Full wwPDB EM Validation Report ⓘ

Jun 24, 2025 – 08:11 pm BST

PDB ID	:	9QEG / pdb_00009qeg
EMDB ID	:	EMD-53066
Title	:	Cryo-EM structure of the 70S ribosome of a MLSb sensitive S. aureus strain "KES34" in complex with solithromycin
Authors	:	Rivalta, A.; Yonath, A.
Deposited on	:	2025-03-10
Resolution	:	2.21 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:

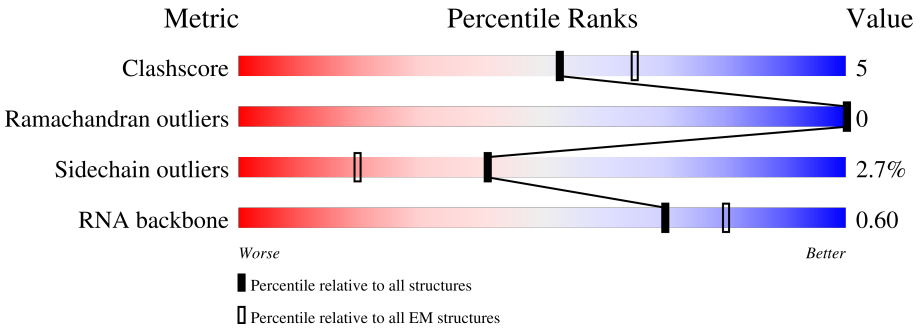
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

1 Overall quality at a glance

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

The reported resolution of this entry is 2.21 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	1	52	83% 10% 8%
2	2	45	84% 13%
3	3	66	91% 8%
4	4	37	84% 16%
5	B	115	57% 36% 6%
6	C	277	92% 7%
7	D	220	89% 9%

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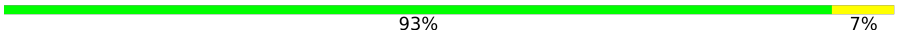
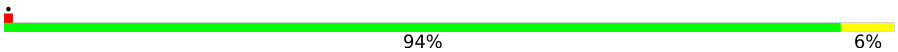
Mol	Chain	Length	Quality of chain
8	E	207	
9	G	178	
10	H	145	
11	I	122	
12	J	146	
13	K	144	
14	L	122	
15	M	119	
16	N	116	
17	O	118	
18	P	102	
19	Q	117	
20	R	91	
21	S	105	
22	T	217	
23	U	94	
24	V	62	
25	W	73	
26	X	59	
27	Z	57	
28	F	179	
29	11	15	
30	A	2923	
31	Ae	166	
32	Af	98	

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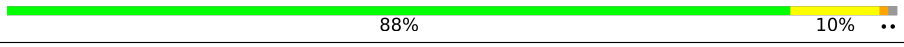
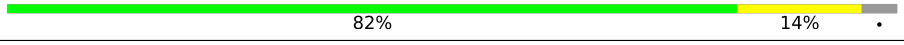
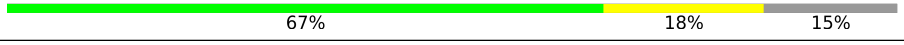
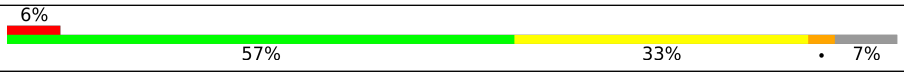
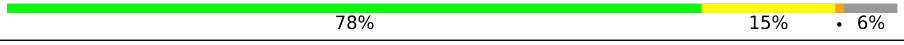
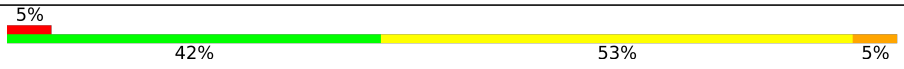
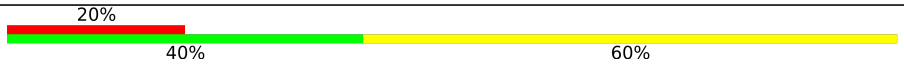
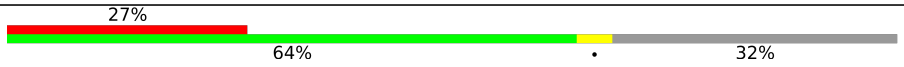
Mol	Chain	Length	Quality of chain
33	Ag	156	
34	Ai	132	
35	Al	137	
36	Ao	89	
37	Ap	91	
38	Aq	87	
39	Ar	80	
40	At	83	
41	Aa	1552	
42	Aj	102	
43	Ac	217	
44	Am	121	
45	Ak	129	
46	Ab	255	
47	Ah	132	
48	Ad	200	
49	An	61	
50	As	92	
51	d	19	
52	8	71	
53	9	5	
54	13	84	

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 130300 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 bL33A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	48	355	218	70	64	3	0	0

- Molecule 2 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	2	44	368	225	89	53	1	0	0

- Molecule 3 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	3	65	508	315	108	83	2	0	0

- Molecule 4 is a protein called Large ribosomal subunit protein bL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	4	37	280	175	57	43	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	B	113	2408	1076	430	789	113	0	0

- Molecule 6 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	C	274	2037	1271	406	355	5	0	0

- Molecule 7 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	215	Total	C	N	O	S	0	0
			1582	994	296	287	5		

- Molecule 8 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	206	Total	C	N	O	S	0	0
			1510	955	282	271	2		

- Molecule 9 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	160	Total	C	N	O	S	0	0
			944	572	191	180	1		

- Molecule 10 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	145	Total	C	N	O	S	0	0
			1140	712	208	217	3		

- Molecule 11 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	122	Total	C	N	O	S	0	0
			865	543	163	156	3		

- Molecule 12 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	146	Total	C	N	O	S	0	0
			1057	659	213	184	1		

- Molecule 13 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	137	Total	C	N	O	S	0	0
			1024	660	193	168	3		

- Molecule 14 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	118	Total	C	N	O	S	0	0
			901	559	179	162	1		

- Molecule 15 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	M	119	Total	C	N	O	0	0
			801	497	162	142		

- Molecule 16 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	N	111	Total	C	N	O	0	0
			800	504	159	137		

- Molecule 17 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	116	Total	C	N	O	S	0	0
			943	593	189	157	4		

- Molecule 18 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	P	102	Total	C	N	O	S	0	0
			752	480	138	133	1		

- Molecule 19 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Q	111	Total	C	N	O	S	0	0
			814	511	158	143	2		

- Molecule 20 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	R	89	Total	C	N	O	S	0	0
			664	422	118	120	4		

- Molecule 21 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	93	Total	C	N	O	S	0	0
			635	403	121	110	1		

- Molecule 22 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	T	90	Total	C	N	O	0	0
			600	385	109	106		

- Molecule 23 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	U	79	Total	C	N	O	0	0
			575	356	115	104		

- Molecule 24 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	V	50	Total	C	N	O	0	0
			360	223	76	61		

- Molecule 25 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	W	64	Total	C	N	O	0	0
			473	295	96	82		

- Molecule 26 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	X	58	Total	C	N	O	0	0
			438	273	84	81		

- Molecule 27 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	42	Total	C	N	O	S	0	0
			333	205	71	53	4		

- Molecule 28 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	F	149	Total	C	N	O	S	0	0
			914	580	165	166	3		

- Molecule 29 is a RNA chain called E-site tRNA molecule.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	11	15	Total	C	N	O	P	0	0
			322	143	61	103	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	A	2586	Total	C	N	O	P	2	0
			55514	24786	10184	17956	2588		

- Molecule 31 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Ae	156	Total	C	N	O	S	0	0
			1130	716	211	201	2		

- Molecule 32 is a protein called Small ribosomal subunit protein bS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Af	95	Total	C	N	O	S	0	0
			734	466	136	130	2		

- Molecule 33 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Ag	154	Total	C	N	O	S	0	0
			1222	761	234	223	4		

- Molecule 34 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Ai	127	Total	C	N	O	S	0	0
			975	606	195	173	1		

- Molecule 35 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Al	134	Total	C	N	O	S	0	0
			1011	628	204	177	2		

- Molecule 36 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Ao	88	Total	C	N	O	S	0	0
			727	449	150	127	1		

- Molecule 37 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Ap	89	Total	C	N	O	S	0	0
			679	428	125	125	1		

- Molecule 38 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	Aq	74	Total	C	N	O	0	0
			551	351	106	94		

- Molecule 39 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Ar	54	Total	C	N	O	S	0	0
			445	284	86	73	2		

- Molecule 40 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	At	81	Total	C	N	O	S	0	0
			593	363	118	110	2		

- Molecule 41 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Aa	1440	Total	C	N	O	P	0	0
			30880	13790	5653	9997	1440		

- Molecule 42 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	Aj	96	Total 720	C 452	N 133	O 135	0	0

- Molecule 43 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Ac	202	Total 1477	C 935	N 275	O 266	S 1	0	0

- Molecule 44 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Am	114	Total 845	C 526	N 168	O 150	S 1	0	0

- Molecule 45 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Ak	112	Total 759	C 467	N 146	O 144	S 2	0	0

- Molecule 46 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	Ab	104	Total 629	C 397	N 117	O 115	0	0

- Molecule 47 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Ah	131	Total 1032	C 652	N 183	O 193	S 4	0	0

- Molecule 48 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Ad	199	Total 1502	C 954	N 283	O 263	S 2	0	0

- Molecule 49 is a protein called Small ribosomal subunit protein uS14B.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	An	60	Total	C	N	O	S	0	0
			502	317	100	80	5		

- Molecule 50 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	As	82	Total	C	N	O	S	0	0
			617	399	114	102	2		

- Molecule 51 is a RNA chain called mRNA molecule.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	d	19	Total	C	N	O	P	0	0
			412	184	79	130	19		

- Molecule 52 is a RNA chain called P-site tRNA molecule.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	8	71	Total	C	N	O	P	0	0
			1519	677	279	492	71		

- Molecule 53 is a RNA chain called A-site tRNA molecule.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	9	5	Total	C	N	O	P	0	0
			106	48	20	33	5		

- Molecule 54 is a protein called Large ribosomal subunit protein bL31B.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	13	57	Total	C	N	O	0	0
			382	245	74	63		

- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
55	1	1	Total	Zn	0
			1	1	
55	4	1	Total	Zn	0
			1	1	
55	Z	1	Total	Zn	0
			1	1	

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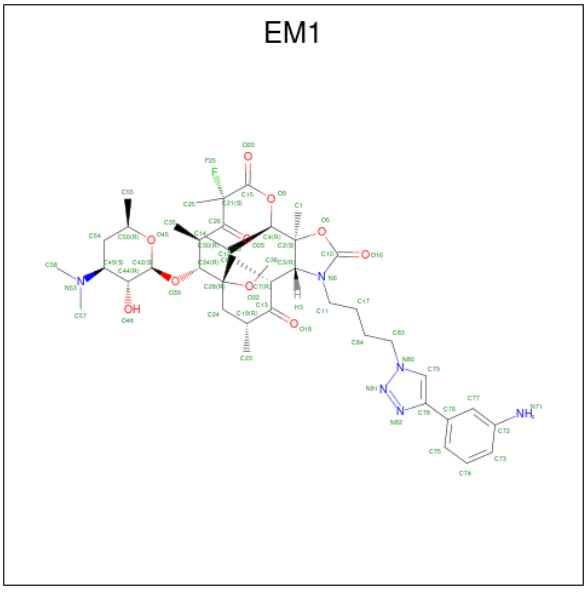
Mol	Chain	Residues	Atoms		AltConf
55	An	1	Total 1	Zn 1	0

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
56	C	1	Total 1	Mg 1	0
56	D	1	Total 1	Mg 1	0
56	A	170	Total 170	Mg 170	0
56	Aa	59	Total 59	Mg 59	0

- Molecule 57 is (3aS,4R,7S,9R,10R,11R,13R,15R,15aR)-1-{4-[4-(3-aminophenyl)-1H-1,2,3-triazol-1-yl]butyl}-4-ethyl-7-fluoro-11-methoxy-3a ,7,9,11,13,15-hexamethyl-2,6,8,14-tetraoxotetradecahydro-2H-oxacyclotetradecino[4,3-d][1,3]oxazol-10-yl 3,4,6-trideoxy-3-(dimethylamino)-beta-D-xylo-hexopyranoside (CCD ID: EM1) (formula: $C_{43}H_{65}FN_6O_{10}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
57	A	1	Total 60	C 43	F 1	N 6	O 10	0

- Molecule 58 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
58	A	15	Total K 15 15	0
58	Aa	3	Total K 3 3	0

- Molecule 59 is water.

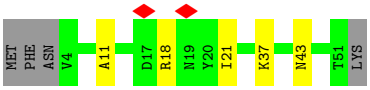
Mol	Chain	Residues	Atoms	AltConf
59	C	16	Total O 16 16	0
59	D	2	Total O 2 2	0
59	J	7	Total O 7 7	0
59	N	3	Total O 3 3	0
59	O	2	Total O 2 2	0
59	P	1	Total O 1 1	0
59	R	1	Total O 1 1	0
59	A	574	Total O 574 574	0
59	Aa	15	Total O 15 15	0

3 Residue-property plots (i)

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

• Molecule 1: Large ribosomal subunit protein bL33A

Chain 1:



• Molecule 2: Large ribosomal subunit protein bL34

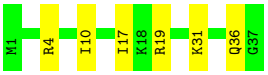
Chain 2:

• Molecule 3: Large ribosomal subunit protein bL35

Chain 3:

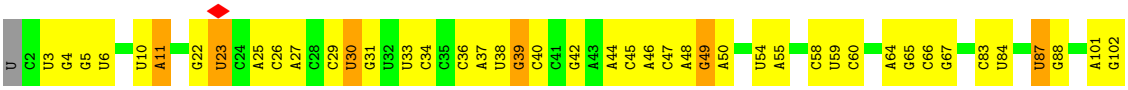
• Molecule 4: Large ribosomal subunit protein bL36

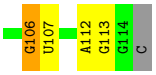
Chain 4:



• Molecule 5: 5S ribosomal RNA

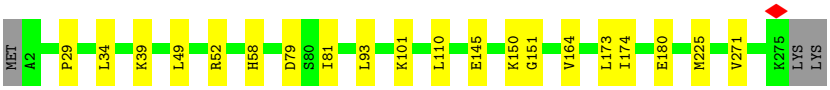
Chain B:





• Molecule 6: Large ribosomal subunit protein uL2

Chain C:



• Molecule 7: Large ribosomal subunit protein uL3

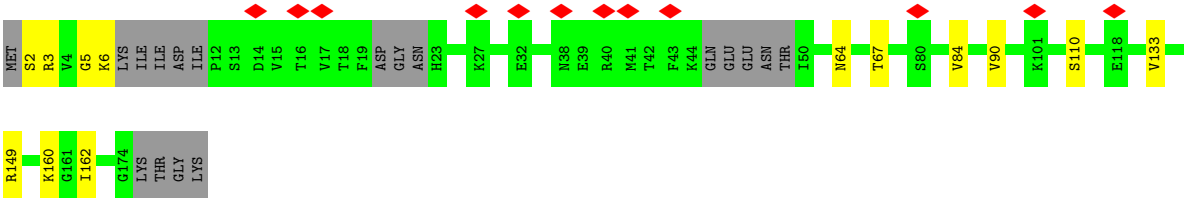
Chain D:

• Molecule 8: Large ribosomal subunit protein uL4

Chain E:

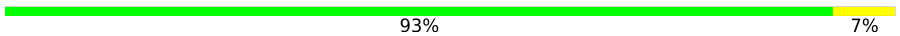
• Molecule 9: Large ribosomal subunit protein uL6

Chain G:



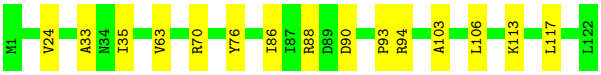
• Molecule 10: Large ribosomal subunit protein uL13

Chain H:



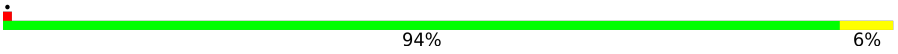
• Molecule 11: Large ribosomal subunit protein uL14

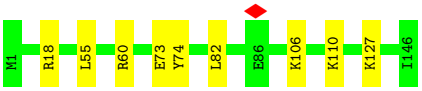
Chain I:



• Molecule 12: Large ribosomal subunit protein uL15

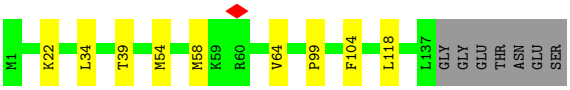
Chain J:





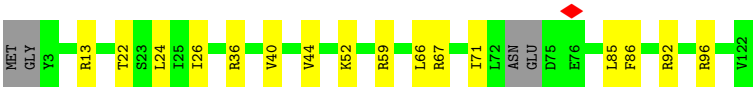
• Molecule 13: Large ribosomal subunit protein uL16

Chain K:



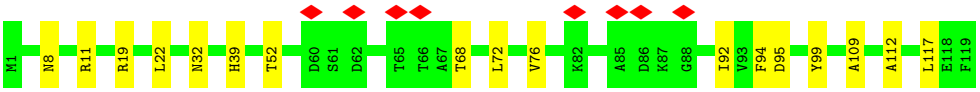
• Molecule 14: Large ribosomal subunit protein bL17

Chain L:



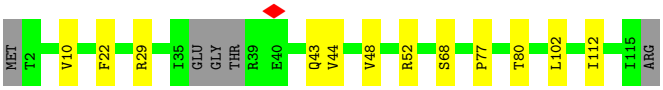
• Molecule 15: Large ribosomal subunit protein uL18

Chain M:



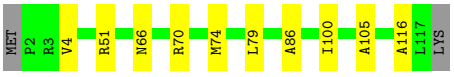
• Molecule 16: Large ribosomal subunit protein bL19

Chain N:



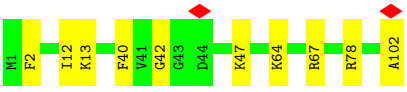
• Molecule 17: Large ribosomal subunit protein bL20

Chain O:



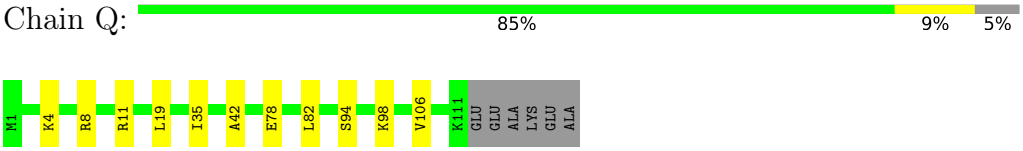
• Molecule 18: Large ribosomal subunit protein bL21

Chain P:



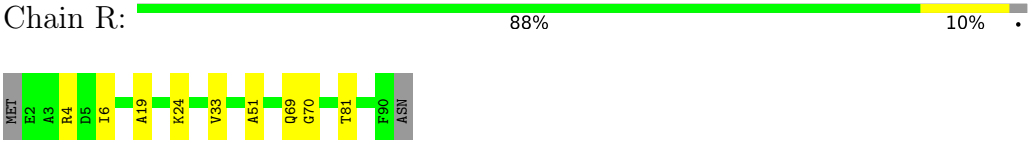
• Molecule 19: Large ribosomal subunit protein uL22

Chain Q:



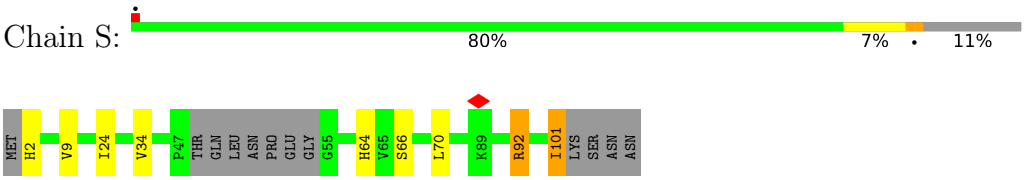
• Molecule 20: Large ribosomal subunit protein uL23

Chain R:



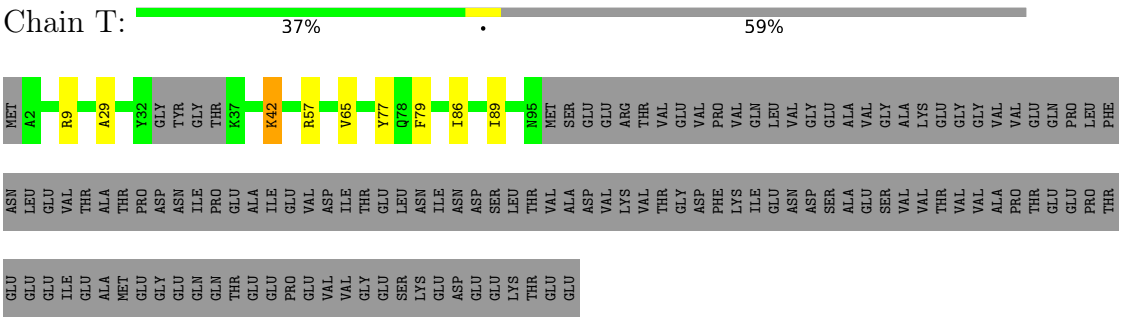
• Molecule 21: Large ribosomal subunit protein uL24

Chain S:



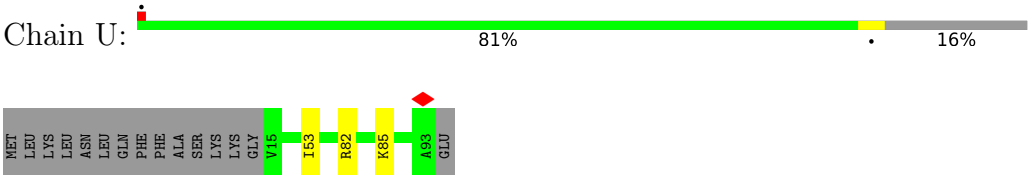
• Molecule 22: 50S ribosomal protein L25

Chain T:



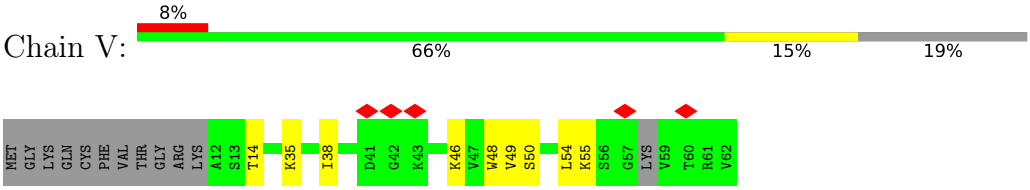
• Molecule 23: Large ribosomal subunit protein bL27

Chain U:



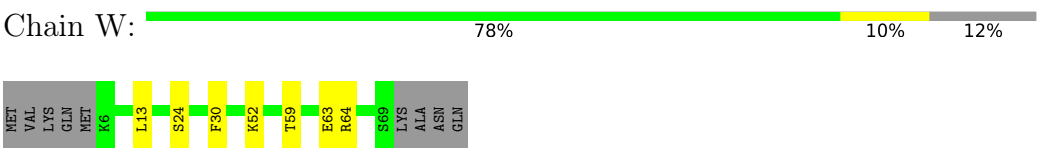
• Molecule 24: Large ribosomal subunit protein bL28

Chain V:



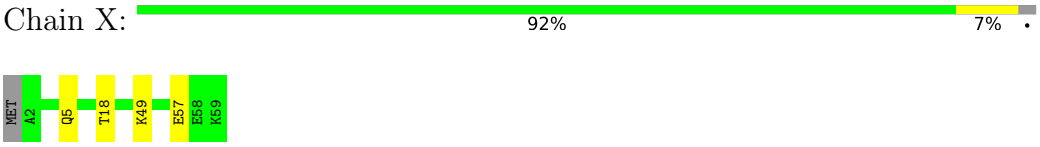
• Molecule 25: Large ribosomal subunit protein uL29

Chain W:



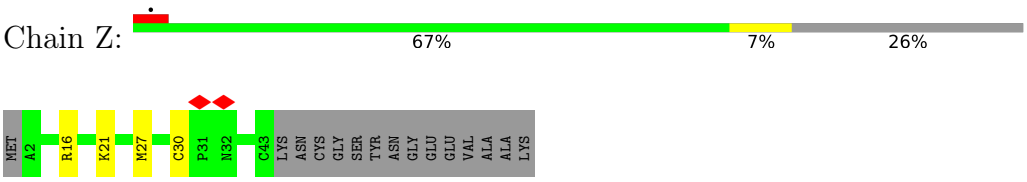
• Molecule 26: Large ribosomal subunit protein uL30

Chain X:



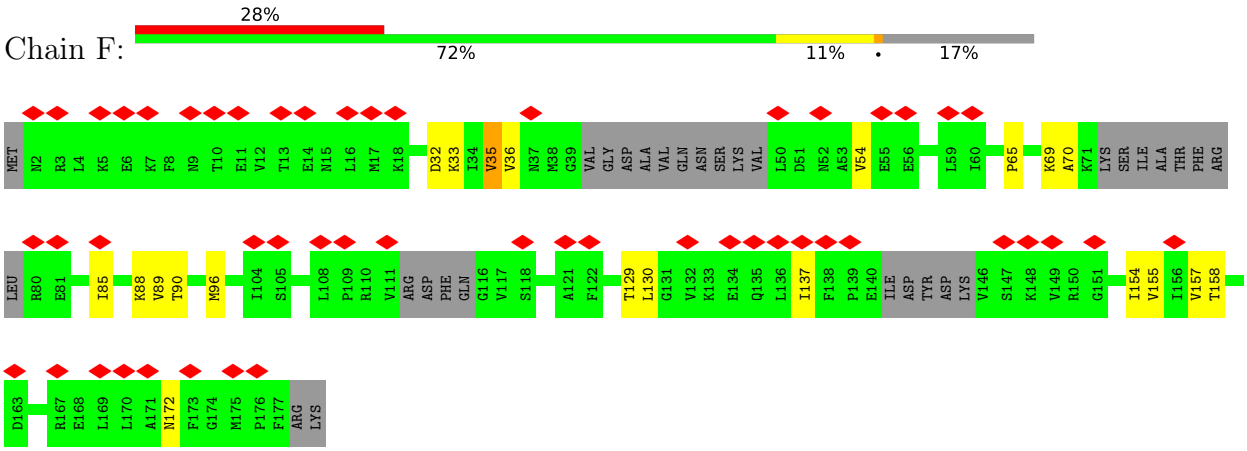
• Molecule 27: Large ribosomal subunit protein bL32

Chain Z:



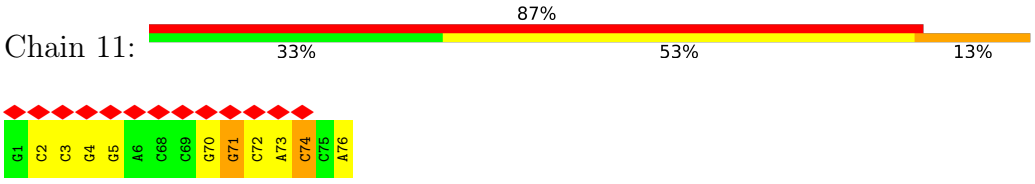
• Molecule 28: Large ribosomal subunit protein uL5

Chain F:



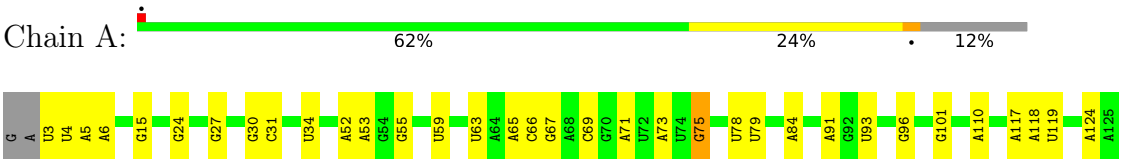
• Molecule 29: E-site tRNA molecule

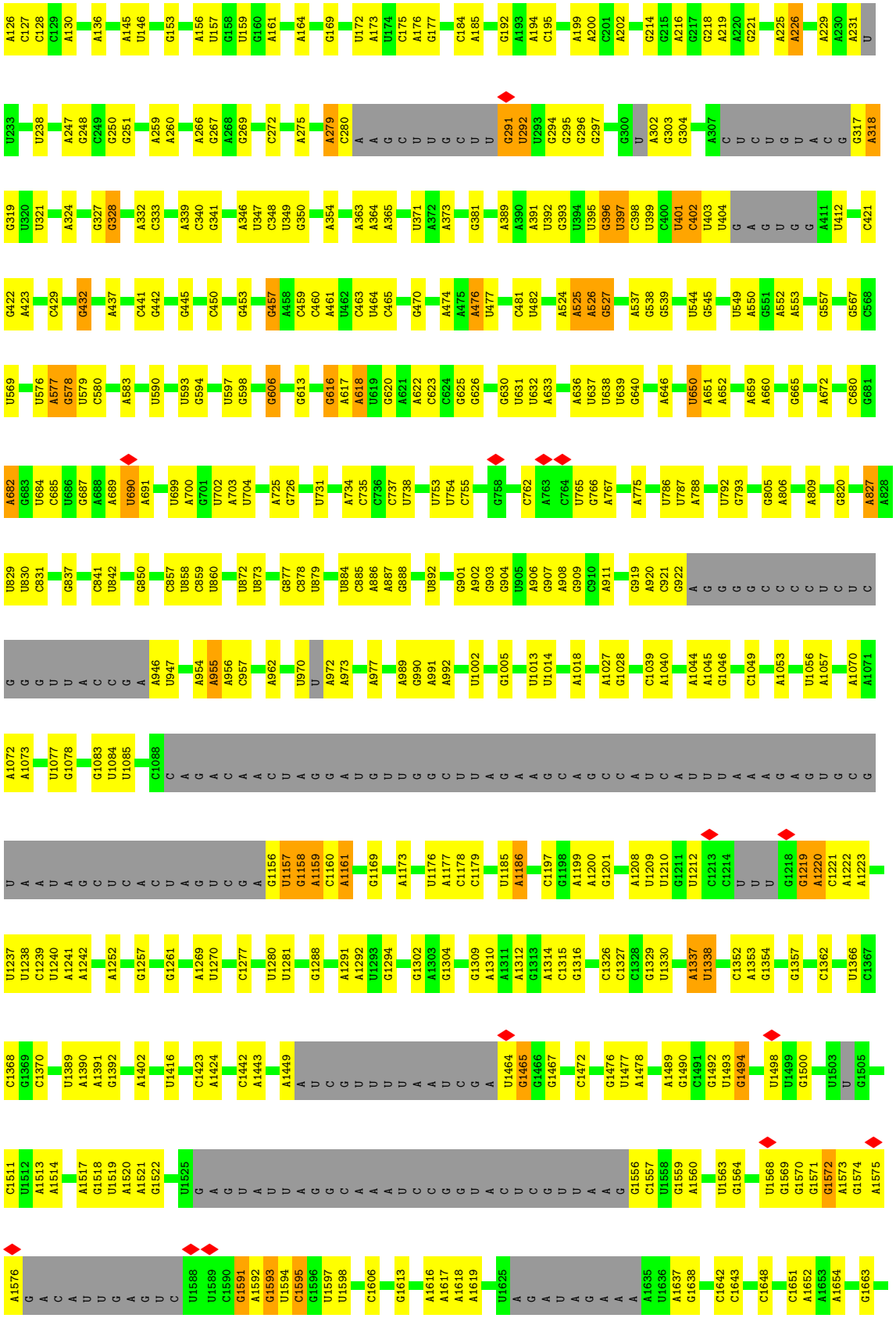
Chain 11:

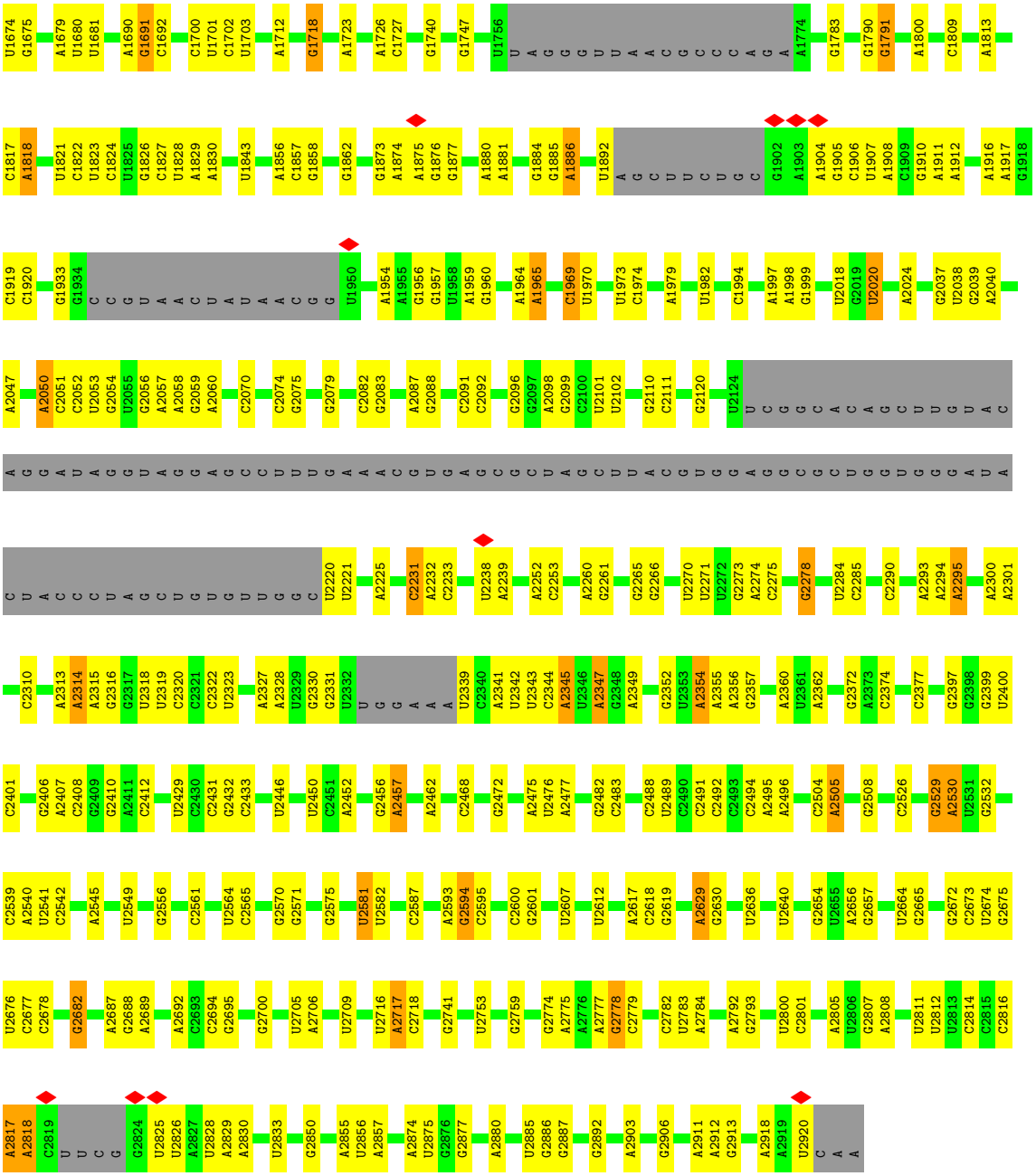


• Molecule 30: 23S ribosomal RNA

Chain A:

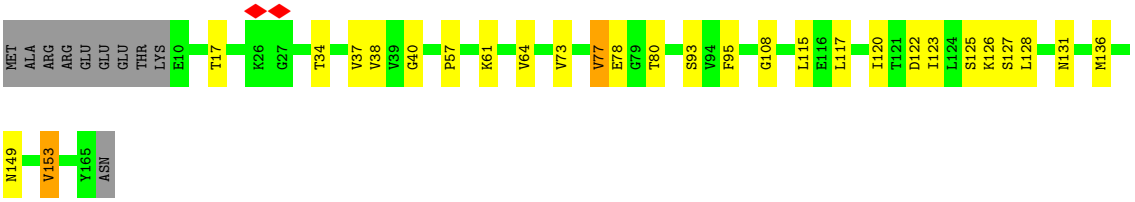






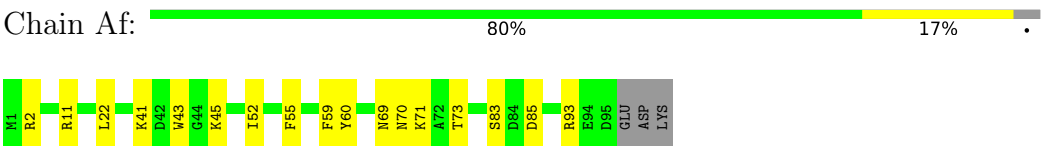
• Molecule 31: Small ribosomal subunit protein uS5

Chain Ae:



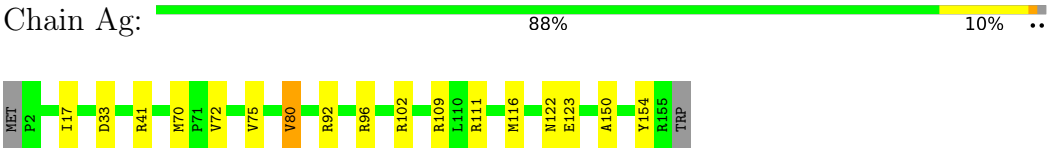
• Molecule 32: Small ribosomal subunit protein bS6

Chain Af:



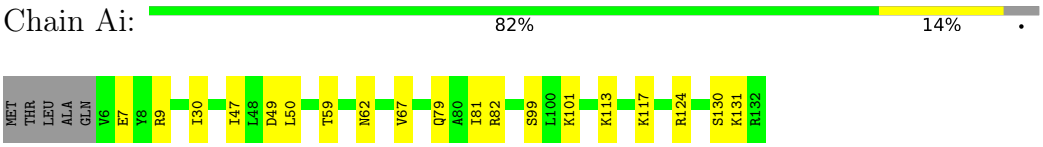
• Molecule 33: Small ribosomal subunit protein uS7

Chain Ag:



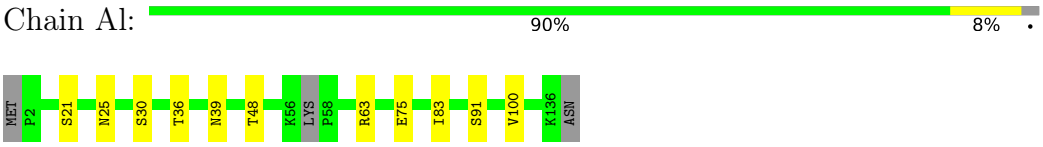
• Molecule 34: Small ribosomal subunit protein uS9

Chain Ai:



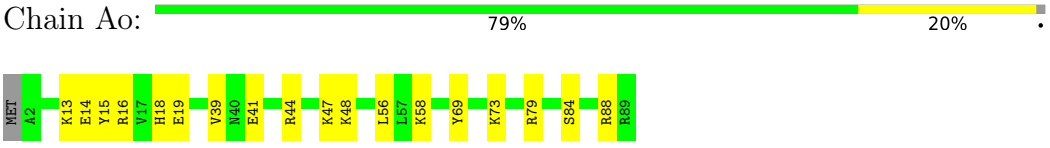
• Molecule 35: Small ribosomal subunit protein uS12

Chain Al:



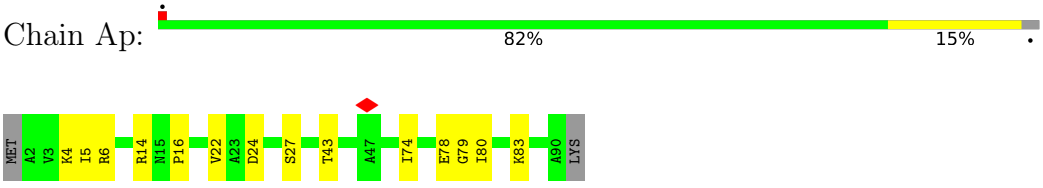
• Molecule 36: Small ribosomal subunit protein uS15

Chain Ao:



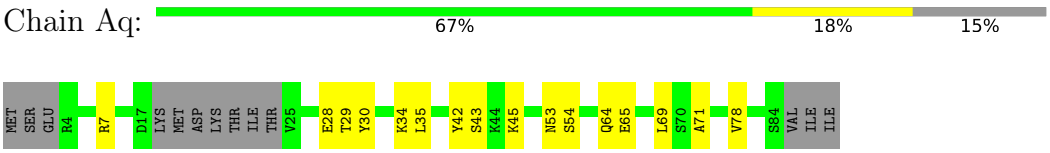
• Molecule 37: Small ribosomal subunit protein bS16

Chain Ap:



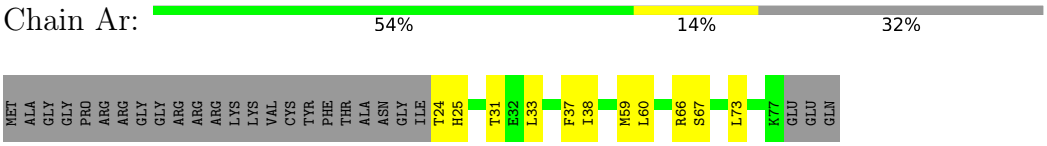
• Molecule 38: Small ribosomal subunit protein uS17

Chain Aq:



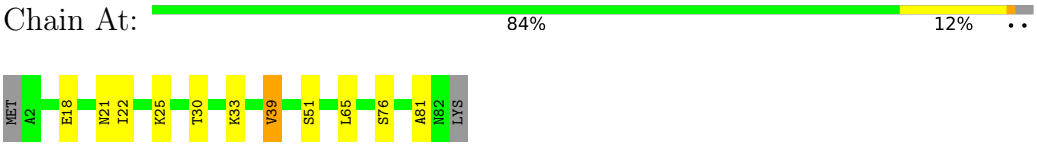
• Molecule 39: Small ribosomal subunit protein bS18

Chain Ar:



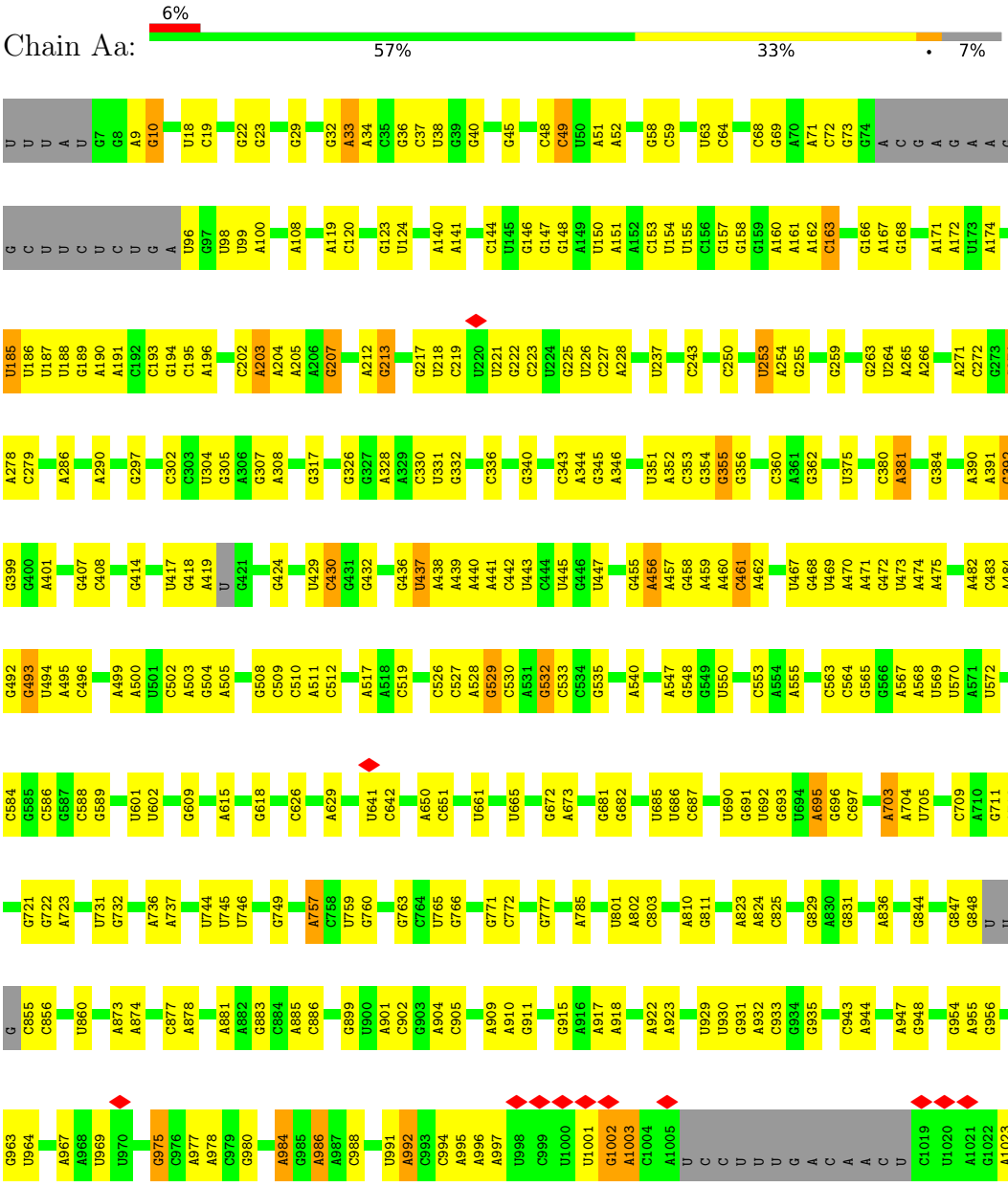
• Molecule 40: Small ribosomal subunit protein bS20

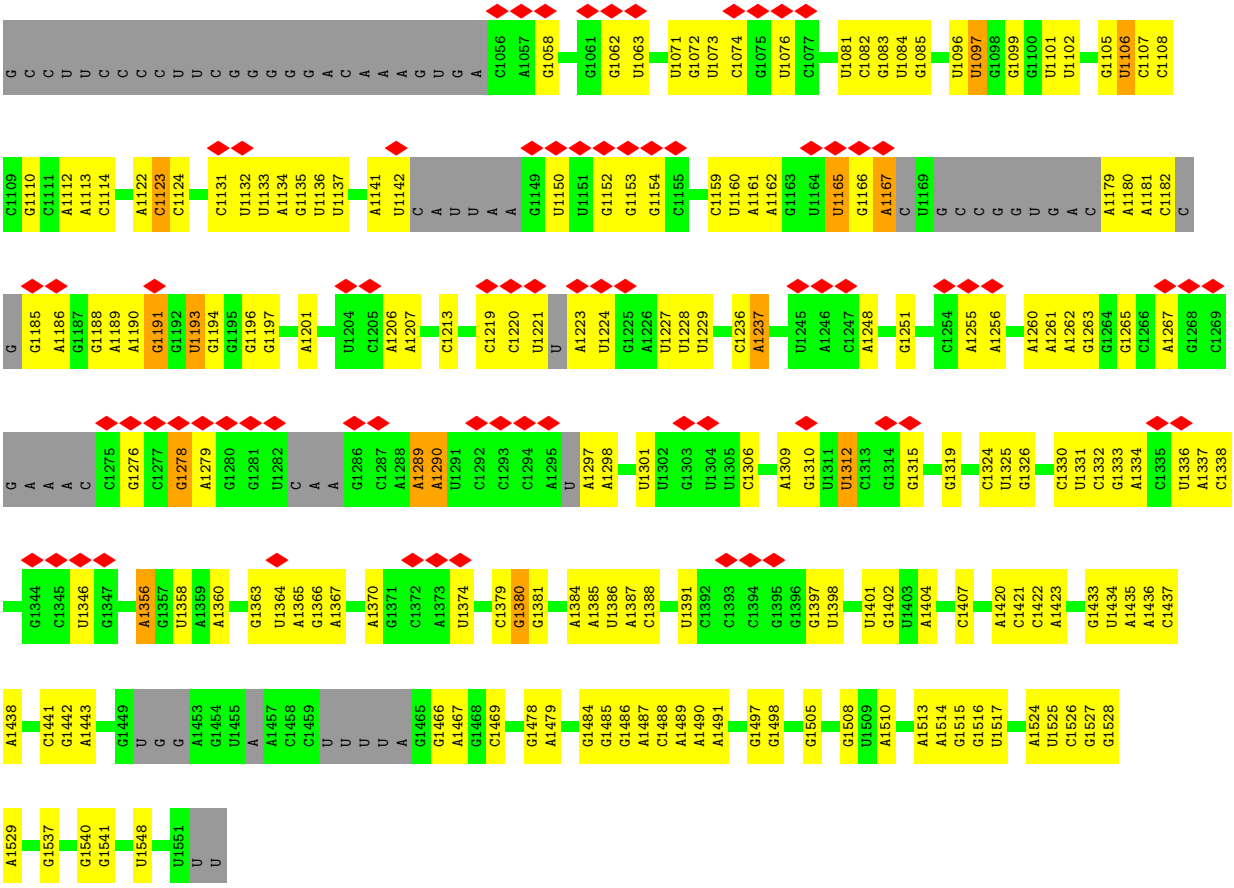
Chain At:



• Molecule 41: 16S ribosomal RNA

Chain Aa:



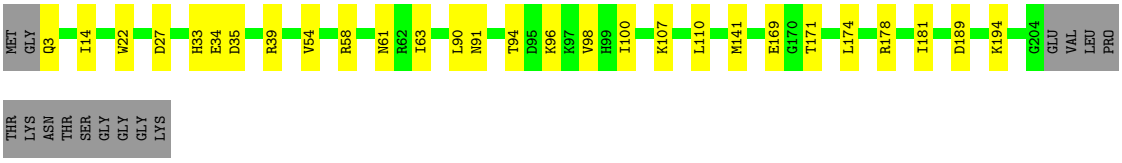


• Molecule 42: Small ribosomal subunit protein uS10

Chain Aj:

• Molecule 43: Small ribosomal subunit protein uS3

Chain Ac:

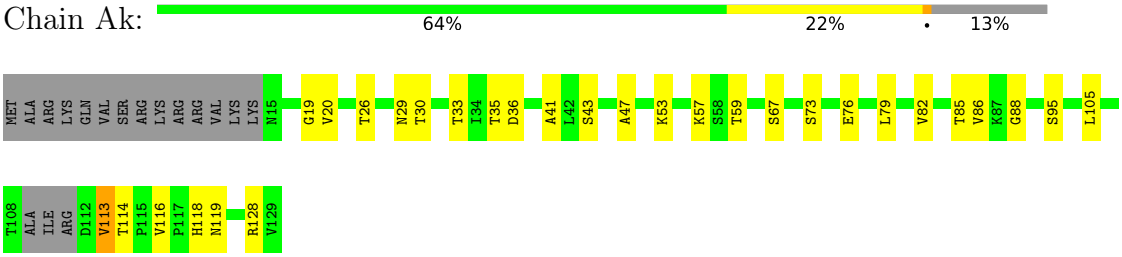


• Molecule 44: Small ribosomal subunit protein uS13

Chain Am:

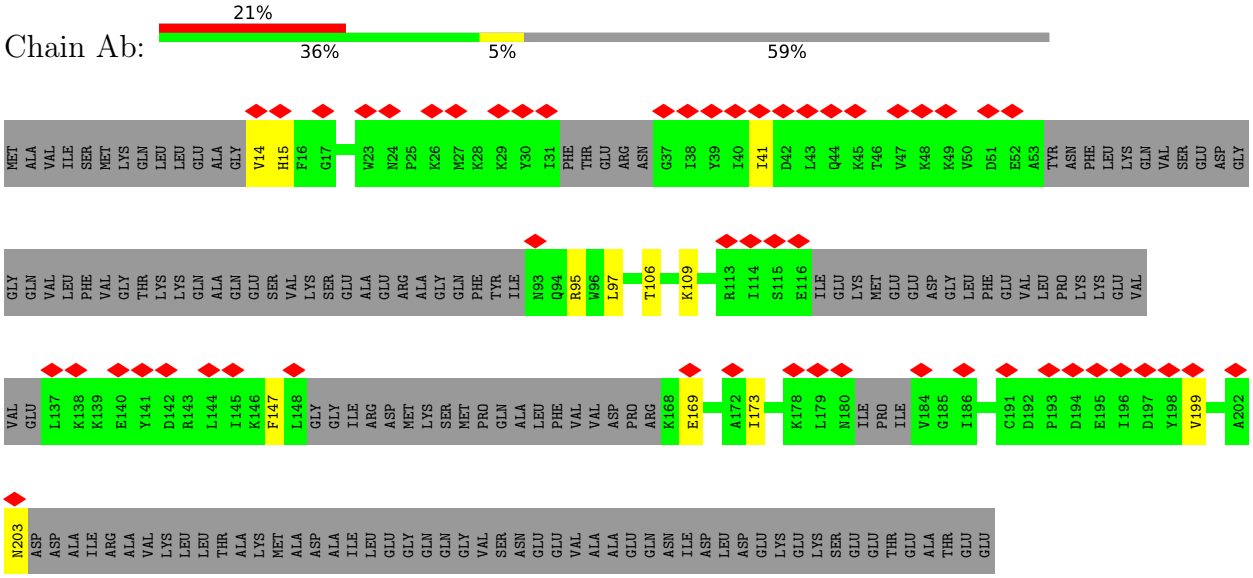
• Molecule 45: Small ribosomal subunit protein uS11

Chain Ak:



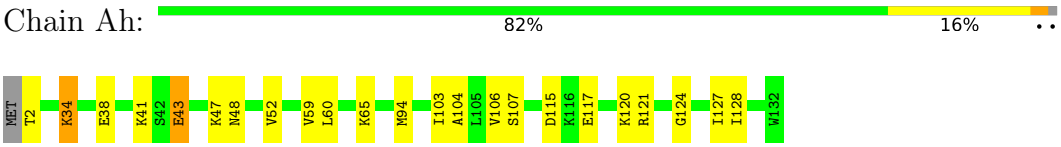
• Molecule 46: Small ribosomal subunit protein uS2

Chain Ab:



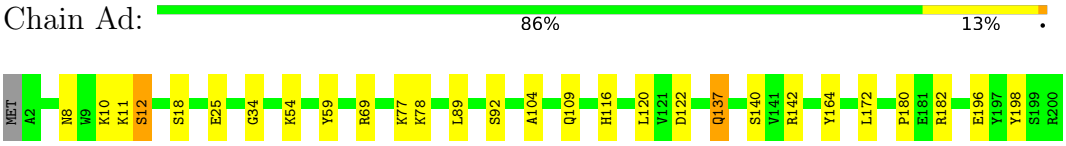
• Molecule 47: Small ribosomal subunit protein uS8

Chain Ah:



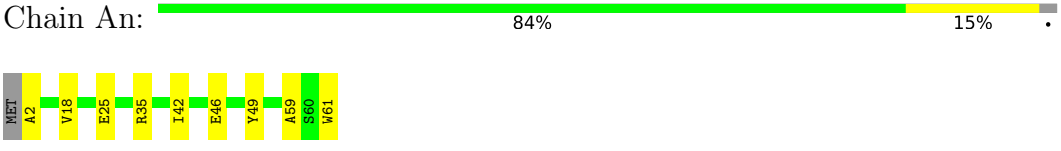
• Molecule 48: Small ribosomal subunit protein uS4

Chain Ad:



• Molecule 49: Small ribosomal subunit protein uS14B

Chain An:

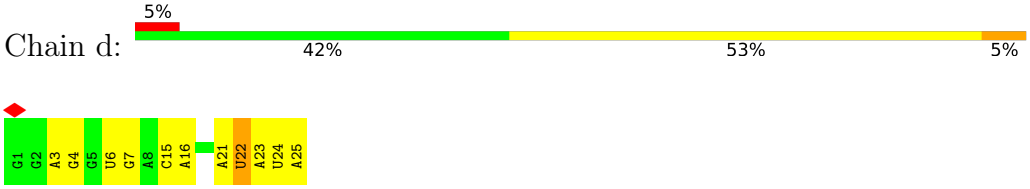


• Molecule 50: Small ribosomal subunit protein uS19

Chain As:

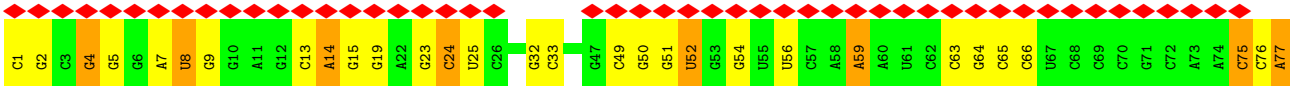
• Molecule 51: mRNA molecule

Chain d:



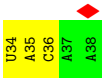
• Molecule 52: P-site tRNA molecule

Chain 8:



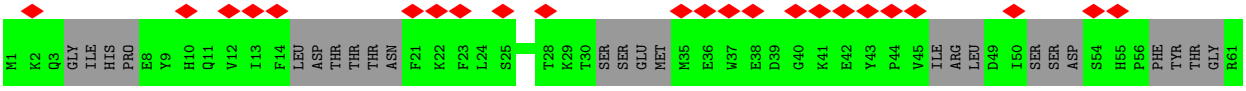
• Molecule 53: A-site tRNA molecule

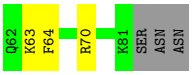
Chain 9:



• Molecule 54: Large ribosomal subunit protein bL31B

Chain 13:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	408831	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.00	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	67.143	Depositor
Minimum map value	-30.208	Depositor
Average map value	0.061	Depositor
Map value standard deviation	1.435	Depositor
Recommended contour level	3	Depositor
Map size (Å)	362.56, 362.56, 362.56	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.824, 0.824, 0.824	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: 2MG, 5MU, UR3, EM1, PSU, MG, ZN, MA6, G7M, H2U, 2MA, 5MC, 4OC, OMG, K

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	0.13	0/360	0.30	0/489
2	2	0.16	0/372	0.33	0/487
3	3	0.17	0/513	0.35	0/678
4	4	0.15	0/283	0.32	0/376
5	B	0.14	0/2692	0.27	0/4193
6	C	0.15	0/2072	0.33	0/2792
7	D	0.16	0/1606	0.39	0/2159
8	E	0.16	0/1533	0.33	0/2077
9	G	0.14	0/953	0.31	0/1301
10	H	0.19	0/1162	0.38	0/1566
11	I	0.15	0/871	0.33	0/1177
12	J	0.15	0/1071	0.35	0/1433
13	K	0.17	0/1048	0.35	0/1420
14	L	0.18	0/904	0.34	0/1209
15	M	0.15	0/810	0.32	0/1102
16	N	0.13	0/811	0.29	0/1099
17	O	0.19	0/955	0.35	0/1265
18	P	0.14	0/762	0.31	0/1025
19	Q	0.18	0/822	0.37	0/1113
20	R	0.15	0/671	0.33	0/904
21	S	0.14	0/642	0.31	0/868
22	T	0.14	0/606	0.32	0/828
23	U	0.15	0/581	0.34	0/776
24	V	0.13	0/363	0.31	0/489
25	W	0.11	0/474	0.24	0/637
26	X	0.16	0/440	0.34	0/594
27	Z	0.17	0/339	0.36	0/451
28	F	0.13	0/923	0.31	0/1260
29	11	0.13	0/358	0.24	0/552
30	A	0.19	0/61919	0.35	0/96529
31	Ae	0.19	0/1144	0.33	0/1547
32	Af	0.16	0/745	0.30	0/1006

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	Ag	0.24	0/1240	0.30	0/1668
34	Ai	0.24	0/991	0.31	0/1334
35	Al	0.21	0/1027	0.33	0/1381
36	Ao	0.18	0/736	0.29	0/984
37	Ap	0.24	0/690	0.38	0/934
38	Aq	0.19	0/558	0.36	0/753
39	Ar	0.19	0/452	0.30	0/604
40	At	0.21	0/593	0.26	0/794
41	Aa	0.26	0/34383	0.32	0/53582
42	Aj	0.23	0/729	0.35	0/986
43	Ac	0.25	0/1499	0.31	0/2036
44	Am	0.21	0/851	0.31	0/1145
45	Ak	0.14	0/772	0.28	0/1050
46	Ab	0.10	0/630	0.24	0/858
47	Ah	0.22	0/1044	0.32	0/1401
48	Ad	0.18	0/1532	0.29	0/2071
49	An	0.25	0/512	0.29	0/678
50	As	0.24	0/634	0.29	0/858
51	d	0.15	0/461	0.31	0/715
52	8	0.14	0/1695	0.27	0/2634
53	9	0.14	0/118	0.31	0/181
54	13	0.13	0/386	0.23	0/515
All	All	0.21	0/140338	0.33	0/210564

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	355	0	316	4	0
2	2	368	0	409	5	0
3	3	508	0	544	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	4	280	0	302	4	0
5	B	2408	0	1217	34	0
6	C	2037	0	2106	11	0
7	D	1582	0	1604	12	0
8	E	1510	0	1533	14	0
9	G	944	0	636	10	0
10	H	1140	0	1130	10	0
11	I	865	0	886	9	0
12	J	1057	0	1084	6	0
13	K	1024	0	1023	8	0
14	L	901	0	942	8	0
15	M	801	0	712	12	0
16	N	800	0	767	7	0
17	O	943	0	1014	7	0
18	P	752	0	761	7	0
19	Q	814	0	854	9	0
20	R	664	0	666	5	0
21	S	635	0	605	6	0
22	T	600	0	540	5	0
23	U	575	0	568	2	0
24	V	360	0	353	4	0
25	W	473	0	472	4	0
26	X	438	0	472	2	0
27	Z	333	0	348	2	0
28	F	914	0	695	12	0
29	11	322	0	167	7	0
30	A	55514	0	27922	397	0
31	Ae	1130	0	1188	15	0
32	Af	734	0	705	10	0
33	Ag	1222	0	1255	12	0
34	Ai	975	0	979	12	0
35	Al	1011	0	1036	4	0
36	Ao	727	0	754	8	0
37	Ap	679	0	684	9	0
38	Aq	551	0	528	10	0
39	Ar	445	0	482	5	0
40	At	593	0	634	5	0
41	Aa	30880	0	15569	314	0
42	Aj	720	0	698	9	0
43	Ac	1477	0	1437	20	0
44	Am	845	0	865	17	0
45	Ak	759	0	706	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	Ab	629	0	463	6	0
47	Ah	1032	0	1082	13	0
48	Ad	1502	0	1440	16	0
49	An	502	0	523	8	0
50	As	617	0	591	7	0
51	d	412	0	207	5	0
52	8	1519	0	775	18	0
53	9	106	0	55	2	0
54	13	382	0	288	2	0
55	1	1	0	0	0	0
55	4	1	0	0	0	0
55	An	1	0	0	0	0
55	Z	1	0	0	0	0
56	A	170	0	0	0	0
56	Aa	59	0	0	0	0
56	C	1	0	0	0	0
56	D	1	0	0	0	0
57	A	60	0	65	0	0
58	A	15	0	0	0	0
58	Aa	3	0	0	0	0
59	A	574	0	0	1	0
59	Aa	15	0	0	0	0
59	C	16	0	0	0	0
59	D	2	0	0	0	0
59	J	7	0	0	0	0
59	N	3	0	0	0	0
59	O	2	0	0	0	0
59	P	1	0	0	0	0
59	R	1	0	0	0	0
All	All	130300	0	83657	1058	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 5.

All (1058) 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)
44:Am:79:ARG:HH12	50:As:69:HIS:HE1	1.20	0.85
7:D:3:LYS:HD2	7:D:109:THR:HG22	1.58	0.85
30:A:788:A:O2'	30:A:1703:U:OP1	1.96	0.82
10:H:126:TYR:HH	10:H:133:HIS:HE2	1.23	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:87:U:H3	30:A:1002:U:H3	1.27	0.79
52:8:52:U:H3	52:8:64:G:H1	1.33	0.77
47:Ah:34:LYS:HG2	47:Ah:60:LEU:HD21	1.68	0.75
10:H:1:MET:SD	10:H:1:MET:N	2.51	0.75
41:Aa:1058:G:H21	41:Aa:1223:A:H2	1.33	0.74
30:A:159:U:H3	30:A:169:G:H1	1.35	0.74
41:Aa:672:G:H22	41:Aa:749:G:H1	1.33	0.74
41:Aa:685:U:H3	41:Aa:721:G:H22	1.36	0.73
41:Aa:18:U:H2'	41:Aa:19:C:C6	2.24	0.73
30:A:1886:A:N6	30:A:1910:G:O2'	2.22	0.72
18:P:47:LYS:HD2	18:P:102:ALA:HB1	1.72	0.71
41:Aa:161:A:N1	41:Aa:355:G:O2'	2.22	0.71
43:Ac:94:THR:HG22	43:Ac:96:LYS:HG3	1.73	0.71
52:8:19:G:H21	52:8:59:A:H5'	1.55	0.71
32:Af:2:ARG:HG2	32:Af:93:ARG:HH21	1.55	0.70
14:L:13:ARG:NH2	30:A:2717:A:OP2	2.25	0.70
25:W:52:LYS:NZ	30:A:75:G:O2'	2.22	0.70
44:Am:11:ARG:HA	44:Am:45:VAL:HG22	1.74	0.70
41:Aa:665:U:H3	41:Aa:757:A:H62	1.37	0.70
41:Aa:184:A:N1	41:Aa:207:G:O6	2.24	0.69
30:A:221:G:H22	30:A:238:U:H4'	1.56	0.69
30:A:2355:A:H2'	30:A:2356:A:C8	2.27	0.69
4:4:31:LYS:HE2	30:A:2505:A:H5'	1.75	0.69
31:Ae:115:LEU:HD13	31:Ae:123:ILE:HG21	1.73	0.69
34:Ai:79:GLN:HG2	34:Ai:82:ARG:HH21	1.58	0.69
12:J:18:ARG:NH2	30:A:1288:G:N7	2.41	0.68
41:Aa:955:A:H2'	41:Aa:956:G:C8	2.29	0.68
28:F:35:VAL:HG23	28:F:155:VAL:HB	1.75	0.68
24:V:35:LYS:HD2	24:V:46:LYS:HE3	1.75	0.67
41:Aa:1188:G:N2	41:Aa:1191:G:OP2	2.27	0.67
41:Aa:1058:G:N2	41:Aa:1221:U:O2	2.28	0.67
41:Aa:681:G:H2'	41:Aa:682:G:C8	2.30	0.67
34:Ai:50:LEU:HA	34:Ai:82:ARG:HB2	1.76	0.67
33:Ag:102:ARG:NH2	41:Aa:948:G:OP1	2.28	0.67
41:Aa:1179:A:H2'	41:Aa:1180:A:C8	2.30	0.66
30:A:275:A:H8	30:A:304:G:H21	1.42	0.66
44:Am:16:VAL:HG13	44:Am:34:LEU:HD12	1.76	0.66
5:B:39:G:N7	28:F:69:LYS:NZ	2.40	0.66
30:A:672:A:H61	30:A:682:A:H5"	1.61	0.66
47:Ah:47:LYS:HG3	47:Ah:65:LYS:HG3	1.77	0.66
52:8:63:C:H2'	52:8:64:G:C8	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:A:2318:U:H2'	30:A:2319:U:C6	2.31	0.65
41:Aa:1484:G:H2'	41:Aa:1485:G:C8	2.31	0.65
52:8:19:G:N2	52:8:59:A:OP2	2.29	0.65
18:P:67:ARG:NH2	30:A:1261:G:OP1	2.29	0.65
30:A:1916:A:H2'	30:A:1917:A:C8	2.32	0.64
30:A:75:G:H22	30:A:110:A:H2	1.45	0.64
41:Aa:831:G:HO2'	47:Ah:2:THR:N	1.96	0.64
45:Ak:19:GLY:HA2	45:Ak:36:ASP:HA	1.79	0.64
31:Ae:108:GLY:HA2	41:Aa:9:A:H1'	1.79	0.64
41:Aa:1336:U:H2'	41:Aa:1337:A:H8	1.63	0.64
8:E:174:GLN:NE2	8:E:185:ASP:OD2	2.30	0.63
41:Aa:1135:G:N2	41:Aa:1136:U:O4	2.32	0.63
30:A:921:C:H42	30:A:946:A:H61	1.45	0.63
41:Aa:99:U:H2'	41:Aa:100:A:C8	2.34	0.63
41:Aa:1435:A:H2'	41:Aa:1436:A:H8	1.64	0.63
15:M:8:ASN:OD1	15:M:11:ARG:NH2	2.29	0.63
32:Af:69:ASN:O	32:Af:70:ASN:ND2	2.32	0.63
37:Ap:14:ARG:NH2	41:Aa:401:A:OP1	2.32	0.62
41:Aa:721:G:H2'	41:Aa:722:G:C8	2.33	0.62
30:A:291:G:H2'	30:A:292:U:C6	2.35	0.62
50:As:65:ASP:HA	54:13:70:ARG:HG3	1.80	0.62
5:B:38:U:N3	5:B:42:G:OP2	2.20	0.62
17:O:74:MET:HE2	17:O:79:LEU:HA	1.82	0.62
30:A:1442:C:H2'	30:A:1443:A:H8	1.64	0.62
47:Ah:117:GLU:OE1	47:Ah:121:ARG:NH2	2.26	0.62
26:X:18:THR:OG1	26:X:49:LYS:NZ	2.31	0.62
34:Ai:113:LYS:NZ	41:Aa:1381:G:N7	2.48	0.62
41:Aa:148:G:H1	41:Aa:174:A:H61	1.48	0.62
41:Aa:461:C:H5	41:Aa:487:U:H3	1.46	0.62
14:L:24:LEU:HD23	14:L:44:VAL:HG21	1.81	0.61
30:A:631:U:H2'	30:A:632:U:C6	2.34	0.61
30:A:1513:A:H2'	30:A:1514:A:C8	2.36	0.61
28:F:36:VAL:HG22	28:F:154:ILE:HD12	1.82	0.61
30:A:172:U:H2'	30:A:173:A:H8	1.65	0.61
38:Aq:29:THR:HG22	38:Aq:30:TYR:H	1.66	0.61
21:S:92:ARG:HB3	21:S:101:ILE:HG13	1.83	0.61
30:A:830:U:H2'	30:A:831:C:C6	2.36	0.61
28:F:129:THR:HG22	28:F:155:VAL:HG22	1.82	0.61
30:A:702:U:H2'	30:A:703:A:C8	2.36	0.61
41:Aa:147:G:H2'	41:Aa:148:G:C8	2.35	0.61
30:A:787:U:H2'	30:A:788:A:C8	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:A:172:U:H2'	30:A:173:A:C8	2.36	0.60
44:Am:3:ARG:O	44:Am:57:ARG:NH1	2.34	0.60
9:G:3:ARG:NH2	30:A:1156:G:O3'	2.33	0.60
31:Ae:38:VAL:HG12	31:Ae:117:LEU:HD12	1.83	0.60
41:Aa:1236:C:N4	44:Am:103:LYS:HG3	2.16	0.60
30:A:2618:C:H2'	30:A:2619:G:C8	2.36	0.60
41:Aa:1276:G:N2	41:Aa:1279:A:OP2	2.25	0.60
41:Aa:963:G:H21	41:Aa:1237:A:H62	1.49	0.60
9:G:110:SER:OG	30:A:2694:C:N3	2.33	0.60
30:A:901:G:H2'	30:A:902:A:C8	2.36	0.60
30:A:2825:U:H2'	30:A:2826:U:C6	2.37	0.60
43:Ac:27:ASP:OD2	43:Ac:27:ASP:N	2.35	0.60
41:Aa:1370:A:OP2	49:An:35:ARG:NH2	2.36	0.59
30:A:1675:G:H1'	30:A:1679:A:N6	2.18	0.59
34:Ai:101:LYS:NZ	41:Aa:1188:G:N7	2.42	0.59
30:A:684:U:H2'	30:A:685:C:C6	2.36	0.59
30:A:1594:U:HO2'	30:A:1595:C:H6	1.48	0.59
41:Aa:1490:A:H2'	41:Aa:1491:A:H8	1.65	0.59
5:B:22:G:H4'	5:B:23:U:H5	1.68	0.59
41:Aa:1097:U:H3	41:Aa:1110:G:H22	1.49	0.59
41:Aa:1228:U:H2'	41:Aa:1229:U:C6	2.37	0.59
32:Af:69:ASN:HB2	32:Af:71:LYS:NZ	2.18	0.59
4:4:17:ILE:HD12	4:4:19:ARG:HG3	1.85	0.59
30:A:1823:U:H2'	30:A:1824:C:C6	2.37	0.59
30:A:2260:A:H2'	30:A:2261:G:C8	2.38	0.59
53:9:34:U:H2'	53:9:35:A:C8	2.38	0.58
31:Ae:108:GLY:HA3	41:Aa:10:G:H5'	1.85	0.58
38:Aq:45:LYS:NZ	41:Aa:286:A:OP2	2.36	0.58
12:J:110:LYS:HE2	12:J:127:LYS:HD3	1.83	0.58
30:A:632:U:H2'	30:A:633:A:C8	2.38	0.58
30:A:754:U:H2'	30:A:755:C:C6	2.38	0.58
41:Aa:1025:A:HO2'	41:Aa:1227:U:HO2'	1.50	0.58
41:Aa:1366:G:H2'	41:Aa:1367:A:C8	2.39	0.58
30:A:302:A:H2'	30:A:303:G:H8	1.69	0.58
41:Aa:744:U:H2'	41:Aa:745:U:C6	2.39	0.58
41:Aa:1297:A:H2'	41:Aa:1298:A:C8	2.38	0.58
14:L:52:LYS:NZ	14:L:96:ARG:O	2.37	0.58
30:A:302:A:H2'	30:A:303:G:C8	2.39	0.58
30:A:858:U:H2'	30:A:859:C:C6	2.38	0.58
43:Ac:90:LEU:HD12	43:Ac:100:ILE:HD11	1.85	0.58
30:A:1442:C:H2'	30:A:1443:A:C8	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:A:1829:A:H2'	30:A:1830:A:C8	2.39	0.57
8:E:148:GLN:NE2	8:E:191:SER:OG	2.37	0.57
30:A:1353:A:H2'	30:A:1354:G:C8	2.39	0.57
33:Ag:92:ARG:NH2	41:Aa:1387:A:OP1	2.37	0.57
41:Aa:1133:U:O4	41:Aa:1134:A:N6	2.38	0.57
45:Ak:20:VAL:N	45:Ak:35:THR:O	2.26	0.57
28:F:70:ALA:HB2	28:F:85:ILE:HD11	1.84	0.57
41:Aa:499:A:H2'	41:Aa:500:A:H8	1.69	0.57
41:Aa:777:G:H4'	41:Aa:1524:A:H4'	1.86	0.57
41:Aa:1306:C:H4'	41:Aa:1312:U:O4	2.04	0.57
30:A:221:G:N2	30:A:238:U:H4'	2.19	0.57
41:Aa:1213:C:OP1	49:An:2:ALA:N	2.38	0.57
41:Aa:1497:G:H2'	41:Aa:1498:G:C8	2.40	0.57
8:E:27:GLU:CD	8:E:27:GLU:H	2.12	0.57
32:Af:22:LEU:H	32:Af:22:LEU:HD23	1.68	0.57
41:Aa:824:A:OP1	41:Aa:1537:G:O2'	2.21	0.57
10:H:1:MET:HA	30:A:1039:C:C5	2.40	0.57
21:S:9:VAL:HG12	21:S:70:LEU:HD23	1.87	0.57
41:Aa:991:U:H4'	41:Aa:992:A:H5'	1.87	0.57
13:K:58:MET:HE1	13:K:64:VAL:HG22	1.87	0.57
41:Aa:32:G:O2'	41:Aa:49:C:N4	2.38	0.57
41:Aa:955:A:H2'	41:Aa:956:G:H8	1.69	0.57
28:F:129:THR:HG21	30:A:2330:G:H21	1.70	0.56
30:A:1241:A:H2'	30:A:1242:A:C8	2.40	0.56
41:Aa:186:U:H2'	41:Aa:187:U:C6	2.40	0.56
41:Aa:1058:G:N1	41:Aa:1221:U:N3	2.53	0.56
17:O:105:ALA:HB1	18:P:40:PHE:HZ	1.70	0.56
41:Aa:1333:G:H2'	41:Aa:1334:A:C8	2.41	0.56
9:G:2:SER:HB2	9:G:5:GLY:H	1.70	0.56
24:V:35:LYS:HG3	24:V:48:TRP:CE2	2.40	0.56
30:A:2354:A:H2'	30:A:2355:A:C8	2.41	0.56
30:A:1791:G:N7	59:A:3211:HOH:O	2.33	0.56
16:N:22:PHE:O	16:N:52:ARG:NH1	2.38	0.56
16:N:102:LEU:HD11	16:N:112:ILE:HD11	1.88	0.56
38:Aq:71:ALA:HB2	41:Aa:274:G:H3'	1.88	0.56
41:Aa:345:G:H2'	41:Aa:346:A:C8	2.41	0.56
41:Aa:532:G:H2'	41:Aa:533:C:C6	2.41	0.56
52:8:4:G:H2'	52:8:5:G:H8	1.71	0.56
30:A:687:G:N2	30:A:690:U:OP2	2.36	0.56
41:Aa:736:A:H2'	41:Aa:737:A:C8	2.41	0.56
41:Aa:1435:A:H2'	41:Aa:1436:A:C8	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:A:441:C:H2'	30:A:442:G:H8	1.71	0.56
30:A:1571:G:N2	30:A:1593:G:O6	2.39	0.55
41:Aa:473:U:O2'	41:Aa:475:A:N7	2.27	0.55
50:As:12:ASP:OD2	50:As:35:SER:OG	2.24	0.55
30:A:1357:G:C2	30:A:1366:U:H5"	2.41	0.55
30:A:1712:A:O2'	30:A:1718:G:N7	2.32	0.55
30:A:877:G:H2'	30:A:878:C:C6	2.41	0.55
2:2:2:VAL:N	30:A:1663:G:HO2'	2.05	0.55
18:P:78:ARG:NH2	30:A:606:G:OP2	2.31	0.55
20:R:69:GLN:NE2	20:R:70:GLY:O	2.39	0.55
30:A:1884:G:N2	30:A:1912:A:C2	2.72	0.55
41:Aa:1180:A:H2'	41:Aa:1181:A:O4'	2.06	0.55
11:I:88:ARG:HG2	11:I:94:ARG:HD3	1.89	0.55
30:A:3:U:H2'	30:A:4:U:C6	2.42	0.55
30:A:2618:C:H2'	30:A:2619:G:H8	1.71	0.55
43:Ac:22:TRP:HB3	43:Ac:58:ARG:HB2	1.89	0.55
11:I:113:LYS:HZ2	11:I:117:LEU:HD11	1.72	0.55
30:A:2331:G:H1	30:A:2339:U:H3	1.55	0.55
11:I:35:ILE:HG21	11:I:103:ALA:HB3	1.88	0.55
26:X:5:GLN:HB3	26:X:57:GLU:HG3	1.87	0.55
30:A:1575:A:H2'	30:A:1576:A:C8	2.42	0.55
30:A:259:A:H2'	30:A:260:A:C8	2.42	0.55
30:A:1044:A:H2'	30:A:1045:A:C8	2.41	0.55
41:Aa:1153:G:H2'	41:Aa:1154:G:H8	1.71	0.55
41:Aa:553:C:OP1	48:Ad:54:LYS:NZ	2.39	0.54
41:Aa:1401:U:H2'	41:Aa:1402:G:C8	2.41	0.54
41:Aa:1420:A:H2'	41:Aa:1421:C:C6	2.43	0.54
30:A:2052:C:H2'	30:A:2053:U:C6	2.42	0.54
30:A:2101:U:H2'	30:A:2102:U:C6	2.42	0.54
32:Af:69:ASN:HB2	32:Af:71:LYS:HZ3	1.71	0.54
8:E:174:GLN:HE22	8:E:185:ASP:CG	2.16	0.54
13:K:54:MET:O	13:K:58:MET:HG3	2.08	0.54
30:A:259:A:H2'	30:A:260:A:H8	1.73	0.54
41:Aa:1489:A:H2'	41:Aa:1490:A:C8	2.42	0.54
48:Ad:8:ASN:O	48:Ad:12:SER:OG	2.23	0.54
41:Aa:1082:C:H2'	41:Aa:1083:G:H8	1.71	0.54
41:Aa:1336:U:H2'	41:Aa:1337:A:C8	2.41	0.54
36:Ao:41:GLU:HA	36:Ao:44:ARG:HE	1.71	0.54
41:Aa:390:A:H2'	41:Aa:391:A:C8	2.43	0.54
30:A:525:A:H1'	30:A:526:A:H5"	1.89	0.54
30:A:632:U:H2'	30:A:633:A:H8	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:Ai:131:LYS:O	41:Aa:975:2MG:O2'	2.26	0.54
44:Am:79:ARG:HH12	50:As:69:HIS:CE1	2.12	0.54
6:C:150:LYS:HD2	30:A:2231:C:H4'	1.90	0.54
41:Aa:499:A:H2'	41:Aa:500:A:C8	2.43	0.54
45:Ak:35:THR:HB	45:Ak:41:ALA:HA	1.88	0.54
52:8:15:G:N2	52:8:49:C:O2	2.38	0.54
30:A:2232:A:H2'	30:A:2233:C:C6	2.42	0.54
30:A:2654:G:O2'	30:A:2808:A:N1	2.38	0.54
30:A:69:C:H4'	30:A:75:G:N7	2.23	0.54
30:A:156:A:O2'	30:A:157:U:H5"	2.08	0.54
30:A:2705:U:H2'	30:A:2706:A:C8	2.42	0.54
30:A:2817:A:O2'	30:A:2818:A:O5'	2.22	0.54
41:Aa:1161:A:HO2'	41:Aa:1162:A:H8	1.56	0.54
3:3:60:GLN:HE21	3:3:60:GLN:HA	1.73	0.54
6:C:180:GLU:OE2	30:A:1826:G:O2'	2.24	0.54
19:Q:8:ARG:NH1	30:A:539:G:OP1	2.36	0.54
30:A:955:A:H2'	30:A:956:A:C8	2.43	0.54
30:A:1329:G:H2'	30:A:1330:U:C6	2.43	0.54
17:O:66:ASN:O	17:O:70:ARG:HG2	2.09	0.53
19:Q:35:ILE:HG13	27:Z:27:MET:HE1	1.89	0.53
30:A:395:U:H2'	30:A:396:G:H8	1.73	0.53
30:A:1823:U:H2'	30:A:1824:C:H6	1.71	0.53
30:A:2270:U:H2'	30:A:2271:U:C6	2.43	0.53
41:Aa:222:G:H2'	41:Aa:223:C:C6	2.42	0.53
30:A:2817:A:H5"	30:A:2912:A:H2	1.73	0.53
32:Af:45:LYS:HE2	32:Af:59:PHE:CZ	2.44	0.53
41:Aa:917:A:H2'	41:Aa:918:A:C8	2.44	0.53
30:A:422:G:H2'	30:A:423:A:C8	2.44	0.53
30:A:2672:G:H4'	30:A:2759:G:O2'	2.08	0.53
36:Ao:18:HIS:ND1	36:Ao:19:GLU:O	2.41	0.53
41:Aa:302:C:OP1	41:Aa:618:G:O2'	2.22	0.53
9:G:3:ARG:NH1	30:A:2778:G:OP2	2.41	0.53
7:D:156:MET:O	30:A:2079:G:H4'	2.08	0.53
41:Aa:307:G:H2'	41:Aa:308:A:C8	2.44	0.53
41:Aa:1107:C:H2'	41:Aa:1108:C:H6	1.74	0.53
42:Aj:24:LYS:HG2	42:Aj:90:LEU:HD11	1.91	0.53
41:Aa:1137:U:N3	41:Aa:1290:A:OP1	2.40	0.53
6:C:29:PRO:HG2	6:C:34:LEU:HD11	1.90	0.53
41:Aa:1423:A:H61	41:Aa:1498:G:H1	1.54	0.53
47:Ah:43:GLU:HG2	47:Ah:103:ILE:HG21	1.91	0.53
30:A:2220:U:H2'	30:A:2221:U:H6	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:3:ARG:HD2	30:A:2778:G:C8	2.44	0.53
43:Ac:35:ASP:O	43:Ac:39:ARG:HG3	2.08	0.53
30:A:577:A:H4'	30:A:578:G:C8	2.44	0.52
30:A:2232:A:H2'	30:A:2233:C:H6	1.74	0.52
41:Aa:1261:A:H2'	41:Aa:1262:A:C8	2.44	0.52
41:Aa:1488:C:H2'	41:Aa:1489:A:H8	1.73	0.52
15:M:92:ILE:HD13	15:M:117:LEU:HD13	1.91	0.52
30:A:2294:A:H5"	30:A:2295:A:H5'	1.91	0.52
41:Aa:160:A:H2'	41:Aa:161:A:O4'	2.10	0.52
45:Ak:85:THR:HB	45:Ak:113:VAL:HG21	1.91	0.52
1:1:21:ILE:HD13	30:A:2446:U:H5"	1.90	0.52
14:L:59:ARG:HA	14:L:86:PHE:CZ	2.44	0.52
28:F:32:ASP:N	28:F:157:VAL:O	2.42	0.52
5:B:6:U:OP1	15:M:11:ARG:NH1	2.38	0.52
30:A:1337:A:H4'	30:A:1338:U:H5"	1.92	0.52
30:A:1353:A:H2'	30:A:1354:G:H8	1.74	0.52
41:Aa:873:A:H2'	41:Aa:874:A:C8	2.44	0.52
41:Aa:1437:C:H2'	41:Aa:1438:A:H8	1.75	0.52
49:An:42:ILE:O	49:An:46:GLU:HG3	2.09	0.52
51:d:22:U:H2'	51:d:23:A:C8	2.45	0.52
11:I:88:ARG:NE	11:I:90:ASP:OD2	2.41	0.52
30:A:441:C:H2'	30:A:442:G:C8	2.44	0.52
41:Aa:190:A:H2'	41:Aa:191:A:H8	1.75	0.52
15:M:32:ASN:HA	15:M:95:ASP:HB3	1.92	0.52
30:A:200:A:N6	30:A:2457:A:O2'	2.43	0.52
41:Aa:1524:A:H2'	41:Aa:1525:U:C6	2.45	0.52
8:E:205:VAL:HG23	8:E:206:LEU:HD12	1.92	0.52
29:11:72:C:H2'	29:11:73:A:H8	1.75	0.52
30:A:625:G:H2'	30:A:626:G:C8	2.45	0.52
30:A:954:A:H2'	30:A:957:C:C5	2.45	0.52
41:Aa:1107:C:H2'	41:Aa:1108:C:C6	2.45	0.52
41:Aa:1443:A:OP2	41:Aa:1478:G:N1	2.35	0.52
51:d:6:U:H2'	51:d:7:G:C8	2.45	0.52
19:Q:4:LYS:HG3	19:Q:106:VAL:HG22	1.92	0.52
30:A:1880:A:H2'	30:A:1881:A:C8	2.45	0.52
6:C:164:VAL:HA	6:C:174:ILE:HD13	1.92	0.51
30:A:2231:C:H2'	30:A:2232:A:C8	2.45	0.51
30:A:2300:A:H2'	30:A:2301:A:C8	2.45	0.51
34:Ai:7:GLU:OE1	34:Ai:9:ARG:NH2	2.43	0.51
5:B:83:C:H2'	5:B:84:U:O4'	2.09	0.51
19:Q:42:ALA:HB2	30:A:2037:G:H5"	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:A:78:U:H2'	30:A:79:U:C6	2.45	0.51
30:A:579:U:H2'	30:A:580:C:C6	2.45	0.51
41:Aa:271:A:H2'	41:Aa:272:C:C6	2.45	0.51
43:Ac:39:ARG:NH2	43:Ac:54:VAL:O	2.43	0.51
51:d:23:A:H2'	51:d:24:U:O4'	2.10	0.51
41:Aa:959:U:H2'	41:Aa:960:G:C8	2.45	0.51
43:Ac:174:LEU:HD23	43:Ac:181:ILE:HD13	1.91	0.51
37:Ap:24:ASP:OD2	41:Aa:237:U:O2'	2.26	0.51
15:M:112:ALA:HB1	15:M:117:LEU:HD12	1.91	0.51
30:A:1160:C:H2'	30:A:1161:A:C8	2.45	0.51
41:Aa:1423:A:N1	41:Aa:1498:G:N2	2.54	0.51
30:A:346:A:H2'	30:A:347:U:C6	2.46	0.51
30:A:651:A:H2'	30:A:652:A:C8	2.46	0.51
30:A:1072:A:N6	30:A:1169:G:H2'	2.26	0.51
30:A:1423:C:H2'	30:A:1424:A:C8	2.45	0.51
30:A:1477:U:H2'	30:A:1478:A:C8	2.46	0.51
30:A:2327:A:H2'	30:A:2328:A:C8	2.46	0.51
41:Aa:1434:U:H2'	41:Aa:1435:A:C8	2.45	0.51
25:W:59:THR:O	25:W:63:GLU:HG3	2.11	0.51
30:A:1464:U:H2'	30:A:1465:G:C8	2.45	0.51
41:Aa:190:A:H2'	41:Aa:191:A:C8	2.46	0.51
41:Aa:509:C:H2'	41:Aa:510:C:C6	2.46	0.51
30:A:991:A:H2'	30:A:992:A:C8	2.45	0.51
41:Aa:929:U:H2'	41:Aa:930:U:C6	2.46	0.51
41:Aa:1525:U:H2'	41:Aa:1526:C:C6	2.46	0.51
5:B:40:C:O2	28:F:90:THR:HG22	2.11	0.51
10:H:2:ARG:HB3	10:H:3:GLN:HG3	1.93	0.51
30:A:525:A:N3	30:A:527:G:H5"	2.26	0.51
11:I:88:ARG:NH1	11:I:93:PRO:O	2.44	0.50
30:A:2098:A:H2'	30:A:2099:G:C8	2.45	0.50
41:Aa:155:U:O2	41:Aa:166:G:N2	2.39	0.50
41:Aa:29:G:O2'	41:Aa:304:U:OP1	2.27	0.50
41:Aa:483:C:H2'	41:Aa:484:A:H8	1.76	0.50
41:Aa:995:A:H2'	41:Aa:996:A:C8	2.46	0.50
43:Ac:33:HIS:NE2	49:An:25:GLU:HB2	2.26	0.50
30:A:363:A:H4'	30:A:365:A:C8	2.46	0.50
30:A:1556:G:H2'	30:A:1557:C:C6	2.46	0.50
30:A:618:A:OP2	30:A:2526:C:O2'	2.25	0.50
34:Ai:49:ASP:O	34:Ai:82:ARG:HD3	2.11	0.50
41:Aa:690:U:H2'	41:Aa:691:G:H8	1.76	0.50
41:Aa:917:A:H2'	41:Aa:918:A:H8	1.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:Aa:1058:G:C2	41:Aa:1221:U:O2	2.64	0.50
45:Ak:47:ALA:HB3	45:Ak:57:LYS:HG2	1.92	0.50
21:S:2:HIS:O	21:S:92:ARG:NH1	2.41	0.50
30:A:766:G:H2'	30:A:767:A:C8	2.47	0.50
30:A:1513:A:H2'	30:A:1514:A:H8	1.77	0.50
30:A:1813:A:H1'	30:A:1965:A:N6	2.27	0.50
2:2:15:LYS:NZ	30:A:124:A:OP1	2.38	0.50
16:N:43:GLN:NE2	41:Aa:354:G:OP1	2.44	0.50
30:A:2231:C:H2'	30:A:2232:A:H8	1.75	0.50
30:A:2539:C:H2'	30:A:2540:A:O4'	2.11	0.50
41:Aa:345:G:H2'	41:Aa:346:A:H8	1.77	0.50
41:Aa:407:G:H2'	41:Aa:408:C:C6	2.46	0.50
41:Aa:650:A:H2'	41:Aa:651:C:H6	1.76	0.50
5:B:4:G:H2'	5:B:5:G:H8	1.76	0.50
30:A:2343:U:H2'	30:A:2344:C:C6	2.47	0.50
52:8:65:C:H2'	52:8:66:C:C6	2.47	0.50
14:L:36:ARG:O	14:L:40:VAL:HG23	2.12	0.50
28:F:32:ASP:H	28:F:158:THR:HA	1.77	0.50
30:A:363:A:H4'	30:A:365:A:N7	2.27	0.50
30:A:5:A:H2'	30:A:6:A:C8	2.47	0.50
41:Aa:73:G:H1	41:Aa:96:U:H3	1.60	0.49
30:A:1238:U:H2'	30:A:1239:C:H6	1.77	0.49
30:A:1238:U:H2'	30:A:1239:C:C6	2.47	0.49
30:A:2356:A:H2'	30:A:2357:G:C8	2.47	0.49
41:Aa:1324:C:H2'	41:Aa:1325:U:C6	2.47	0.49
47:Ah:41:LYS:NZ	47:Ah:47:LYS:O	2.45	0.49
30:A:1390:A:H2'	30:A:1391:A:C8	2.48	0.49
30:A:1969:C:OP2	30:A:1970:U:O2'	2.29	0.49
40:At:30:THR:OG1	41:Aa:1469:C:OP1	2.27	0.49
48:Ad:11:LYS:HE2	48:Ad:59:TYR:CZ	2.47	0.49
30:A:1618:A:H2'	30:A:1619:A:C8	2.48	0.49
41:Aa:704:A:H2'	41:Aa:705:U:H6	1.77	0.49
46:Ab:15:HIS:O	46:Ab:41:ILE:N	2.35	0.49
27:Z:16:ARG:NH2	30:A:1302:G:OP1	2.39	0.49
30:A:903:G:N3	30:A:2295:A:H2'	2.28	0.49
41:Aa:445:U:O2'	48:Ad:116:HIS:ND1	2.33	0.49
41:Aa:1422:C:H2'	41:Aa:1423:A:C8	2.48	0.49
43:Ac:61:ASN:HA	43:Ac:96:LYS:NZ	2.27	0.49
30:A:765:U:H2'	30:A:766:G:C8	2.48	0.49
30:A:841:C:H2'	30:A:842:U:C6	2.48	0.49
30:A:1959:A:H2'	30:A:1960:G:O4'	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:Aa:716:A:H2'	41:Aa:717:U:C6	2.48	0.49
30:A:460:C:H2'	30:A:461:A:C8	2.48	0.49
30:A:684:U:H2'	30:A:685:C:H6	1.77	0.49
41:Aa:909:A:H2'	41:Aa:910:A:C8	2.47	0.49
11:I:63:VAL:HG12	11:I:106:LEU:HD11	1.95	0.49
41:Aa:470:A:H2'	41:Aa:471:A:C8	2.48	0.49
21:S:24:ILE:N	21:S:34:VAL:O	2.46	0.49
30:A:921:C:H2'	30:A:922:G:C8	2.48	0.49
41:Aa:1083:G:H2'	41:Aa:1084:U:C6	2.48	0.49
7:D:2:THR:HB	7:D:213:THR:HB	1.95	0.48
30:A:398:C:H2'	30:A:399:U:O4'	2.13	0.48
30:A:1876:G:H2'	30:A:1877:G:H8	1.78	0.48
30:A:2705:U:H2'	30:A:2706:A:H8	1.77	0.48
32:Af:11:ARG:HE	32:Af:85:ASP:HA	1.78	0.48
41:Aa:184:A:H2	41:Aa:207:G:H1	1.60	0.48
41:Aa:1441:C:H2'	41:Aa:1442:G:O4'	2.13	0.48
50:As:50:ALA:HB1	50:As:57:HIS:HB3	1.94	0.48
53:9:34:U:H2'	53:9:35:A:H8	1.77	0.48
30:A:422:G:H2'	30:A:423:A:H8	1.78	0.48
30:A:639:U:H2'	30:A:640:G:H8	1.79	0.48
30:A:2313:A:H4'	30:A:2314:A:O4'	2.13	0.48
41:Aa:1337:A:H2'	41:Aa:1338:C:H6	1.79	0.48
41:Aa:1437:C:H2'	41:Aa:1438:A:C8	2.48	0.48
48:Ad:104:ALA:HB1	48:Ad:109:GLN:HB3	1.94	0.48
30:A:2617:A:H2'	30:A:2618:C:H6	1.78	0.48
37:Ap:6:ARG:HB2	41:Aa:384:G:H5"	1.95	0.48
39:Ar:37:PHE:CG	39:Ar:60:LEU:HD21	2.47	0.48
41:Aa:502:C:O2'	41:Aa:504:G:H1'	2.13	0.48
41:Aa:996:A:H2'	41:Aa:997:A:C8	2.48	0.48
41:Aa:1527:G:H2'	41:Aa:1529:MA6:OP2	2.13	0.48
1:1:11:ALA:HB2	1:1:18:ARG:HG3	1.96	0.48
24:V:14:THR:HG21	30:A:192:G:OP2	2.14	0.48
30:A:2431:C:H2'	30:A:2432:G:O4'	2.13	0.48
38:Aq:29:THR:HB	38:Aq:42:TYR:CE1	2.49	0.48
44:Am:15:VAL:HG22	44:Am:43:THR:O	2.13	0.48
45:Ak:29:ASN:OD1	45:Ak:30:THR:N	2.46	0.48
30:A:1518:G:H2'	30:A:1519:U:O4'	2.13	0.48
30:A:2457:A:H2'	30:A:2457:A:N3	2.28	0.48
30:A:2829:A:H2'	30:A:2830:A:C8	2.48	0.48
38:Aq:34:LYS:NZ	38:Aq:35:LEU:HB2	2.29	0.48
41:Aa:331:U:H2'	41:Aa:332:G:O4'	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:Aa:1312:U:C5	44:Am:17:ILE:HG13	2.47	0.48
5:B:48:A:H5'	15:M:68:THR:HG23	1.96	0.48
20:R:19:ALA:HB1	20:R:24:LYS:HB2	1.95	0.48
30:A:2091:C:H2'	30:A:2092:C:C6	2.49	0.48
41:Aa:456:A:H2'	41:Aa:457:A:O4'	2.14	0.48
41:Aa:855:C:H2'	41:Aa:856:C:C6	2.49	0.48
5:B:112:A:H2'	5:B:113:G:H8	1.78	0.48
29:11:3:C:H2'	29:11:4:G:H8	1.78	0.48
30:A:954:A:H2'	30:A:957:C:H5	1.77	0.48
30:A:1160:C:H2'	30:A:1161:A:H8	1.79	0.48
35:Al:63:ARG:NH2	41:Aa:530:C:H41	2.11	0.48
41:Aa:588:C:H2'	41:Aa:589:G:O4'	2.14	0.48
41:Aa:1312:U:C4	44:Am:17:ILE:HG13	2.49	0.48
41:Aa:1366:G:H2'	41:Aa:1367:A:H8	1.79	0.48
17:O:4:VAL:HG22	30:A:1238:U:H1'	1.94	0.48
30:A:317:G:HO2'	30:A:318:A:H8	1.59	0.48
30:A:638:U:H2'	30:A:639:U:C6	2.49	0.48
30:A:1352:C:H2'	30:A:1353:A:C8	2.48	0.48
30:A:2343:U:H2'	30:A:2344:C:H6	1.79	0.48
30:A:2811:U:H2'	30:A:2812:U:C6	2.48	0.48
30:A:250:G:H4'	30:A:432:G:C5	2.48	0.48
30:A:2406:G:H2'	30:A:2407:A:C8	2.49	0.48
30:A:2570:G:H2'	30:A:2571:G:C8	2.49	0.48
41:Aa:436:G:H5"	48:Ad:10:LYS:HG3	1.96	0.48
41:Aa:1325:U:H2'	41:Aa:1326:G:O4'	2.14	0.48
41:Aa:1490:A:H2'	41:Aa:1491:A:C8	2.46	0.48
41:Aa:1260:A:H2'	41:Aa:1261:A:C8	2.49	0.47
52:8:13:C:H2'	52:8:14:A:H5"	1.94	0.47
30:A:127:C:H2'	30:A:128:C:C6	2.49	0.47
30:A:1280:U:H2'	30:A:1281:U:C6	2.49	0.47
41:Aa:153:C:H2'	41:Aa:154:U:C6	2.49	0.47
41:Aa:932:A:H2'	41:Aa:933:C:C6	2.48	0.47
41:Aa:1071:U:H2'	41:Aa:1072:G:H8	1.79	0.47
41:Aa:1433:G:H2'	41:Aa:1434:U:C6	2.49	0.47
41:Aa:1488:C:H2'	41:Aa:1489:A:C8	2.49	0.47
48:Ad:78:LYS:HE2	48:Ad:78:LYS:HB3	1.58	0.47
41:Aa:547:A:H2'	41:Aa:548:G:C8	2.49	0.47
52:8:7:A:H3'	52:8:8:U:H5'	1.95	0.47
41:Aa:963:G:H2'	41:Aa:964:U:C6	2.49	0.47
43:Ac:63:ILE:HD12	43:Ac:94:THR:HG21	1.95	0.47
5:B:4:G:H2'	5:B:5:G:C8	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:36:C:H2'	5:B:37:A:C8	2.49	0.47
6:C:81:ILE:HD11	6:C:110:LEU:HD23	1.95	0.47
30:A:886:A:H2'	30:A:887:A:H8	1.79	0.47
30:A:1326:C:H2'	30:A:1327:C:H6	1.80	0.47
30:A:2676:U:H2'	30:A:2677:C:H6	1.80	0.47
30:A:2856:U:H2'	30:A:2857:A:C8	2.50	0.47
41:Aa:457:A:H2'	41:Aa:458:G:O4'	2.14	0.47
43:Ac:34:GLU:HG2	43:Ac:58:ARG:HH22	1.79	0.47
30:A:318:A:H2'	30:A:319:G:C8	2.50	0.47
30:A:537:A:H2'	30:A:538:G:O4'	2.14	0.47
41:Aa:351:U:O3'	41:Aa:352:A:H8	1.98	0.47
41:Aa:1181:A:H2'	41:Aa:1182:C:C6	2.50	0.47
45:Ak:79:LEU:HD12	45:Ak:105:LEU:HD11	1.97	0.47
46:Ab:95:ARG:HD3	46:Ab:147:PHE:CZ	2.50	0.47
6:C:39:LYS:NZ	6:C:58:HIS:O	2.45	0.47
30:A:55:G:O2'	30:A:126:A:N1	2.41	0.47
30:A:348:C:H2'	30:A:349:U:C6	2.49	0.47
30:A:1362:C:OP1	30:A:1691:G:O2'	2.29	0.47
30:A:2344:C:H3'	30:A:2345:A:H5"	1.96	0.47
33:Ag:109:ARG:HG3	33:Ag:116:MET:HE1	1.95	0.47
41:Aa:904:A:H2'	41:Aa:905:C:C6	2.49	0.47
41:Aa:954:G:C2	41:Aa:955:A:C8	3.03	0.47
41:Aa:967:A:C6	50:As:55:ARG:HG2	2.50	0.47
41:Aa:1337:A:H2'	41:Aa:1338:C:C6	2.50	0.47
41:Aa:1489:A:H2'	41:Aa:1490:A:H8	1.79	0.47
47:Ah:106:VAL:HG13	47:Ah:127:ILE:HD13	1.96	0.47
5:B:3:U:OP1	5:B:60:C:H5'	2.15	0.47
15:M:11:ARG:HG3	15:M:99:TYR:CE1	2.50	0.47
30:A:1907:U:H2'	30:A:1908:A:C8	2.50	0.47
30:A:2885:U:H5"	30:A:2886:G:H2'	1.95	0.47
34:Ai:124:ARG:HG3	41:Aa:1358:U:H4'	1.96	0.47
41:Aa:1159:C:H2'	41:Aa:1160:U:C6	2.50	0.47
11:I:24:VAL:HG13	11:I:33:ALA:HB2	1.97	0.47
30:A:689:A:H4'	30:A:690:U:C5	2.50	0.47
30:A:787:U:H2'	30:A:788:A:H8	1.77	0.47
41:Aa:22:G:H2'	41:Aa:23:G:C8	2.50	0.47
41:Aa:148:G:H1	41:Aa:174:A:N6	2.12	0.47
41:Aa:343:C:H2'	41:Aa:344:A:H8	1.80	0.47
41:Aa:550:U:H5'	48:Ad:34:GLY:HA3	1.97	0.47
42:Aj:24:LYS:HB2	42:Aj:24:LYS:HE2	1.65	0.47
13:K:58:MET:HE1	13:K:64:VAL:CG2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Q:82:LEU:HB2	19:Q:98:LYS:HB2	1.95	0.47
41:Aa:155:U:H3	41:Aa:166:G:H1	1.62	0.47
41:Aa:1134:A:O2'	41:Aa:1135:G:H5'	2.15	0.47
41:Aa:1167:A:H62	41:Aa:1188:G:H21	1.61	0.47
47:Ah:107:SER:HB2	47:Ah:128:ILE:HD11	1.96	0.47
51:d:15:C:H2'	51:d:16:A:O4'	2.15	0.47
52:8:4:G:H2'	52:8:5:G:C8	2.50	0.47
22:T:79:PHE:HD1	22:T:86:ILE:HD13	1.80	0.46
29:11:3:C:H2'	29:11:4:G:C8	2.50	0.46
30:A:590:U:OP1	30:A:1257:G:O2'	2.26	0.46
30:A:1617:A:H2'	30:A:1618:A:C8	2.50	0.46
30:A:1648:C:O2'	30:A:1654:A:N1	2.47	0.46
30:A:1817:C:H2'	30:A:1818:A:C5	2.50	0.46
30:A:1857:C:H2'	30:A:1858:G:H8	1.80	0.46
42:Aj:57:LYS:HE3	42:Aj:58:TYR:CZ	2.49	0.46
5:B:58:C:H2'	5:B:59:U:C6	2.50	0.46
34:Ai:67:VAL:HG11	34:Ai:81:ILE:HG12	1.97	0.46
41:Aa:495:A:H2'	41:Aa:496:C:O4'	2.15	0.46
41:Aa:744:U:H2'	41:Aa:745:U:H6	1.79	0.46
41:Aa:759:U:H2'	41:Aa:760:G:O4'	2.15	0.46
30:A:194:A:H2'	30:A:195:C:C6	2.51	0.46
30:A:1873:G:C6	30:A:1874:A:C6	3.04	0.46
36:Ao:69:TYR:CZ	36:Ao:73:LYS:HD3	2.50	0.46
41:Aa:391:A:OP1	41:Aa:462:A:O2'	2.30	0.46
43:Ac:63:ILE:HB	43:Ac:98:VAL:HG22	1.97	0.46
48:Ad:164:TYR:CD2	48:Ad:180:PRO:HB3	2.51	0.46
10:H:1:MET:HA	30:A:1039:C:C4	2.50	0.46
30:A:613:G:H2'	30:A:2057:A:N7	2.30	0.46
30:A:907:G:H2'	30:A:908:A:O4'	2.16	0.46
30:A:1222:A:H2'	30:A:1223:A:C8	2.50	0.46
33:Ag:41:ARG:NH2	41:Aa:1301:U:OP1	2.40	0.46
33:Ag:70:MET:HG2	33:Ag:96:ARG:O	2.15	0.46
36:Ao:79:ARG:HG3	36:Ao:79:ARG:HH11	1.80	0.46
41:Aa:326:G:HO2'	41:Aa:1479:A:HO2'	1.62	0.46
41:Aa:392:G:H2'	41:Aa:393:C:C6	2.51	0.46
41:Aa:455:G:O6	41:Aa:493:G:O2'	2.27	0.46
4:4:4:ARG:O	4:4:36:GLN:HA	2.16	0.46
5:B:25:A:H5"	15:M:39:HIS:CE1	2.51	0.46
10:H:3:GLN:NE2	18:P:13:LYS:O	2.43	0.46
22:T:29:ALA:HA	22:T:89:ILE:O	2.16	0.46
30:A:1053:A:N3	30:A:1197:C:O2'	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:A:1157:U:O2'	30:A:1158:G:OP1	2.27	0.46
41:Aa:996:A:H2'	41:Aa:997:A:H8	1.80	0.46
41:Aa:1123:C:O2	43:Ac:178:ARG:HG2	2.16	0.46
30:A:66:C:H2'	30:A:67:G:H8	1.81	0.46
30:A:1072:A:H2'	30:A:1073:A:C8	2.51	0.46
41:Aa:250:C:O2'	41:Aa:253:U:OP1	2.26	0.46
48:Ad:122:ASP:OD1	48:Ad:137:GLN:HG3	2.15	0.46
10:H:126:TYR:OH	10:H:133:HIS:NE2	2.27	0.46
14:L:66:LEU:HD11	14:L:85:LEU:HD22	1.97	0.46
30:A:291:G:O2'	30:A:292:U:OP1	2.28	0.46
30:A:437:A:H1'	30:A:457:G:O4'	2.16	0.46
33:Ag:33:ASP:OD1	41:Aa:1360:A:O2'	2.32	0.46
41:Aa:193:C:H2'	41:Aa:194:G:H8	1.80	0.46
41:Aa:959:U:H2'	41:Aa:960:G:H8	1.81	0.46
8:E:81:PRO:HB3	8:E:89:VAL:HG23	1.98	0.46
30:A:1637:A:H2'	30:A:1638:G:C8	2.51	0.46
30:A:2342:U:H2'	30:A:2343:U:C6	2.51	0.46
31:Ae:93:SER:HB3	31:Ae:128:LEU:O	2.15	0.46
33:Ag:111:ARG:HD2	33:Ag:123:GLU:HG2	1.98	0.46
38:Aq:29:THR:HG22	38:Aq:30:TYR:N	2.28	0.46
41:Aa:171:A:H2'	41:Aa:172:A:C8	2.50	0.46
41:Aa:278:A:H2'	41:Aa:279:C:C6	2.50	0.46
41:Aa:563:C:H2'	41:Aa:564:C:C6	2.50	0.46
41:Aa:771:G:H2'	41:Aa:772:C:C6	2.51	0.46
29:11:73:A:C2'	29:11:74:C:H5'	2.45	0.46
30:A:1723:A:H2	30:A:1791:G:C8	2.33	0.46
37:Ap:79:GLY:O	37:Ap:83:LYS:HG3	2.16	0.46
41:Aa:343:C:H2'	41:Aa:344:A:C8	2.51	0.46
41:Aa:1433:G:H2'	41:Aa:1434:U:H6	1.80	0.46
50:As:4:SER:HB2	50:As:7:LYS:HD3	1.96	0.46
5:B:30:U:C2	5:B:49:G:N2	2.84	0.46
20:R:4:ARG:HG2	25:W:30:PHE:CG	2.51	0.46
29:11:72:C:C2	29:11:73:A:C8	3.04	0.46
30:A:340:C:H2'	30:A:341:G:O4'	2.16	0.46
30:A:391:A:H2'	30:A:392:U:H6	1.81	0.46
30:A:1572:G:C6	30:A:1591:G:C6	3.04	0.46
30:A:2488:C:H2'	30:A:2489:U:C6	2.50	0.46
30:A:2564:U:H2'	30:A:2565:C:C6	2.50	0.46
32:Af:43:TRP:HB2	32:Af:60:TYR:HB2	1.97	0.46
41:Aa:217:G:H2'	41:Aa:218:U:O4'	2.16	0.46
41:Aa:885:A:H2'	41:Aa:886:C:C6	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:Aa:1073:U:H2'	41:Aa:1074:C:C6	2.51	0.46
42:Aj:11:LYS:HB2	42:Aj:97:ASP:OD2	2.16	0.46
5:B:65:G:H2'	5:B:66:C:C6	2.51	0.45
9:G:64:ASN:HA	9:G:67:THR:HG22	1.98	0.45
30:A:734:A:H2'	30:A:735:C:C6	2.51	0.45
30:A:1680:U:H2'	30:A:1681:U:C6	2.51	0.45
30:A:1876:G:H2'	30:A:1877:G:C8	2.52	0.45
35:Al:25:ASN:HB2	35:Al:39:ASN:HD22	1.81	0.45
41:Aa:471:A:H2'	41:Aa:472:G:O4'	2.16	0.45
30:A:689:A:H2'	30:A:691:A:C8	2.51	0.45
30:A:1352:C:H2'	30:A:1353:A:H8	1.82	0.45
30:A:2594:G:H2'	30:A:2595:C:C6	2.51	0.45
41:Aa:695:A:C2	41:Aa:712:A:C5	3.05	0.45
41:Aa:1002:G:O2'	41:Aa:1003:A:N7	2.49	0.45
47:Ah:41:LYS:HZ3	47:Ah:48:ASN:HA	1.81	0.45
5:B:58:C:H2'	5:B:59:U:H6	1.80	0.45
30:A:689:A:H4'	30:A:690:U:H5	1.81	0.45
30:A:1240:U:H2'	30:A:1241:A:C8	2.51	0.45
30:A:1674:U:H2'	30:A:1675:G:O4'	2.17	0.45
30:A:1973:U:H2'	30:A:1974:C:C6	2.52	0.45
37:Ap:4:LYS:HB3	37:Ap:4:LYS:HE2	1.75	0.45
41:Aa:1379:C:H2'	41:Aa:1380:G:C8	2.52	0.45
7:D:194:VAL:HG11	16:N:10:VAL:HG11	1.97	0.45
30:A:27:G:N2	30:A:557:G:H1'	2.31	0.45
30:A:279:A:H2'	30:A:280:C:C6	2.52	0.45
30:A:332:A:H2'	30:A:333:C:C6	2.52	0.45
30:A:2495:A:O2'	30:A:2496:A:H8	2.00	0.45
40:At:18:GLU:OE1	41:Aa:330:C:H4'	2.17	0.45
5:B:46:A:H2'	5:B:47:C:C6	2.51	0.45
5:B:106:G:H2'	5:B:107:U:C6	2.52	0.45
7:D:59:TYR:HB3	7:D:74:GLU:OE1	2.17	0.45
30:A:650:U:C5	30:A:665:G:C5	3.04	0.45
30:A:1476:G:H2'	30:A:1477:U:C6	2.52	0.45
30:A:1597:U:H2'	30:A:1598:U:C6	2.52	0.45
30:A:2051:C:H2'	30:A:2052:C:C6	2.51	0.45
30:A:2496:A:N6	30:A:2508:G:O2'	2.49	0.45
30:A:2677:C:H2'	30:A:2678:C:H6	1.82	0.45
30:A:2877:G:N2	30:A:2880:A:OP2	2.36	0.45
31:Ae:37:VAL:HG11	31:Ae:64:VAL:HG22	1.97	0.45
35:Al:83:ILE:HD13	41:Aa:529:G:H4'	1.98	0.45
38:Aq:28:GLU:HA	38:Aq:43:SER:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:At:39:VAL:HG11	40:At:81:ALA:HB1	1.98	0.45
41:Aa:265:A:H2'	41:Aa:266:A:C8	2.52	0.45
41:Aa:877:C:H2'	41:Aa:878:A:O4'	2.17	0.45
41:Aa:1082:C:H2'	41:Aa:1083:G:C8	2.51	0.45
42:Aj:40:ILE:HB	42:Aj:73:LEU:HB3	1.98	0.45
44:Am:45:VAL:HA	44:Am:48:LEU:HG	1.98	0.45
28:F:35:VAL:HG21	30:A:2341:A:H5'	1.98	0.45
30:A:901:G:H2'	30:A:902:A:H8	1.79	0.45
30:A:1493:U:H2'	30:A:1494:G:O4'	2.17	0.45
30:A:1821:U:H2'	30:A:1822:C:C6	2.51	0.45
41:Aa:58:G:H2'	41:Aa:59:C:C6	2.51	0.45
41:Aa:398:C:H2'	41:Aa:399:G:C8	2.51	0.45
7:D:5:ILE:HG22	7:D:211:ILE:HB	1.99	0.45
30:A:680:C:O2'	30:A:684:U:OP1	2.27	0.45
30:A:1979:A:N3	30:A:2587:C:O2'	2.46	0.45
41:Aa:381:A:O2'	41:Aa:459:A:N7	2.49	0.45
28:F:54:VAL:HG13	28:F:65:PRO:HG2	1.99	0.45
30:A:946:A:H2'	30:A:947:U:C6	2.52	0.45
30:A:2664:U:H2'	30:A:2665:G:O4'	2.17	0.45
39:Ar:59:MET:HE2	39:Ar:59:MET:HB2	1.85	0.45
41:Aa:1062:G:H2'	41:Aa:1063:U:C6	2.51	0.45
30:A:2260:A:H2'	30:A:2261:G:H8	1.81	0.45
41:Aa:695:A:N6	41:Aa:709:C:O4'	2.50	0.45
47:Ah:34:LYS:O	47:Ah:38:GLU:HG2	2.17	0.45
5:B:59:U:H2'	5:B:60:C:C6	2.51	0.45
30:A:970:U:O2'	30:A:972:A:OP2	2.32	0.45
30:A:1314:A:H2'	30:A:1315:C:C6	2.52	0.45
30:A:2477:A:O2'	52:8:77:A:N1	2.43	0.45
41:Aa:202:C:H2'	41:Aa:203:A:O4'	2.17	0.45
41:Aa:722:G:H2'	41:Aa:723:A:C8	2.52	0.45
41:Aa:1420:A:H2'	41:Aa:1421:C:H6	1.81	0.45
13:K:54:MET:HE1	13:K:104:PHE:CD2	2.52	0.44
30:A:2050:A:H2'	30:A:2051:C:C6	2.52	0.44
30:A:2110:G:H2'	30:A:2111:C:C6	2.52	0.44
30:A:2617:A:H2'	30:A:2618:C:C6	2.51	0.44
41:Aa:63:U:H2'	41:Aa:64:C:C6	2.52	0.44
41:Aa:482:A:H2'	41:Aa:483:C:C6	2.52	0.44
43:Ac:194:LYS:HD3	43:Ac:194:LYS:HA	1.78	0.44
44:Am:86:TYR:O	44:Am:90:ARG:HG2	2.17	0.44
52:8:1:C:H2'	52:8:2:G:H8	1.82	0.44
52:8:24:C:H2'	52:8:25:U:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:8:32:G:H2’	52:8:33:C:H6	1.82	0.44
12:J:74:TYR:CZ	12:J:127:LYS:HD2	2.52	0.44
30:A:754:U:H2’	30:A:755:C:H6	1.82	0.44
30:A:1240:U:H2’	30:A:1241:A:H8	1.83	0.44
30:A:2220:U:H2’	30:A:2221:U:C6	2.52	0.44
30:A:2318:U:OP1	30:A:2407:A:O2’	2.35	0.44
30:A:2482:G:H2’	30:A:2483:C:C6	2.52	0.44
37:Ap:78:GLU:HB2	37:Ap:80:ILE:HD12	1.99	0.44
41:Aa:803:C:O2’	45:Ak:128:ARG:O	2.33	0.44
8:E:53:ASN:O	8:E:57:VAL:HG23	2.17	0.44
30:A:1013:U:H2’	30:A:1014:U:C6	2.52	0.44
30:A:1563:U:H2’	30:A:1564:G:C8	2.53	0.44
30:A:1700:C:H2’	30:A:1701:U:H6	1.82	0.44
30:A:2549:U:O2’	30:A:2674:U:OP1	2.29	0.44
41:Aa:317:G:O2’	41:Aa:615:A:N1	2.49	0.44
41:Aa:765:U:H2’	41:Aa:766:G:O4’	2.17	0.44
48:Ad:182:ARG:O	48:Ad:182:ARG:NH1	2.50	0.44
13:K:39:THR:OG1	13:K:99:PRO:HD3	2.18	0.44
30:A:884:U:H2’	30:A:885:C:C6	2.51	0.44
35:Al:25:ASN:HB2	35:Al:39:ASN:ND2	2.32	0.44
38:Aq:65:GLU:OE1	41:Aa:243:C:O2’	2.28	0.44
40:At:25:LYS:HG3	40:At:65:LEU:HD22	1.99	0.44
41:Aa:263:G:H2’	41:Aa:264:U:C6	2.52	0.44
41:Aa:986:A:O2’	41:Aa:988:C:OP2	2.28	0.44
41:Aa:1106:U:H2’	41:Aa:1107:C:C6	2.51	0.44
41:Aa:1131:C:H2’	41:Aa:1132:U:C6	2.52	0.44
48:Ad:120:LEU:HD11	48:Ad:142:ARG:HA	1.98	0.44
9:G:84:VAL:HA	9:G:133:VAL:O	2.18	0.44
13:K:34:LEU:HD13	13:K:118:LEU:HB3	1.98	0.44
14:L:26:ILE:HG13	14:L:71:ILE:HG12	1.99	0.44
30:A:52:A:H2’	30:A:53:A:C8	2.53	0.44
30:A:569:U:H4’	30:A:598:G:H4’	1.99	0.44
30:A:1821:U:H2’	30:A:1822:C:H6	1.82	0.44
30:A:1916:A:H2’	30:A:1917:A:H8	1.80	0.44
41:Aa:697:C:OP2	45:Ak:57:LYS:NZ	2.46	0.44
54:13:63:LYS:HG3	54:13:64:PHE:CD2	2.52	0.44
14:L:22:THR:HG21	14:L:67:ARG:HB2	1.99	0.44
30:A:3:U:H2’	30:A:4:U:H6	1.81	0.44
30:A:622:A:H2’	30:A:623:C:C6	2.52	0.44
30:A:702:U:H2’	30:A:703:A:H8	1.82	0.44
30:A:1045:A:H2’	30:A:1046:G:O4’	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:A:1519:U:H2'	30:A:1520:A:C8	2.53	0.44
41:Aa:692:U:H2'	41:Aa:693:G:O4'	2.18	0.44
41:Aa:1167:A:H61	41:Aa:1190:A:H2'	1.81	0.44
11:I:86:ILE:HG22	11:I:94:ARG:HG3	1.99	0.44
30:A:30:G:H2'	30:A:31:C:C6	2.53	0.44
30:A:766:G:H2'	30:A:767:A:H8	1.82	0.44
30:A:859:C:H2'	30:A:860:U:H6	1.83	0.44
30:A:1158:G:O2'	30:A:1159:A:OP1	2.32	0.44
30:A:2270:U:H2'	30:A:2271:U:H6	1.82	0.44
30:A:2673:C:H2'	30:A:2674:U:O4'	2.18	0.44
41:Aa:441:A:H2'	41:Aa:442:C:C6	2.52	0.44
41:Aa:947:A:N3	41:Aa:1386:U:O2'	2.43	0.44
41:Aa:1081:U:H2'	41:Aa:1082:C:C6	2.52	0.44
30:A:78:U:H2'	30:A:79:U:H6	1.82	0.44
30:A:1521:A:N6	30:A:1559:G:O2'	2.48	0.44
30:A:2494:C:H2'	30:A:2495:A:O4'	2.18	0.44
30:A:2676:U:H2'	30:A:2677:C:C6	2.53	0.44
38:Aq:7:ARG:HB2	38:Aq:64:GLN:HE21	1.83	0.44
41:Aa:36:G:H2'	41:Aa:37:C:C6	2.53	0.44
46:Ab:109:LYS:NZ	46:Ab:109:LYS:HB3	2.33	0.44
8:E:117:LYS:HG3	8:E:192:LEU:HD13	2.00	0.44
30:A:339:A:H2'	30:A:340:C:C6	2.53	0.44
30:A:395:U:H2'	30:A:396:G:C8	2.52	0.44
30:A:725:A:H2'	30:A:726:G:C8	2.52	0.44
41:Aa:166:G:H2'	41:Aa:167:A:H8	1.83	0.44
41:Aa:187:U:H2'	41:Aa:188:U:C6	2.53	0.44
41:Aa:1255:A:H2'	41:Aa:1256:A:H8	1.83	0.44
9:G:90:VAL:O	9:G:160:LYS:HA	2.17	0.43
30:A:1252:A:H4'	30:A:1277:C:H4'	2.00	0.43
41:Aa:123:G:H2'	41:Aa:124:U:C6	2.53	0.43
41:Aa:140:A:H2'	41:Aa:141:A:C8	2.52	0.43
41:Aa:162:A:C5	41:Aa:163:C:H1'	2.53	0.43
41:Aa:225:G:H2'	41:Aa:226:U:C6	2.53	0.43
41:Aa:1423:A:N6	41:Aa:1498:G:H1	2.16	0.43
52:8:1:C:H2'	52:8:2:G:C8	2.53	0.43
25:W:13:LEU:O	25:W:64:ARG:NH2	2.44	0.43
30:A:229:A:O2'	30:A:231:A:N1	2.46	0.43
30:A:349:U:H2'	30:A:350:G:O4'	2.17	0.43
34:Ai:30:ILE:HD13	34:Ai:50:LEU:HD11	2.00	0.43
34:Ai:59:THR:O	34:Ai:62:ASN:HB2	2.18	0.43
36:Ao:39:VAL:HB	36:Ao:56:LEU:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:Aa:1364:U:H2'	41:Aa:1365:A:H8	1.83	0.43
30:A:460:C:H2'	30:A:461:A:H8	1.83	0.43
30:A:464:U:H2'	30:A:465:C:C6	2.54	0.43
30:A:639:U:H2'	30:A:640:G:C8	2.52	0.43
41:Aa:9:A:N6	48:Ad:196:GLU:O	2.51	0.43
41:Aa:417:U:H2'	41:Aa:418:G:O4'	2.18	0.43
41:Aa:1153:G:H2'	41:Aa:1154:G:C8	2.51	0.43
41:Aa:1255:A:H2'	41:Aa:1256:A:C8	2.53	0.43
41:Aa:1265:G:H2'	41:Aa:1289:A:H61	1.82	0.43
6:C:79:ASP:N	6:C:93:LEU:O	2.46	0.43
8:E:154:VAL:HB	8:E:175:VAL:HG22	1.99	0.43
11:I:70:ARG:HB2	11:I:76:TYR:CE2	2.54	0.43
30:A:476:A:H5"	30:A:477:U:OP2	2.18	0.43
30:A:597:U:H2'	30:A:598:G:O4'	2.19	0.43
30:A:878:C:H2'	30:A:879:U:C6	2.53	0.43
30:A:1219:G:O2'	30:A:1220:A:H8	2.00	0.43
30:A:1570:G:H2'	30:A:1571:G:C8	2.53	0.43
30:A:2774:G:O6	30:A:2782:C:H5"	2.19	0.43
41:Aa:1081:U:H2'	41:Aa:1082:C:H6	1.82	0.43
6:C:225:MET:HG2	30:A:827:A:C2	2.53	0.43
30:A:332:A:H2'	30:A:333:C:H6	1.82	0.43
30:A:1208:A:H2'	30:A:1209:U:C6	2.53	0.43
30:A:2495:A:HO2'	30:A:2496:A:H8	1.64	0.43
31:Ae:40:GLY:HA3	31:Ae:117:LEU:HB3	2.01	0.43
36:Ao:13:LYS:HG2	36:Ao:16:ARG:NH2	2.34	0.43
41:Aa:568:A:H4'	41:Aa:569:U:H5"	1.99	0.43
41:Aa:703:A:H2'	41:Aa:704:A:C8	2.53	0.43
41:Aa:984:A:H5'	41:Aa:984:A:H8	1.83	0.43
41:Aa:1122:A:OP1	41:Aa:1193:U:O2'	2.27	0.43
2:2:30:LYS:HB3	2:2:30:LYS:HE3	1.81	0.43
6:C:145:GLU:HG2	6:C:151:GLY:C	2.43	0.43
12:J:73:GLU:O	12:J:106:LYS:HB3	2.18	0.43
18:P:2:PHE:CE1	18:P:42:GLY:HA3	2.53	0.43
19:Q:4:LYS:HB3	19:Q:4:LYS:HE2	1.56	0.43
30:A:886:A:H2'	30:A:887:A:C8	2.54	0.43
30:A:1563:U:H2'	30:A:1564:G:H8	1.83	0.43
30:A:2273:G:H2'	30:A:2274:A:C8	2.54	0.43
31:Ae:95:PHE:O	31:Ae:125:SER:HA	2.18	0.43
7:D:142:SER:OG	30:A:2020:U:H4'	2.19	0.43
8:E:110:LEU:HD23	8:E:110:LEU:HA	1.91	0.43
30:A:637:U:H2'	30:A:638:U:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:A:805:G:H2'	30:A:806:A:O4'	2.18	0.43
30:A:1084:U:H2'	30:A:1085:U:O4'	2.17	0.43
41:Aa:1365:A:H2'	41:Aa:1366:G:C8	2.53	0.43
30:A:59:U:H1'	30:A:73:A:H2'	2.00	0.43
30:A:2278:OMG:HM23	30:A:2278:OMG:H1'	1.73	0.43
30:A:2341:A:H2'	30:A:2342:U:C6	2.54	0.43
41:Aa:963:G:H2'	41:Aa:964:U:H6	1.83	0.43
41:Aa:1319:G:N7	44:Am:98:ARG:NH2	2.67	0.43
3:3:41:LYS:HB2	3:3:41:LYS:HE2	1.73	0.43
3:3:60:GLN:NE2	30:A:636:A:O2'	2.32	0.43
16:N:77:PRO:O	16:N:80:THR:HG22	2.19	0.43
41:Aa:271:A:H2'	41:Aa:272:C:C5	2.54	0.43
41:Aa:493:G:O2'	41:Aa:494:U:OP2	2.36	0.43
41:Aa:931:G:H2'	41:Aa:932:A:C8	2.53	0.43
41:Aa:1024:G:H8	41:Aa:1024:G:OP2	2.01	0.43
41:Aa:1487:A:H2'	41:Aa:1488:C:O4'	2.18	0.43
30:A:247:A:H2'	30:A:248:G:O4'	2.18	0.43
30:A:906:A:H2'	30:A:907:G:O4'	2.19	0.43
33:Ag:150:ALA:O	45:Ak:59:THR:HG21	2.18	0.43
41:Aa:150:U:H2'	41:Aa:151:A:H8	1.84	0.43
41:Aa:430:C:P	41:Aa:430:C:H6	2.42	0.43
41:Aa:437:U:H4'	41:Aa:438:A:O5'	2.18	0.43
41:Aa:682:G:H21	45:Ak:118:HIS:HB2	1.84	0.43
41:Aa:847:G:H2'	41:Aa:848:G:C8	2.54	0.43
52:8:19:G:O6	52:8:56:U:O2'	2.36	0.43
8:E:157:GLU:HG2	8:E:201:LYS:HE2	2.00	0.42
12:J:55:LEU:HD23	12:J:60:ARG:HB3	2.01	0.42
30:A:421:C:H2'	30:A:422:G:H8	1.83	0.42
30:A:1185:U:H4'	30:A:1186:A:O4'	2.19	0.42
30:A:1269:A:H2'	30:A:1270:U:C6	2.54	0.42
30:A:1315:C:H2'	30:A:1316:G:H8	1.84	0.42
30:A:1326:C:H2'	30:A:1327:C:C6	2.54	0.42
30:A:1391:A:H2'	30:A:1392:G:O4'	2.19	0.42
30:A:1973:U:H2'	30:A:1974:C:H6	1.84	0.42
30:A:2601:G7M:O5'	30:A:2601:G7M:H8	2.19	0.42
39:Ar:66:ARG:NE	41:Aa:744:U:OP1	2.48	0.42
41:Aa:276:U:H2'	41:Aa:277:U:C6	2.54	0.42
41:Aa:1023:A:C2	41:Aa:1229:U:H1'	2.54	0.42
46:Ab:169:GLU:O	46:Ab:173:ILE:HG12	2.19	0.42
2:2:26:LYS:NZ	30:A:214:G:OP1	2.46	0.42
4:4:10:ILE:HG23	30:A:2504:C:N4	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:11:A:P	23:U:82:ARG:HH11	2.42	0.42
19:Q:94:SER:HB3	30:A:2040:A:O2'	2.19	0.42
23:U:53:ILE:HG12	23:U:85:LYS:HG3	2.01	0.42
39:Ar:37:PHE:CD1	39:Ar:60:LEU:HD21	2.54	0.42
41:Aa:1083:G:H2'	41:Aa:1084:U:H6	1.83	0.42
41:Aa:1189:A:H2'	41:Aa:1190:A:O4'	2.19	0.42
42:Aj:66:GLU:HB3	49:An:59:ALA:HB2	2.01	0.42
48:Ad:18:SER:OG	48:Ad:25:GLU:OE1	2.25	0.42
30:A:65:A:H2'	30:A:66:C:C6	2.54	0.42
30:A:391:A:H2'	30:A:392:U:C6	2.54	0.42
30:A:737:C:H2'	30:A:738:U:C6	2.54	0.42
30:A:1642:C:H2'	30:A:1643:C:H6	1.84	0.42
30:A:2330:G:O6	30:A:2341:A:N6	2.53	0.42
30:A:2529:G:H5"	30:A:2530:2MA:H5"	2.00	0.42
31:Ae:131:ASN:HA	31:Ae:136:MET:HE2	2.00	0.42
41:Aa:1141:A:H2'	41:Aa:1142:U:C6	2.54	0.42
42:Aj:18:ILE:HD13	42:Aj:72:ARG:HG2	2.02	0.42
43:Ac:141:MET:HG3	43:Ac:169:GLU:OE1	2.19	0.42
5:B:65:G:H2'	5:B:66:C:H6	1.85	0.42
22:T:9:ARG:HG2	22:T:42:LYS:HG2	2.01	0.42
30:A:4:U:H2'	30:A:5:A:C8	2.54	0.42
30:A:127:C:H2'	30:A:128:C:H6	1.84	0.42
30:A:266:A:H1'	30:A:476:A:N3	2.34	0.42
30:A:1726:A:H2'	30:A:1727:C:C6	2.55	0.42
38:Aq:53:ASN:N	38:Aq:53:ASN:HD22	2.18	0.42
10:H:43:VAL:HG22	17:O:100:ILE:HG13	2.00	0.42
15:M:19:ARG:NH1	15:M:22:LEU:O	2.49	0.42
30:A:616:G:O6	30:A:2056:G:O2'	2.35	0.42
30:A:920:A:H2'	30:A:921:C:C6	2.55	0.42
30:A:2682:G:N2	30:A:2692:A:OP2	2.38	0.42
44:Am:90:ARG:HB2	44:Am:97:VAL:HG12	2.01	0.42
45:Ak:88:GLY:H	45:Ak:114:THR:HG23	1.84	0.42
8:E:7:LEU:HD23	8:E:13:LYS:HA	2.02	0.42
30:A:296:G:O2'	30:A:297:G:H5'	2.19	0.42
30:A:2038:U:H2'	30:A:2039:G:O4'	2.20	0.42
39:Ar:38:ILE:HD13	39:Ar:73:LEU:HD22	2.01	0.42
41:Aa:439:A:H2'	41:Aa:440:A:O4'	2.20	0.42
47:Ah:104:ALA:HB3	47:Ah:115:ASP:HB3	2.01	0.42
1:1:43:ASN:OD1	30:A:2397:G:O2'	2.37	0.42
8:E:125:VAL:HA	8:E:194:ILE:O	2.20	0.42
9:G:2:SER:O	9:G:6:LYS:N	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:57:ARG:HH21	22:T:77:TYR:HE1	1.67	0.42
29:11:70:G:H2'	29:11:71:G:C8	2.54	0.42
30:A:328:G:N2	30:A:399:U:H1'	2.35	0.42
30:A:396:G:O2'	30:A:397:U:OP1	2.27	0.42
30:A:403:U:H2'	30:A:404:U:C6	2.55	0.42
30:A:544:U:H2'	30:A:545:G:O4'	2.20	0.42
30:A:659:A:H2'	30:A:660:A:C8	2.55	0.42
30:A:786:U:H2'	30:A:787:U:C6	2.55	0.42
30:A:2372:G:N3	30:A:2408:C:H2'	2.34	0.42
41:Aa:1333:G:H2'	41:Aa:1334:A:H8	1.85	0.42
43:Ac:189:ASP:OD1	43:Ac:194:LYS:HE2	2.20	0.42
5:B:59:U:H2'	5:B:60:C:H6	1.85	0.42
30:A:175:C:H2'	30:A:176:A:O4'	2.20	0.42
30:A:2284:U:O2'	30:A:2285:C:H5'	2.20	0.42
30:A:2541:U:H2'	30:A:2542:C:C6	2.54	0.42
31:Ae:126:LYS:NZ	41:Aa:10:G:OP2	2.40	0.42
31:Ae:149:ASN:O	31:Ae:153:VAL:HG13	2.20	0.42
41:Aa:626:C:N4	41:Aa:629:A:OP2	2.52	0.42
41:Aa:899:G:O2'	41:Aa:915:G:O6	2.29	0.42
44:Am:10:PRO:HB2	44:Am:13:LYS:HD2	2.01	0.42
16:N:29:ARG:NH1	16:N:44:VAL:HG11	2.35	0.42
30:A:625:G:H2'	30:A:626:G:H8	1.84	0.42
30:A:2098:A:H2'	30:A:2099:G:H8	1.83	0.42
30:A:2319:U:H2'	30:A:2320:C:C6	2.55	0.42
30:A:2817:A:H5"	30:A:2912:A:C2	2.53	0.42
33:Ag:80:VAL:HG11	33:Ag:154:TYR:CE1	2.55	0.42
37:Ap:74:ILE:O	37:Ap:78:GLU:HG2	2.20	0.42
41:Aa:212:A:H4'	41:Aa:213:G:OP1	2.20	0.42
41:Aa:305:G:H4'	41:Aa:565:G:H4'	2.01	0.42
41:Aa:1101:U:H2'	41:Aa:1102:U:C6	2.55	0.42
41:Aa:1312:U:OP1	44:Am:13:LYS:HE3	2.19	0.42
5:B:112:A:H2'	5:B:113:G:C8	2.55	0.42
20:R:6:ILE:HG23	20:R:33:VAL:HG21	2.02	0.42
41:Aa:511:A:H2'	41:Aa:512:C:C6	2.54	0.42
41:Aa:745:U:H2'	41:Aa:746:U:C6	2.55	0.42
41:Aa:1136:U:HO2'	41:Aa:1137:U:P	2.43	0.42
41:Aa:1324:C:H2'	41:Aa:1325:U:H6	1.82	0.42
47:Ah:94:MET:HE3	47:Ah:124:GLY:HA2	2.02	0.42
15:M:94:PHE:CZ	15:M:109:ALA:HB2	2.55	0.41
21:S:64:HIS:CD2	30:A:371:U:H4'	2.55	0.41
30:A:972:A:H2'	30:A:973:A:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:Aa:1114:C:H4'	46:Ab:97:LEU:HD13	2.01	0.41
42:Aj:63:GLU:OE2	49:An:49:TYR:OH	2.27	0.41
7:D:107:VAL:HG21	7:D:193:LYS:HA	2.00	0.41
21:S:70:LEU:HD23	21:S:70:LEU:HA	1.89	0.41
30:A:266:A:H2'	30:A:267:G:O4'	2.20	0.41
30:A:703:A:H2'	30:A:704:U:C6	2.55	0.41
30:A:2274:A:H2'	30:A:2275:C:H6	1.85	0.41
30:A:2400:U:H2'	30:A:2401:C:C6	2.55	0.41
31:Ae:57:PRO:O	31:Ae:61:LYS:HG2	2.20	0.41
36:Ao:47:LYS:HB2	36:Ao:47:LYS:HE2	1.70	0.41
41:Aa:33:A:H2'	41:Aa:34:A:C8	2.55	0.41
41:Aa:184:A:N1	41:Aa:207:G:C6	2.87	0.41
46:Ab:14:VAL:C	46:Ab:203:ASN:HB3	2.44	0.41
28:F:33:LYS:HA	28:F:96:MET:SD	2.61	0.41
30:A:145:A:H2'	30:A:146:U:C6	2.55	0.41
30:A:1209:U:H2'	30:A:1210:U:C6	2.55	0.41
30:A:1237:U:H2'	30:A:1238:U:C6	2.56	0.41
30:A:2874:A:H2'	30:A:2875:U:C6	2.55	0.41
31:Ae:149:ASN:OD1	31:Ae:149:ASN:N	2.43	0.41
41:Aa:23:G:O2'	41:Aa:922:A:N1	2.49	0.41
41:Aa:1365:A:H2'	41:Aa:1366:G:H8	1.86	0.41
45:Ak:35:THR:OG1	45:Ak:36:ASP:N	2.53	0.41
5:B:26:C:H2'	5:B:27:A:O4'	2.20	0.41
5:B:30:U:H2'	5:B:31:G:H8	1.85	0.41
5:B:58:C:C2	5:B:59:U:C5	3.09	0.41
6:C:49:LEU:HD21	6:C:52:ARG:HA	2.02	0.41
7:D:134:HIS:CD2	7:D:168:LYS:HB3	2.56	0.41
24:V:49:VAL:HG12	24:V:54:LEU:HG	2.02	0.41
30:A:2327:A:H2'	30:A:2328:A:H8	1.84	0.41
31:Ae:120:ILE:HG22	31:Ae:122:ASP:H	1.86	0.41
36:Ao:14:GLU:HG2	36:Ao:15:TYR:CD2	2.55	0.41
41:Aa:98:U:H2'	41:Aa:99:U:C6	2.55	0.41
41:Aa:601:U:H2'	41:Aa:602:U:C6	2.55	0.41
41:Aa:994:C:H2'	41:Aa:995:A:H8	1.84	0.41
41:Aa:1248:A:H2	41:Aa:1251:G:N3	2.18	0.41
41:Aa:1385:A:H2'	41:Aa:1386:U:O4'	2.20	0.41
47:Ah:52:VAL:HB	47:Ah:59:VAL:HB	2.01	0.41
5:B:48:A:OP1	15:M:68:THR:HG22	2.20	0.41
5:B:66:C:H2'	5:B:67:G:O4'	2.20	0.41
17:O:86:ALA:HB2	17:O:116:ALA:HB2	2.03	0.41
30:A:1157:U:H2'	30:A:1158:G:H8	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:A:2053:U:H2'	30:A:2054:G:O4'	2.20	0.41
30:A:2800:U:H2'	30:A:2801:C:H6	1.85	0.41
32:Af:52:ILE:O	32:Af:55:PHE:HB2	2.20	0.41
41:Aa:1185:G:H2'	41:Aa:1186:A:H8	1.84	0.41
5:B:29:C:O2'	5:B:30:U:H5'	2.20	0.41
8:E:131:PHE:CZ	8:E:138:GLU:HG2	2.55	0.41
20:R:51:ALA:N	20:R:81:THR:O	2.51	0.41
30:A:4:U:H2'	30:A:5:A:H8	1.84	0.41
30:A:753:U:H2'	30:A:754:U:C6	2.55	0.41
30:A:1492:G:H2'	30:A:1493:U:C6	2.55	0.41
30:A:2581:U:H2'	30:A:2582:U:C6	2.56	0.41
31:Ae:77:VAL:HG22	31:Ae:78:GLU:HG2	2.02	0.41
34:Ai:117:LYS:HE2	41:Aa:1197:G:H5'	2.01	0.41
41:Aa:527:C:H2'	41:Aa:528:A:O4'	2.21	0.41
41:Aa:1196:G:H21	49:An:61:TRP:C	2.28	0.41
13:K:54:MET:HE3	13:K:54:MET:HB2	1.91	0.41
30:A:2677:C:H2'	30:A:2678:C:C6	2.56	0.41
32:Af:41:LYS:HB3	32:Af:41:LYS:HE3	1.62	0.41
37:Ap:16:PRO:HD2	37:Ap:43:THR:HG21	2.01	0.41
40:At:21:ASN:HB3	40:At:65:LEU:HD21	2.02	0.41
41:Aa:71:A:H2'	41:Aa:72:C:C6	2.56	0.41
41:Aa:1201:A:OP2	43:Ac:3:GLN:NE2	2.54	0.41
5:B:106:G:H2'	5:B:107:U:H6	1.86	0.41
7:D:159:ASP:HA	7:D:160:ALA:HA	1.81	0.41
10:H:56:ILE:HA	10:H:124:PHE:O	2.20	0.41
30:A:1304:G:O2'	30:A:2039:G:O6	2.36	0.41
30:A:1368:C:H2'	30:A:1370:C:C5	2.55	0.41
37:Ap:5:ILE:HG12	37:Ap:22:VAL:HG22	2.02	0.41
41:Aa:185:U:H2'	41:Aa:186:U:C6	2.56	0.41
41:Aa:407:G:H2'	41:Aa:408:C:H6	1.86	0.41
41:Aa:901:A:H2'	41:Aa:902:C:C6	2.56	0.41
41:Aa:1113:A:H2'	41:Aa:1114:C:C6	2.56	0.41
41:Aa:1236:C:C4	44:Am:103:LYS:HG3	2.56	0.41
41:Aa:1466:G:H2'	41:Aa:1467:A:H8	1.86	0.41
44:Am:14:ARG:HE	44:Am:42:ASP:HA	1.85	0.41
5:B:44:A:C5	5:B:45:C:C5	3.09	0.41
5:B:101:A:H2'	5:B:102:G:O4'	2.21	0.41
15:M:72:LEU:O	15:M:76:VAL:HG23	2.20	0.41
16:N:48:VAL:HG11	16:N:112:ILE:HD12	2.03	0.41
17:O:51:ARG:HD3	30:A:1200:A:C5	2.56	0.41
30:A:463:C:H2'	30:A:464:U:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:A:620:G:O2'	30:A:1292:A:OP1	2.36	0.41
30:A:1701:U:H2'	30:A:1702:C:H6	1.85	0.41
30:A:2290:C:H4'	30:A:2356:A:H4'	2.03	0.41
30:A:2322:C:O2'	30:A:2323:U:H5'	2.21	0.41
30:A:2347:A:N6	30:A:2360:A:O2'	2.54	0.41
30:A:2491:C:H2'	30:A:2492:C:O4'	2.20	0.41
33:Ag:41:ARG:HH22	41:Aa:1301:U:P	2.42	0.41
41:Aa:810:A:H2'	41:Aa:811:G:O4'	2.21	0.41
41:Aa:1356:A:N1	41:Aa:1384:A:H5"	2.36	0.41
41:Aa:1397:G:H2'	41:Aa:1398:U:C6	2.56	0.41
43:Ac:107:LYS:HE3	43:Ac:110:LEU:HD12	2.03	0.41
45:Ak:53:LYS:HA	45:Ak:53:LYS:HD3	1.99	0.41
51:d:3:A:H2'	51:d:4:G:C8	2.56	0.41
6:C:173:LEU:HD11	6:C:271:VAL:HG21	2.03	0.41
12:J:82:LEU:HD23	12:J:82:LEU:HA	1.92	0.41
30:A:459:C:H2'	30:A:460:C:C6	2.56	0.41
41:Aa:38:U:O2'	41:Aa:508:G:H4'	2.21	0.41
41:Aa:68:C:H2'	41:Aa:69:G:C8	2.56	0.41
41:Aa:468:G:H2'	41:Aa:469:U:C6	2.56	0.41
41:Aa:686:U:H2'	41:Aa:687:C:C6	2.56	0.41
41:Aa:1165:U:H2'	41:Aa:1166:G:O4'	2.21	0.41
41:Aa:1331:U:H2'	41:Aa:1332:C:C5	2.56	0.41
48:Ad:69:ARG:HD3	48:Ad:198:TYR:CE1	2.56	0.41
13:K:22:LYS:NZ	30:A:909:G:N7	2.62	0.40
19:Q:78:GLU:O	30:A:24:G:O2'	2.39	0.40
29:11:70:G:H2'	29:11:71:G:H8	1.86	0.40
30:A:1919:C:H2'	30:A:1920:C:H6	1.85	0.40
30:A:2051:C:H2'	30:A:2052:C:H6	1.86	0.40
33:Ag:122:ASN:HD22	33:Ag:122:ASN:HA	1.71	0.40
41:Aa:586:C:O2'	41:Aa:736:A:N3	2.47	0.40
41:Aa:1084:U:H2'	41:Aa:1085:G:O4'	2.21	0.40
41:Aa:1124:C:O2'	43:Ac:14:ILE:HD12	2.21	0.40
3:3:53:SER:HB2	30:A:879:U:O3'	2.20	0.40
10:H:20:ASP:OD2	10:H:59:ASN:HB2	2.20	0.40
30:A:1702:C:H2'	30:A:1703:U:C6	2.56	0.40
30:A:2675:G:H2'	30:A:2676:U:C6	2.56	0.40
30:A:2777:A:H1'	30:A:2779:C:N4	2.36	0.40
41:Aa:227:C:H2'	41:Aa:228:A:O4'	2.22	0.40
41:Aa:1435:A:H2	41:Aa:1486:G:H22	1.68	0.40
43:Ac:91:ASN:HD21	43:Ac:98:VAL:HB	1.86	0.40
18:P:64:LYS:HB2	18:P:64:LYS:HE3	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Q:19:LEU:HD23	19:Q:19:LEU:HA	1.88	0.40
22:T:65:VAL:O	22:T:65:VAL:HG23	2.19	0.40
30:A:226:A:N1	30:A:453:G:O2'	2.46	0.40
30:A:524:A:N1	30:A:545:G:H4'	2.37	0.40
30:A:765:U:H2'	30:A:766:G:H8	1.86	0.40
30:A:1028:G:N3	30:A:1028:G:H2'	2.35	0.40
30:A:2074:C:H2'	30:A:2075:G:H8	1.87	0.40
30:A:2629:A:P	52:8:75:C:H5"	2.61	0.40
33:Ag:92:ARG:O	33:Ag:96:ARG:HG3	2.21	0.40
41:Aa:218:U:H2'	41:Aa:219:C:O4'	2.22	0.40
41:Aa:1278:G:H8	41:Aa:1278:G:OP2	2.04	0.40
41:Aa:1515:G:H4'	41:Aa:1516:G:C4	2.57	0.40
2:2:9:ASN:HB3	2:2:12:LYS:HB3	2.03	0.40
3:3:52:LYS:O	3:3:56:LYS:HG3	2.21	0.40
7:D:67:LYS:HE3	30:A:2850:G:H5'	2.03	0.40
7:D:72:PRO:HG3	30:A:2814:C:H1'	2.04	0.40
30:A:401:U:H2'	30:A:402:C:C6	2.56	0.40
41:Aa:254:A:C2	41:Aa:290:A:C5	3.09	0.40
41:Aa:277:U:H2'	41:Aa:278:A:C8	2.57	0.40
41:Aa:1326:G:H4'	49:An:18:VAL:HG11	2.03	0.40
52:8:51:G:C2'	52:8:52:U:H5'	2.52	0.40
1:1:37:LYS:HA	1:1:37:LYS:HD2	1.96	0.40
9:G:149:ARG:HG3	9:G:162:ILE:O	2.21	0.40
30:A:346:A:H2'	30:A:347:U:H6	1.87	0.40
30:A:2293:A:H4'	30:A:2294:A:N3	2.37	0.40
30:A:2688:G:H2'	30:A:2689:A:C8	2.56	0.40
41:Aa:469:U:H2'	41:Aa:470:A:H8	1.86	0.40
42:Aj:59:LYS:HE2	42:Aj:62:ARG:NH2	2.36	0.40
48:Ad:172:LEU:HD23	48:Ad:172:LEU:HA	1.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	46/52 (88%)	45 (98%)	1 (2%)	0	100	100
2	2	42/45 (93%)	42 (100%)	0	0	100	100
3	3	63/66 (96%)	62 (98%)	1 (2%)	0	100	100
4	4	35/37 (95%)	35 (100%)	0	0	100	100
6	C	272/277 (98%)	269 (99%)	3 (1%)	0	100	100
7	D	213/220 (97%)	203 (95%)	10 (5%)	0	100	100
8	E	204/207 (99%)	201 (98%)	3 (2%)	0	100	100
9	G	152/178 (85%)	133 (88%)	19 (12%)	0	100	100
10	H	143/145 (99%)	138 (96%)	5 (4%)	0	100	100
11	I	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
12	J	144/146 (99%)	140 (97%)	4 (3%)	0	100	100
13	K	135/144 (94%)	133 (98%)	2 (2%)	0	100	100
14	L	114/122 (93%)	112 (98%)	2 (2%)	0	100	100
15	M	117/119 (98%)	111 (95%)	6 (5%)	0	100	100
16	N	107/116 (92%)	105 (98%)	2 (2%)	0	100	100
17	O	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
18	P	100/102 (98%)	99 (99%)	1 (1%)	0	100	100
19	Q	109/117 (93%)	108 (99%)	1 (1%)	0	100	100
20	R	87/91 (96%)	85 (98%)	2 (2%)	0	100	100
21	S	89/105 (85%)	83 (93%)	6 (7%)	0	100	100
22	T	86/217 (40%)	83 (96%)	3 (4%)	0	100	100
23	U	77/94 (82%)	75 (97%)	2 (3%)	0	100	100
24	V	46/62 (74%)	46 (100%)	0	0	100	100
25	W	62/73 (85%)	59 (95%)	3 (5%)	0	100	100
26	X	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
27	Z	40/57 (70%)	40 (100%)	0	0	100	100
28	F	139/179 (78%)	130 (94%)	9 (6%)	0	100	100
31	Ae	154/166 (93%)	147 (96%)	7 (4%)	0	100	100
32	Af	93/98 (95%)	89 (96%)	4 (4%)	0	100	100
33	Ag	152/156 (97%)	151 (99%)	1 (1%)	0	100	100
34	Ai	125/132 (95%)	119 (95%)	6 (5%)	0	100	100
35	Al	130/137 (95%)	124 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	Ao	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
37	Ap	87/91 (96%)	82 (94%)	5 (6%)	0	100	100
38	Aq	70/87 (80%)	64 (91%)	6 (9%)	0	100	100
39	Ar	52/80 (65%)	51 (98%)	1 (2%)	0	100	100
40	At	79/83 (95%)	76 (96%)	3 (4%)	0	100	100
42	Aj	90/102 (88%)	86 (96%)	4 (4%)	0	100	100
43	Ac	200/217 (92%)	194 (97%)	6 (3%)	0	100	100
44	Am	112/121 (93%)	109 (97%)	3 (3%)	0	100	100
45	Ak	108/129 (84%)	106 (98%)	2 (2%)	0	100	100
46	Ab	92/255 (36%)	87 (95%)	5 (5%)	0	100	100
47	Ah	129/132 (98%)	124 (96%)	5 (4%)	0	100	100
48	Ad	197/200 (98%)	190 (96%)	7 (4%)	0	100	100
49	An	58/61 (95%)	58 (100%)	0	0	100	100
50	As	80/92 (87%)	79 (99%)	1 (1%)	0	100	100
54	13	43/84 (51%)	42 (98%)	1 (2%)	0	100	100
All	All	5049/5782 (87%)	4883 (97%)	166 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	33/50 (66%)	33 (100%)	0	100	100
2	2	38/40 (95%)	38 (100%)	0	100	100
3	3	51/57 (90%)	51 (100%)	0	100	100
4	4	31/35 (89%)	31 (100%)	0	100	100
6	C	206/224 (92%)	205 (100%)	1 (0%)	86	93
7	D	160/177 (90%)	158 (99%)	2 (1%)	65	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	E	150/169 (89%)	148 (99%)	2 (1%)	65 77
9	G	44/155 (28%)	44 (100%)	0	100 100
10	H	121/123 (98%)	121 (100%)	0	100 100
11	I	85/100 (85%)	85 (100%)	0	100 100
12	J	100/112 (89%)	100 (100%)	0	100 100
13	K	95/119 (80%)	95 (100%)	0	100 100
14	L	88/102 (86%)	87 (99%)	1 (1%)	70 81
15	M	57/95 (60%)	56 (98%)	1 (2%)	54 67
16	N	73/102 (72%)	72 (99%)	1 (1%)	62 75
17	O	96/98 (98%)	96 (100%)	0	100 100
18	P	73/86 (85%)	72 (99%)	1 (1%)	62 75
19	Q	80/94 (85%)	79 (99%)	1 (1%)	65 77
20	R	66/82 (80%)	66 (100%)	0	100 100
21	S	54/90 (60%)	51 (94%)	3 (6%)	17 20
22	T	49/190 (26%)	48 (98%)	1 (2%)	50 63
23	U	53/75 (71%)	53 (100%)	0	100 100
24	V	32/52 (62%)	29 (91%)	3 (9%)	7 6
25	W	42/66 (64%)	41 (98%)	1 (2%)	44 56
26	X	49/53 (92%)	49 (100%)	0	100 100
27	Z	37/50 (74%)	35 (95%)	2 (5%)	18 21
28	F	54/158 (34%)	48 (89%)	6 (11%)	5 4
31	Ae	114/131 (87%)	107 (94%)	7 (6%)	15 17
32	Af	68/86 (79%)	66 (97%)	2 (3%)	37 48
33	Ag	129/132 (98%)	125 (97%)	4 (3%)	35 45
34	Ai	97/109 (89%)	94 (97%)	3 (3%)	35 45
35	Al	106/119 (89%)	99 (93%)	7 (7%)	14 15
36	Ao	78/81 (96%)	74 (95%)	4 (5%)	20 24
37	Ap	69/77 (90%)	68 (99%)	1 (1%)	62 75
38	Aq	50/82 (61%)	47 (94%)	3 (6%)	16 18
39	Ar	48/68 (71%)	43 (90%)	5 (10%)	5 5
40	At	61/69 (88%)	56 (92%)	5 (8%)	9 8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
42	Aj	72/91 (79%)	69 (96%)	3 (4%)	25 32
43	Ac	135/175 (77%)	134 (99%)	1 (1%)	81 89
44	Am	82/104 (79%)	77 (94%)	5 (6%)	15 17
45	Ak	70/104 (67%)	58 (83%)	12 (17%)	1 1
46	Ab	32/221 (14%)	30 (94%)	2 (6%)	15 16
47	Ah	112/113 (99%)	109 (97%)	3 (3%)	40 51
48	Ad	142/175 (81%)	136 (96%)	6 (4%)	25 32
49	An	52/53 (98%)	52 (100%)	0	100 100
50	As	59/80 (74%)	59 (100%)	0	100 100
54	13	22/75 (29%)	22 (100%)	0	100 100
All	All	3615/4899 (74%)	3516 (97%)	99 (3%)	41 51

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	C	101	LYS
7	D	107	VAL
7	D	200	ASN
8	E	124	THR
8	E	191	SER
14	L	92	ARG
15	M	52	THR
16	N	68	SER
18	P	12	ILE
19	Q	11	ARG
21	S	66	SER
21	S	92	ARG
21	S	101	ILE
22	T	42	LYS
24	V	38	ILE
24	V	50	SER
24	V	55	LYS
25	W	24	SER
27	Z	21	LYS
27	Z	30	CYS
28	F	35	VAL
28	F	88	LYS
28	F	89	VAL

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Mol	Chain	Res	Type
28	F	130	LEU
28	F	137	ILE
28	F	172	ASN
31	Ae	17	THR
31	Ae	34	THR
31	Ae	73	VAL
31	Ae	77	VAL
31	Ae	80	THR
31	Ae	127	SER
31	Ae	153	VAL
32	Af	73	THR
32	Af	83	SER
33	Ag	17	ILE
33	Ag	72	VAL
33	Ag	75	VAL
33	Ag	80	VAL
34	Ai	47	ILE
34	Ai	99	SER
34	Ai	130	SER
35	Al	21	SER
35	Al	30	SER
35	Al	36	THR
35	Al	48	THR
35	Al	75	GLU
35	Al	91	SER
35	Al	100	VAL
36	Ao	48	LYS
36	Ao	58	LYS
36	Ao	84	SER
36	Ao	88	ARG
37	Ap	27	SER
38	Aq	54	SER
38	Aq	69	LEU
38	Aq	78	VAL
39	Ar	24	THR
39	Ar	25	HIS
39	Ar	31	THR
39	Ar	33	LEU
39	Ar	67	SER
40	At	22	ILE
40	At	33	LYS
40	At	39	VAL

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Mol	Chain	Res	Type
40	At	51	SER
40	At	76	SER
42	Aj	6	ILE
42	Aj	18	ILE
42	Aj	77	VAL
43	Ac	171	THR
44	Am	7	VAL
44	Am	15	VAL
44	Am	16	VAL
44	Am	45	VAL
44	Am	114	LYS
45	Ak	26	THR
45	Ak	33	THR
45	Ak	43	SER
45	Ak	67	SER
45	Ak	73	SER
45	Ak	76	GLU
45	Ak	82	VAL
45	Ak	86	VAL
45	Ak	95	SER
45	Ak	113	VAL
45	Ak	116	VAL
45	Ak	119	ASN
46	Ab	106	THR
46	Ab	199	VAL
47	Ah	34	LYS
47	Ah	43	GLU
47	Ah	120	LYS
48	Ad	12	SER
48	Ad	77	LYS
48	Ad	89	LEU
48	Ad	92	SER
48	Ad	137	GLN
48	Ad	140	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
2	2	27	ASN
3	3	21	GLN
3	3	35	ASN
3	3	60	GLN

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Mol	Chain	Res	Type
7	D	134	HIS
7	D	136	GLN
7	D	167	GLN
7	D	200	ASN
8	E	148	GLN
8	E	174	GLN
9	G	111	HIS
11	I	45	ASN
12	J	104	ASN
13	K	35	GLN
14	L	106	GLN
15	M	37	ASN
15	M	39	HIS
16	N	113	GLN
17	O	52	GLN
17	O	108	GLN
19	Q	65	ASN
20	R	47	ASN
23	U	58	ASN
23	U	86	GLN
24	V	30	ASN
25	W	40	GLN
28	F	63	GLN
28	F	127	ASN
33	Ag	19	ASN
33	Ag	130	ASN
34	Ai	29	ASN
34	Ai	52	GLN
34	Ai	128	GLN
35	Al	39	ASN
36	Ao	5	GLN
36	Ao	9	ASN
38	Aq	53	ASN
40	At	3	ASN
43	Ac	3	GLN
43	Ac	91	ASN
43	Ac	101	ASN
44	Am	104	ASN
45	Ak	18	ASN
45	Ak	119	ASN
47	Ah	18	ASN
47	Ah	22	HIS

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Mol	Chain	Res	Type
48	Ad	146	GLN
50	As	69	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
29	11	13/15 (86%)	5 (38%)	0
30	A	2562/2923 (87%)	303 (11%)	9 (0%)
41	Aa	1423/1552 (91%)	171 (12%)	0
5	B	112/115 (97%)	15 (13%)	0
51	d	17/19 (89%)	3 (17%)	0
52	8	67/71 (94%)	13 (19%)	0
53	9	4/5 (80%)	1 (25%)	0
All	All	4198/4700 (89%)	511 (12%)	9 (0%)

All (511) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	B	10	U
5	B	11	A
5	B	23	U
5	B	30	U
5	B	33	U
5	B	34	C
5	B	39	G
5	B	49	G
5	B	50	A
5	B	54	U
5	B	55	A
5	B	64	A
5	B	87	U
5	B	88	G
5	B	106	G
29	11	2	C
29	11	5	G
29	11	71	G
29	11	74	C
29	11	76	A
30	A	15	G
30	A	34	U
30	A	63	U

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Mol	Chain	Res	Type
30	A	71	A
30	A	75	G
30	A	84	A
30	A	91	A
30	A	93	U
30	A	96	G
30	A	101	G
30	A	117	A
30	A	118	A
30	A	119	U
30	A	130	A
30	A	136	A
30	A	153	G
30	A	161	A
30	A	164	A
30	A	177	G
30	A	184	C
30	A	185	A
30	A	199	A
30	A	202	A
30	A	216	A
30	A	218	G
30	A	219	A
30	A	225	A
30	A	226	A
30	A	251	G
30	A	269	G
30	A	272	C
30	A	279	A
30	A	292	U
30	A	294	G
30	A	295	G
30	A	318	A
30	A	321	U
30	A	324	A
30	A	327	G
30	A	328	G
30	A	354	A
30	A	364	A
30	A	373	A
30	A	381	G
30	A	389	A

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Mol	Chain	Res	Type
30	A	393	G
30	A	397	U
30	A	401	U
30	A	402	C
30	A	412	U
30	A	429	C
30	A	432	G
30	A	445	G
30	A	450	C
30	A	457	G
30	A	470	G
30	A	474	A
30	A	476	A
30	A	481	C
30	A	482	U
30	A	526	A
30	A	527	G
30	A	549	U
30	A	550	A
30	A	552	A
30	A	553	A
30	A	567	G
30	A	576	U
30	A	577	A
30	A	578	G
30	A	583	A
30	A	593	U
30	A	594	G
30	A	606	G
30	A	616	G
30	A	617	A
30	A	618	A
30	A	630	G
30	A	646	A
30	A	650	U
30	A	682	A
30	A	690	U
30	A	699	U
30	A	700	A
30	A	731	U
30	A	762	C
30	A	775	A

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Mol	Chain	Res	Type
30	A	792	5MU
30	A	793	G
30	A	820	G
30	A	827	A
30	A	829	U
30	A	837	G
30	A	850	G
30	A	857	C
30	A	872	U
30	A	873	U
30	A	888	G
30	A	892	U
30	A	904	G
30	A	911	A
30	A	919	G
30	A	955	A
30	A	962	A
30	A	977	A
30	A	989	A
30	A	990	G
30	A	1005	G
30	A	1018	A
30	A	1027	A
30	A	1040	A
30	A	1049	C
30	A	1056	U
30	A	1057	A
30	A	1070	A
30	A	1077	U
30	A	1078	G
30	A	1083	G
30	A	1158	G
30	A	1159	A
30	A	1161	A
30	A	1173	A
30	A	1176	U
30	A	1177	A
30	A	1178	C
30	A	1179	C
30	A	1186	A
30	A	1199	A
30	A	1201	G

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Mol	Chain	Res	Type
30	A	1212	U
30	A	1219	G
30	A	1220	A
30	A	1221	C
30	A	1291	A
30	A	1294	G
30	A	1309	G
30	A	1310	A
30	A	1312	A
30	A	1337	A
30	A	1338	U
30	A	1389	U
30	A	1402	A
30	A	1416	U
30	A	1449	A
30	A	1465	G
30	A	1467	G
30	A	1472	C
30	A	1489	A
30	A	1490	G
30	A	1494	G
30	A	1498	U
30	A	1500	G
30	A	1511	C
30	A	1517	A
30	A	1522	G
30	A	1560	A
30	A	1568	U
30	A	1569	G
30	A	1572	G
30	A	1573	A
30	A	1574	G
30	A	1591	G
30	A	1592	A
30	A	1593	G
30	A	1595	C
30	A	1606	C
30	A	1613	G
30	A	1616	A
30	A	1651	C
30	A	1652	A
30	A	1690	A

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Mol	Chain	Res	Type
30	A	1691	G
30	A	1692	C
30	A	1718	G
30	A	1740	G
30	A	1747	G
30	A	1783	G
30	A	1790	G
30	A	1791	G
30	A	1800	A
30	A	1809	C
30	A	1818	A
30	A	1827	C
30	A	1828	U
30	A	1843	U
30	A	1856	A
30	A	1862	G
30	A	1875	A
30	A	1885	G
30	A	1886	A
30	A	1892	U
30	A	1904	A
30	A	1906	C
30	A	1911	A
30	A	1933	G
30	A	1954	A
30	A	1956	G
30	A	1957	G
30	A	1964	A
30	A	1965	A
30	A	1969	C
30	A	1982	U
30	A	1994	C
30	A	1997	A
30	A	1998	A
30	A	1999	G
30	A	2018	U
30	A	2020	U
30	A	2024	A
30	A	2047	A
30	A	2050	A
30	A	2058	A
30	A	2059	G

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Mol	Chain	Res	Type
30	A	2060	A
30	A	2070	C
30	A	2082	C
30	A	2083	G
30	A	2087	A
30	A	2088	G
30	A	2096	G
30	A	2120	G
30	A	2225	A
30	A	2231	C
30	A	2238	U
30	A	2239	A
30	A	2252	A
30	A	2253	C
30	A	2265	G
30	A	2266	G
30	A	2295	A
30	A	2310	C
30	A	2314	A
30	A	2315	A
30	A	2316	G
30	A	2345	A
30	A	2347	A
30	A	2349	A
30	A	2352	G
30	A	2354	A
30	A	2362	A
30	A	2374	C
30	A	2377	C
30	A	2399	G
30	A	2410	G
30	A	2412	C
30	A	2429	U
30	A	2433	C
30	A	2450	U
30	A	2452	A
30	A	2456	G
30	A	2457	A
30	A	2462	A
30	A	2468	C
30	A	2475	A
30	A	2505	A

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Mol	Chain	Res	Type
30	A	2529	G
30	A	2532	G
30	A	2545	A
30	A	2556	G
30	A	2561	C
30	A	2575	G
30	A	2581	U
30	A	2593	A
30	A	2594	G
30	A	2600	C
30	A	2612	U
30	A	2629	A
30	A	2630	G
30	A	2636	U
30	A	2640	U
30	A	2656	A
30	A	2657	G
30	A	2682	G
30	A	2687	A
30	A	2695	G
30	A	2700	G
30	A	2709	U
30	A	2716	U
30	A	2717	A
30	A	2718	C
30	A	2741	G
30	A	2753	U
30	A	2775	A
30	A	2778	G
30	A	2784	A
30	A	2792	A
30	A	2793	G
30	A	2805	A
30	A	2807	G
30	A	2816	C
30	A	2817	A
30	A	2818	A
30	A	2828	U
30	A	2833	U
30	A	2855	A
30	A	2887	G
30	A	2892	G

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Mol	Chain	Res	Type
30	A	2903	A
30	A	2906	G
30	A	2911	A
30	A	2913	G
30	A	2918	A
30	A	2920	U
41	Aa	10	G
41	Aa	33	A
41	Aa	40	G
41	Aa	45	G
41	Aa	48	C
41	Aa	49	C
41	Aa	51	A
41	Aa	52	A
41	Aa	108	A
41	Aa	119	A
41	Aa	120	C
41	Aa	144	C
41	Aa	146	G
41	Aa	157	G
41	Aa	158	G
41	Aa	163	C
41	Aa	168	G
41	Aa	182	A
41	Aa	183	U
41	Aa	184	A
41	Aa	185	U
41	Aa	189	G
41	Aa	195	C
41	Aa	196	A
41	Aa	203	A
41	Aa	204	A
41	Aa	205	A
41	Aa	207	G
41	Aa	213	G
41	Aa	221	U
41	Aa	253	U
41	Aa	255	G
41	Aa	259	G
41	Aa	274	G
41	Aa	275	C
41	Aa	297	G

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Mol	Chain	Res	Type
41	Aa	328	A
41	Aa	336	C
41	Aa	340	G
41	Aa	353	C
41	Aa	355	G
41	Aa	356	G
41	Aa	360	C
41	Aa	362	G
41	Aa	375	U
41	Aa	380	C
41	Aa	381	A
41	Aa	392	G
41	Aa	414	G
41	Aa	419	A
41	Aa	424	G
41	Aa	429	U
41	Aa	430	C
41	Aa	432	G
41	Aa	437	U
41	Aa	443	U
41	Aa	447	U
41	Aa	456	A
41	Aa	460	A
41	Aa	461	C
41	Aa	467	U
41	Aa	474	A
41	Aa	492	G
41	Aa	493	G
41	Aa	503	A
41	Aa	505	A
41	Aa	517	A
41	Aa	519	C
41	Aa	526	C
41	Aa	529	G
41	Aa	532	G
41	Aa	535	G7M
41	Aa	540	A
41	Aa	555	A
41	Aa	567	A
41	Aa	570	U
41	Aa	572	U
41	Aa	580	A

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Mol	Chain	Res	Type
41	Aa	581	A
41	Aa	584	C
41	Aa	609	G
41	Aa	641	U
41	Aa	642	C
41	Aa	661	U
41	Aa	673	A
41	Aa	695	A
41	Aa	696	G
41	Aa	703	A
41	Aa	711	G
41	Aa	731	U
41	Aa	732	G
41	Aa	757	A
41	Aa	763	G
41	Aa	785	A
41	Aa	801	U
41	Aa	802	A
41	Aa	823	A
41	Aa	825	C
41	Aa	829	G
41	Aa	836	A
41	Aa	844	G
41	Aa	860	U
41	Aa	881	A
41	Aa	883	G
41	Aa	911	G
41	Aa	923	A
41	Aa	935	G
41	Aa	943	C
41	Aa	944	A
41	Aa	969	U
41	Aa	977	A
41	Aa	978	A
41	Aa	980	G
41	Aa	984	A
41	Aa	986	A
41	Aa	992	A
41	Aa	1001	U
41	Aa	1002	G
41	Aa	1003	A
41	Aa	1024	G

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Mol	Chain	Res	Type
41	Aa	1027	A
41	Aa	1076	U
41	Aa	1096	U
41	Aa	1097	U
41	Aa	1099	G
41	Aa	1105	G
41	Aa	1106	U
41	Aa	1112	A
41	Aa	1123	C
41	Aa	1150	U
41	Aa	1152	G
41	Aa	1165	U
41	Aa	1167	A
41	Aa	1191	G
41	Aa	1193	U
41	Aa	1194	G
41	Aa	1206	A
41	Aa	1207	A
41	Aa	1219	C
41	Aa	1220	C
41	Aa	1224	U
41	Aa	1237	A
41	Aa	1263	G
41	Aa	1267	A
41	Aa	1278	G
41	Aa	1289	A
41	Aa	1290	A
41	Aa	1309	A
41	Aa	1310	G
41	Aa	1312	U
41	Aa	1315	G
41	Aa	1330	C
41	Aa	1346	U
41	Aa	1356	A
41	Aa	1363	G
41	Aa	1374	U
41	Aa	1380	G
41	Aa	1388	C
41	Aa	1391	U
41	Aa	1404	A
41	Aa	1407	C
41	Aa	1505	G

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Mol	Chain	Res	Type
41	Aa	1508	G
41	Aa	1510	A
41	Aa	1513	A
41	Aa	1514	A
41	Aa	1517	U
41	Aa	1528	G
41	Aa	1540	G
41	Aa	1541	G
41	Aa	1548	U
51	d	21	A
51	d	22	U
51	d	25	A
52	8	4	G
52	8	8	U
52	8	9	G
52	8	14	A
52	8	23	G
52	8	24	C
52	8	50	G
52	8	52	U
52	8	54	G
52	8	59	A
52	8	75	C
52	8	76	C
52	8	77	A
53	9	36	C

All (9) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	A	291	G
30	A	396	G
30	A	525	A
30	A	793	G
30	A	809	A
30	A	1157	U
30	A	1158	G
30	A	1905	G
30	A	2783	U

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

17 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	$\#\|Z\| > 2$
41	4OC	Aa	1412	41	20,23,24	0.32	0	26,32,35	0.54	0
30	2MG	A	2472	30	18,26,27	0.92	1 (5%)	16,38,41	0.66	0
41	MA6	Aa	1529	41	18,26,27	0.77	0	19,38,41	0.75	0
30	OMG	A	2278	52,30	18,26,27	0.94	1 (5%)	19,38,41	0.59	0
41	5MC	Aa	976	41	18,22,23	0.28	0	26,32,35	0.43	0
30	PSU	A	2607	30	18,21,22	0.61	1 (5%)	22,30,33	0.75	1 (4%)
30	5MU	A	792	30	19,22,23	0.44	0	28,32,35	0.65	0
30	PSU	A	2632	30	18,21,22	0.48	0	22,30,33	0.61	0
30	H2U	A	2476	30	18,21,22	0.49	0	21,30,33	0.86	1 (4%)
41	UR3	Aa	1509	41	19,22,23	0.30	0	26,32,35	0.37	0
30	2MA	A	2530	30,56	19,25,26	1.06	2 (10%)	21,37,40	3.02	4 (19%)
30	G7M	A	2601	30,56	20,26,27	0.55	0	17,39,42	0.33	0
41	G7M	Aa	535	41	20,26,27	0.59	0	17,39,42	0.48	0
41	MA6	Aa	1530	41	18,26,27	0.75	0	19,38,41	0.73	0
41	2MG	Aa	975	41	18,26,27	0.98	2 (11%)	16,38,41	0.67	0
30	PSU	A	2484	30	18,21,22	0.52	0	22,30,33	0.59	0
30	5MU	A	1966	30	19,22,23	0.51	0	28,32,35	0.49	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	4OC	Aa	1412	41	-	0/9/29/30	0/2/2/2
30	2MG	A	2472	30	-	0/5/27/28	0/3/3/3
41	MA6	Aa	1529	41	-	0/7/29/30	0/3/3/3
30	OMG	A	2278	52,30	-	1/5/27/28	0/3/3/3
41	5MC	Aa	976	41	-	0/7/25/26	0/2/2/2
30	PSU	A	2607	30	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	5MU	A	792	30	-	0/7/25/26	0/2/2/2
30	PSU	A	2632	30	-	0/7/25/26	0/2/2/2
30	H2U	A	2476	30	-	0/7/38/39	0/2/2/2
41	UR3	Aa	1509	41	-	0/7/25/26	0/2/2/2
30	2MA	A	2530	30,56	-	2/3/25/26	0/3/3/3
30	G7M	A	2601	30,56	-	0/3/25/26	0/3/3/3
41	G7M	Aa	535	41	-	2/3/25/26	0/3/3/3
41	MA6	Aa	1530	41	-	2/7/29/30	0/3/3/3
41	2MG	Aa	975	41	-	0/5/27/28	0/3/3/3
30	PSU	A	2484	30	-	0/7/25/26	0/2/2/2
30	5MU	A	1966	30	-	0/7/25/26	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	Aa	975	2MG	C5-C6	-2.51	1.42	1.47
30	A	2530	2MA	C6-N6	-2.35	1.25	1.34
30	A	2278	OMG	C5-C6	-2.32	1.42	1.47
30	A	2607	PSU	O4'-C1'	-2.17	1.40	1.43
30	A	2530	2MA	C6-N1	2.11	1.37	1.33
30	A	2472	2MG	C5-C6	-2.11	1.43	1.47
41	Aa	975	2MG	C8-N7	-2.07	1.31	1.35

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	2530	2MA	C5-C6-N1	-12.10	113.06	121.01
30	A	2530	2MA	C2-N3-C4	-4.06	112.22	115.52
30	A	2530	2MA	C2-N1-C6	3.60	123.70	118.08
30	A	2607	PSU	O4'-C1'-C2'	2.57	108.77	105.14
30	A	2530	2MA	N6-C6-N1	2.50	123.87	117.07
30	A	2476	H2U	C5-C4-N3	-2.36	114.00	116.65

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
41	Aa	535	G7M	O4'-C4'-C5'-O5'
41	Aa	535	G7M	C3'-C4'-C5'-O5'
30	A	2278	OMG	C1'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
41	Aa	1530	MA6	O4'-C4'-C5'-O5'
41	Aa	1530	MA6	C3'-C4'-C5'-O5'
30	A	2530	2MA	C4'-C5'-O5'-P
30	A	2530	2MA	O4'-C4'-C5'-O5'

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
41	Aa	1529	MA6	1	0
30	A	2278	OMG	1	0
30	A	2530	2MA	1	0
30	A	2601	G7M	1	0
41	Aa	975	2MG	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 254 ligands modelled in this entry, 253 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
57	EM1	A	3001	-	58,64,64	0.51	0	71,97,97	0.42	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	EM1	A	3001	-	-	1/71/112/112	0/4/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

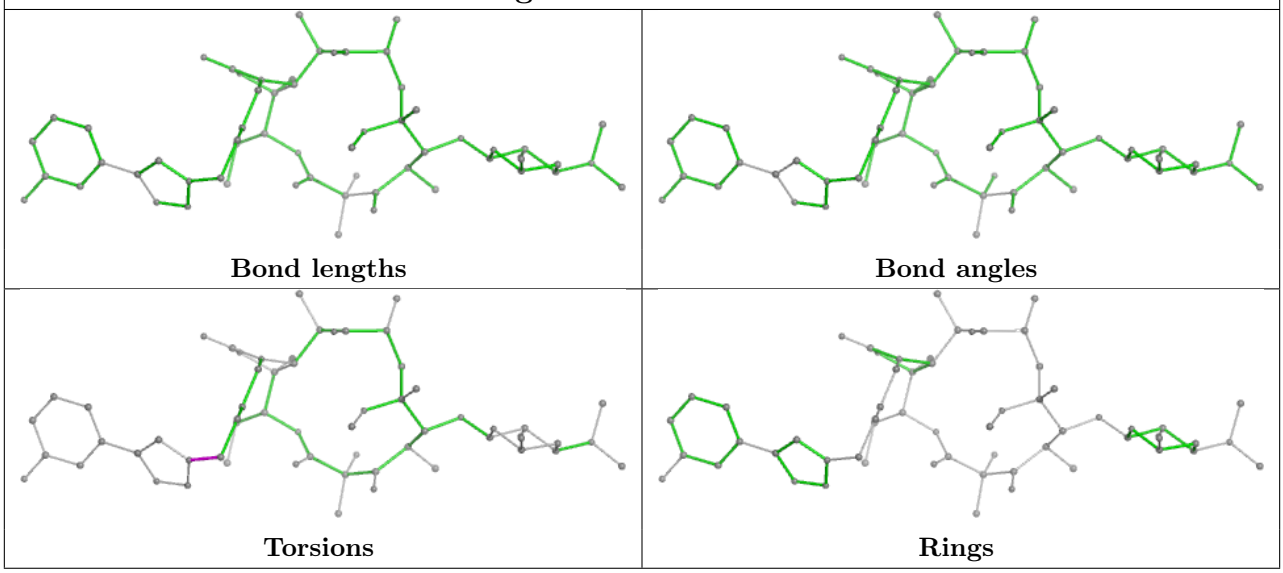
Mol	Chain	Res	Type	Atoms
57	A	3001	EM1	C84-C83-N80-N81

There are no ring outliers.

No monomer is involved in short contacts.

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

Ligand EM1 A 3001



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
52	8	3
51	d	1
29	11	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	d	8:A	O3'	15:C	P	14.91
1	11	6:A	O3'	68:C	P	14.41
1	8	19:G	O3'	22:A	P	10.42
1	8	15:G	O3'	19:G	P	8.49
1	8	47:G	O3'	49:C	P	6.61

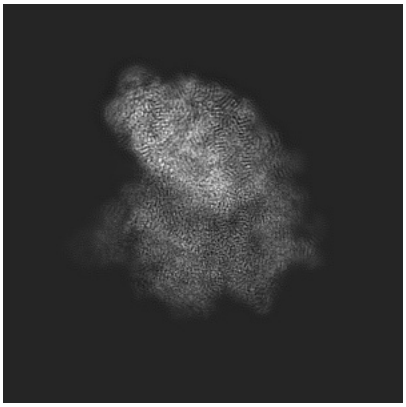
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-53066. These allow visual inspection of the internal detail of the map and identification of artifacts.

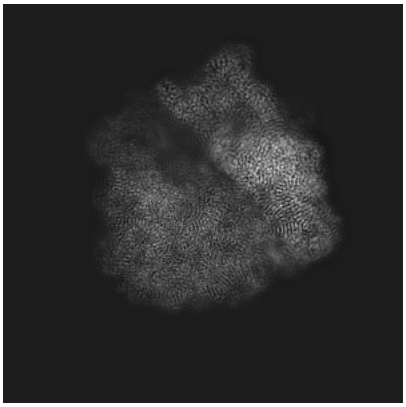
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

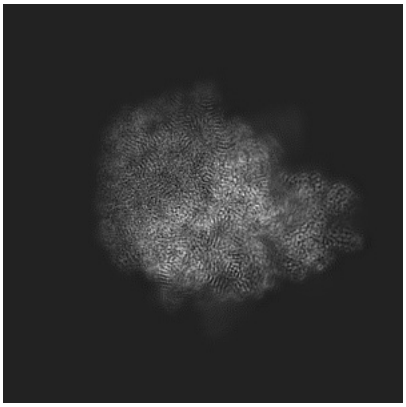
6.1.1 Primary map



X



Y

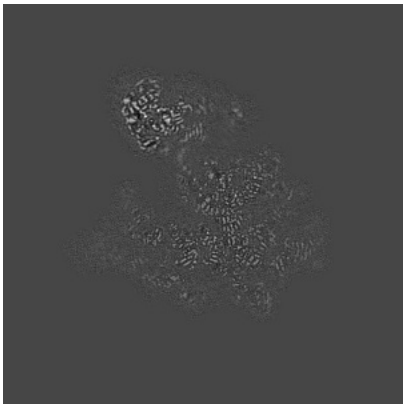


Z

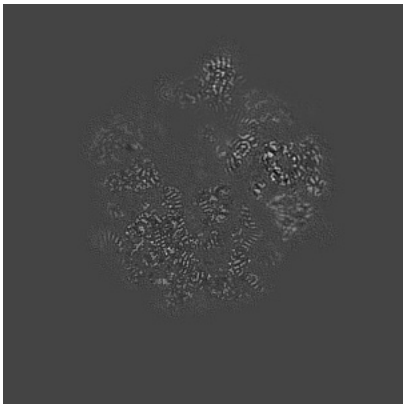
The images above show the map projected in three orthogonal directions.

6.2 Central slices

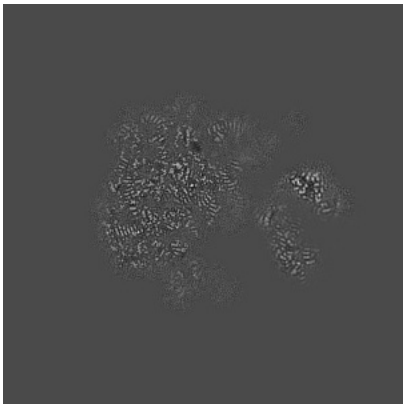
6.2.1 Primary map



X Index: 220



Y Index: 220



Z Index: 220

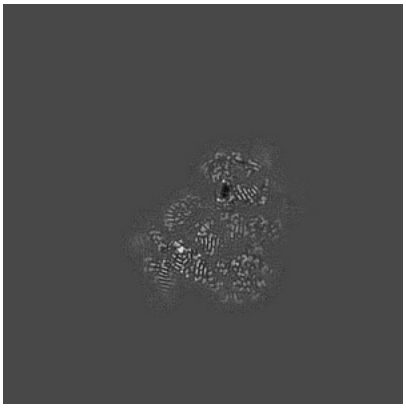
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 192

Y Index: 235

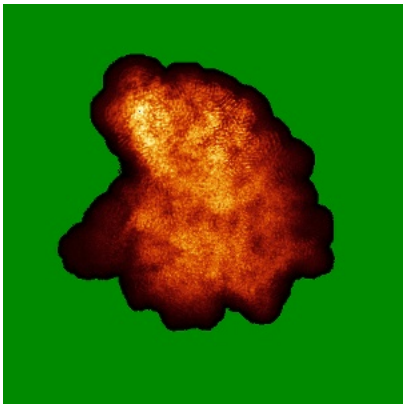


Z Index: 318

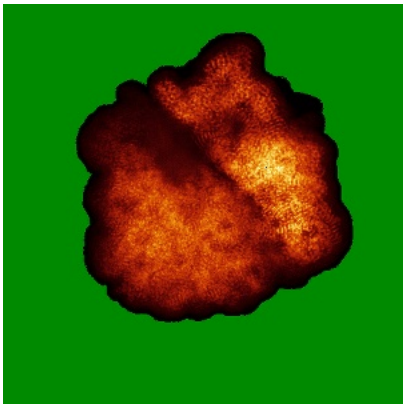
The images above show the largest variance slices of the map in three orthogonal directions.

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

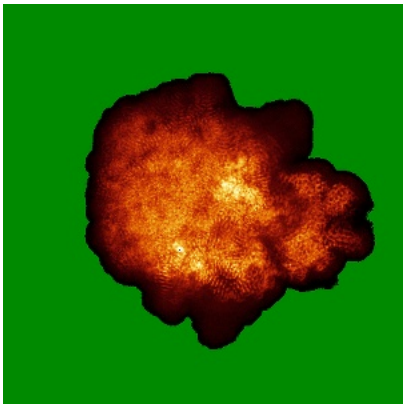
6.4.1 Primary map



X



Y

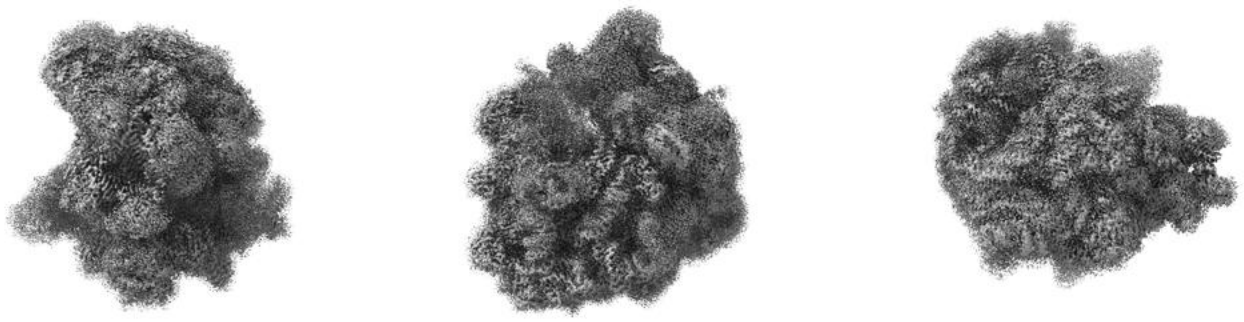


Z

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 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

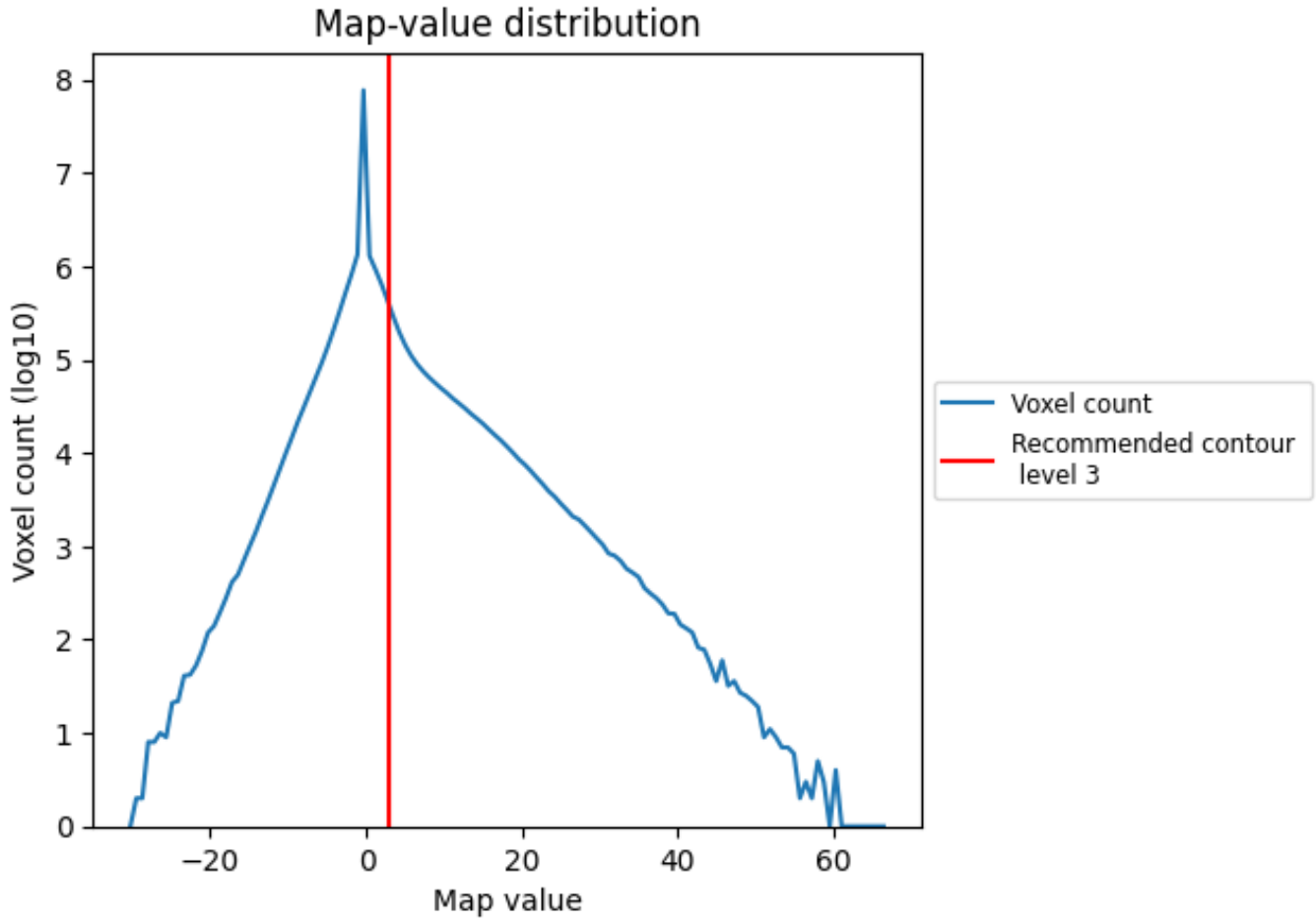
6.6 Mask visualisation (i)

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

7 Map analysis

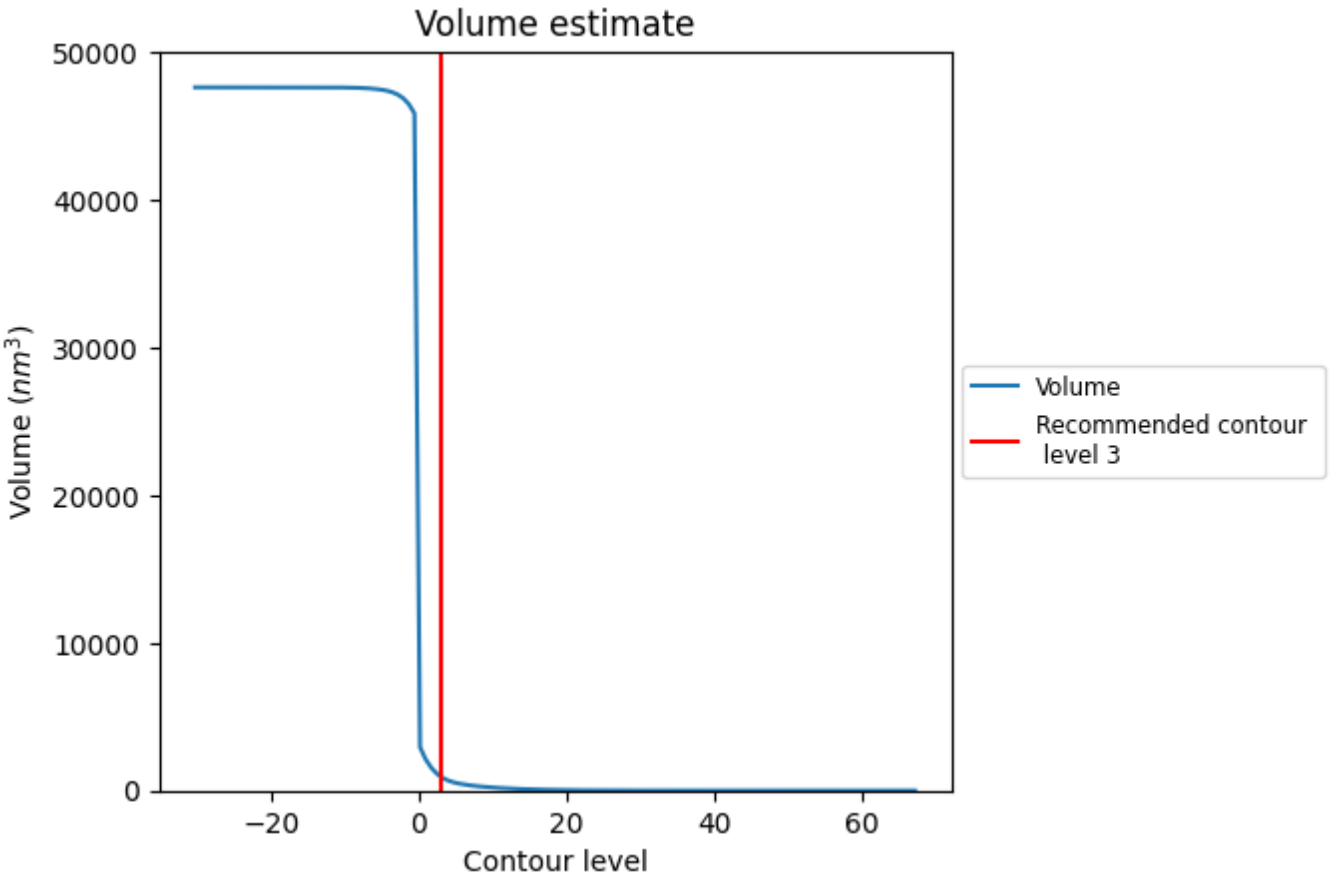
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

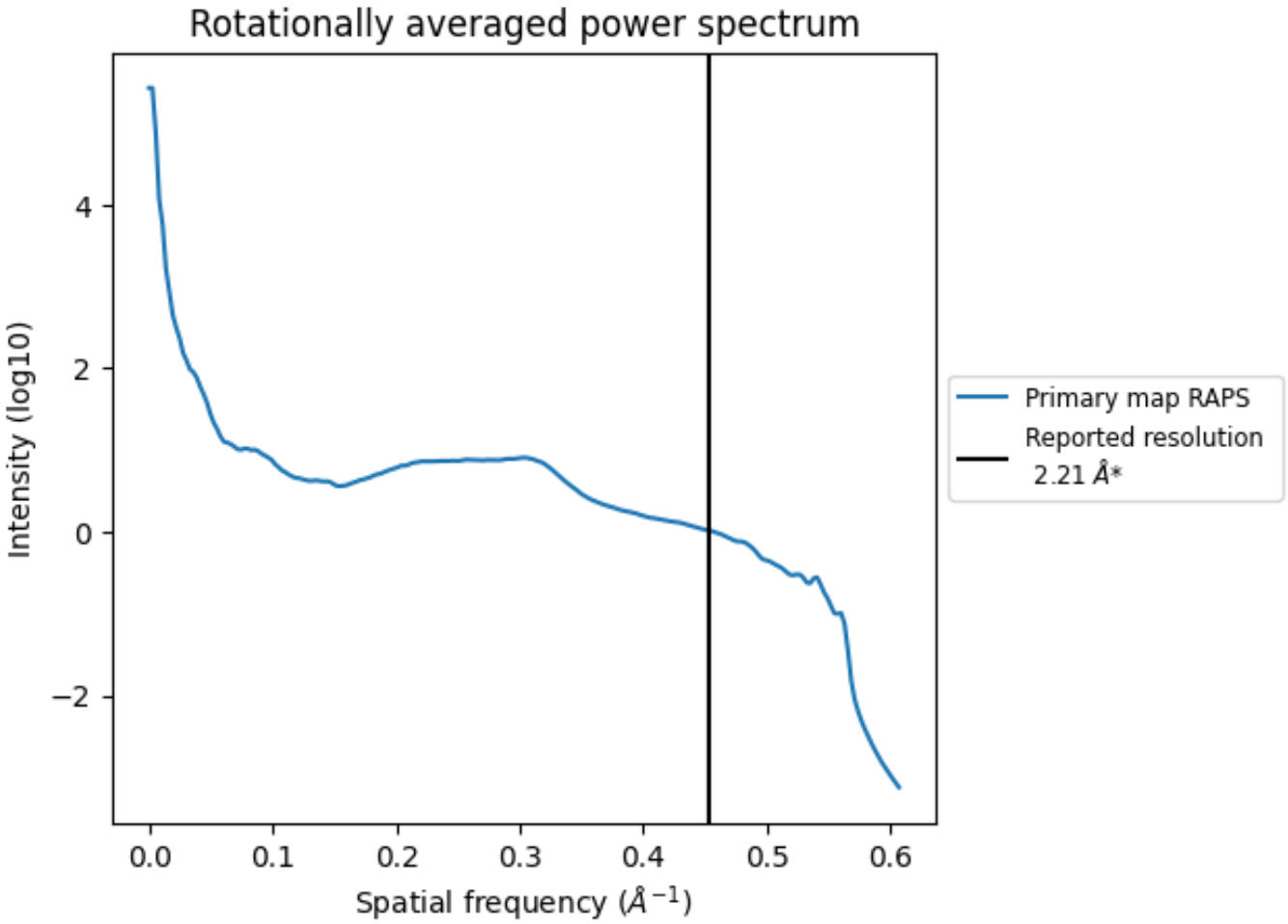
7.2 Volume estimate



The volume at the recommended contour level is 955 nm^3; this corresponds to an approximate mass of 863 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.452 Å^{-1}

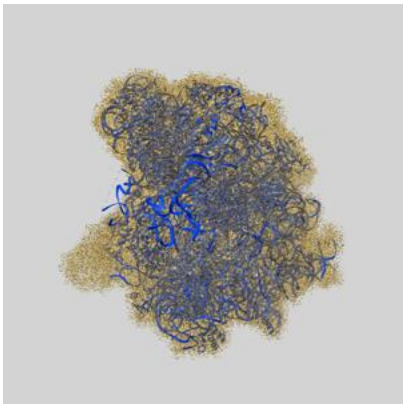
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

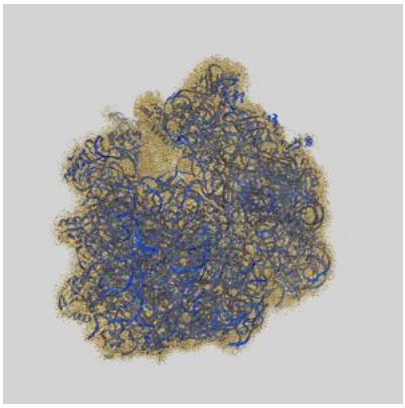
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-53066 and PDB model 9QEG. Per-residue inclusion information can be found in section 3 on page 15.

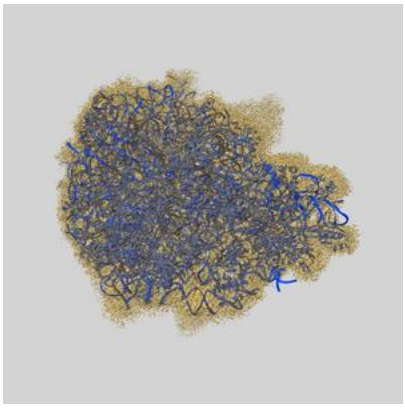
9.1 Map-model overlay



X



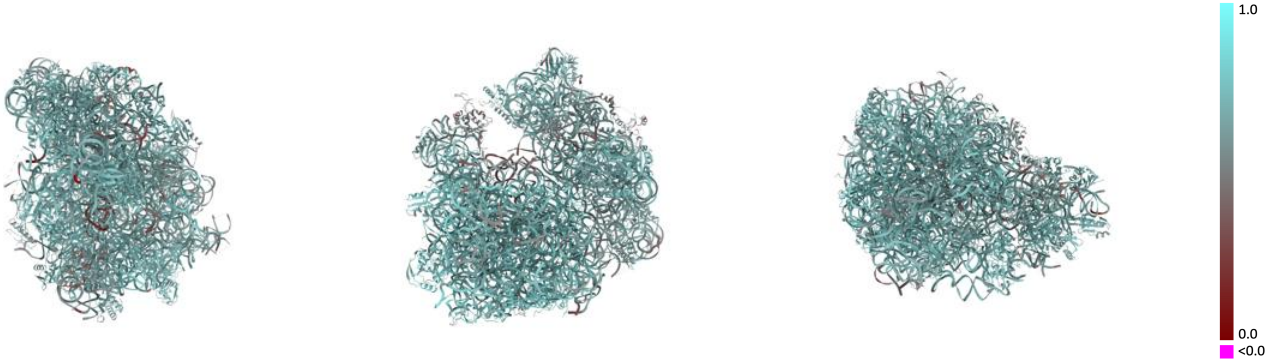
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

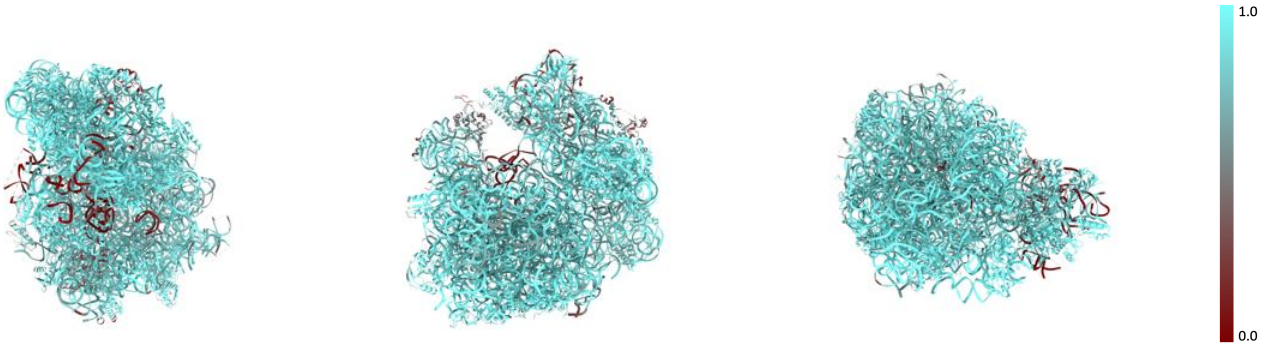
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

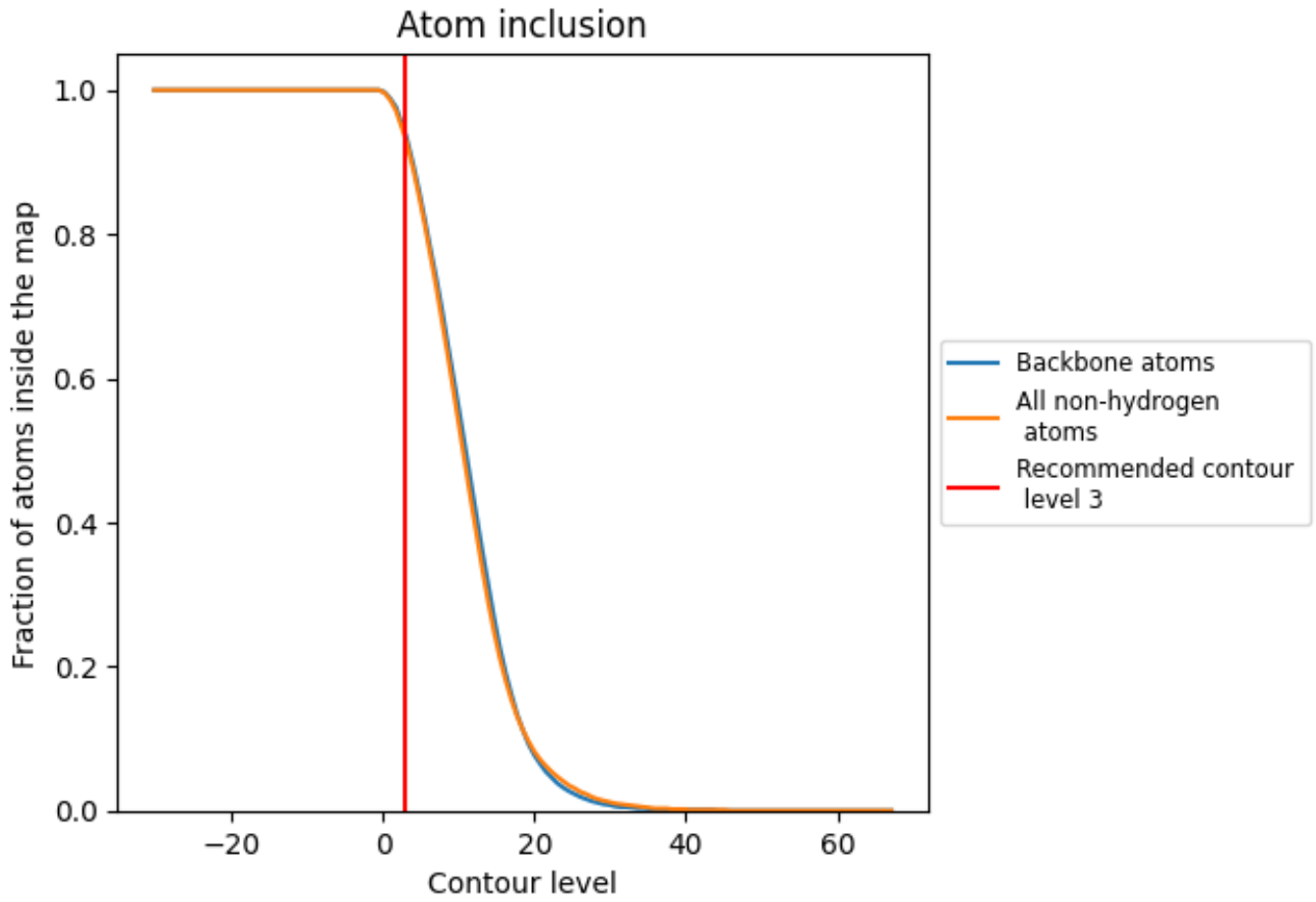
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 93% 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 (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9320	0.7030
1	0.8840	0.6800
11	0.2360	0.4530
13	0.6190	0.5520
2	0.9910	0.8090
3	0.9960	0.7950
4	0.9750	0.7430
8	0.3500	0.4210
9	0.5470	0.4800
A	0.9580	0.7340
Aa	0.9110	0.6620
Ab	0.4820	0.5090
Ac	0.9930	0.6940
Ad	0.9880	0.6740
Ae	0.9710	0.6700
Af	0.9590	0.6110
Ag	0.9770	0.6760
Ah	0.9850	0.7030
Ai	0.9950	0.7020
Aj	0.9890	0.6800
Ak	0.9560	0.5860
Al	0.9910	0.7080
Am	0.9900	0.7040
An	0.9920	0.7280
Ao	0.9800	0.6920
Ap	0.9830	0.7060
Aq	0.9890	0.6450
Ar	0.9910	0.6890
As	0.9980	0.7180
At	0.9900	0.6940
B	0.8760	0.6300
C	0.9890	0.7810
D	0.9890	0.7830
E	0.9670	0.7630
F	0.5770	0.5070

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Chain	Atom inclusion	Q-score
G	0.7990	0.6130
H	0.9750	0.7770
I	0.9800	0.7680
J	0.9640	0.7500
K	0.9810	0.7680
L	0.9860	0.7830
M	0.8780	0.6560
N	0.9760	0.7650
O	0.9870	0.7910
P	0.9740	0.7720
Q	0.9790	0.7880
R	0.9680	0.7520
S	0.9220	0.6950
T	0.8980	0.6790
U	0.9780	0.7810
V	0.8850	0.7030
W	0.9300	0.7170
X	0.9650	0.7680
Z	0.9350	0.7500
d	0.7430	0.4670