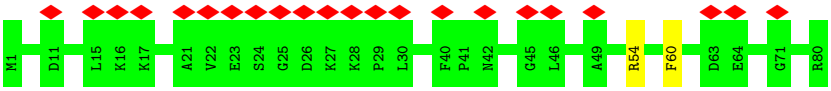
• Molecule 52: Small ribosomal subunit protein uS17



• Molecule 53: 30S ribosomal protein S18

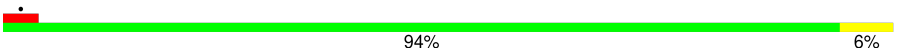


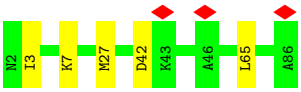
• Molecule 54: Small ribosomal subunit protein uS19



• Molecule 55: 30S ribosomal protein S20

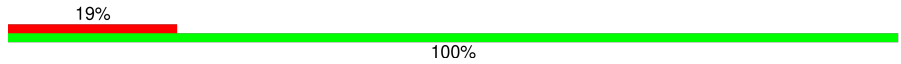
Chain st:

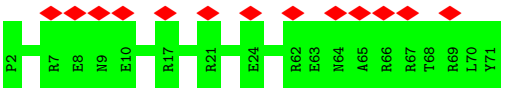




• Molecule 56: Small ribosomal subunit protein bS21

Chain su:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	34210	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 ($e^-/Å^2$)	56.8	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	5.343	Depositor
Minimum map value	-3.544	Depositor
Average map value	0.018	Depositor
Map value standard deviation	0.230	Depositor
Recommended contour level	0.85	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, 4SU, NA, H2U, MG, FME, PSU, 5MU, 4OC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	1	0.27	0/1361	0.51	0/1796
2	13	0.47	0/1152	0.55	0/1551
3	14	0.43	0/947	0.61	0/1268
4	15	0.42	0/1062	0.60	0/1413
5	16	0.42	0/1093	0.62	0/1460
6	17	0.43	0/973	0.61	0/1301
7	18	0.35	0/902	0.57	0/1209
8	19	0.46	0/929	0.57	0/1242
9	2	0.46	0/2121	0.60	0/2852
10	20	0.52	0/960	0.55	0/1278
11	21	0.45	0/829	0.55	0/1107
12	22	0.42	0/864	0.55	0/1156
13	23	0.39	0/744	0.55	0/994
14	24	0.38	0/787	0.54	0/1051
15	25	0.38	0/766	0.51	0/1025
16	27	0.45	0/582	0.60	0/769
17	28	0.41	0/635	0.58	0/848
18	29	0.34	0/510	0.58	0/677
19	3	0.46	0/1586	0.58	0/2134
20	30	0.38	0/453	0.63	0/605
21	31	0.27	0/531	0.52	0/709
22	32	0.43	0/450	0.59	0/599
23	33	0.38	0/416	0.53	0/554
24	34	0.45	0/380	0.67	0/498
25	35	0.43	0/513	0.56	0/676
26	36	0.41	0/303	0.56	0/397
27	4	0.40	0/1571	0.54	0/2113
28	5	0.31	0/1434	0.55	0/1926
29	6	0.35	0/1343	0.57	0/1816
30	9	0.48	1/1122 (0.1%)	0.71	3/1515 (0.2%)
31	M	0.43	0/219	0.70	0/339
32	R1	0.84	1/69796 (0.0%)	0.85	16/108886 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	R2	0.62	0/2847	0.86	2/4440 (0.0%)
34	R3	0.63	0/36961	0.82	4/57654 (0.0%)
35	T	0.41	0/1716	0.77	0/2672
36	Y	0.38	2/4285 (0.0%)	0.70	4/5774 (0.1%)
37	sb	0.30	0/1735	0.50	0/2338
38	sc	0.31	0/1651	0.55	0/2225
39	sd	0.35	0/1665	0.60	2/2227 (0.1%)
40	se	0.37	0/1169	0.60	1/1573 (0.1%)
41	sf	0.37	0/835	0.57	0/1128
42	sg	0.28	0/1195	0.52	0/1602
43	sh	0.36	0/989	0.51	0/1326
44	si	0.32	0/1034	0.63	0/1375
45	sj	0.30	0/796	0.59	0/1077
46	sk	0.34	0/885	0.57	0/1195
47	sl	0.38	0/969	0.62	0/1300
48	sm	0.28	0/892	0.59	0/1193
49	sn	0.31	0/817	0.58	0/1088
50	so	0.32	0/722	0.58	0/964
51	sp	0.36	0/659	0.57	0/884
52	sq	0.36	0/657	0.61	1/881 (0.1%)
53	sr	0.35	0/544	0.58	0/731
54	ss	0.28	0/660	0.53	0/887
55	st	0.31	0/671	0.55	1/888 (0.1%)
56	su	0.34	0/598	0.61	0/792
All	All	0.67	4/162286 (0.0%)	0.78	34/241978 (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
30	9	0	2
35	T	9	0
39	sd	0	1
40	se	0	2
41	sf	0	1
47	sl	0	1
49	sn	0	1
All	All	9	8

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	Y	152	PRO	CB-CG	-12.05	0.89	1.50
30	9	118	PRO	CG-CD	-10.34	1.16	1.50
32	R1	1142	A	N9-C4	-5.25	1.34	1.37
36	Y	152	PRO	CG-CD	-5.15	1.33	1.50

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	Y	152	PRO	CB-CG-CD	18.82	179.88	106.50
36	Y	152	PRO	N-CD-CG	-17.73	76.60	103.20
36	Y	152	PRO	CA-CB-CG	-15.85	73.88	104.00
30	9	118	PRO	N-CD-CG	-12.38	84.64	103.20
32	R1	1314	C	C2-N1-C1'	6.63	126.09	118.80
32	R1	12	U	C2-N1-C1'	6.60	125.62	117.70
39	sd	49	ASP	CB-CG-OD2	6.45	124.10	118.30
32	R1	1313	U	C2-N1-C1'	6.40	125.38	117.70
30	9	118	PRO	CA-CB-CG	-6.27	92.09	104.00
52	sq	14	ASP	CB-CG-OD1	5.98	123.68	118.30
55	st	42	ASP	CB-CG-OD1	5.96	123.66	118.30
36	Y	152	PRO	CA-N-CD	-5.85	103.31	111.50
34	R3	1158	C	C2-N1-C1'	5.69	125.06	118.80
30	9	118	PRO	N-CA-CB	-5.62	96.42	102.60
32	R1	2178	C	N3-C2-O2	-5.62	117.97	121.90
32	R1	2174	C	N3-C2-O2	-5.62	117.97	121.90
32	R1	12	U	N3-C2-O2	-5.59	118.29	122.20
33	R2	12	C	N1-C2-O2	5.50	122.20	118.90
40	se	141	ASP	CB-CG-OD1	5.43	123.19	118.30
32	R1	2550	G	N3-C4-N9	5.39	129.23	126.00
32	R1	2177	C	C6-N1-C2	-5.37	118.15	120.30
34	R3	1443	C	C2-N1-C1'	5.34	124.67	118.80
39	sd	98	ASP	CB-CG-OD2	5.34	123.10	118.30
33	R2	12	C	C2-N1-C1'	5.29	124.62	118.80
34	R3	73	C	C2-N1-C1'	5.29	124.61	118.80
32	R1	955	U	N3-C2-O2	-5.24	118.54	122.20
32	R1	12	U	N1-C2-O2	5.18	126.43	122.80
34	R3	509	A	N7-C8-N9	5.13	116.36	113.80
32	R1	1917	U	N3-C2-O2	-5.08	118.64	122.20
32	R1	1313	U	N3-C2-O2	-5.07	118.65	122.20
32	R1	528	A	C2-N3-C4	-5.07	108.06	110.60
32	R1	1914	C	N1-C2-O2	5.07	121.94	118.90
32	R1	2164	C	N1-C2-O2	5.02	121.91	118.90
32	R1	1314	C	C6-N1-C1'	-5.01	114.79	120.80

All (9) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
35	T	8	4SU	C2',C1'
35	T	20	H2U	C2'
35	T	32	4OC	C2'
35	T	54	5MU	C4',C3',C2'
35	T	55	PSU	C4',C2'

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	9	7	ASP	Peptide
30	9	8	LYS	Peptide
39	sd	29	THR	Peptide
40	se	120	HIS	Peptide
40	se	121	ASN	Peptide
41	sf	94	HIS	Peptide
47	sl	86	VAL	Peptide
49	sn	86	ALA	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1353	0	1159	34	0
2	13	1129	0	1162	26	0
3	14	938	0	1012	15	0
4	15	1053	0	1129	25	0
5	16	1074	0	1157	17	0
6	17	960	0	1000	14	0
7	18	892	0	923	24	0
8	19	917	0	965	20	0
9	2	2082	0	2157	46	0
10	20	947	0	1022	16	0
11	21	816	0	839	16	0
12	22	857	0	922	21	0
13	23	738	0	807	12	0
14	24	779	0	834	11	0
15	25	753	0	780	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	27	575	0	592	13	0
17	28	625	0	655	4	0
18	29	509	0	543	8	0
19	3	1565	0	1616	28	0
20	30	449	0	491	10	0
21	31	522	0	524	15	0
22	32	444	0	461	13	0
23	33	409	0	440	11	0
24	34	377	0	418	8	0
25	35	504	0	574	9	0
26	36	302	0	343	7	0
27	4	1552	0	1619	26	0
28	5	1410	0	1447	35	0
29	6	1323	0	1374	23	0
30	9	1111	0	1148	33	0
31	M	195	0	99	0	0
32	R1	62318	0	31345	548	0
33	R2	2546	0	1292	26	0
34	R3	33012	0	16619	290	0
35	T	1639	0	843	25	0
36	Y	4210	0	4176	166	0
37	sb	1704	0	1732	0	0
38	sc	1624	0	1699	0	0
39	sd	1643	0	1710	0	0
40	se	1156	0	1199	0	0
41	sf	817	0	808	0	0
42	sg	1181	0	1238	0	0
43	sh	979	0	1034	0	0
44	si	1022	0	1070	0	0
45	sj	786	0	828	0	0
46	sk	869	0	878	0	0
47	sl	955	0	1019	0	0
48	sm	883	0	944	0	0
49	sn	805	0	847	0	0
50	so	714	0	737	0	0
51	sp	649	0	666	0	0
52	sq	648	0	691	0	0
53	sr	535	0	552	0	0
54	ss	645	0	677	0	0
55	st	665	0	714	0	0
56	su	590	0	629	0	0
57	17	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	32	1	0	0	0	0
57	4	1	0	0	0	0
57	R1	179	0	0	0	0
57	R3	68	0	0	0	0
58	T	10	0	10	0	0
59	Y	62	0	24	5	0
60	Y	2	0	0	0	0
All	All	150079	0	102193	1466	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (1466) 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)
20:30:2:LYS:NZ	20:30:58:GLU:OE2	1.94	0.99
36:Y:306:PHE:HD2	36:Y:424:ARG:HD2	1.28	0.98
32:R1:1847:G:HO2'	32:R1:1848:A:H8	1.03	0.94
2:13:96:ARG:NH2	32:R1:2639:A:O3'	2.01	0.93
36:Y:215:LEU:O	36:Y:219:CYS:HB2	1.70	0.92
32:R1:306:U:H3	32:R1:310:A:H62	1.23	0.87
32:R1:284:U:H3	32:R1:356:G:H1	0.86	0.86
7:18:33:ARG:NH2	33:R2:52:A:N7	2.23	0.85
36:Y:481:LEU:HD21	36:Y:488:LEU:HD22	1.56	0.85
19:3:11:MET:CE	32:R1:2682:A:C8	2.61	0.83
4:15:76:GLU:OE2	32:R1:636:G:N2	2.10	0.83
28:5:104:THR:HG23	28:5:105:ILE:HG23	1.62	0.82
19:3:11:MET:HE2	32:R1:2682:A:C8	2.16	0.80
19:3:133:THR:HG22	19:3:134:HIS:H	1.47	0.80
32:R1:2124:G:N2	32:R1:2175:C:O2	2.15	0.80
34:R3:1139:G:H4'	34:R3:1140:C:H5'	1.63	0.79
36:Y:311:GLN:HE21	36:Y:458:ASN:HB2	1.49	0.78
16:27:43:THR:HG21	32:R1:2336:A:H61	1.49	0.78
19:3:59:ARG:NH1	32:R1:2831:G:OP2	2.15	0.78
34:R3:509:A:H8	34:R3:543:U:HO2'	1.30	0.77
9:2:269:ARG:NH2	32:R1:1799:G:OP2	2.18	0.77
34:R3:673:A:H2'	34:R3:674:G:C8	2.20	0.76
34:R3:687:A:N6	34:R3:703:G:O2'	2.19	0.76
34:R3:1040:U:H2'	34:R3:1041:G:H8	1.51	0.75
29:6:21:GLN:NE2	29:6:40:VAL:O	2.19	0.75
34:R3:417:G:N2	34:R3:426:U:O2	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:15:51:GLU:OE2	4:15:56:PRO:HA	1.87	0.74
15:25:32:GLY:HA3	15:25:93:ARG:HB2	1.69	0.74
5:16:123:LYS:NZ	32:R1:2483:C:N3	2.35	0.74
24:34:19:ARG:NH1	32:R1:125:A:OP2	2.19	0.74
11:21:80:ARG:NH2	32:R1:572:A:OP2	2.20	0.74
36:Y:11:PHE:HD2	59:Y:601:ATP:C4	2.05	0.74
1:1:31:LYS:NZ	1:1:178:VAL:O	2.22	0.73
32:R1:1070:A:OP2	32:R1:1075:C:N4	2.17	0.73
19:3:11:MET:HE1	32:R1:2682:A:C8	2.24	0.73
9:2:5:CYS:SG	9:2:12:ARG:NH2	2.61	0.73
36:Y:306:PHE:CD2	36:Y:424:ARG:HD2	2.19	0.73
2:13:128:ASN:O	2:13:128:ASN:ND2	2.21	0.73
32:R1:848:C:H2'	32:R1:849:A:H8	1.54	0.72
8:19:43:GLU:OE2	8:19:86:LYS:NZ	2.22	0.72
32:R1:1450:G:N2	32:R1:1452:G:O6	2.18	0.72
36:Y:35:ALA:O	36:Y:40:LYS:NZ	2.19	0.71
34:R3:790:A:OP1	35:T:38:A:O2'	2.08	0.71
7:18:61:GLN:N	7:18:61:GLN:OE1	2.24	0.71
21:31:44:PHE:HD1	21:31:45:THR:HG23	1.56	0.71
7:18:24:THR:HG22	7:18:42:PRO:HD3	1.73	0.71
8:19:55:HIS:HA	19:3:13:ARG:HH21	1.56	0.70
32:R1:285:G:H1	32:R1:355:U:H3	1.39	0.70
16:27:42:GLY:HA2	32:R1:2330:G:H21	1.56	0.70
2:13:17:VAL:HG23	2:13:137:PRO:HB2	1.72	0.70
32:R1:1437:C:HO2'	32:R1:1516:G:HO2'	1.34	0.70
36:Y:352:GLY:HA3	36:Y:358:LYS:HB2	1.73	0.70
32:R1:1073:A:N6	32:R1:1074:G:O6	2.25	0.70
9:2:216:ARG:NH2	32:R1:781:A:OP1	2.25	0.70
27:4:48:THR:HG23	27:4:50:ALA:H	1.55	0.70
10:20:49:ARG:O	10:20:53:LYS:NZ	2.25	0.69
28:5:70:ARG:NH1	32:R1:2298:A:OP1	2.23	0.69
28:5:132:ARG:HE	32:R1:2305:U:H4'	1.57	0.69
32:R1:1044:C:O2'	32:R1:1111:A:N6	2.23	0.69
12:22:5:ALA:HB2	12:22:54:ALA:HB2	1.74	0.69
19:3:11:MET:HE1	32:R1:2682:A:N7	2.08	0.69
32:R1:2123:G:N2	32:R1:2124:G:O6	2.25	0.69
36:Y:132:GLU:O	36:Y:136:GLY:N	2.26	0.69
32:R1:2303:G:H2'	32:R1:2304:G:H8	1.57	0.69
32:R1:843:G:C2	32:R1:936:A:C2	2.80	0.69
36:Y:236:ASN:H	36:Y:239:GLU:HB2	1.58	0.69
34:R3:1261:A:N6	34:R3:1274:A:O2'	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:T:54:5MU:H4'	35:T:55:PSU:OP2	1.93	0.68
32:R1:1936:A:H2	32:R1:1943:U:H3	1.40	0.68
32:R1:2115:G:N3	32:R1:2117:A:N6	2.41	0.68
2:13:39:LYS:NZ	32:R1:1007:C:OP1	2.26	0.68
7:18:102:ARG:HG2	33:R2:49:C:OP1	1.94	0.68
29:6:34:ARG:HD3	29:6:70:LEU:HD21	1.76	0.68
10:20:25:GLY:O	10:20:29:ARG:NH1	2.25	0.68
11:21:46:GLU:N	11:21:46:GLU:OE1	2.27	0.68
1:1:59:VAL:H	1:1:165:ASN:HD21	1.40	0.68
32:R1:827:U:O2'	32:R1:2068:U:N3	2.25	0.68
36:Y:99:ARG:HG3	36:Y:119:LEU:HD12	1.75	0.68
9:2:179:GLU:OE2	9:2:269:ARG:NH1	2.26	0.67
29:6:22:VAL:HG22	29:6:35:THR:HG22	1.76	0.67
32:R1:141:G:N2	32:R1:141:G:OP2	2.27	0.67
24:34:41:ARG:HB3	24:34:41:ARG:CZ	2.24	0.67
21:31:59:ARG:HA	21:31:62:LYS:HD3	1.76	0.67
4:15:41:ARG:NH2	32:R1:807:U:OP2	2.28	0.67
27:4:111:GLU:HG3	27:4:115:GLN:HE21	1.60	0.67
33:R2:5:U:OP1	33:R2:61:G:O2'	2.10	0.67
30:9:5:LEU:HD21	30:9:12:LEU:HD12	1.76	0.67
34:R3:1125:U:H2'	34:R3:1126:U:H2'	1.76	0.67
34:R3:1040:U:H2'	34:R3:1041:G:C8	2.30	0.66
15:25:30:ILE:HG22	15:25:91:PHE:HB2	1.76	0.66
32:R1:219:A:N3	32:R1:234:U:O2'	2.22	0.66
32:R1:1466:U:HO2'	32:R1:1546:G:HO2'	1.24	0.66
32:R1:704:G:O2'	32:R1:727:A:N6	2.29	0.66
36:Y:303:GLN:O	36:Y:472:GLU:HG2	1.96	0.66
36:Y:404:TRP:O	36:Y:407:GLN:OE1	2.14	0.66
25:35:7:ARG:NH1	32:R1:243:U:OP2	2.29	0.66
30:9:99:ILE:O	30:9:103:VAL:HG23	1.96	0.66
32:R1:1270:C:H5"	32:R1:1271:G:H5'	1.78	0.66
34:R3:419:C:O2	34:R3:425:G:N2	2.29	0.66
11:21:6:GLN:HB2	11:21:11:GLN:HG2	1.76	0.65
34:R3:78:A:H62	34:R3:79:G:H21	1.43	0.65
34:R3:1013:G:N2	34:R3:1016:A:OP2	2.29	0.65
32:R1:1087:G:H22	32:R1:1102:C:H42	1.43	0.65
1:1:38:PHE:HB3	1:1:40:GLU:HG3	1.77	0.65
19:3:45:TYR:HH	32:R1:2636:C:HO2'	1.41	0.65
36:Y:142:VAL:HG21	36:Y:167:ALA:HB2	1.79	0.65
16:27:37:ILE:HG22	16:27:38:VAL:HG23	1.76	0.65
34:R3:1316:G:N2	34:R3:1319:A:OP2	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:22:4:ILE:H	12:22:4:ILE:HD12	1.62	0.65
14:24:85:ARG:NH2	14:24:99:SER:O	2.26	0.65
22:32:15:ARG:NH1	32:R1:1266:G:OP2	2.30	0.65
32:R1:2156:G:O6	32:R1:2157:G:N2	2.28	0.65
1:1:58:ASN:ND2	36:Y:125:GLU:OE1	2.30	0.65
3:14:31:ARG:NH1	32:R1:1996:C:OP1	2.30	0.65
32:R1:1236:G:O2'	32:R1:1237:A:O5'	2.14	0.65
3:14:70:ARG:NH1	32:R1:2684:U:O4'	2.29	0.65
32:R1:880:G:H2'	32:R1:881:G:H8	1.61	0.65
34:R3:674:G:H2'	34:R3:675:A:H8	1.62	0.64
32:R1:1527:G:N1	32:R1:1544:A:OP2	2.30	0.64
9:2:144:GLU:HB2	9:2:187:CYS:HB3	1.79	0.64
28:5:59:ILE:O	28:5:101:ARG:NH2	2.30	0.64
1:1:8:MET:CE	32:R1:2175:C:H5'	2.28	0.64
36:Y:33:ILE:HD12	36:Y:237:TYR:HE1	1.62	0.64
9:2:257:ARG:NH1	9:2:263:ASP:OD2	2.31	0.64
36:Y:213:HIS:O	36:Y:217:MET:HG2	1.98	0.64
18:29:3:ALA:HA	18:29:6:LEU:HD12	1.79	0.64
20:30:40:THR:HG22	20:30:42:ALA:H	1.61	0.64
36:Y:8:THR:HA	36:Y:18:GLU:HA	1.79	0.64
15:25:69:GLU:OE2	15:25:71:LYS:NZ	2.26	0.64
36:Y:470:ASP:OD1	36:Y:470:ASP:N	2.30	0.64
30:9:9:VAL:HB	30:9:12:LEU:O	1.98	0.64
1:1:168:ASN:ND2	32:R1:2178:C:O2'	2.31	0.63
28:5:61:GLY:O	28:5:94:ARG:NH2	2.31	0.63
32:R1:1085:A:H2'	32:R1:1086:A:N3	2.14	0.63
32:R1:1171:G:H1'	32:R1:1179:G:H22	1.62	0.63
36:Y:184:ASN:O	36:Y:185:ASN:ND2	2.31	0.63
1:1:12:ARG:NH2	32:R1:2107:G:OP1	2.32	0.63
25:35:8:GLY:O	25:35:12:ARG:NH1	2.31	0.63
32:R1:1086:A:H5"	32:R1:1087:G:H5'	1.80	0.63
35:T:56:C:N3	36:Y:419:ARG:NH2	2.47	0.63
32:R1:227:A:O2'	32:R1:228:C:O5'	2.16	0.63
6:17:53:THR:HG21	32:R1:2840:C:H5"	1.80	0.63
28:5:51:ASN:OD1	28:5:149:ARG:NH2	2.32	0.63
29:6:116:LEU:HD13	29:6:120:ILE:HG22	1.80	0.63
34:R3:415:A:H2'	34:R3:416:G:H8	1.64	0.63
34:R3:811:C:O2'	34:R3:901:A:N1	2.32	0.63
34:R3:1323:G:H2'	34:R3:1324:A:C8	2.34	0.63
27:4:152:GLU:OE1	27:4:152:GLU:N	2.32	0.62
34:R3:516:U:HO2'	34:R3:519:C:H5	1.45	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:R1:1721:G:O2'	32:R1:1739:A:N6	2.32	0.62
32:R1:1521:G:H3'	32:R1:1522:A:H5"	1.80	0.62
36:Y:407:GLN:OE1	36:Y:407:GLN:N	2.32	0.62
17:28:2:ARG:NH1	32:R1:1365:A:OP1	2.31	0.62
28:5:79:ARG:H	28:5:82:TYR:HD2	1.47	0.62
15:25:42:LEU:HD13	15:25:47:VAL:HG21	1.81	0.62
19:3:10:GLY:H	19:3:197:THR:HG23	1.65	0.62
34:R3:991:U:O4	34:R3:1212:U:O2'	2.16	0.62
13:23:11:LEU:O	18:29:29:ARG:NH1	2.32	0.62
34:R3:427:U:O2'	34:R3:541:G:OP1	2.16	0.62
36:Y:147:GLU:N	36:Y:147:GLU:OE2	2.33	0.62
9:2:71:ASP:OD1	9:2:188:ARG:NH2	2.32	0.62
32:R1:2508:G:H1	32:R1:2580:U:H5	1.46	0.62
34:R3:1218:C:H2'	34:R3:1219:A:C8	2.35	0.62
12:22:59:GLU:HA	12:22:64:ALA:HA	1.82	0.61
36:Y:325:LEU:HA	36:Y:373:SER:HB3	1.81	0.61
3:14:17:ARG:HH12	3:14:47:ILE:HG23	1.65	0.61
34:R3:416:G:H2'	34:R3:417:G:C8	2.35	0.61
36:Y:281:GLN:O	36:Y:285:ARG:NH1	2.33	0.61
1:1:60:ARG:HD3	1:1:164:ARG:HB3	1.82	0.61
32:R1:2124:G:H2'	32:R1:2125:G:O4'	2.00	0.61
34:R3:620:C:HO2'	34:R3:621:A:H8	1.49	0.61
30:9:133:GLN:HE22	30:9:139:PHE:HE1	1.47	0.61
36:Y:179:LEU:HD21	36:Y:207:ILE:HG12	1.83	0.61
21:31:16:CYS:HB3	21:31:20:ASN:HB2	1.81	0.61
32:R1:1509:A:H2'	32:R1:1510:G:H8	1.65	0.61
34:R3:80:A:H2'	34:R3:81:A:H4'	1.83	0.61
12:22:34:ASP:OD2	22:32:36:LYS:NZ	2.27	0.61
32:R1:370:G:O2'	32:R1:424:G:OP1	2.14	0.61
32:R1:1536:C:O2'	32:R1:1537:G:N2	2.34	0.61
32:R1:284:U:O4	32:R1:356:G:O6	2.19	0.61
32:R1:1779:U:H5	32:R1:1784:A:N7	1.98	0.61
32:R1:2328:A:H2'	32:R1:2329:U:C6	2.35	0.61
6:17:22:ARG:HG3	6:17:70:THR:HA	1.83	0.61
34:R3:494:G:H2'	34:R3:496:A:H8	1.66	0.61
34:R3:1356:G:H2'	34:R3:1357:A:C8	2.36	0.61
32:R1:1509:A:H2'	32:R1:1510:G:C8	2.36	0.61
36:Y:466:THR:HA	36:Y:469:LEU:HD12	1.83	0.61
23:33:34:GLU:OE1	23:33:49:LYS:HG3	2.00	0.60
32:R1:1645:G:H5"	32:R1:1646:C:H5'	1.83	0.60
32:R1:2103:C:H2'	32:R1:2104:C:H6	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:9:104:THR:HG22	30:9:110:VAL:H	1.66	0.60
19:3:151:THR:OG1	32:R1:2032:G:N2	2.35	0.60
20:30:10:ARG:HB2	20:30:53:MET:HB2	1.83	0.60
26:36:3:VAL:HG21	32:R1:2539:C:H5'	1.84	0.60
32:R1:1363:C:O2'	32:R1:1809:A:N3	2.32	0.60
36:Y:406:SER:HB3	36:Y:409:LYS:HE2	1.83	0.60
32:R1:700:G:O2'	32:R1:1632:A:N3	2.27	0.60
32:R1:2258:C:O2'	32:R1:2427:C:OP2	2.19	0.60
34:R3:908:A:H2'	34:R3:909:A:H8	1.66	0.60
36:Y:457:PRO:O	36:Y:484:TYR:OH	2.19	0.60
2:13:125:TYR:OH	2:13:132:HIS:NE2	2.29	0.60
24:34:24:THR:HG23	24:34:27:GLY:H	1.65	0.60
32:R1:1607:C:N4	32:R1:1622:G:OP2	2.35	0.60
5:16:20:LEU:HD22	15:25:81:PRO:HG2	1.84	0.59
32:R1:2120:G:H2'	32:R1:2121:G:C8	2.37	0.59
36:Y:254:ASP:OD1	36:Y:258:LYS:NZ	2.32	0.59
19:3:46:ARG:NH2	19:3:88:GLU:O	2.35	0.59
4:15:110:VAL:HB	4:15:127:VAL:HG12	1.84	0.59
12:22:4:ILE:HG13	12:22:106:VAL:HG22	1.84	0.59
15:25:77:VAL:HG12	15:25:89:ILE:HG12	1.85	0.59
1:1:211:LYS:HE3	1:1:223:ALA:HB2	1.84	0.59
35:T:7:U:O2'	35:T:21:A:N1	2.34	0.59
25:35:14:LYS:HB2	25:35:22:LYS:HE2	1.83	0.59
32:R1:976:G:HO2'	32:R1:1155:A:HO2'	1.50	0.59
32:R1:2303:G:H2'	32:R1:2304:G:C8	2.37	0.59
32:R1:2682:A:H61	32:R1:2728:U:H1'	1.67	0.59
5:16:51:ARG:NH1	32:R1:2483:C:O2'	2.35	0.59
27:4:111:GLU:O	27:4:115:GLN:HG3	2.02	0.59
32:R1:1236:G:HO2'	32:R1:1237:A:P	2.26	0.59
32:R1:2848:G:O2'	32:R1:2868:A:N6	2.36	0.59
34:R3:978:A:O2'	34:R3:1322:C:N3	2.35	0.59
32:R1:481:G:O2'	32:R1:506:G:N2	2.36	0.59
32:R1:2006:C:O2'	32:R1:2823:A:N3	2.36	0.59
32:R1:2107:G:H2'	32:R1:2108:A:H8	1.68	0.59
3:14:70:ARG:NH2	32:R1:2683:C:O2	2.35	0.59
9:2:153:LEU:HD13	9:2:175:LEU:HD21	1.85	0.59
4:15:123:ARG:NE	4:15:143:GLU:OE1	2.36	0.58
34:R3:296:U:O2'	34:R3:556:C:O2	2.19	0.58
32:R1:2291:U:OP1	32:R1:2380:C:O2'	2.20	0.58
34:R3:620:C:O2'	34:R3:621:A:H8	1.86	0.58
35:T:47:U:O2'	35:T:50:U:OP1	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:Y:89:HIS:CD2	36:Y:92:LEU:HB3	2.38	0.58
36:Y:212:ARG:NH2	36:Y:238:ASP:OD1	2.29	0.58
34:R3:1250:A:H2'	34:R3:1251:A:C8	2.38	0.58
32:R1:306:U:H3	32:R1:310:A:N6	1.96	0.58
10:20:48:ASP:OD1	32:R1:559:G:N2	2.34	0.58
34:R3:362:G:N2	34:R3:365:U:OP2	2.35	0.58
36:Y:187:ASP:HB3	36:Y:354:ASN:ND2	2.18	0.58
23:33:22:THR:HG21	32:R1:2286:G:O6	2.03	0.58
28:5:102:LEU:HD12	28:5:106:ALA:HB3	1.86	0.58
32:R1:2705:A:O2'	32:R1:2852:G:OP1	2.19	0.58
36:Y:352:GLY:H	36:Y:358:LYS:HD3	1.69	0.58
14:24:81:ARG:NH2	32:R1:301:G:OP2	2.37	0.58
34:R3:1143:G:H2'	34:R3:1144:G:H8	1.69	0.58
8:19:105:LYS:O	8:19:108:ARG:NH1	2.34	0.58
11:21:68:ARG:NH1	32:R1:1223:G:OP1	2.37	0.58
32:R1:613:A:H4'	32:R1:614:A:C8	2.38	0.58
32:R1:891:G:HO2'	32:R1:892:A:H8	1.49	0.58
34:R3:517:G:N2	34:R3:530:G:OP1	2.34	0.58
1:1:175:ILE:O	1:1:188:ASN:ND2	2.34	0.58
3:14:21:CYS:HA	3:14:41:ILE:HG22	1.85	0.58
34:R3:77:A:H2'	34:R3:78:A:H8	1.69	0.58
34:R3:714:G:H2'	34:R3:715:A:C8	2.39	0.58
36:Y:89:HIS:HD2	36:Y:92:LEU:HB3	1.68	0.58
15:25:9:ARG:HG2	15:25:41:GLU:HB3	1.86	0.58
25:35:4:LYS:NZ	32:R1:253:C:OP2	2.34	0.58
30:9:30:LEU:HB3	30:9:36:ALA:HB3	1.86	0.58
18:29:1:MET:HB3	18:29:2:LYS:HD2	1.84	0.57
32:R1:880:G:H2'	32:R1:881:G:C8	2.39	0.57
34:R3:335:C:O2'	34:R3:1433:A:N3	2.35	0.57
34:R3:1041:G:H2'	34:R3:1042:A:C8	2.38	0.57
34:R3:1162:C:H2'	34:R3:1163:A:H8	1.67	0.57
21:31:16:CYS:SG	21:31:17:SER:N	2.77	0.57
32:R1:1009:A:N3	32:R1:1153:C:O2'	2.33	0.57
9:2:239:PHE:O	9:2:241:LYS:HG3	2.04	0.57
32:R1:288:U:H2'	32:R1:289:G:H8	1.69	0.57
14:24:6:ARG:NH2	32:R1:99:U:O2	2.37	0.57
32:R1:299:A:N3	32:R1:319:G:O2'	2.33	0.57
32:R1:2166:U:O4	32:R1:2170:A:N6	2.38	0.57
12:22:88:ARG:NH1	12:22:94:ASP:OD2	2.33	0.57
32:R1:2457:U:H5	32:R1:2494:G:H1	1.52	0.57
34:R3:458:U:H2'	34:R3:459:A:C8	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:R1:1858:A:N6	32:R1:1884:G:O2'	2.36	0.57
22:32:3:GLN:NE2	32:R1:2016:U:O2	2.36	0.57
4:15:1:MET:CE	27:4:184:ASP:HA	2.34	0.57
30:9:22:LYS:HE3	32:R1:2093:G:H5'	1.86	0.57
32:R1:1779:U:OP2	32:R1:1784:A:N6	2.38	0.57
6:17:106:ASP:OD1	6:17:106:ASP:N	2.38	0.57
34:R3:1006:G:O6	34:R3:1024:G:N2	2.35	0.57
34:R3:1323:G:H2'	34:R3:1324:A:H8	1.69	0.57
3:14:17:ARG:HH12	3:14:47:ILE:CG2	2.17	0.56
8:19:94:ALA:HB2	32:R1:2848:G:C8	2.40	0.56
23:33:5:ARG:NH1	32:R1:2285:C:OP2	2.37	0.56
12:22:49:LYS:NZ	32:R1:488:G:O2'	2.38	0.56
32:R1:2119:A:N6	32:R1:2169:A:H61	2.03	0.56
34:R3:1144:G:N2	34:R3:1146:A:H62	2.03	0.56
2:13:65:THR:OG1	32:R1:1141:U:OP2	2.22	0.56
4:15:1:MET:HE3	27:4:184:ASP:HB2	1.87	0.56
32:R1:172:A:H2'	32:R1:173:A:H8	1.71	0.56
32:R1:1048:A:OP2	32:R1:1110:G:N2	2.34	0.56
32:R1:1913:A:N7	34:R3:1492:A:O2'	2.36	0.56
34:R3:673:A:H2'	34:R3:674:G:H8	1.67	0.56
36:Y:195:GLU:HG2	36:Y:214:PHE:HD1	1.68	0.56
18:29:2:LYS:HG3	18:29:52:ARG:HD3	1.87	0.56
32:R1:1534:U:H2'	32:R1:1536:C:H1'	1.86	0.56
21:31:26:SER:OG	28:5:139:GLU:OE2	2.21	0.56
32:R1:833:A:H2'	32:R1:834:G:H8	1.70	0.56
35:T:16:C:OP2	35:T:60:U:O2'	2.23	0.56
36:Y:327:LYS:HD2	36:Y:371:PRO:HA	1.87	0.56
32:R1:2473:U:OP1	32:R1:2529:G:N2	2.39	0.56
8:19:33:GLU:OE2	8:19:38:ARG:NE	2.28	0.56
21:31:44:PHE:CD1	21:31:45:THR:HG23	2.39	0.56
30:9:73:ASN:HA	30:9:108:VAL:HG21	1.87	0.56
32:R1:2303:G:O6	32:R1:2314:A:N6	2.39	0.56
34:R3:418:C:OP1	34:R3:513:C:O2'	2.23	0.56
3:14:63:VAL:HG12	3:14:107:LEU:HD21	1.86	0.56
8:19:94:ALA:HB2	32:R1:2848:G:H8	1.69	0.56
9:2:16:VAL:HB	9:2:203:VAL:HG22	1.87	0.56
9:2:143:VAL:HB	9:2:153:LEU:HB2	1.88	0.56
11:21:48:LYS:NZ	11:21:49:ILE:H	2.04	0.56
28:5:3:LEU:HG	28:5:100:GLU:HB2	1.88	0.56
28:5:114:ARG:NE	28:5:114:ARG:O	2.37	0.56
32:R1:1:G:H2'	32:R1:2:G:H8	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:2:220:ARG:NH1	32:R1:1789:A:OP2	2.39	0.56
15:25:43:ASP:OD1	15:25:44:HIS:N	2.39	0.56
32:R1:1068:G:N2	32:R1:1096:A:OP1	2.39	0.56
34:R3:420:U:O2'	34:R3:422:C:OP1	2.19	0.56
35:T:44:A:N6	35:T:45:G:O6	2.39	0.56
36:Y:179:LEU:HD12	36:Y:182:PRO:HB3	1.87	0.56
32:R1:1061:U:O2'	32:R1:1070:A:O3'	2.21	0.55
36:Y:89:HIS:CD2	36:Y:92:LEU:H	2.25	0.55
13:23:67:VAL:HG22	13:23:76:ARG:HB3	1.88	0.55
19:3:26:VAL:HG22	19:3:188:LEU:HD22	1.87	0.55
29:6:23:ILE:HG12	29:6:71:LEU:HD21	1.87	0.55
32:R1:2141:G:H2'	32:R1:2142:A:H8	1.71	0.55
32:R1:1060:U:H3	32:R1:1088:A:H8	1.54	0.55
32:R1:2164:C:H2'	32:R1:2165:C:O4'	2.06	0.55
34:R3:420:U:O2	34:R3:424:G:N2	2.39	0.55
1:1:47:ASN:HA	1:1:170:ILE:HG22	1.88	0.55
1:1:197:LYS:HD3	1:1:208:TYR:HE2	1.71	0.55
28:5:107:VAL:HG11	28:5:175:PRO:HG2	1.88	0.55
34:R3:438:U:O2'	34:R3:439:U:O5'	2.25	0.55
36:Y:482:GLU:HG3	36:Y:483:LEU:HD22	1.88	0.55
7:18:27:VAL:HA	7:18:93:ASP:HB3	1.87	0.55
30:9:73:ASN:HB2	30:9:108:VAL:HG11	1.89	0.55
32:R1:1:G:H2'	32:R1:2:G:C8	2.42	0.55
1:1:186:LYS:O	1:1:190:GLU:HG2	2.06	0.55
9:2:229:HIS:CD2	9:2:246:PRO:HB3	2.42	0.55
16:27:56:ASP:HB3	16:27:58:THR:HG23	1.88	0.55
32:R1:1196:C:HO2'	32:R1:1227:G:HO2'	1.54	0.55
34:R3:77:A:H2'	34:R3:78:A:C8	2.41	0.55
8:19:90:ALA:HB2	8:19:112:ARG:HA	1.89	0.55
24:34:43:THR:OG1	24:34:44:VAL:N	2.38	0.55
32:R1:404:A:H1'	32:R1:406:G:C5	2.42	0.55
32:R1:2581:G:OP2	32:R1:2581:G:N2	2.35	0.55
32:R1:278:A:C6	32:R1:362:A:C8	2.95	0.55
32:R1:631:A:N3	32:R1:2415:G:O2'	2.34	0.55
32:R1:2103:C:H2'	32:R1:2104:C:C6	2.42	0.55
32:R1:2116:G:O6	32:R1:2171:A:N6	2.40	0.55
32:R1:2304:G:H22	32:R1:2312:U:H3	1.54	0.55
23:33:42:VAL:HG23	23:33:44:GLN:HG2	1.89	0.55
32:R1:286:U:H2'	32:R1:287:G:H8	1.72	0.55
34:R3:923:A:O2'	34:R3:1399:C:OP2	2.20	0.55
13:23:82:LYS:NZ	32:R1:1340:U:OP2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:34:41:ARG:HB3	24:34:41:ARG:NH1	2.22	0.54
32:R1:547:A:H4'	32:R1:548:G:C8	2.41	0.54
32:R1:2327:A:H2'	32:R1:2328:A:C8	2.42	0.54
34:R3:946:A:H2'	34:R3:947:G:C8	2.41	0.54
19:3:180:VAL:HG22	19:3:187:LEU:HD12	1.88	0.54
27:4:136:GLN:NE2	27:4:140:ASP:OD1	2.40	0.54
32:R1:1417:C:O2'	32:R1:1587:G:O2'	2.22	0.54
36:Y:41:SER:O	36:Y:45:LYS:HG2	2.07	0.54
4:15:29:LYS:O	4:15:30:THR:OG1	2.18	0.54
9:2:244:VAL:HG12	9:2:250:GLN:HA	1.89	0.54
9:2:270:ARG:NH2	32:R1:1798:U:OP2	2.31	0.54
29:6:88:LEU:HG	29:6:161:VAL:HG22	1.90	0.54
32:R1:286:U:H2'	32:R1:287:G:C8	2.42	0.54
32:R1:1528:A:OP2	32:R1:1543:G:N2	2.39	0.54
32:R1:1720:U:H2'	32:R1:1721:G:O4'	2.08	0.54
34:R3:946:A:H2'	34:R3:947:G:H8	1.72	0.54
34:R3:1071:C:H2'	34:R3:1072:G:H8	1.72	0.54
7:18:60:GLU:HG2	7:18:61:GLN:OE1	2.07	0.54
23:33:34:GLU:OE1	23:33:49:LYS:HA	2.07	0.54
33:R2:28:C:H2'	33:R2:29:A:C8	2.43	0.54
34:R3:1210:C:HO2'	34:R3:1213:A:HO2'	1.53	0.54
36:Y:76:PHE:HB3	36:Y:79:PHE:HE1	1.72	0.54
8:19:1:SER:HA	8:19:4:ILE:HB	1.87	0.54
32:R1:843:G:N1	32:R1:936:A:C6	2.76	0.54
32:R1:2246:G:H2'	32:R1:2247:A:H8	1.72	0.54
36:Y:264:GLU:O	36:Y:267:SER:OG	2.20	0.54
9:2:132:ARG:NH2	9:2:186:ASP:OD1	2.35	0.54
22:32:12:ARG:NH1	32:R1:1263:U:OP1	2.41	0.54
36:Y:8:THR:HG23	36:Y:18:GLU:HB2	1.90	0.54
11:21:49:ILE:HG12	11:21:53:PHE:O	2.08	0.54
28:5:57:ALA:HB2	28:5:64:PRO:HD3	1.89	0.54
29:6:172:GLU:HA	29:6:172:GLU:OE2	2.08	0.54
34:R3:486:U:H2'	34:R3:487:A:H8	1.73	0.54
32:R1:2135:A:H3'	32:R1:2136:G:C8	2.42	0.54
34:R3:79:G:H2'	34:R3:80:A:C5	2.43	0.54
34:R3:147:G:H2'	34:R3:148:G:C8	2.43	0.54
34:R3:415:A:H2'	34:R3:416:G:C8	2.43	0.54
7:18:117:PHE:O	32:R1:2377:A:O2'	2.25	0.54
32:R1:1064:C:N4	32:R1:1069:A:OP2	2.41	0.54
32:R1:1802:A:H2'	32:R1:1803:A:C8	2.42	0.54
6:17:2:ARG:HA	6:17:5:LYS:HE2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:R1:139:U:H2'	32:R1:140:C:H5	1.73	0.54
32:R1:1746:A:H2'	32:R1:1747:U:C6	2.42	0.54
32:R1:2857:G:N2	32:R1:2860:A:OP2	2.32	0.54
34:R3:380:G:N2	34:R3:383:A:OP2	2.32	0.54
6:17:4:ARG:O	32:R1:2873:A:O2'	2.26	0.53
32:R1:704:G:H2'	32:R1:726:G:H22	1.73	0.53
32:R1:1019:U:OP1	32:R1:1035:U:O2'	2.21	0.53
34:R3:674:G:H2'	34:R3:675:A:C8	2.43	0.53
2:13:32:LEU:HD22	2:13:54:ILE:HG21	1.89	0.53
8:19:89:GLY:O	8:19:112:ARG:NH1	2.42	0.53
29:6:74:MET:O	29:6:78:VAL:HG22	2.09	0.53
32:R1:78:U:H2'	32:R1:79:C:C6	2.44	0.53
32:R1:693:A:O2'	32:R1:1353:A:N3	2.39	0.53
36:Y:389:GLN:NE2	59:Y:602:ATP:O2G	2.33	0.53
1:1:49:GLY:N	1:1:208:TYR:O	2.41	0.53
1:1:170:ILE:HD12	32:R1:2177:C:H6	1.73	0.53
8:19:18:SER:O	8:19:18:SER:OG	2.26	0.53
30:9:87:GLU:CD	30:9:87:GLU:H	2.11	0.53
32:R1:1076:C:H2'	32:R1:1077:A:C4	2.43	0.53
34:R3:1025:U:O2'	34:R3:1026:G:H5'	2.09	0.53
4:15:1:MET:HE1	27:4:184:ASP:HA	1.90	0.53
32:R1:593:U:H2'	32:R1:594:U:C6	2.43	0.53
32:R1:1715:G:N2	32:R1:1744:A:OP2	2.38	0.53
32:R1:2788:C:O2'	32:R1:2809:A:N3	2.36	0.53
35:T:6:G:O2'	35:T:49:G:O4'	2.26	0.53
2:13:27:ARG:NH2	32:R1:1143:A:OP1	2.42	0.53
14:24:71:ILE:HD12	14:24:102:ILE:HD11	1.91	0.53
23:33:14:ALA:HB2	23:33:46:VAL:HG21	1.90	0.53
36:Y:429:GLN:HA	36:Y:432:ILE:HB	1.90	0.53
9:2:106:PRO:HD2	9:2:109:LEU:HD22	1.91	0.53
34:R3:1452:C:H4'	34:R3:1453:G:C2	2.44	0.53
32:R1:1475:G:HO2'	32:R1:1476:U:H6	1.57	0.53
34:R3:423:G:N2	34:R3:424:G:N3	2.54	0.53
16:27:40:GLN:NE2	16:27:57:HIS:O	2.42	0.53
34:R3:96:U:H2'	34:R3:97:G:H8	1.73	0.53
12:22:59:GLU:OE2	12:22:66:ILE:HB	2.09	0.53
34:R3:1095:U:P	34:R3:1108:G:H1	2.32	0.53
2:13:114:LEU:O	2:13:118:MET:HG3	2.08	0.53
8:19:52:ARG:NH2	32:R1:2720:U:OP1	2.42	0.53
8:19:108:ARG:NH2	34:R3:1464:U:OP2	2.42	0.53
11:21:79:ARG:NH2	32:R1:572:A:OP2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:5:7:TYR:HB2	28:5:172:PHE:HZ	1.74	0.53
29:6:27:GLY:HA3	29:6:78:VAL:HB	1.89	0.53
32:R1:955:U:H5	32:R1:962:G:H1	1.57	0.53
34:R3:180:U:H2'	34:R3:181:A:C8	2.43	0.53
36:Y:323:GLU:O	36:Y:375:THR:OG1	2.20	0.53
36:Y:349:ALA:HB3	36:Y:505:ILE:HD13	1.91	0.53
32:R1:704:G:H2'	32:R1:726:G:N2	2.25	0.52
32:R1:2135:A:H3'	32:R1:2136:G:H8	1.73	0.52
34:R3:908:A:H2'	34:R3:909:A:C8	2.43	0.52
34:R3:1533:C:HO2'	34:R3:1535:C:N4	2.07	0.52
10:20:51:GLN:HA	10:20:54:ARG:HG2	1.91	0.52
28:5:33:ILE:HG23	28:5:90:LEU:HB2	1.91	0.52
32:R1:45:G:H5"	32:R1:46:G:H5'	1.91	0.52
32:R1:2154:A:HO2'	32:R1:2155:U:H6	1.56	0.52
32:R1:2183:A:H2'	32:R1:2184:A:H8	1.72	0.52
7:18:62:LEU:HD13	7:18:70:ALA:HA	1.91	0.52
10:20:65:ASN:ND2	32:R1:1010:A:OP1	2.34	0.52
20:30:10:ARG:HG2	20:30:10:ARG:HH11	1.73	0.52
32:R1:1266:G:O2'	32:R1:2012:G:O6	2.21	0.52
32:R1:1443:U:H2'	32:R1:1444:G:H8	1.74	0.52
32:R1:2127:G:H21	32:R1:2173:A:H1'	1.74	0.52
34:R3:1218:C:H2'	34:R3:1219:A:H8	1.72	0.52
2:13:98:GLU:O	2:13:102:GLU:HG3	2.10	0.52
9:2:123:ILE:HG23	9:2:191:LEU:HD11	1.90	0.52
27:4:30:GLN:OE1	32:R1:659:G:N2	2.37	0.52
32:R1:742:A:H2'	32:R1:743:A:C8	2.45	0.52
34:R3:321:A:H2'	34:R3:322:C:H6	1.74	0.52
1:1:38:PHE:HZ	32:R1:2125:G:O3'	1.92	0.52
7:18:55:GLU:HG3	7:18:57:ALA:H	1.75	0.52
7:18:94:ARG:HG2	7:18:97:PHE:O	2.10	0.52
11:21:15:SER:OG	11:21:16:GLU:N	2.41	0.52
17:28:42:GLU:OE1	17:28:44:ARG:NH1	2.41	0.52
29:6:85:LYS:HG3	29:6:131:VAL:HG22	1.91	0.52
30:9:132:PHE:HB2	30:9:140:ALA:HB3	1.91	0.52
32:R1:270:A:N1	32:R1:369:U:O2'	2.43	0.52
34:R3:456:A:H61	34:R3:475:C:N4	2.07	0.52
34:R3:1062:U:H2'	34:R3:1063:C:C6	2.44	0.52
34:R3:1297:G:H4'	34:R3:1298:U:O5'	2.08	0.52
32:R1:2831:G:N2	32:R1:2884:U:OP2	2.41	0.52
34:R3:695:A:H2'	34:R3:696:A:C8	2.45	0.52
34:R3:766:A:OP2	34:R3:812:G:N2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:9:44:ILE:HD12	30:9:44:ILE:H	1.74	0.52
32:R1:287:G:H2'	32:R1:288:U:C6	2.45	0.52
34:R3:126:G:OP1	34:R3:605:U:O2'	2.12	0.52
34:R3:418:C:H2'	34:R3:419:C:O4'	2.09	0.52
34:R3:1038:C:H2'	34:R3:1039:G:H8	1.74	0.52
36:Y:214:PHE:O	36:Y:218:VAL:HG22	2.09	0.52
27:4:45:ALA:HB2	27:4:89:PRO:HD3	1.91	0.52
32:R1:394:C:H2'	32:R1:395:U:O4'	2.10	0.52
34:R3:518:C:H4'	34:R3:519:C:O2	2.10	0.52
34:R3:1294:G:H2'	34:R3:1295:U:C6	2.44	0.52
32:R1:639:U:H2'	32:R1:640:C:C6	2.45	0.52
32:R1:833:A:H2'	32:R1:834:G:C8	2.45	0.52
7:18:35:ILE:HB	7:18:102:ARG:HH21	1.75	0.52
32:R1:1076:C:H2'	32:R1:1077:A:C8	2.45	0.52
32:R1:2645:G:OP2	32:R1:2645:G:N2	2.34	0.52
34:R3:745:G:H2'	34:R3:746:A:H8	1.75	0.52
27:4:95:LYS:O	32:R1:659:G:O2'	2.28	0.51
30:9:27:ARG:NH1	32:R1:2092:U:OP2	2.43	0.51
32:R1:1059:G:H5"	32:R1:1060:U:H2'	1.92	0.51
32:R1:2038:G:H2'	32:R1:2039:U:O4'	2.09	0.51
32:R1:2125:G:H22	32:R1:2174:C:H42	1.58	0.51
32:R1:2184:A:H2'	32:R1:2185:U:C6	2.45	0.51
34:R3:1314:C:H2'	34:R3:1315:U:H6	1.75	0.51
9:2:123:ILE:HG23	9:2:191:LEU:CD1	2.40	0.51
35:T:19:G:H5'	35:T:20:H2U:HN3	1.75	0.51
16:27:70:GLU:OE2	16:27:81:SER:OG	2.21	0.51
32:R1:851:C:H2'	32:R1:852:U:C6	2.46	0.51
32:R1:974:G:C6	32:R1:1186:G:C6	2.98	0.51
32:R1:2113:U:OP1	32:R1:2115:G:N1	2.43	0.51
7:18:63:LYS:NZ	33:R2:51:G:OP1	2.42	0.51
9:2:75:ALA:HB1	9:2:93:VAL:HG13	1.93	0.51
19:3:39:ASP:OD1	19:3:40:LEU:N	2.44	0.51
19:3:149:ASN:ND2	32:R1:2575:C:OP1	2.43	0.51
32:R1:577:G:O2'	32:R1:1254:A:OP1	2.28	0.51
32:R1:1682:G:H2'	32:R1:1683:U:C6	2.45	0.51
32:R1:2246:G:H2'	32:R1:2247:A:C8	2.45	0.51
34:R3:35:G:H2'	34:R3:36:C:C6	2.46	0.51
34:R3:457:G:N2	34:R3:475:C:O2	2.44	0.51
3:14:42:THR:HG22	3:14:57:VAL:HG22	1.92	0.51
15:25:4:ILE:HG13	15:25:63:ILE:HG13	1.92	0.51
27:4:123:LYS:HA	27:4:123:LYS:HE3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:5:37:MET:SD	28:5:52:ALA:HB1	2.50	0.51
32:R1:2314:A:H2'	32:R1:2315:G:H8	1.76	0.51
34:R3:745:G:H2'	34:R3:746:A:C8	2.46	0.51
9:2:208:GLY:HA2	9:2:211:ARG:HB2	1.92	0.51
32:R1:2649:C:H2'	32:R1:2650:U:C6	2.45	0.51
32:R1:2798:U:H5"	32:R1:2799:A:OP1	2.10	0.51
34:R3:71:A:N6	34:R3:100:G:N3	2.50	0.51
34:R3:500:G:H2'	34:R3:501:C:C6	2.46	0.51
34:R3:1034:G:C6	34:R3:1035:A:C6	2.98	0.51
1:1:46:VAL:HG12	1:1:212:VAL:HG22	1.91	0.51
32:R1:475:C:O2	32:R1:479:A:N6	2.43	0.51
32:R1:818:G:N1	32:R1:1188:U:OP2	2.24	0.51
32:R1:1087:G:C8	32:R1:1089:A:H5"	2.45	0.51
32:R1:2155:U:H3'	32:R1:2156:G:H8	1.76	0.51
36:Y:408:TRP:CD1	36:Y:454:MET:HG3	2.46	0.51
32:R1:355:U:H2'	32:R1:356:G:H8	1.76	0.51
34:R3:938:A:N3	34:R3:1376:U:O2'	2.38	0.51
36:Y:269:VAL:HG21	36:Y:289:ILE:HD11	1.92	0.51
36:Y:354:ASN:H	36:Y:358:LYS:HZ3	1.59	0.51
36:Y:471:MET:O	36:Y:474:ILE:HG22	2.10	0.51
1:1:30:LEU:HD22	1:1:216:THR:HG23	1.91	0.51
32:R1:12:U:O2	32:R1:12:U:H2'	2.10	0.51
32:R1:1912:A:H62	32:R1:1917:U:H5	1.57	0.51
15:25:80:HIS:CD2	15:25:81:PRO:HD2	2.45	0.51
32:R1:1056:G:N1	32:R1:1102:C:OP2	2.30	0.51
32:R1:1338:G:O2'	32:R1:1393:A:N1	2.41	0.51
4:15:81:ASP:HB3	4:15:100:ILE:HD13	1.92	0.50
6:17:69:ARG:O	6:17:70:THR:OG1	2.25	0.50
13:23:64:LYS:HA	13:23:79:ASP:HB3	1.93	0.50
32:R1:547:A:H5"	32:R1:548:G:H5'	1.93	0.50
32:R1:1410:G:H2'	32:R1:1411:U:C6	2.46	0.50
36:Y:349:ALA:O	36:Y:351:LEU:HD23	2.11	0.50
16:27:29:GLU:OE2	32:R1:922:C:O2'	2.20	0.50
32:R1:1094:U:C4	32:R1:1096:A:H5"	2.45	0.50
34:R3:376:G:H1	34:R3:387:U:H3	1.58	0.50
34:R3:422:C:H5'	34:R3:423:G:H5"	1.93	0.50
34:R3:1340:A:HO2'	35:T:31:G:HO2'	1.58	0.50
15:25:80:HIS:ND1	15:25:83:LYS:HB2	2.26	0.50
19:3:110:THR:HG21	19:3:169:ARG:HE	1.76	0.50
25:35:31:ILE:HG13	25:35:31:ILE:O	2.10	0.50
32:R1:1036:G:C6	32:R1:1120:G:C6	2.99	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:R1:2247:A:H2'	32:R1:2248:C:H6	1.76	0.50
33:R2:28:C:H2'	33:R2:29:A:H8	1.74	0.50
34:R3:321:A:H2'	34:R3:322:C:C6	2.46	0.50
34:R3:1352:C:H2'	34:R3:1353:G:C8	2.46	0.50
34:R3:1513:A:H2'	34:R3:1514:G:C8	2.46	0.50
35:T:21:A:O2'	35:T:46:A:N6	2.41	0.50
35:T:53:G:H2'	35:T:54:5MU:C6	2.45	0.50
1:1:58:ASN:OD1	1:1:165:ASN:ND2	2.45	0.50
22:32:30:ASP:OD1	22:32:31:LYS:N	2.40	0.50
30:9:25:TYR:HE1	30:9:29:PHE:HD2	1.57	0.50
32:R1:2291:U:H2'	32:R1:2292:U:C6	2.47	0.50
34:R3:1300:G:H1'	34:R3:1303:C:N4	2.26	0.50
36:Y:184:ASN:OD1	36:Y:468:HIS:NE2	2.45	0.50
4:15:92:LEU:O	4:15:96:LYS:HG2	2.11	0.50
5:16:42:THR:HG22	5:16:43:ALA:H	1.76	0.50
32:R1:2102:G:H2'	32:R1:2103:C:C6	2.46	0.50
34:R3:509:A:H8	34:R3:543:U:O2'	1.93	0.50
36:Y:392:GLU:O	36:Y:396:GLU:HG2	2.10	0.50
26:36:23:ILE:HB	26:36:38:GLY:HA3	1.92	0.50
4:15:64:PHE:HB3	25:35:24:LYS:HD2	1.93	0.50
5:16:41:LEU:HD11	5:16:124:LEU:HD22	1.93	0.50
14:24:48:VAL:HG22	14:24:50:ALA:H	1.76	0.50
15:25:62:THR:HG23	15:25:62:THR:O	2.11	0.50
15:25:30:ILE:HD11	15:25:38:LEU:HD23	1.94	0.50
32:R1:1300:G:H4'	32:R1:1301:A:H5"	1.93	0.50
32:R1:1583:A:O2'	32:R1:1585:C:N4	2.45	0.50
34:R3:56:U:H2'	34:R3:57:G:H8	1.76	0.50
34:R3:593:U:H2'	34:R3:594:U:C6	2.47	0.50
14:24:82:VAL:HG13	14:24:93:ARG:HB3	1.94	0.50
19:3:56:LYS:HD2	19:3:59:ARG:HG3	1.93	0.50
20:30:10:ARG:HG2	20:30:10:ARG:NH1	2.27	0.50
32:R1:2128:G:H1	32:R1:2160:C:H42	1.60	0.50
10:20:48:ASP:HA	10:20:51:GLN:HG3	1.94	0.49
13:23:23:ALA:HB1	13:23:29:THR:HB	1.92	0.49
32:R1:415:A:H2'	32:R1:416:U:C6	2.47	0.49
34:R3:210:C:O2'	34:R3:211:G:N2	2.45	0.49
36:Y:481:LEU:O	36:Y:481:LEU:HD23	2.12	0.49
11:21:5:PHE:HB3	11:21:59:ILE:HD12	1.93	0.49
32:R1:151:C:H2'	32:R1:152:A:H8	1.77	0.49
32:R1:1668:A:N3	32:R1:1670:C:N4	2.60	0.49
32:R1:1900:A:H1'	32:R1:1970:A:H2'	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:R1:2071:A:H2'	32:R1:2072:C:C6	2.47	0.49
34:R3:82:G:N2	34:R3:85:U:OP2	2.45	0.49
35:T:10:A:H2'	35:T:11:G:C8	2.48	0.49
36:Y:44:MET:SD	36:Y:178:LEU:HB3	2.52	0.49
36:Y:419:ARG:HH22	36:Y:429:GLN:HB3	1.77	0.49
6:17:38:LEU:HB3	6:17:39:PRO:HD3	1.95	0.49
12:22:23:LEU:HD21	22:32:21:LEU:HB2	1.95	0.49
23:33:6:GLU:OE1	23:33:26:LYS:HD2	2.13	0.49
32:R1:1085:A:H2'	32:R1:1086:A:C4	2.47	0.49
34:R3:1143:G:H2'	34:R3:1144:G:C8	2.47	0.49
4:15:96:LYS:HB3	4:15:101:ILE:HG13	1.94	0.49
26:36:25:VAL:HB	26:36:35:GLN:HB2	1.94	0.49
32:R1:2113:U:H2'	32:R1:2114:A:C8	2.47	0.49
33:R2:60:C:H2'	33:R2:61:G:H8	1.75	0.49
34:R3:113:G:H1'	34:R3:354:G:H5'	1.95	0.49
34:R3:212:G:C2	34:R3:213:G:C8	3.00	0.49
36:Y:196:GLN:O	36:Y:200:GLU:HG2	2.13	0.49
36:Y:338:LEU:HD13	36:Y:513:VAL:HG11	1.94	0.49
2:13:31:GLU:HG2	2:13:142:ILE:HG13	1.93	0.49
32:R1:602:A:O2'	32:R1:604:G:O2'	2.29	0.49
36:Y:325:LEU:O	36:Y:337:ASN:N	2.46	0.49
36:Y:357:GLY:HA2	36:Y:360:THR:HG22	1.94	0.49
4:15:85:VAL:HG23	4:15:86:GLU:N	2.28	0.49
32:R1:1054:A:N6	32:R1:1106:G:O6	2.46	0.49
32:R1:1182:G:H2'	32:R1:1183:U:O4'	2.13	0.49
34:R3:263:A:H2'	34:R3:264:C:C5	2.47	0.49
34:R3:501:C:H2'	34:R3:502:A:H8	1.77	0.49
30:9:14:SER:O	30:9:14:SER:OG	2.27	0.49
32:R1:639:U:H2'	32:R1:640:C:H6	1.78	0.49
29:6:137:LYS:HA	29:6:140:ILE:HG22	1.94	0.49
32:R1:271:G:C4	32:R1:367:G:N2	2.81	0.49
32:R1:2183:A:H2'	32:R1:2184:A:C8	2.47	0.49
26:36:3:VAL:HG12	26:36:36:ARG:HB3	1.93	0.49
32:R1:171:U:H2'	32:R1:172:A:H8	1.77	0.49
32:R1:1539:U:H2'	32:R1:1540:G:H8	1.78	0.49
34:R3:417:G:H2'	34:R3:418:C:C6	2.48	0.49
34:R3:1315:U:H3'	34:R3:1316:G:H8	1.77	0.49
36:Y:29:ARG:HG2	36:Y:205:MET:HE2	1.94	0.49
36:Y:400:THR:HG23	36:Y:403:GLU:HB3	1.95	0.49
2:13:108:MET:HE2	32:R1:1138:G:H21	1.77	0.49
5:16:86:LYS:HG2	5:16:87:GLY:H	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:2:92:LEU:HD21	9:2:100:ARG:HD3	1.95	0.49
9:2:219:VAL:HG21	32:R1:782:A:N7	2.28	0.49
12:22:5:ALA:HB1	12:22:50:VAL:HG22	1.95	0.49
19:3:133:THR:HG22	19:3:134:HIS:N	2.23	0.49
32:R1:546:U:H4'	32:R1:548:G:H1	1.78	0.49
32:R1:2540:C:O2'	32:R1:2740:A:N3	2.36	0.49
34:R3:593:U:H2'	34:R3:594:U:H6	1.78	0.49
36:Y:80:THR:HG22	36:Y:83:ASP:OD2	2.13	0.49
2:13:128:ASN:HD22	2:13:128:ASN:C	2.07	0.48
7:18:80:GLU:O	7:18:84:GLU:HG3	2.13	0.48
12:22:93:ALA:HB2	32:R1:1614:A:N1	2.27	0.48
19:3:4:LEU:HD13	19:3:29:VAL:HG11	1.94	0.48
32:R1:306:U:H2'	32:R1:307:G:O4'	2.12	0.48
32:R1:834:G:H1'	32:R1:2358:A:N3	2.28	0.48
32:R1:1563:U:H2'	32:R1:1564:C:C6	2.48	0.48
34:R3:1095:U:OP2	34:R3:1108:G:N1	2.41	0.48
36:Y:118:ASP:O	36:Y:121:VAL:HG22	2.13	0.48
36:Y:138:LEU:HD11	36:Y:170:LEU:HD11	1.95	0.48
3:14:15:GLY:HA2	3:14:47:ILE:HD11	1.93	0.48
8:19:105:LYS:HA	8:19:108:ARG:HD3	1.94	0.48
32:R1:570:G:H2'	32:R1:2030:A:N7	2.28	0.48
32:R1:2107:G:C6	32:R1:2183:A:C6	3.01	0.48
32:R1:2522:U:O2'	32:R1:2647:U:OP1	2.25	0.48
32:R1:2649:C:H2'	32:R1:2650:U:H6	1.78	0.48
36:Y:354:ASN:H	36:Y:358:LYS:NZ	2.10	0.48
18:29:42:LEU:O	18:29:46:VAL:HG22	2.12	0.48
36:Y:9:MET:SD	36:Y:11:PHE:CE1	3.06	0.48
3:14:92:GLU:HG3	3:14:111:LYS:HE3	1.94	0.48
32:R1:1889:A:H2'	32:R1:1890:A:C8	2.48	0.48
32:R1:2114:A:H61	32:R1:2119:A:H61	1.61	0.48
34:R3:181:A:H2'	34:R3:182:A:C8	2.49	0.48
36:Y:181:GLN:H	36:Y:208:ILE:HG23	1.78	0.48
9:2:261:ARG:O	9:2:264:LYS:HE2	2.13	0.48
32:R1:1873:G:H2'	32:R1:1874:C:C6	2.49	0.48
34:R3:80:A:H2	34:R3:91:U:C4	2.31	0.48
34:R3:204:G:C5	34:R3:465:A:N1	2.81	0.48
34:R3:572:A:H5'	34:R3:573:A:OP2	2.13	0.48
9:2:97:ASP:N	9:2:97:ASP:OD1	2.43	0.48
17:28:51:SER:OG	17:28:52:ALA:N	2.47	0.48
28:5:101:ARG:HA	28:5:104:THR:HG22	1.94	0.48
29:6:174:LYS:HD2	32:R1:2529:G:H4'	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:R1:1636:U:H2'	32:R1:1637:A:H8	1.79	0.48
36:Y:326:THR:HB	36:Y:372:ASP:HB3	1.94	0.48
36:Y:370:GLN:N	36:Y:371:PRO:HD3	2.28	0.48
4:15:74:THR:HA	4:15:107:PHE:O	2.13	0.48
14:24:85:ARG:HG2	14:24:94:PHE:CD1	2.48	0.48
30:9:43:ASN:HA	30:9:46:PHE:HD2	1.78	0.48
32:R1:134:G:H2'	32:R1:135:U:C6	2.49	0.48
32:R1:1539:U:H2'	32:R1:1540:G:C8	2.48	0.48
34:R3:1019:A:H2'	34:R3:1020:G:O4'	2.14	0.48
35:T:65:C:H2'	35:T:66:C:C6	2.49	0.48
1:1:42:VAL:N	1:1:176:GLY:O	2.46	0.48
1:1:168:ASN:ND2	32:R1:2179:C:H5'	2.29	0.48
3:14:25:LEU:HD22	32:R1:2562:U:H4'	1.95	0.48
4:15:85:VAL:HG23	4:15:86:GLU:H	1.79	0.48
5:16:59:ARG:NE	5:16:59:ARG:HA	2.28	0.48
12:22:61:ASN:HD21	32:R1:495:G:H21	1.61	0.48
34:R3:1055:A:C6	34:R3:1206:G:C5	3.02	0.48
34:R3:1305:G:O2'	34:R3:1306:A:H8	1.96	0.48
11:21:23:GLU:OE2	32:R1:993:G:N2	2.47	0.48
22:32:15:ARG:NH2	32:R1:1264:A:OP1	2.41	0.48
25:35:51:LYS:HE3	25:35:51:LYS:HB3	1.60	0.48
28:5:136:ILE:HG13	28:5:137:PHE:CD1	2.49	0.48
32:R1:310:A:O2'	32:R1:311:A:H2'	2.14	0.48
32:R1:1016:G:O6	32:R1:1147:A:N6	2.47	0.48
32:R1:1889:A:H2'	32:R1:1890:A:H8	1.79	0.48
32:R1:2725:A:O2'	32:R1:2726:A:O5'	2.32	0.48
34:R3:460:A:H2'	34:R3:461:A:H8	1.79	0.48
34:R3:922:G:H2'	34:R3:923:A:C8	2.49	0.48
36:Y:327:LYS:HE2	36:Y:329:PHE:HE1	1.78	0.48
36:Y:525:ARG:NH2	36:Y:530:GLU:HA	2.29	0.48
7:18:100:HIS:ND1	33:R2:48:U:H4'	2.29	0.48
10:20:32:ARG:HD2	32:R1:581:C:OP2	2.14	0.48
12:22:55:ILE:O	12:22:59:GLU:HG3	2.13	0.48
22:32:43:THR:HG23	22:32:47:TYR:O	2.14	0.48
32:R1:1490:A:H5'	32:R1:1491:G:OP2	2.14	0.48
32:R1:1536:C:H4'	32:R1:1537:G:C2	2.49	0.48
32:R1:2157:G:H2'	32:R1:2158:A:C4	2.49	0.48
34:R3:1038:C:H2'	34:R3:1039:G:C8	2.49	0.48
34:R3:1071:C:H2'	34:R3:1072:G:C8	2.49	0.48
36:Y:525:ARG:NH2	36:Y:530:GLU:HG2	2.29	0.48
2:13:7:LYS:HG2	32:R1:538:A:H4'	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:32:7:PRO:HD2	32:R1:1263:U:O2'	2.14	0.47
32:R1:4:U:H2'	32:R1:5:A:H8	1.79	0.47
32:R1:2542:A:H5"	32:R1:2766:A:O2'	2.14	0.47
34:R3:1251:A:H2'	34:R3:1252:A:C8	2.49	0.47
34:R3:1355:G:H2'	34:R3:1356:G:H8	1.79	0.47
36:Y:358:LYS:HE3	59:Y:602:ATP:O3B	2.14	0.47
1:1:59:VAL:H	1:1:165:ASN:ND2	2.07	0.47
1:1:205:LYS:NZ	32:R1:1876:A:OP1	2.46	0.47
2:13:26:GLY:HA3	32:R1:1140:C:H5'	1.96	0.47
7:18:60:GLU:N	7:18:60:GLU:OE1	2.44	0.47
9:2:222:THR:HG23	32:R1:1826:G:OP1	2.14	0.47
32:R1:774:G:O2'	32:R1:775:G:H5"	2.13	0.47
32:R1:2064:C:H2'	32:R1:2065:C:C6	2.48	0.47
32:R1:2125:G:N2	32:R1:2174:C:H42	2.12	0.47
34:R3:894:G:C6	34:R3:895:G:N7	2.81	0.47
34:R3:1287:A:H2'	34:R3:1288:A:C8	2.49	0.47
36:Y:348:LEU:HD21	36:Y:506:LEU:HD13	1.96	0.47
15:25:51:GLN:OE1	15:25:57:TYR:OH	2.31	0.47
32:R1:476:G:N1	32:R1:479:A:OP2	2.46	0.47
34:R3:384:G:H2'	34:R3:385:C:C6	2.48	0.47
34:R3:1287:A:H2	34:R3:1353:G:H1'	1.79	0.47
36:Y:462:MET:HB3	36:Y:465:PRO:HB3	1.96	0.47
36:Y:488:LEU:HD12	36:Y:489:ILE:N	2.29	0.47
32:R1:780:G:C2	32:R1:782:A:C2	3.03	0.47
32:R1:1874:C:H2'	32:R1:1875:G:O4'	2.15	0.47
34:R3:1266:G:N2	34:R3:1269:A:OP2	2.23	0.47
7:18:60:GLU:H	7:18:60:GLU:CD	2.18	0.47
14:24:5:ARG:NH1	14:24:93:ARG:HD3	2.29	0.47
32:R1:358:U:H2'	32:R1:359:G:C8	2.50	0.47
9:2:209:ALA:HA	9:2:212:TRP:CE2	2.50	0.47
13:23:21:SER:O	13:23:25:GLU:HG3	2.14	0.47
28:5:99:PHE:HE1	28:5:174:PHE:HE1	1.62	0.47
32:R1:191:A:H2'	32:R1:192:C:C6	2.50	0.47
32:R1:463:G:N2	32:R1:466:A:OP2	2.35	0.47
32:R1:1288:G:N2	32:R1:1288:G:OP2	2.48	0.47
32:R1:1410:G:H2'	32:R1:1411:U:H6	1.80	0.47
33:R2:51:G:C2	33:R2:52:A:C2	3.02	0.47
34:R3:297:G:N2	34:R3:300:A:OP2	2.46	0.47
34:R3:1432:G:H1'	34:R3:1468:A:H62	1.80	0.47
4:15:109:LYS:HE2	4:15:128:THR:HG22	1.95	0.47
6:17:114:GLU:OE1	6:17:118:ARG:NE	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:19:1:SER:O	8:19:1:SER:OG	2.32	0.47
9:2:140:VAL:HG11	9:2:189:ALA:HB1	1.96	0.47
14:24:37:GLY:N	14:24:61:GLU:OE1	2.41	0.47
15:25:20:LEU:HD21	15:25:41:GLU:HB2	1.96	0.47
32:R1:414:C:H2'	32:R1:415:A:H8	1.80	0.47
32:R1:848:C:H2'	32:R1:849:A:C8	2.43	0.47
32:R1:2111:U:C2	32:R1:2118:U:H4'	2.50	0.47
34:R3:945:G:C2	34:R3:946:A:C8	3.03	0.47
34:R3:975:A:H8	34:R3:1357:A:HO2'	1.62	0.47
34:R3:1077:G:N1	34:R3:1080:A:OP2	2.48	0.47
34:R3:1282:C:H2'	34:R3:1283:U:C6	2.50	0.47
34:R3:1432:G:H1'	34:R3:1468:A:N6	2.29	0.47
36:Y:360:THR:HA	36:Y:363:LYS:HE2	1.97	0.47
9:2:207:ALA:HB2	32:R1:1790:C:O2'	2.14	0.47
32:R1:1412:U:H2'	32:R1:1413:A:C8	2.49	0.47
32:R1:1477:A:N6	32:R1:1514:G:O2'	2.48	0.47
36:Y:91:GLU:OE1	36:Y:91:GLU:N	2.47	0.47
36:Y:148:GLN:NE2	36:Y:148:GLN:O	2.45	0.47
36:Y:216:ASN:OD1	36:Y:236:ASN:HB3	2.14	0.47
5:16:66:ARG:NH1	5:16:104:GLU:OE2	2.40	0.47
7:18:40:ILE:HG12	7:18:47:VAL:HG12	1.97	0.47
29:6:138:GLN:NE2	32:R1:2745:C:O2	2.47	0.47
32:R1:365:U:H2'	32:R1:366:C:C6	2.50	0.47
32:R1:2532:G:O2'	32:R1:2657:A:N1	2.46	0.47
32:R1:2804:U:H2'	32:R1:2805:C:C6	2.50	0.47
33:R2:32:U:C4	33:R2:51:G:N2	2.83	0.47
35:T:15:C:H3'	35:T:16:C:H5"	1.97	0.47
36:Y:258:LYS:HD2	36:Y:294:LEU:HA	1.97	0.47
7:18:58:ILE:O	7:18:62:LEU:HG	2.15	0.47
9:2:12:ARG:HD2	32:R1:728:G:H4'	1.97	0.47
20:30:23:LEU:HD11	20:30:53:MET:CE	2.45	0.47
32:R1:172:A:H2'	32:R1:173:A:C8	2.48	0.47
32:R1:827:U:O2'	32:R1:2068:U:C2	2.68	0.47
32:R1:1296:G:OP1	32:R1:2709:G:O2'	2.26	0.47
32:R1:2297:A:H61	32:R1:2319:G:H1'	1.80	0.47
32:R1:2804:U:H2'	32:R1:2805:C:H6	1.79	0.47
34:R3:1034:G:H2'	34:R3:1035:A:C8	2.50	0.47
6:17:32:GLU:HB2	6:17:118:ARG:HD2	1.97	0.46
32:R1:918:A:N3	33:R2:80:U:O2'	2.43	0.46
32:R1:1871:A:H8	32:R1:1872:A:C8	2.33	0.46
34:R3:501:C:O2	34:R3:549:C:O2'	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:R3:1211:U:H5”	34:R3:1212:U:OP1	2.15	0.46
35:T:67:C:H2’	35:T:68:C:C6	2.50	0.46
30:9:96:THR:H	30:9:99:ILE:HD11	1.80	0.46
32:R1:933:A:H5’	32:R1:934:U:OP2	2.16	0.46
32:R1:2107:G:O6	32:R1:2183:A:N6	2.48	0.46
34:R3:1533:C:O2’	34:R3:1535:C:N4	2.48	0.46
36:Y:461:ILE:HA	36:Y:489:ILE:O	2.15	0.46
19:3:113:SER:OG	19:3:114:LYS:N	2.48	0.46
30:9:3:VAL:CG1	30:9:36:ALA:HB1	2.45	0.46
30:9:9:VAL:HG11	30:9:12:LEU:HG	1.97	0.46
32:R1:1106:G:H2’	32:R1:1107:G:H8	1.79	0.46
32:R1:1796:U:H2’	32:R1:1797:G:C8	2.51	0.46
32:R1:2098:U:O3’	32:R1:2099:U:H5’	2.15	0.46
32:R1:2590:A:H2’	32:R1:2591:C:H6	1.81	0.46
33:R2:48:U:H2’	33:R2:49:C:C6	2.50	0.46
36:Y:265:LEU:O	36:Y:269:VAL:HG23	2.16	0.46
36:Y:458:ASN:OD1	36:Y:459:ILE:HG13	2.15	0.46
8:19:27:VAL:HG13	8:19:80:VAL:HG13	1.97	0.46
28:5:3:LEU:HD23	28:5:3:LEU:HA	1.77	0.46
32:R1:721:A:H2’	32:R1:722:A:C8	2.51	0.46
33:R2:111:U:H2’	33:R2:112:G:H8	1.80	0.46
34:R3:210:C:O2’	34:R3:211:G:H5”	2.15	0.46
34:R3:459:A:H2’	34:R3:460:A:H8	1.80	0.46
34:R3:839:C:H2’	34:R3:840:C:C6	2.50	0.46
36:Y:140:LEU:HD11	36:Y:146:VAL:O	2.14	0.46
4:15:21:ARG:HA	32:R1:811:U:H2’	1.98	0.46
22:32:52:LYS:NZ	22:32:55:ALA:HA	2.30	0.46
32:R1:1796:U:H2’	32:R1:1797:G:H8	1.78	0.46
34:R3:842:U:OP2	34:R3:846:G:N2	2.48	0.46
34:R3:967:C:OP2	34:R3:968:A:O2’	2.24	0.46
34:R3:1356:G:H2’	34:R3:1357:A:H8	1.79	0.46
34:R3:1410:A:H2’	34:R3:1411:C:C6	2.51	0.46
5:16:90:GLU:HA	5:16:90:GLU:OE2	2.15	0.46
13:23:37:ASP:OD1	13:23:37:ASP:N	2.49	0.46
15:25:5:ASN:OD1	15:25:5:ASN:N	2.48	0.46
29:6:9:VAL:HA	29:6:48:THR:HG22	1.97	0.46
32:R1:1038:G:H2’	32:R1:1039:A:C8	2.50	0.46
34:R3:604:G:C6	34:R3:635:A:N1	2.83	0.46
1:1:6:LYS:HG2	1:1:9:ARG:HD2	1.97	0.46
11:21:31:GLU:HA	11:21:31:GLU:OE2	2.16	0.46
32:R1:554:U:H2’	32:R1:555:G:O4’	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:R3:458:U:O2	34:R3:474:G:N2	2.49	0.46
36:Y:226:ASP:OD1	36:Y:301:SER:HB2	2.16	0.46
13:23:34:VAL:HG23	13:23:81:LYS:HB3	1.97	0.46
16:27:50:ASN:HB2	16:27:82:ILE:HB	1.98	0.46
19:3:149:ASN:OD1	19:3:150:GLN:N	2.46	0.46
24:34:34:ARG:HB2	24:34:42:LEU:HD13	1.97	0.46
32:R1:1969:A:H2'	32:R1:1972:G:H21	1.79	0.46
32:R1:2102:G:H2'	32:R1:2103:C:H6	1.81	0.46
34:R3:204:G:H2'	34:R3:205:A:H8	1.81	0.46
35:T:18:G:N1	35:T:57:A:N7	2.64	0.46
36:Y:198:LEU:HD23	36:Y:198:LEU:HA	1.79	0.46
30:9:90:LEU:HD11	30:9:146:VAL:HG21	1.98	0.46
32:R1:4:U:H2'	32:R1:5:A:C8	2.51	0.46
32:R1:358:U:H2'	32:R1:359:G:H8	1.80	0.46
34:R3:457:G:C2	34:R3:458:U:H1'	2.51	0.46
34:R3:494:G:O2'	34:R3:496:A:H1'	2.16	0.46
34:R3:713:G:H2'	34:R3:714:G:C8	2.51	0.46
36:Y:308:ARG:H	36:Y:453:MET:CE	2.28	0.46
36:Y:323:GLU:HB3	36:Y:375:THR:OG1	2.15	0.46
36:Y:350:VAL:HG23	36:Y:506:LEU:O	2.16	0.46
8:19:50:ARG:NH1	8:19:55:HIS:O	2.49	0.46
10:20:85:ALA:HB2	10:20:115:ALA:HB2	1.97	0.46
11:21:77:PHE:HD1	11:21:84:ARG:HG3	1.81	0.46
29:6:3:VAL:HG23	32:R1:2751:G:H4'	1.98	0.46
32:R1:281:C:H2'	32:R1:282:A:C8	2.51	0.46
34:R3:78:A:H62	34:R3:79:G:N2	2.12	0.46
34:R3:1031:C:O3'	34:R3:1033:G:N2	2.49	0.46
4:15:1:MET:CE	27:4:184:ASP:HB2	2.46	0.45
15:25:56:PHE:CE1	15:25:61:LEU:HD21	2.51	0.45
32:R1:528:A:C2	32:R1:2043:C:H4'	2.51	0.45
32:R1:1918:A:O2'	32:R1:1919:A:N7	2.46	0.45
36:Y:89:HIS:HB2	36:Y:172:ALA:HB2	1.98	0.45
2:13:96:ARG:HH22	32:R1:2640:G:P	2.38	0.45
5:16:71:LYS:HB3	5:16:93:VAL:O	2.16	0.45
29:6:59:ASP:O	29:6:63:GLN:HG2	2.16	0.45
32:R1:721:A:H2'	32:R1:722:A:H8	1.81	0.45
32:R1:2127:G:H1'	32:R1:2173:A:H2	1.82	0.45
34:R3:204:G:C4	34:R3:205:A:C8	3.04	0.45
34:R3:459:A:H2'	34:R3:460:A:C8	2.52	0.45
34:R3:821:G:H2'	34:R3:822:U:C6	2.51	0.45
34:R3:1033:G:H2'	34:R3:1034:G:C8	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:R3:1314:C:H2'	34:R3:1315:U:C6	2.50	0.45
8:19:63:ILE:HA	8:19:68:GLY:HA2	1.99	0.45
12:22:70:LYS:HB3	12:22:70:LYS:HE3	1.66	0.45
18:29:47:ARG:NH2	32:R1:61:C:OP2	2.50	0.45
21:31:35:ASP:OD1	21:31:35:ASP:N	2.48	0.45
32:R1:962:G:H21	32:R1:2250:G:H1	1.64	0.45
32:R1:2118:U:O4	32:R1:2148:G:N2	2.29	0.45
32:R1:2175:C:H5"	32:R1:2176:A:OP2	2.16	0.45
34:R3:1301:U:O2'	34:R3:1302:C:O5'	2.35	0.45
34:R3:1513:A:H2'	34:R3:1514:G:H8	1.81	0.45
4:15:58:TYR:HD1	4:15:58:TYR:H	1.65	0.45
4:15:110:VAL:O	4:15:128:THR:HG23	2.15	0.45
4:15:122:VAL:HG13	4:15:125:LEU:HD12	1.97	0.45
32:R1:281:C:H2'	32:R1:282:A:H8	1.82	0.45
32:R1:287:G:H2'	32:R1:288:U:H6	1.80	0.45
32:R1:372:G:O2'	32:R1:373:U:P	2.75	0.45
32:R1:742:A:H2'	32:R1:743:A:H8	1.82	0.45
32:R1:1070:A:N1	32:R1:1096:A:H2	2.14	0.45
32:R1:1928:A:H2'	32:R1:1929:G:O4'	2.17	0.45
32:R1:2134:A:C6	32:R1:2157:G:H4'	2.51	0.45
33:R2:60:C:H2'	33:R2:61:G:C8	2.51	0.45
34:R3:746:A:H2'	34:R3:747:A:C8	2.52	0.45
34:R3:1157:A:N7	34:R3:1180:A:N6	2.64	0.45
34:R3:1365:G:C6	34:R3:1366:C:C4	3.05	0.45
35:T:13:A:H2'	35:T:14:G:O4'	2.17	0.45
36:Y:435:PRO:O	36:Y:438:VAL:HG22	2.17	0.45
5:16:106:ASP:OD2	5:16:107:GLY:N	2.49	0.45
21:31:30:HIS:CE1	21:31:32:LEU:HD21	2.52	0.45
22:32:28:SER:HB3	22:32:39:ARG:HD2	1.97	0.45
22:32:51:ARG:NH1	22:32:53:VAL:HG12	2.32	0.45
27:4:149:ILE:HD11	27:4:175:ILE:HG21	1.98	0.45
30:9:11:ASN:O	30:9:11:ASN:ND2	2.49	0.45
30:9:125:THR:HA	30:9:146:VAL:HG13	1.98	0.45
32:R1:30:G:H2'	32:R1:31:C:C6	2.52	0.45
32:R1:546:U:O2'	32:R1:547:A:O4'	2.14	0.45
32:R1:645:C:H2'	32:R1:647:G:N7	2.31	0.45
32:R1:859:G:O2'	32:R1:916:G:O6	2.27	0.45
34:R3:78:A:C5	34:R3:79:G:H1'	2.52	0.45
34:R3:394:G:H2'	34:R3:395:C:H5'	1.98	0.45
34:R3:1261:A:O2'	34:R3:1283:U:H5"	2.17	0.45
36:Y:40:LYS:HG3	36:Y:208:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:Y:265:LEU:HD22	36:Y:285:ARG:HB3	1.97	0.45
32:R1:573:U:N3	32:R1:2031:A:OP1	2.49	0.45
32:R1:686:U:H2'	32:R1:788:A:N1	2.32	0.45
32:R1:1693:U:H5"	32:R1:1694:C:H5	1.80	0.45
32:R1:2097:A:H2'	32:R1:2098:U:C6	2.52	0.45
33:R2:14:U:OP2	33:R2:70:C:O2'	2.30	0.45
32:R1:891:G:O2'	32:R1:892:A:H8	1.99	0.45
32:R1:983:A:N6	32:R1:984:A:N1	2.64	0.45
32:R1:1020:A:H4'	32:R1:1021:A:O5'	2.16	0.45
36:Y:17:PHE:HB2	36:Y:20:ILE:HD11	1.97	0.45
2:13:39:LYS:NZ	32:R1:1007:C:P	2.90	0.45
17:28:17:ARG:HD3	17:28:17:ARG:HA	1.69	0.45
19:3:130:GLN:OE1	32:R1:2578:G:N2	2.50	0.45
32:R1:2098:U:H2'	32:R1:2099:U:O4'	2.16	0.45
32:R1:2168:G:H2'	32:R1:2169:A:C8	2.51	0.45
34:R3:456:A:H61	34:R3:475:C:H42	1.63	0.45
34:R3:600:A:H2'	34:R3:601:G:H8	1.82	0.45
34:R3:1010:U:H2'	34:R3:1011:C:H6	1.82	0.45
36:Y:11:PHE:CD2	59:Y:601:ATP:C4	2.95	0.45
36:Y:203:SER:HB2	36:Y:205:MET:SD	2.56	0.45
23:33:16:THR:HG21	23:33:41:VAL:HG11	1.99	0.45
29:6:63:GLN:HA	29:6:66:THR:HG22	1.99	0.45
32:R1:1469:A:H2'	32:R1:1470:A:C8	2.52	0.45
32:R1:2156:G:H2'	32:R1:2157:G:H5'	1.99	0.45
34:R3:1118:U:H2'	34:R3:1119:C:H6	1.81	0.45
36:Y:459:ILE:HG23	36:Y:487:THR:HB	1.98	0.45
9:2:74:PRO:HD2	9:2:96:LYS:HG3	1.98	0.45
21:31:41:HIS:HD2	21:31:43:PHE:HB3	1.82	0.45
27:4:170:ARG:NH1	27:4:176:ASP:OD1	2.49	0.45
30:9:70:GLU:HB2	30:9:134:VAL:HG21	1.99	0.45
32:R1:164:C:H2'	32:R1:165:A:O4'	2.17	0.45
32:R1:196:A:O2'	32:R1:805:G:O6	2.26	0.45
32:R1:843:G:N1	32:R1:936:A:N1	2.65	0.45
32:R1:2196:C:H2'	32:R1:2197:U:C6	2.51	0.45
33:R2:2:G:H2'	33:R2:3:C:C6	2.52	0.45
36:Y:2:LEU:HD21	36:Y:47:LEU:HD11	1.99	0.45
9:2:264:LYS:H	9:2:264:LYS:HG3	1.56	0.44
12:22:89:ALA:HB1	32:R1:748:G:C8	2.52	0.44
23:33:22:THR:HG22	23:33:23:THR:H	1.81	0.44
24:34:3:ARG:HD3	24:34:3:ARG:HA	1.68	0.44
32:R1:404:A:O2'	32:R1:405:U:O5'	2.27	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:R1:730:A:OP1	32:R1:1775:U:O2'	2.23	0.44
34:R3:471:U:H2'	34:R3:472:U:C6	2.52	0.44
34:R3:1131:G:H2'	34:R3:1132:C:H5"	1.97	0.44
2:13:42:ALA:O	10:20:63:ARG:HG2	2.17	0.44
2:13:64:VAL:HG12	2:13:68:LYS:HB2	1.99	0.44
9:2:206:LYS:HB2	32:R1:729:G:C6	2.51	0.44
34:R3:581:G:N1	34:R3:759:A:OP2	2.37	0.44
2:13:92:MET:SD	2:13:95:ARG:NH2	2.89	0.44
12:22:5:ALA:O	32:R1:494:G:O2'	2.29	0.44
19:3:114:LYS:NZ	32:R1:2681:C:OP2	2.44	0.44
27:4:45:ALA:HB3	32:R1:38:A:H4'	1.98	0.44
32:R1:1057:A:N7	32:R1:1086:A:C4	2.85	0.44
6:17:36:THR:HG23	6:17:41:ALA:HB2	1.99	0.44
13:23:61:LEU:HD11	32:R1:1340:U:C2'	2.47	0.44
29:6:53:PRO:HG3	29:6:61:TRP:CE2	2.52	0.44
32:R1:1086:A:H1'	32:R1:1103:A:N6	2.32	0.44
32:R1:1923:U:OP1	35:T:24:U:O2'	2.36	0.44
32:R1:2143:C:N4	32:R1:2144:G:O6	2.51	0.44
32:R1:2725:A:O2'	32:R1:2726:A:H2'	2.17	0.44
33:R2:106:G:H2'	33:R2:107:G:O4'	2.18	0.44
36:Y:142:VAL:HG11	36:Y:163:ARG:HB3	1.99	0.44
36:Y:157:ALA:HB3	36:Y:160:TRP:CZ3	2.53	0.44
27:4:188:MET:HB3	27:4:193:VAL:HG23	1.98	0.44
32:R1:549:G:H2'	32:R1:550:C:C6	2.53	0.44
32:R1:1111:A:N3	32:R1:1111:A:H2'	2.31	0.44
32:R1:1395:A:O2'	32:R1:1396:U:H5"	2.17	0.44
32:R1:2812:G:H2'	32:R1:2813:A:C8	2.52	0.44
36:Y:9:MET:SD	36:Y:11:PHE:CD1	3.10	0.44
36:Y:22:VAL:HG11	36:Y:230:LEU:HD11	1.99	0.44
36:Y:334:LEU:HD12	36:Y:334:LEU:H	1.82	0.44
1:1:6:LYS:HG3	1:1:8:MET:H	1.81	0.44
1:1:67:HIS:CD2	1:1:184:LYS:HB3	2.52	0.44
10:20:5:ARG:HD2	32:R1:1250:G:H5"	1.99	0.44
34:R3:223:A:H2'	34:R3:224:U:H6	1.81	0.44
34:R3:246:A:C2	34:R3:282:A:C5	3.05	0.44
34:R3:1009:U:H2'	34:R3:1010:U:H6	1.82	0.44
34:R3:1326:U:C2	34:R3:1327:C:C5	3.06	0.44
36:Y:306:PHE:CE2	36:Y:308:ARG:HG3	2.52	0.44
10:20:8:ILE:HA	10:20:8:ILE:HD13	1.83	0.44
18:29:8:GLU:O	18:29:60:LYS:NZ	2.48	0.44
21:31:3:LYS:HD3	21:31:3:LYS:HA	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:4:146:VAL:HG23	27:4:167:VAL:HG13	2.00	0.44
32:R1:355:U:H2'	32:R1:356:G:C8	2.51	0.44
32:R1:882:G:H2'	32:R1:883:G:H8	1.83	0.44
32:R1:1383:A:H1'	32:R1:1405:U:O2'	2.17	0.44
32:R1:2577:A:H2'	32:R1:2614:A:N6	2.32	0.44
9:2:13:ARG:NH2	32:R1:1693:U:O2'	2.51	0.44
9:2:177:SER:OG	32:R1:1799:G:N7	2.49	0.44
19:3:149:ASN:HB3	32:R1:2572:A:OP2	2.17	0.44
20:30:6:ILE:HD13	20:30:26:LEU:HD22	1.99	0.44
20:30:23:LEU:HD11	20:30:53:MET:HE1	1.98	0.44
28:5:28:PRO:HB2	28:5:168:LEU:HD22	1.99	0.44
32:R1:3:U:H2'	32:R1:4:U:C6	2.53	0.44
32:R1:414:C:H2'	32:R1:415:A:C8	2.53	0.44
32:R1:1000:A:H2'	32:R1:1001:A:C8	2.53	0.44
32:R1:2515:C:H2'	32:R1:2516:A:H8	1.82	0.44
34:R3:779:C:H2'	34:R3:780:A:O4'	2.18	0.44
34:R3:983:A:H5'	34:R3:984:C:OP2	2.17	0.44
36:Y:212:ARG:HG2	36:Y:237:TYR:CE2	2.53	0.44
4:15:56:PRO:HB2	4:15:58:TYR:CE1	2.53	0.44
28:5:131:VAL:CG2	28:5:151:LEU:H	2.31	0.44
32:R1:511:U:H4'	32:R1:1235:G:H4'	1.99	0.44
32:R1:898:C:H2'	32:R1:899:A:O4'	2.18	0.44
32:R1:2144:G:N2	32:R1:2146:C:O2'	2.51	0.44
32:R1:2158:A:H4'	32:R1:2159:G:O4'	2.18	0.44
32:R1:2834:G:H2'	32:R1:2879:A:N6	2.33	0.44
34:R3:193:C:H2'	34:R3:194:C:C6	2.52	0.44
34:R3:1410:A:H2'	34:R3:1411:C:H6	1.83	0.44
36:Y:195:GLU:HG2	36:Y:214:PHE:CD1	2.50	0.44
36:Y:306:PHE:HB3	36:Y:424:ARG:HG3	1.98	0.44
36:Y:393:TYR:CZ	36:Y:394:GLU:HG3	2.53	0.44
4:15:76:GLU:HG2	32:R1:636:G:H1	1.83	0.43
5:16:1:MET:CE	5:16:44:ARG:HE	2.30	0.43
28:5:73:VAL:HG12	28:5:78:ILE:HD11	2.00	0.43
32:R1:579:G:H2'	32:R1:580:U:C6	2.53	0.43
32:R1:843:G:N2	32:R1:936:A:N3	2.66	0.43
32:R1:2177:C:H2'	32:R1:2178:C:O4'	2.18	0.43
34:R3:26:A:H61	34:R3:558:G:H1'	1.83	0.43
34:R3:50:A:O2'	34:R3:360:G:N2	2.51	0.43
6:17:49:GLU:O	6:17:53:THR:HG23	2.18	0.43
25:35:31:ILE:HD11	32:R1:2391:G:H5'	2.00	0.43
28:5:24:VAL:O	28:5:27:VAL:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:R3:1530:G:H2'	34:R3:1531:A:H8	1.82	0.43
36:Y:66:ILE:HG22	36:Y:176:ILE:HG21	2.01	0.43
36:Y:68:LYS:HB3	36:Y:68:LYS:HE3	1.83	0.43
36:Y:144:ILE:HG23	36:Y:145:PRO:HD2	2.00	0.43
12:22:26:GLY:O	12:22:70:LYS:NZ	2.42	0.43
32:R1:1327:A:H2'	32:R1:1328:A:O4'	2.18	0.43
32:R1:2141:G:H2'	32:R1:2142:A:C8	2.52	0.43
32:R1:2143:C:H2'	32:R1:2144:G:C8	2.53	0.43
32:R1:2314:A:H2'	32:R1:2315:G:C8	2.53	0.43
33:R2:48:U:H2'	33:R2:49:C:H6	1.83	0.43
34:R3:187:G:O2'	34:R3:189:A:N7	2.42	0.43
34:R3:419:C:H1'	34:R3:425:G:N2	2.32	0.43
34:R3:481:G:O2'	34:R3:483:C:N4	2.51	0.43
34:R3:966:G:C2	35:T:34:C:H5'	2.54	0.43
34:R3:1163:A:H2'	34:R3:1164:G:H8	1.83	0.43
36:Y:13:SER:HB3	36:Y:430:ASP:OD1	2.18	0.43
36:Y:36:ASN:ND2	36:Y:469:LEU:HD23	2.33	0.43
36:Y:462:MET:O	36:Y:490:PHE:HA	2.18	0.43
8:19:27:VAL:HA	8:19:82:SER:O	2.19	0.43
10:20:67:ALA:O	10:20:71:ASN:ND2	2.51	0.43
12:22:3:THR:HG21	12:22:58:ALA:HA	2.00	0.43
28:5:59:ILE:HG21	28:5:151:LEU:HD21	2.01	0.43
32:R1:44:A:H2'	32:R1:45:G:O4'	2.18	0.43
32:R1:1511:G:H2'	32:R1:1512:C:C6	2.53	0.43
32:R1:2324:U:H3'	32:R1:2325:G:C5'	2.49	0.43
32:R1:2461:A:H2'	32:R1:2462:C:C6	2.52	0.43
34:R3:662:U:H2'	34:R3:663:A:C8	2.53	0.43
34:R3:1157:A:C2	34:R3:1181:G:C5	3.07	0.43
34:R3:1219:A:H2'	34:R3:1220:G:H8	1.83	0.43
19:3:197:THR:O	32:R1:2820:A:N6	2.51	0.43
21:31:41:HIS:CD2	21:31:43:PHE:HB3	2.53	0.43
27:4:200:LEU:HD12	27:4:200:LEU:HA	1.84	0.43
29:6:136:ASP:HB3	29:6:139:VAL:HB	2.01	0.43
32:R1:538:A:N6	32:R1:555:G:O2'	2.47	0.43
32:R1:1866:A:C6	32:R1:1876:A:N7	2.86	0.43
32:R1:1923:U:H2'	32:R1:1924:C:C6	2.53	0.43
34:R3:180:U:H2'	34:R3:181:A:H8	1.83	0.43
35:T:63:G:H2'	35:T:64:G:H8	1.84	0.43
2:13:96:ARG:NH2	32:R1:2640:G:P	2.92	0.43
30:9:5:LEU:HD23	30:9:8:LYS:O	2.18	0.43
32:R1:421:C:O2'	32:R1:422:A:P	2.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:R1:1060:U:O4'	32:R1:1062:G:H5'	2.17	0.43
32:R1:2158:A:H5"	32:R1:2159:G:O5'	2.19	0.43
34:R3:1121:U:C2	34:R3:1122:U:C5	3.06	0.43
34:R3:1157:A:H4'	34:R3:1158:C:O5'	2.17	0.43
36:Y:106:PRO:HA	36:Y:107:GLU:HA	1.58	0.43
36:Y:267:SER:O	36:Y:271:ARG:HG3	2.19	0.43
1:1:29:LEU:HA	1:1:32:GLU:HG2	2.01	0.43
1:1:51:ASP:OD1	1:1:51:ASP:N	2.50	0.43
6:17:97:ILE:HD11	6:17:113:ILE:HD12	2.01	0.43
10:20:79:ILE:HD13	10:20:79:ILE:HA	1.86	0.43
13:23:61:LEU:HD11	32:R1:1340:U:H2'	2.00	0.43
32:R1:1084:A:N7	32:R1:1085:A:N6	2.67	0.43
34:R3:1355:G:H2'	34:R3:1356:G:C8	2.53	0.43
36:Y:82:LEU:HD12	36:Y:82:LEU:HA	1.64	0.43
14:24:84:PHE:CE1	14:24:93:ARG:HG2	2.53	0.43
27:4:171:ASP:OD2	27:4:172:ALA:N	2.52	0.43
32:R1:81:G:H2'	32:R1:82:U:O4'	2.19	0.43
32:R1:843:G:N2	32:R1:936:A:C4	2.87	0.43
32:R1:2547:A:H2'	32:R1:2548:U:C6	2.54	0.43
34:R3:1412:C:H2'	34:R3:1413:A:C8	2.54	0.43
34:R3:1452:C:H4'	34:R3:1453:G:N2	2.34	0.43
34:R3:1530:G:H2'	34:R3:1531:A:C8	2.54	0.43
36:Y:29:ARG:HD3	36:Y:205:MET:HE1	2.01	0.43
36:Y:33:ILE:HD12	36:Y:237:TYR:CE1	2.49	0.43
36:Y:142:VAL:HG13	36:Y:163:ARG:HD2	2.01	0.43
7:18:33:ARG:HG2	7:18:34:HIS:CD2	2.54	0.43
7:18:51:ALA:HB3	7:18:78:VAL:HG13	2.01	0.43
11:21:74:ILE:HB	11:21:87:GLN:HB3	2.00	0.43
32:R1:64:A:H2'	32:R1:65:U:C6	2.54	0.43
32:R1:161:A:H3'	32:R1:162:U:H5"	2.01	0.43
32:R1:1076:C:H2'	32:R1:1077:A:N9	2.34	0.43
32:R1:1421:G:H1'	32:R1:1494:A:H61	1.84	0.43
32:R1:2233:U:H2'	32:R1:2234:G:C8	2.54	0.43
32:R1:2326:C:O2'	32:R1:2327:A:OP1	2.26	0.43
32:R1:2583:G:H2'	32:R1:2584:U:O4'	2.18	0.43
32:R1:2725:A:O2'	32:R1:2726:A:C8	2.71	0.43
33:R2:72:G:H21	33:R2:104:A:H62	1.66	0.43
34:R3:90:C:H2'	34:R3:91:U:C5	2.54	0.43
34:R3:166:U:H2'	34:R3:167:A:H8	1.84	0.43
34:R3:1316:G:H22	34:R3:1319:A:P	2.42	0.43
9:2:66:PHE:HB3	9:2:150:GLY:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:3:155:VAL:HG21	32:R1:2618:G:H21	1.84	0.43
28:5:136:ILE:HG13	28:5:137:PHE:HD1	1.84	0.43
32:R1:593:U:H2'	32:R1:594:U:H6	1.83	0.43
32:R1:1979:U:O2'	32:R1:1980:G:H5'	2.19	0.43
33:R2:13:G:O2'	33:R2:15:A:H2'	2.19	0.43
34:R3:269:C:N4	34:R3:270:A:H62	2.17	0.43
34:R3:460:A:H2'	34:R3:461:A:C8	2.54	0.43
34:R3:769:G:H4'	34:R3:1513:A:H4'	2.01	0.43
34:R3:865:A:H2'	34:R3:866:C:C6	2.53	0.43
34:R3:925:G:C6	34:R3:927:G:N7	2.87	0.43
34:R3:1315:U:H3'	34:R3:1316:G:C8	2.54	0.43
36:Y:504:ARG:NH2	36:Y:515:ASP:OD2	2.49	0.43
2:13:78:THR:HB	32:R1:2641:G:H5"	1.99	0.42
5:16:47:GLU:OE2	5:16:50:ARG:NH2	2.39	0.42
15:25:2:PHE:HB3	15:25:50:MET:SD	2.58	0.42
16:27:18:ALA:O	16:27:20:ARG:NH1	2.52	0.42
21:31:59:ARG:O	21:31:62:LYS:HG2	2.19	0.42
27:4:45:ALA:HA	27:4:87:ALA:O	2.19	0.42
32:R1:2122:U:O4	32:R1:2176:A:N6	2.52	0.42
32:R1:2157:G:H2'	32:R1:2158:A:N3	2.33	0.42
34:R3:56:U:H2'	34:R3:57:G:C8	2.54	0.42
34:R3:1120:C:H2'	34:R3:1121:U:H6	1.84	0.42
36:Y:2:LEU:HD12	36:Y:60:LEU:HD13	2.00	0.42
7:18:30:ARG:NH2	33:R2:48:U:OP1	2.52	0.42
9:2:48:ILE:HD13	9:2:48:ILE:HG21	1.76	0.42
26:36:32:LYS:HD3	32:R1:2478:A:H5'	2.01	0.42
32:R1:288:U:H2'	32:R1:289:G:C8	2.51	0.42
32:R1:619:G:OP2	32:R1:620:G:N2	2.52	0.42
32:R1:1548:A:H2'	32:R1:1549:A:C8	2.54	0.42
32:R1:2499:C:N4	32:R1:2500:U:O4	2.52	0.42
34:R3:78:A:N6	34:R3:79:G:H21	2.13	0.42
36:Y:89:HIS:HD2	36:Y:92:LEU:H	1.64	0.42
36:Y:452:LEU:HD23	36:Y:452:LEU:HA	1.83	0.42
14:24:60:LYS:HB2	14:24:60:LYS:HE3	1.72	0.42
23:33:33:LEU:HD23	23:33:33:LEU:HA	1.87	0.42
27:4:146:VAL:HA	27:4:185:LYS:O	2.19	0.42
32:R1:1055:G:N2	32:R1:1085:A:N3	2.68	0.42
32:R1:1104:C:H2'	32:R1:1105:U:O4'	2.18	0.42
32:R1:1794:A:H2'	32:R1:1795:C:H6	1.84	0.42
34:R3:20:U:H2'	34:R3:21:G:O4'	2.19	0.42
34:R3:151:A:C5	34:R3:152:A:C8	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:R3:222:C:H2'	34:R3:223:A:H8	1.84	0.42
34:R3:686:U:H2'	34:R3:687:A:H8	1.83	0.42
34:R3:898:G:N2	34:R3:901:A:OP2	2.48	0.42
34:R3:993:G:O2'	34:R3:994:A:N7	2.53	0.42
34:R3:1107:C:C4	34:R3:1108:G:C8	3.08	0.42
34:R3:1225:A:H2'	34:R3:1225:A:N3	2.33	0.42
36:Y:81:VAL:HA	36:Y:84:THR:HG22	2.01	0.42
36:Y:177:LEU:HD12	36:Y:177:LEU:HA	1.82	0.42
2:13:30:THR:HG21	32:R1:1005:C:O2'	2.19	0.42
2:13:64:VAL:CG1	2:13:68:LYS:HB2	2.50	0.42
3:14:15:GLY:O	3:14:47:ILE:HG12	2.19	0.42
9:2:86:ARG:NH1	32:R1:1817:G:OP1	2.50	0.42
9:2:97:ASP:HB3	32:R1:1490:A:H8	1.84	0.42
9:2:259:ASN:ND2	9:2:262:THR:OG1	2.52	0.42
13:23:65:GLY:H	13:23:79:ASP:HB3	1.84	0.42
23:33:4:ILE:HD13	23:33:4:ILE:HA	1.86	0.42
32:R1:30:G:O2'	32:R1:1214:A:N3	2.43	0.42
32:R1:151:C:H2'	32:R1:152:A:C8	2.54	0.42
32:R1:171:U:H2'	32:R1:172:A:C8	2.53	0.42
32:R1:1169:A:H2'	32:R1:1170:C:O4'	2.19	0.42
32:R1:1873:G:H2'	32:R1:1874:C:H6	1.84	0.42
34:R3:773:G:O6	34:R3:807:A:N6	2.52	0.42
36:Y:16:LEU:HD13	36:Y:39:GLY:HA3	2.00	0.42
1:1:59:VAL:N	1:1:165:ASN:HD21	2.11	0.42
10:20:51:GLN:O	10:20:55:GLN:HB3	2.20	0.42
28:5:91:ARG:CZ	33:R2:45:A:H1'	2.49	0.42
29:6:125:PRO:HG2	29:6:129:GLU:OE2	2.19	0.42
32:R1:134:G:H2'	32:R1:135:U:H6	1.85	0.42
32:R1:284:U:O2	32:R1:356:G:N2	2.31	0.42
32:R1:2273:A:H2'	32:R1:2274:A:C8	2.55	0.42
32:R1:2698:U:H2'	32:R1:2699:C:C6	2.55	0.42
34:R3:868:C:H2'	34:R3:869:G:O4'	2.20	0.42
34:R3:1248:A:C6	34:R3:1290:G:C2	3.08	0.42
34:R3:1260:G:H4'	34:R3:1283:U:O2'	2.19	0.42
35:T:29:G:C4	35:T:42:G:N2	2.88	0.42
3:14:41:ILE:HG13	3:14:58:LEU:O	2.19	0.42
12:22:18:ARG:HG3	12:22:76:VAL:HG22	2.02	0.42
32:R1:2557:G:H2'	32:R1:2558:C:C6	2.54	0.42
32:R1:2576:G:O2'	32:R1:2579:C:OP2	2.35	0.42
34:R3:504:C:C2	34:R3:542:G:N2	2.87	0.42
34:R3:676:A:H2'	34:R3:677:U:H6	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:Y:20:ILE:HD13	36:Y:230:LEU:HD23	2.00	0.42
36:Y:389:GLN:HB3	36:Y:463:ASP:OD2	2.19	0.42
36:Y:462:MET:HB2	36:Y:490:PHE:HB2	2.02	0.42
36:Y:488:LEU:HD11	36:Y:490:PHE:HB3	2.00	0.42
6:17:72:ASP:O	6:17:76:VAL:HG23	2.20	0.42
20:30:13:ILE:HD12	32:R1:989:G:C8	2.55	0.42
30:9:53:GLU:O	30:9:57:LYS:HD2	2.19	0.42
32:R1:628:G:C6	32:R1:636:G:C2	3.08	0.42
32:R1:1103:A:H5"	32:R1:1104:C:C5	2.55	0.42
32:R1:1485:U:H2'	32:R1:1486:U:H6	1.85	0.42
32:R1:2136:G:H2'	32:R1:2137:U:O4'	2.19	0.42
34:R3:131:A:H2'	34:R3:132:C:C6	2.54	0.42
34:R3:176:C:H2'	34:R3:177:G:N3	2.35	0.42
34:R3:235:C:H2'	34:R3:236:A:C8	2.54	0.42
34:R3:839:C:H2'	34:R3:840:C:H6	1.85	0.42
34:R3:922:G:N3	34:R3:1398:A:H2	2.18	0.42
34:R3:1176:A:H2'	34:R3:1177:G:C8	2.55	0.42
36:Y:7:VAL:HG23	36:Y:8:THR:H	1.83	0.42
36:Y:399:LEU:HD13	36:Y:407:GLN:NE2	2.35	0.42
4:15:10:GLU:HG3	32:R1:1175:A:N1	2.34	0.42
5:16:86:LYS:NZ	32:R1:955:U:OP1	2.40	0.42
9:2:246:PRO:HG2	9:2:247:TRP:CZ3	2.54	0.42
28:5:39:VAL:HG22	28:5:84:ILE:O	2.19	0.42
32:R1:1593:A:H2'	32:R1:1594:U:C6	2.55	0.42
34:R3:392:C:H2'	34:R3:393:A:H5"	2.02	0.42
36:Y:227:TYR:HE2	36:Y:231:ARG:NH2	2.18	0.42
36:Y:366:VAL:HG11	36:Y:386:TYR:CE2	2.55	0.42
1:1:45:ALA:HB2	1:1:172:HIS:HB3	2.00	0.42
11:21:48:LYS:HZ2	11:21:49:ILE:H	1.65	0.42
16:27:55:ARG:NH1	32:R1:2364:C:OP1	2.48	0.42
28:5:59:ILE:HD11	28:5:134:GLN:HB2	2.02	0.42
32:R1:1094:U:N3	32:R1:1096:A:H3'	2.35	0.42
32:R1:1412:U:H2'	32:R1:1413:A:H8	1.83	0.42
32:R1:1667:G:O2'	32:R1:1991:U:O4	2.33	0.42
32:R1:1794:A:H2'	32:R1:1795:C:C6	2.54	0.42
32:R1:2155:U:OP2	32:R1:2157:G:N1	2.53	0.42
32:R1:2328:A:H2'	32:R1:2329:U:H6	1.80	0.42
32:R1:2572:A:OP1	32:R1:2574:G:H4'	2.20	0.42
34:R3:1343:G:H2'	34:R3:1344:C:C6	2.55	0.42
34:R3:1507:A:H2'	34:R3:1508:A:C8	2.55	0.42
35:T:20:H2U:OP2	35:T:20:H2U:O2	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:Y:449:PHE:O	36:Y:453:MET:HG3	2.19	0.42
2:13:36:LEU:O	2:13:51:GLY:HA3	2.20	0.42
3:14:71:ARG:HD3	3:14:71:ARG:HA	1.74	0.42
15:25:62:THR:HA	15:25:70:ILE:O	2.20	0.42
28:5:116:LEU:N	28:5:175:PRO:O	2.50	0.42
30:9:3:VAL:HG13	30:9:36:ALA:HB1	2.02	0.42
30:9:45:GLU:O	30:9:50:ARG:HG3	2.20	0.42
32:R1:160:A:N3	32:R1:2208:C:O2'	2.46	0.42
32:R1:1441:G:H2'	32:R1:1442:U:C6	2.54	0.42
32:R1:1443:U:H2'	32:R1:1444:G:C8	2.53	0.42
32:R1:2144:G:N1	32:R1:2148:G:O6	2.52	0.42
34:R3:391:G:H2'	34:R3:392:C:O4'	2.20	0.42
34:R3:573:A:N3	34:R3:883:C:O2'	2.42	0.42
34:R3:984:C:H2'	34:R3:985:C:H6	1.85	0.42
34:R3:1414:U:H2'	34:R3:1415:G:H8	1.85	0.42
12:22:87:PRO:HB3	32:R1:1614:A:C6	2.54	0.41
27:4:118:LEU:HD11	27:4:188:MET:HG3	2.01	0.41
30:9:76:GLU:O	30:9:143:ILE:HG22	2.20	0.41
32:R1:1989:G:H2'	32:R1:1990:C:O4'	2.20	0.41
34:R3:355:C:C4	34:R3:356:A:N7	2.88	0.41
36:Y:9:MET:CE	36:Y:11:PHE:HE1	2.33	0.41
36:Y:70:ARG:O	36:Y:165:LEU:HD23	2.20	0.41
6:17:12:ARG:HG2	6:17:16:HIS:CE1	2.55	0.41
15:25:4:ILE:HD11	15:25:63:ILE:HD11	2.01	0.41
22:32:11:LYS:HE3	22:32:11:LYS:HB3	1.87	0.41
30:9:84:ALA:HB2	30:9:90:LEU:HD23	2.02	0.41
32:R1:640:C:H2'	32:R1:641:U:H6	1.85	0.41
32:R1:703:U:H2'	32:R1:704:G:O4'	2.20	0.41
32:R1:843:G:C6	32:R1:936:A:N1	2.88	0.41
32:R1:971:G:O2'	32:R1:983:A:N3	2.43	0.41
32:R1:1817:G:N3	32:R1:1817:G:H2'	2.35	0.41
34:R3:976:G:OP2	34:R3:1358:U:O2'	2.38	0.41
36:Y:80:THR:OG1	36:Y:151:GLY:O	2.26	0.41
36:Y:414:ASP:OD1	36:Y:417:ALA:N	2.41	0.41
36:Y:512:ARG:HE	36:Y:512:ARG:HB2	1.73	0.41
10:20:19:GLN:H	10:20:19:GLN:HG3	1.74	0.41
15:25:86:LEU:HD13	15:25:89:ILE:HD11	2.01	0.41
16:27:72:LYS:HB3	16:27:72:LYS:HE2	1.73	0.41
28:5:22:ASN:N	28:5:22:ASN:OD1	2.52	0.41
28:5:169:LEU:O	28:5:174:PHE:HB2	2.21	0.41
32:R1:963:U:H2'	32:R1:964:C:H6	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:R1:2031:A:N3	32:R1:2455:G:O2'	2.37	0.41
34:R3:79:G:H2'	34:R3:80:A:N7	2.35	0.41
34:R3:351:G:H8	34:R3:351:G:OP2	2.03	0.41
34:R3:580:C:H2'	34:R3:581:G:O4'	2.21	0.41
34:R3:1283:U:H2'	34:R3:1284:C:C6	2.55	0.41
36:Y:196:GLN:OE1	36:Y:197:VAL:HG23	2.19	0.41
36:Y:418:VAL:HG23	36:Y:454:MET:CE	2.51	0.41
36:Y:507:GLU:OE2	36:Y:523:TYR:OH	2.21	0.41
9:2:140:VAL:HG12	9:2:141:HIS:H	1.85	0.41
10:20:5:ARG:NH1	32:R1:1251:C:OP2	2.53	0.41
32:R1:2236:U:H2'	32:R1:2237:G:O4'	2.20	0.41
32:R1:2766:A:H2'	32:R1:2766:A:N3	2.36	0.41
32:R1:2898:U:H2'	32:R1:2899:A:H8	1.85	0.41
34:R3:1178:G:N2	34:R3:1181:G:OP2	2.53	0.41
34:R3:1306:A:N6	34:R3:1331:G:O2'	2.53	0.41
34:R3:1327:C:C2	34:R3:1328:C:C5	3.08	0.41
9:2:198:GLU:HG2	9:2:201:LEU:HD12	2.03	0.41
20:30:38:GLU:O	20:30:43:ILE:HG21	2.20	0.41
21:31:7:PRO:HG2	28:5:61:GLY:HA2	2.03	0.41
21:31:30:HIS:ND1	21:31:30:HIS:O	2.52	0.41
28:5:35:LEU:H	28:5:35:LEU:HD23	1.85	0.41
30:9:46:PHE:O	30:9:50:ARG:HB2	2.19	0.41
32:R1:116:C:O2'	32:R1:126:A:N3	2.43	0.41
32:R1:2175:C:H2'	32:R1:2176:A:O4'	2.21	0.41
32:R1:2364:C:H2'	32:R1:2365:G:O4'	2.21	0.41
32:R1:2532:G:N2	32:R1:2663:G:O2'	2.52	0.41
32:R1:2800:A:C2	32:R1:2895:G:H1'	2.55	0.41
34:R3:524:G:H2'	34:R3:525:C:C6	2.55	0.41
36:Y:197:VAL:HG13	36:Y:201:ARG:HH12	1.84	0.41
7:18:30:ARG:HH22	33:R2:48:U:P	2.44	0.41
8:19:47:ILE:HD11	8:19:61:ARG:HD2	2.01	0.41
9:2:219:VAL:HG21	32:R1:782:A:C8	2.56	0.41
11:21:79:ARG:H	11:21:79:ARG:HG3	1.62	0.41
16:27:30:SER:O	16:27:30:SER:OG	2.35	0.41
24:34:31:LEU:HG	24:34:42:LEU:HD12	2.03	0.41
32:R1:359:G:H2'	32:R1:360:U:C6	2.56	0.41
32:R1:2859:G:H2'	32:R1:2860:A:C8	2.55	0.41
34:R3:474:G:N3	34:R3:474:G:H2'	2.34	0.41
34:R3:842:U:H5"	34:R3:846:G:C6	2.55	0.41
34:R3:1238:A:H2	34:R3:1241:G:N3	2.19	0.41
34:R3:1325:C:H2'	34:R3:1326:U:H6	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:R3:1442:G:H2'	34:R3:1443:C:C6	2.55	0.41
36:Y:191:ILE:HG22	36:Y:195:GLU:OE1	2.20	0.41
36:Y:315:LEU:HD21	36:Y:381:ASN:HB2	2.01	0.41
36:Y:325:LEU:HD13	36:Y:338:LEU:HD23	2.03	0.41
5:16:69:PRO:HA	5:16:94:ALA:HB2	2.02	0.41
9:2:70:LYS:HB2	9:2:101:ARG:NH2	2.35	0.41
27:4:145:ASP:HB3	27:4:184:ASP:HB3	2.01	0.41
32:R1:1075:C:H5'	32:R1:1076:C:C5	2.56	0.41
32:R1:1385:A:O2'	32:R1:1396:U:O2	2.37	0.41
32:R1:1715:G:HO2'	32:R1:1716:U:H6	1.63	0.41
33:R2:3:C:H2'	33:R2:4:C:C6	2.56	0.41
34:R3:424:G:H2'	34:R3:425:G:C4	2.56	0.41
34:R3:575:G:O2'	34:R3:821:G:OP2	2.20	0.41
34:R3:984:C:H2'	34:R3:985:C:C6	2.56	0.41
34:R3:1213:A:N6	34:R3:1215:G:N3	2.68	0.41
36:Y:5:SER:HB2	36:Y:57:ASN:OD1	2.19	0.41
32:R1:1057:A:N3	32:R1:1057:A:H2'	2.35	0.41
32:R1:1444:G:C4	32:R1:1445:G:C8	3.09	0.41
32:R1:2097:A:H2'	32:R1:2098:U:H6	1.86	0.41
34:R3:604:G:H2'	34:R3:605:U:O4'	2.20	0.41
1:1:31:LYS:HE3	1:1:31:LYS:HB3	1.63	0.41
3:14:8:LEU:HD22	3:14:84:CYS:HB3	2.02	0.41
7:18:74:VAL:HG13	7:18:106:LEU:HD13	2.02	0.41
9:2:47:ARG:NH1	32:R1:774:G:OP1	2.54	0.41
11:21:80:ARG:NH1	32:R1:571:U:OP1	2.54	0.41
16:27:65:GLY:HA3	16:27:83:GLU:O	2.21	0.41
19:3:56:LYS:HE3	32:R1:2830:C:H5"	2.03	0.41
25:35:3:ILE:HD11	32:R1:592:A:C2	2.56	0.41
26:36:4:ARG:HB3	32:R1:2466:C:OP1	2.21	0.41
30:9:76:GLU:HA	30:9:142:VAL:HG13	2.03	0.41
30:9:129:GLU:OE1	30:9:129:GLU:N	2.54	0.41
32:R1:222:A:H61	32:R1:232:G:H1'	1.86	0.41
32:R1:272:A:H2'	32:R1:273:G:H8	1.84	0.41
32:R1:851:C:H2'	32:R1:852:U:H6	1.86	0.41
32:R1:852:U:H2'	32:R1:853:C:C6	2.56	0.41
32:R1:1197:G:H2'	32:R1:1198:U:H6	1.86	0.41
32:R1:1310:G:N2	32:R1:1313:U:C4	2.89	0.41
32:R1:2078:C:H2'	32:R1:2079:U:C6	2.56	0.41
32:R1:2247:A:H2'	32:R1:2248:C:C6	2.54	0.41
32:R1:2281:A:C2'	32:R1:2282:G:H5'	2.50	0.41
32:R1:2304:G:N2	32:R1:2312:U:H3	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:R3:320:A:H2'	34:R3:321:A:C8	2.56	0.41
34:R3:1096:C:H2'	34:R3:1097:C:C6	2.56	0.41
34:R3:1118:U:H1'	34:R3:1179:A:C5	2.55	0.41
34:R3:1118:U:H1'	34:R3:1179:A:C4	2.56	0.41
34:R3:1442:G:H2'	34:R3:1443:C:H6	1.85	0.41
34:R3:1512:U:H2'	34:R3:1513:A:C8	2.55	0.41
35:T:50:U:H3	35:T:64:G:H1	1.68	0.41
36:Y:191:ILE:O	36:Y:195:GLU:HG3	2.21	0.41
36:Y:497:PHE:O	36:Y:501:LEU:HB2	2.20	0.41
1:1:196:LEU:HD23	1:1:196:LEU:HA	1.88	0.41
18:29:57:LEU:HD23	18:29:57:LEU:HA	1.79	0.41
27:4:44:ARG:HH11	27:4:87:ALA:CB	2.34	0.41
32:R1:1631:G:N1	32:R1:1634:A:OP2	2.52	0.41
33:R2:44:G:H1'	33:R2:47:C:H42	1.86	0.41
34:R3:208:U:O2'	34:R3:211:G:N1	2.50	0.41
34:R3:257:G:H2'	34:R3:258:G:H8	1.86	0.41
34:R3:456:A:H2'	34:R3:457:G:O4'	2.20	0.41
34:R3:472:U:H2'	34:R3:473:U:C6	2.56	0.41
34:R3:951:G:C6	34:R3:1231:G:C6	3.09	0.41
1:1:179:ASP:OD1	1:1:179:ASP:N	2.54	0.40
15:25:56:PHE:HD2	15:25:57:TYR:CE1	2.38	0.40
26:36:11:CYS:HG	26:36:33:HIS:CE1	2.38	0.40
30:9:30:LEU:HD23	30:9:30:LEU:HA	1.89	0.40
32:R1:271:G:C6	32:R1:367:G:N1	2.89	0.40
32:R1:852:U:H2'	32:R1:853:C:H6	1.85	0.40
32:R1:1910:G:N2	32:R1:1921:G:C4	2.90	0.40
32:R1:2262:U:H2'	32:R1:2263:C:H6	1.86	0.40
32:R1:2379:G:H2'	32:R1:2380:C:C6	2.56	0.40
33:R2:45:A:C4	33:R2:46:A:C8	3.10	0.40
34:R3:371:A:O2'	34:R3:373:A:N7	2.48	0.40
34:R3:420:U:H2'	34:R3:422:C:O4'	2.21	0.40
36:Y:84:THR:O	36:Y:168:GLN:NE2	2.51	0.40
36:Y:403:GLU:O	36:Y:407:GLN:OE1	2.39	0.40
19:3:4:LEU:HD12	19:3:101:PHE:CE2	2.56	0.40
29:6:157:LYS:HE2	29:6:157:LYS:HB3	1.90	0.40
32:R1:629:G:N3	32:R1:639:U:O2'	2.54	0.40
32:R1:1178:C:H2'	32:R1:1179:G:H8	1.84	0.40
34:R3:190:A:H2'	34:R3:191:G:O4'	2.20	0.40
34:R3:923:A:H2'	34:R3:924:C:C6	2.57	0.40
34:R3:1162:C:H2'	34:R3:1163:A:C8	2.51	0.40
35:T:14:G:C2	35:T:59:A:N1	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:Y:40:LYS:H	36:Y:40:LYS:HG2	1.64	0.40
36:Y:257:LYS:HD2	36:Y:257:LYS:HA	1.92	0.40
1:1:194:VAL:O	1:1:198:LYS:HG3	2.21	0.40
5:16:57:VAL:C	5:16:58:LYS:HG3	2.42	0.40
12:22:20:VAL:HG11	12:22:44:ALA:HA	2.03	0.40
13:23:80:TRP:CD1	13:23:80:TRP:N	2.89	0.40
21:31:47:LYS:HE3	28:5:114:ARG:HD2	2.03	0.40
29:6:108:PHE:O	32:R1:2666:C:N4	2.55	0.40
32:R1:231:A:H2'	32:R1:232:G:O4'	2.21	0.40
32:R1:306:U:O4	32:R1:310:A:N7	2.54	0.40
32:R1:376:G:H2'	32:R1:377:G:H8	1.87	0.40
32:R1:967:U:H2'	32:R1:968:C:C6	2.56	0.40
32:R1:1604:C:O2'	32:R1:1610:A:N1	2.46	0.40
32:R1:2186:G:H2'	32:R1:2187:U:O4'	2.22	0.40
32:R1:2505:G:O2'	32:R1:2506:U:H5"	2.21	0.40
34:R3:599:C:H2'	34:R3:600:A:H8	1.87	0.40
34:R3:783:C:H2'	34:R3:784:A:H8	1.86	0.40
34:R3:1160:G:C2	34:R3:1161:C:C6	3.10	0.40
34:R3:1516:G:H2'	34:R3:1518:A:OP2	2.21	0.40
36:Y:116:VAL:HA	36:Y:119:LEU:HB2	2.02	0.40
36:Y:340:LEU:HD13	36:Y:506:LEU:HD13	2.02	0.40
5:16:73:ILE:HG13	5:16:93:VAL:HG13	2.04	0.40
8:19:28:LYS:HD3	8:19:39:LEU:HD21	2.02	0.40
32:R1:312:G:C2	32:R1:313:G:C8	3.10	0.40
32:R1:2315:G:H2'	32:R1:2316:G:H8	1.87	0.40
32:R1:2902:C:H3'	32:R1:2903:U:H5"	2.02	0.40
34:R3:142:G:O2'	34:R3:196:A:N1	2.45	0.40
34:R3:162:A:H2'	34:R3:163:C:O4'	2.21	0.40
34:R3:1165:U:H2'	34:R3:1166:G:O4'	2.20	0.40
34:R3:1534:A:C6	34:R3:1535:C:H1'	2.56	0.40
36:Y:275:ASN:O	36:Y:279:SER:HB3	2.21	0.40
36:Y:340:LEU:HD13	36:Y:506:LEU:CD1	2.51	0.40
36:Y:351:LEU:HA	36:Y:491:VAL:HG23	2.04	0.40
2:13:82:GLY:HA2	32:R1:1131:G:OP1	2.20	0.40
7:18:85:LYS:HB2	7:18:85:LYS:HE2	1.86	0.40
27:4:172:ALA:HB1	27:4:196:VAL:HG23	2.02	0.40
29:6:163:TYR:HB2	29:6:166:GLU:HB3	2.04	0.40
32:R1:48:G:N1	32:R1:177:G:OP2	2.49	0.40
32:R1:580:U:H2'	32:R1:581:C:C6	2.57	0.40
32:R1:1482:G:H2'	32:R1:1483:G:H8	1.86	0.40
32:R1:1636:U:H2'	32:R1:1637:A:C8	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:R3:299:G:H2'	34:R3:300:A:C8	2.56	0.40
34:R3:337:G:H2'	34:R3:338:A:C8	2.57	0.40
34:R3:961:U:OP2	34:R3:1223:C:O2'	2.30	0.40
34:R3:1020:G:H2'	34:R3:1021:A:C8	2.57	0.40
36:Y:41:SER:N	59:Y:601:ATP:O1A	2.45	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	218/220 (99%)	199 (91%)	19 (9%)	0	100	100
2	13	140/142 (99%)	134 (96%)	6 (4%)	0	100	100
3	14	120/122 (98%)	109 (91%)	11 (9%)	0	100	100
4	15	142/144 (99%)	127 (89%)	15 (11%)	0	100	100
5	16	134/136 (98%)	126 (94%)	8 (6%)	0	100	100
6	17	118/120 (98%)	107 (91%)	11 (9%)	0	100	100
7	18	114/116 (98%)	109 (96%)	5 (4%)	0	100	100
8	19	112/114 (98%)	100 (89%)	12 (11%)	0	100	100
9	2	269/271 (99%)	247 (92%)	22 (8%)	0	100	100
10	20	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
11	21	101/103 (98%)	91 (90%)	10 (10%)	0	100	100
12	22	108/110 (98%)	101 (94%)	7 (6%)	0	100	100
13	23	91/93 (98%)	81 (89%)	10 (11%)	0	100	100
14	24	100/102 (98%)	86 (86%)	14 (14%)	0	100	100
15	25	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
16	27	73/75 (97%)	70 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	28	75/77 (97%)	73 (97%)	2 (3%)	0	100	100
18	29	61/63 (97%)	61 (100%)	0	0	100	100
19	3	207/209 (99%)	186 (90%)	21 (10%)	0	100	100
20	30	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
21	31	64/66 (97%)	57 (89%)	7 (11%)	0	100	100
22	32	54/56 (96%)	49 (91%)	5 (9%)	0	100	100
23	33	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
24	34	44/46 (96%)	39 (89%)	5 (11%)	0	100	100
25	35	62/64 (97%)	56 (90%)	6 (10%)	0	100	100
26	36	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
27	4	199/201 (99%)	186 (94%)	13 (6%)	0	100	100
28	5	175/177 (99%)	158 (90%)	17 (10%)	0	100	100
29	6	174/176 (99%)	164 (94%)	10 (6%)	0	100	100
30	9	147/149 (99%)	129 (88%)	16 (11%)	2 (1%)	9	34
36	Y	528/530 (100%)	475 (90%)	49 (9%)	4 (1%)	16	46
37	sb	216/218 (99%)	193 (89%)	22 (10%)	1 (0%)	25	56
38	sc	204/206 (99%)	193 (95%)	11 (5%)	0	100	100
39	sd	203/205 (99%)	185 (91%)	17 (8%)	1 (0%)	25	56
40	se	155/157 (99%)	129 (83%)	24 (16%)	2 (1%)	10	36
41	sf	98/100 (98%)	88 (90%)	10 (10%)	0	100	100
42	sg	149/151 (99%)	146 (98%)	3 (2%)	0	100	100
43	sh	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
44	si	125/127 (98%)	111 (89%)	12 (10%)	2 (2%)	8	32
45	sj	96/98 (98%)	86 (90%)	9 (9%)	1 (1%)	13	42
46	sk	114/116 (98%)	105 (92%)	9 (8%)	0	100	100
47	sl	121/123 (98%)	97 (80%)	24 (20%)	0	100	100
48	sm	112/114 (98%)	96 (86%)	16 (14%)	0	100	100
49	sn	98/100 (98%)	81 (83%)	17 (17%)	0	100	100
50	so	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
51	sp	80/82 (98%)	68 (85%)	12 (15%)	0	100	100
52	sq	78/80 (98%)	68 (87%)	10 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
53	sr	63/65 (97%)	59 (94%)	4 (6%)	0	100 100
54	ss	78/80 (98%)	73 (94%)	5 (6%)	0	100 100
55	st	83/85 (98%)	79 (95%)	3 (4%)	1 (1%)	11 38
56	su	68/70 (97%)	65 (96%)	3 (4%)	0	100 100
All	All	6331/6433 (98%)	5781 (91%)	536 (8%)	14 (0%)	45 71

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
36	Y	145	PRO
36	Y	433	LYS
37	sb	11	ALA
44	si	57	VAL
30	9	8	LYS
30	9	9	VAL
36	Y	93	TRP
36	Y	253	ALA
39	sd	30	LYS
40	se	122	VAL
40	se	121	ASN
44	si	114	LYS
55	st	3	ILE
45	sj	57	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	1	106/171 (62%)	105 (99%)	1 (1%)	75 85
2	13	116/116 (100%)	113 (97%)	3 (3%)	41 66
3	14	103/103 (100%)	98 (95%)	5 (5%)	21 49
4	15	103/103 (100%)	101 (98%)	2 (2%)	52 72
5	16	109/109 (100%)	105 (96%)	4 (4%)	29 56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	17	100/100 (100%)	98 (98%)	2 (2%)	50 71
7	18	86/86 (100%)	84 (98%)	2 (2%)	45 68
8	19	99/99 (100%)	95 (96%)	4 (4%)	27 55
9	2	216/216 (100%)	210 (97%)	6 (3%)	38 64
10	20	89/89 (100%)	89 (100%)	0	100 100
11	21	84/84 (100%)	84 (100%)	0	100 100
12	22	93/93 (100%)	93 (100%)	0	100 100
13	23	80/80 (100%)	77 (96%)	3 (4%)	28 56
14	24	83/83 (100%)	81 (98%)	2 (2%)	44 68
15	25	78/78 (100%)	77 (99%)	1 (1%)	65 79
16	27	57/57 (100%)	52 (91%)	5 (9%)	8 28
17	28	67/67 (100%)	66 (98%)	1 (2%)	60 77
18	29	55/55 (100%)	55 (100%)	0	100 100
19	3	164/164 (100%)	160 (98%)	4 (2%)	44 68
20	30	48/48 (100%)	48 (100%)	0	100 100
21	31	59/59 (100%)	57 (97%)	2 (3%)	32 59
22	32	47/47 (100%)	47 (100%)	0	100 100
23	33	45/45 (100%)	44 (98%)	1 (2%)	47 69
24	34	38/38 (100%)	36 (95%)	2 (5%)	19 47
25	35	51/51 (100%)	51 (100%)	0	100 100
26	36	34/34 (100%)	33 (97%)	1 (3%)	37 63
27	4	165/165 (100%)	161 (98%)	4 (2%)	44 68
28	5	148/148 (100%)	143 (97%)	5 (3%)	32 59
29	6	137/137 (100%)	133 (97%)	4 (3%)	37 63
30	9	114/114 (100%)	109 (96%)	5 (4%)	24 52
36	Y	456/456 (100%)	438 (96%)	18 (4%)	27 55
37	sb	180/180 (100%)	177 (98%)	3 (2%)	56 74
38	sc	170/170 (100%)	169 (99%)	1 (1%)	84 90
39	sd	172/172 (100%)	168 (98%)	4 (2%)	45 68
40	se	119/119 (100%)	118 (99%)	1 (1%)	79 87
41	sf	87/87 (100%)	84 (97%)	3 (3%)	32 59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	sg	124/124 (100%)	120 (97%)	4 (3%)	34	61
43	sh	104/104 (100%)	101 (97%)	3 (3%)	37	63
44	si	105/105 (100%)	99 (94%)	6 (6%)	17	44
45	sj	86/86 (100%)	84 (98%)	2 (2%)	45	68
46	sk	89/89 (100%)	86 (97%)	3 (3%)	32	59
47	sl	103/103 (100%)	100 (97%)	3 (3%)	37	63
48	sm	92/92 (100%)	88 (96%)	4 (4%)	25	53
49	sn	83/83 (100%)	79 (95%)	4 (5%)	21	50
50	so	76/76 (100%)	76 (100%)	0	100	100
51	sp	65/65 (100%)	63 (97%)	2 (3%)	35	61
52	sq	74/74 (100%)	73 (99%)	1 (1%)	62	78
53	sr	56/56 (100%)	55 (98%)	1 (2%)	54	74
54	ss	71/71 (100%)	69 (97%)	2 (3%)	38	64
55	st	65/65 (100%)	62 (95%)	3 (5%)	23	52
56	su	60/60 (100%)	60 (100%)	0	100	100
All	All	5211/5276 (99%)	5074 (97%)	137 (3%)	42	66

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	218	MET
2	13	1	MET
2	13	49	ASP
2	13	128	ASN
3	14	18	ARG
3	14	23	LYS
3	14	32	TYR
3	14	73	ASP
3	14	89	ASN
4	15	42	SER
4	15	48	ARG
5	16	13	HIS
5	16	34	LYS
5	16	70	ASP
5	16	136	MET
6	17	2	ARG
6	17	100	CYS

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Mol	Chain	Res	Type
7	18	81	ARG
7	18	85	LYS
8	19	65	ASN
8	19	70	GLU
8	19	108	ARG
8	19	110	LYS
9	2	37	SER
9	2	38	LYS
9	2	65	ASP
9	2	156	SER
9	2	212	TRP
9	2	258	SER
13	23	3	ARG
13	23	5	GLU
13	23	78	SER
14	24	29	SER
14	24	80	ASP
15	25	5	ASN
16	27	30	SER
16	27	50	ASN
16	27	53	CYS
16	27	62	LYS
16	27	76	ASN
17	28	34	SER
19	3	89	GLU
19	3	95	SER
19	3	181	ASP
19	3	200	ASP
21	31	16	CYS
21	31	44	PHE
23	33	52	LYS
24	34	14	ARG
24	34	41	ARG
26	36	12	ARG
27	4	44	ARG
27	4	55	SER
27	4	114	ARG
27	4	127	GLU
28	5	5	ASP
28	5	55	ASP
28	5	112	ASP
28	5	113	PHE

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Mol	Chain	Res	Type
28	5	174	PHE
29	6	29	ASN
29	6	44	HIS
29	6	124	CYS
29	6	166	GLU
30	9	11	ASN
30	9	14	SER
30	9	42	LYS
30	9	75	LEU
30	9	112	LYS
36	Y	68	LYS
36	Y	79	PHE
36	Y	127	ASP
36	Y	150	TYR
36	Y	171	PHE
36	Y	196	GLN
36	Y	227	TYR
36	Y	335	PHE
36	Y	340	LEU
36	Y	351	LEU
36	Y	377	LYS
36	Y	402	PHE
36	Y	408	TRP
36	Y	426	LEU
36	Y	494	ASP
36	Y	495	ARG
36	Y	504	ARG
36	Y	512	ARG
37	sb	20	ARG
37	sb	22	TRP
37	sb	89	PHE
38	sc	133	MET
39	sd	25	ARG
39	sd	28	ASP
39	sd	31	CYS
39	sd	112	GLU
40	se	72	ASN
41	sf	11	HIS
41	sf	63	ASN
41	sf	82	ASP
42	sg	11	LYS
42	sg	33	ASP

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Mol	Chain	Res	Type
42	sg	95	ARG
42	sg	96	ARG
43	sh	47	ASP
43	sh	88	LYS
43	sh	112	ASP
44	si	17	ARG
44	si	30	ASN
44	si	48	ARG
44	si	55	ASP
44	si	89	TYR
44	si	126	PHE
45	sj	14	ASP
45	sj	66	GLU
46	sk	39	ASN
46	sk	69	CYS
46	sk	120	CYS
47	sl	11	ARG
47	sl	37	TYR
47	sl	113	ARG
48	sm	46	GLU
48	sm	62	PHE
48	sm	92	ARG
48	sm	106	ARG
49	sn	17	ASP
49	sn	20	PHE
49	sn	63	CYS
49	sn	88	MET
51	sp	12	LYS
51	sp	44	SER
52	sq	50	ASN
53	sr	10	CYS
54	ss	54	ARG
54	ss	60	PHE
55	st	7	LYS
55	st	27	MET
55	st	65	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	58	ASN
1	1	165	ASN

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Mol	Chain	Res	Type
1	1	168	ASN
2	13	128	ASN
19	3	49	GLN
36	Y	36	ASN
36	Y	89	HIS
36	Y	185	ASN
36	Y	311	GLN
36	Y	354	ASN
41	sf	17	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
31	M	8/9 (88%)	1 (12%)	0
32	R1	2901/2903 (99%)	490 (16%)	10 (0%)
33	R2	118/119 (99%)	17 (14%)	1 (0%)
34	R3	1536/1539 (99%)	284 (18%)	3 (0%)
35	T	75/77 (97%)	22 (29%)	3 (4%)
All	All	4638/4647 (99%)	814 (17%)	17 (0%)

All (814) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
31	M	7	A
32	R1	10	A
32	R1	34	U
32	R1	35	G
32	R1	36	G
32	R1	45	G
32	R1	46	G
32	R1	50	U
32	R1	51	G
32	R1	63	A
32	R1	71	A
32	R1	74	A
32	R1	75	G
32	R1	96	C
32	R1	102	U
32	R1	103	A
32	R1	118	A
32	R1	119	A

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Mol	Chain	Res	Type
32	R1	120	U
32	R1	125	A
32	R1	131	A
32	R1	138	U
32	R1	139	U
32	R1	140	C
32	R1	141	G
32	R1	142	A
32	R1	162	U
32	R1	166	U
32	R1	181	A
32	R1	196	A
32	R1	199	A
32	R1	203	A
32	R1	204	A
32	R1	215	G
32	R1	216	A
32	R1	218	A
32	R1	221	A
32	R1	222	A
32	R1	223	A
32	R1	226	A
32	R1	228	C
32	R1	230	G
32	R1	233	A
32	R1	241	A
32	R1	248	G
32	R1	255	A
32	R1	265	A
32	R1	266	G
32	R1	273	G
32	R1	278	A
32	R1	284	U
32	R1	291	G
32	R1	323	C
32	R1	324	A
32	R1	329	G
32	R1	330	A
32	R1	361	G
32	R1	362	A
32	R1	369	U
32	R1	371	A

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Mol	Chain	Res	Type
32	R1	372	G
32	R1	373	U
32	R1	386	G
32	R1	387	U
32	R1	395	U
32	R1	396	G
32	R1	404	A
32	R1	405	U
32	R1	406	G
32	R1	411	G
32	R1	417	C
32	R1	422	A
32	R1	424	G
32	R1	443	A
32	R1	448	U
32	R1	457	A
32	R1	466	A
32	R1	473	G
32	R1	481	G
32	R1	491	G
32	R1	505	A
32	R1	506	G
32	R1	509	C
32	R1	510	C
32	R1	531	C
32	R1	532	A
32	R1	533	G
32	R1	545	U
32	R1	546	U
32	R1	547	A
32	R1	548	G
32	R1	553	G
32	R1	557	C
32	R1	562	U
32	R1	563	A
32	R1	573	U
32	R1	575	A
32	R1	586	A
32	R1	603	A
32	R1	613	A
32	R1	614	A
32	R1	627	A

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Mol	Chain	Res	Type
32	R1	634	C
32	R1	637	A
32	R1	644	A
32	R1	645	C
32	R1	647	G
32	R1	653	U
32	R1	654	A
32	R1	669	G
32	R1	670	A
32	R1	686	U
32	R1	730	A
32	R1	738	G
32	R1	747	U
32	R1	764	A
32	R1	765	C
32	R1	775	G
32	R1	776	G
32	R1	782	A
32	R1	784	G
32	R1	785	G
32	R1	805	G
32	R1	812	C
32	R1	819	A
32	R1	827	U
32	R1	845	A
32	R1	846	U
32	R1	847	U
32	R1	857	G
32	R1	859	G
32	R1	877	A
32	R1	883	G
32	R1	885	C
32	R1	886	A
32	R1	887	U
32	R1	888	C
32	R1	889	C
32	R1	891	G
32	R1	893	C
32	R1	894	U
32	R1	896	A
32	R1	910	A
32	R1	914	G

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Mol	Chain	Res	Type
32	R1	927	A
32	R1	932	U
32	R1	941	A
32	R1	945	A
32	R1	946	C
32	R1	953	G
32	R1	961	C
32	R1	973	A
32	R1	974	G
32	R1	983	A
32	R1	985	C
32	R1	989	G
32	R1	995	C
32	R1	996	A
32	R1	1005	C
32	R1	1006	C
32	R1	1012	U
32	R1	1013	C
32	R1	1021	A
32	R1	1022	G
32	R1	1023	U
32	R1	1026	G
32	R1	1033	U
32	R1	1040	A
32	R1	1046	A
32	R1	1051	G
32	R1	1057	A
32	R1	1058	U
32	R1	1060	U
32	R1	1062	G
32	R1	1064	C
32	R1	1065	U
32	R1	1066	U
32	R1	1067	A
32	R1	1069	A
32	R1	1070	A
32	R1	1071	G
32	R1	1072	C
32	R1	1073	A
32	R1	1074	G
32	R1	1075	C
32	R1	1076	C

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Mol	Chain	Res	Type
32	R1	1077	A
32	R1	1079	C
32	R1	1080	A
32	R1	1085	A
32	R1	1088	A
32	R1	1089	A
32	R1	1090	A
32	R1	1091	G
32	R1	1094	U
32	R1	1095	A
32	R1	1096	A
32	R1	1099	G
32	R1	1103	A
32	R1	1104	C
32	R1	1106	G
32	R1	1107	G
32	R1	1110	G
32	R1	1111	A
32	R1	1112	G
32	R1	1132	U
32	R1	1133	A
32	R1	1134	A
32	R1	1135	C
32	R1	1139	G
32	R1	1142	A
32	R1	1169	A
32	R1	1173	U
32	R1	1175	A
32	R1	1176	U
32	R1	1178	C
32	R1	1180	U
32	R1	1204	A
32	R1	1211	C
32	R1	1212	G
32	R1	1237	A
32	R1	1253	A
32	R1	1256	G
32	R1	1265	A
32	R1	1271	G
32	R1	1272	A
32	R1	1273	U
32	R1	1300	G

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Mol	Chain	Res	Type
32	R1	1301	A
32	R1	1325	U
32	R1	1341	G
32	R1	1345	C
32	R1	1352	U
32	R1	1365	A
32	R1	1368	G
32	R1	1378	A
32	R1	1379	U
32	R1	1383	A
32	R1	1386	C
32	R1	1395	A
32	R1	1416	G
32	R1	1427	A
32	R1	1428	C
32	R1	1434	A
32	R1	1452	G
32	R1	1453	A
32	R1	1458	U
32	R1	1461	C
32	R1	1475	G
32	R1	1482	G
32	R1	1490	A
32	R1	1508	A
32	R1	1509	A
32	R1	1515	A
32	R1	1522	A
32	R1	1523	U
32	R1	1524	G
32	R1	1529	G
32	R1	1535	A
32	R1	1536	C
32	R1	1537	G
32	R1	1558	C
32	R1	1559	U
32	R1	1560	G
32	R1	1566	A
32	R1	1569	A
32	R1	1578	U
32	R1	1583	A
32	R1	1584	U
32	R1	1585	C

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Mol	Chain	Res	Type
32	R1	1608	A
32	R1	1610	A
32	R1	1634	A
32	R1	1647	U
32	R1	1648	U
32	R1	1649	G
32	R1	1654	A
32	R1	1674	G
32	R1	1675	C
32	R1	1677	A
32	R1	1693	U
32	R1	1698	A
32	R1	1713	A
32	R1	1715	G
32	R1	1716	U
32	R1	1729	U
32	R1	1730	C
32	R1	1738	G
32	R1	1744	A
32	R1	1758	U
32	R1	1764	C
32	R1	1773	A
32	R1	1776	G
32	R1	1781	U
32	R1	1782	U
32	R1	1791	A
32	R1	1800	C
32	R1	1801	A
32	R1	1802	A
32	R1	1808	A
32	R1	1816	C
32	R1	1829	A
32	R1	1870	C
32	R1	1871	A
32	R1	1884	G
32	R1	1901	A
32	R1	1903	G
32	R1	1906	G
32	R1	1914	C
32	R1	1919	A
32	R1	1927	A
32	R1	1929	G

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Mol	Chain	Res	Type
32	R1	1930	G
32	R1	1937	A
32	R1	1938	A
32	R1	1955	U
32	R1	1960	A
32	R1	1966	A
32	R1	1967	C
32	R1	1970	A
32	R1	1971	U
32	R1	1972	G
32	R1	1991	U
32	R1	1992	G
32	R1	1993	U
32	R1	1996	C
32	R1	1997	C
32	R1	2002	G
32	R1	2022	U
32	R1	2023	C
32	R1	2030	A
32	R1	2031	A
32	R1	2033	A
32	R1	2043	C
32	R1	2055	C
32	R1	2056	G
32	R1	2060	A
32	R1	2061	G
32	R1	2062	A
32	R1	2069	G
32	R1	2072	C
32	R1	2093	G
32	R1	2096	C
32	R1	2100	G
32	R1	2110	G
32	R1	2111	U
32	R1	2112	G
32	R1	2114	A
32	R1	2115	G
32	R1	2118	U
32	R1	2119	A
32	R1	2120	G
32	R1	2121	G
32	R1	2122	U

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Mol	Chain	Res	Type
32	R1	2123	G
32	R1	2124	G
32	R1	2126	A
32	R1	2127	G
32	R1	2129	C
32	R1	2132	U
32	R1	2133	G
32	R1	2136	G
32	R1	2138	G
32	R1	2140	G
32	R1	2145	C
32	R1	2146	C
32	R1	2147	A
32	R1	2148	G
32	R1	2149	U
32	R1	2153	C
32	R1	2156	G
32	R1	2157	G
32	R1	2158	A
32	R1	2161	C
32	R1	2163	A
32	R1	2166	U
32	R1	2167	U
32	R1	2172	U
32	R1	2173	A
32	R1	2174	C
32	R1	2176	A
32	R1	2178	C
32	R1	2182	U
32	R1	2188	U
32	R1	2189	U
32	R1	2193	G
32	R1	2198	A
32	R1	2203	U
32	R1	2204	G
32	R1	2211	A
32	R1	2214	C
32	R1	2219	U
32	R1	2225	A
32	R1	2238	G
32	R1	2239	G
32	R1	2243	U

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Mol	Chain	Res	Type
32	R1	2250	G
32	R1	2266	A
32	R1	2278	A
32	R1	2282	G
32	R1	2283	C
32	R1	2287	A
32	R1	2300	C
32	R1	2302	U
32	R1	2305	U
32	R1	2307	G
32	R1	2309	A
32	R1	2322	A
32	R1	2325	G
32	R1	2327	A
32	R1	2331	G
32	R1	2345	G
32	R1	2347	C
32	R1	2359	C
32	R1	2361	G
32	R1	2371	G
32	R1	2383	G
32	R1	2385	C
32	R1	2402	U
32	R1	2403	C
32	R1	2406	A
32	R1	2423	U
32	R1	2429	G
32	R1	2430	A
32	R1	2431	U
32	R1	2441	U
32	R1	2448	A
32	R1	2449	U
32	R1	2459	A
32	R1	2474	U
32	R1	2476	A
32	R1	2502	G
32	R1	2503	A
32	R1	2504	U
32	R1	2505	G
32	R1	2506	U
32	R1	2518	A
32	R1	2520	C

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Mol	Chain	Res	Type
32	R1	2530	A
32	R1	2535	G
32	R1	2547	A
32	R1	2554	U
32	R1	2562	U
32	R1	2566	A
32	R1	2567	G
32	R1	2572	A
32	R1	2573	C
32	R1	2582	G
32	R1	2602	A
32	R1	2604	U
32	R1	2609	U
32	R1	2613	U
32	R1	2615	U
32	R1	2629	U
32	R1	2630	G
32	R1	2661	G
32	R1	2681	C
32	R1	2682	A
32	R1	2689	U
32	R1	2690	U
32	R1	2714	G
32	R1	2724	U
32	R1	2727	A
32	R1	2732	G
32	R1	2733	A
32	R1	2744	G
32	R1	2748	A
32	R1	2764	A
32	R1	2765	A
32	R1	2777	G
32	R1	2778	A
32	R1	2779	U
32	R1	2791	G
32	R1	2793	C
32	R1	2794	C
32	R1	2799	A
32	R1	2800	A
32	R1	2807	U
32	R1	2808	G
32	R1	2818	U

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Mol	Chain	Res	Type
32	R1	2820	A
32	R1	2835	A
32	R1	2837	A
32	R1	2848	G
32	R1	2849	U
32	R1	2861	U
32	R1	2867	G
32	R1	2868	A
32	R1	2883	A
32	R1	2887	A
32	R1	2903	U
33	R2	9	G
33	R2	12	C
33	R2	13	G
33	R2	25	U
33	R2	35	C
33	R2	42	C
33	R2	44	G
33	R2	45	A
33	R2	67	G
33	R2	87	U
33	R2	88	C
33	R2	89	U
33	R2	90	C
33	R2	108	A
33	R2	109	A
33	R2	117	G
33	R2	119	A
34	R3	4	U
34	R3	6	G
34	R3	7	A
34	R3	9	G
34	R3	22	G
34	R3	32	A
34	R3	39	G
34	R3	47	C
34	R3	48	C
34	R3	51	A
34	R3	64	G
34	R3	68	G
34	R3	70	U
34	R3	71	A

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Mol	Chain	Res	Type
34	R3	73	C
34	R3	81	A
34	R3	82	G
34	R3	83	C
34	R3	84	U
34	R3	86	G
34	R3	87	C
34	R3	88	U
34	R3	89	U
34	R3	93	U
34	R3	94	G
34	R3	95	C
34	R3	96	U
34	R3	121	U
34	R3	128	G
34	R3	130	A
34	R3	131	A
34	R3	135	C
34	R3	153	C
34	R3	154	U
34	R3	155	A
34	R3	160	A
34	R3	163	C
34	R3	164	G
34	R3	171	A
34	R3	174	A
34	R3	183	C
34	R3	184	G
34	R3	186	C
34	R3	190	A
34	R3	197	A
34	R3	202	G
34	R3	208	U
34	R3	210	C
34	R3	211	G
34	R3	216	U
34	R3	226	G
34	R3	240	G
34	R3	245	U
34	R3	247	G
34	R3	251	G
34	R3	266	G

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Mol	Chain	Res	Type
34	R3	267	C
34	R3	279	A
34	R3	280	C
34	R3	281	G
34	R3	289	G
34	R3	293	G
34	R3	305	G
34	R3	319	G
34	R3	321	A
34	R3	328	C
34	R3	329	A
34	R3	330	C
34	R3	341	C
34	R3	344	A
34	R3	345	C
34	R3	347	G
34	R3	351	G
34	R3	352	C
34	R3	354	G
34	R3	356	A
34	R3	367	U
34	R3	372	C
34	R3	373	A
34	R3	378	G
34	R3	387	U
34	R3	391	G
34	R3	392	C
34	R3	393	A
34	R3	394	G
34	R3	398	U
34	R3	401	C
34	R3	404	G
34	R3	406	G
34	R3	413	G
34	R3	414	A
34	R3	415	A
34	R3	420	U
34	R3	421	U
34	R3	422	C
34	R3	423	G
34	R3	424	G
34	R3	425	G

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Mol	Chain	Res	Type
34	R3	429	U
34	R3	439	U
34	R3	448	A
34	R3	451	A
34	R3	459	A
34	R3	464	U
34	R3	465	A
34	R3	467	U
34	R3	468	A
34	R3	472	U
34	R3	474	G
34	R3	476	U
34	R3	478	A
34	R3	479	U
34	R3	482	A
34	R3	484	G
34	R3	485	U
34	R3	486	U
34	R3	487	A
34	R3	492	C
34	R3	493	A
34	R3	495	A
34	R3	497	G
34	R3	500	G
34	R3	518	C
34	R3	524	G
34	R3	527	G
34	R3	529	G
34	R3	531	U
34	R3	532	A
34	R3	533	A
34	R3	540	G
34	R3	547	A
34	R3	550	G
34	R3	559	A
34	R3	562	U
34	R3	564	C
34	R3	572	A
34	R3	573	A
34	R3	575	G
34	R3	576	C
34	R3	577	G

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Mol	Chain	Res	Type
34	R3	592	G
34	R3	596	A
34	R3	607	A
34	R3	614	C
34	R3	615	G
34	R3	621	A
34	R3	622	A
34	R3	633	G
34	R3	665	A
34	R3	682	G
34	R3	686	U
34	R3	703	G
34	R3	713	G
34	R3	718	A
34	R3	721	G
34	R3	723	U
34	R3	724	G
34	R3	731	G
34	R3	734	G
34	R3	755	G
34	R3	777	A
34	R3	793	U
34	R3	815	A
34	R3	817	C
34	R3	818	G
34	R3	819	A
34	R3	821	G
34	R3	829	G
34	R3	841	C
34	R3	842	U
34	R3	843	U
34	R3	846	G
34	R3	851	G
34	R3	858	G
34	R3	872	A
34	R3	885	G
34	R3	889	A
34	R3	902	G
34	R3	926	G
34	R3	932	C
34	R3	934	C
34	R3	935	A

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Mol	Chain	Res	Type
34	R3	954	G
34	R3	960	U
34	R3	961	U
34	R3	965	U
34	R3	966	G
34	R3	969	A
34	R3	971	G
34	R3	975	A
34	R3	976	G
34	R3	977	A
34	R3	982	U
34	R3	992	U
34	R3	993	G
34	R3	1004	A
34	R3	1026	G
34	R3	1027	C
34	R3	1028	C
34	R3	1029	U
34	R3	1031	C
34	R3	1033	G
34	R3	1036	A
34	R3	1039	G
34	R3	1045	C
34	R3	1053	G
34	R3	1064	G
34	R3	1084	G
34	R3	1085	U
34	R3	1094	G
34	R3	1095	U
34	R3	1101	A
34	R3	1130	A
34	R3	1132	C
34	R3	1137	C
34	R3	1138	G
34	R3	1139	G
34	R3	1140	C
34	R3	1159	U
34	R3	1167	A
34	R3	1168	U
34	R3	1171	A
34	R3	1174	G
34	R3	1182	G

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Mol	Chain	Res	Type
34	R3	1184	G
34	R3	1196	A
34	R3	1200	C
34	R3	1212	U
34	R3	1225	A
34	R3	1227	A
34	R3	1236	A
34	R3	1238	A
34	R3	1241	G
34	R3	1250	A
34	R3	1256	A
34	R3	1261	A
34	R3	1268	G
34	R3	1275	A
34	R3	1279	G
34	R3	1280	A
34	R3	1282	C
34	R3	1285	A
34	R3	1286	U
34	R3	1287	A
34	R3	1289	A
34	R3	1298	U
34	R3	1300	G
34	R3	1301	U
34	R3	1303	C
34	R3	1312	G
34	R3	1317	C
34	R3	1323	G
34	R3	1336	C
34	R3	1338	G
34	R3	1340	A
34	R3	1346	A
34	R3	1353	G
34	R3	1363	A
34	R3	1368	A
34	R3	1370	G
34	R3	1378	C
34	R3	1379	G
34	R3	1398	A
34	R3	1419	G
34	R3	1441	A
34	R3	1442	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	R3	1446	A
34	R3	1448	C
34	R3	1452	C
34	R3	1453	G
34	R3	1455	G
34	R3	1487	G
34	R3	1492	A
34	R3	1493	A
34	R3	1497	G
34	R3	1499	A
34	R3	1502	A
34	R3	1506	U
34	R3	1517	G
34	R3	1529	G
34	R3	1530	G
34	R3	1533	C
34	R3	1537	U
34	R3	1539	C
35	T	8	4SU
35	T	9	G
35	T	15	C
35	T	16	C
35	T	17	U
35	T	18	G
35	T	19	G
35	T	20	H2U
35	T	22	G
35	T	23	C
35	T	45	G
35	T	46	A
35	T	47	U
35	T	48	C
35	T	51	C
35	T	54	5MU
35	T	55	PSU
35	T	56	C
35	T	57	A
35	T	60	U
35	T	61	C
35	T	71	C

All (17) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
32	R1	227	A
32	R1	372	G
32	R1	404	A
32	R1	421	C
32	R1	784	G
32	R1	1020	A
32	R1	1236	G
32	R1	1715	G
32	R1	2326	C
32	R1	2798	U
33	R2	66	A
34	R3	391	G
34	R3	438	U
34	R3	1297	G
35	T	8	4SU
35	T	17	U
35	T	55	PSU

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
35	4OC	T	32	35	20,23,24	2.56	5 (25%)	25,32,35	1.02	1 (4%)
35	H2U	T	20	35	18,21,22	4.26	5 (27%)	19,30,33	4.21	6 (31%)
35	4SU	T	8	35	18,21,22	3.48	7 (38%)	25,30,33	2.23	6 (24%)
35	5MU	T	54	35	19,22,23	2.26	6 (31%)	27,32,35	2.28	7 (25%)
35	PSU	T	55	35	18,21,22	2.30	9 (50%)	21,30,33	2.29	5 (23%)

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
35	4OC	T	32	35	1/1/5/6	1/9/29/30	0/2/2/2
35	H2U	T	20	35	1/1/8/9	6/7/38/39	0/2/2/2
35	4SU	T	8	35	2/2/5/5	0/7/25/26	0/2/2/2
35	5MU	T	54	35	3/3/5/5	3/7/25/26	0/2/2/2
35	PSU	T	55	35	2/2/5/5	2/7/25/26	0/2/2/2

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	T	20	H2U	O4-C4	10.33	1.43	1.23
35	T	8	4SU	O2-C2	9.67	1.40	1.23
35	T	20	H2U	C2-N1	9.01	1.48	1.35
35	T	32	4OC	O2-C2	8.79	1.40	1.23
35	T	20	H2U	O2-C2	7.99	1.37	1.23
35	T	8	4SU	C4-S4	7.08	1.81	1.68
35	T	20	H2U	C2-N3	6.64	1.49	1.38
35	T	8	4SU	C4-N3	-5.34	1.32	1.37
35	T	20	H2U	C4-N3	5.27	1.46	1.37
35	T	54	5MU	C4-C5	-4.70	1.37	1.44
35	T	32	4OC	C4-N4	4.60	1.45	1.36
35	T	54	5MU	C2-N1	-4.23	1.31	1.38
35	T	8	4SU	C2-N1	-4.00	1.32	1.38
35	T	55	PSU	C2-N1	-3.98	1.31	1.36
35	T	54	5MU	C6-C5	3.97	1.41	1.34
35	T	32	4OC	C2-N1	-3.89	1.31	1.40
35	T	55	PSU	C2-N3	-3.79	1.31	1.37
35	T	54	5MU	C4-N3	-3.74	1.31	1.38
35	T	54	5MU	C6-N1	-3.74	1.31	1.38
35	T	55	PSU	O4-C4	-3.58	1.16	1.23
35	T	55	PSU	C4-N3	-3.52	1.32	1.38
35	T	8	4SU	C2-N3	-3.43	1.32	1.38
35	T	55	PSU	C6-C5	3.36	1.39	1.35
35	T	55	PSU	C6-N1	-3.14	1.31	1.36
35	T	54	5MU	O2-C2	-2.86	1.18	1.23
35	T	8	4SU	C5-C4	-2.85	1.39	1.42
35	T	32	4OC	C6-N1	-2.54	1.32	1.38
35	T	8	4SU	C6-N1	-2.44	1.32	1.38
35	T	55	PSU	C4-C5	-2.30	1.38	1.44
35	T	32	4OC	C2-N3	-2.28	1.31	1.36
35	T	55	PSU	O2-C2	-2.26	1.18	1.23
35	T	55	PSU	C1'-C5	2.20	1.55	1.50

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	T	20	H2U	O2-C2-N1	-11.80	108.92	123.10
35	T	20	H2U	O4-C4-N3	-7.48	108.77	120.30
35	T	55	PSU	N1-C2-N3	7.15	122.71	115.17
35	T	20	H2U	O2-C2-N3	-6.76	109.03	121.49
35	T	8	4SU	C4-N3-C2	-6.47	121.11	127.31
35	T	20	H2U	O4-C4-C5	-6.37	109.17	122.20
35	T	20	H2U	N3-C2-N1	-5.86	110.75	116.65
35	T	8	4SU	N3-C2-N1	5.67	122.27	114.89
35	T	54	5MU	O4-C4-C5	-4.91	119.30	124.92
35	T	54	5MU	C4-N3-C2	-4.81	121.03	127.34
35	T	54	5MU	N3-C2-N1	4.74	121.07	114.89
35	T	54	5MU	C5-C4-N3	4.53	119.27	115.32
35	T	55	PSU	C4-N3-C2	-4.42	120.28	126.37
35	T	8	4SU	C5-C4-N3	4.40	118.85	114.75
35	T	20	H2U	C5-C4-N3	-4.12	112.31	116.69
35	T	54	5MU	C5-C6-N1	-3.94	119.03	123.31
35	T	55	PSU	O2-C2-N1	-3.82	118.85	122.79
35	T	8	4SU	C5-C4-S4	-2.98	120.91	124.31
35	T	54	5MU	C1'-N1-C6	-2.96	116.27	121.15
35	T	8	4SU	O2-C2-N1	-2.96	118.94	122.80
35	T	54	5MU	C1'-N1-C2	2.80	122.62	117.59
35	T	55	PSU	C6-N1-C2	-2.68	120.21	122.69
35	T	32	4OC	C5-C4-N3	-2.65	118.45	122.60
35	T	8	4SU	C6-C5-C4	-2.23	118.02	119.95
35	T	55	PSU	C5-C6-N1	-2.01	119.35	122.14

All (9) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
35	T	20	H2U	C2'
35	T	32	4OC	C2'
35	T	54	5MU	C4'
35	T	54	5MU	C3'
35	T	54	5MU	C2'
35	T	55	PSU	C4'
35	T	55	PSU	C2'
35	T	8	4SU	C2'
35	T	8	4SU	C1'

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	T	20	H2U	O4'-C1'-N1-C2
35	T	20	H2U	O4'-C1'-N1-C6
35	T	54	5MU	C4'-C5'-O5'-P
35	T	55	PSU	C4'-C5'-O5'-P
35	T	20	H2U	O4'-C4'-C5'-O5'
35	T	20	H2U	C2'-C1'-N1-C6
35	T	32	4OC	C3'-C2'-O2'-CM2
35	T	20	H2U	C4'-C5'-O5'-P
35	T	20	H2U	C3'-C4'-C5'-O5'
35	T	55	PSU	O4'-C1'-C5-C6
35	T	54	5MU	C2'-C1'-N1-C6
35	T	54	5MU	C3'-C4'-C5'-O5'

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	T	20	H2U	2	0
35	T	54	5MU	2	0
35	T	55	PSU	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 255 ligands modelled in this entry, 252 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
59	ATP	Y	601	60	28,33,33	0.68	0	34,52,52	0.59	1 (2%)
59	ATP	Y	602	60	28,33,33	0.82	0	34,52,52	0.60	1 (2%)
58	FME	T	101	35	8,9,10	0.97	0	8,9,11	1.06	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
59	ATP	Y	601	60	-	8/18/38/38	0/3/3/3
59	ATP	Y	602	60	-	5/18/38/38	0/3/3/3
58	FME	T	101	35	-	3/7/9/11	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	Y	601	ATP	C5-C6-N6	2.32	123.84	120.31
59	Y	602	ATP	C5-C6-N6	2.30	123.82	120.31

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	T	101	FME	O1-CN-N-CA
59	Y	601	ATP	PB-O3B-PG-O2G
59	Y	601	ATP	C5'-O5'-PA-O2A
59	Y	601	ATP	C5'-O5'-PA-O3A
59	Y	602	ATP	C5'-O5'-PA-O1A
59	Y	602	ATP	O4'-C4'-C5'-O5'
58	T	101	FME	CA-CB-CG-SD
59	Y	602	ATP	C3'-C4'-C5'-O5'
58	T	101	FME	CB-CG-SD-CE
59	Y	602	ATP	PA-O3A-PB-O2B
59	Y	601	ATP	C5'-O5'-PA-O1A
59	Y	601	ATP	PG-O3B-PB-O2B
59	Y	601	ATP	PB-O3B-PG-O1G
59	Y	601	ATP	PB-O3B-PG-O3G
59	Y	601	ATP	O4'-C4'-C5'-O5'
59	Y	602	ATP	PA-O3A-PB-O1B

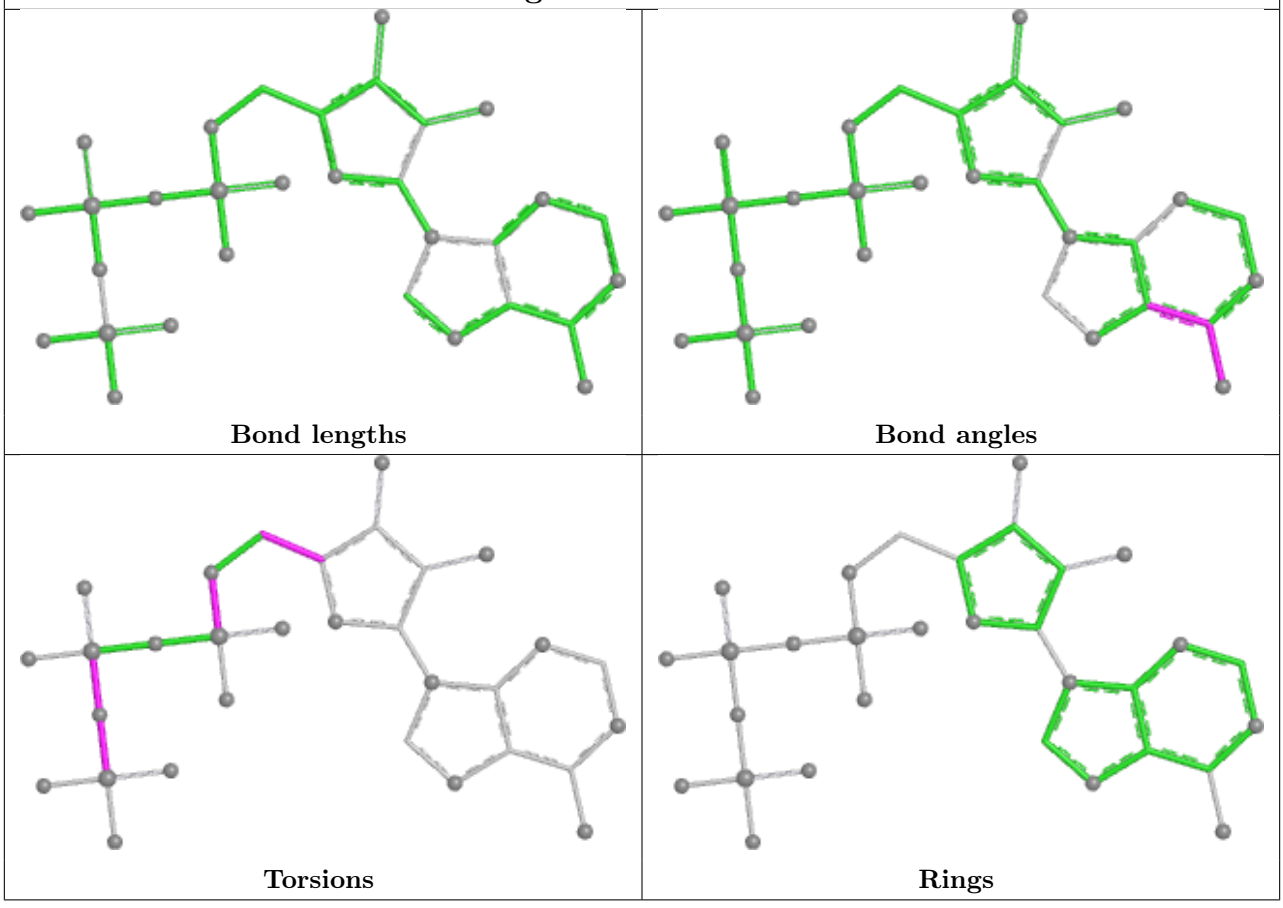
There are no ring outliers.

2 monomers are involved in 5 short contacts:

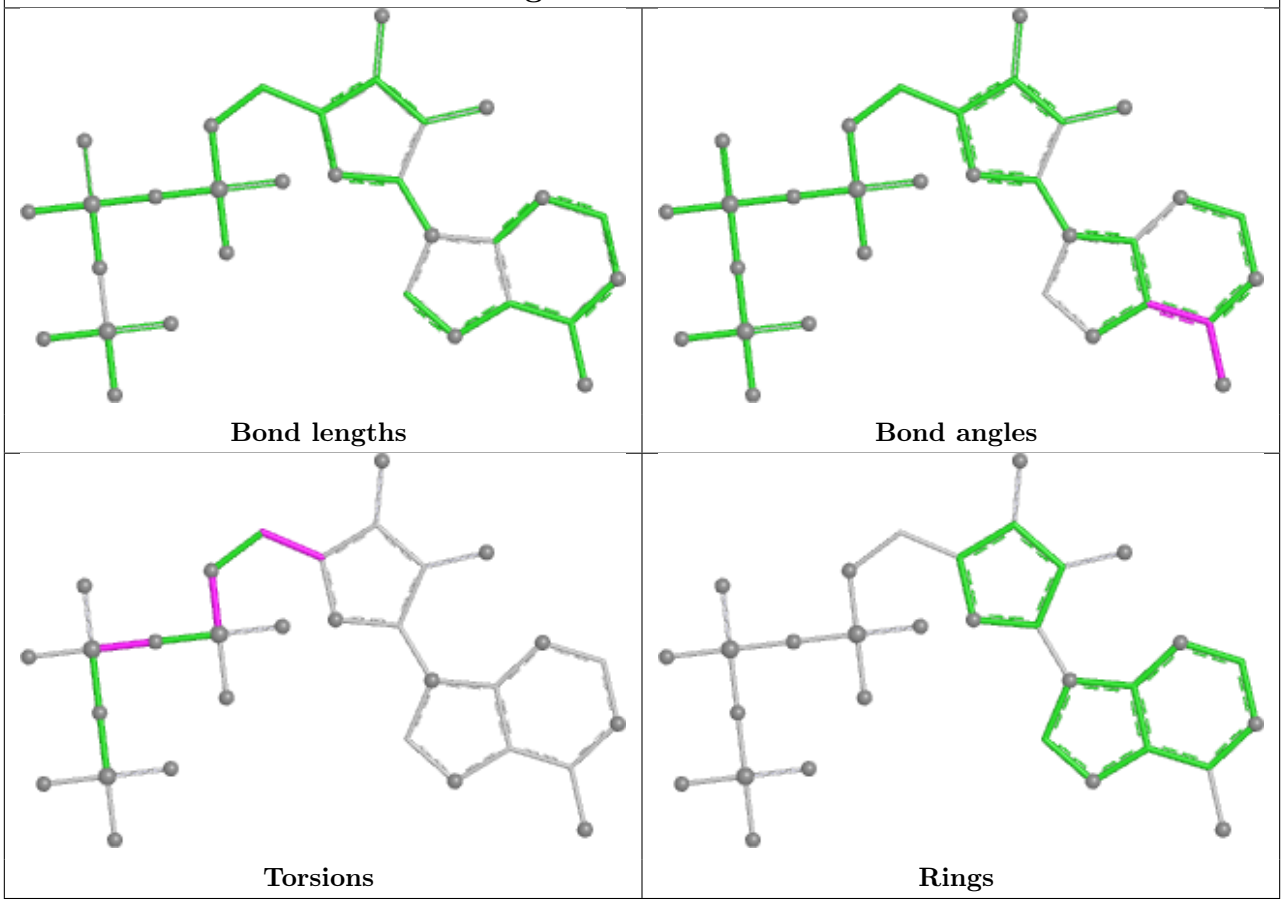
Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	Y	601	ATP	3	0
59	Y	602	ATP	2	0

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

Ligand ATP Y 601



Ligand ATP Y 602



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
34	R3	2
32	R1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	R3	1301:U	O3'	1302:C	P	4.44
1	R3	1533:C	O3'	1534:A	P	3.87
1	R1	2098:U	O3'	2099:U	P	3.33

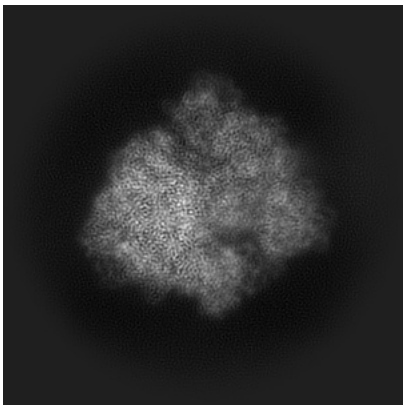
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-40928. These allow visual inspection of the internal detail of the map and identification of artifacts.

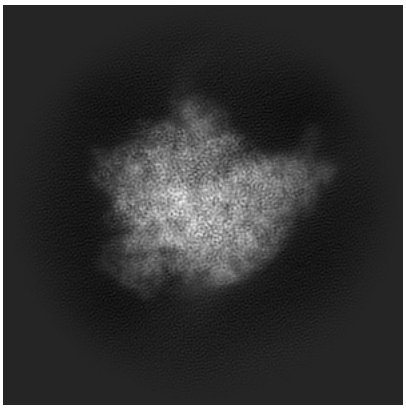
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

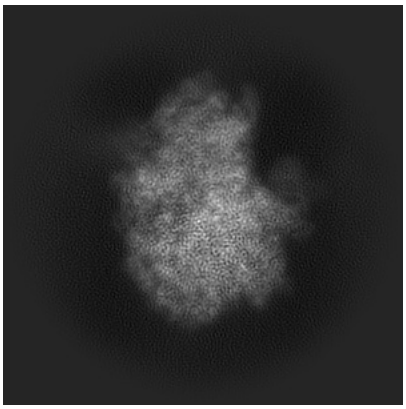
6.1.1 Primary map



X

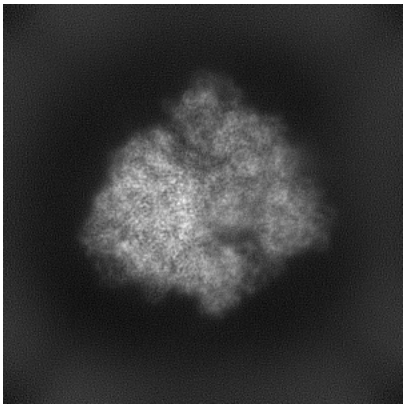


Y

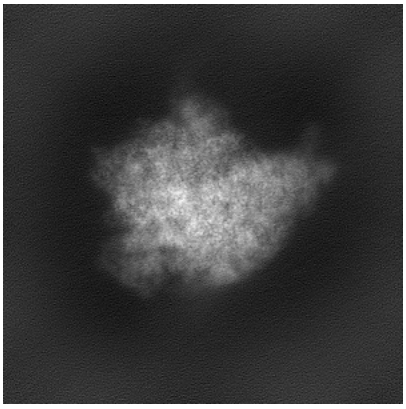


Z

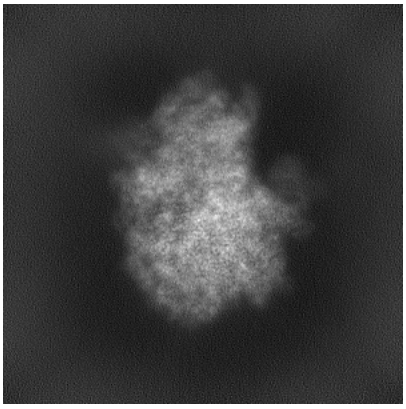
6.1.2 Raw map



X



Y

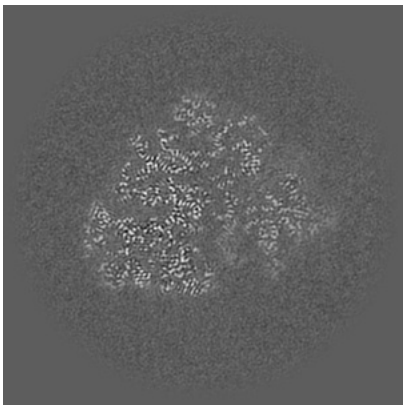


Z

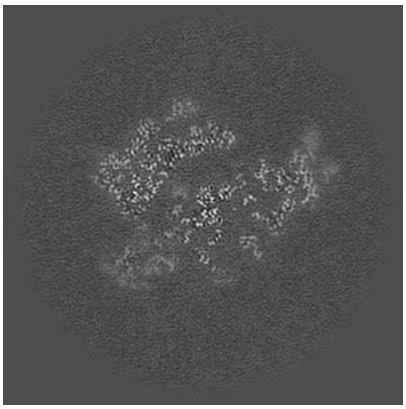
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



X Index: 200



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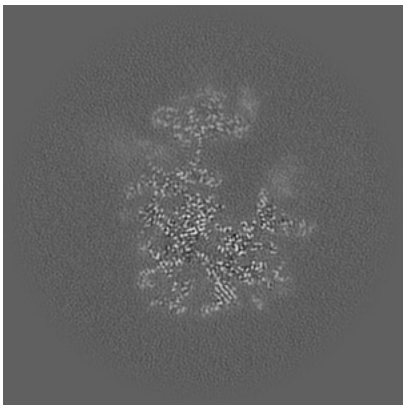
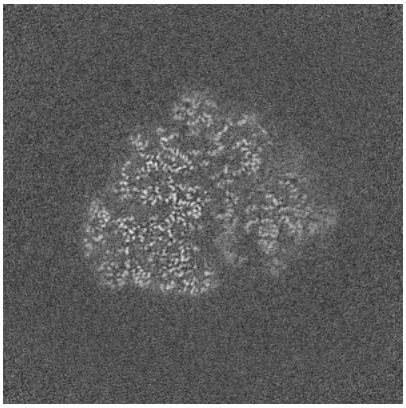
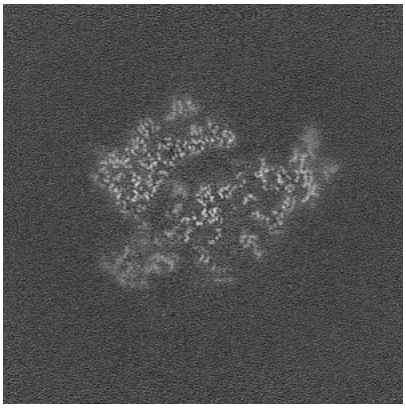


Z Index: 200

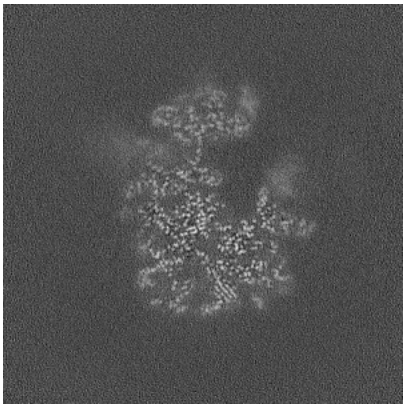
6.2.2 Raw map



X Index: 200



Y Index: 200

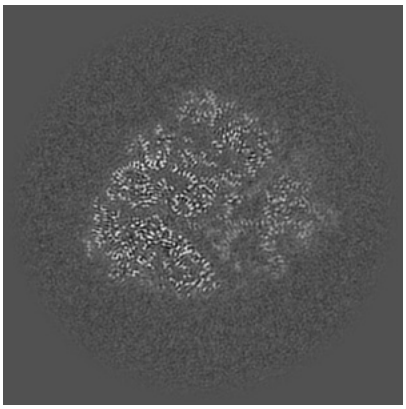


Z Index: 200

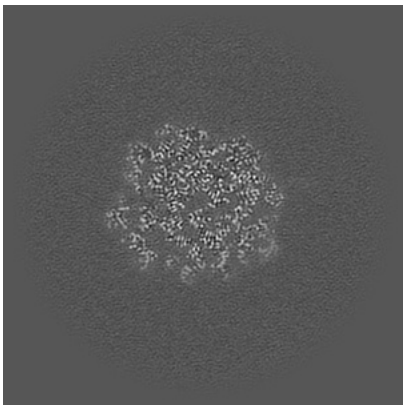
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

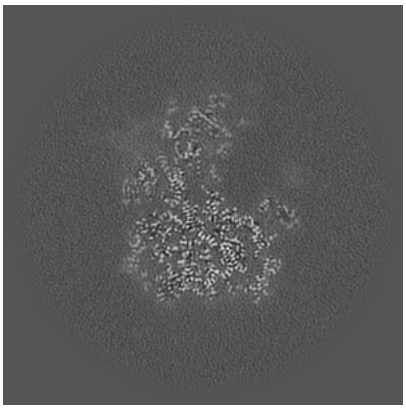
6.3.1 Primary map



X Index: 206

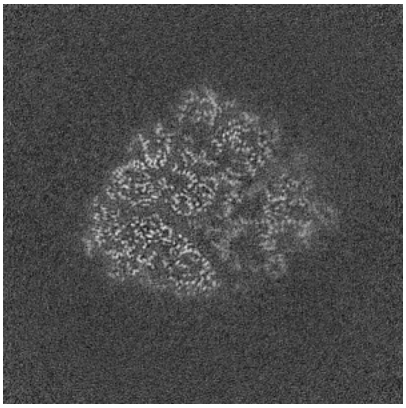


Y Index: 156

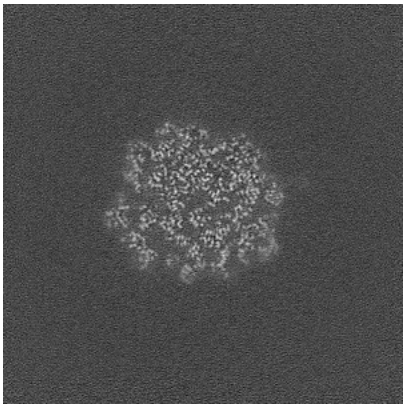


Z Index: 217

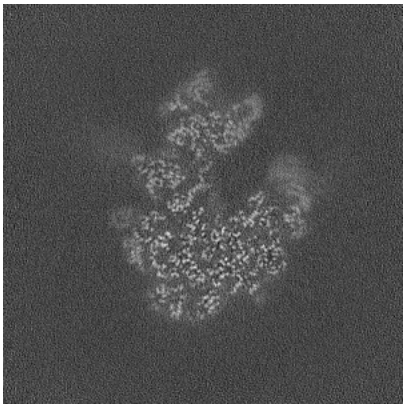
6.3.2 Raw map



X Index: 206



Y Index: 156

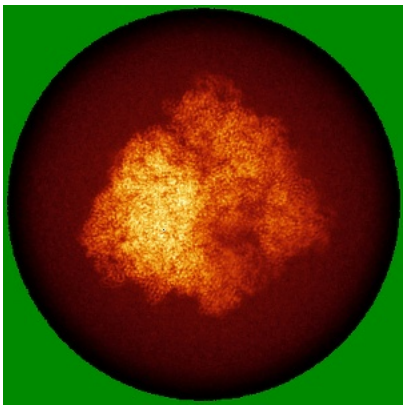


Z Index: 185

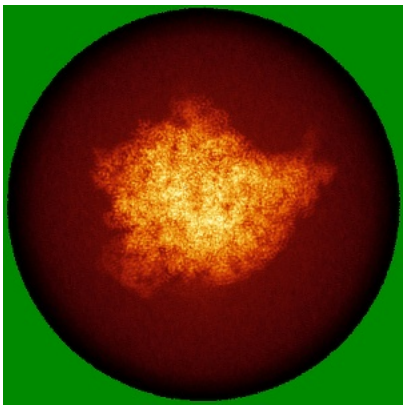
The images above show the largest variance slices of the map in three orthogonal directions.

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

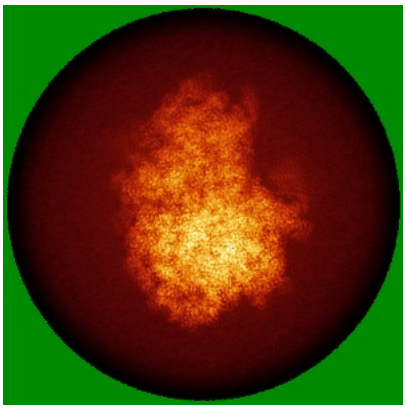
6.4.1 Primary map



X

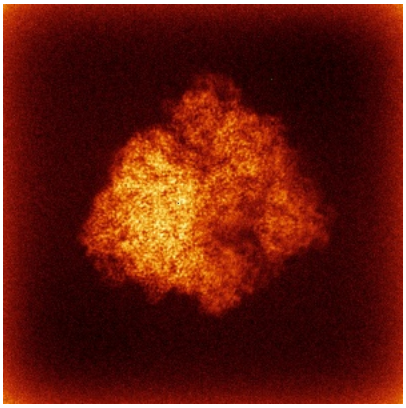


Y

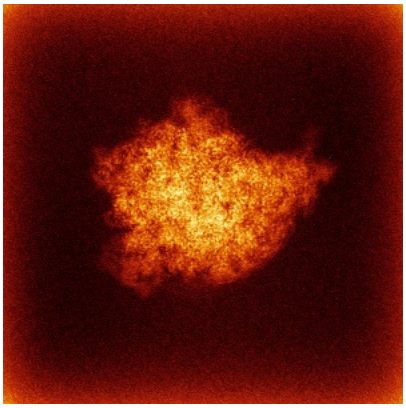


Z

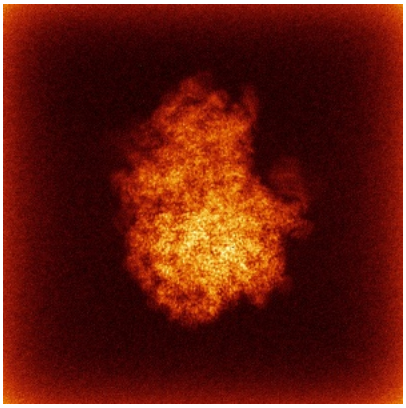
6.4.2 Raw map



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 0.85. 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.

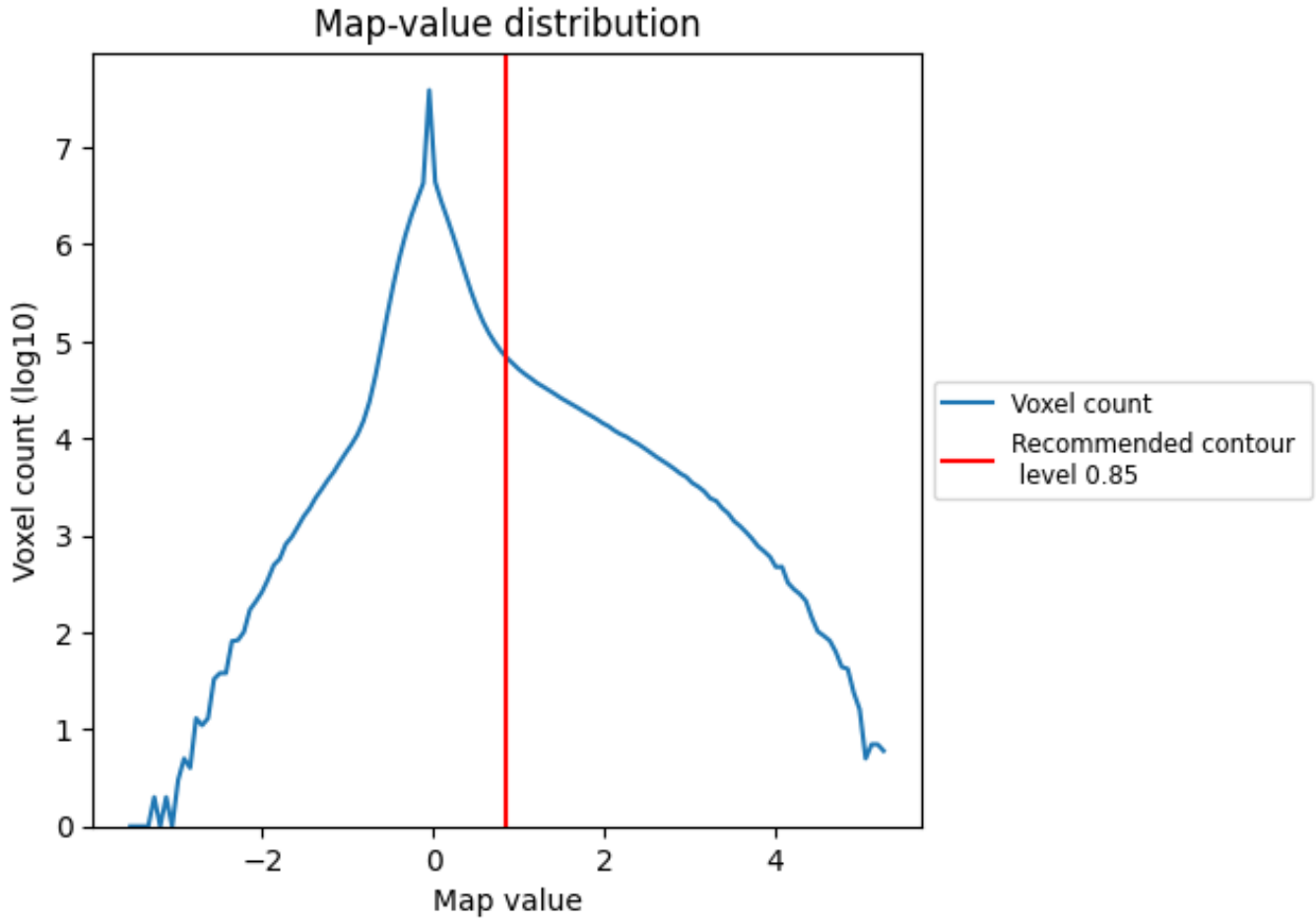
6.6 Mask visualisation (i)

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

7 Map analysis

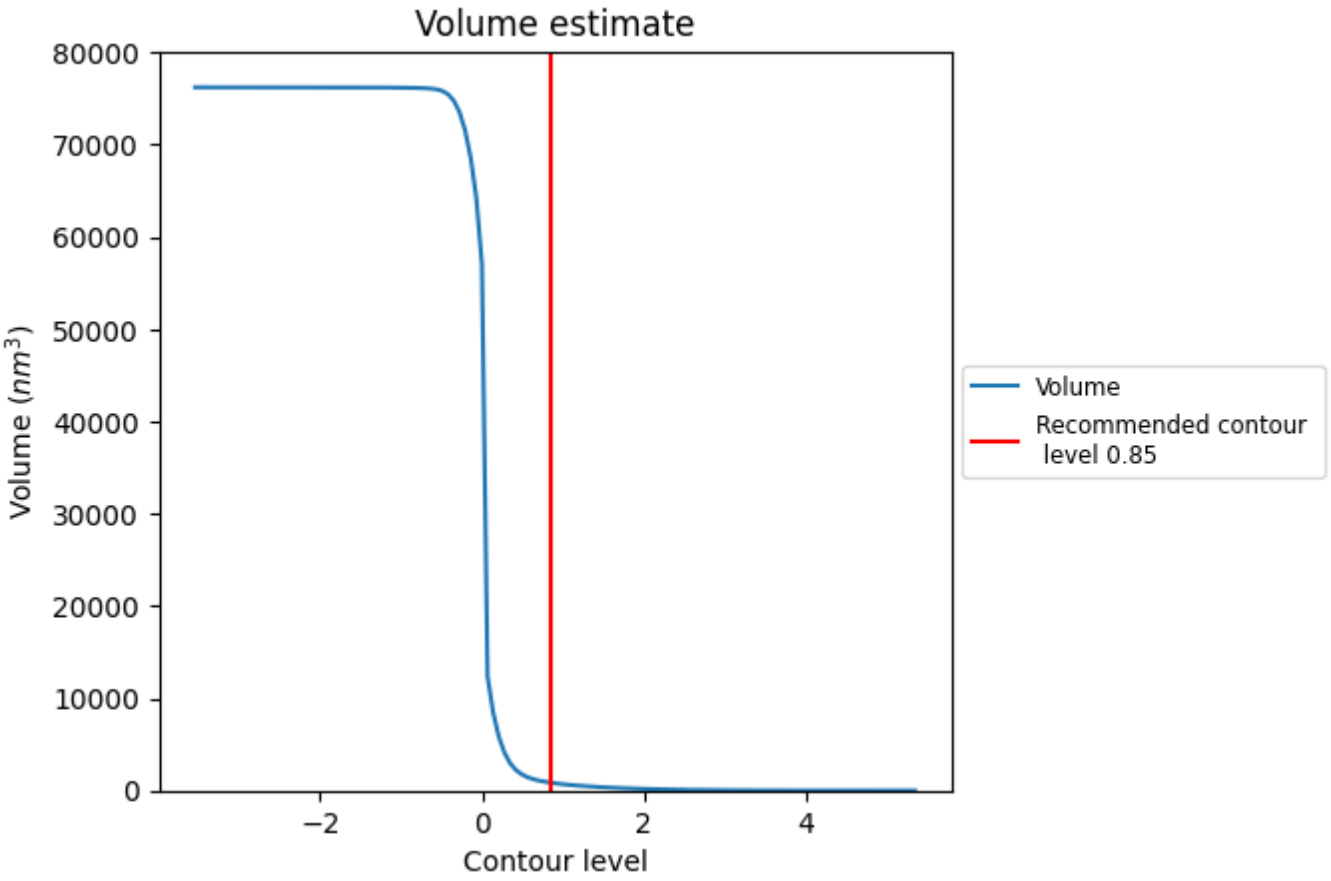
This section contains the results of statistical analysis of the map.

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.

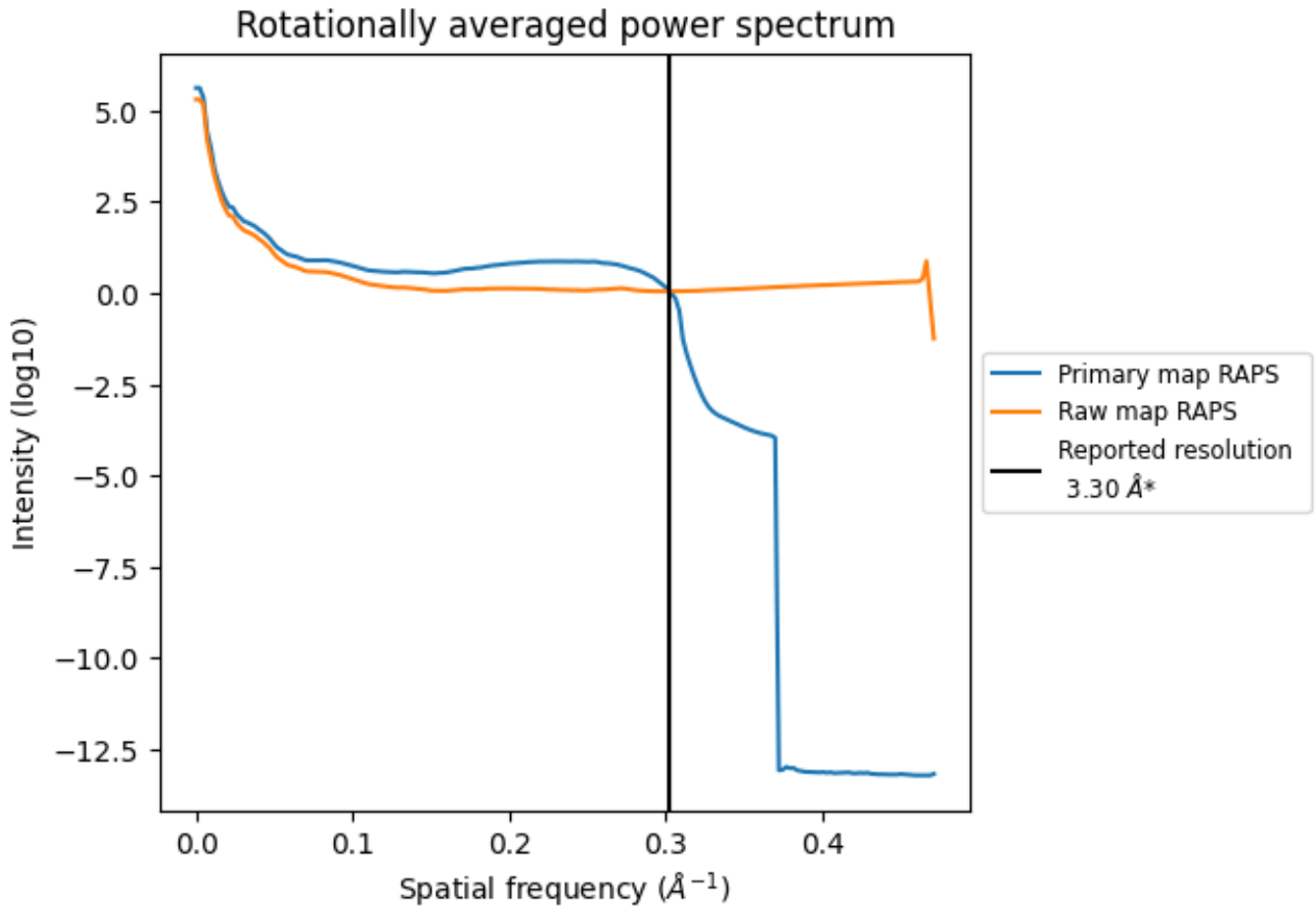
7.2 Volume estimate



The volume at the recommended contour level is 845 nm^3; this corresponds to an approximate mass of 763 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)

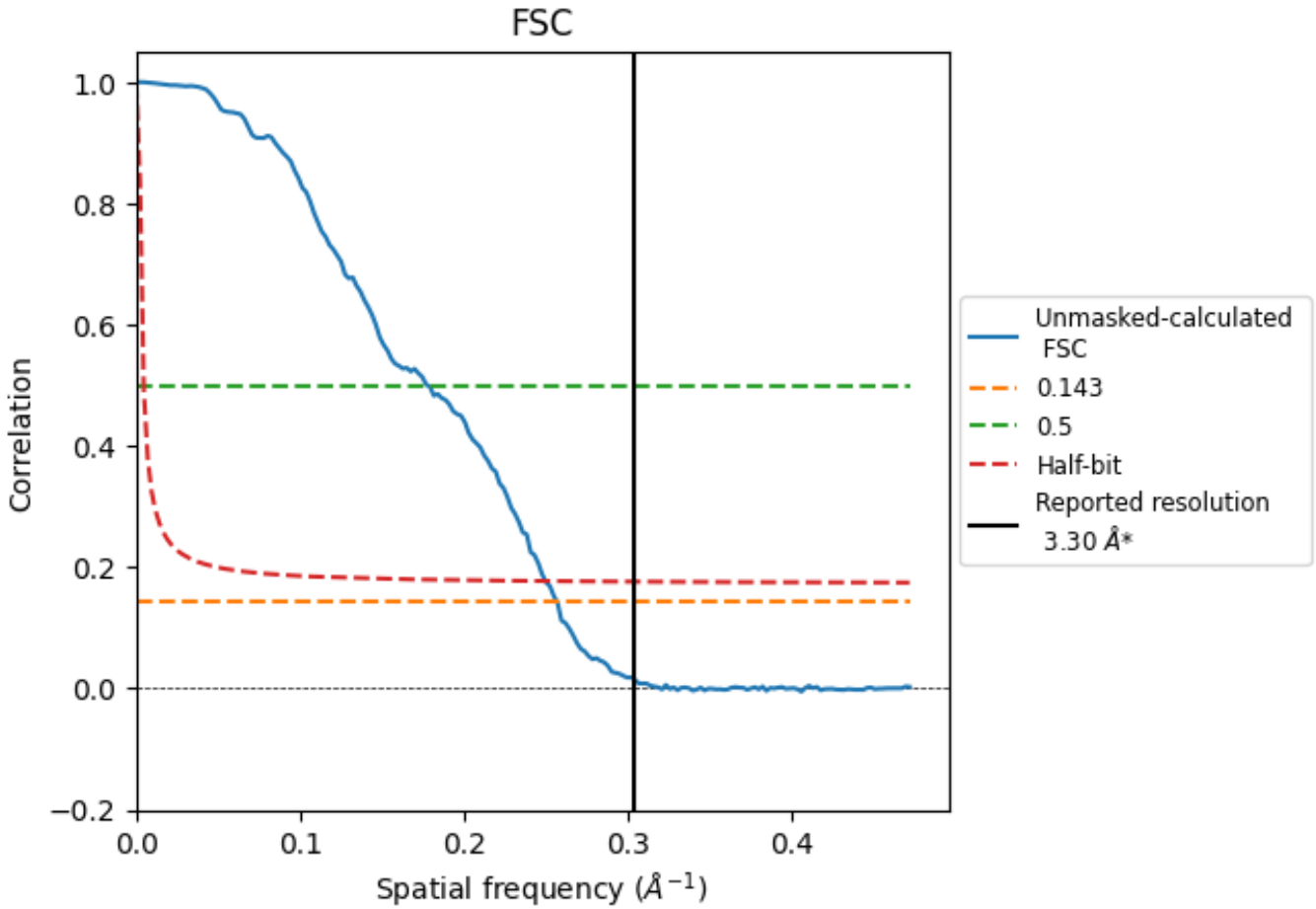


*Reported resolution corresponds to spatial frequency of 0.303 $Å^{-1}$

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 0.303 Å^{-1}

8.2 Resolution estimates (i)

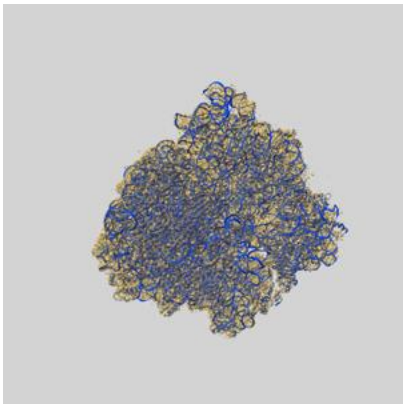
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.90	5.63	4.01

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.90 differs from the reported value 3.3 by more than 10 %

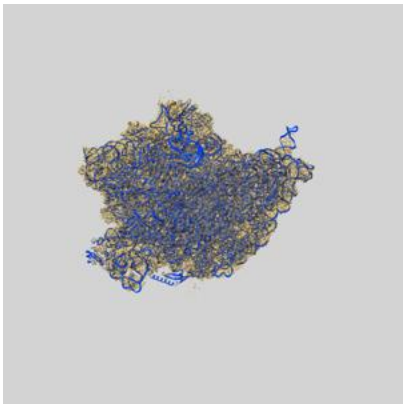
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-40928 and PDB model 9NL7. Per-residue inclusion information can be found in section 3 on page 17.

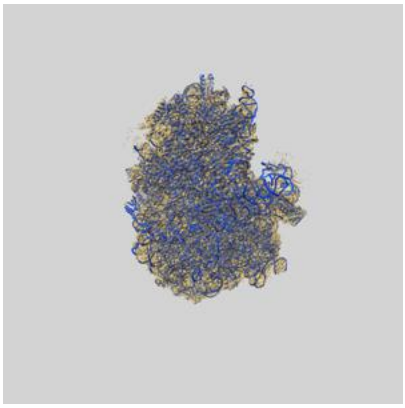
9.1 Map-model overlay



X



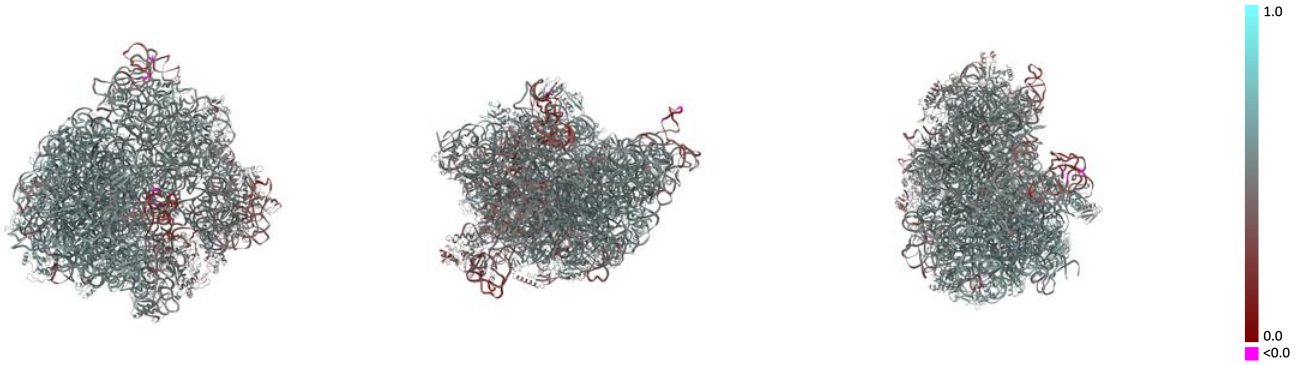
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.85 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

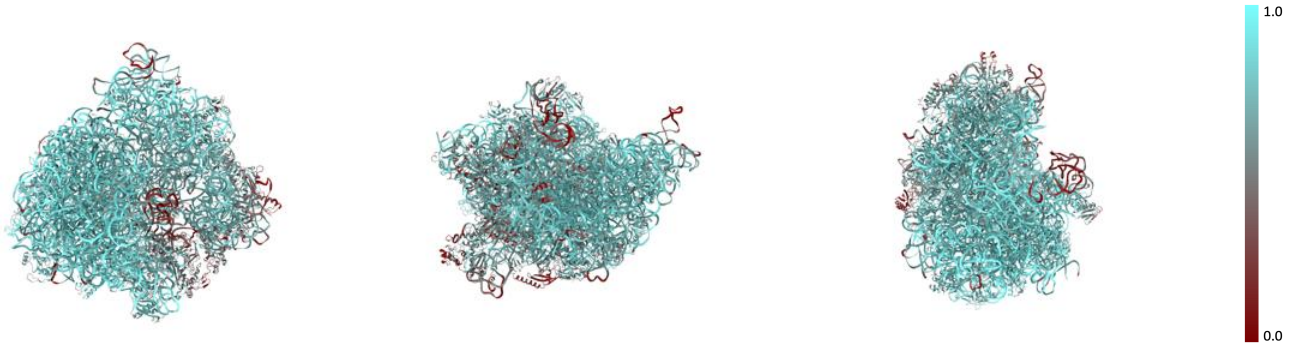
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

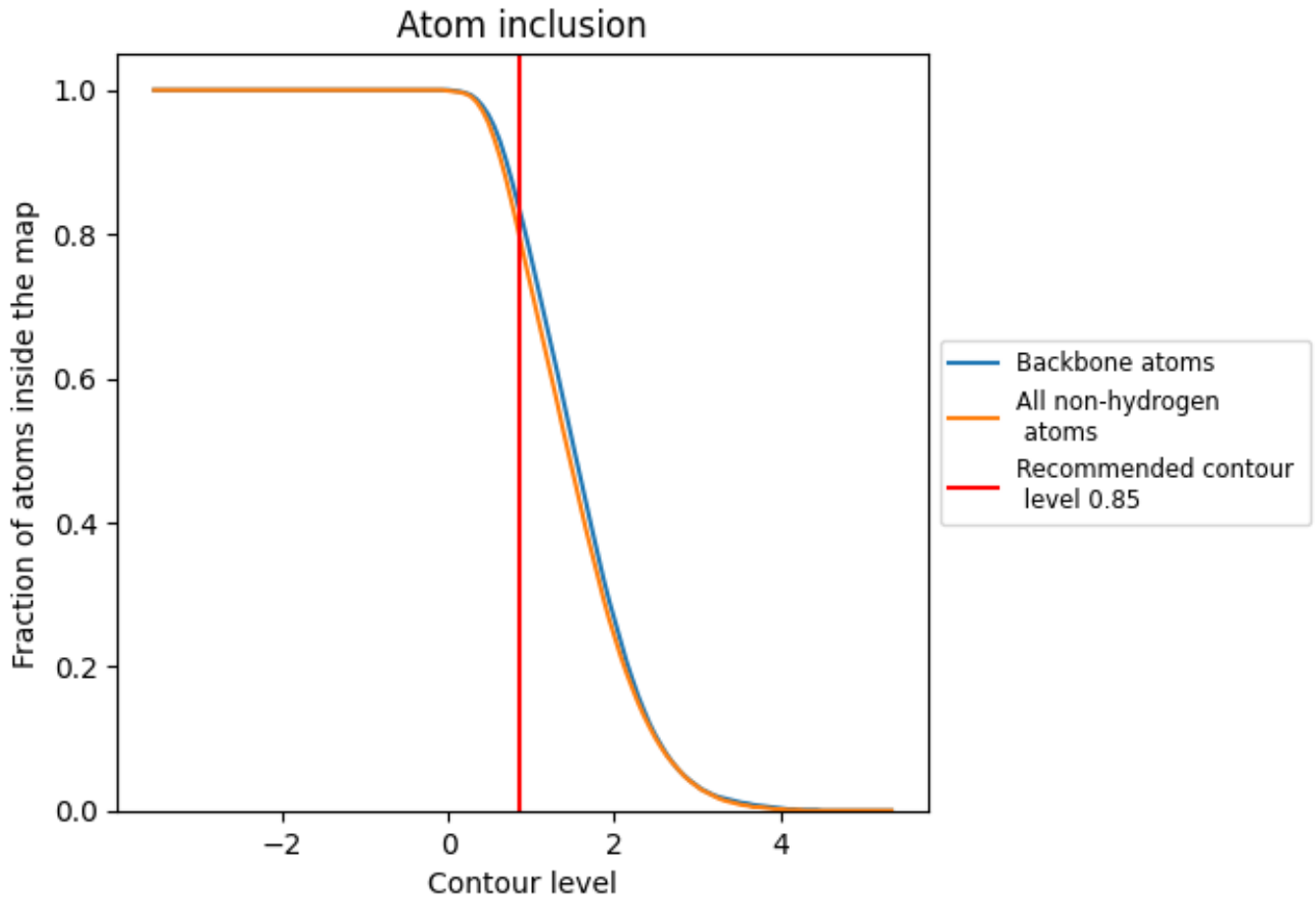
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.85).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 80% 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 (0.85) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8020	0.5200
1	0.4220	0.4240
13	0.8690	0.5770
14	0.8230	0.5680
15	0.8560	0.5700
16	0.8330	0.5740
17	0.8810	0.5800
18	0.7440	0.5450
19	0.8180	0.5670
2	0.8650	0.5790
20	0.8850	0.5820
21	0.8130	0.5600
22	0.8420	0.5660
23	0.7960	0.5660
24	0.7740	0.5430
25	0.7370	0.5560
27	0.8530	0.5800
28	0.8450	0.5780
29	0.7200	0.5310
3	0.8530	0.5760
30	0.8240	0.5690
31	0.2470	0.3900
32	0.8280	0.5620
33	0.6830	0.5540
34	0.8700	0.5820
35	0.8980	0.5880
36	0.8630	0.5850
4	0.7880	0.5570
5	0.5180	0.4660
6	0.6510	0.5250
9	0.2720	0.4150
M	0.5740	0.4860
R1	0.8760	0.5300
R2	0.8540	0.5050
R3	0.8270	0.4990

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Chain	Atom inclusion	Q-score
T	0.5540	0.4110
Y	0.5230	0.4710
sb	0.5860	0.4850
sc	0.6470	0.5210
sd	0.7120	0.5240
se	0.7660	0.5380
sf	0.6560	0.5180
sg	0.5590	0.4950
sh	0.7650	0.5580
si	0.6130	0.4980
sj	0.4640	0.4480
sk	0.7050	0.5400
sl	0.7310	0.5430
sm	0.5480	0.4850
sn	0.6380	0.4830
so	0.7610	0.5530
sp	0.7610	0.5330
sq	0.7140	0.5400
sr	0.7120	0.5280
ss	0.5480	0.4700
st	0.7720	0.5470
su	0.5770	0.5060