



Full wwPDB EM Validation Report ⓘ

Mar 24, 2025 – 02:39 PM EDT

PDB ID : 9NLQ
EMDB ID : EMD-29408
Title : E. coli initiation complex with EQ2-YbiT in Hydrolytic 1/PtIM(a) conformation
Authors : Singh, S.; Hunt, J.F.
Deposited on : 2025-03-03
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:

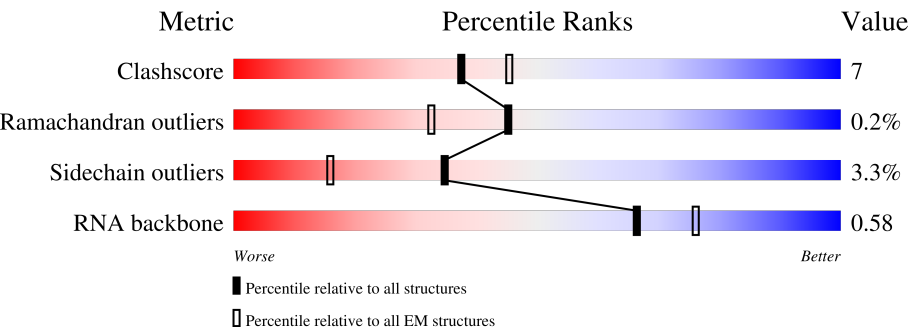
EMDB validation analysis : 0.0.1.dev117
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA,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





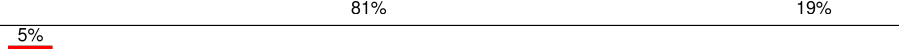
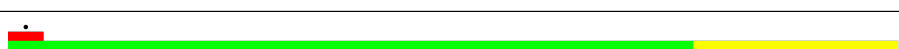

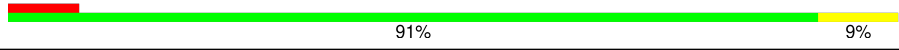

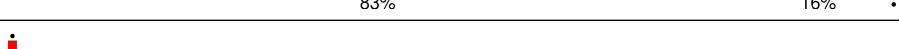



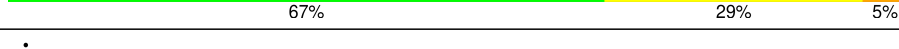

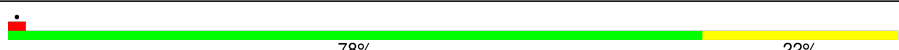


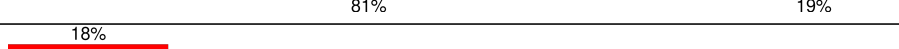







Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	220	<div><div>94%</div><div><div></div><div></div><div></div><div></div></div><div>79%21%</div></div>
2	13	142	<div><div></div><div></div><div></div><div></div></div> <div>77%22%</div> <div></div>
3	14	122	<div><div></div><div></div><div></div><div></div></div> <div>79%21%</div> <div></div>
4	15	144	<div><div></div><div></div><div></div><div></div></div> <div>81%18%</div> <div></div>
5	16	136	<div><div></div><div></div><div></div><div></div></div> <div>78%22%</div> <div></div>
6	17	120	<div><div></div><div></div><div></div><div></div></div> <div>82%17%</div> <div></div>
7	18	116	<div><div>7%</div><div></div><div></div><div></div></div> <div>73%26%</div> <div></div>

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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	77	
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	
34	R3	1539	
35	T	77	
36	Y	530	
37	sb	218	
38	sc	206	
39	sd	205	
40	se	157	
41	sf	100	
42	sg	151	
43	sh	129	
44	si	127	
45	sj	98	
46	sk	116	
47	sl	123	
48	sm	114	
49	sn	100	
50	so	88	
51	sp	82	
52	sq	80	
53	sr	65	
54	ss	79	
55	st	85	
56	su	65	

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 149989 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	27	77	Total	C	N	O	S		
			588	363	118	106	1	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 31 is a 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	527	Total	C	N	O	S		0	0
			4170	2636	715	800	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 30S ribosomal protein S19.

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

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

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

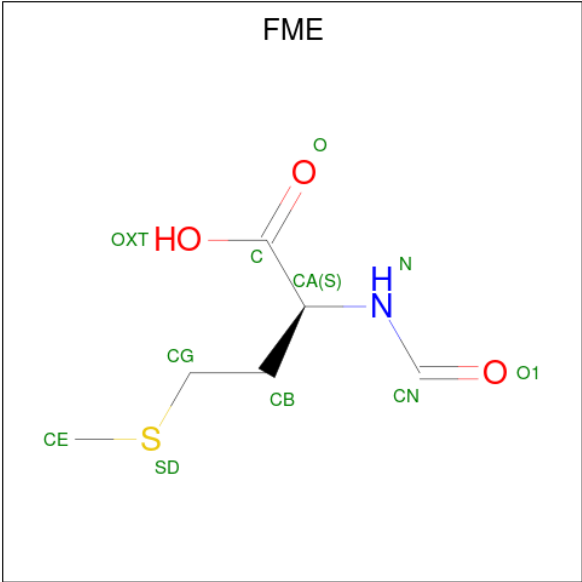
- Molecule 56 is a protein called Small ribosomal subunit protein bS21.

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

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

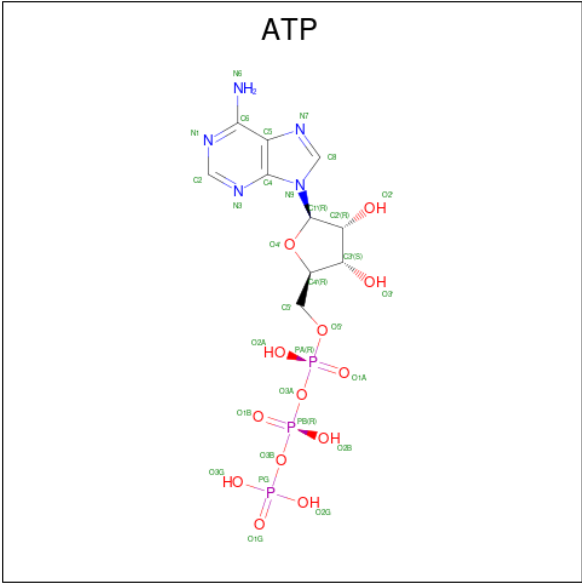
Mol	Chain	Residues	Atoms		AltConf
57	15	1	Total	Mg	0
			1	1	
57	17	1	Total	Mg	0
			1	1	
57	32	1	Total	Mg	0
			1	1	
57	M	1	Total	Mg	0
			1	1	
57	R1	184	Total	Mg	0
			184	184	
57	R3	53	Total	Mg	0
			53	53	

- Molecule 58 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: C₆H₁₁NO₃S).



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

- Molecule 59 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

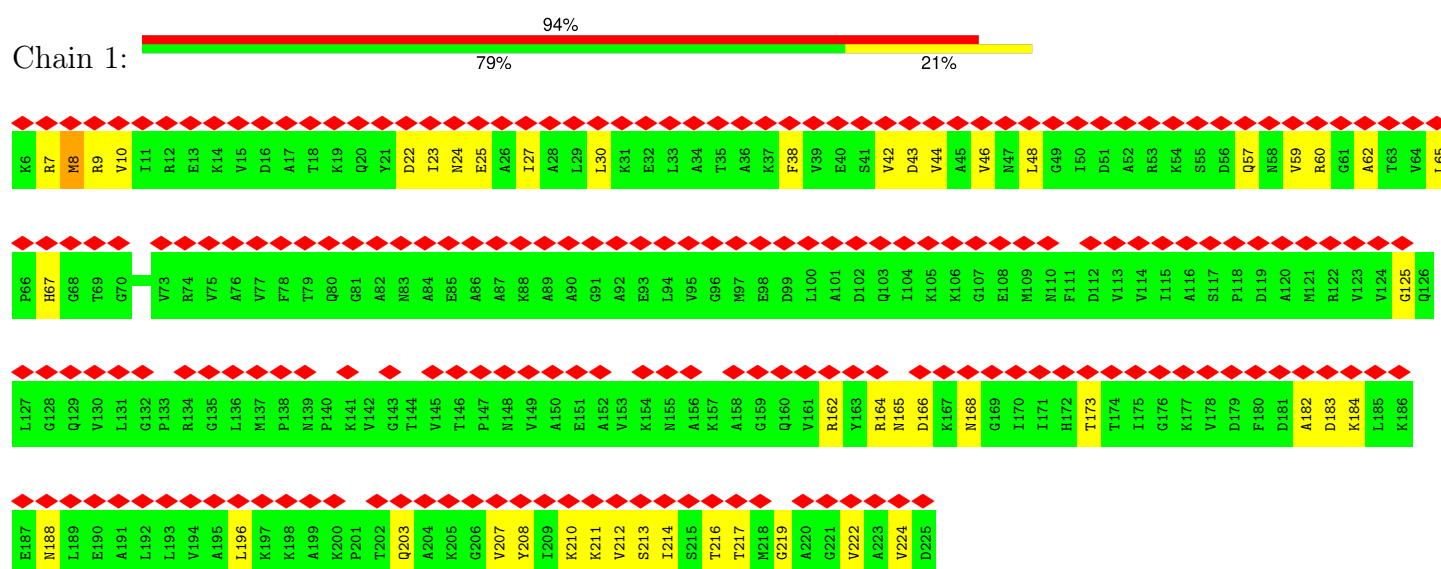
- Molecule 60 is SODIUM ION (three-letter code: NA) (formula: Na).

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

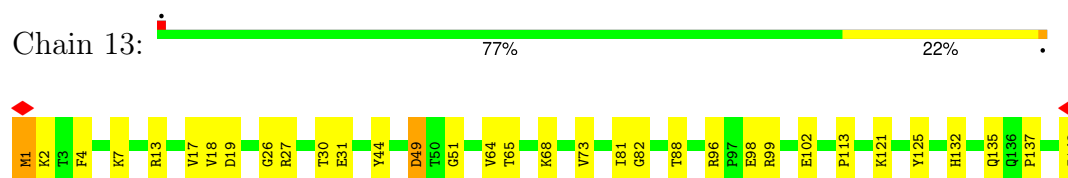
3 Residue-property plots

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

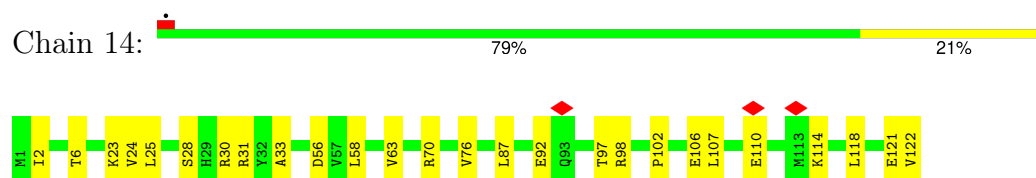
• Molecule 1: Large ribosomal subunit protein uL1



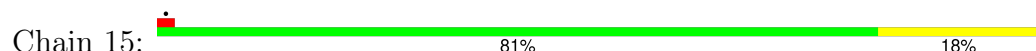
• Molecule 2: Large ribosomal subunit protein uL13

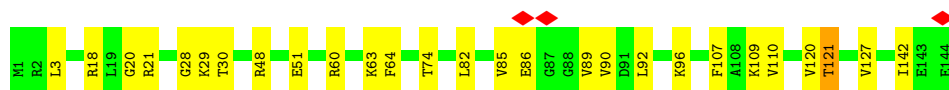


• Molecule 3: 50S ribosomal protein L14

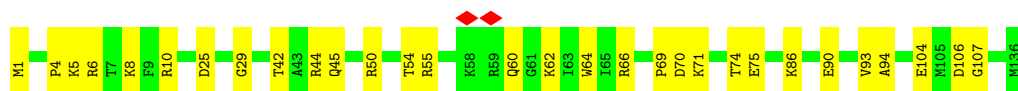
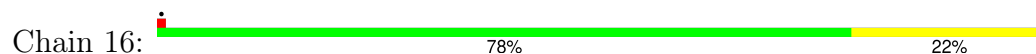


• Molecule 4: Large ribosomal subunit protein uL15

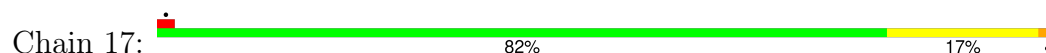




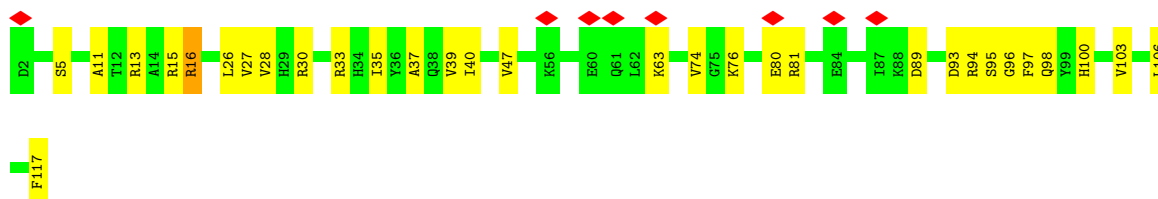
- Molecule 5: 50S ribosomal protein L16



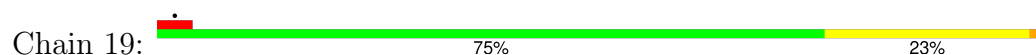
- Molecule 6: Large ribosomal subunit protein bL17



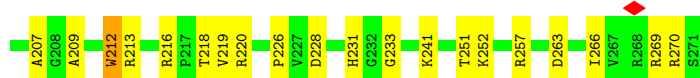
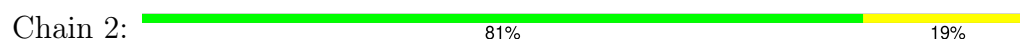
- Molecule 7: Large ribosomal subunit protein uL18




- Molecule 8: 50S ribosomal protein L19

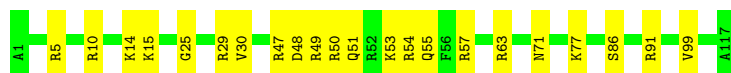


- Molecule 9: 50S ribosomal protein L2




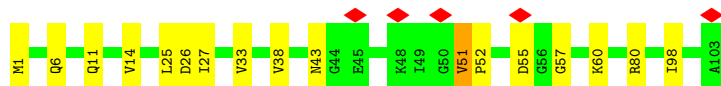
- Molecule 10: Large ribosomal subunit protein bL20

Chain 20:  81% 19%




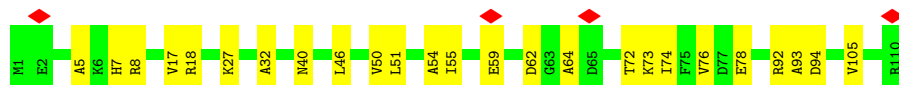
- Molecule 11: Large ribosomal subunit protein bL21

Chain 21:  5% 83% 16%




- Molecule 12: Large ribosomal subunit protein uL22

Chain 22:  77% 23%



- Molecule 13: Large ribosomal subunit protein uL23

Chain 23:  78% 22%




- Molecule 14: Large ribosomal subunit protein uL24

Chain 24:  8% 91% 9%




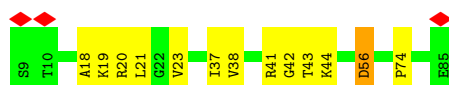
- Molecule 15: Large ribosomal subunit protein bL25

Chain 25:  10% 81% 19%




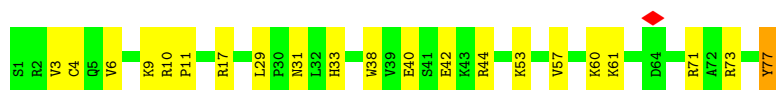
- Molecule 16: Large ribosomal subunit protein bL27

Chain 27:  83% 16%




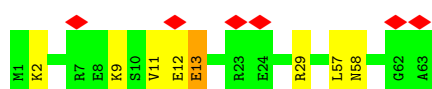
- Molecule 17: 50S ribosomal protein L28

Chain 28:  73% 26%




- Molecule 18: Large ribosomal subunit protein uL29

Chain 29:  10% 87% 11%




- Molecule 19: 50S ribosomal protein L3

Chain 3:  77% 22%




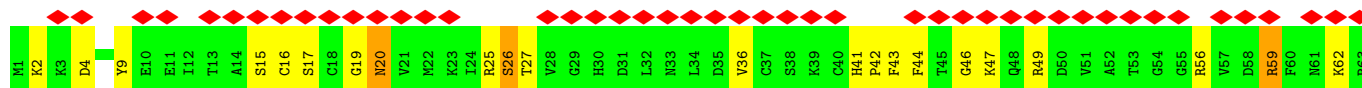
- Molecule 20: 50S ribosomal protein L30

Chain 30:  78% 22%



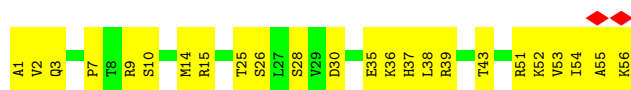
- Molecule 21: Large ribosomal subunit protein bL31

Chain 31:  74% 67% 29% 5%

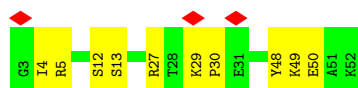
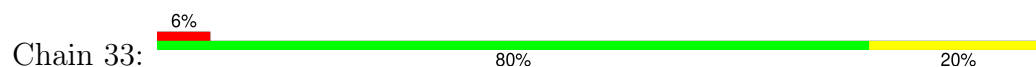


- Molecule 22: 50S ribosomal protein L32

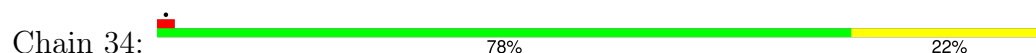
Chain 32:  57% 43%



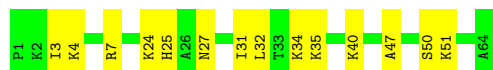
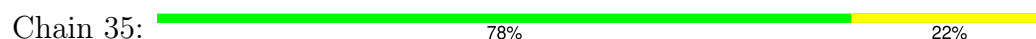
- Molecule 23: Large ribosomal subunit protein bL33



- Molecule 24: 50S ribosomal protein L34



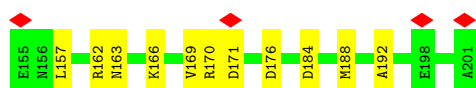
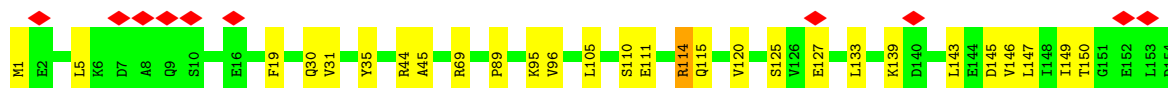
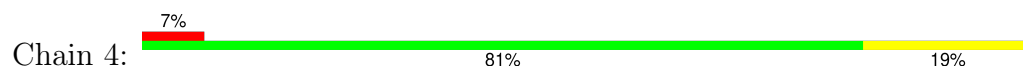
- Molecule 25: Large ribosomal subunit protein bL35



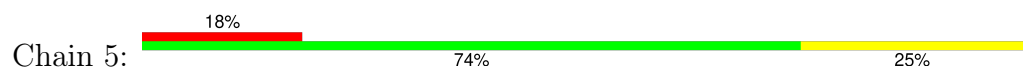
- Molecule 26: 50S ribosomal protein L36

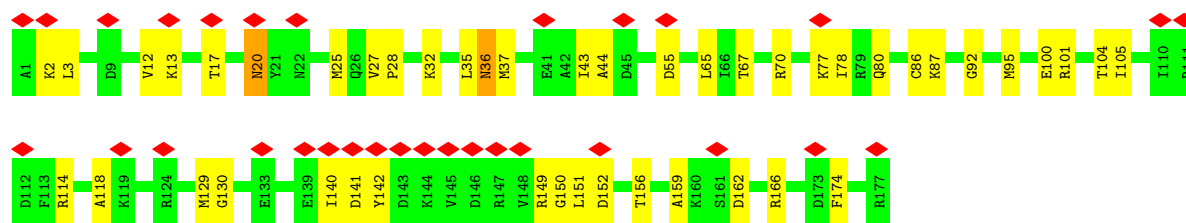


- Molecule 27: Large ribosomal subunit protein uL4

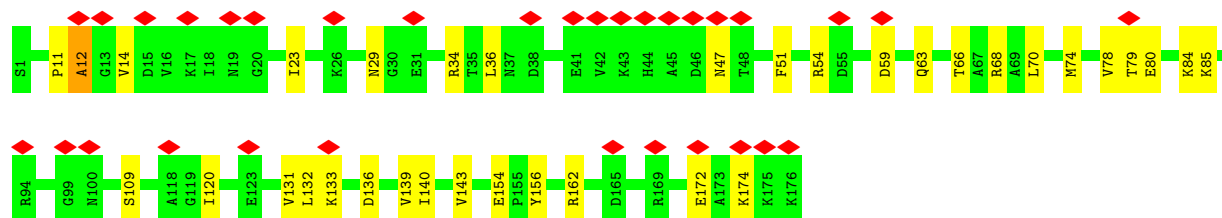
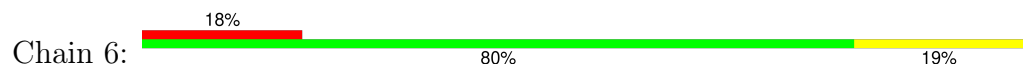


- Molecule 28: 50S ribosomal protein L5

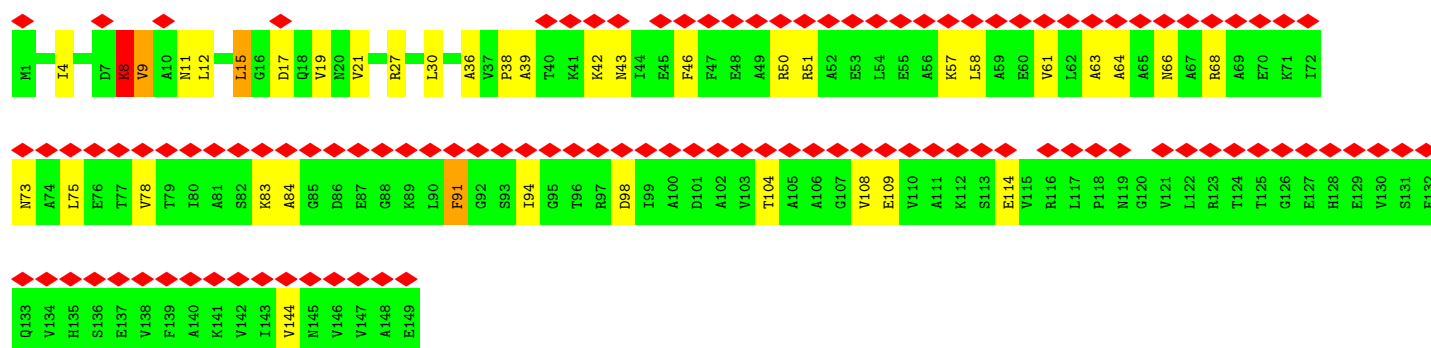




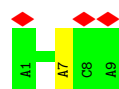
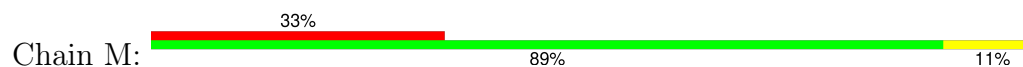
- Molecule 29: Large ribosomal subunit protein uL6



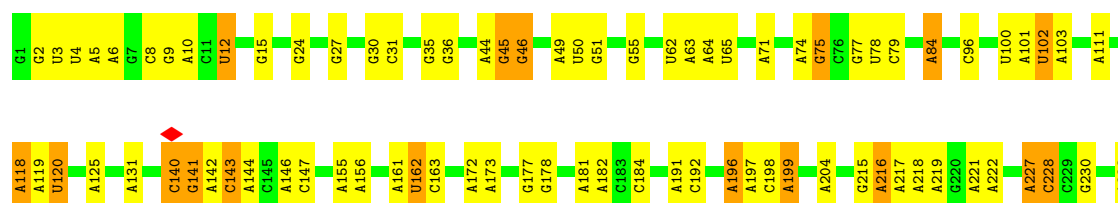
- Molecule 30: Large ribosomal subunit protein bL9



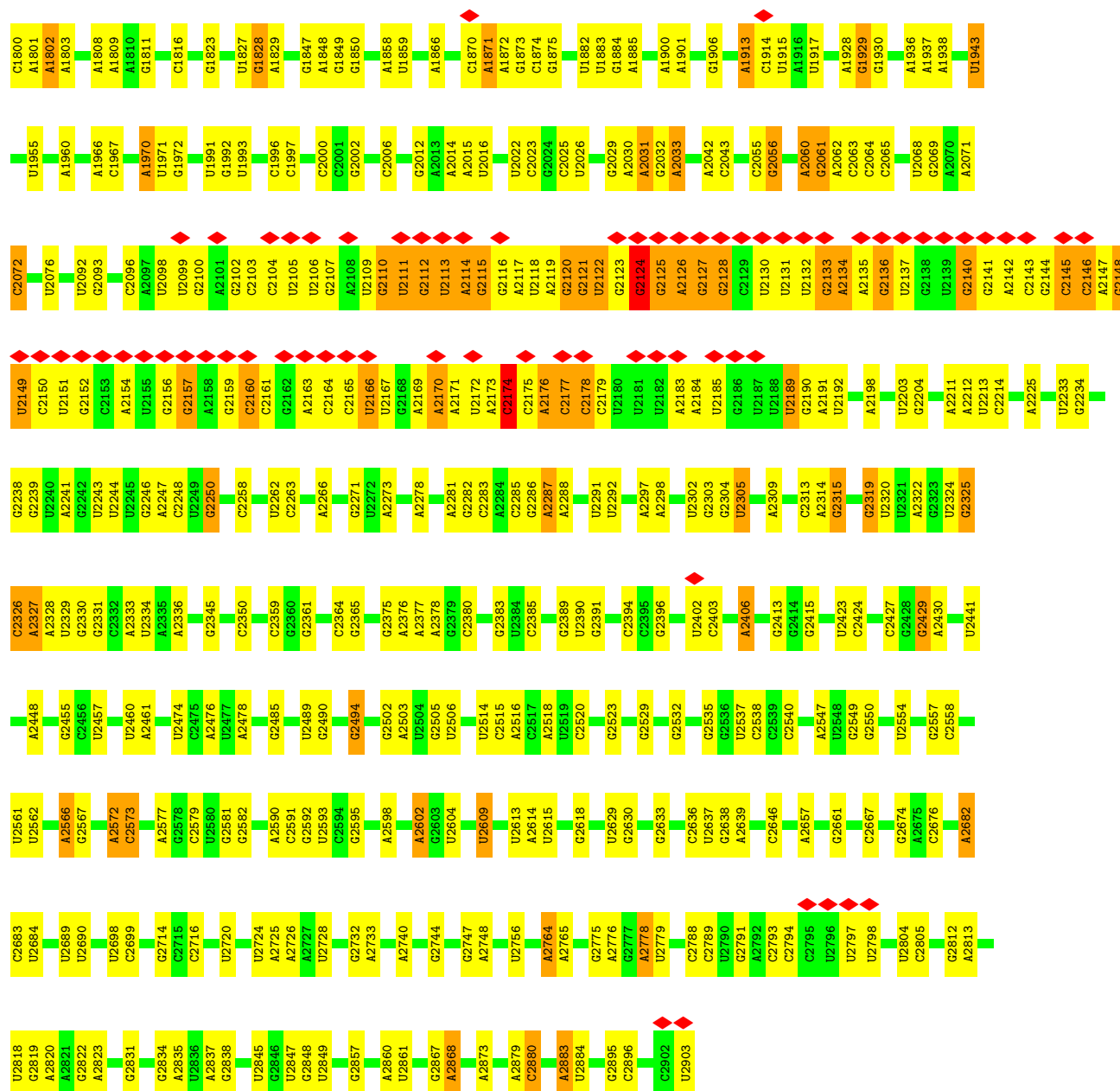
- Molecule 31: mRNA



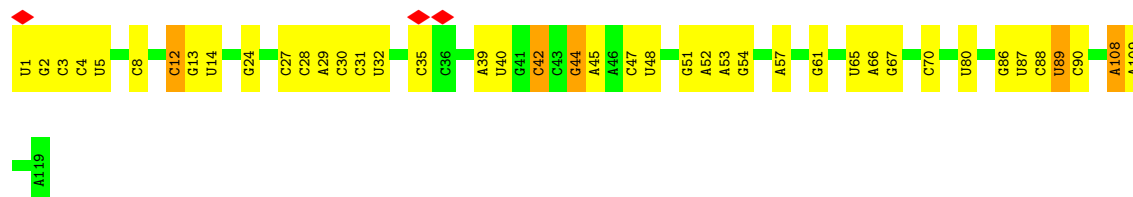
- Molecule 32: 23S ribosomal RNA





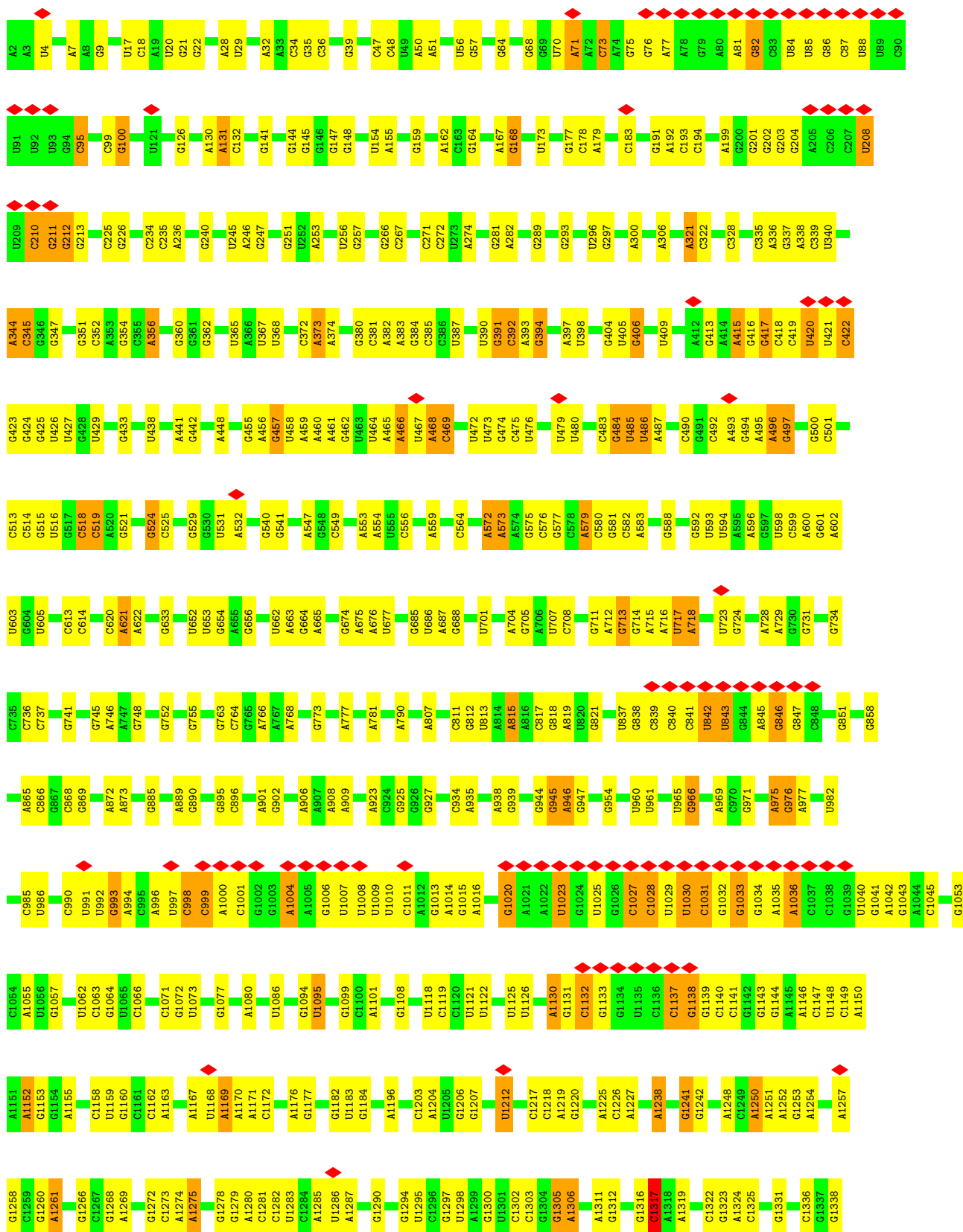


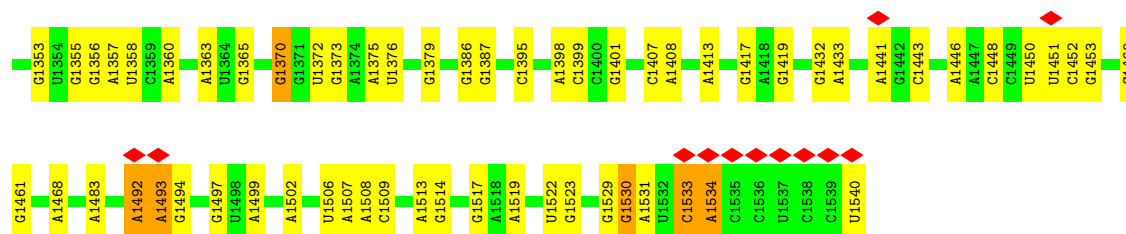
• Molecule 33: 5S ribosomal RNA



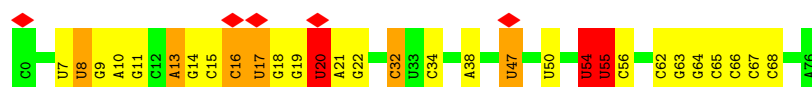
• Molecule 34: 16S ribosomal RNA



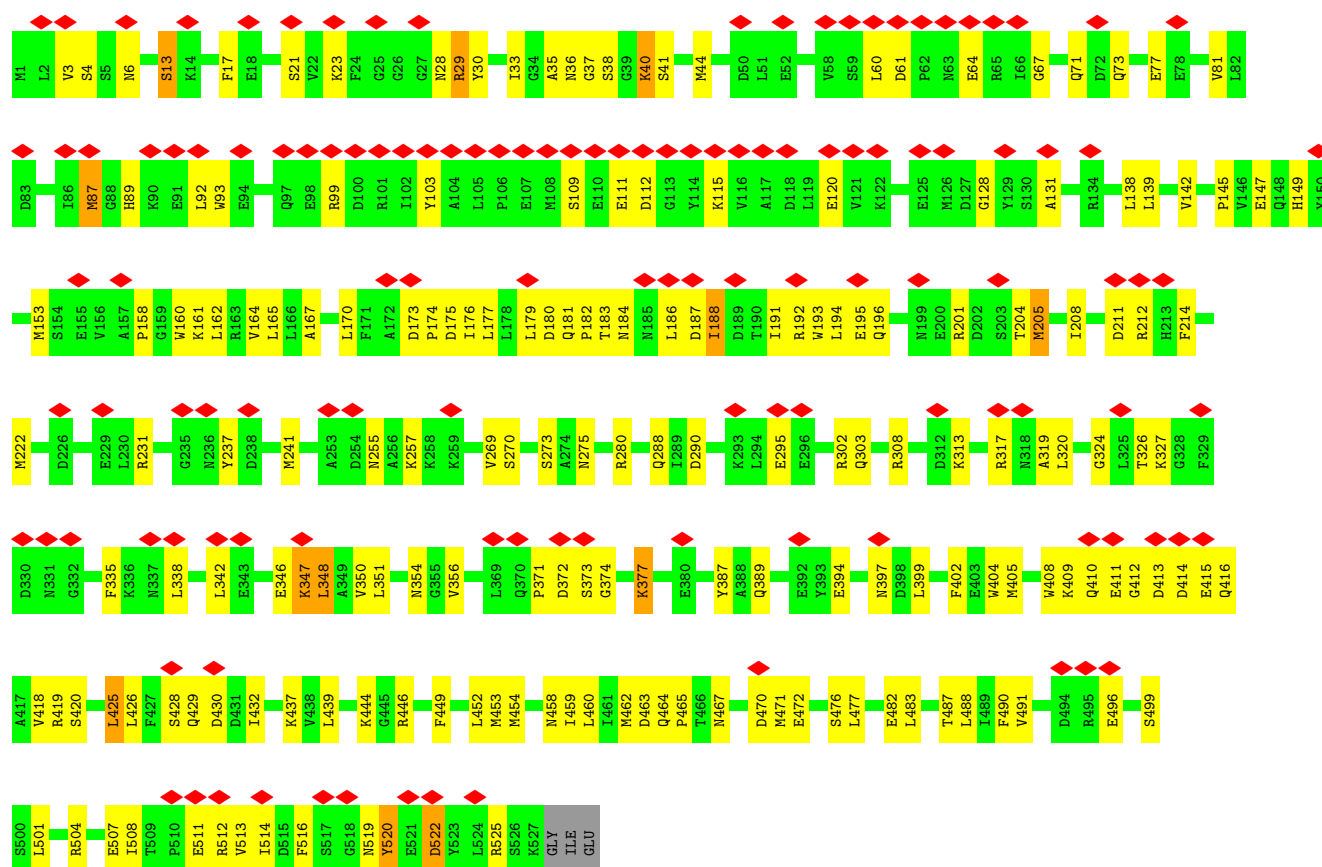




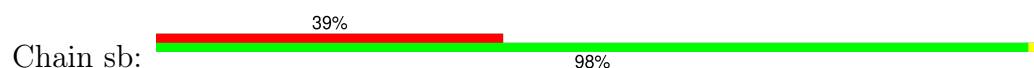
• Molecule 35: tRNA

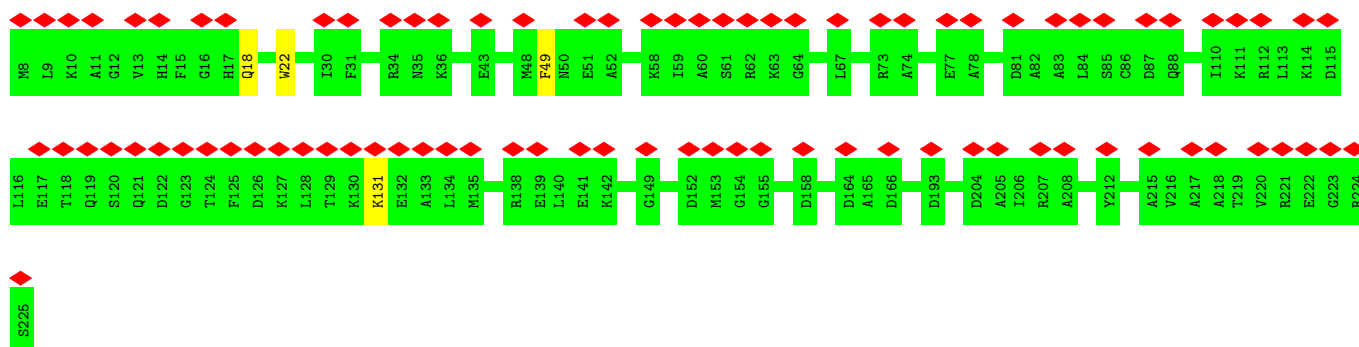


• Molecule 36: Probable ATP-binding protein YbiT



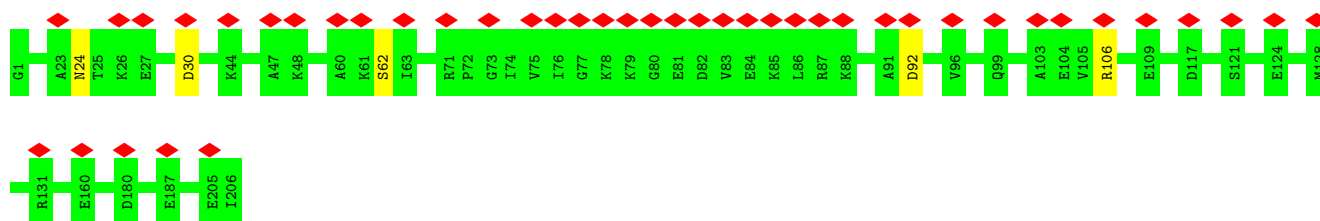
• Molecule 37: Small ribosomal subunit protein uS2





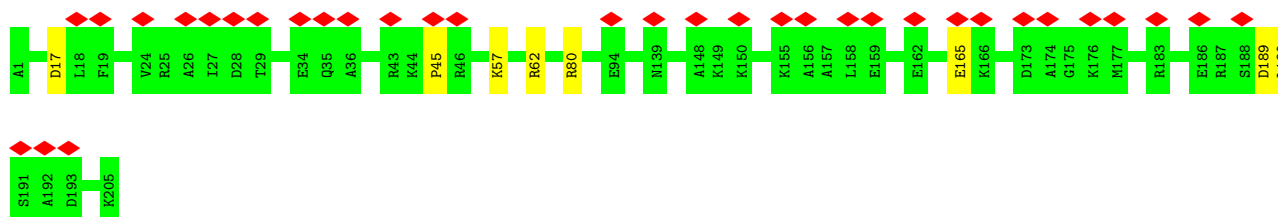
- Molecule 38: Small ribosomal subunit protein uS3

Chain sc: 21% 98%



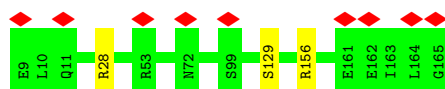
- Molecule 39: 30S ribosomal protein S4

Chain sd: 17% 96%



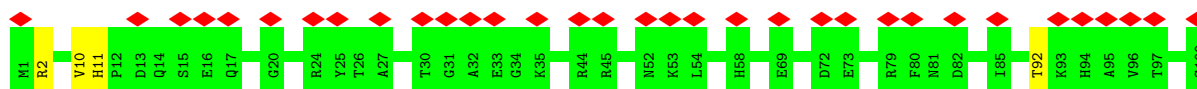
- Molecule 40: Small ribosomal subunit protein uS5

Chain se: 6% 98%

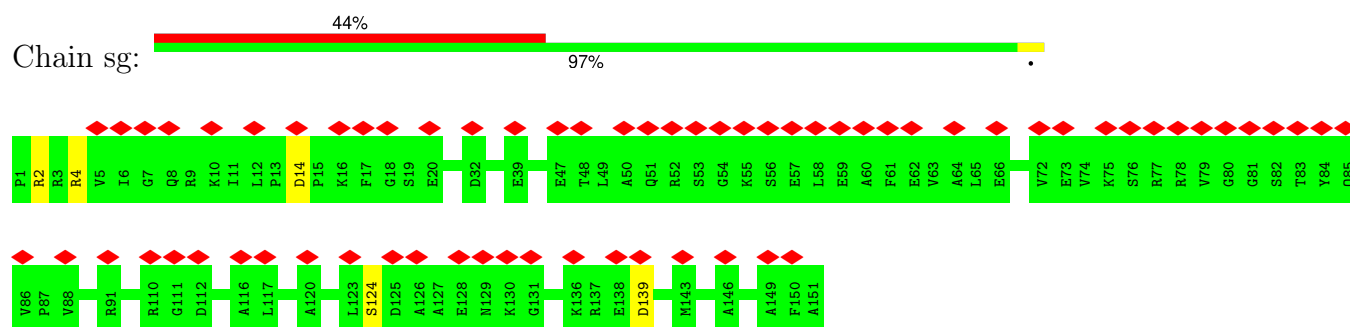


- Molecule 41: 30S ribosomal protein S6, non-modified isoform

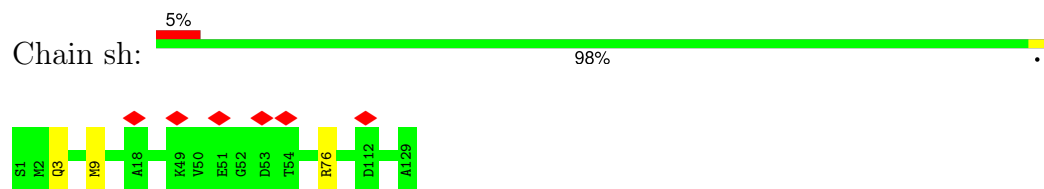
Chain sf: 33% 96%



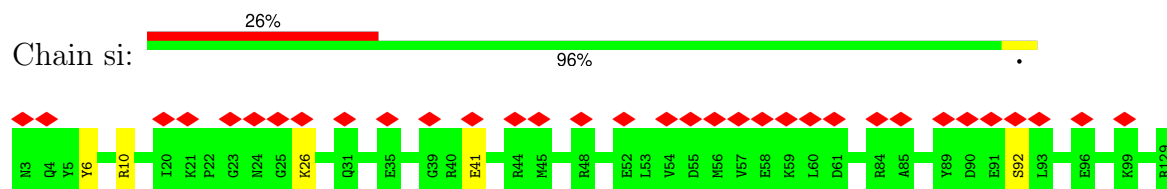
- Molecule 42: 30S ribosomal protein S7



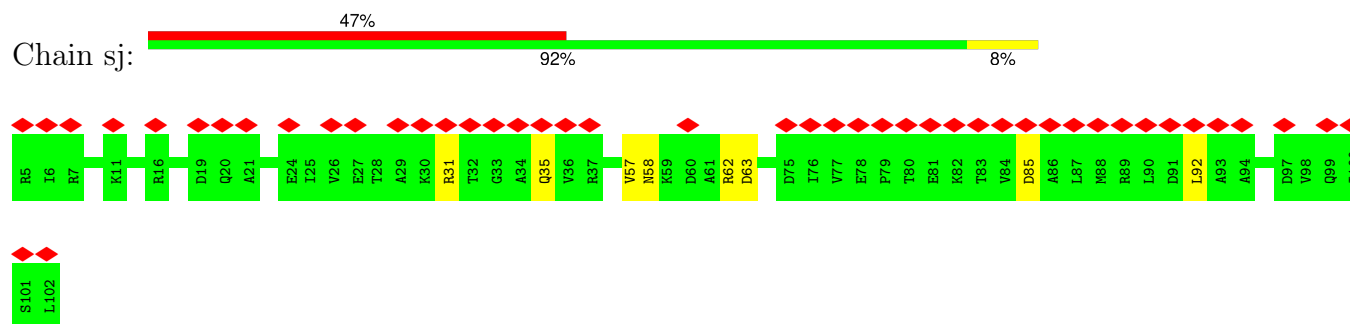
- Molecule 43: 30S ribosomal protein S8



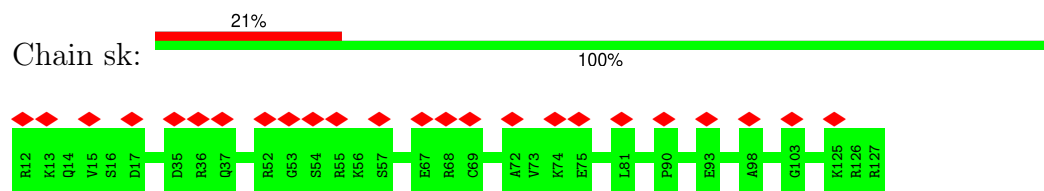
- Molecule 44: Small ribosomal subunit protein uS9



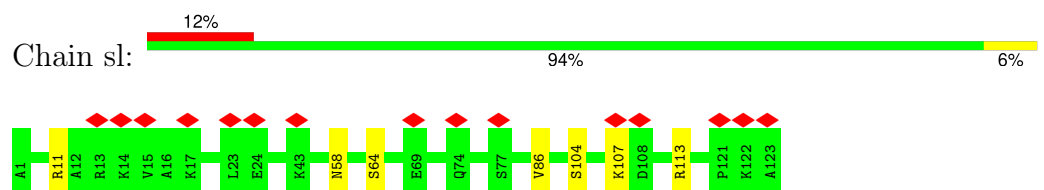
- Molecule 45: 30S ribosomal protein S10



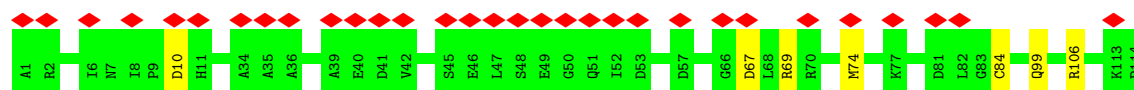
- Molecule 46: Small ribosomal subunit protein uS11



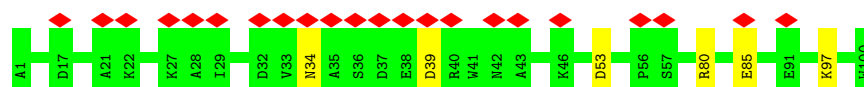
- Molecule 47: Small ribosomal subunit protein uS12



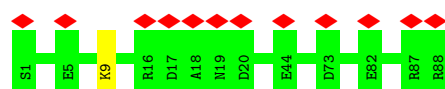
• Molecule 48: 30S ribosomal protein S13



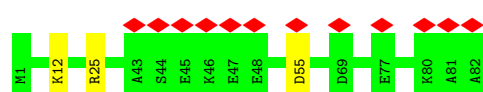
• Molecule 49: Small ribosomal subunit protein uS14



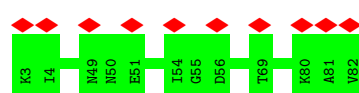
• Molecule 50: Small ribosomal subunit protein uS15



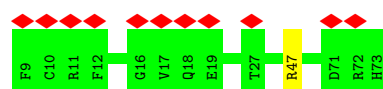
• Molecule 51: Small ribosomal subunit protein bS16



• Molecule 52: Small ribosomal subunit protein uS17

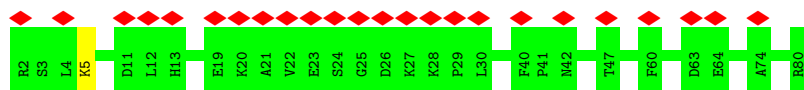


• Molecule 53: 30S ribosomal protein S18



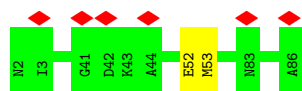
• Molecule 54: 30S ribosomal protein S19





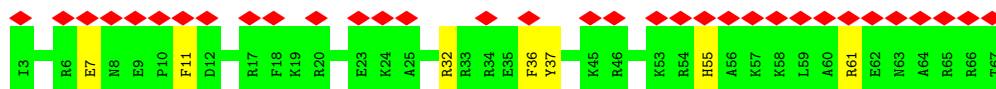
- Molecule 55: 30S ribosomal protein S20

Chain st: 7% 98%



- Molecule 56: Small ribosomal subunit protein bS21

Chain su: 51% 89% 11%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	40604	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	56.8	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	6.138	Depositor
Minimum map value	-3.742	Depositor
Average map value	0.016	Depositor
Map value standard deviation	0.237	Depositor
Recommended contour level	0.9	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: 4OC, PSU, ATP, 4SU, H2U, MG, FME, 5MU, NA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.24	0/1361	0.50	0/1796
2	13	0.31	0/1152	0.51	0/1551
3	14	0.30	0/947	0.60	0/1268
4	15	0.30	0/1062	0.57	0/1413
5	16	0.30	0/1093	0.58	0/1460
6	17	0.30	0/973	0.61	1/1301 (0.1%)
7	18	0.27	0/902	0.55	0/1209
8	19	0.30	0/929	0.62	1/1242 (0.1%)
9	2	0.30	0/2121	0.58	0/2852
10	20	0.34	0/960	0.54	0/1278
11	21	0.31	0/829	0.57	0/1107
12	22	0.28	0/864	0.53	0/1156
13	23	0.28	0/744	0.54	0/994
14	24	0.28	0/787	0.52	0/1051
15	25	0.28	0/766	0.50	0/1025
16	27	0.32	0/595	0.56	0/787
17	28	0.28	0/635	0.57	0/848
18	29	0.24	0/510	0.50	0/677
19	3	0.32	0/1586	0.53	0/2134
20	30	0.28	0/453	0.55	0/605
21	31	0.26	0/531	0.55	0/709
22	32	0.30	0/450	0.58	0/599
23	33	0.31	0/416	0.56	0/554
24	34	0.29	0/380	0.65	0/498
25	35	0.29	0/513	0.54	0/676
26	36	0.28	0/303	0.57	0/397
27	4	0.29	0/1571	0.50	0/2113
28	5	0.27	0/1434	0.53	0/1926
29	6	0.31	0/1343	0.64	3/1816 (0.2%)
30	9	0.26	0/1122	0.55	1/1515 (0.1%)
31	M	0.23	0/219	0.71	0/339
32	R1	0.44	0/69797	0.79	14/108890 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	R2	0.35	0/2847	0.83	0/4440
34	R3	0.33	0/36963	0.78	5/57662 (0.0%)
35	T	0.29	0/1716	0.76	1/2672 (0.0%)
36	Y	0.27	0/4245	0.56	2/5723 (0.0%)
37	sb	0.25	0/1735	0.50	0/2338
38	sc	0.25	0/1651	0.53	0/2225
39	sd	0.30	1/1665 (0.1%)	0.62	3/2227 (0.1%)
40	se	0.28	0/1169	0.56	0/1573
41	sf	0.26	0/835	0.63	1/1128 (0.1%)
42	sg	0.24	0/1195	0.53	0/1602
43	sh	0.27	0/989	0.51	0/1326
44	si	0.26	0/1034	0.61	0/1375
45	sj	0.26	0/796	0.61	1/1077 (0.1%)
46	sk	0.25	0/885	0.53	0/1195
47	sl	0.28	0/969	0.62	0/1300
48	sm	0.25	0/892	0.59	0/1193
49	sn	0.26	0/817	0.59	0/1088
50	so	0.24	0/722	0.53	0/964
51	sp	0.27	0/659	0.55	0/884
52	sq	0.27	0/657	0.55	0/881
53	sr	0.26	0/544	0.51	0/731
54	ss	0.26	0/652	0.51	0/877
55	st	0.25	0/671	0.47	0/888
56	su	0.26	0/550	0.68	0/728
All	All	0.37	1/162206 (0.0%)	0.73	33/241883 (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
29	6	0	1
30	9	0	1
35	T	7	0
41	sf	0	2
47	sl	0	1
49	sn	0	1
56	su	0	1
All	All	7	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	sd	45	PRO	CG-CD	-6.29	1.29	1.50

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	sd	45	PRO	N-CD-CG	-11.10	86.55	103.20
29	6	11	PRO	N-CD-CG	-10.04	88.14	103.20
36	Y	348	LEU	CA-CB-CG	8.17	134.09	115.30
29	6	11	PRO	CA-CB-CG	-7.57	89.62	104.00
8	19	113	LEU	CA-CB-CG	7.21	131.88	115.30
32	R1	62	U	C2-N1-C1'	6.79	125.85	117.70
32	R1	12	U	C2-N1-C1'	6.64	125.67	117.70
32	R1	2174	C	N3-C2-O2	-6.61	117.27	121.90
29	6	11	PRO	CA-N-CD	-6.55	102.33	111.50
30	9	15	LEU	CA-CB-CG	6.50	130.24	115.30
45	sj	92	LEU	CA-CB-CG	6.43	130.09	115.30
32	R1	1313	U	C2-N1-C1'	6.33	125.29	117.70
39	sd	45	PRO	CA-CB-CG	-6.30	92.03	104.00
41	sf	10	VAL	C-N-CA	-6.16	106.30	121.70
32	R1	2174	C	N1-C2-O2	6.10	122.56	118.90
39	sd	45	PRO	CA-N-CD	-5.82	103.35	111.50
32	R1	2124	G	N1-C6-O6	-5.77	116.44	119.90
6	17	117	ASP	CB-CG-OD1	5.74	123.46	118.30
36	Y	425	LEU	CA-CB-CG	5.65	128.29	115.30
32	R1	62	U	N1-C2-O2	5.61	126.72	122.80
32	R1	2178	C	N3-C2-O2	-5.40	118.12	121.90
32	R1	1314	C	C2-N1-C1'	5.39	124.73	118.80
32	R1	12	U	N3-C2-O2	-5.26	118.52	122.20
34	R3	1317	C	N1-C2-O2	5.23	122.04	118.90
34	R3	73	C	C2-N1-C1'	5.20	124.52	118.80
34	R3	998	C	C2-N1-C1'	5.17	124.49	118.80
35	T	17	U	OP2-P-O3'	5.17	116.58	105.20
32	R1	12	U	N1-C2-O2	5.17	126.42	122.80
32	R1	2124	G	C5-C6-O6	5.14	131.68	128.60
34	R3	998	C	N1-C2-O2	5.14	121.98	118.90
32	R1	955	U	N3-C2-O2	-5.09	118.64	122.20
34	R3	1132	C	C2-N1-C1'	5.08	124.39	118.80
32	R1	2573	C	C2-N1-C1'	5.07	124.38	118.80

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
35	T	8	4SU	C2',C1'

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

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
29	6	12	ALA	Peptide
30	9	8	LYS	Peptide
41	sf	11	HIS	Peptide
41	sf	92	THR	Peptide
47	sl	86	VAL	Peptide
49	sn	85	GLU	Peptide
56	su	7	GLU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1353	0	1159	30	0
2	13	1129	0	1162	25	0
3	14	938	0	1012	21	0
4	15	1053	0	1129	19	0
5	16	1074	0	1157	18	0
6	17	960	0	1000	14	0
7	18	892	0	923	21	0
8	19	917	0	965	18	0
9	2	2082	0	2157	33	0
10	20	947	0	1022	17	0
11	21	816	0	839	14	0
12	22	857	0	922	16	0
13	23	738	0	807	12	0
14	24	779	0	834	5	0
15	25	753	0	780	10	0
16	27	588	0	604	12	0
17	28	625	0	655	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	29	509	0	543	6	0
19	3	1565	0	1616	37	0
20	30	449	0	491	7	0
21	31	522	0	524	14	0
22	32	444	0	461	19	0
23	33	409	0	440	6	0
24	34	377	0	418	8	0
25	35	504	0	574	10	0
26	36	302	0	343	4	0
27	4	1552	0	1619	26	0
28	5	1410	0	1447	31	0
29	6	1323	0	1374	18	0
30	9	1111	0	1148	22	0
31	M	195	0	99	0	0
32	R1	62318	0	31344	563	0
33	R2	2546	0	1292	32	0
34	R3	33012	0	16617	277	0
35	T	1639	0	843	18	0
36	Y	4170	0	4132	128	0
37	sb	1704	0	1732	0	0
38	sc	1624	0	1699	0	0
39	sd	1643	0	1710	0	0
40	se	1156	0	1199	0	0
41	sf	817	0	808	0	0
42	sg	1181	0	1240	0	0
43	sh	979	0	1034	0	0
44	si	1022	0	1070	0	0
45	sj	786	0	828	0	0
46	sk	869	0	878	0	0
47	sl	955	0	1019	0	0
48	sm	883	0	944	0	0
49	sn	805	0	847	0	0
50	so	714	0	737	0	0
51	sp	649	0	666	0	0
52	sq	648	0	691	0	0
53	sr	535	0	552	0	0
54	ss	637	0	665	0	0
55	st	665	0	714	0	0
56	su	544	0	579	0	0
57	15	1	0	0	0	0
57	17	1	0	0	0	0
57	32	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	M	1	0	0	0	0
57	R1	184	0	0	0	0
57	R3	53	0	0	0	0
58	T	10	0	10	1	0
59	Y	62	0	24	3	0
60	Y	2	0	0	0	0
All	All	149989	0	102098	1373	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 7.

All (1373) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:R1:1847:G:HO2'	32:R1:1848:A:H8	1.04	0.98
11:21:51:VAL:HG12	11:21:52:PRO:HD2	1.48	0.96
8:19:113:LEU:HD12	8:19:114:ASN:H	1.37	0.90
34:R3:409:U:H3	34:R3:433:G:H1	1.22	0.88
32:R1:284:U:H3	32:R1:356:G:H1	1.23	0.86
36:Y:347:LYS:HZ1	36:Y:501:LEU:HB2	1.40	0.85
36:Y:73:GLN:HE21	36:Y:184:ASN:HD22	1.24	0.84
32:R1:1417:C:O2	32:R1:1581:G:N2	2.11	0.81
32:R1:2391:G:O2'	32:R1:2429:G:N2	2.13	0.81
34:R3:75:G:N2	34:R3:95:C:O2	2.11	0.80
32:R1:1091:G:N1	32:R1:1100:C:N3	2.28	0.78
32:R1:1533:C:N3	32:R1:1538:G:N1	2.30	0.78
34:R3:674:G:H2'	34:R3:675:A:H8	1.49	0.77
34:R3:1356:G:H2'	34:R3:1357:A:H8	1.50	0.77
13:23:6:ARG:NH2	13:23:37:ASP:OD1	2.19	0.76
32:R1:306:U:H3	32:R1:310:A:H62	1.34	0.76
36:Y:40:LYS:HB3	36:Y:208:ILE:HD11	1.68	0.75
36:Y:255:ASN:ND2	36:Y:295:GLU:O	2.18	0.75
32:R1:2166:U:O4	32:R1:2170:A:N6	2.20	0.74
34:R3:202:G:H21	34:R3:466:A:H61	1.34	0.74
34:R3:938:A:N3	34:R3:1376:U:O2'	2.20	0.74
32:R1:1270:C:H5''	32:R1:1271:G:H5'	1.70	0.74
34:R3:1133:G:N1	34:R3:1141:C:N3	2.34	0.73
32:R1:1048:A:OP2	32:R1:1110:G:N2	2.20	0.73
20:30:40:THR:HG22	20:30:42:ALA:H	1.52	0.73
36:Y:347:LYS:NZ	36:Y:501:LEU:HB2	2.03	0.73
32:R1:1091:G:N2	32:R1:1100:C:O2	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:Y:29:ARG:HB3	36:Y:205:MET:HE3	1.70	0.73
21:31:16:CYS:SG	21:31:17:SER:N	2.62	0.73
34:R3:297:G:N2	34:R3:300:A:OP2	2.22	0.73
32:R1:545:U:O2	32:R1:549:G:N2	2.22	0.72
34:R3:461:A:H2'	34:R3:462:G:H8	1.54	0.72
3:14:28:SER:OG	32:R1:2566:A:N1	2.22	0.72
20:30:11:SER:OG	32:R1:989:G:OP2	2.06	0.72
22:32:9:ARG:NH2	32:R1:516:C:OP1	2.23	0.72
9:2:71:ASP:OD2	9:2:188:ARG:NH2	2.23	0.72
32:R1:881:G:O6	32:R1:895:U:O2	2.08	0.71
30:9:73:ASN:HB3	30:9:108:VAL:HG21	1.72	0.71
35:T:50:U:H3	35:T:64:G:H1	1.38	0.71
34:R3:75:G:N1	34:R3:95:C:N3	2.30	0.71
2:13:44:TYR:O	10:20:63:ARG:NH1	2.24	0.71
32:R1:481:G:O2'	32:R1:506:G:N2	2.23	0.71
34:R3:1357:A:H61	34:R3:1365:G:H1	1.38	0.71
33:R2:65:U:H3'	33:R2:108:A:H61	1.55	0.71
8:19:105:LYS:O	8:19:108:ARG:NH1	2.22	0.71
36:Y:425:LEU:HD13	36:Y:446:ARG:HG2	1.73	0.71
32:R1:2144:G:N2	32:R1:2146:C:O2'	2.23	0.70
34:R3:1356:G:H2'	34:R3:1357:A:C8	2.26	0.70
19:3:5:VAL:H	19:3:32:ASN:HD21	1.39	0.70
32:R1:2156:G:N7	32:R1:2157:G:N2	2.37	0.70
36:Y:387:TYR:HB3	36:Y:462:MET:HA	1.73	0.70
1:1:27:ILE:HD12	1:1:182:ALA:HB1	1.72	0.70
8:19:52:ARG:NH2	32:R1:2720:U:OP1	2.25	0.70
32:R1:1779:U:OP2	32:R1:1784:A:N6	2.25	0.70
3:14:98:ARG:NH1	34:R3:339:C:OP2	2.25	0.69
34:R3:1015:G:N2	34:R3:1218:C:O2	2.25	0.69
10:20:47:ARG:NH1	32:R1:560:C:O2'	2.26	0.69
1:1:30:LEU:HD21	1:1:42:VAL:HG11	1.75	0.69
34:R3:1323:G:H2'	34:R3:1324:A:C8	2.28	0.69
6:17:4:ARG:O	32:R1:2873:A:O2'	2.09	0.69
4:15:48:ARG:HD2	32:R1:666:A:H4'	1.76	0.68
11:21:6:GLN:HB3	11:21:11:GLN:HG3	1.75	0.68
6:17:17:ARG:NH2	32:R1:2002:G:OP1	2.27	0.68
19:3:59:ARG:NH1	32:R1:2831:G:OP2	2.26	0.68
33:R2:14:U:OP2	33:R2:70:C:O2'	2.10	0.68
7:18:30:ARG:NH2	33:R2:48:U:OP1	2.27	0.68
6:17:22:ARG:HG3	6:17:70:THR:HA	1.75	0.68
32:R1:958:U:H2'	33:R2:89:U:H1'	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:R1:1079:C:O2	32:R1:1080:A:N6	2.24	0.67
32:R1:2297:A:N6	32:R1:2319:G:O2'	2.27	0.67
19:3:77:ARG:NH1	19:3:200:ASP:OD1	2.27	0.67
9:2:216:ARG:NH2	32:R1:781:A:OP1	2.27	0.67
25:35:4:LYS:NZ	32:R1:253:C:OP2	2.26	0.67
4:15:127:VAL:HG21	4:15:142:ILE:HD13	1.75	0.67
36:Y:320:LEU:HB2	36:Y:342:LEU:HD22	1.76	0.67
14:24:39:ASN:HB3	14:24:62:ALA:HB3	1.77	0.67
32:R1:729:G:H5''	32:R1:730:A:H5''	1.77	0.67
32:R1:1521:G:H3'	32:R1:1522:A:H5''	1.76	0.67
16:27:18:ALA:O	16:27:20:ARG:NH1	2.28	0.67
19:3:33:ARG:NH2	19:3:53:GLY:O	2.28	0.67
29:6:79:THR:HG22	29:6:80:GLU:HG3	1.75	0.67
1:1:44:VAL:HG12	1:1:214:ILE:HG12	1.77	0.67
4:15:48:ARG:NH2	25:35:4:LYS:O	2.27	0.66
30:9:94:ILE:HG23	30:9:98:ASP:HB2	1.76	0.66
36:Y:77:GLU:OE2	36:Y:161:LYS:NZ	2.24	0.66
34:R3:212:G:H2'	34:R3:213:G:H8	1.59	0.66
12:22:5:ALA:HB2	12:22:54:ALA:HB2	1.77	0.66
34:R3:1218:C:H2'	34:R3:1219:A:C8	2.31	0.66
32:R1:389:G:C8	32:R1:2413:G:H4'	2.30	0.66
34:R3:1306:A:N6	34:R3:1331:G:O2'	2.28	0.66
28:5:20:ASN:ND2	28:5:20:ASN:O	2.28	0.65
32:R1:918:A:N3	33:R2:80:U:O2'	2.28	0.65
16:27:37:ILE:HG22	16:27:38:VAL:HG13	1.77	0.65
32:R1:2126:A:N6	32:R1:2163:A:O2'	2.28	0.65
32:R1:270:A:N1	32:R1:369:U:O2'	2.29	0.65
32:R1:2523:G:HO2'	32:R1:2764:A:HO2'	1.44	0.65
10:20:49:ARG:O	10:20:53:LYS:NZ	2.29	0.65
34:R3:790:A:OP1	35:T:38:A:O2'	2.13	0.65
34:R3:1040:U:H2'	34:R3:1041:G:C8	2.31	0.65
29:6:85:LYS:HG2	29:6:131:VAL:HG22	1.79	0.65
30:9:8:LYS:HA	30:9:15:LEU:HB3	1.79	0.65
12:22:8:ARG:NH1	32:R1:494:G:OP1	2.30	0.65
32:R1:886:A:H2'	32:R1:888:C:H5	1.62	0.64
36:Y:179:LEU:HD12	36:Y:208:ILE:HG21	1.78	0.64
11:21:80:ARG:NH2	32:R1:572:A:OP2	2.31	0.64
34:R3:1137:C:O2'	34:R3:1138:G:N2	2.30	0.64
36:Y:67:GLY:O	36:Y:176:ILE:HA	1.97	0.64
12:22:72:THR:HG22	12:22:73:LYS:HG3	1.79	0.64
27:4:163:ASN:ND2	32:R1:320:A:N3	2.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:R3:1009:U:H3	34:R3:1020:G:H1	1.43	0.64
8:19:113:LEU:CD1	8:19:114:ASN:H	2.10	0.64
14:24:81:ARG:NH2	32:R1:301:G:OP2	2.31	0.64
32:R1:1668:A:N3	32:R1:1670:C:N4	2.46	0.64
7:18:76:LYS:NZ	7:18:80:GLU:OE2	2.31	0.64
30:9:78:VAL:HB	30:9:144:VAL:HG22	1.80	0.64
4:15:74:THR:HG23	4:15:107:PHE:HB2	1.80	0.63
36:Y:350:VAL:HB	36:Y:491:VAL:HG12	1.80	0.63
16:27:21:LEU:HD21	16:27:41:ARG:HH21	1.63	0.63
34:R3:1133:G:N2	34:R3:1141:C:O2	2.19	0.63
35:T:47:U:O2'	35:T:50:U:OP1	2.14	0.63
27:4:143:LEU:HB3	27:4:146:VAL:HG21	1.79	0.63
9:2:231:HIS:HA	9:2:241:LYS:HE3	1.81	0.63
34:R3:1013:G:N2	34:R3:1016:A:OP2	2.30	0.63
34:R3:356:A:N3	34:R3:368:U:O2'	2.29	0.63
9:2:144:GLU:HB2	9:2:187:CYS:HB2	1.80	0.63
34:R3:674:G:H2'	34:R3:675:A:C8	2.34	0.63
33:R2:30:C:H1'	33:R2:57:A:H61	1.64	0.63
34:R3:1086:U:H3	34:R3:1099:G:H22	1.46	0.63
36:Y:347:LYS:HB3	36:Y:490:PHE:HE1	1.64	0.63
6:17:30:ARG:NH1	6:17:74:GLU:OE1	2.31	0.62
28:5:104:THR:HG23	28:5:105:ILE:HG23	1.81	0.62
32:R1:2112:G:HO2'	32:R1:2115:G:N2	1.96	0.62
32:R1:177:G:OP2	32:R1:177:G:N2	2.29	0.62
32:R1:1089:A:N6	32:R1:1098:A:OP1	2.31	0.62
34:R3:1218:C:H2'	34:R3:1219:A:H8	1.63	0.62
36:Y:139:LEU:HD11	36:Y:164:VAL:HG13	1.79	0.62
9:2:97:ASP:N	9:2:97:ASP:OD1	2.32	0.62
25:35:34:LYS:NZ	32:R1:2390:U:OP2	2.31	0.62
34:R3:1533:C:H5'	34:R3:1534:A:H5'	1.82	0.62
1:1:207:VAL:O	1:1:210:LYS:NZ	2.33	0.62
4:15:110:VAL:HB	4:15:127:VAL:HG12	1.81	0.62
32:R1:2130:U:O2'	32:R1:2134:A:O2'	2.18	0.62
15:25:77:VAL:HG23	15:25:89:ILE:HG12	1.81	0.62
19:3:151:THR:OG1	32:R1:2032:G:N2	2.33	0.62
34:R3:993:G:O2'	34:R3:994:A:N7	2.32	0.62
1:1:8:MET:HG2	1:1:9:ARG:HG3	1.82	0.61
32:R1:1044:C:O2'	32:R1:1111:A:N6	2.33	0.61
4:15:18:ARG:NH2	32:R1:1250:G:N7	2.41	0.61
32:R1:704:G:H2'	32:R1:726:G:H22	1.65	0.61
19:3:64:GLU:OE2	32:R1:2633:G:O2'	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:R1:1069:A:H1'	32:R1:1096:A:H4'	1.82	0.61
34:R3:392:C:HO2'	34:R3:483:C:HO2'	1.49	0.61
34:R3:714:G:H2'	34:R3:715:A:C8	2.35	0.61
21:31:25:ARG:O	28:5:101:ARG:NH2	2.30	0.61
27:4:45:ALA:HB2	27:4:89:PRO:HD3	1.83	0.61
9:2:106:PRO:HD2	9:2:109:LEU:HD22	1.82	0.61
32:R1:2328:A:H2'	32:R1:2329:U:C6	2.35	0.61
36:Y:308:ARG:HD2	36:Y:483:LEU:HD22	1.82	0.61
11:21:51:VAL:HG12	11:21:52:PRO:CD	2.28	0.61
34:R3:1323:G:H2'	34:R3:1324:A:H8	1.64	0.61
32:R1:962:G:H21	32:R1:2250:G:H1	1.49	0.60
32:R1:1533:C:O2	32:R1:1538:G:N2	2.17	0.60
34:R3:713:G:H2'	34:R3:714:G:C8	2.36	0.60
2:13:65:THR:OG1	32:R1:1141:U:OP2	2.18	0.60
9:2:116:GLN:O	9:2:127:ASN:ND2	2.27	0.60
32:R1:2174:C:H2'	32:R1:2175:C:C6	2.37	0.60
34:R3:1071:C:H2'	34:R3:1072:G:H8	1.66	0.60
36:Y:13:SER:O	36:Y:13:SER:OG	2.17	0.60
10:20:49:ARG:NH1	32:R1:993:G:OP1	2.28	0.60
32:R1:745:G:HO2'	32:R1:748:G:HO2'	1.37	0.60
32:R1:2595:G:N2	32:R1:2598:A:OP2	2.30	0.60
33:R2:52:A:O2'	33:R2:53:A:H8	1.85	0.60
36:Y:6:ASN:H	36:Y:21:SER:HG	1.50	0.60
1:1:48:LEU:HD11	1:1:196:LEU:HD11	1.82	0.60
8:19:91:VAL:HG11	8:19:96:LEU:HD21	1.83	0.60
13:23:8:LEU:O	18:29:29:ARG:NH2	2.34	0.60
32:R1:2006:C:O2'	32:R1:2823:A:N3	2.34	0.60
32:R1:1447:C:O2'	32:R1:1544:A:N3	2.28	0.60
7:18:35:ILE:HD11	7:18:106:LEU:HD22	1.84	0.60
11:21:14:VAL:HG11	11:21:98:ILE:HD12	1.83	0.60
14:24:5:ARG:NH1	32:R1:84:A:OP1	2.34	0.60
34:R3:1522:U:H2'	34:R3:1523:G:H8	1.66	0.60
36:Y:162:LEU:HD23	36:Y:186:LEU:HD21	1.84	0.60
32:R1:219:A:N3	32:R1:234:U:O2'	2.30	0.60
32:R1:890:C:H3'	32:R1:891:G:H4'	1.83	0.60
32:R1:1509:A:H2'	32:R1:1510:G:C8	2.36	0.60
36:Y:87:MET:HA	36:Y:93:TRP:HB2	1.84	0.60
34:R3:82:G:H22	34:R3:85:U:P	2.25	0.60
36:Y:36:ASN:OD1	36:Y:446:ARG:NH2	2.35	0.60
33:R2:1:U:H2'	33:R2:2:G:H8	1.65	0.60
34:R3:1034:G:H2'	34:R3:1035:A:C8	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:R1:1114:C:H2'	32:R1:1115:G:C8	2.37	0.59
19:3:38:LYS:NZ	19:3:81:GLU:OE1	2.35	0.59
32:R1:1534:U:H2'	32:R1:1536:C:H1'	1.84	0.59
34:R3:337:G:H2'	34:R3:338:A:C8	2.38	0.59
36:Y:158:PRO:HA	36:Y:161:LYS:HB2	1.84	0.59
3:14:70:ARG:NH2	32:R1:2683:C:O2	2.35	0.59
19:3:155:VAL:HG21	32:R1:2618:G:H21	1.67	0.59
33:R2:31:C:H1'	33:R2:53:A:H61	1.67	0.59
29:6:154:GLU:HG2	29:6:156:TYR:H	1.67	0.59
34:R3:1144:G:H21	34:R3:1146:A:H62	1.51	0.59
36:Y:335:PHE:HB2	36:Y:338:LEU:HD23	1.84	0.59
32:R1:1019:U:OP1	32:R1:1035:U:O2'	2.17	0.59
32:R1:2646:C:OP2	32:R1:2732:G:O2'	2.21	0.59
36:Y:410:GLN:HG2	36:Y:411:GLU:H	1.68	0.59
2:13:17:VAL:HG23	2:13:137:PRO:HB2	1.84	0.59
2:13:18:VAL:HG11	2:13:142:ILE:HD13	1.85	0.59
17:28:38:TRP:NE1	17:28:40:GLU:OE1	2.30	0.59
32:R1:955:U:H5	32:R1:962:G:H1	1.49	0.59
34:R3:1530:G:H2'	34:R3:1531:A:H8	1.67	0.59
32:R1:184:C:O2'	32:R1:217:A:N3	2.36	0.59
34:R3:745:G:H2'	34:R3:746:A:H8	1.68	0.59
34:R3:1077:G:N2	34:R3:1080:A:OP2	2.32	0.59
9:2:270:ARG:NH1	32:R1:1798:U:OP2	2.36	0.58
34:R3:417:G:H2'	34:R3:418:C:C6	2.38	0.58
36:Y:162:LEU:HD21	36:Y:181:GLN:NE2	2.18	0.58
2:13:4:PHE:O	10:20:63:ARG:NH2	2.36	0.58
32:R1:370:G:O2'	32:R1:424:G:OP1	2.20	0.58
32:R1:1900:A:H1'	32:R1:1970:A:H2'	1.85	0.58
1:1:67:HIS:ND1	1:1:188:ASN:OD1	2.37	0.58
30:9:64:ALA:O	30:9:68:ARG:HG3	2.03	0.58
32:R1:1802:A:H2'	32:R1:1803:A:C8	2.37	0.58
32:R1:2141:G:H1	32:R1:2151:U:H1'	1.69	0.58
35:T:7:U:O2'	35:T:21:A:N1	2.31	0.58
1:1:214:ILE:HD12	1:1:224:VAL:HG21	1.86	0.58
9:2:220:ARG:NH1	32:R1:1789:A:OP2	2.37	0.58
36:Y:181:GLN:CD	36:Y:194:LEU:HD22	2.24	0.58
19:3:56:LYS:HB2	19:3:59:ARG:HB2	1.85	0.58
32:R1:882:G:H2'	32:R1:883:G:C8	2.39	0.58
1:1:42:VAL:HG12	1:1:216:THR:HA	1.84	0.58
32:R1:1266:G:O2'	32:R1:2012:G:O6	2.20	0.58
34:R3:416:G:H2'	34:R3:417:G:C8	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:21:55:ASP:N	11:21:55:ASP:OD1	2.37	0.58
19:3:26:VAL:HG22	19:3:188:LEU:HD22	1.85	0.58
28:5:13:LYS:O	28:5:17:THR:HG23	2.04	0.58
34:R3:159:G:N2	34:R3:162:A:OP2	2.36	0.58
34:R3:380:G:N2	34:R3:383:A:OP2	2.32	0.58
17:28:3:VAL:HG22	17:28:10:ARG:HG2	1.84	0.58
34:R3:337:G:H2'	34:R3:338:A:H8	1.68	0.58
36:Y:347:LYS:HZ1	36:Y:501:LEU:HD12	1.68	0.58
8:19:28:LYS:HE3	8:19:39:LEU:HD23	1.86	0.57
27:4:30:GLN:OE1	32:R1:659:G:N2	2.36	0.57
28:5:150:GLY:O	32:R1:2305:U:N3	2.36	0.57
29:6:109:SER:OG	32:R1:2667:C:N3	2.33	0.57
36:Y:408:TRP:O	36:Y:409:LYS:HG2	2.04	0.57
1:1:168:ASN:ND2	32:R1:2178:C:O2'	2.37	0.57
2:13:68:LYS:NZ	32:R1:1022:G:O6	2.28	0.57
8:19:79:VAL:HG23	19:3:19:GLY:HA3	1.87	0.57
20:30:39:ASP:OD1	20:30:44:ARG:NH1	2.34	0.57
23:33:29:LYS:HG2	23:33:30:PRO:HD2	1.86	0.57
30:9:104:THR:HG22	30:9:109:GLU:HA	1.86	0.57
32:R1:631:A:N3	32:R1:2415:G:O2'	2.32	0.57
1:1:162:ARG:O	1:1:173:THR:OG1	2.21	0.57
8:19:90:ALA:HB2	8:19:112:ARG:HA	1.85	0.57
29:6:120:ILE:HD11	29:6:140:ILE:HB	1.86	0.57
32:R1:1063:G:N7	32:R1:1076:C:O2'	2.36	0.57
36:Y:439:LEU:O	36:Y:444:LYS:NZ	2.31	0.57
3:14:102:PRO:HB3	3:14:121:GLU:HB3	1.86	0.57
34:R3:71:A:H62	34:R3:100:G:H1'	1.69	0.57
32:R1:1936:A:H2	32:R1:1943:U:H3	1.53	0.57
24:34:31:LEU:HD22	24:34:42:LEU:HD13	1.86	0.57
32:R1:463:G:N2	32:R1:466:A:OP2	2.36	0.57
32:R1:882:G:H2'	32:R1:883:G:H8	1.69	0.57
36:Y:402:PHE:HE1	36:Y:419:ARG:HB2	1.69	0.57
36:Y:511:GLU:OE1	36:Y:511:GLU:N	2.38	0.57
17:28:11:PRO:HB3	17:28:29:LEU:HD23	1.87	0.57
28:5:32:LYS:HG2	28:5:156:THR:HB	1.85	0.57
32:R1:1746:A:H2'	32:R1:1747:U:C6	2.40	0.57
34:R3:201:G:HO2'	34:R3:469:C:HO2'	1.51	0.57
36:Y:413:ASP:OD1	36:Y:413:ASP:N	2.35	0.57
32:R1:284:U:O4	32:R1:356:G:O6	2.23	0.57
32:R1:1071:G:H1'	32:R1:1089:A:H5''	1.86	0.57
34:R3:1162:C:H2'	34:R3:1163:A:H8	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:R3:1355:G:H2'	34:R3:1356:G:C8	2.40	0.57
34:R3:1241:G:H2'	34:R3:1242:G:H8	1.70	0.56
28:5:44:ALA:HB1	36:Y:413:ASP:HB2	1.86	0.56
32:R1:2457:U:H5	32:R1:2494:G:H1	1.53	0.56
30:9:38:PRO:O	30:9:43:ASN:ND2	2.30	0.56
32:R1:1509:A:H2'	32:R1:1510:G:H8	1.69	0.56
32:R1:2324:U:H3'	32:R1:2325:G:H5'	1.86	0.56
34:R3:147:G:H2'	34:R3:148:G:C8	2.40	0.56
34:R3:1004:A:O2'	34:R3:1036:A:N1	2.38	0.56
34:R3:1253:G:H2'	34:R3:1254:A:H8	1.70	0.56
36:Y:319:ALA:HB3	36:Y:342:LEU:HD23	1.88	0.56
7:18:27:VAL:HA	7:18:93:ASP:HB3	1.86	0.56
32:R1:161:A:H3'	32:R1:162:U:H5''	1.87	0.56
32:R1:848:C:H2'	32:R1:849:A:H8	1.71	0.56
32:R1:1069:A:H2'	32:R1:1072:C:H5'	1.87	0.56
17:28:9:LYS:NZ	32:R1:397:U:OP2	2.30	0.56
21:31:26:SER:OG	21:31:27:THR:N	2.39	0.56
24:34:7:PRO:HG3	32:R1:1612:C:H5'	1.87	0.56
32:R1:545:U:H3'	32:R1:546:U:O4'	2.05	0.56
32:R1:1181:U:H2'	32:R1:1182:G:C8	2.41	0.56
32:R1:2246:G:H2'	32:R1:2247:A:H8	1.70	0.56
9:2:159:THR:HG23	9:2:176:ARG:HG2	1.87	0.56
27:4:44:ARG:NH2	32:R1:1248:G:OP1	2.32	0.56
34:R3:211:G:N1	34:R3:212:G:N3	2.54	0.56
19:3:178:VAL:HG12	19:3:179:ARG:HG3	1.88	0.56
21:31:16:CYS:HB3	21:31:20:ASN:HB3	1.86	0.56
32:R1:1715:G:HO2'	32:R1:1716:U:H6	1.51	0.56
32:R1:1992:G:N2	32:R1:1996:C:O2'	2.38	0.56
7:18:40:ILE:HG12	7:18:47:VAL:HG12	1.88	0.56
28:5:12:VAL:HG13	28:5:27:VAL:HG11	1.88	0.56
34:R3:736:C:H2'	34:R3:737:C:C6	2.41	0.56
34:R3:976:G:OP2	34:R3:1358:U:O2'	2.23	0.56
32:R1:818:G:N1	32:R1:1188:U:OP2	2.22	0.56
32:R1:1068:G:N2	32:R1:1095:A:O2'	2.38	0.56
32:R1:2135:A:H62	32:R1:2156:G:H21	1.54	0.56
5:16:50:ARG:O	5:16:54:THR:HG23	2.04	0.55
34:R3:745:G:H2'	34:R3:746:A:C8	2.41	0.55
36:Y:187:ASP:O	36:Y:188:ILE:HB	2.05	0.55
32:R1:807:U:O2'	32:R1:2060:A:N1	2.33	0.55
32:R1:1417:C:N3	32:R1:1581:G:N1	2.38	0.55
34:R3:736:C:H2'	34:R3:737:C:H6	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:2:12:ARG:HD2	32:R1:728:G:H4'	1.87	0.55
30:9:57:LYS:O	30:9:61:VAL:HG13	2.06	0.55
36:Y:175:ASP:HA	36:Y:204:THR:HG23	1.87	0.55
32:R1:700:G:O2'	32:R1:1632:A:N3	2.31	0.55
34:R3:1355:G:H2'	34:R3:1356:G:H8	1.70	0.55
36:Y:44:MET:SD	36:Y:177:LEU:HB3	2.46	0.55
8:19:33:GLU:OE2	8:19:38:ARG:NH2	2.32	0.55
32:R1:1590:A:H2'	32:R1:1591:A:H8	1.70	0.55
32:R1:2105:U:H2'	32:R1:2106:U:C6	2.40	0.55
4:15:20:GLY:HA2	4:15:28:GLY:HA2	1.88	0.55
32:R1:1417:C:O5'	32:R1:1587:G:N2	2.38	0.55
36:Y:170:LEU:HA	36:Y:173:ASP:OD2	2.06	0.55
4:15:29:LYS:O	4:15:30:THR:OG1	2.22	0.55
7:18:30:ARG:HH22	33:R2:48:U:P	2.30	0.55
32:R1:75:G:H22	32:R1:111:A:H2	1.55	0.55
36:Y:354:ASN:ND2	59:Y:602:ATP:O1G	2.38	0.55
16:27:74:PRO:HB3	33:R2:12:C:N4	2.22	0.55
32:R1:2148:G:H2'	32:R1:2149:U:C6	2.42	0.55
3:14:121:GLU:HG2	3:14:122:VAL:HG23	1.88	0.55
32:R1:1363:C:O2'	32:R1:1809:A:N3	2.30	0.55
27:4:111:GLU:OE2	27:4:115:GLN:NE2	2.40	0.54
10:20:48:ASP:HA	10:20:51:GLN:HG3	1.89	0.54
17:28:71:ARG:NH1	17:28:77:TYR:OH	2.40	0.54
18:29:9:LYS:HG2	18:29:12:GLU:HB2	1.88	0.54
32:R1:1779:U:H5	32:R1:1784:A:N7	2.04	0.54
32:R1:2532:G:O2'	32:R1:2657:A:N1	2.40	0.54
34:R3:56:U:H2'	34:R3:57:G:H8	1.73	0.54
34:R3:944:G:N1	34:R3:1338:G:OP2	2.34	0.54
34:R3:1357:A:N6	34:R3:1365:G:H1	2.06	0.54
34:R3:1432:G:O2'	34:R3:1468:A:N6	2.40	0.54
1:1:59:VAL:H	1:1:165:ASN:ND2	2.05	0.54
34:R3:208:U:O2'	34:R3:212:G:N2	2.39	0.54
34:R3:613:C:H2'	34:R3:614:C:C6	2.42	0.54
34:R3:662:U:H2'	34:R3:663:A:C8	2.42	0.54
12:22:5:ALA:O	32:R1:494:G:O2'	2.25	0.54
25:35:7:ARG:NH1	32:R1:243:U:OP2	2.40	0.54
32:R1:227:A:O2'	32:R1:228:C:O5'	2.22	0.54
34:R3:409:U:O4	34:R3:433:G:O6	2.26	0.54
34:R3:716:A:H2'	34:R3:717:U:O4'	2.07	0.54
32:R1:1432:G:H2'	32:R1:1433:A:C8	2.43	0.54
22:32:2:VAL:HG13	32:R1:2015:A:C6	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:R3:1010:U:H2'	34:R3:1011:C:C6	2.42	0.54
36:Y:320:LEU:H	36:Y:342:LEU:HB2	1.72	0.54
13:23:34:VAL:HG23	13:23:81:LYS:HB3	1.90	0.54
34:R3:178:C:H2'	34:R3:179:A:H8	1.73	0.54
35:T:55:PSU:OP2	35:T:55:PSU:H4'	2.08	0.54
20:30:44:ARG:NH1	20:30:58:GLU:OE2	2.40	0.54
27:4:145:ASP:HB3	27:4:184:ASP:HB2	1.90	0.54
32:R1:827:U:O2'	32:R1:2068:U:N3	2.41	0.54
32:R1:2114:A:N7	32:R1:2167:U:H4'	2.23	0.54
7:18:13:ARG:HH11	7:18:13:ARG:HG2	1.73	0.53
32:R1:2113:U:OP1	32:R1:2169:A:N6	2.41	0.53
32:R1:2258:C:O2'	32:R1:2427:C:OP2	2.19	0.53
34:R3:846:G:H2'	34:R3:847:G:C8	2.42	0.53
36:Y:269:VAL:O	36:Y:273:SER:HB3	2.08	0.53
36:Y:303:GLN:HB2	36:Y:426:LEU:HD21	1.89	0.53
2:13:135:GLN:NE2	32:R1:6:A:N3	2.56	0.53
32:R1:1009:A:N3	32:R1:1153:C:O2'	2.38	0.53
32:R1:1794:A:H2'	32:R1:1795:C:C6	2.43	0.53
32:R1:2113:U:OP1	32:R1:2114:A:N6	2.41	0.53
34:R3:1016:A:O2'	34:R3:1217:C:O2'	2.23	0.53
7:18:16:ARG:HD2	32:R1:2334:U:C4	2.44	0.53
11:21:43:ASN:OD1	11:21:43:ASN:N	2.40	0.53
32:R1:2112:G:O2'	32:R1:2115:G:N2	2.41	0.53
19:3:181:ASP:HB2	19:3:186:LEU:HB2	1.89	0.53
29:6:12:ALA:O	29:6:14:VAL:N	2.40	0.53
32:R1:1114:C:H2'	32:R1:1115:G:H8	1.71	0.53
32:R1:2331:G:O2'	32:R1:2336:A:N1	2.40	0.53
32:R1:2602:A:H5'	36:Y:275:ASN:HD21	1.73	0.53
1:1:57:GLN:NE2	1:1:203:GLN:O	2.41	0.53
19:3:45:TYR:OH	32:R1:2636:C:O2'	2.20	0.53
30:9:15:LEU:O	30:9:15:LEU:HD12	2.09	0.53
32:R1:1441:G:H2'	32:R1:1442:U:C6	2.44	0.53
32:R1:2140:G:N2	32:R1:2141:G:N3	2.57	0.53
34:R3:890:G:O2'	34:R3:906:A:N6	2.42	0.53
7:18:15:ARG:NH2	7:18:95:SER:OG	2.42	0.53
32:R1:303:G:H2'	32:R1:304:U:C6	2.44	0.53
32:R1:2064:C:H2'	32:R1:2065:C:C6	2.44	0.53
32:R1:2246:G:H2'	32:R1:2247:A:C8	2.43	0.53
34:R3:620:C:O2'	34:R3:621:A:H8	1.92	0.53
5:16:75:GLU:HB3	5:16:90:GLU:HG3	1.90	0.53
21:31:44:PHE:O	21:31:47:LYS:NZ	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:R1:1482:G:H2'	32:R1:1483:G:H8	1.72	0.53
34:R3:1450:U:O2'	34:R3:1453:G:O6	2.26	0.53
17:28:31:ASN:OD1	17:28:33:HIS:NE2	2.42	0.53
24:34:45:SER:O	24:34:45:SER:OG	2.27	0.53
34:R3:76:G:H2'	34:R3:77:A:C8	2.43	0.53
34:R3:1492:A:O2'	34:R3:1493:A:OP1	2.21	0.53
36:Y:192:ARG:O	36:Y:195:GLU:HG3	2.08	0.53
33:R2:1:U:H2'	33:R2:2:G:C8	2.45	0.52
34:R3:76:G:H2'	34:R3:77:A:H8	1.72	0.52
7:18:28:VAL:HG11	7:18:103:VAL:HG12	1.90	0.52
11:21:1:MET:HB2	11:21:43:ASN:HB3	1.90	0.52
34:R3:1149:C:H2'	34:R3:1150:A:C8	2.44	0.52
4:15:21:ARG:HA	32:R1:811:U:H2'	1.92	0.52
4:15:82:LEU:HB3	4:15:120:VAL:HG11	1.91	0.52
4:15:89:VAL:HA	4:15:121:THR:HG23	1.91	0.52
32:R1:286:U:H2'	32:R1:287:G:C8	2.44	0.52
32:R1:2112:G:HO2'	32:R1:2115:G:H1	1.56	0.52
32:R1:2324:U:H3'	32:R1:2325:G:C5'	2.38	0.52
32:R1:2637:U:H2'	32:R1:2638:G:O4'	2.10	0.52
36:Y:425:LEU:HD12	36:Y:425:LEU:O	2.09	0.52
11:21:38:VAL:HG11	11:21:57:GLY:HA3	1.91	0.52
29:6:66:THR:OG1	32:R1:2747:G:O2'	2.25	0.52
32:R1:282:A:H2'	32:R1:283:G:C8	2.44	0.52
32:R1:1386:C:H2'	32:R1:1387:A:C8	2.44	0.52
32:R1:1417:C:HO2'	32:R1:1587:G:HO2'	1.58	0.52
32:R1:1803:A:H2	32:R1:1823:G:H1'	1.74	0.52
10:20:5:ARG:NH2	32:R1:585:G:N7	2.58	0.52
21:31:41:HIS:HD2	21:31:43:PHE:HB3	1.75	0.52
25:35:25:HIS:CE1	25:35:47:ALA:HB2	2.44	0.52
28:5:140:ILE:HG22	28:5:142:TYR:H	1.75	0.52
34:R3:235:C:H2'	34:R3:236:A:H8	1.74	0.52
36:Y:496:GLU:HA	36:Y:499:SER:HB3	1.92	0.52
3:14:6:THR:HG23	32:R1:1666:G:H4'	1.91	0.52
32:R1:554:U:H2'	32:R1:555:G:O4'	2.09	0.52
32:R1:2857:G:N2	32:R1:2860:A:OP2	2.40	0.52
34:R3:501:C:O2	34:R3:549:C:O2'	2.28	0.52
13:23:27:SER:O	13:23:27:SER:OG	2.28	0.52
29:6:136:ASP:O	29:6:140:ILE:HG22	2.10	0.52
32:R1:619:G:OP2	32:R1:620:G:N2	2.42	0.52
32:R1:1098:A:H3'	32:R1:1099:G:H8	1.74	0.52
32:R1:1178:C:N4	32:R1:1180:U:O4	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:R1:2327:A:H2'	32:R1:2328:A:C8	2.44	0.52
34:R3:212:G:H2'	34:R3:213:G:C8	2.44	0.52
34:R3:599:C:H2'	34:R3:600:A:H8	1.75	0.52
15:25:42:LEU:HD13	15:25:47:VAL:HG21	1.91	0.52
21:31:46:GLY:HA2	21:31:49:ARG:HE	1.75	0.52
36:Y:211:ASP:HB3	36:Y:214:PHE:HB3	1.92	0.52
9:2:153:LEU:HD13	9:2:175:LEU:HD21	1.91	0.52
19:3:136:ASN:OD1	32:R1:2579:C:O2'	2.27	0.52
32:R1:593:U:H2'	32:R1:594:U:C6	2.44	0.52
32:R1:1681:G:O2'	32:R1:1762:A:N3	2.40	0.52
34:R3:484:G:H4'	34:R3:485:U:H5''	1.92	0.52
34:R3:811:C:O2'	34:R3:901:A:N1	2.43	0.52
34:R3:996:A:H2'	34:R3:997:U:C6	2.45	0.52
30:9:50:ARG:HH21	30:9:51:ARG:HH12	1.58	0.51
32:R1:2291:U:H2'	32:R1:2292:U:C6	2.45	0.51
27:4:157:LEU:HG	27:4:169:VAL:HG21	1.92	0.51
29:6:136:ASP:HB3	29:6:139:VAL:HB	1.92	0.51
9:2:226:PRO:HD3	9:2:233:GLY:H	1.75	0.51
28:5:43:ILE:HD11	28:5:78:ILE:HG22	1.92	0.51
32:R1:30:G:O2'	32:R1:1214:A:N3	2.35	0.51
32:R1:743:A:O2'	32:R1:1659:G:OP1	2.27	0.51
32:R1:2025:C:H2'	32:R1:2026:U:C6	2.44	0.51
34:R3:999:C:H2'	34:R3:1000:A:C8	2.45	0.51
36:Y:459:ILE:HA	36:Y:487:THR:O	2.10	0.51
32:R1:357:C:H2'	32:R1:358:U:C6	2.46	0.51
32:R1:644:A:H2'	32:R1:645:C:O4'	2.10	0.51
32:R1:2177:C:H2'	32:R1:2178:C:C6	2.45	0.51
34:R3:455:G:H2'	34:R3:456:A:C8	2.45	0.51
34:R3:600:A:H2'	34:R3:601:G:H8	1.73	0.51
36:Y:409:LYS:HE3	36:Y:412:GLY:O	2.09	0.51
36:Y:465:PRO:HB2	36:Y:477:LEU:HD21	1.93	0.51
6:17:92:GLY:HA3	32:R1:2880:C:H1'	1.92	0.51
34:R3:620:C:HO2'	34:R3:621:A:H8	1.58	0.51
34:R3:975:A:H8	34:R3:1357:A:HO2'	1.58	0.51
34:R3:1261:A:N6	34:R3:1274:A:O2'	2.41	0.51
9:2:209:ALA:HA	9:2:212:TRP:CE2	2.46	0.51
24:34:34:ARG:NE	24:34:42:LEU:O	2.44	0.51
30:9:12:LEU:HD21	30:9:19:VAL:HG21	1.93	0.51
32:R1:5:A:H2'	32:R1:6:A:H8	1.76	0.51
28:5:92:GLY:H	28:5:95:MET:HE2	1.76	0.51
32:R1:1077:A:H61	32:R1:1089:A:P	2.34	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:R1:2124:G:O2'	32:R1:2125:G:O5'	2.28	0.51
32:R1:2537:U:H2'	32:R1:2538:C:C6	2.46	0.51
34:R3:473:U:H2'	34:R3:474:G:C8	2.46	0.51
36:Y:452:LEU:HD13	36:Y:460:LEU:HD22	1.93	0.51
36:Y:158:PRO:HB2	36:Y:184:ASN:HB3	1.93	0.51
36:Y:347:LYS:HB3	36:Y:490:PHE:CE1	2.45	0.51
8:19:21:PRO:HD3	8:19:49:ILE:HG13	1.93	0.51
32:R1:2106:U:H2'	32:R1:2107:G:H8	1.76	0.51
1:1:8:MET:N	1:1:8:MET:SD	2.83	0.51
12:22:93:ALA:HB2	32:R1:1614:A:C2	2.46	0.51
34:R3:923:A:O2'	34:R3:1399:C:OP2	2.23	0.51
5:16:45:GLN:NE2	32:R1:2485:G:OP1	2.39	0.50
19:3:18:ASP:OD1	19:3:18:ASP:N	2.36	0.50
32:R1:1170:C:H2'	32:R1:1171:G:C8	2.46	0.50
32:R1:1597:A:H5''	32:R1:1598:A:H5'	1.93	0.50
34:R3:126:G:OP1	34:R3:605:U:O2'	2.27	0.50
10:20:51:GLN:HA	10:20:54:ARG:HG2	1.92	0.50
23:33:4:ILE:HD12	23:33:27:ARG:NH2	2.26	0.50
32:R1:64:A:H2'	32:R1:65:U:C6	2.46	0.50
32:R1:2834:G:H2'	32:R1:2879:A:H61	1.76	0.50
34:R3:1040:U:H2'	34:R3:1041:G:H8	1.75	0.50
32:R1:1682:G:H2'	32:R1:1683:U:C6	2.46	0.50
32:R1:2314:A:H2'	32:R1:2315:G:H8	1.77	0.50
36:Y:463:ASP:O	36:Y:491:VAL:HG22	2.12	0.50
36:Y:470:ASP:O	36:Y:471:MET:HB3	2.10	0.50
10:20:10:ARG:NH1	32:R1:1216:G:OP1	2.41	0.50
22:32:25:THR:OG1	22:32:26:SER:N	2.45	0.50
29:6:34:ARG:NE	29:6:70:LEU:HD21	2.25	0.50
32:R1:2:G:H2'	32:R1:3:U:C6	2.47	0.50
34:R3:999:C:H2'	34:R3:1000:A:H8	1.77	0.50
19:3:45:TYR:HH	32:R1:2636:C:HO2'	1.57	0.50
22:32:7:PRO:HD2	32:R1:1263:U:O2'	2.12	0.50
27:4:95:LYS:O	32:R1:659:G:O2'	2.29	0.50
32:R1:851:C:H2'	32:R1:852:U:C6	2.46	0.50
32:R1:1771:C:H2'	32:R1:1772:A:H8	1.77	0.50
32:R1:1913:A:N1	34:R3:1492:A:H2'	2.26	0.50
34:R3:652:U:O4	34:R3:752:G:O2'	2.19	0.50
36:Y:504:ARG:HG3	36:Y:504:ARG:O	2.11	0.50
28:5:130:GLY:HA3	32:R1:2305:U:H5''	1.93	0.50
32:R1:5:A:H2'	32:R1:6:A:C8	2.47	0.50
32:R1:639:U:H2'	32:R1:640:C:C6	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:R1:1541:C:H2'	32:R1:1542:U:C6	2.47	0.50
34:R3:1395:C:HO2'	34:R3:1401:G:HO2'	1.59	0.50
35:T:62:C:H2'	35:T:63:G:H8	1.76	0.50
4:15:64:PHE:HB3	25:35:24:LYS:HD2	1.92	0.50
7:18:63:LYS:HD2	7:18:63:LYS:C	2.32	0.50
32:R1:1418:G:H1'	32:R1:1580:A:H61	1.76	0.50
32:R1:1528:A:OP2	32:R1:1543:G:N2	2.37	0.50
32:R1:2127:G:H2'	32:R1:2128:G:C8	2.46	0.50
1:1:183:ASP:OD1	1:1:184:LYS:N	2.45	0.50
7:18:117:PHE:O	32:R1:2377:A:O2'	2.22	0.50
22:32:3:GLN:NE2	32:R1:2016:U:O2	2.40	0.50
34:R3:766:A:OP2	34:R3:812:G:N2	2.45	0.50
34:R3:1144:G:N2	34:R3:1146:A:H62	2.09	0.50
34:R3:1162:C:H2'	34:R3:1163:A:C8	2.46	0.50
36:Y:394:GLU:HB3	36:Y:404:TRP:HH2	1.77	0.50
5:16:29:GLY:N	5:16:104:GLU:OE2	2.35	0.50
9:2:228:ASP:OD2	32:R1:780:G:N1	2.28	0.50
32:R1:570:G:H2'	32:R1:2030:A:N7	2.27	0.50
32:R1:774:G:O2'	32:R1:775:G:O5'	2.29	0.50
8:19:83:ILE:O	8:19:83:ILE:HG22	2.11	0.49
22:32:54:ILE:HG22	22:32:56:LYS:H	1.75	0.49
27:4:149:ILE:HG23	27:4:188:MET:HG3	1.94	0.49
34:R3:676:A:H2'	34:R3:677:U:H6	1.77	0.49
35:T:15:C:H3'	35:T:16:C:H5''	1.93	0.49
9:2:52:HIS:CE1	9:2:218:THR:HG1	2.29	0.49
28:5:3:LEU:HD12	28:5:100:GLU:HG3	1.95	0.49
32:R1:100:U:H4'	32:R1:101:A:O4'	2.12	0.49
32:R1:1527:G:N1	32:R1:1544:A:OP2	2.29	0.49
32:R1:1570:A:H2'	32:R1:1571:A:C8	2.47	0.49
32:R1:1874:C:H2'	32:R1:1875:G:O4'	2.12	0.49
32:R1:2071:A:H2'	32:R1:2072:C:C6	2.47	0.49
32:R1:2540:C:O2'	32:R1:2740:A:N3	2.43	0.49
34:R3:415:A:H61	34:R3:427:U:H3	1.58	0.49
34:R3:593:U:H2'	34:R3:594:U:H6	1.76	0.49
34:R3:1533:C:O2'	34:R3:1534:A:N7	2.42	0.49
32:R1:2233:U:H2'	32:R1:2234:G:C8	2.47	0.49
32:R1:2375:G:N2	32:R1:2378:A:OP2	2.38	0.49
32:R1:2557:G:H2'	32:R1:2558:C:C6	2.47	0.49
2:13:27:ARG:NH2	32:R1:1143:A:OP1	2.46	0.49
5:16:42:THR:HA	5:16:93:VAL:HA	1.93	0.49
32:R1:639:U:H2'	32:R1:640:C:H6	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:R1:1073:A:H4'	32:R1:2474:U:H5''	1.94	0.49
32:R1:2031:A:N3	32:R1:2455:G:O2'	2.38	0.49
34:R3:167:A:H2'	34:R3:168:G:C8	2.47	0.49
34:R3:167:A:H2'	34:R3:168:G:H8	1.77	0.49
34:R3:841:C:O2'	34:R3:843:U:O4'	2.30	0.49
36:Y:372:ASP:OD1	36:Y:373:SER:N	2.46	0.49
32:R1:12:U:O2	32:R1:12:U:H2'	2.13	0.49
32:R1:629:G:N3	32:R1:639:U:O2'	2.45	0.49
34:R3:1041:G:H2'	34:R3:1042:A:C8	2.48	0.49
36:Y:183:THR:HG22	36:Y:467:ASN:O	2.12	0.49
3:14:87:LEU:HG	3:14:92:GLU:O	2.13	0.49
9:2:144:GLU:HA	9:2:151:GLY:HA2	1.95	0.49
15:25:30:ILE:HD11	15:25:40:ILE:HD13	1.93	0.49
32:R1:881:G:O6	32:R1:895:U:C2	2.65	0.49
36:Y:109:SER:H	36:Y:112:ASP:HB2	1.77	0.49
11:21:80:ARG:NH1	32:R1:571:U:OP1	2.45	0.49
26:36:19:ARG:NE	32:R1:2756:U:OP2	2.46	0.49
32:R1:198:C:O2'	32:R1:199:A:H5'	2.12	0.49
32:R1:577:G:O2'	32:R1:1254:A:OP1	2.30	0.49
32:R1:2029:G:N1	32:R1:2033:A:OP2	2.30	0.49
32:R1:2100:G:H1	32:R1:2189:U:H3	1.60	0.49
32:R1:2106:U:H2'	32:R1:2107:G:C8	2.47	0.49
32:R1:2848:G:O2'	32:R1:2868:A:N6	2.43	0.49
33:R2:65:U:H3'	33:R2:108:A:N6	2.26	0.49
34:R3:427:U:O2'	34:R3:541:G:OP1	2.28	0.49
34:R3:460:A:H2'	34:R3:461:A:H8	1.76	0.49
34:R3:461:A:H2'	34:R3:462:G:C8	2.41	0.49
34:R3:1253:G:H2'	34:R3:1254:A:C8	2.48	0.49
36:Y:60:LEU:HD23	36:Y:60:LEU:H	1.78	0.49
32:R1:2111:U:H5''	32:R1:2145:C:H41	1.77	0.49
34:R3:600:A:H2'	34:R3:601:G:C8	2.47	0.49
34:R3:1266:G:N2	34:R3:1269:A:OP2	2.26	0.49
5:16:6:ARG:HH12	5:16:8:LYS:HA	1.78	0.49
10:20:25:GLY:O	10:20:29:ARG:NH1	2.44	0.49
32:R1:703:U:H2'	32:R1:704:G:O4'	2.13	0.49
32:R1:2064:C:H2'	32:R1:2065:C:H6	1.77	0.49
36:Y:405:MET:HG3	36:Y:454:MET:HE1	1.95	0.49
28:5:141:ASP:OD1	28:5:141:ASP:N	2.39	0.49
32:R1:2120:G:H2'	32:R1:2121:G:C8	2.48	0.49
1:1:48:LEU:HD21	1:1:196:LEU:HD21	1.95	0.48
11:21:27:ILE:HD13	11:21:33:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:28:57:VAL:HG13	17:28:61:LYS:HD3	1.93	0.48
32:R1:1583:A:O2'	32:R1:1585:C:N4	2.45	0.48
32:R1:1590:A:H2'	32:R1:1591:A:C8	2.47	0.48
30:9:30:LEU:HB3	30:9:36:ALA:HB3	1.94	0.48
32:R1:580:U:H2'	32:R1:581:C:C6	2.48	0.48
32:R1:2682:A:H61	32:R1:2728:U:H1'	1.77	0.48
34:R3:687:A:N6	34:R3:701:U:O4'	2.46	0.48
36:Y:61:ASP:OD1	36:Y:61:ASP:N	2.43	0.48
32:R1:1068:G:O2'	32:R1:1096:A:H1'	2.13	0.48
32:R1:2291:U:OP1	32:R1:2380:C:O2'	2.30	0.48
34:R3:1137:C:H4'	34:R3:1138:G:C2	2.48	0.48
34:R3:1386:G:H2'	34:R3:1387:G:H8	1.79	0.48
34:R3:1407:C:H2'	34:R3:1408:A:H8	1.78	0.48
10:20:91:ARG:NH2	32:R1:1153:C:OP1	2.43	0.48
12:22:17:VAL:HG12	12:22:76:VAL:HG11	1.95	0.48
1:1:211:LYS:NZ	32:R1:2177:C:O3'	2.45	0.48
2:13:49:ASP:OD2	2:13:121:LYS:NZ	2.24	0.48
19:3:149:ASN:OD1	19:3:150:GLN:N	2.34	0.48
27:4:69:ARG:O	32:R1:674:G:H4'	2.13	0.48
32:R1:1079:C:H2'	32:R1:1080:A:N7	2.29	0.48
32:R1:1171:G:O2'	32:R1:1172:C:O5'	2.23	0.48
2:13:81:ILE:HG13	19:3:156:PHE:HB3	1.95	0.48
5:16:6:ARG:HG3	5:16:6:ARG:O	2.12	0.48
13:23:11:LEU:HD13	13:23:51:PHE:HE2	1.78	0.48
22:32:10:SER:O	22:32:14:MET:HG3	2.13	0.48
27:4:162:ARG:NH2	32:R1:340:A:O2'	2.46	0.48
28:5:162:ASP:OD1	28:5:162:ASP:N	2.47	0.48
32:R1:1409:U:H2'	32:R1:1410:G:H8	1.78	0.48
33:R2:5:U:OP1	33:R2:61:G:O2'	2.22	0.48
34:R3:1305:G:O2'	34:R3:1306:A:H8	1.97	0.48
3:14:110:GLU:HG2	3:14:110:GLU:O	2.14	0.48
32:R1:2:G:H2'	32:R1:3:U:H6	1.79	0.48
32:R1:282:A:H2'	32:R1:283:G:H8	1.79	0.48
32:R1:2537:U:H2'	32:R1:2538:C:H6	1.78	0.48
34:R3:362:G:N2	34:R3:365:U:OP2	2.45	0.48
34:R3:441:A:H1'	34:R3:497:G:N2	2.28	0.48
34:R3:579:A:H2'	34:R3:580:C:C6	2.49	0.48
34:R3:846:G:H2'	34:R3:847:G:H8	1.79	0.48
34:R3:1219:A:H2'	34:R3:1220:G:C8	2.49	0.48
34:R3:1250:A:H2	34:R3:1370:G:H1'	1.79	0.48
36:Y:499:SER:HB2	36:Y:520:TYR:HE2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:28:9:LYS:HE3	17:28:53:LYS:HD2	1.96	0.48
19:3:108:ASP:OD2	19:3:173:GLN:NE2	2.42	0.48
32:R1:704:G:H2'	32:R1:726:G:N2	2.28	0.48
32:R1:820:A:H4'	32:R1:836:G:H22	1.78	0.48
33:R2:44:G:H1'	33:R2:47:C:H42	1.78	0.48
34:R3:1121:U:H2'	34:R3:1122:U:C6	2.49	0.48
36:Y:350:VAL:O	36:Y:491:VAL:HA	2.13	0.48
32:R1:146:A:H2'	32:R1:147:C:C6	2.49	0.48
32:R1:278:A:C6	32:R1:362:A:C8	3.02	0.48
32:R1:859:G:O2'	32:R1:916:G:O6	2.20	0.48
32:R1:2577:A:H2'	32:R1:2614:A:N6	2.29	0.48
34:R3:253:A:N6	34:R3:274:A:N1	2.62	0.48
36:Y:416:GLN:C	36:Y:418:VAL:H	2.17	0.48
5:16:4:PRO:HG2	5:16:70:ASP:HA	1.96	0.48
32:R1:1631:G:N2	32:R1:1634:A:OP2	2.39	0.48
32:R1:1796:U:H2'	32:R1:1797:G:H8	1.79	0.48
32:R1:2834:G:H1'	32:R1:2883:A:N6	2.29	0.48
34:R3:515:G:H2'	34:R3:516:U:O4'	2.13	0.48
36:Y:81:VAL:HG12	36:Y:139:LEU:HD21	1.95	0.48
6:17:114:GLU:OE1	6:17:118:ARG:NE	2.45	0.47
12:22:7:HIS:HB2	12:22:50:VAL:HG22	1.96	0.47
28:5:114:ARG:HA	28:5:114:ARG:HD2	1.73	0.47
32:R1:987:C:O2'	32:R1:1000:A:N3	2.36	0.47
34:R3:191:G:H2'	34:R3:192:A:H8	1.79	0.47
36:Y:519:ASN:O	36:Y:520:TYR:HB3	2.13	0.47
23:33:12:SER:HB2	23:33:48:TYR:CZ	2.49	0.47
32:R1:78:U:H2'	32:R1:79:C:C6	2.49	0.47
32:R1:1522:A:H8	32:R1:1522:A:OP1	1.97	0.47
32:R1:776:G:N2	32:R1:2241:A:OP1	2.44	0.47
32:R1:881:G:C6	32:R1:895:U:O2	2.67	0.47
32:R1:886:A:H2'	32:R1:888:C:C5	2.46	0.47
35:T:20:H2U:O4'	35:T:20:H2U:N3	2.47	0.47
36:Y:429:GLN:HA	36:Y:432:ILE:HG12	1.95	0.47
32:R1:146:A:H2'	32:R1:147:C:H6	1.80	0.47
32:R1:1746:A:H2'	32:R1:1747:U:H6	1.77	0.47
32:R1:2515:C:H2'	32:R1:2516:A:H8	1.80	0.47
34:R3:34:C:H2'	34:R3:35:G:H8	1.79	0.47
36:Y:182:PRO:O	36:Y:183:THR:OG1	2.24	0.47
1:1:166:ASP:OD1	32:R1:2122:U:O2'	2.28	0.47
19:3:149:ASN:HB3	32:R1:2572:A:OP2	2.14	0.47
32:R1:359:G:H2'	32:R1:360:U:C6	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:R3:50:A:O2'	34:R3:360:G:N2	2.47	0.47
34:R3:728:A:H2'	34:R3:729:A:C8	2.50	0.47
34:R3:1169:A:H2'	34:R3:1170:A:C8	2.49	0.47
34:R3:1203:C:H2'	34:R3:1204:A:C8	2.49	0.47
9:2:140:VAL:HG23	9:2:191:LEU:HA	1.96	0.47
13:23:87:LEU:HD12	13:23:91:GLN:HG2	1.96	0.47
16:27:23:VAL:HG13	16:27:38:VAL:HG12	1.95	0.47
32:R1:172:A:H2'	32:R1:173:A:H8	1.80	0.47
32:R1:1754:A:N1	32:R1:2716:C:O2'	2.38	0.47
32:R1:1847:G:H21	32:R1:1848:A:H62	1.61	0.47
34:R3:945:G:C2	34:R3:946:A:C8	3.03	0.47
1:1:7:ARG:HA	1:1:10:VAL:HG12	1.96	0.47
1:1:62:ALA:HB2	1:1:162:ARG:HG2	1.96	0.47
19:3:48:ILE:HG23	19:3:84:LEU:HD21	1.97	0.47
30:9:9:VAL:HG12	30:9:11:ASN:H	1.79	0.47
32:R1:155:A:H2'	32:R1:156:A:C8	2.50	0.47
32:R1:307:G:N2	32:R1:310:A:OP2	2.45	0.47
32:R1:752:A:H62	32:R1:2609:U:H3	1.62	0.47
32:R1:1020:A:H4'	32:R1:1021:A:O5'	2.15	0.47
32:R1:2159:G:H2'	32:R1:2160:C:O4'	2.15	0.47
32:R1:2639:A:N6	32:R1:2775:G:O2'	2.48	0.47
34:R3:20:U:H2'	34:R3:21:G:O4'	2.15	0.47
34:R3:296:U:O2'	34:R3:556:C:O2	2.32	0.47
13:23:54:GLU:N	13:23:54:GLU:OE1	2.47	0.47
27:4:31:VAL:HG22	27:4:96:VAL:HG11	1.97	0.47
32:R1:1589:U:H2'	32:R1:1590:A:H8	1.78	0.47
34:R3:837:U:H2'	34:R3:838:G:H8	1.80	0.47
36:Y:35:ALA:HA	36:Y:470:ASP:OD1	2.15	0.47
36:Y:504:ARG:HH11	36:Y:516:PHE:HB2	1.80	0.47
4:15:85:VAL:HG23	4:15:86:GLU:N	2.30	0.47
21:31:62:LYS:HB2	21:31:62:LYS:HE3	1.66	0.47
22:32:52:LYS:HZ2	22:32:55:ALA:HA	1.80	0.47
34:R3:56:U:H2'	34:R3:57:G:C8	2.49	0.47
34:R3:384:G:H2'	34:R3:385:C:C6	2.49	0.47
34:R3:715:A:H2'	34:R3:716:A:C8	2.50	0.47
9:2:120:ASP:HB3	30:9:91:PHE:HE2	1.80	0.47
32:R1:4:U:H2'	32:R1:5:A:H8	1.80	0.47
32:R1:1386:C:H2'	32:R1:1387:A:H8	1.79	0.47
32:R1:1563:U:H2'	32:R1:1564:C:C6	2.50	0.47
32:R1:2114:A:H61	32:R1:2119:A:N6	2.13	0.47
32:R1:2698:U:H2'	32:R1:2699:C:C6	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:R3:592:G:H2'	34:R3:593:U:C6	2.50	0.47
34:R3:768:A:H4'	34:R3:1523:G:N2	2.29	0.47
36:Y:347:LYS:H	36:Y:488:LEU:HD23	1.80	0.47
36:Y:415:GLU:HG3	36:Y:419:ARG:HH21	1.79	0.47
6:17:5:LYS:NZ	32:R1:2000:C:OP1	2.48	0.46
25:35:32:LEU:O	25:35:40:LYS:HE2	2.15	0.46
32:R1:871:U:H2'	32:R1:872:U:C6	2.51	0.46
32:R1:2895:G:H2'	32:R1:2896:C:C6	2.50	0.46
34:R3:516:U:O2'	34:R3:519:C:H5	1.99	0.46
36:Y:222:MET:HE3	36:Y:237:TYR:HD2	1.80	0.46
1:1:22:ASP:OD1	1:1:23:ILE:N	2.48	0.46
6:17:57:THR:O	6:17:57:THR:OG1	2.26	0.46
7:18:13:ARG:HG2	7:18:13:ARG:NH1	2.30	0.46
9:2:251:THR:OG1	9:2:252:LYS:N	2.48	0.46
14:24:3:LYS:HD3	14:24:82:VAL:HB	1.96	0.46
20:30:6:ILE:HD13	20:30:26:LEU:HD22	1.97	0.46
27:4:105:LEU:HD23	27:4:105:LEU:HA	1.80	0.46
32:R1:1636:U:O2'	32:R1:1760:C:O2	2.22	0.46
32:R1:1730:C:O2'	32:R1:1731:G:N7	2.48	0.46
34:R3:420:U:H2'	34:R3:422:C:H1'	1.97	0.46
34:R3:588:G:N2	34:R3:653:U:O4	2.46	0.46
34:R3:1176:A:H2'	34:R3:1177:G:C8	2.50	0.46
36:Y:89:HIS:ND1	36:Y:92:LEU:HB2	2.30	0.46
36:Y:348:LEU:HD12	36:Y:348:LEU:O	2.15	0.46
2:13:64:VAL:CG1	2:13:68:LYS:HB2	2.46	0.46
4:15:51:GLU:OE2	4:15:60:ARG:NH2	2.48	0.46
27:4:44:ARG:HH22	32:R1:1248:G:P	2.36	0.46
28:5:70:ARG:HD2	32:R1:2298:A:OP1	2.16	0.46
32:R1:3:U:H2'	32:R1:4:U:C6	2.51	0.46
32:R1:227:A:HO2'	32:R1:228:C:P	2.38	0.46
32:R1:586:A:N1	32:R1:809:G:O2'	2.44	0.46
32:R1:1113:U:H2'	32:R1:1114:C:H6	1.80	0.46
32:R1:1645:G:H5''	32:R1:1646:C:H5'	1.98	0.46
33:R2:5:U:O2'	33:R2:27:C:O2	2.34	0.46
34:R3:460:A:H2'	34:R3:461:A:C8	2.50	0.46
34:R3:1095:U:OP1	34:R3:1108:G:N2	2.33	0.46
35:T:20:H2U:OP2	35:T:20:H2U:O2	2.33	0.46
19:3:1:MET:SD	19:3:1:MET:N	2.82	0.46
28:5:25:MET:CE	33:R2:54:G:H21	2.29	0.46
32:R1:645:C:H2'	32:R1:647:G:C8	2.50	0.46
34:R3:193:C:H2'	34:R3:194:C:C6	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:R3:382:A:H2'	34:R3:383:A:C8	2.50	0.46
34:R3:868:C:H2'	34:R3:869:G:O4'	2.14	0.46
36:Y:71:GLN:N	36:Y:179:LEU:HD23	2.30	0.46
36:Y:522:ASP:N	36:Y:522:ASP:OD1	2.48	0.46
19:3:83:ARG:NH1	32:R1:2637:U:H5''	2.31	0.46
26:36:32:LYS:HD3	32:R1:2478:A:H5'	1.97	0.46
28:5:70:ARG:O	28:5:80:GLN:NE2	2.34	0.46
32:R1:4:U:H2'	32:R1:5:A:C8	2.51	0.46
32:R1:1771:C:H2'	32:R1:1772:A:C8	2.50	0.46
32:R1:2812:G:H2'	32:R1:2813:A:C8	2.50	0.46
32:R1:2847:U:H2'	32:R1:2848:G:O4'	2.15	0.46
33:R2:3:C:H2'	33:R2:4:C:C6	2.50	0.46
34:R3:1006:G:O6	34:R3:1023:U:O2	2.33	0.46
32:R1:306:U:H2'	32:R1:307:G:O4'	2.16	0.46
32:R1:594:U:H2'	32:R1:595:C:C6	2.50	0.46
32:R1:891:G:H2'	32:R1:892:A:H8	1.81	0.46
32:R1:2136:G:H2'	32:R1:2137:U:C6	2.50	0.46
34:R3:381:C:H2'	34:R3:382:A:O4'	2.16	0.46
36:Y:165:LEU:HD23	36:Y:165:LEU:HA	1.78	0.46
2:13:113:PRO:HD3	32:R1:529:A:OP2	2.16	0.46
6:17:36:THR:HG23	6:17:41:ALA:HB2	1.96	0.46
9:2:219:VAL:HG21	32:R1:782:A:N7	2.30	0.46
13:23:69:ARG:NH2	13:23:72:GLN:HA	2.31	0.46
27:4:147:LEU:HD11	27:4:170:ARG:HD2	1.97	0.46
32:R1:45:G:H5''	32:R1:46:G:H5'	1.97	0.46
32:R1:140:C:H2'	32:R1:141:G:H5'	1.97	0.46
32:R1:2126:A:N7	32:R1:2163:A:H4'	2.31	0.46
34:R3:1316:G:N1	34:R3:1319:A:OP2	2.48	0.46
3:14:25:LEU:HD22	32:R1:2562:U:H4'	1.97	0.46
13:23:26:LYS:HE2	13:23:26:LYS:HB2	1.70	0.46
15:25:32:GLY:HA3	15:25:93:ARG:HB2	1.98	0.46
29:6:23:ILE:HD12	29:6:23:ILE:N	2.31	0.46
32:R1:721:A:H2'	32:R1:722:A:C8	2.51	0.46
32:R1:1042:G:H2'	32:R1:1043:C:C6	2.50	0.46
32:R1:1171:G:H2'	32:R1:1172:C:C6	2.50	0.46
3:14:97:THR:O	3:14:118:LEU:HD22	2.16	0.46
5:16:106:ASP:OD2	5:16:107:GLY:N	2.49	0.46
6:17:37:THR:HA	6:17:110:MET:HA	1.97	0.46
9:2:207:ALA:HB2	32:R1:1790:C:O2'	2.15	0.46
32:R1:394:C:H2'	32:R1:395:U:O4'	2.16	0.46
32:R1:1168:G:H2'	32:R1:1169:A:H8	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:R1:1281:G:H2'	32:R1:1282:U:C6	2.51	0.46
32:R1:2243:U:H2'	32:R1:2244:U:C6	2.51	0.46
34:R3:598:U:H2'	34:R3:599:C:H6	1.81	0.46
34:R3:685:G:N2	34:R3:704:A:OP2	2.34	0.46
7:18:33:ARG:HD3	33:R2:52:A:H62	1.81	0.46
30:9:83:LYS:O	30:9:91:PHE:HB3	2.16	0.46
32:R1:1113:U:H2'	32:R1:1114:C:C6	2.50	0.46
32:R1:2175:C:H2'	32:R1:2176:A:N9	2.31	0.46
32:R1:2178:C:H2'	32:R1:2179:C:C6	2.50	0.46
34:R3:131:A:H2'	34:R3:132:C:C6	2.51	0.46
34:R3:688:G:O2'	34:R3:704:A:N1	2.45	0.46
34:R3:1417:G:O2'	34:R3:1483:A:N6	2.49	0.46
35:T:32:4OC:O5'	35:T:32:4OC:H6	2.15	0.46
1:1:42:VAL:HG12	1:1:216:THR:HG23	1.97	0.45
12:22:18:ARG:HG3	12:22:76:VAL:HG22	1.97	0.45
16:27:19:LYS:HA	16:27:19:LYS:HD3	1.79	0.45
19:3:2:ILE:HG13	19:3:3:GLY:H	1.81	0.45
22:32:37:HIS:ND1	22:32:38:LEU:O	2.48	0.45
27:4:139:LYS:HE3	27:4:139:LYS:HB2	1.80	0.45
30:9:63:ALA:HA	30:9:66:ASN:ND2	2.31	0.45
32:R1:411:G:OP2	32:R1:2406:A:O2'	2.32	0.45
32:R1:878:A:H3'	32:R1:879:G:H8	1.81	0.45
32:R1:1072:C:OP2	32:R1:1075:C:N4	2.44	0.45
32:R1:1328:A:O2'	32:R1:1329:U:O5'	2.32	0.45
32:R1:2788:C:H2'	32:R1:2789:C:C6	2.51	0.45
2:13:13:ARG:HD3	2:13:51:GLY:O	2.16	0.45
3:14:2:ILE:HD12	3:14:6:THR:HG21	1.98	0.45
8:19:88:ARG:NH2	8:19:113:LEU:O	2.49	0.45
9:2:116:GLN:H	9:2:127:ASN:ND2	2.13	0.45
11:21:14:VAL:HG21	11:21:98:ILE:HD12	1.97	0.45
19:3:23:PRO:HB3	32:R1:2682:A:C2	2.51	0.45
32:R1:813:U:H2'	32:R1:814:C:C6	2.51	0.45
32:R1:1209:U:O2'	32:R1:1237:A:N1	2.41	0.45
32:R1:2103:C:H2'	32:R1:2104:C:C6	2.52	0.45
32:R1:2233:U:H2'	32:R1:2234:G:H8	1.81	0.45
34:R3:390:U:H2'	34:R3:391:G:C8	2.51	0.45
34:R3:1014:A:C2	34:R3:1219:A:H1'	2.51	0.45
34:R3:1225:A:H2'	34:R3:1225:A:N3	2.30	0.45
34:R3:1372:U:H2'	34:R3:1373:G:O4'	2.15	0.45
3:14:70:ARG:HG3	3:14:76:VAL:HG22	1.98	0.45
13:23:54:GLU:HG2	13:23:88:LYS:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:34:21:ARG:HG3	24:34:43:THR:HG21	1.98	0.45
32:R1:2329:U:H2'	32:R1:2330:G:C8	2.52	0.45
34:R3:1130:A:C8	34:R3:1146:A:N1	2.85	0.45
36:Y:470:ASP:C	36:Y:472:GLU:H	2.19	0.45
24:34:42:LEU:HD23	24:34:42:LEU:HA	1.82	0.45
32:R1:155:A:H2'	32:R1:156:A:H8	1.80	0.45
32:R1:1484:U:H2'	32:R1:1485:U:C6	2.52	0.45
19:3:27:ILE:HG12	19:3:201:LEU:HD12	1.99	0.45
27:4:143:LEU:HB3	27:4:146:VAL:CG2	2.45	0.45
32:R1:356:G:H2'	32:R1:357:C:C6	2.51	0.45
32:R1:514:A:N3	32:R1:581:C:O2'	2.41	0.45
32:R1:645:C:H2'	32:R1:647:G:N7	2.32	0.45
34:R3:1530:G:H2'	34:R3:1531:A:C8	2.50	0.45
2:13:26:GLY:O	32:R1:1143:A:N6	2.49	0.45
32:R1:8:C:H2'	32:R1:9:G:O4'	2.17	0.45
32:R1:351:C:H2'	32:R1:352:A:H8	1.82	0.45
32:R1:2175:C:H2'	32:R1:2176:A:C4	2.52	0.45
35:T:64:G:H2'	35:T:65:C:H6	1.81	0.45
36:Y:389:GLN:NE2	36:Y:464:GLN:OE1	2.49	0.45
18:29:2:LYS:HG2	32:R1:77:G:H5''	1.98	0.45
19:3:164:GLN:NE2	32:R1:2822:G:OP1	2.46	0.45
32:R1:1016:G:O6	32:R1:1147:A:N6	2.50	0.45
32:R1:2581:G:OP2	32:R1:2581:G:N2	2.46	0.45
32:R1:2818:U:H2'	32:R1:2819:G:H8	1.82	0.45
36:Y:327:LYS:HD3	36:Y:371:PRO:HA	1.97	0.45
21:31:15:SER:OG	21:31:19:GLY:O	2.35	0.45
22:32:30:ASP:N	22:32:35:GLU:O	2.34	0.45
26:36:37:GLN:HG2	26:36:37:GLN:O	2.17	0.45
28:5:77:LYS:HB2	28:5:77:LYS:HE3	1.70	0.45
32:R1:1378:A:O2'	32:R1:1380:G:OP2	2.35	0.45
32:R1:1505:A:H2'	32:R1:1506:U:O4'	2.17	0.45
32:R1:2105:U:H2'	32:R1:2106:U:H6	1.80	0.45
34:R3:235:C:H2'	34:R3:236:A:C8	2.52	0.45
34:R3:1294:G:H2'	34:R3:1295:U:C6	2.52	0.45
34:R3:1316:G:H2'	34:R3:1317:C:H5''	1.99	0.45
36:Y:181:GLN:NE2	36:Y:194:LEU:HD22	2.32	0.45
8:19:52:ARG:NH2	32:R1:2720:U:H5''	2.32	0.45
32:R1:2364:C:H2'	32:R1:2365:G:O4'	2.17	0.45
33:R2:88:C:H5''	33:R2:89:U:OP1	2.17	0.45
36:Y:324:GLY:O	36:Y:374:GLY:HA3	2.16	0.45
36:Y:449:PHE:O	36:Y:453:MET:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:27:42:GLY:HA2	32:R1:2330:G:H21	1.81	0.45
21:31:41:HIS:ND1	21:31:42:PRO:HD2	2.32	0.45
28:5:36:ASN:ND2	32:R1:2313:C:O4'	2.50	0.45
32:R1:851:C:H2'	32:R1:852:U:H6	1.81	0.45
32:R1:2063:C:H1'	58:T:101:FME:HG2	1.99	0.45
36:Y:186:LEU:HB2	36:Y:191:ILE:HG13	1.97	0.45
36:Y:428:SER:O	36:Y:432:ILE:HG23	2.17	0.45
29:6:51:PHE:CD1	29:6:68:ARG:HB2	2.52	0.44
29:6:63:GLN:HA	29:6:66:THR:HG22	1.99	0.44
32:R1:528:A:C2	32:R1:2042:A:H2'	2.52	0.44
32:R1:978:G:O4'	32:R1:1001:A:H2	2.00	0.44
32:R1:1048:A:N3	32:R1:1048:A:H2'	2.32	0.44
34:R3:1055:A:C6	34:R3:1206:G:C5	3.05	0.44
12:22:51:LEU:O	12:22:55:ILE:HG12	2.18	0.44
16:27:18:ALA:HB1	32:R1:2271:G:OP1	2.18	0.44
17:28:42:GLU:OE2	17:28:44:ARG:NE	2.48	0.44
32:R1:1057:A:O2'	32:R1:1058:U:H5'	2.17	0.44
32:R1:1858:A:H2'	32:R1:1859:U:O4'	2.17	0.44
34:R3:664:G:H22	34:R3:741:G:H1	1.65	0.44
34:R3:1015:G:H2'	34:R3:1016:A:C8	2.52	0.44
36:Y:356:VAL:HG11	36:Y:508:ILE:HG23	2.00	0.44
7:18:15:ARG:NH2	33:R2:8:C:OP1	2.49	0.44
7:18:94:ARG:HG2	7:18:97:PHE:O	2.18	0.44
32:R1:1159:U:C2	32:R1:1160:G:C8	3.05	0.44
32:R1:1495:A:N3	32:R1:1578:U:O2'	2.44	0.44
9:2:119:VAL:HG23	9:2:133:ASN:OD1	2.18	0.44
12:22:27:LYS:HB2	12:22:32:ALA:HB2	1.99	0.44
12:22:46:LEU:O	12:22:50:VAL:HG23	2.17	0.44
28:5:65:LEU:HD13	33:R2:42:C:C5	2.53	0.44
29:6:139:VAL:O	29:6:143:VAL:HG23	2.16	0.44
34:R3:707:U:H2'	34:R3:708:C:H6	1.82	0.44
5:16:8:LYS:HE2	32:R1:869:G:H1'	1.98	0.44
5:16:62:LYS:HG2	5:16:64:TRP:CZ2	2.52	0.44
5:16:71:LYS:HB3	5:16:93:VAL:O	2.17	0.44
17:28:6:VAL:O	17:28:73:ARG:NH2	2.50	0.44
22:32:37:HIS:CD2	22:32:43:THR:HG22	2.53	0.44
32:R1:3:U:H2'	32:R1:4:U:H6	1.83	0.44
32:R1:44:A:H2'	32:R1:45:G:O4'	2.17	0.44
32:R1:723:C:H2'	32:R1:724:U:O4'	2.18	0.44
32:R1:856:G:H2'	32:R1:857:G:C8	2.53	0.44
32:R1:2804:U:H2'	32:R1:2805:C:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:R3:707:U:H2'	34:R3:708:C:C6	2.52	0.44
34:R3:909:A:N3	34:R3:1413:A:O2'	2.37	0.44
34:R3:1513:A:H2'	34:R3:1514:G:C8	2.52	0.44
35:T:10:A:H2'	35:T:11:G:C8	2.53	0.44
3:14:63:VAL:HG12	3:14:107:LEU:HD21	2.00	0.44
12:22:59:GLU:HA	12:22:64:ALA:HA	1.98	0.44
12:22:62:ASP:OD1	12:22:62:ASP:N	2.51	0.44
15:25:55:GLU:O	15:25:59:GLU:HG3	2.18	0.44
30:9:19:VAL:HG23	30:9:21:VAL:HG13	1.99	0.44
32:R1:2326:C:O2'	32:R1:2327:A:OP1	2.25	0.44
34:R3:210:C:H4'	34:R3:211:G:N2	2.33	0.44
34:R3:839:C:H2'	34:R3:840:C:C6	2.52	0.44
5:16:69:PRO:HA	5:16:94:ALA:HB2	2.00	0.44
16:27:44:LYS:HB3	16:27:44:LYS:HE2	1.74	0.44
21:31:59:ARG:NH1	34:R3:1311:A:OP1	2.50	0.44
23:33:13:SER:OG	23:33:49:LYS:NZ	2.51	0.44
32:R1:247:G:OP2	32:R1:249:C:N4	2.51	0.44
32:R1:1181:U:H2'	32:R1:1182:G:H8	1.83	0.44
32:R1:2128:G:N1	32:R1:2161:C:O2	2.51	0.44
32:R1:2314:A:H2'	32:R1:2315:G:C8	2.52	0.44
34:R3:393:A:H3'	34:R3:394:G:H5''	1.99	0.44
34:R3:939:G:N3	34:R3:1375:A:H2	2.16	0.44
36:Y:402:PHE:CE1	36:Y:419:ARG:HB2	2.51	0.44
1:1:213:SER:HA	1:1:222:VAL:O	2.17	0.44
32:R1:1511:G:H2'	32:R1:1512:C:C6	2.53	0.44
32:R1:1538:G:H2'	32:R1:1539:U:C6	2.52	0.44
32:R1:1751:U:H2'	32:R1:1752:C:C6	2.53	0.44
32:R1:2812:G:H2'	32:R1:2813:A:H8	1.83	0.44
33:R2:30:C:H2'	33:R2:31:C:H5'	2.00	0.44
34:R3:484:G:O4'	34:R3:486:U:H5''	2.18	0.44
36:Y:28:ASN:ND2	36:Y:30:TYR:OH	2.51	0.44
8:19:3:ILE:HG21	19:3:186:LEU:HD21	2.00	0.44
19:3:105:LYS:O	19:3:177:VAL:HG12	2.18	0.44
23:33:5:ARG:NH1	32:R1:2285:C:OP2	2.45	0.44
27:4:150:THR:HA	27:4:192:ALA:HB2	2.00	0.44
30:9:84:ALA:HA	30:9:91:PHE:H	1.82	0.44
32:R1:49:A:H4'	32:R1:50:U:H5''	2.00	0.44
32:R1:885:C:H5''	32:R1:887:U:C6	2.53	0.44
32:R1:2592:G:H2'	32:R1:2593:U:O4'	2.18	0.44
34:R3:17:U:H2'	34:R3:18:C:C6	2.53	0.44
34:R3:1130:A:C4	34:R3:1131:G:C8	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:14:114:LYS:O	3:14:118:LEU:HD12	2.18	0.43
9:2:123:ILE:HG23	9:2:191:LEU:HD11	2.00	0.43
32:R1:2102:G:H2'	32:R1:2103:C:H6	1.81	0.43
34:R3:234:C:H2'	34:R3:235:C:H6	1.83	0.43
34:R3:1007:U:H2'	34:R3:1008:U:C6	2.53	0.43
36:Y:38:SER:O	36:Y:38:SER:OG	2.34	0.43
8:19:36:LYS:HB3	8:19:36:LYS:HE3	1.90	0.43
14:24:85:ARG:HH21	14:24:101:THR:HG23	1.83	0.43
19:3:5:VAL:H	19:3:32:ASN:ND2	2.13	0.43
32:R1:1173:U:O2	32:R1:1176:U:N3	2.52	0.43
32:R1:1395:A:O2'	32:R1:1396:U:H5''	2.18	0.43
32:R1:1873:G:H2'	32:R1:1874:C:C6	2.53	0.43
32:R1:2523:G:O2'	32:R1:2764:A:O2'	2.18	0.43
34:R3:711:G:H2'	34:R3:712:A:C8	2.54	0.43
34:R3:1007:U:H2'	34:R3:1008:U:H6	1.83	0.43
36:Y:193:TRP:O	36:Y:196:GLN:HG3	2.18	0.43
11:21:60:LYS:HB2	11:21:60:LYS:HE3	1.78	0.43
17:28:60:LYS:NZ	32:R1:371:A:O2'	2.33	0.43
28:5:44:ALA:O	36:Y:414:ASP:N	2.51	0.43
32:R1:983:A:N6	32:R1:984:A:N1	2.67	0.43
32:R1:1469:A:H2'	32:R1:1470:A:C8	2.53	0.43
32:R1:2102:G:H2'	32:R1:2103:C:C6	2.53	0.43
32:R1:2514:U:H2'	32:R1:2515:C:C6	2.53	0.43
34:R3:335:C:C2	34:R3:336:A:C8	3.07	0.43
36:Y:326:THR:HA	36:Y:335:PHE:O	2.18	0.43
10:20:77:LYS:HE2	10:20:77:LYS:HB2	1.71	0.43
16:27:74:PRO:HB3	33:R2:12:C:H41	1.83	0.43
30:9:58:LEU:O	30:9:61:VAL:HG22	2.19	0.43
32:R1:215:G:H4'	32:R1:216:A:H4'	2.01	0.43
32:R1:415:A:H2'	32:R1:416:U:C6	2.53	0.43
34:R3:598:U:H2'	34:R3:599:C:C6	2.53	0.43
34:R3:1031:C:H4'	34:R3:1033:G:H21	1.84	0.43
34:R3:1057:G:C6	34:R3:1204:A:N1	2.86	0.43
1:1:125:GLY:HA3	36:Y:103:TYR:HE1	1.83	0.43
26:36:6:SER:O	26:36:6:SER:OG	2.29	0.43
32:R1:143:C:H2'	32:R1:144:A:C8	2.53	0.43
32:R1:283:G:H2'	32:R1:284:U:O4'	2.19	0.43
32:R1:634:C:H2'	32:R1:635:C:C6	2.52	0.43
32:R1:1292:G:H2'	32:R1:1293:C:C6	2.54	0.43
34:R3:28:A:H2'	34:R3:29:U:O4'	2.18	0.43
34:R3:718:A:H2'	34:R3:718:A:N3	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:R3:1071:C:H2'	34:R3:1072:G:C8	2.50	0.43
36:Y:35:ALA:HB2	36:Y:302:ARG:HG2	1.99	0.43
2:13:7:LYS:HG2	32:R1:538:A:H4'	2.00	0.43
4:15:63:LYS:HD3	32:R1:2394:C:H5''	2.01	0.43
21:31:16:CYS:SG	21:31:36:VAL:HA	2.59	0.43
24:34:46:LYS:HE3	24:34:46:LYS:HB3	1.86	0.43
27:4:110:SER:HB3	27:4:114:ARG:HH12	1.83	0.43
28:5:32:LYS:NZ	32:R1:2315:G:OP1	2.42	0.43
32:R1:307:G:N1	32:R1:310:A:OP2	2.48	0.43
32:R1:1087:G:H8	32:R1:1088:A:H4'	1.84	0.43
32:R1:2121:G:H8	32:R1:2121:G:OP2	2.02	0.43
34:R3:191:G:H2'	34:R3:192:A:C8	2.53	0.43
34:R3:1219:A:H2'	34:R3:1220:G:H8	1.83	0.43
36:Y:111:GLU:O	36:Y:115:LYS:HG2	2.18	0.43
7:18:37:ALA:HB2	7:18:106:LEU:HD21	2.00	0.43
9:2:266:ILE:HG21	9:2:269:ARG:HD2	2.00	0.43
30:9:27:ARG:NH1	32:R1:2092:U:OP2	2.51	0.43
32:R1:2174:C:H2'	32:R1:2175:C:N1	2.34	0.43
32:R1:2247:A:H2'	32:R1:2248:C:H6	1.83	0.43
34:R3:925:G:C2	34:R3:927:G:C8	3.06	0.43
34:R3:1118:U:H2'	34:R3:1119:C:H6	1.84	0.43
34:R3:1260:G:O2'	34:R3:1275:A:N6	2.51	0.43
34:R3:1261:A:O2'	34:R3:1283:U:H5''	2.19	0.43
3:14:70:ARG:NH1	32:R1:2684:U:O4'	2.52	0.43
9:2:257:ARG:HD2	9:2:269:ARG:NH1	2.34	0.43
28:5:65:LEU:HD23	28:5:67:THR:HG22	1.99	0.43
32:R1:351:C:H2'	32:R1:352:A:C8	2.54	0.43
32:R1:2143:C:H2'	32:R1:2144:G:O4'	2.19	0.43
32:R1:2149:U:H2'	32:R1:2150:C:O4'	2.18	0.43
32:R1:2286:G:H4'	32:R1:2287:A:O4'	2.19	0.43
33:R2:28:C:H2'	33:R2:29:A:C8	2.54	0.43
34:R3:193:C:H2'	34:R3:194:C:H6	1.83	0.43
34:R3:426:U:H2'	34:R3:427:U:C6	2.53	0.43
34:R3:593:U:H2'	34:R3:594:U:C6	2.53	0.43
34:R3:1027:C:C2	34:R3:1034:G:N2	2.85	0.43
34:R3:1062:U:H2'	34:R3:1063:C:C6	2.54	0.43
1:1:216:THR:HB	1:1:219:GLY:H	1.83	0.43
2:13:1:MET:HB2	2:13:2:LYS:H	1.67	0.43
11:21:25:LEU:HD12	11:21:27:ILE:HD12	2.00	0.43
27:4:35:TYR:OH	27:4:176:ASP:OD2	2.31	0.43
28:5:87:LYS:HD3	32:R1:2313:C:H5''	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:R1:30:G:H2'	32:R1:31:C:C6	2.54	0.43
32:R1:196:A:O2'	32:R1:805:G:O6	2.37	0.43
32:R1:2590:A:H2'	32:R1:2591:C:H6	1.84	0.43
34:R3:815:A:N7	34:R3:1509:C:O2'	2.43	0.43
1:1:46:VAL:HG12	1:1:212:VAL:HG13	2.01	0.43
4:15:85:VAL:HG21	4:15:90:VAL:HG22	2.01	0.43
8:19:51:ASN:O	32:R1:2845:U:H5''	2.19	0.43
9:2:10:PRO:O	32:R1:729:G:N2	2.51	0.43
10:20:51:GLN:O	10:20:55:GLN:N	2.52	0.43
16:27:43:THR:H	32:R1:2331:G:H4'	1.83	0.43
32:R1:414:C:H2'	32:R1:415:A:H8	1.84	0.43
32:R1:1170:C:N4	32:R1:1171:G:O6	2.52	0.43
32:R1:1871:A:H8	32:R1:1872:A:C8	2.36	0.43
32:R1:1928:A:H2'	32:R1:1929:G:O4'	2.19	0.43
32:R1:2725:A:O2'	32:R1:2726:A:C8	2.72	0.43
34:R3:1000:A:H2'	34:R3:1001:C:C6	2.53	0.43
36:Y:37:GLY:HA2	59:Y:601:ATP:H3'	2.00	0.43
36:Y:139:LEU:HB3	36:Y:149:HIS:NE2	2.34	0.43
19:3:43:ASP:N	19:3:43:ASP:OD1	2.52	0.42
24:34:37:LYS:NZ	32:R1:468:G:OP2	2.52	0.42
32:R1:27:G:N2	32:R1:512:G:H1'	2.34	0.42
32:R1:404:A:H1'	32:R1:406:G:C4	2.53	0.42
32:R1:458:G:O2'	32:R1:469:G:O6	2.25	0.42
32:R1:755:U:H2'	32:R1:756:A:C8	2.54	0.42
32:R1:1361:G:H2'	32:R1:1362:C:C6	2.54	0.42
32:R1:1499:C:C2	32:R1:1500:G:C8	3.07	0.42
34:R3:391:G:H2'	34:R3:392:C:O4'	2.19	0.42
36:Y:73:GLN:NE2	36:Y:184:ASN:HD22	2.04	0.42
2:13:73:VAL:HG22	2:13:88:THR:HG22	2.01	0.42
3:14:23:LYS:NZ	32:R1:2561:U:O2	2.52	0.42
12:22:78:GLU:O	32:R1:24:G:O2'	2.36	0.42
18:29:2:LYS:HD2	32:R1:102:U:N3	2.34	0.42
32:R1:2183:A:H2'	32:R1:2184:A:C8	2.54	0.42
32:R1:2184:A:H2'	32:R1:2185:U:O4'	2.19	0.42
34:R3:1072:G:H2'	34:R3:1073:U:C6	2.53	0.42
34:R3:1171:A:H2'	34:R3:1172:C:C6	2.54	0.42
36:Y:482:GLU:HB3	36:Y:501:LEU:HD13	2.00	0.42
7:18:11:ALA:HB2	7:18:96:GLY:N	2.33	0.42
18:29:13:GLU:HB3	18:29:57:LEU:HD11	2.02	0.42
19:3:25:THR:OG1	19:3:191:GLY:O	2.32	0.42
32:R1:1159:U:N3	32:R1:1160:G:N7	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:R2:32:U:C2	33:R2:51:G:N2	2.87	0.42
34:R3:393:A:C6	34:R3:394:G:N2	2.88	0.42
34:R3:553:A:H2'	34:R3:554:A:H8	1.84	0.42
34:R3:773:G:O6	34:R3:807:A:N6	2.53	0.42
34:R3:908:A:H2'	34:R3:909:A:H8	1.84	0.42
35:T:64:G:H2'	35:T:65:C:C6	2.54	0.42
2:13:64:VAL:HG13	2:13:68:LYS:HE3	2.00	0.42
12:22:74:ILE:HD12	12:22:105:VAL:HG22	2.00	0.42
27:4:1:MET:HE1	27:4:19:PHE:C	2.40	0.42
28:5:152:ASP:OD1	32:R1:2304:G:O2'	2.31	0.42
29:6:23:ILE:HD13	29:6:36:LEU:HG	2.01	0.42
32:R1:579:G:H2'	32:R1:580:U:C6	2.54	0.42
32:R1:1036:G:C6	32:R1:1120:G:C6	3.07	0.42
32:R1:1110:G:H8	32:R1:1110:G:OP2	2.02	0.42
32:R1:1182:G:H2'	32:R1:1183:U:O4'	2.18	0.42
32:R1:1482:G:O2'	32:R1:1483:G:O5'	2.35	0.42
32:R1:1494:A:H2'	32:R1:1495:A:C8	2.54	0.42
32:R1:1507:C:H5'	32:R1:1508:A:OP2	2.19	0.42
34:R3:373:A:C2	34:R3:374:A:C8	3.07	0.42
34:R3:456:A:N6	34:R3:457:G:C6	2.87	0.42
36:Y:179:LEU:HD12	36:Y:179:LEU:HA	1.78	0.42
36:Y:409:LYS:HB3	36:Y:454:MET:SD	2.59	0.42
2:13:98:GLU:O	2:13:102:GLU:HG3	2.18	0.42
6:17:44:LEU:HD23	6:17:113:ILE:HD13	2.01	0.42
13:23:3:ARG:O	13:23:4:GLU:HB3	2.19	0.42
15:25:80:HIS:CE1	15:25:83:LYS:HD2	2.54	0.42
30:9:4:ILE:HG13	30:9:39:ALA:HB2	2.02	0.42
32:R1:30:G:H2'	32:R1:31:C:H6	1.85	0.42
32:R1:1022:G:H22	32:R1:1142:A:H2	1.64	0.42
32:R1:1128:G:N7	32:R1:2489:U:O2'	2.53	0.42
32:R1:2134:A:O2'	32:R1:2159:G:N2	2.52	0.42
32:R1:2154:A:P	32:R1:2154:A:H8	2.42	0.42
36:Y:142:VAL:HG11	36:Y:167:ALA:HB2	2.02	0.42
1:1:60:ARG:HG2	1:1:164:ARG:HG2	2.02	0.42
9:2:7:PRO:HB3	9:2:13:ARG:HG3	2.01	0.42
22:32:53:VAL:O	22:32:54:ILE:HD13	2.20	0.42
28:5:28:PRO:HB3	28:5:159:ALA:HA	2.01	0.42
30:9:46:PHE:HB3	30:9:51:ARG:HH12	1.84	0.42
32:R1:852:U:H2'	32:R1:853:C:C6	2.54	0.42
32:R1:886:A:C2	32:R1:887:U:H4'	2.55	0.42
32:R1:1429:G:H2'	32:R1:1430:G:H8	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:R2:86:G:C6	33:R2:88:C:H1'	2.54	0.42
34:R3:203:G:HO2'	34:R3:204:G:H8	1.63	0.42
34:R3:524:G:H2'	34:R3:525:C:C6	2.55	0.42
36:Y:394:GLU:HB3	36:Y:404:TRP:CH2	2.53	0.42
36:Y:513:VAL:HG23	36:Y:513:VAL:O	2.19	0.42
2:13:30:THR:HG21	32:R1:1005:C:O2'	2.20	0.42
6:17:59:SER:OG	6:17:60:VAL:N	2.53	0.42
32:R1:1176:U:H2'	32:R1:1177:G:C5	2.54	0.42
33:R2:28:C:H2'	33:R2:29:A:H8	1.83	0.42
34:R3:1507:A:H2'	34:R3:1508:A:C8	2.55	0.42
5:16:74:THR:HG21	5:16:86:LYS:HE3	2.01	0.42
18:29:9:LYS:HE2	18:29:11:VAL:HB	2.01	0.42
32:R1:1059:G:N2	32:R1:1081:U:H3	2.17	0.42
32:R1:1091:G:O6	32:R1:1100:C:N4	2.36	0.42
34:R3:202:G:O2'	34:R3:468:A:N3	2.42	0.42
34:R3:676:A:H2'	34:R3:677:U:C6	2.55	0.42
34:R3:1147:C:H2'	34:R3:1148:U:C6	2.55	0.42
35:T:13:A:H2'	35:T:14:G:O4'	2.20	0.42
36:Y:338:LEU:HD13	36:Y:338:LEU:HA	1.80	0.42
1:1:65:LEU:HD21	1:1:188:ASN:HB3	2.01	0.42
19:3:137:SER:O	19:3:137:SER:OG	2.38	0.42
22:32:51:ARG:CZ	22:32:53:VAL:HG12	2.50	0.42
32:R1:1747:U:H2'	32:R1:1748:C:C6	2.55	0.42
32:R1:2098:U:H2'	32:R1:2099:U:C6	2.55	0.42
32:R1:2133:G:O2'	32:R1:2134:A:O4'	2.31	0.42
32:R1:2391:G:H2'	32:R1:2424:C:H41	1.85	0.42
34:R3:382:A:H2'	34:R3:383:A:H8	1.84	0.42
34:R3:985:C:H2'	34:R3:986:U:C6	2.55	0.42
5:16:5:LYS:H	5:16:5:LYS:HG2	1.77	0.42
7:18:100:HIS:ND1	33:R2:48:U:H4'	2.35	0.42
15:25:76:ASP:HB3	15:25:90:ASP:HB2	2.02	0.42
32:R1:638:G:H2'	32:R1:639:U:C6	2.55	0.42
32:R1:981:A:OP2	32:R1:982:C:N4	2.44	0.42
32:R1:1093:G:N1	32:R1:1099:G:O6	2.53	0.42
32:R1:1198:U:H2'	32:R1:1199:U:C6	2.55	0.42
32:R1:1326:U:H2'	32:R1:1327:A:H8	1.84	0.42
32:R1:2014:A:H2'	32:R1:2015:A:C8	2.54	0.42
32:R1:2109:U:H2'	32:R1:2110:G:C8	2.55	0.42
32:R1:2191:A:H2'	32:R1:2192:U:C6	2.55	0.42
32:R1:2282:G:H4'	32:R1:2389:G:O2'	2.19	0.42
32:R1:2460:U:C2	32:R1:2461:A:C8	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:R1:2818:U:H2'	32:R1:2819:G:C8	2.55	0.42
34:R3:144:G:H2'	34:R3:145:G:C8	2.55	0.42
34:R3:455:G:H2'	34:R3:456:A:H8	1.84	0.42
34:R3:1125:U:H2'	34:R3:1126:U:H2'	2.01	0.42
34:R3:1130:A:H61	34:R3:1144:G:H1'	1.85	0.42
36:Y:175:ASP:CA	36:Y:204:THR:HG23	2.50	0.42
36:Y:397:ASN:ND2	36:Y:399:LEU:HG	2.34	0.42
2:13:4:PHE:CD2	10:20:99:VAL:HG11	2.55	0.41
3:14:31:ARG:HH22	32:R1:2676:C:P	2.42	0.41
32:R1:453:A:N3	32:R1:457:A:O2'	2.53	0.41
32:R1:729:G:H5''	32:R1:730:A:C5'	2.48	0.41
32:R1:1625:C:H2'	32:R1:1626:A:O4'	2.20	0.41
32:R1:1827:U:H2'	32:R1:1828:G:O4'	2.20	0.41
32:R1:2590:A:H2'	32:R1:2591:C:C6	2.55	0.41
34:R3:1272:G:H2'	34:R3:1273:C:C6	2.55	0.41
34:R3:1324:A:H2'	34:R3:1325:C:H6	1.86	0.41
2:13:82:GLY:HA2	32:R1:1131:G:OP1	2.20	0.41
12:22:92:ARG:NH2	12:22:94:ASP:OD2	2.48	0.41
16:27:56:ASP:N	16:27:56:ASP:OD1	2.53	0.41
22:32:15:ARG:NH1	32:R1:1266:G:OP2	2.54	0.41
34:R3:246:A:C2	34:R3:282:A:C5	3.07	0.41
34:R3:418:C:H2'	34:R3:419:C:O4'	2.20	0.41
36:Y:145:PRO:HB2	36:Y:147:GLU:OE1	2.20	0.41
5:16:25:ASP:O	5:16:66:ARG:NH1	2.53	0.41
10:20:57:ARG:NH2	32:R1:998:C:OP2	2.52	0.41
15:25:68:LYS:HB2	15:25:68:LYS:HE3	1.89	0.41
32:R1:191:A:H2'	32:R1:192:C:C6	2.55	0.41
32:R1:1796:U:H2'	32:R1:1797:G:C8	2.55	0.41
32:R1:2122:U:H5'	32:R1:2123:G:OP2	2.21	0.41
36:Y:41:SER:HB3	59:Y:601:ATP:O1B	2.19	0.41
36:Y:64:GLU:O	36:Y:174:PRO:HG2	2.20	0.41
3:14:106:GLU:N	3:14:106:GLU:OE1	2.54	0.41
5:16:1:MET:SD	5:16:44:ARG:HG2	2.61	0.41
7:18:74:VAL:HG13	7:18:106:LEU:HD13	2.02	0.41
32:R1:1664:A:H61	32:R1:1996:C:H42	1.69	0.41
34:R3:895:G:H2'	34:R3:896:C:C6	2.56	0.41
34:R3:1238:A:OP2	36:Y:317:ARG:NH1	2.38	0.41
19:3:204:LYS:HB2	19:3:204:LYS:HE2	1.91	0.41
20:30:4:ILE:HD11	20:30:56:VAL:HG21	2.02	0.41
22:32:52:LYS:NZ	22:32:55:ALA:HA	2.35	0.41
29:6:74:MET:O	29:6:78:VAL:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:R1:310:A:O2'	32:R1:311:A:H2'	2.20	0.41
32:R1:2489:U:H2'	32:R1:2490:G:O4'	2.21	0.41
34:R3:553:A:H2'	34:R3:554:A:C8	2.55	0.41
36:Y:313:LYS:O	36:Y:458:ASN:ND2	2.54	0.41
3:14:24:VAL:HG13	3:14:33:ALA:HB2	2.02	0.41
4:15:3:LEU:HD23	32:R1:1203:U:H5'	2.01	0.41
19:3:99:GLU:H	19:3:99:GLU:HG3	1.69	0.41
25:35:3:ILE:HD11	32:R1:592:A:C2	2.55	0.41
28:5:35:LEU:HB3	28:5:151:LEU:HD23	2.03	0.41
32:R1:372:G:O2'	32:R1:373:U:P	2.79	0.41
32:R1:876:C:H2'	32:R1:877:A:O4'	2.21	0.41
32:R1:1412:U:H2'	32:R1:1413:A:H8	1.85	0.41
32:R1:1542:U:H2'	32:R1:1543:G:O4'	2.20	0.41
32:R1:2303:G:O6	32:R1:2314:A:N6	2.54	0.41
34:R3:405:U:H3'	34:R3:406:G:H5'	2.02	0.41
34:R3:763:G:H2'	34:R3:764:C:C6	2.56	0.41
34:R3:865:A:H2'	34:R3:866:C:C6	2.55	0.41
34:R3:1273:C:H2'	34:R3:1274:A:O4'	2.20	0.41
36:Y:99:ARG:NH1	36:Y:120:GLU:OE1	2.54	0.41
32:R1:419:U:H2'	32:R1:420:C:C6	2.55	0.41
32:R1:523:C:O2	32:R1:554:U:O2'	2.38	0.41
32:R1:1409:U:H2'	32:R1:1410:G:C8	2.55	0.41
32:R1:2837:A:H2'	32:R1:2838:G:H8	1.86	0.41
34:R3:271:C:H2'	34:R3:272:C:C6	2.56	0.41
34:R3:456:A:C6	34:R3:457:G:C5	3.09	0.41
34:R3:518:C:H4'	34:R3:519:C:O2	2.21	0.41
34:R3:966:G:N2	35:T:34:C:H5'	2.35	0.41
3:14:30:ARG:HD2	32:R1:2674:G:H4'	2.01	0.41
22:32:36:LYS:HB3	22:32:36:LYS:HE2	1.87	0.41
23:33:27:ARG:HH11	23:33:27:ARG:HG3	1.86	0.41
25:35:27:ASN:O	25:35:35:LYS:HE2	2.20	0.41
32:R1:118:A:H2'	32:R1:120:U:O4	2.20	0.41
32:R1:340:A:H2'	32:R1:341:C:O4'	2.20	0.41
32:R1:704:G:H1'	32:R1:727:A:N6	2.36	0.41
32:R1:784:G:H5'	32:R1:785:G:OP1	2.21	0.41
32:R1:2114:A:C5	32:R1:2167:U:H4'	2.55	0.41
32:R1:2895:G:H2'	32:R1:2896:C:H6	1.84	0.41
34:R3:335:C:O2'	34:R3:1433:A:N3	2.42	0.41
36:Y:138:LEU:HD21	36:Y:170:LEU:HB2	2.03	0.41
2:13:31:GLU:HG2	2:13:142:ILE:HG13	2.02	0.41
5:16:10:ARG:NH1	32:R1:2278:A:OP1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:17:38:LEU:HB3	6:17:39:PRO:HD3	2.03	0.41
15:25:51:GLN:HE22	15:25:79:ARG:NH1	2.19	0.41
21:31:41:HIS:CD2	21:31:43:PHE:HB3	2.55	0.41
32:R1:363:G:H2'	32:R1:364:C:H6	1.86	0.41
32:R1:440:C:H2'	32:R1:441:U:H6	1.86	0.41
32:R1:628:G:C6	32:R1:636:G:C2	3.09	0.41
32:R1:1042:G:H2'	32:R1:1043:C:H6	1.85	0.41
32:R1:1300:G:H4'	32:R1:1301:A:H5''	2.03	0.41
32:R1:1418:G:N2	32:R1:1579:A:C8	2.89	0.41
32:R1:1882:U:H2'	32:R1:1883:U:C6	2.56	0.41
32:R1:2638:G:H1'	32:R1:2778:A:N6	2.35	0.41
34:R3:256:U:H2'	34:R3:257:G:C8	2.56	0.41
34:R3:344:A:H5''	34:R3:345:C:H5	1.86	0.41
34:R3:602:A:H2'	34:R3:603:U:C6	2.55	0.41
34:R3:613:C:H2'	34:R3:614:C:H6	1.85	0.41
34:R3:966:G:C2	35:T:34:C:H5'	2.55	0.41
35:T:65:C:H2'	35:T:66:C:H6	1.86	0.41
35:T:67:C:H2'	35:T:68:C:C6	2.56	0.41
22:32:28:SER:HB3	22:32:39:ARG:HG2	2.03	0.41
29:6:172:GLU:HG3	29:6:174:LYS:H	1.86	0.41
32:R1:597:G:H2'	32:R1:598:U:C6	2.56	0.41
32:R1:2060:A:O2'	32:R1:2061:G:OP2	2.33	0.41
32:R1:2116:G:H1	32:R1:2171:A:N6	2.19	0.41
32:R1:2281:A:O2'	32:R1:2282:G:H5'	2.21	0.41
34:R3:35:G:H2'	34:R3:36:C:C6	2.56	0.41
34:R3:582:C:C2	34:R3:583:A:C8	3.09	0.41
34:R3:704:A:C4	34:R3:705:G:C8	3.09	0.41
1:1:38:PHE:HE1	32:R1:2127:G:H4'	1.86	0.40
2:13:99:ARG:HA	2:13:99:ARG:HD2	1.90	0.40
3:14:76:VAL:HG21	32:R1:2684:U:H4'	2.03	0.40
6:17:36:THR:OG1	6:17:37:THR:N	2.54	0.40
7:18:26:LEU:HD12	7:18:39:VAL:HG22	2.04	0.40
9:2:43:ASN:OD1	9:2:43:ASN:N	2.54	0.40
13:23:49:LYS:HE3	13:23:49:LYS:HB2	1.83	0.40
17:28:17:ARG:HA	17:28:17:ARG:HD2	1.83	0.40
27:4:5:LEU:HD22	27:4:120:VAL:HG22	2.02	0.40
29:6:59:ASP:OD1	29:6:59:ASP:N	2.54	0.40
32:R1:177:G:H3'	32:R1:178:G:H8	1.85	0.40
32:R1:1419:A:C8	32:R1:1579:A:N6	2.89	0.40
32:R1:1849:G:H2'	32:R1:1850:G:H8	1.86	0.40
34:R3:991:U:O4	34:R3:1212:U:O2'	2.28	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:R3:1225:A:H5''	34:R3:1226:C:OP2	2.21	0.40
34:R3:1460:C:C2	34:R3:1461:G:C8	3.09	0.40
36:Y:482:GLU:HB3	36:Y:501:LEU:CD1	2.51	0.40
36:Y:504:ARG:HD2	36:Y:516:PHE:CG	2.55	0.40
4:15:109:LYS:HE2	32:R1:636:G:N7	2.36	0.40
9:2:110:LYS:HB3	9:2:110:LYS:HE2	1.79	0.40
10:20:14:LYS:HE2	10:20:14:LYS:HB2	1.83	0.40
10:20:30:VAL:HG13	32:R1:580:U:O3'	2.22	0.40
15:25:30:ILE:HD12	15:25:38:LEU:HD23	2.03	0.40
20:30:51:SER:O	20:30:51:SER:OG	2.30	0.40
25:35:50:SER:OG	25:35:51:LYS:N	2.54	0.40
27:4:127:GLU:HG2	27:4:133:LEU:HD13	2.02	0.40
27:4:150:THR:O	27:4:171:ASP:HA	2.21	0.40
32:R1:284:U:N3	32:R1:285:G:N7	2.70	0.40
32:R1:849:A:H2'	32:R1:850:U:H6	1.86	0.40
32:R1:852:U:H2'	32:R1:853:C:H6	1.85	0.40
32:R1:878:A:N6	32:R1:899:A:O2'	2.54	0.40
32:R1:2100:G:C6	32:R1:2190:G:C6	3.09	0.40
32:R1:2262:U:H2'	32:R1:2263:C:H6	1.85	0.40
32:R1:2549:G:C2	32:R1:2550:G:N7	2.89	0.40
33:R2:39:A:H2'	33:R2:40:U:C6	2.57	0.40
34:R3:99:C:O2'	34:R3:100:G:OP2	2.40	0.40
34:R3:201:G:O2'	34:R3:469:C:O2'	2.31	0.40
34:R3:1251:A:H2'	34:R3:1252:A:C8	2.56	0.40
36:Y:347:LYS:HG2	36:Y:488:LEU:HD21	2.03	0.40
8:19:94:ALA:HB2	32:R1:2848:G:C8	2.56	0.40
32:R1:64:A:H2'	32:R1:65:U:H6	1.86	0.40
32:R1:589:U:H2'	32:R1:590:A:C8	2.56	0.40
32:R1:827:U:O2'	32:R1:2068:U:C2	2.74	0.40
32:R1:1000:A:H2'	32:R1:1001:A:C8	2.56	0.40
34:R3:335:C:H2'	34:R3:336:A:H8	1.85	0.40
34:R3:991:U:C4	34:R3:1212:U:H1'	2.56	0.40
34:R3:1152:A:H2'	34:R3:1153:G:C8	2.57	0.40
34:R3:1206:G:C6	34:R3:1207:G:C5	3.09	0.40
36:Y:317:ARG:H	36:Y:317:ARG:HG2	1.58	0.40
36:Y:346:GLU:HG2	36:Y:347:LYS:HG3	2.04	0.40
2:13:125:TYR:OH	2:13:132:HIS:NE2	2.46	0.40
4:15:92:LEU:O	4:15:96:LYS:HD2	2.21	0.40
8:19:30:TRP:CE3	8:19:37:LYS:HD3	2.56	0.40
9:2:81:GLU:OE1	9:2:102:TYR:OH	2.21	0.40
19:3:4:LEU:HD12	19:3:4:LEU:HA	1.96	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:32:1:ALA:N	32:R1:2056:G:H21	2.20	0.40
27:4:145:ASP:HA	27:4:166:LYS:HB3	2.04	0.40
28:5:2:LYS:HE2	28:5:2:LYS:HB3	1.82	0.40
32:R1:181:A:H2'	32:R1:182:A:H8	1.86	0.40
32:R1:843:G:H2'	32:R1:844:A:C8	2.56	0.40
32:R1:1292:G:H2'	32:R1:1293:C:H6	1.87	0.40
32:R1:1536:C:HO2'	32:R1:1537:G:N2	2.20	0.40
32:R1:1858:A:C6	32:R1:1885:A:C8	3.10	0.40
34:R3:580:C:H2'	34:R3:581:G:O4'	2.22	0.40
34:R3:842:U:H3'	34:R3:843:U:H4'	2.03	0.40
34:R3:990:C:H2'	34:R3:991:U:C6	2.57	0.40
34:R3:1010:U:H2'	34:R3:1011:C:H6	1.86	0.40
34:R3:1028:C:O2'	34:R3:1030:U:O4	2.36	0.40
36:Y:3:VAL:HG12	36:Y:23:LYS:HG3	2.03	0.40
36:Y:160:TRP:O	36:Y:164:VAL:HG23	2.21	0.40
36:Y:514:ILE:H	36:Y:514:ILE:HG12	1.75	0.40
1:1:217:THR:O	32:R1:2124:G:N2	2.55	0.40
9:2:131:MET:CE	9:2:173:LEU:HD21	2.52	0.40
21:31:2:LYS:HE2	33:R2:40:U:H2'	2.03	0.40
22:32:54:ILE:HG22	22:32:56:LYS:N	2.35	0.40
28:5:118:ALA:O	28:5:166:ARG:NE	2.34	0.40
32:R1:248:G:H5'	32:R1:250:G:N7	2.37	0.40
32:R1:947:A:H2'	32:R1:948:C:C6	2.57	0.40
32:R1:1219:U:H2'	32:R1:1220:G:C8	2.57	0.40
32:R1:1417:C:H2'	32:R1:1418:G:C8	2.57	0.40
32:R1:1496:A:H2'	32:R1:1498:C:C5	2.57	0.40
32:R1:2130:U:H1'	32:R1:2159:G:C6	2.57	0.40
33:R2:31:C:H2'	33:R2:32:U:H6	1.86	0.40
34:R3:321:A:H2'	34:R3:322:C:H6	1.86	0.40
34:R3:494:G:O2'	34:R3:496:A:H1'	2.21	0.40
34:R3:572:A:H5'	34:R3:573:A:OP2	2.21	0.40
36:Y:33:ILE:HG22	36:Y:302:ARG:HH21	1.87	0.40
36:Y:128:GLY:HA2	36:Y:131:ALA:HB2	2.03	0.40
36:Y:351:LEU:HD23	36:Y:507:GLU:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	202 (93%)	16 (7%)	0	100	100
2	13	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
3	14	120/122 (98%)	108 (90%)	12 (10%)	0	100	100
4	15	142/144 (99%)	131 (92%)	11 (8%)	0	100	100
5	16	134/136 (98%)	123 (92%)	11 (8%)	0	100	100
6	17	118/120 (98%)	106 (90%)	12 (10%)	0	100	100
7	18	114/116 (98%)	108 (95%)	6 (5%)	0	100	100
8	19	112/114 (98%)	103 (92%)	9 (8%)	0	100	100
9	2	269/271 (99%)	245 (91%)	24 (9%)	0	100	100
10	20	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
11	21	101/103 (98%)	93 (92%)	7 (7%)	1 (1%)	13	42
12	22	108/110 (98%)	98 (91%)	10 (9%)	0	100	100
13	23	91/93 (98%)	79 (87%)	12 (13%)	0	100	100
14	24	100/102 (98%)	89 (89%)	11 (11%)	0	100	100
15	25	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
16	27	75/77 (97%)	70 (93%)	5 (7%)	0	100	100
17	28	75/77 (97%)	72 (96%)	3 (4%)	0	100	100
18	29	61/63 (97%)	60 (98%)	1 (2%)	0	100	100
19	3	207/209 (99%)	190 (92%)	17 (8%)	0	100	100
20	30	56/58 (97%)	51 (91%)	5 (9%)	0	100	100
21	31	64/66 (97%)	55 (86%)	9 (14%)	0	100	100
22	32	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
23	33	48/50 (96%)	43 (90%)	5 (10%)	0	100	100
24	34	44/46 (96%)	39 (89%)	5 (11%)	0	100	100
25	35	62/64 (97%)	58 (94%)	3 (5%)	1 (2%)	8	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	36	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
27	4	199/201 (99%)	185 (93%)	14 (7%)	0	100	100
28	5	175/177 (99%)	166 (95%)	9 (5%)	0	100	100
29	6	174/176 (99%)	160 (92%)	14 (8%)	0	100	100
30	9	147/149 (99%)	129 (88%)	16 (11%)	2 (1%)	9	34
36	Y	525/530 (99%)	445 (85%)	75 (14%)	5 (1%)	13	42
37	sb	216/218 (99%)	196 (91%)	19 (9%)	1 (0%)	25	56
38	sc	204/206 (99%)	194 (95%)	10 (5%)	0	100	100
39	sd	203/205 (99%)	187 (92%)	16 (8%)	0	100	100
40	se	155/157 (99%)	130 (84%)	25 (16%)	0	100	100
41	sf	98/100 (98%)	87 (89%)	11 (11%)	0	100	100
42	sg	149/151 (99%)	135 (91%)	14 (9%)	0	100	100
43	sh	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
44	si	125/127 (98%)	104 (83%)	20 (16%)	1 (1%)	16	46
45	sj	96/98 (98%)	88 (92%)	7 (7%)	1 (1%)	13	42
46	sk	114/116 (98%)	106 (93%)	8 (7%)	0	100	100
47	sl	121/123 (98%)	94 (78%)	27 (22%)	0	100	100
48	sm	112/114 (98%)	99 (88%)	13 (12%)	0	100	100
49	sn	98/100 (98%)	78 (80%)	19 (19%)	1 (1%)	13	42
50	so	86/88 (98%)	82 (95%)	4 (5%)	0	100	100
51	sp	80/82 (98%)	69 (86%)	11 (14%)	0	100	100
52	sq	78/80 (98%)	65 (83%)	13 (17%)	0	100	100
53	sr	63/65 (97%)	61 (97%)	2 (3%)	0	100	100
54	ss	77/79 (98%)	71 (92%)	6 (8%)	0	100	100
55	st	83/85 (98%)	81 (98%)	2 (2%)	0	100	100
56	su	63/65 (97%)	42 (67%)	21 (33%)	0	100	100
All	All	6324/6429 (98%)	5720 (90%)	591 (9%)	13 (0%)	45	71

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	21	51	VAL
36	Y	188	ILE

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Mol	Chain	Res	Type
30	9	9	VAL
36	Y	420	SER
36	Y	377	LYS
30	9	8	LYS
36	Y	40	LYS
36	Y	347	LYS
37	sb	18	GLN
44	si	41	GLU
49	sn	97	LYS
25	35	31	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%)	101 (95%)	5 (5%)	22	51
2	13	116/116 (100%)	112 (97%)	4 (3%)	32	59
3	14	103/103 (100%)	101 (98%)	2 (2%)	52	72
4	15	103/103 (100%)	102 (99%)	1 (1%)	73	84
5	16	109/109 (100%)	107 (98%)	2 (2%)	54	74
6	17	100/100 (100%)	98 (98%)	2 (2%)	50	71
7	18	86/86 (100%)	81 (94%)	5 (6%)	17	44
8	19	99/99 (100%)	94 (95%)	5 (5%)	20	48
9	2	216/216 (100%)	212 (98%)	4 (2%)	52	72
10	20	89/89 (100%)	85 (96%)	4 (4%)	23	52
11	21	84/84 (100%)	83 (99%)	1 (1%)	67	80
12	22	93/93 (100%)	92 (99%)	1 (1%)	70	82
13	23	80/80 (100%)	78 (98%)	2 (2%)	42	67
14	24	83/83 (100%)	82 (99%)	1 (1%)	67	80
15	25	78/78 (100%)	78 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	27	59/59 (100%)	58 (98%)	1 (2%)	56	74
17	28	67/67 (100%)	65 (97%)	2 (3%)	36	62
18	29	55/55 (100%)	53 (96%)	2 (4%)	30	57
19	3	164/164 (100%)	161 (98%)	3 (2%)	54	74
20	30	48/48 (100%)	46 (96%)	2 (4%)	25	53
21	31	59/59 (100%)	53 (90%)	6 (10%)	6	23
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%)	37 (97%)	1 (3%)	41	66
25	35	51/51 (100%)	51 (100%)	0	100	100
26	36	34/34 (100%)	34 (100%)	0	100	100
27	4	165/165 (100%)	163 (99%)	2 (1%)	67	80
28	5	148/148 (100%)	140 (95%)	8 (5%)	18	46
29	6	137/137 (100%)	130 (95%)	7 (5%)	20	48
30	9	114/114 (100%)	109 (96%)	5 (4%)	24	52
36	Y	449/456 (98%)	424 (94%)	25 (6%)	17	45
37	sb	180/180 (100%)	177 (98%)	3 (2%)	56	74
38	sc	170/170 (100%)	165 (97%)	5 (3%)	37	63
39	sd	172/172 (100%)	165 (96%)	7 (4%)	26	54
40	se	119/119 (100%)	116 (98%)	3 (2%)	42	67
41	sf	87/87 (100%)	86 (99%)	1 (1%)	70	82
42	sg	124/124 (100%)	119 (96%)	5 (4%)	27	55
43	sh	104/104 (100%)	101 (97%)	3 (3%)	37	63
44	si	105/105 (100%)	101 (96%)	4 (4%)	28	56
45	sj	86/86 (100%)	80 (93%)	6 (7%)	12	37
46	sk	89/89 (100%)	89 (100%)	0	100	100
47	sl	103/103 (100%)	97 (94%)	6 (6%)	17	44
48	sm	92/92 (100%)	85 (92%)	7 (8%)	11	34
49	sn	83/83 (100%)	79 (95%)	4 (5%)	21	50
50	so	76/76 (100%)	75 (99%)	1 (1%)	65	79
51	sp	65/65 (100%)	62 (95%)	3 (5%)	23	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	sq	74/74 (100%)	74 (100%)	0	100	100
53	sr	56/56 (100%)	55 (98%)	1 (2%)	54	74
54	ss	70/70 (100%)	69 (99%)	1 (1%)	62	78
55	st	65/65 (100%)	63 (97%)	2 (3%)	35	61
56	su	55/55 (100%)	49 (89%)	6 (11%)	5	20
All	All	5200/5272 (99%)	5028 (97%)	172 (3%)	35	60

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	8	MET
1	1	24	ASN
1	1	25	GLU
1	1	43	ASP
1	1	208	TYR
2	13	1	MET
2	13	19	ASP
2	13	49	ASP
2	13	96	ARG
3	14	56	ASP
3	14	58	LEU
4	15	121	THR
5	16	55	ARG
5	16	60	GLN
6	17	5	LYS
6	17	36	THR
7	18	5	SER
7	18	16	ARG
7	18	81	ARG
7	18	89	ASP
7	18	98	GLN
8	19	20	ARG
8	19	23	ASP
8	19	65	ASN
8	19	81	ASP
8	19	105	LYS
9	2	86	ARG
9	2	212	TRP
9	2	213	ARG
9	2	263	ASP

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Mol	Chain	Res	Type
10	20	15	LYS
10	20	50	ARG
10	20	71	ASN
10	20	86	SER
11	21	26	ASP
12	22	40	ASN
13	23	24	MET
13	23	40	LYS
14	24	45	GLN
16	27	56	ASP
17	28	4	CYS
17	28	77	TYR
18	29	13	GLU
18	29	58	ASN
19	3	1	MET
19	3	46	ARG
19	3	137	SER
20	30	10	ARG
20	30	30	ARG
21	31	4	ASP
21	31	9	TYR
21	31	20	ASN
21	31	26	SER
21	31	56	ARG
21	31	59	ARG
23	33	50	GLU
24	34	25	LYS
27	4	114	ARG
27	4	125	SER
28	5	20	ASN
28	5	36	ASN
28	5	37	MET
28	5	55	ASP
28	5	86	CYS
28	5	129	MET
28	5	149	ARG
28	5	174	PHE
29	6	29	ASN
29	6	47	ASN
29	6	54	ARG
29	6	84	LYS
29	6	132	LEU

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Mol	Chain	Res	Type
29	6	133	LYS
29	6	162	ARG
30	9	17	ASP
30	9	42	LYS
30	9	75	LEU
30	9	91	PHE
30	9	114	GLU
36	Y	4	SER
36	Y	13	SER
36	Y	17	PHE
36	Y	29	ARG
36	Y	87	MET
36	Y	153	MET
36	Y	180	ASP
36	Y	201	ARG
36	Y	205	MET
36	Y	212	ARG
36	Y	231	ARG
36	Y	241	MET
36	Y	257	LYS
36	Y	270	SER
36	Y	280	ARG
36	Y	288	GLN
36	Y	290	ASP
36	Y	377	LYS
36	Y	430	ASP
36	Y	437	LYS
36	Y	476	SER
36	Y	512	ARG
36	Y	520	TYR
36	Y	522	ASP
36	Y	525	ARG
37	sb	22	TRP
37	sb	49	PHE
37	sb	131	LYS
38	sc	24	ASN
38	sc	30	ASP
38	sc	62	SER
38	sc	92	ASP
38	sc	106	ARG
39	sd	17	ASP
39	sd	57	LYS

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Mol	Chain	Res	Type
39	sd	62	ARG
39	sd	80	ARG
39	sd	165	GLU
39	sd	189	ASP
39	sd	190	LEU
40	se	28	ARG
40	se	129	SER
40	se	156	ARG
41	sf	2	ARG
42	sg	2	ARG
42	sg	4	ARG
42	sg	14	ASP
42	sg	124	SER
42	sg	139	ASP
43	sh	3	GLN
43	sh	9	MET
43	sh	76	ARG
44	si	6	TYR
44	si	10	ARG
44	si	26	LYS
44	si	92	SER
45	sj	31	ARG
45	sj	35	GLN
45	sj	58	ASN
45	sj	62	ARG
45	sj	63	ASP
45	sj	85	ASP
47	sl	11	ARG
47	sl	58	ASN
47	sl	64	SER
47	sl	104	SER
47	sl	107	LYS
47	sl	113	ARG
48	sm	10	ASP
48	sm	67	ASP
48	sm	69	ARG
48	sm	74	MET
48	sm	84	CYS
48	sm	99	GLN
48	sm	106	ARG
49	sn	34	ASN
49	sn	39	ASP

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Mol	Chain	Res	Type
49	sn	53	ASP
49	sn	80	ARG
50	so	9	LYS
51	sp	12	LYS
51	sp	25	ARG
51	sp	55	ASP
53	sr	47	ARG
54	ss	5	LYS
55	st	52	GLU
55	st	53	MET
56	su	11	PHE
56	su	32	ARG
56	su	36	PHE
56	su	37	TYR
56	su	55	HIS
56	su	61	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
12	22	61	ASN
19	3	32	ASN
21	31	20	ASN
27	4	165	HIS
36	Y	184	ASN
36	Y	216	ASN
37	sb	17	HIS
39	sd	39	GLN
47	sl	58	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
31	M	8/9 (88%)	1 (12%)	0
32	R1	2902/2903 (99%)	471 (16%)	8 (0%)
33	R2	118/119 (99%)	13 (11%)	1 (0%)
34	R3	1538/1539 (99%)	278 (18%)	5 (0%)
35	T	75/77 (97%)	12 (16%)	3 (4%)
All	All	4641/4647 (99%)	775 (16%)	17 (0%)

All (775) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
31	M	7	A
32	R1	10	A
32	R1	15	G
32	R1	35	G
32	R1	36	G
32	R1	45	G
32	R1	46	G
32	R1	51	G
32	R1	55	G
32	R1	63	A
32	R1	71	A
32	R1	74	A
32	R1	75	G
32	R1	84	A
32	R1	96	C
32	R1	102	U
32	R1	103	A
32	R1	118	A
32	R1	119	A
32	R1	120	U
32	R1	125	A
32	R1	131	A
32	R1	140	C
32	R1	141	G
32	R1	142	A
32	R1	143	C
32	R1	162	U
32	R1	163	C
32	R1	196	A
32	R1	197	A
32	R1	199	A
32	R1	204	A
32	R1	216	A
32	R1	218	A
32	R1	221	A
32	R1	222	A
32	R1	228	C
32	R1	230	G
32	R1	233	A
32	R1	248	G
32	R1	255	A
32	R1	265	A

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Mol	Chain	Res	Type
32	R1	266	G
32	R1	278	A
32	R1	281	C
32	R1	284	U
32	R1	310	A
32	R1	311	A
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
32	R1	372	G
32	R1	373	U
32	R1	386	G
32	R1	387	U
32	R1	389	G
32	R1	395	U
32	R1	396	G
32	R1	403	U
32	R1	404	A
32	R1	405	U
32	R1	406	G
32	R1	411	G
32	R1	417	C
32	R1	424	G
32	R1	443	A
32	R1	448	U
32	R1	457	A
32	R1	473	G
32	R1	481	G
32	R1	489	G
32	R1	490	C
32	R1	491	G
32	R1	501	A
32	R1	504	A
32	R1	505	A
32	R1	509	C
32	R1	510	C
32	R1	529	A

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Mol	Chain	Res	Type
32	R1	530	G
32	R1	531	C
32	R1	532	A
32	R1	533	G
32	R1	544	C
32	R1	545	U
32	R1	546	U
32	R1	548	G
32	R1	563	A
32	R1	573	U
32	R1	575	A
32	R1	586	A
32	R1	603	A
32	R1	614	A
32	R1	615	U
32	R1	627	A
32	R1	637	A
32	R1	645	C
32	R1	646	U
32	R1	647	G
32	R1	654	A
32	R1	655	A
32	R1	669	G
32	R1	686	U
32	R1	709	U
32	R1	711	G
32	R1	722	A
32	R1	730	A
32	R1	738	G
32	R1	747	U
32	R1	748	G
32	R1	752	A
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	792	A
32	R1	805	G
32	R1	812	C

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Mol	Chain	Res	Type
32	R1	819	A
32	R1	827	U
32	R1	844	A
32	R1	845	A
32	R1	846	U
32	R1	847	U
32	R1	857	G
32	R1	885	C
32	R1	886	A
32	R1	887	U
32	R1	888	C
32	R1	891	G
32	R1	893	C
32	R1	896	A
32	R1	897	C
32	R1	907	G
32	R1	910	A
32	R1	927	A
32	R1	932	U
32	R1	941	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	989	G
32	R1	990	A
32	R1	995	C
32	R1	996	A
32	R1	999	U
32	R1	1005	C
32	R1	1009	A
32	R1	1012	U
32	R1	1013	C
32	R1	1021	A
32	R1	1023	U
32	R1	1025	G
32	R1	1026	G
32	R1	1033	U
32	R1	1046	A
32	R1	1047	G

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Mol	Chain	Res	Type
32	R1	1054	A
32	R1	1055	G
32	R1	1056	G
32	R1	1060	U
32	R1	1061	U
32	R1	1062	G
32	R1	1063	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
32	R1	1077	A
32	R1	1078	U
32	R1	1079	C
32	R1	1080	A
32	R1	1081	U
32	R1	1082	U
32	R1	1083	U
32	R1	1086	A
32	R1	1088	A
32	R1	1089	A
32	R1	1090	A
32	R1	1095	A
32	R1	1096	A
32	R1	1103	A
32	R1	1104	C
32	R1	1106	G
32	R1	1109	C
32	R1	1111	A
32	R1	1112	G
32	R1	1132	U
32	R1	1133	A
32	R1	1135	C
32	R1	1139	G

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Mol	Chain	Res	Type
32	R1	1172	C
32	R1	1174	U
32	R1	1175	A
32	R1	1176	U
32	R1	1178	C
32	R1	1180	U
32	R1	1210	G
32	R1	1211	C
32	R1	1212	G
32	R1	1236	G
32	R1	1250	G
32	R1	1253	A
32	R1	1256	G
32	R1	1258	U
32	R1	1271	G
32	R1	1272	A
32	R1	1273	U
32	R1	1300	G
32	R1	1301	A
32	R1	1329	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	1395	A
32	R1	1416	G
32	R1	1417	C
32	R1	1428	C
32	R1	1434	A
32	R1	1456	G
32	R1	1458	U
32	R1	1460	U
32	R1	1461	C
32	R1	1475	G
32	R1	1482	G
32	R1	1490	A
32	R1	1494	A
32	R1	1507	C

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Mol	Chain	Res	Type
32	R1	1508	A
32	R1	1509	A
32	R1	1515	A
32	R1	1522	A
32	R1	1524	G
32	R1	1529	G
32	R1	1532	A
32	R1	1535	A
32	R1	1536	C
32	R1	1560	G
32	R1	1569	A
32	R1	1578	U
32	R1	1583	A
32	R1	1584	U
32	R1	1608	A
32	R1	1610	A
32	R1	1647	U
32	R1	1648	U
32	R1	1654	A
32	R1	1672	A
32	R1	1674	G
32	R1	1675	C
32	R1	1694	C
32	R1	1715	G
32	R1	1729	U
32	R1	1730	C
32	R1	1735	A
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	1786	A
32	R1	1800	C
32	R1	1801	A
32	R1	1802	A
32	R1	1808	A
32	R1	1811	G
32	R1	1816	C
32	R1	1828	G

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Mol	Chain	Res	Type
32	R1	1829	A
32	R1	1866	A
32	R1	1870	C
32	R1	1871	A
32	R1	1884	G
32	R1	1901	A
32	R1	1906	G
32	R1	1913	A
32	R1	1914	C
32	R1	1915	U
32	R1	1917	U
32	R1	1929	G
32	R1	1930	G
32	R1	1937	A
32	R1	1938	A
32	R1	1943	U
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	1993	U
32	R1	1997	C
32	R1	2022	U
32	R1	2023	C
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	2076	U
32	R1	2093	G
32	R1	2096	C
32	R1	2110	G

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Mol	Chain	Res	Type
32	R1	2111	U
32	R1	2112	G
32	R1	2113	U
32	R1	2114	A
32	R1	2115	G
32	R1	2117	A
32	R1	2118	U
32	R1	2120	G
32	R1	2121	G
32	R1	2122	U
32	R1	2124	G
32	R1	2125	G
32	R1	2126	A
32	R1	2127	G
32	R1	2128	G
32	R1	2131	U
32	R1	2132	U
32	R1	2133	G
32	R1	2134	A
32	R1	2136	G
32	R1	2140	G
32	R1	2142	A
32	R1	2145	C
32	R1	2146	C
32	R1	2147	A
32	R1	2148	G
32	R1	2149	U
32	R1	2152	G
32	R1	2157	G
32	R1	2160	C
32	R1	2164	C
32	R1	2165	C
32	R1	2166	U
32	R1	2170	A
32	R1	2172	U
32	R1	2173	A
32	R1	2174	C
32	R1	2176	A
32	R1	2177	C
32	R1	2189	U
32	R1	2198	A
32	R1	2203	U

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Mol	Chain	Res	Type
32	R1	2204	G
32	R1	2211	A
32	R1	2212	A
32	R1	2213	U
32	R1	2214	C
32	R1	2225	A
32	R1	2238	G
32	R1	2239	G
32	R1	2250	G
32	R1	2266	A
32	R1	2273	A
32	R1	2283	C
32	R1	2287	A
32	R1	2288	A
32	R1	2302	U
32	R1	2305	U
32	R1	2309	A
32	R1	2315	G
32	R1	2319	G
32	R1	2320	U
32	R1	2322	A
32	R1	2325	G
32	R1	2326	C
32	R1	2327	A
32	R1	2333	A
32	R1	2345	G
32	R1	2350	C
32	R1	2359	C
32	R1	2361	G
32	R1	2376	A
32	R1	2383	G
32	R1	2385	C
32	R1	2396	G
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	2441	U
32	R1	2448	A
32	R1	2476	A

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Mol	Chain	Res	Type
32	R1	2494	G
32	R1	2502	G
32	R1	2503	A
32	R1	2505	G
32	R1	2506	U
32	R1	2518	A
32	R1	2520	C
32	R1	2529	G
32	R1	2535	G
32	R1	2547	A
32	R1	2554	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	2682	A
32	R1	2689	U
32	R1	2690	U
32	R1	2714	G
32	R1	2724	U
32	R1	2733	A
32	R1	2744	G
32	R1	2748	A
32	R1	2764	A
32	R1	2765	A
32	R1	2776	A
32	R1	2778	A
32	R1	2779	U
32	R1	2791	G
32	R1	2793	C
32	R1	2794	C
32	R1	2797	U
32	R1	2798	U

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Mol	Chain	Res	Type
32	R1	2820	A
32	R1	2835	A
32	R1	2849	U
32	R1	2861	U
32	R1	2867	G
32	R1	2868	A
32	R1	2880	C
32	R1	2883	A
32	R1	2884	U
32	R1	2903	U
33	R2	12	C
33	R2	13	G
33	R2	24	G
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	89	U
33	R2	90	C
33	R2	108	A
33	R2	109	A
34	R3	4	U
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
34	R3	73	C
34	R3	81	A
34	R3	82	G
34	R3	84	U
34	R3	86	G
34	R3	87	C

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Mol	Chain	Res	Type
34	R3	88	U
34	R3	95	C
34	R3	100	G
34	R3	130	A
34	R3	131	A
34	R3	141	G
34	R3	154	U
34	R3	155	A
34	R3	164	G
34	R3	168	G
34	R3	173	U
34	R3	177	G
34	R3	183	C
34	R3	199	A
34	R3	208	U
34	R3	210	C
34	R3	211	G
34	R3	212	G
34	R3	225	C
34	R3	226	G
34	R3	240	G
34	R3	245	U
34	R3	247	G
34	R3	251	G
34	R3	266	G
34	R3	267	C
34	R3	281	G
34	R3	289	G
34	R3	293	G
34	R3	306	A
34	R3	321	A
34	R3	328	C
34	R3	340	U
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

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Mol	Chain	Res	Type
34	R3	373	A
34	R3	387	U
34	R3	391	G
34	R3	392	C
34	R3	394	G
34	R3	397	A
34	R3	398	U
34	R3	404	G
34	R3	406	G
34	R3	413	G
34	R3	415	A
34	R3	417	G
34	R3	420	U
34	R3	421	U
34	R3	422	C
34	R3	423	G
34	R3	424	G
34	R3	425	G
34	R3	429	U
34	R3	438	U
34	R3	442	G
34	R3	448	A
34	R3	457	G
34	R3	458	U
34	R3	459	A
34	R3	464	U
34	R3	465	A
34	R3	466	A
34	R3	467	U
34	R3	468	A
34	R3	469	C
34	R3	472	U
34	R3	475	C
34	R3	476	U
34	R3	479	U
34	R3	480	U
34	R3	484	G
34	R3	485	U
34	R3	486	U
34	R3	487	A
34	R3	490	C
34	R3	492	C

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Mol	Chain	Res	Type
34	R3	493	A
34	R3	495	A
34	R3	496	A
34	R3	497	G
34	R3	500	G
34	R3	513	C
34	R3	514	C
34	R3	518	C
34	R3	519	C
34	R3	521	G
34	R3	524	G
34	R3	529	G
34	R3	531	U
34	R3	532	A
34	R3	540	G
34	R3	547	A
34	R3	559	A
34	R3	564	C
34	R3	572	A
34	R3	573	A
34	R3	575	G
34	R3	576	C
34	R3	577	G
34	R3	579	A
34	R3	596	A
34	R3	621	A
34	R3	622	A
34	R3	633	G
34	R3	654	G
34	R3	656	G
34	R3	665	A
34	R3	686	U
34	R3	713	G
34	R3	717	U
34	R3	718	A
34	R3	723	U
34	R3	724	G
34	R3	731	G
34	R3	734	G
34	R3	748	G
34	R3	755	G
34	R3	777	A

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Mol	Chain	Res	Type
34	R3	781	A
34	R3	813	U
34	R3	815	A
34	R3	817	C
34	R3	818	G
34	R3	819	A
34	R3	821	G
34	R3	842	U
34	R3	843	U
34	R3	845	A
34	R3	846	G
34	R3	851	G
34	R3	858	G
34	R3	872	A
34	R3	873	A
34	R3	885	G
34	R3	889	A
34	R3	902	G
34	R3	934	C
34	R3	935	A
34	R3	945	G
34	R3	946	A
34	R3	947	G
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	998	C
34	R3	999	C
34	R3	1004	A
34	R3	1020	G
34	R3	1023	U
34	R3	1025	U

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Mol	Chain	Res	Type
34	R3	1027	C
34	R3	1028	C
34	R3	1029	U
34	R3	1030	U
34	R3	1031	C
34	R3	1032	G
34	R3	1033	G
34	R3	1036	A
34	R3	1043	G
34	R3	1045	C
34	R3	1053	G
34	R3	1064	G
34	R3	1066	C
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	1143	G
34	R3	1152	A
34	R3	1155	A
34	R3	1158	C
34	R3	1159	U
34	R3	1160	G
34	R3	1167	A
34	R3	1168	U
34	R3	1169	A
34	R3	1182	G
34	R3	1183	U
34	R3	1184	G
34	R3	1196	A
34	R3	1212	U
34	R3	1227	A
34	R3	1238	A
34	R3	1241	G
34	R3	1248	A
34	R3	1250	A
34	R3	1257	A

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Mol	Chain	Res	Type
34	R3	1258	G
34	R3	1261	A
34	R3	1268	G
34	R3	1275	A
34	R3	1278	G
34	R3	1279	G
34	R3	1280	A
34	R3	1281	C
34	R3	1282	C
34	R3	1285	A
34	R3	1286	U
34	R3	1287	A
34	R3	1290	G
34	R3	1298	U
34	R3	1300	G
34	R3	1302	C
34	R3	1303	C
34	R3	1306	A
34	R3	1312	G
34	R3	1317	C
34	R3	1322	C
34	R3	1336	C
34	R3	1353	G
34	R3	1360	A
34	R3	1363	A
34	R3	1370	G
34	R3	1379	G
34	R3	1398	A
34	R3	1419	G
34	R3	1441	A
34	R3	1443	C
34	R3	1446	A
34	R3	1448	C
34	R3	1451	U
34	R3	1452	C
34	R3	1492	A
34	R3	1493	A
34	R3	1494	G
34	R3	1497	G
34	R3	1499	A
34	R3	1502	A
34	R3	1506	U

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Mol	Chain	Res	Type
34	R3	1517	G
34	R3	1519	A
34	R3	1529	G
34	R3	1530	G
34	R3	1533	C
34	R3	1534	A
34	R3	1540	U
35	T	9	G
35	T	13	A
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	47	U
35	T	54	5MU
35	T	55	PSU
35	T	56	C

All (17) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
32	R1	227	A
32	R1	372	G
32	R1	774	G
32	R1	784	G
32	R1	1020	A
32	R1	1108	U
32	R1	1328	A
32	R1	2326	C
33	R2	66	A
34	R3	391	G
34	R3	945	G
34	R3	1297	G
34	R3	1305	G
34	R3	1492	A
35	T	17	U
35	T	19	G
35	T	55	PSU

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

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	5MU	T	54	35	19,22,23	2.17	6 (31%)	27,32,35	2.25	8 (29%)
35	4SU	T	8	35	18,21,22	3.84	8 (44%)	25,30,33	2.33	6 (24%)
35	H2U	T	20	35	18,21,22	4.39	5 (27%)	19,30,33	3.81	6 (31%)
35	4OC	T	32	35	20,23,24	3.21	3 (15%)	25,32,35	1.10	3 (12%)
35	PSU	T	55	35	18,21,22	2.19	9 (50%)	21,30,33	2.31	4 (19%)

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

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	T	8	4SU	O2-C2	12.07	1.44	1.23
35	T	32	4OC	O2-C2	11.42	1.45	1.23
35	T	20	H2U	O4-C4	10.38	1.43	1.23
35	T	20	H2U	C2-N1	9.34	1.48	1.35
35	T	20	H2U	O2-C2	8.49	1.38	1.23
35	T	8	4SU	C4-S4	8.00	1.83	1.68
35	T	32	4OC	C4-N4	7.13	1.50	1.36
35	T	20	H2U	C2-N3	6.78	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	T	20	H2U	C4-N3	5.48	1.46	1.37
35	T	54	5MU	C6-C5	4.25	1.41	1.34
35	T	54	5MU	C4-C5	-4.02	1.38	1.44
35	T	8	4SU	C4-N3	-3.95	1.33	1.37
35	T	55	PSU	C2-N1	-3.88	1.31	1.36
35	T	32	4OC	C2-N1	-3.79	1.32	1.40
35	T	54	5MU	C4-N3	-3.62	1.32	1.38
35	T	54	5MU	O2-C2	-3.60	1.16	1.23
35	T	54	5MU	C2-N1	-3.59	1.32	1.38
35	T	55	PSU	C4-N3	-3.50	1.32	1.38
35	T	8	4SU	C2-N3	-3.47	1.31	1.38
35	T	55	PSU	C2-N3	-3.43	1.31	1.37
35	T	54	5MU	C6-N1	-3.17	1.32	1.38
35	T	55	PSU	C1'-C5	3.05	1.57	1.50
35	T	8	4SU	C2-N1	-3.02	1.33	1.38
35	T	55	PSU	O4'-C1'	-2.88	1.39	1.43
35	T	55	PSU	O4-C4	-2.75	1.18	1.23
35	T	8	4SU	C5-C4	-2.68	1.39	1.42
35	T	55	PSU	C6-C5	2.55	1.38	1.35
35	T	8	4SU	C6-N1	-2.38	1.32	1.38
35	T	55	PSU	O2-C2	-2.29	1.18	1.23
35	T	8	4SU	C6-C5	2.19	1.40	1.35
35	T	55	PSU	C6-N1	-2.09	1.32	1.36

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	T	20	H2U	O2-C2-N1	-10.07	111.00	123.10
35	T	8	4SU	C4-N3-C2	-7.16	120.45	127.31
35	T	20	H2U	O4-C4-N3	-7.07	109.41	120.30
35	T	55	PSU	N1-C2-N3	7.04	122.59	115.17
35	T	20	H2U	O4-C4-C5	-6.38	109.14	122.20
35	T	20	H2U	O2-C2-N3	-6.33	109.81	121.49
35	T	8	4SU	N3-C2-N1	5.27	121.75	114.89
35	T	20	H2U	N3-C2-N1	-5.16	111.47	116.65
35	T	8	4SU	C5-C4-N3	5.04	119.43	114.75
35	T	54	5MU	N3-C2-N1	4.99	121.39	114.89
35	T	55	PSU	C4-N3-C2	-4.72	119.87	126.37
35	T	54	5MU	C4-N3-C2	-4.65	121.25	127.34
35	T	54	5MU	O4-C4-C5	-4.31	119.99	124.92
35	T	54	5MU	C5-C4-N3	4.28	119.04	115.32
35	T	55	PSU	O2-C2-N1	-4.10	118.56	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	T	54	5MU	C5-C6-N1	-3.85	119.13	123.31
35	T	20	H2U	C5-C4-N3	-3.72	112.73	116.69
35	T	54	5MU	C1'-N1-C2	3.39	123.68	117.59
35	T	8	4SU	C5-C4-S4	-3.37	120.46	124.31
35	T	54	5MU	C1'-N1-C6	-3.27	115.76	121.15
35	T	8	4SU	O2-C2-N1	-2.86	119.07	122.80
35	T	55	PSU	C6-N1-C2	-2.57	120.31	122.69
35	T	32	4OC	C5-C4-N3	-2.55	118.61	122.60
35	T	32	4OC	O2-C2-N3	-2.40	118.55	122.33
35	T	54	5MU	O2-C2-N3	-2.32	117.21	121.49
35	T	32	4OC	N1-C2-N3	2.21	122.63	118.80
35	T	8	4SU	C5-C6-N1	-2.08	118.47	121.84

All (7) 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	55	PSU	C4'
35	T	8	4SU	C2'
35	T	8	4SU	C1'

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	T	20	H2U	O4'-C4'-C5'-O5'
35	T	20	H2U	C3'-C4'-C5'-O5'
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	54	5MU	C3'-C4'-C5'-O5'
35	T	54	5MU	O4'-C4'-C5'-O5'
35	T	20	H2U	C2'-C1'-N1-C6
35	T	54	5MU	C2'-C1'-N1-C2

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	32	4OC	1	0
35	T	55	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 246 ligands modelled in this entry, 243 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	602	60	28,33,33	0.65	0	34,52,52	0.60	1 (2%)
58	FME	T	101	35	8,9,10	0.95	0	8,9,11	0.97	0
59	ATP	Y	601	60	28,33,33	0.71	0	34,52,52	0.62	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	ATP	Y	602	60	-	3/18/38/38	0/3/3/3
58	FME	T	101	35	-	5/7/9/11	-
59	ATP	Y	601	60	-	5/18/38/38	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	Y	602	ATP	C5-C6-N6	2.31	123.84	120.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	Y	601	ATP	C5-C6-N6	2.30	123.81	120.31

There are no chirality outliers.

All (13) torsion outliers are listed below:

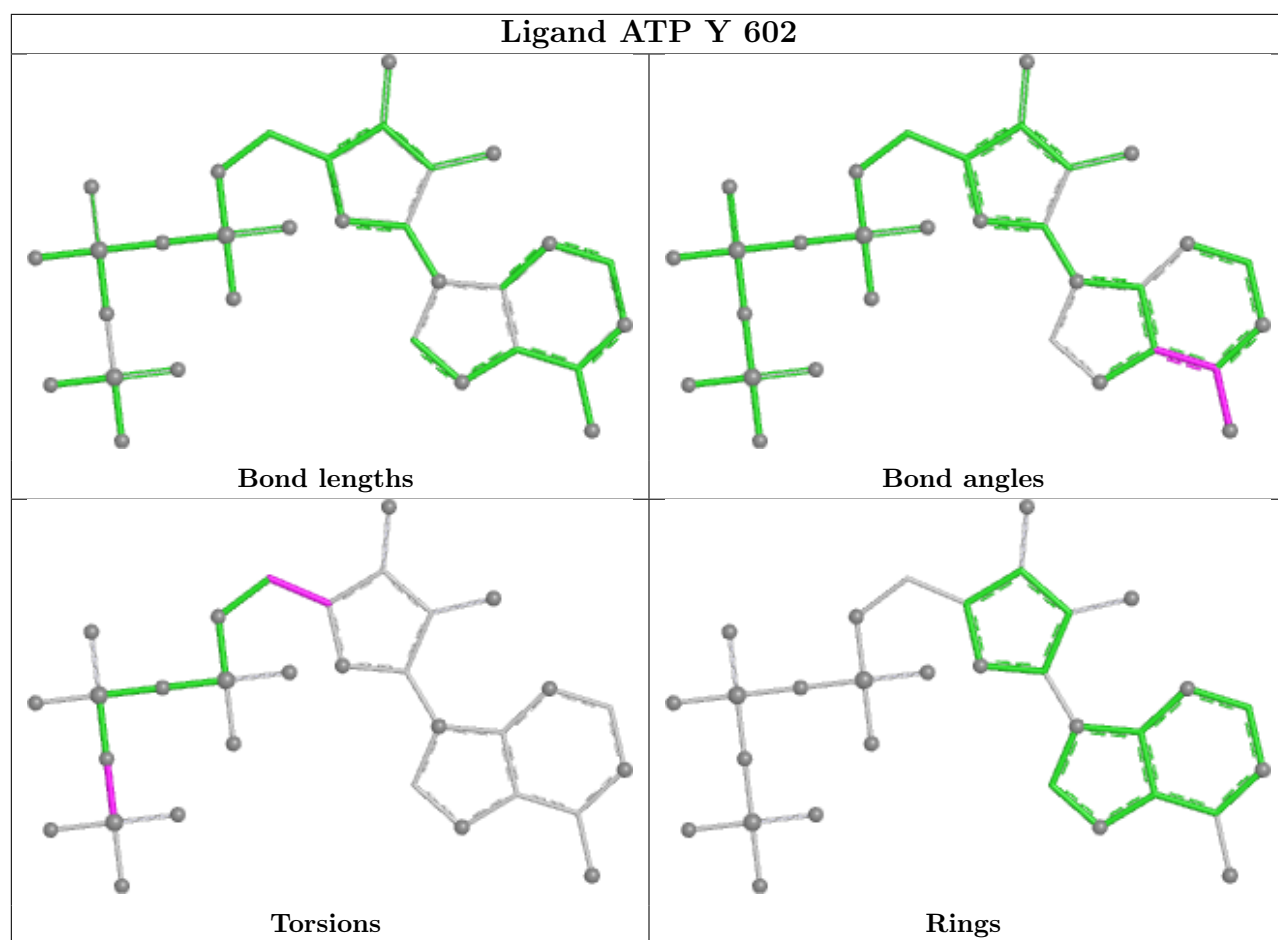
Mol	Chain	Res	Type	Atoms
58	T	101	FME	O1-CN-N-CA
58	T	101	FME	O-C-CA-CB
59	Y	601	ATP	C5'-O5'-PA-O1A
59	Y	601	ATP	C5'-O5'-PA-O2A
59	Y	601	ATP	C5'-O5'-PA-O3A
59	Y	602	ATP	PB-O3B-PG-O2G
58	T	101	FME	CA-CB-CG-SD
59	Y	601	ATP	O4'-C4'-C5'-O5'
59	Y	601	ATP	C3'-C4'-C5'-O5'
59	Y	602	ATP	PB-O3B-PG-O1G
58	T	101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

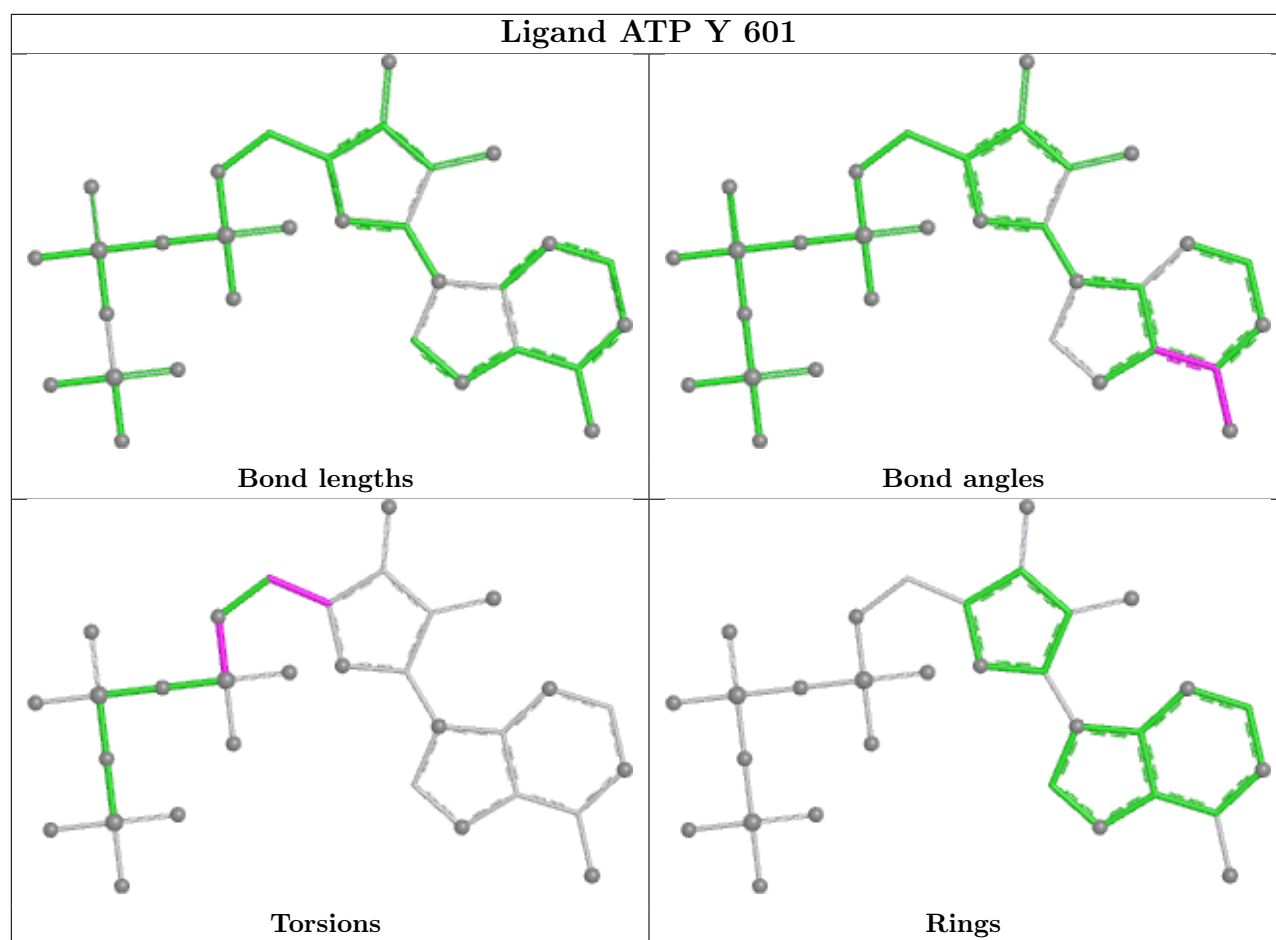
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	Y	602	ATP	1	0
58	T	101	FME	1	0
59	Y	601	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

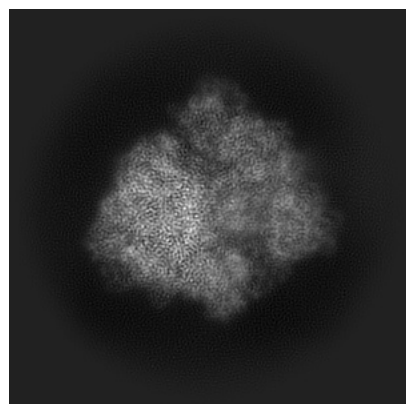
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29408. These allow visual inspection of the internal detail of the map and identification of artifacts.

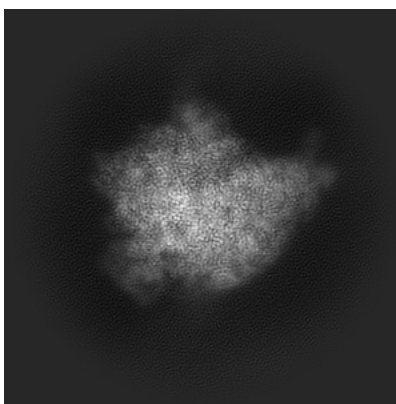
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

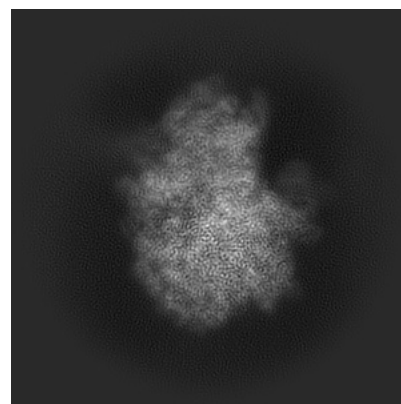
6.1.1 Primary map



X

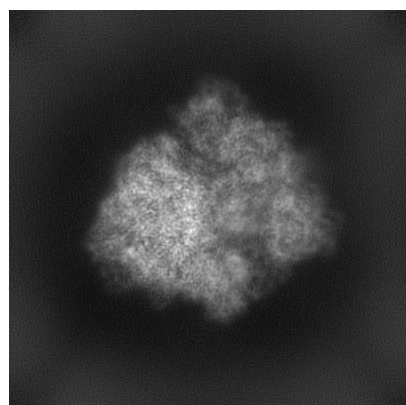


Y

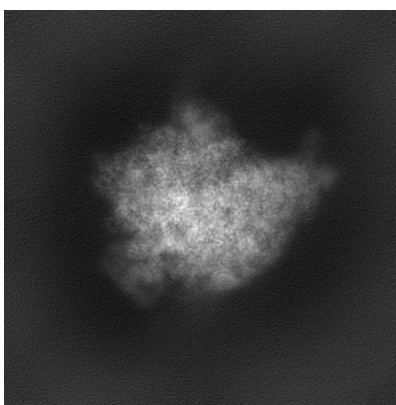


Z

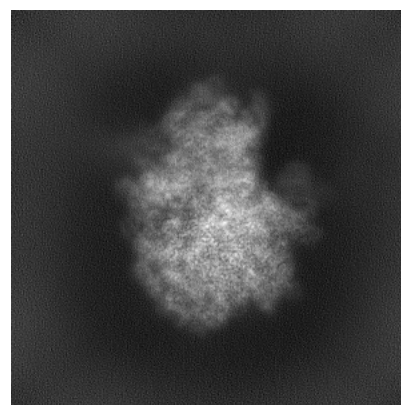
6.1.2 Raw map



X



Y

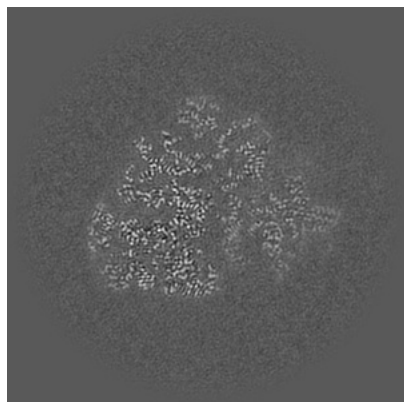


Z

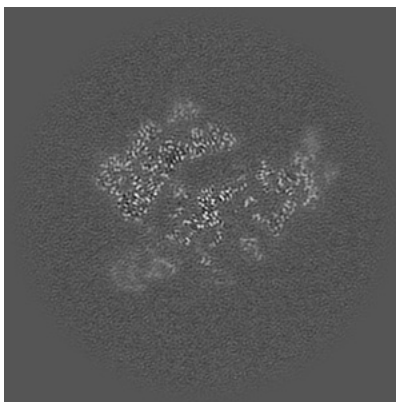
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

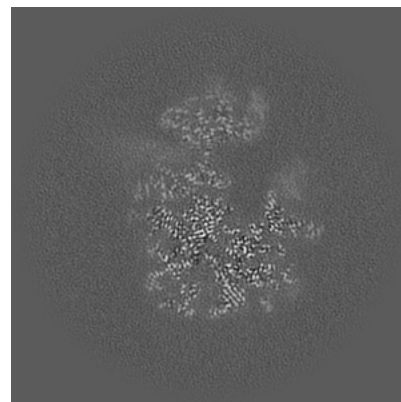
6.2.1 Primary map



X Index: 200

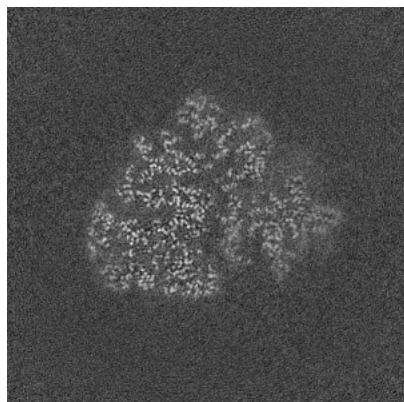


Y Index: 200

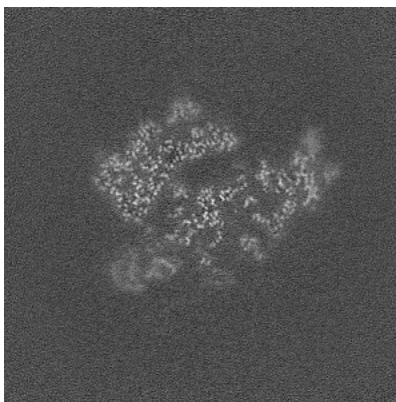


Z Index: 200

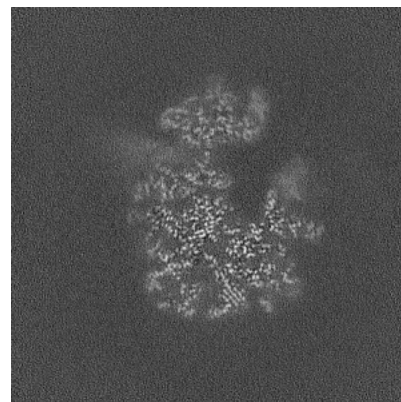
6.2.2 Raw map



X Index: 200



Y Index: 200

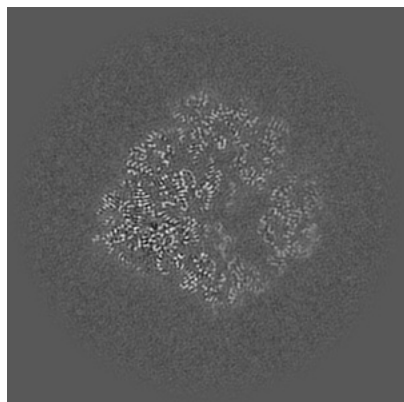


Z Index: 200

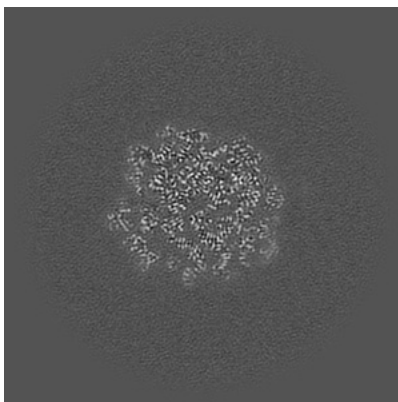
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

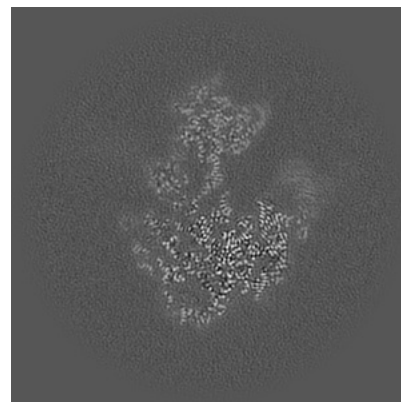
6.3.1 Primary map



X Index: 215

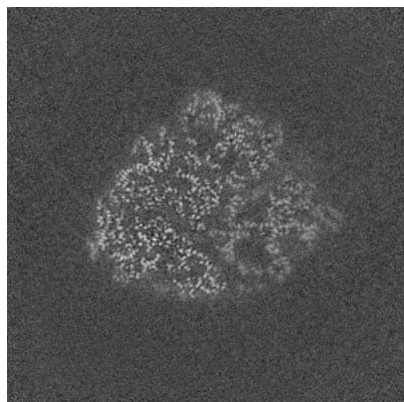


Y Index: 156

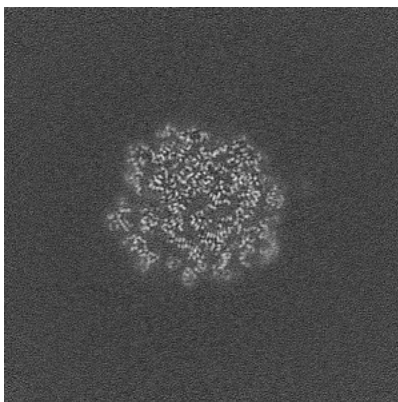


Z Index: 181

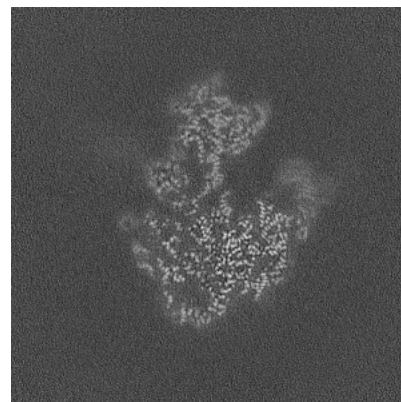
6.3.2 Raw map



X Index: 207



Y Index: 156

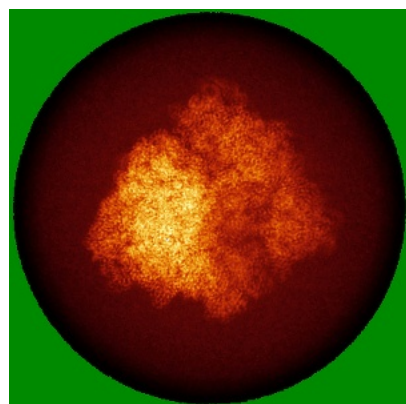


Z Index: 181

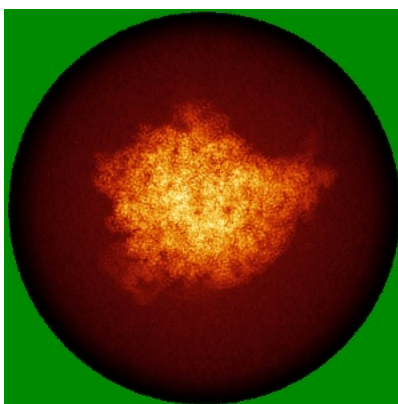
The images above show the largest variance slices of the map in three orthogonal directions.

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

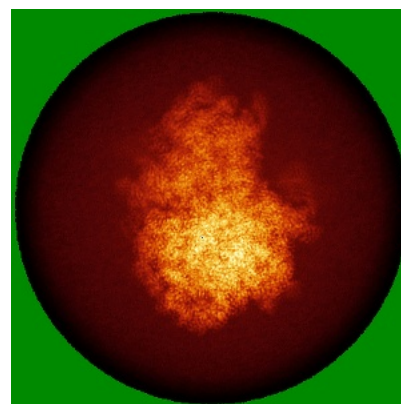
6.4.1 Primary map



X

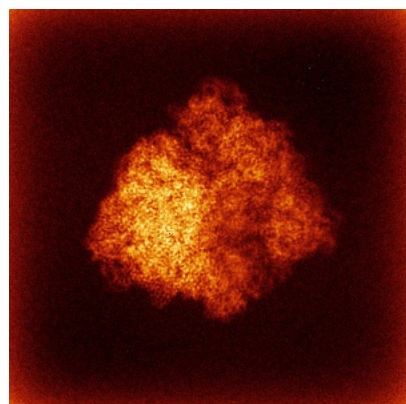


Y

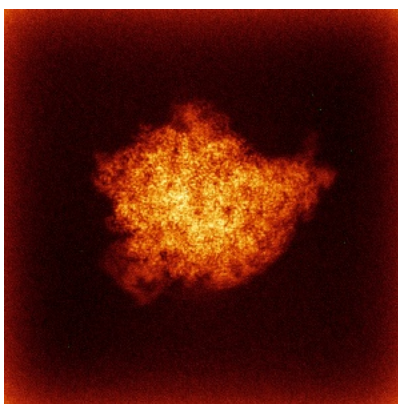


Z

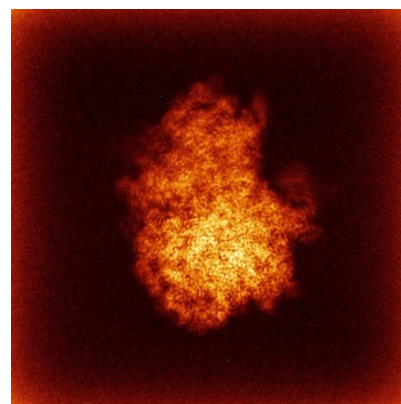
6.4.2 Raw map



X



Y

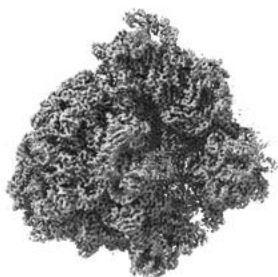


Z

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](#)

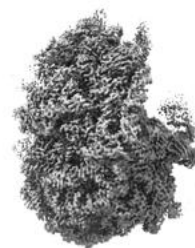
6.5.1 Primary map



X



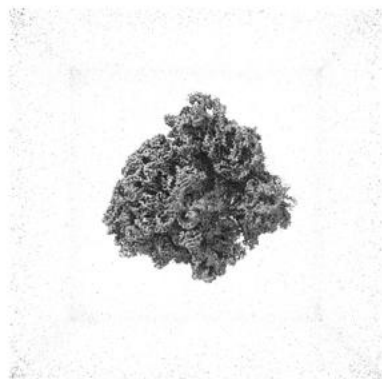
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.9. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

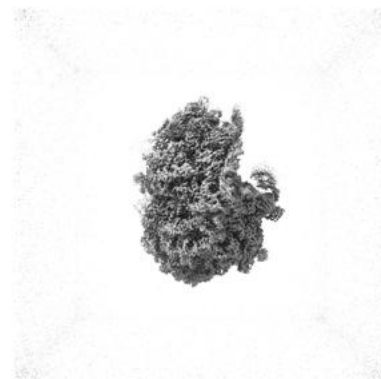
6.5.2 Raw map



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.

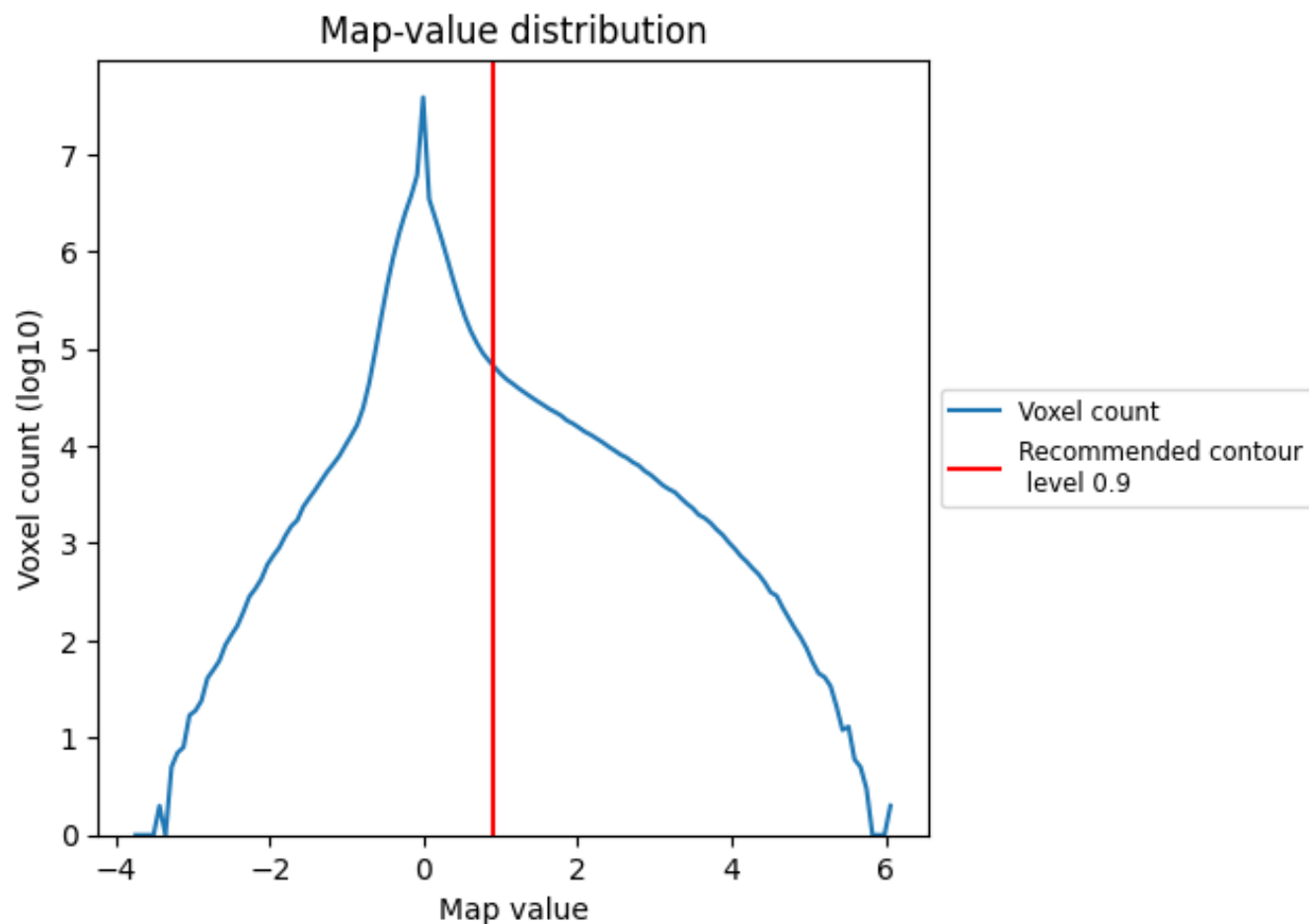
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

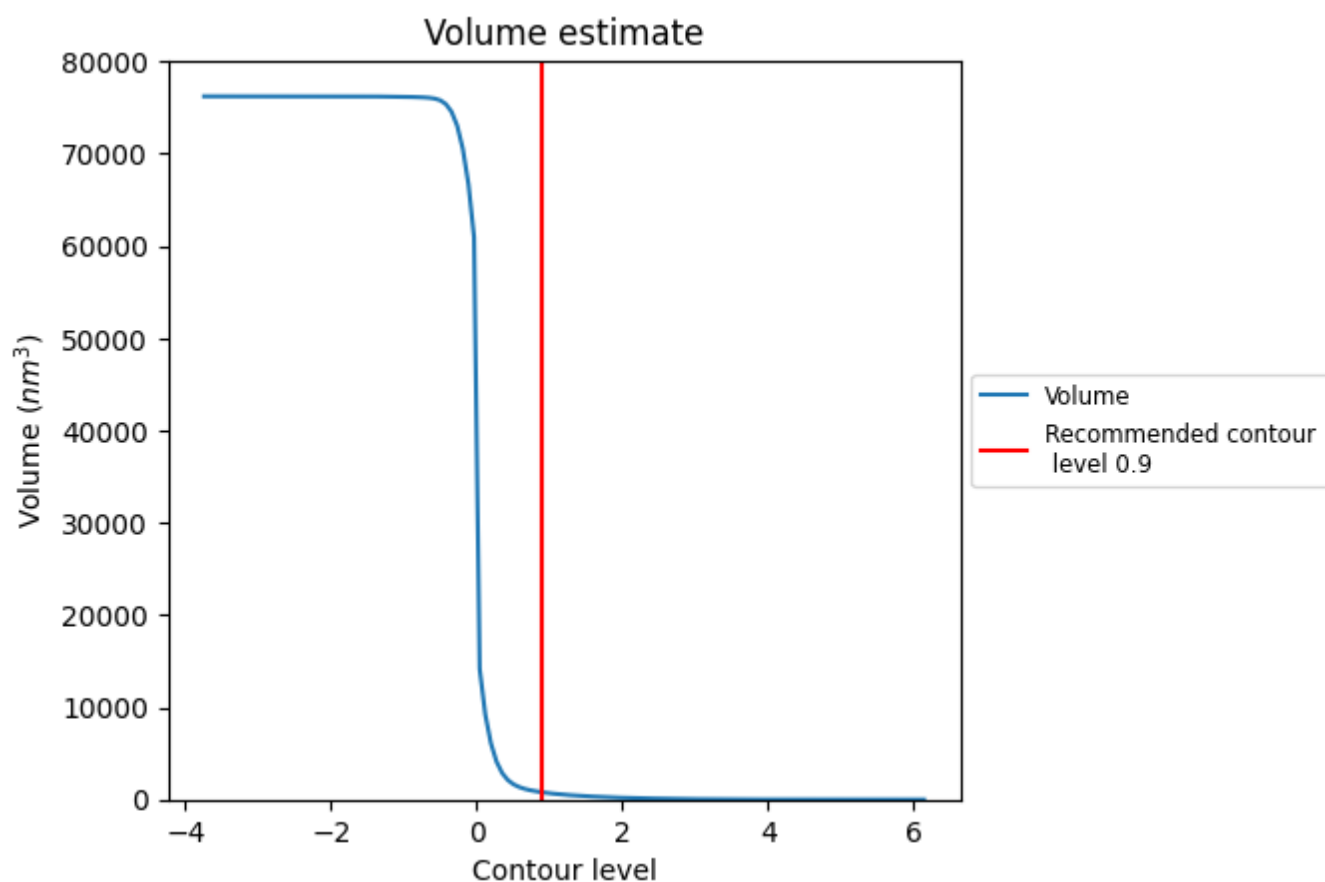
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

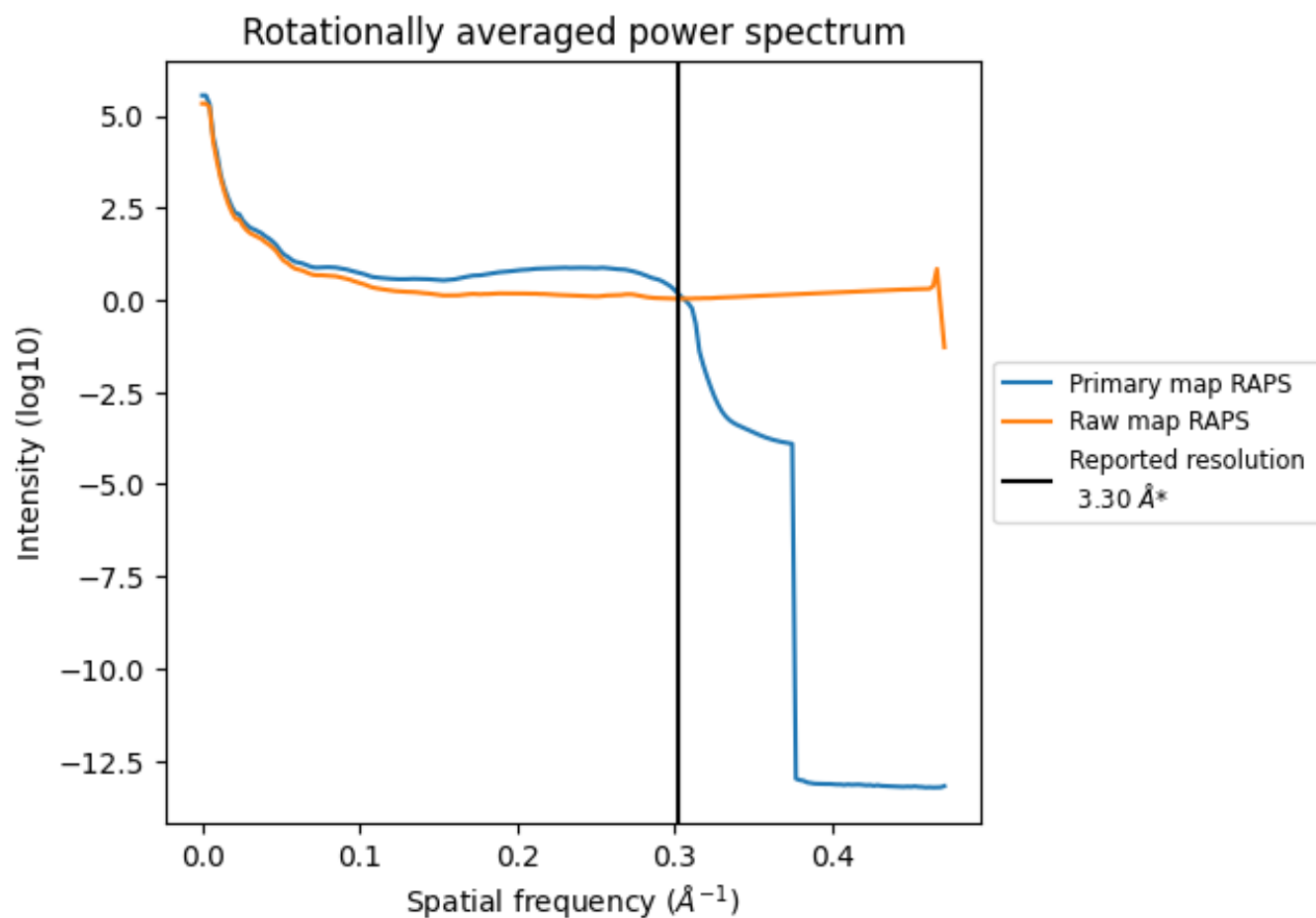
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 784 nm³; this corresponds to an approximate mass of 708 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

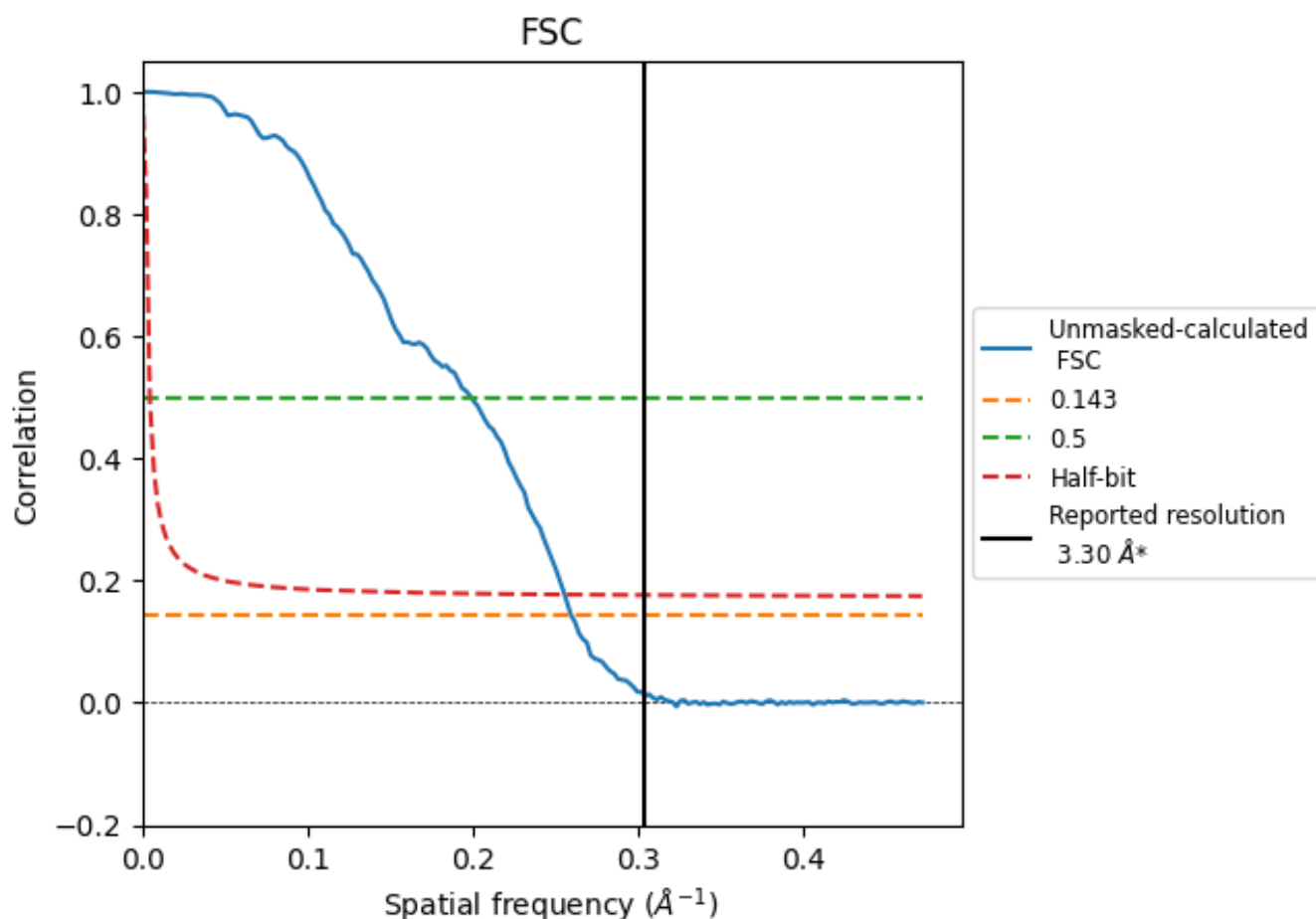


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 \AA^{-1}

8.2 Resolution estimates [i](#)

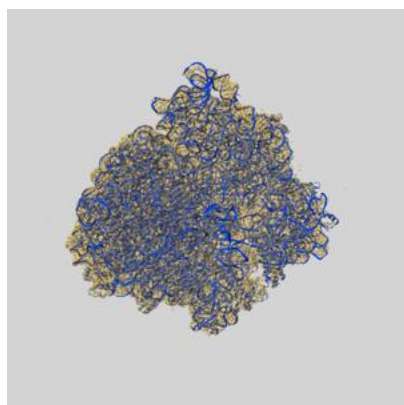
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.86	5.03	3.92

*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 3.86 differs from the reported value 3.3 by more than 10 %

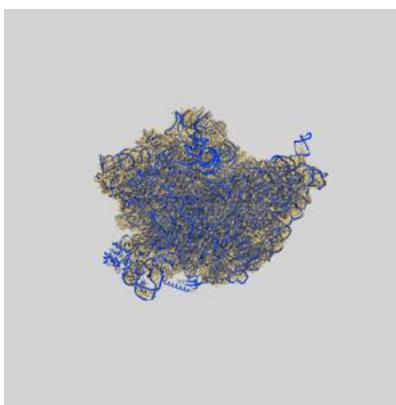
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-29408 and PDB model 9NLQ. Per-residue inclusion information can be found in section 3 on page 17.

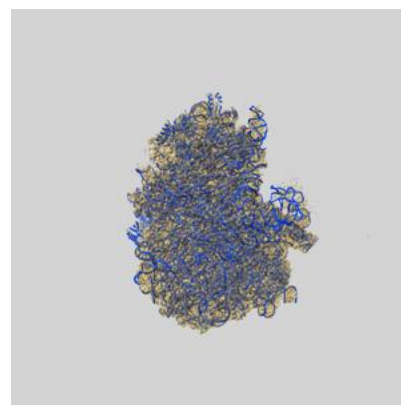
9.1 Map-model overlay [i](#)



X



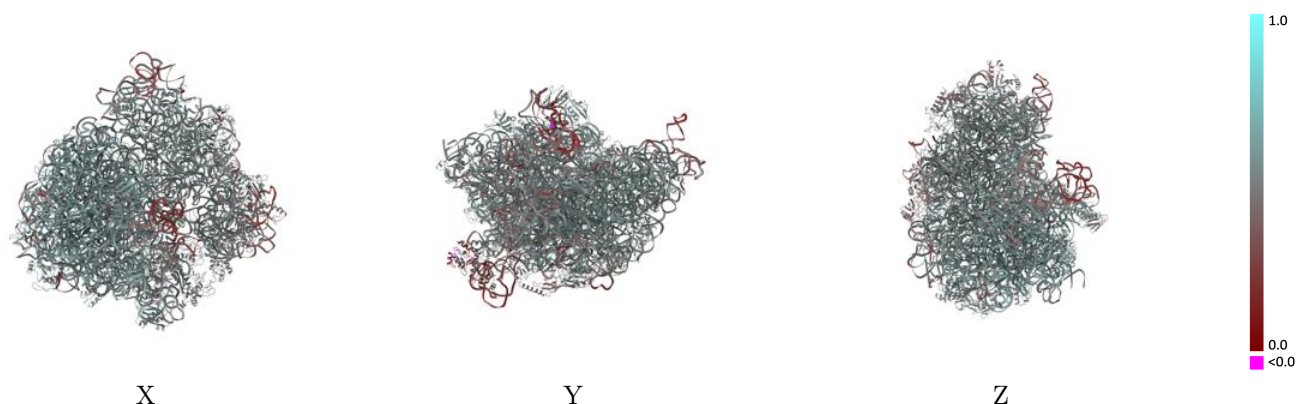
Y



Z

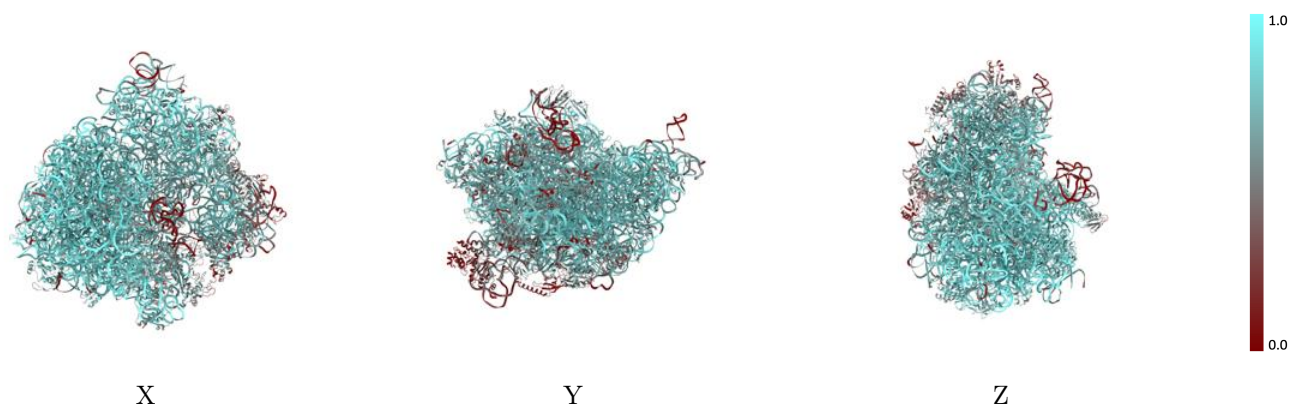
The images above show the 3D surface view of the map at the recommended contour level 0.9 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



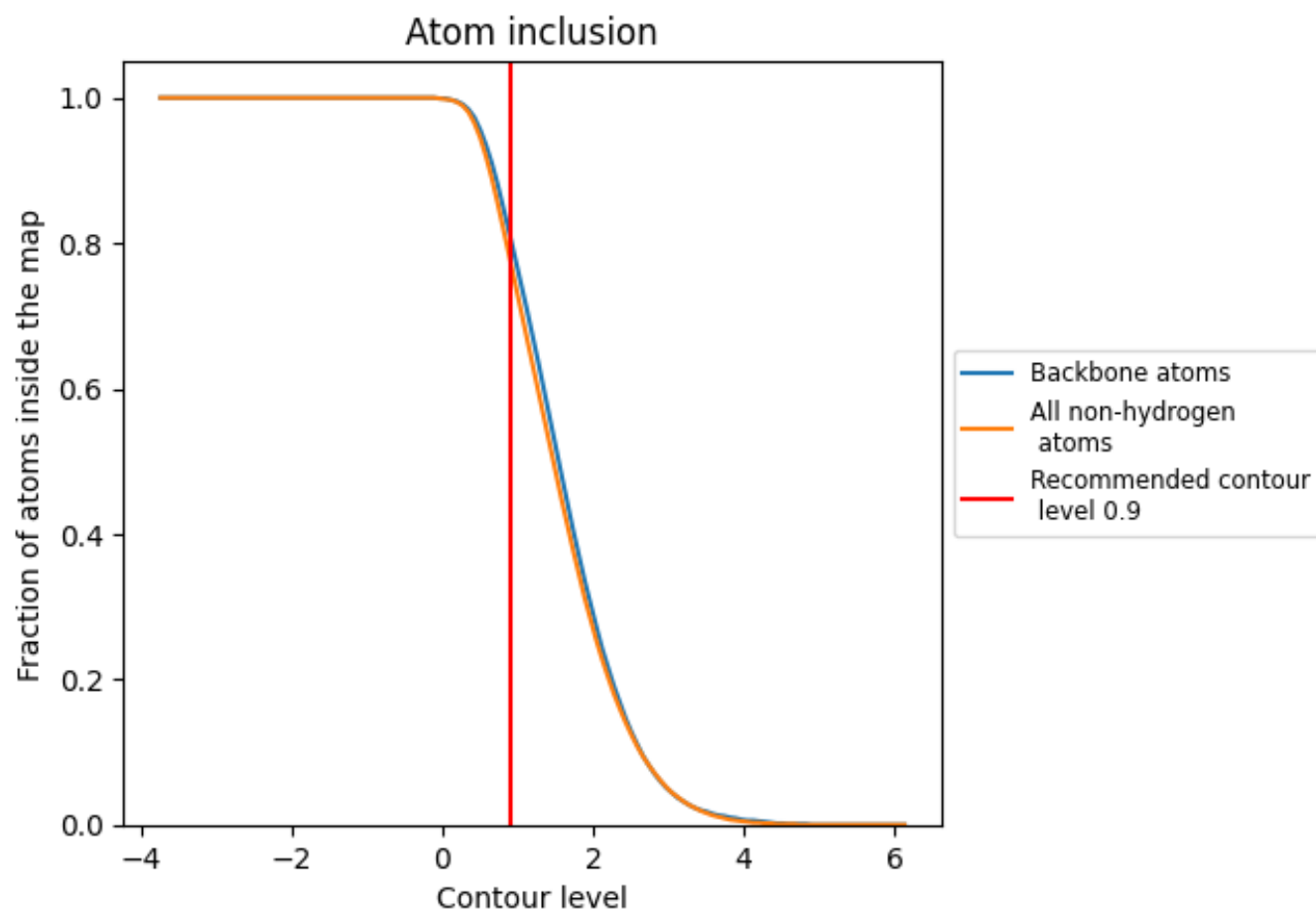
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.9).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 78% 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 (0.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7770	 0.5210
1	 0.0900	 0.3160
13	 0.8550	 0.5820
14	 0.8180	 0.5790
15	 0.8180	 0.5730
16	 0.8220	 0.5780
17	 0.8610	 0.5760
18	 0.7390	 0.5520
19	 0.8100	 0.5800
2	 0.8460	 0.5810
20	 0.8810	 0.5860
21	 0.7930	 0.5690
22	 0.8400	 0.5780
23	 0.7880	 0.5590
24	 0.7170	 0.5400
25	 0.7150	 0.5480
27	 0.8320	 0.5780
28	 0.8170	 0.5810
29	 0.7040	 0.5420
3	 0.8380	 0.5760
30	 0.8100	 0.5730
31	 0.3070	 0.3970
32	 0.8370	 0.5760
33	 0.7530	 0.5610
34	 0.8730	 0.5920
35	 0.8900	 0.6000
36	 0.8220	 0.5870
4	 0.7690	 0.5590
5	 0.5950	 0.5040
6	 0.6150	 0.5160
9	 0.2350	 0.4180
M	 0.5460	 0.4790
R1	 0.8570	 0.5320
R2	 0.8410	 0.5160
R3	 0.8000	 0.4980



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Chain	Atom inclusion	Q-score
T	 0.7290	 0.4890
Y	 0.5700	 0.4930
sb	 0.4820	 0.4610
sc	 0.5920	 0.5240
sd	 0.6240	 0.5160
se	 0.7240	 0.5430
sf	 0.4890	 0.4660
sg	 0.4530	 0.4650
sh	 0.7150	 0.5420
si	 0.5910	 0.4990
sj	 0.4350	 0.4330
sk	 0.5910	 0.5100
sl	 0.7080	 0.5380
sm	 0.5660	 0.5070
sn	 0.6060	 0.4940
so	 0.6430	 0.5380
sp	 0.7290	 0.5430
sq	 0.6600	 0.5300
sr	 0.6210	 0.5130
ss	 0.5220	 0.4800
st	 0.7280	 0.5420
su	 0.3870	 0.4010