



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 03:36 AM UTC

PDB ID : 6W6P / pdb_00006w6p
EMDB ID : EMD-21562
Title : MultiBody Refinement of 70S Ribosome from *Enterococcus faecalis*
Authors : Jogl, G.; Khayat, R.
Deposited on : 2020-03-17
Resolution : 2.90 Å (reported)
Based on initial models : 5LI0, 4YBB

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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

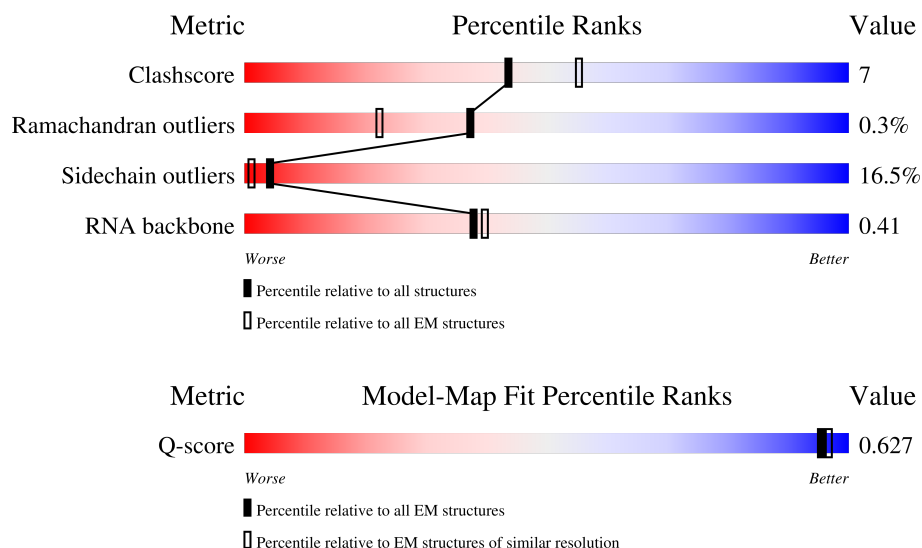
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13054 (2.40 - 3.40)

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

Mol	Chain	Length	Quality of chain
1	a	1548	
2	c	204	
3	d	201	

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Mol	Chain	Length	Quality of chain
4	e	163	
5	f	97	
6	g	154	
7	h	131	
8	i	128	
9	j	99	
10	k	117	
11	l	136	
12	m	112	
13	n	60	
14	o	88	
15	p	89	
16	q	83	
17	r	66	
18	s	78	
19	t	82	
20	A	2908	
21	B	116	
22	C	275	
23	D	207	
24	E	206	
25	F	177	
26	G	176	
27	K	145	
28	L	122	

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Mol	Chain	Length	Quality of chain
29	M	146	
30	N	141	
31	O	124	
32	P	117	
33	Q	114	
34	R	118	
35	S	102	
36	T	112	
37	U	89	
38	V	101	
39	X	76	
40	Y	54	
41	Z	61	
42	0	58	
43	2	56	
44	3	49	
45	4	44	
46	5	64	
47	6	38	

2 Entry composition [i](#)

There are 48 unique types of molecules in this entry. The entry contains 133554 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 RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	1523	Total	C	N	O	P	0	0
			32646	14564	5967	10592	1523		

- Molecule 2 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	c	204	Total	C	N	O	S	0	0
			1610	1012	303	292	3		

- Molecule 3 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	d	201	Total	C	N	O	S	0	0
			1620	1016	303	297	4		

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	e	163	Total	C	N	O	S	0	0
			1204	759	222	221	2		

- Molecule 5 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	f	97	Total	C	N	O	S	0	0
			795	501	137	154	3		

- Molecule 6 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	g	154	Total	C	N	O	S	0	0
			1229	765	236	222	6		

- Molecule 7 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	h	131	Total	C	N	O	S	0	0
			1041	662	184	193	2		

- Molecule 8 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	i	128	Total	C	N	O	S	0	0
			990	615	197	177	1		

- Molecule 9 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	j	99	Total	C	N	O	S	0	0
			800	504	147	147	2		

- Molecule 10 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	k	117	Total	C	N	O	S	0	0
			863	533	165	161	4		

- Molecule 11 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	l	136	Total	C	N	O	S	0	0
			1065	661	214	188	2		

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	m	110	Total	C	N	O	S	0	0
			870	531	178	160	1		

- Molecule 13 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	n	60	Total	C	N	O	S	0	0
			492	310	100	77	5		

- Molecule 14 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	o	88	Total	C	N	O	S	0	0
			741	455	152	133	1		

- Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	p	89	Total	C	N	O	S	0	0
			708	448	131	127	2		

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	q	83	Total	C	N	O	S	0	0
			681	427	127	124	3		

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	r	66	Total	C	N	O	S	0	0
			537	343	99	94	1		

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	s	78	Total	C	N	O	S	0	0
			634	410	113	109	2		

- Molecule 19 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	t	82	Total	C	N	O	S	0	0
			617	377	120	118	2		

- Molecule 20 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	A	2739	Total	C	N	O	P	0	0
			58793	26244	10818	18992	2739		

- Molecule 21 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	B	116	Total	C	N	O	P	0	0
			2480	1106	444	814	116		

- Molecule 22 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	C	275	Total	C	N	O	S	0	0
			2115	1311	416	381	7		

- Molecule 23 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	D	207	Total	C	N	O	S	0	0
			1579	994	292	289	4		

- Molecule 24 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	E	206	Total	C	N	O	S	0	0
			1574	984	290	298	2		

- Molecule 25 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	F	177	Total	C	N	O	S	0	0
			1392	887	239	260	6		

- Molecule 26 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	G	176	Total	C	N	O	S	0	0
			1345	842	244	255	4		

- Molecule 27 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	K	145	Total	C	N	O	S	0	0
			1130	714	205	207	4		

- Molecule 28 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	L	122	Total	C	N	O	S	0	0
			922	574	176	170	2		

- Molecule 29 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	M	146	Total	C	N	O	S	0	0
			1095	677	212	205	1		

- Molecule 30 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	N	141	Total	C	N	O	S	0	0
			1118	710	216	185	7		

- Molecule 31 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	O	124	Total	C	N	O	S	0	0
			991	612	191	185	3		

- Molecule 32 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	P	117	Total	C	N	O	S	0	0
			899	556	175	167	1		

- Molecule 33 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	Q	114	Total	C	N	O	0	0
			924	582	185	157		

- Molecule 34 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	R	118	Total	C	N	O	S	0	0
			950	602	184	160	4		

- Molecule 35 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	S	102	Total	C	N	O	S	0	0
			784	500	139	143	2		

- Molecule 36 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	T	112	Total	C	N	O	S	0	0
			849	532	156	159	2		

- Molecule 37 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	U	89	Total	C	N	O	S	0	0
			720	458	127	132	3		

- Molecule 38 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	V	101	Total	C	N	O	S	0	0
			763	486	135	140	2		

- Molecule 39 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	X	76	Total	C	N	O	0	0
			572	351	109	112		

- Molecule 40 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Y	54	Total	C	N	O	S	0	0
			425	265	86	72	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	51	ALA	THR	conflict	UNP A0A1B4XRZ8

- Molecule 41 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Z	61	Total	C	N	O	S	0	0
			504	314	94	95	1		

- Molecule 42 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	0	58	Total	C	N	O	S	0	0
			435	271	81	82	1		

- Molecule 43 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	2	56	Total	C	N	O	S	0	0
			429	262	88	73	6		

- Molecule 44 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	3	49	Total	C	N	O	S	0	0
			419	253	86	76	4		

- Molecule 45 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	4	44	Total	C	N	O	S	0	0
			374	227	91	54	2		

- Molecule 46 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	5	64	Total	C	N	O	S	0	0
			522	320	122	78	2		

- Molecule 47 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	6	38	Total	C	N	O	S	0	0
			304	188	66	44	6		

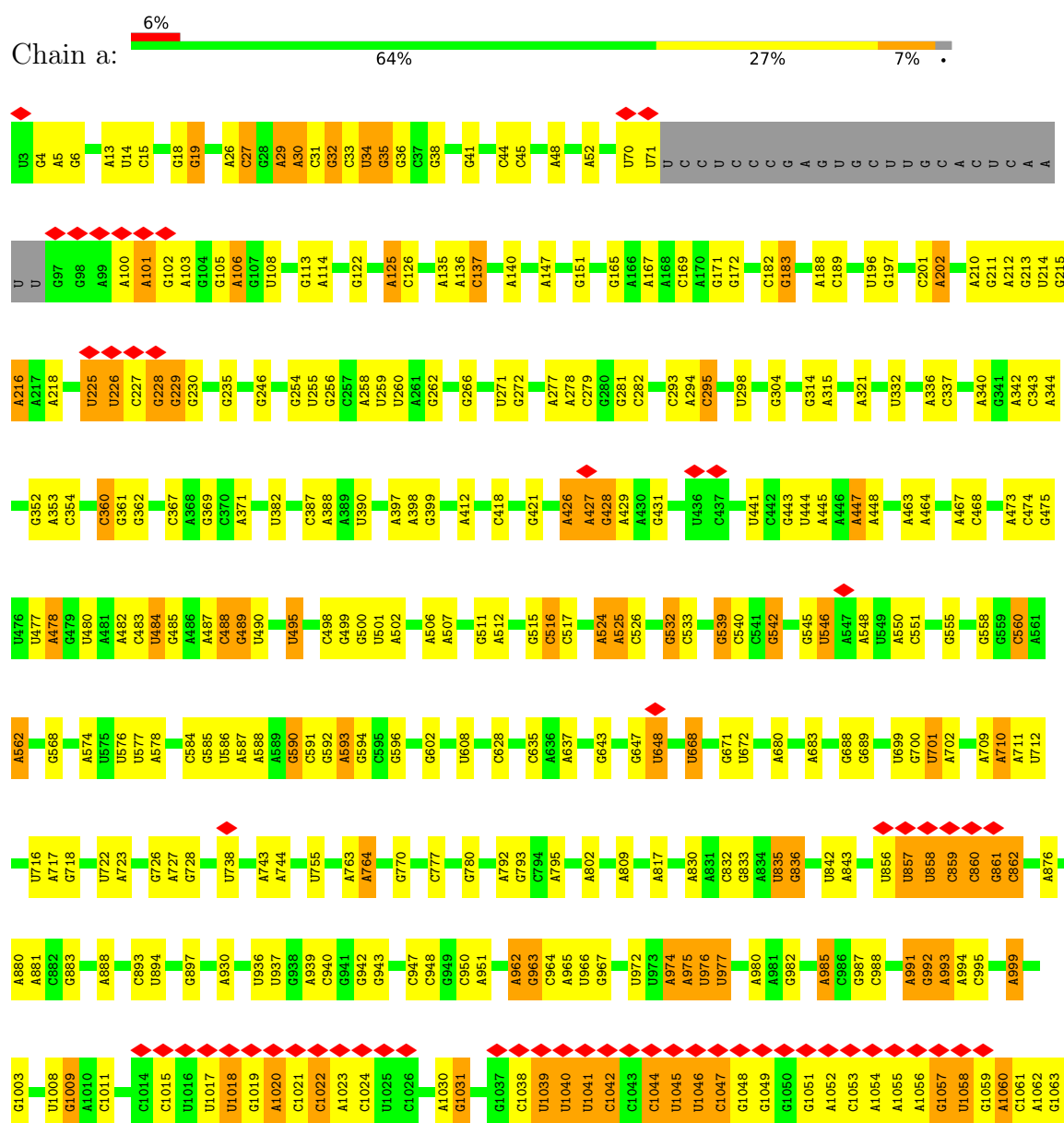
- Molecule 48 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

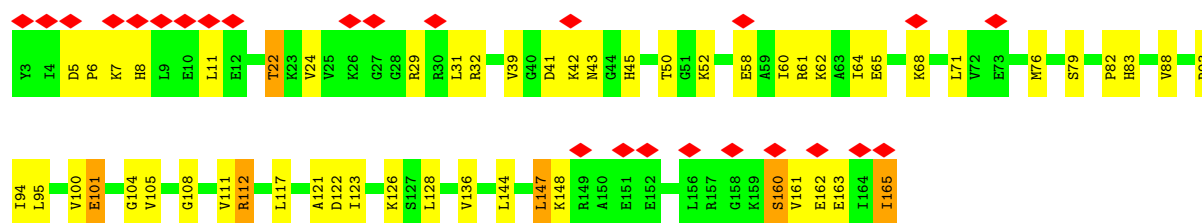
Mol	Chain	Residues	Atoms		AltConf
48	n	1	Total 1	Zn 1	0
48	2	1	Total 1	Zn 1	0
48	3	1	Total 1	Zn 1	0
48	6	1	Total 1	Zn 1	0

3 Residue-property plots

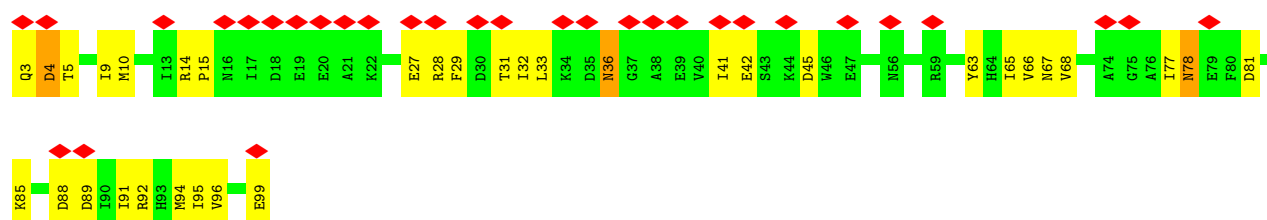
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 16S rRNA





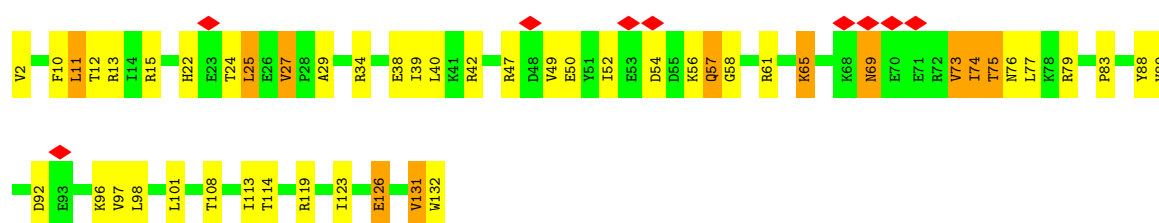
• Molecule 5: 30S ribosomal protein S6



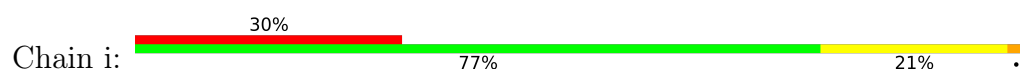
• Molecule 6: 30S ribosomal protein S7

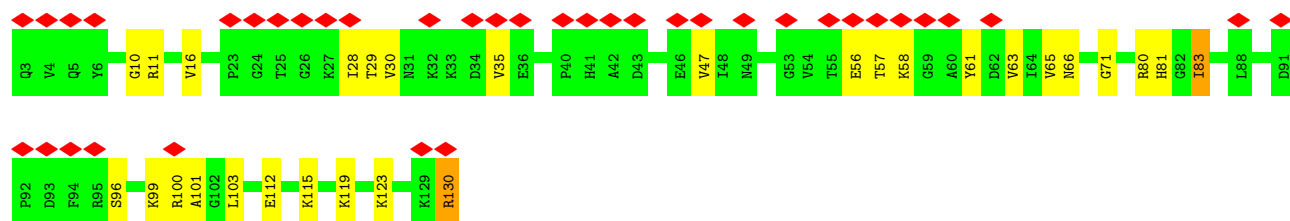


• Molecule 7: 30S ribosomal protein S8

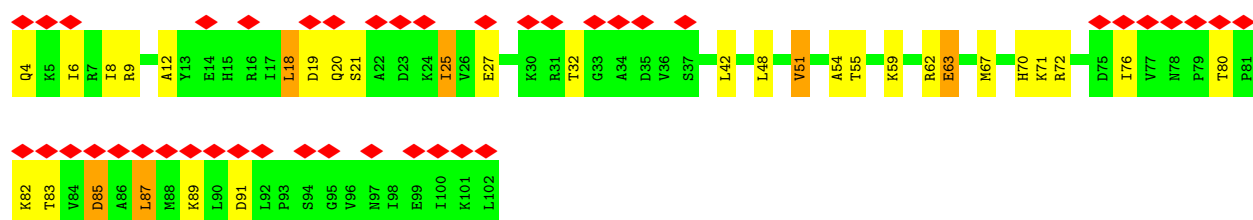
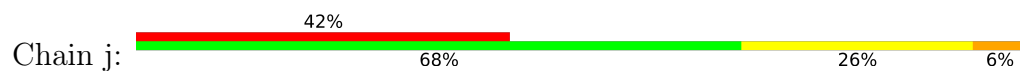


• Molecule 8: 30S ribosomal protein S9

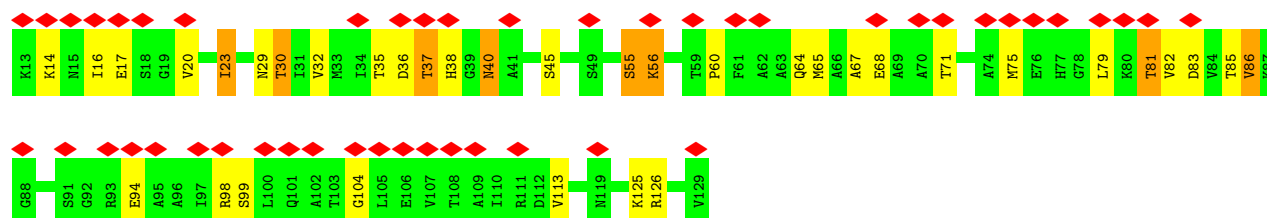
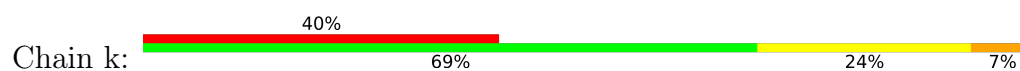




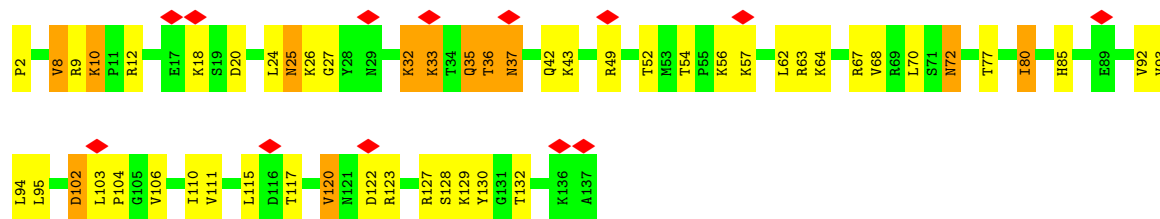
• Molecule 9: 30S ribosomal protein S10



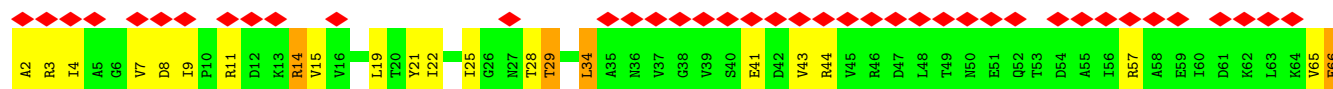
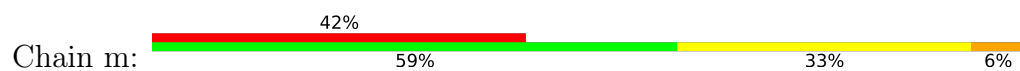
• Molecule 10: 30S ribosomal protein S11

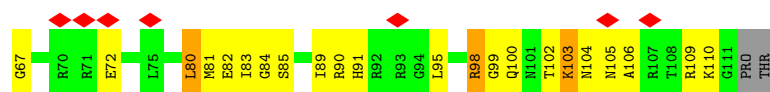


• Molecule 11: 30S ribosomal protein S12

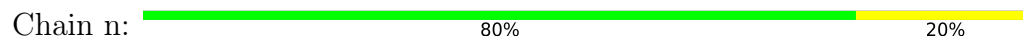


• Molecule 12: 30S ribosomal protein S13

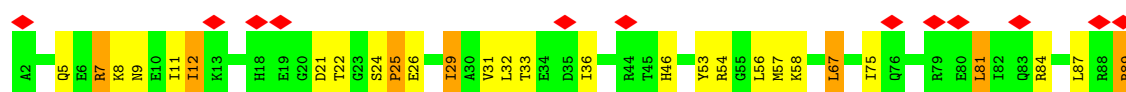




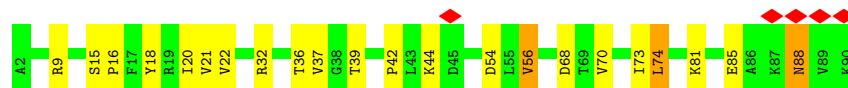
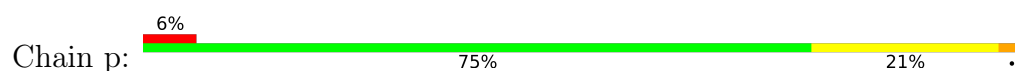
- Molecule 13: 30S ribosomal protein S14 type Z



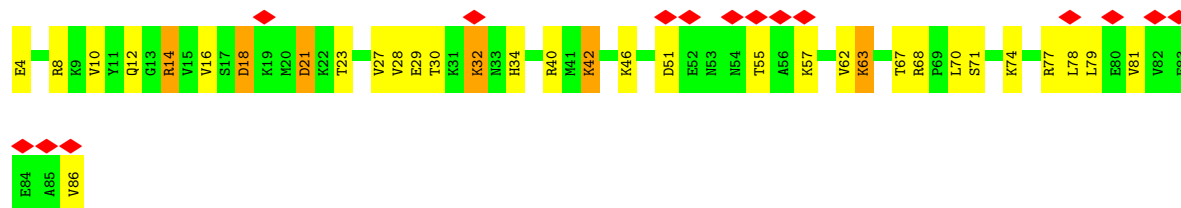
- Molecule 14: 30S ribosomal protein S15



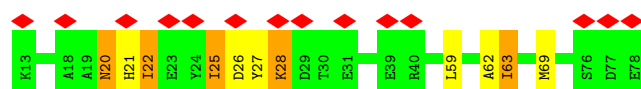
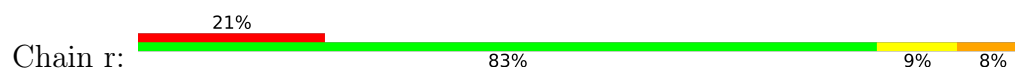
- Molecule 15: 30S ribosomal protein S16



- Molecule 16: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S18

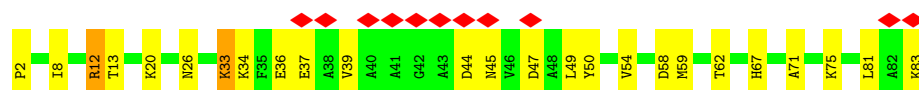


- Molecule 18: 30S ribosomal protein S19

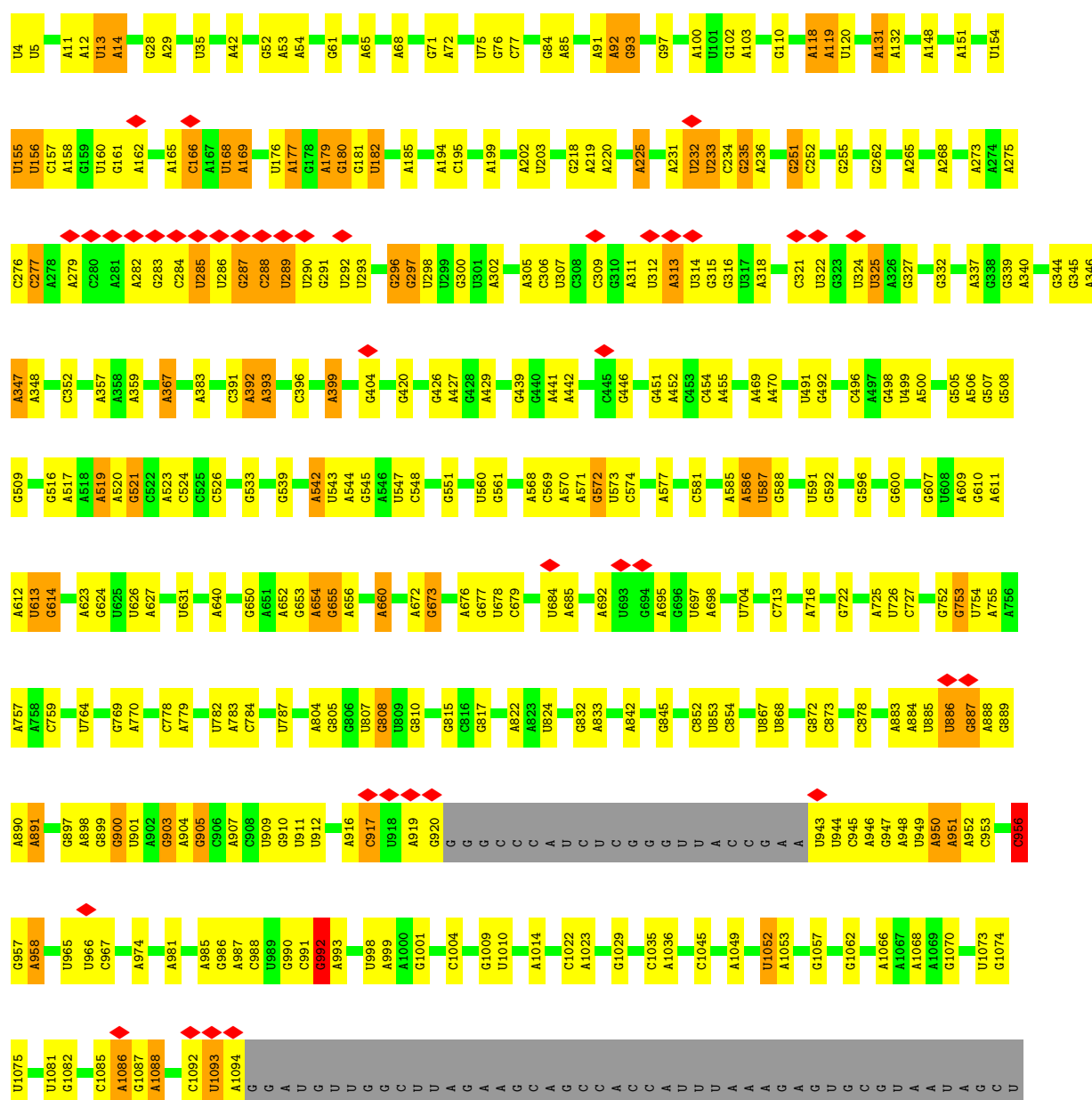




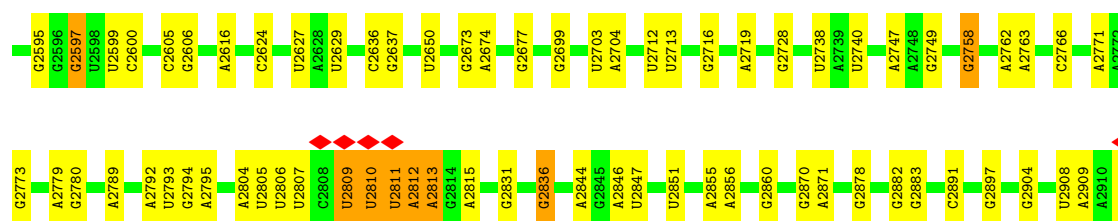
• Molecule 19: 30S ribosomal protein S20



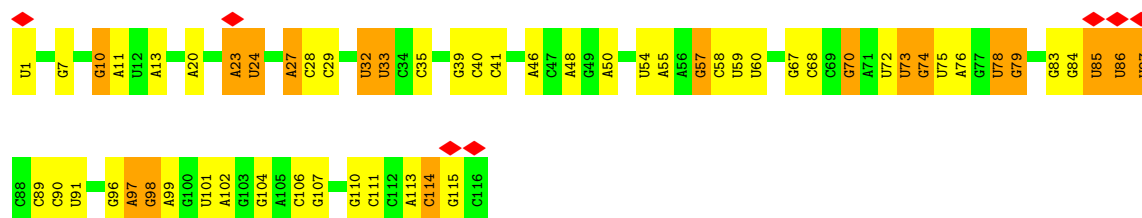
• Molecule 20: 23S rRNA



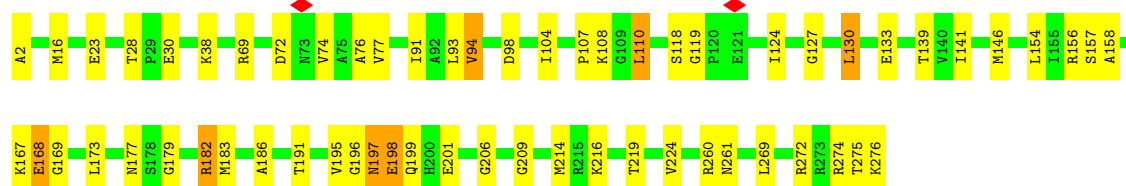
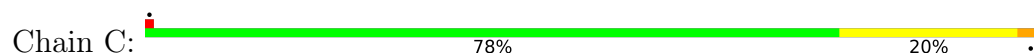




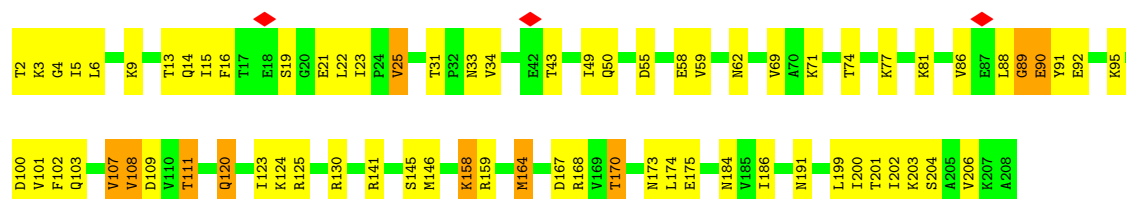
• Molecule 21: 5S rRNA



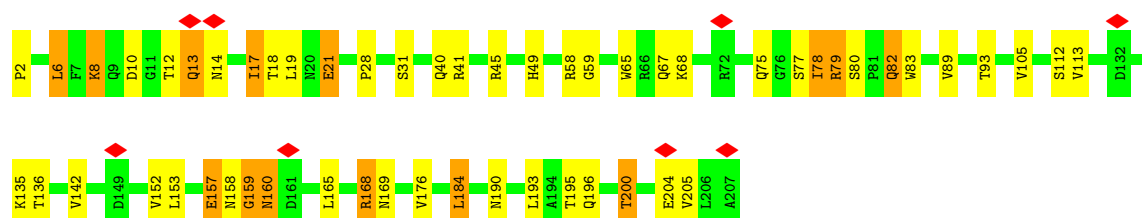
• Molecule 22: 50S ribosomal protein L2



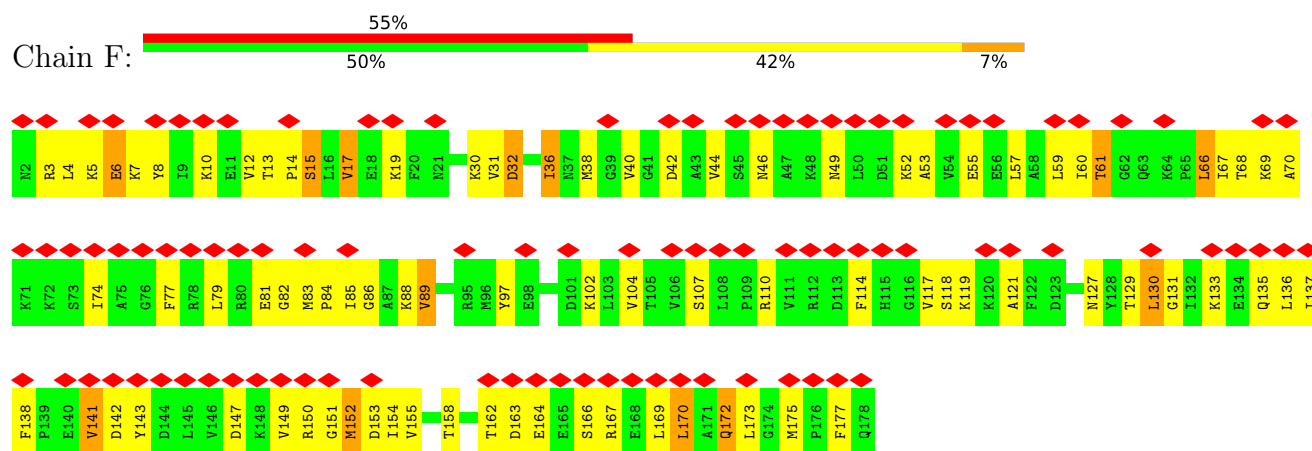
• Molecule 23: 50S ribosomal protein L3



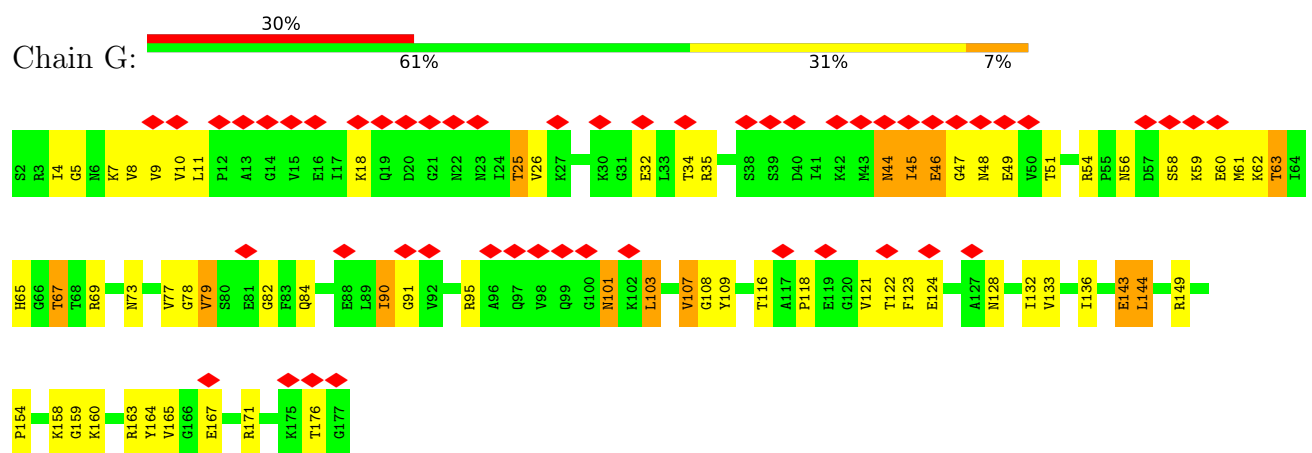
• Molecule 24: 50S ribosomal protein L4



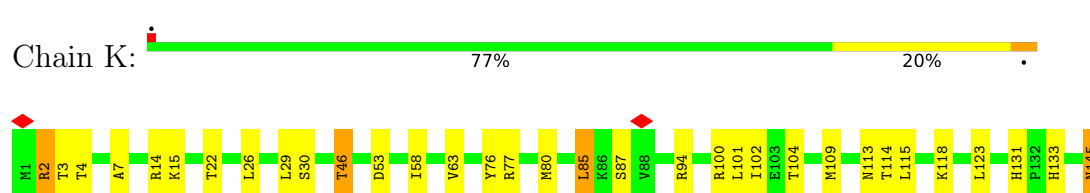
- Molecule 25: 50S ribosomal protein L5



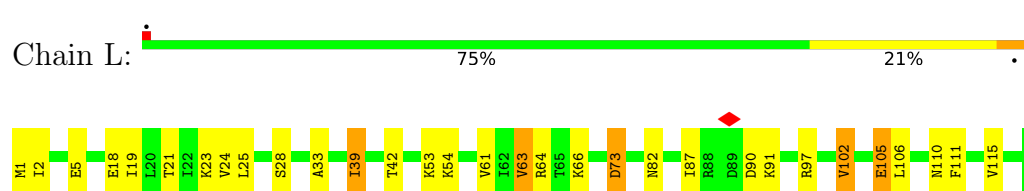
- Molecule 26: 50S ribosomal protein L6



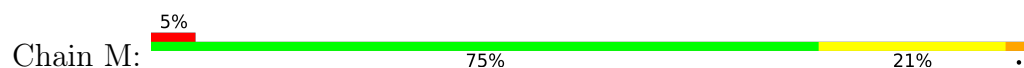
- Molecule 27: 50S ribosomal protein L13

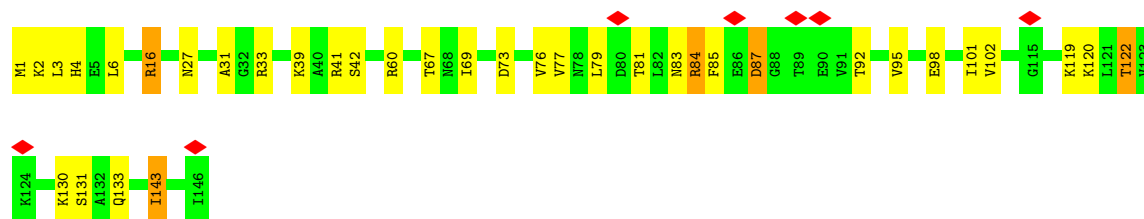


- Molecule 28: 50S ribosomal protein L14

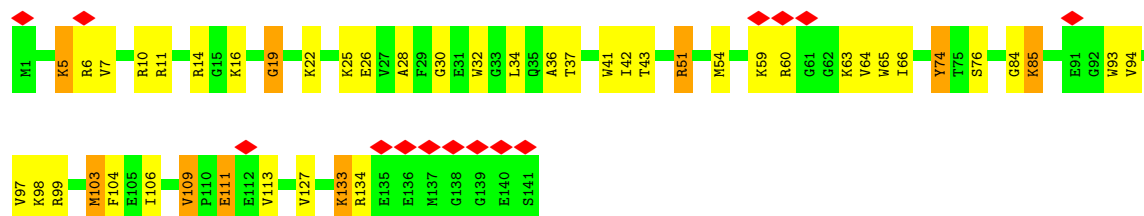


- Molecule 29: 50S ribosomal protein L15

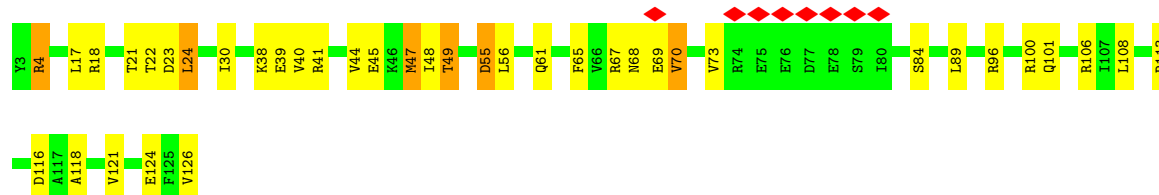




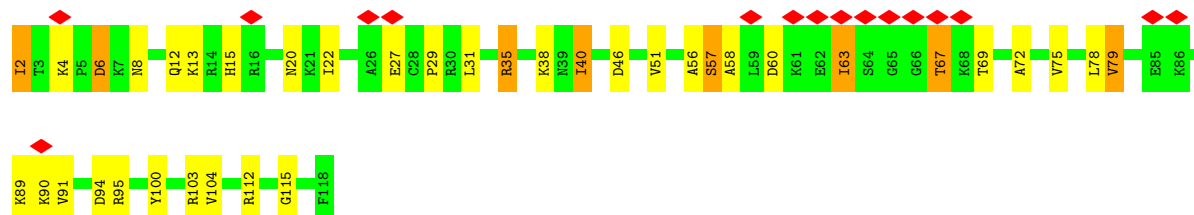
- Molecule 30: 50S ribosomal protein L16



- Molecule 31: 50S ribosomal protein L17



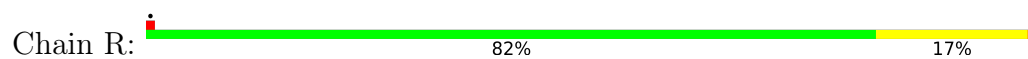
- Molecule 32: 50S ribosomal protein L18



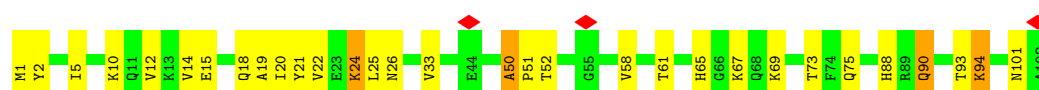
- Molecule 33: 50S ribosomal protein L19



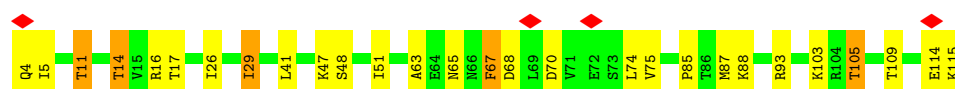
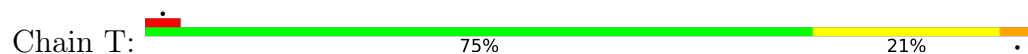
- Molecule 34: 50S ribosomal protein L20



- Molecule 35: 50S ribosomal protein L21



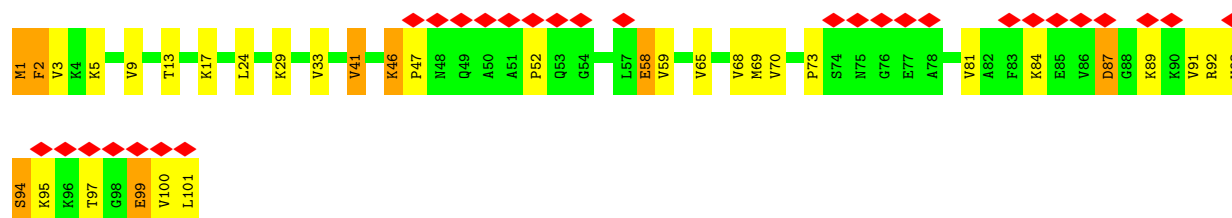
- Molecule 36: 50S ribosomal protein L22



- Molecule 37: 50S ribosomal protein L23



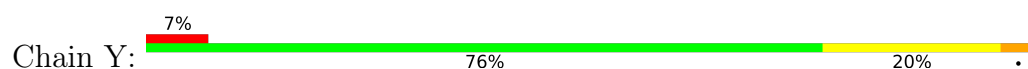
- Molecule 38: 50S ribosomal protein L24

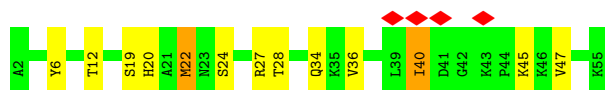


- Molecule 39: 50S ribosomal protein L27

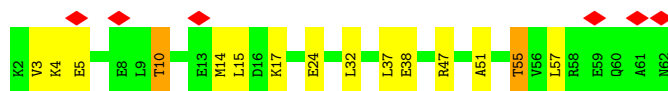
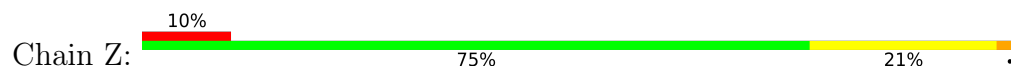


- Molecule 40: 50S ribosomal protein L28





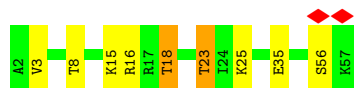
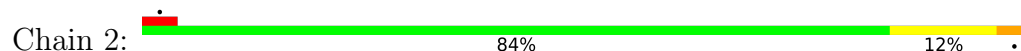
- Molecule 41: 50S ribosomal protein L29



- Molecule 42: 50S ribosomal protein L30



- Molecule 43: 50S ribosomal protein L32



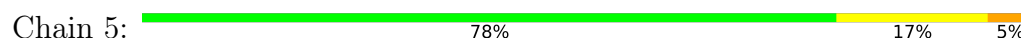
- Molecule 44: 50S ribosomal protein L33



- Molecule 45: 50S ribosomal protein L34



- Molecule 46: 50S ribosomal protein L35



- Molecule 47: 50S ribosomal protein L36



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	335675	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.226	Depositor
Minimum map value	-0.019	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	482.68, 482.68, 482.68	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.097, 1.097, 1.097	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:
ZN

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	a	0.46	0/36547	0.46	2/57003 (0.0%)
2	c	0.28	0/1635	0.44	0/2197
3	d	0.37	0/1650	0.56	0/2217
4	e	0.36	0/1217	0.55	0/1641
5	f	0.31	0/807	0.49	0/1087
6	g	0.25	0/1249	0.44	0/1682
7	h	0.42	0/1054	0.54	0/1417
8	i	0.34	0/1003	0.48	0/1343
9	j	0.29	0/812	0.53	0/1093
10	k	0.29	0/878	0.55	0/1185
11	l	0.43	0/1082	0.62	0/1453
12	m	0.32	0/875	0.50	0/1173
13	n	0.34	0/504	0.49	0/669
14	o	0.36	0/751	0.54	0/1001
15	p	0.47	0/720	0.59	0/966
16	q	0.40	0/689	0.55	0/920
17	r	0.41	0/544	0.50	0/728
18	s	0.35	0/650	0.51	0/872
19	t	0.37	0/620	0.54	0/829
20	A	0.56	0/65858	0.56	3/102721 (0.0%)
21	B	0.44	0/2773	0.55	0/4320
22	C	0.52	0/2150	0.67	1/2892 (0.0%)
23	D	0.50	0/1601	0.66	0/2150
24	E	0.47	0/1596	0.61	0/2159
25	F	0.29	0/1411	0.50	0/1897
26	G	0.33	0/1365	0.58	0/1839
27	K	0.48	0/1151	0.63	0/1554
28	L	0.48	0/929	0.61	0/1247
29	M	0.45	0/1105	0.66	0/1474
30	N	0.44	0/1141	0.63	0/1519
31	O	0.51	0/1000	0.74	0/1341
32	P	0.40	0/908	0.62	0/1216

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Q	0.48	0/938	0.60	1/1262 (0.1%)
34	R	0.52	0/963	0.57	0/1280
35	S	0.46	0/796	0.61	0/1068
36	T	0.46	0/858	0.59	0/1157
37	U	0.45	0/727	0.66	0/972
38	V	0.40	0/772	0.65	0/1035
39	X	0.48	0/578	0.58	0/773
40	Y	0.41	0/431	0.62	0/574
41	Z	0.39	0/505	0.54	0/672
42	0	0.46	0/437	0.57	0/589
43	2	0.49	0/436	0.57	0/578
44	3	0.39	0/423	0.58	0/563
45	4	0.47	0/377	0.59	0/491
46	5	0.43	0/528	0.61	0/689
47	6	0.44	0/309	0.67	0/409
All	All	0.50	0/145353	0.54	7/217917 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
7	h	0	1
11	l	0	1
18	s	0	1
23	D	0	1
30	N	0	2
31	O	0	2
35	S	0	1
36	T	0	1
38	V	0	1
All	All	0	11

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	956	C	N3-C4-N4	-7.21	96.38	118.00
33	Q	52	GLY	N-CA-C	6.62	121.30	110.77
1	a	34	U	O3'-P-O5'	5.99	112.98	104.00
20	A	956	C	C5-C4-N4	5.94	138.03	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	34	U	P-O3'-C3'	-5.74	111.59	120.20
22	C	156	ARG	CB-CG-CD	-5.19	99.36	111.30
20	A	992	G	N9-C1'-C2'	-5.15	106.27	114.00

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
23	D	89	GLY	Peptide
30	N	16	LYS	Peptide
30	N	19	GLY	Peptide
31	O	4	ARG	Peptide
31	O	73	VAL	Peptide
35	S	50	ALA	Peptide
36	T	67	PHE	Peptide
38	V	87	ASP	Peptide
7	h	22	HIS	Peptide
11	l	37	ASN	Peptide
18	s	34	TRP	Peptide

5.2 Too-close contacts

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	a	32646	0	16439	285	0
2	c	1610	0	1653	32	0
3	d	1620	0	1641	48	0
4	e	1204	0	1280	27	0
5	f	795	0	789	18	0
6	g	1229	0	1259	33	0
7	h	1041	0	1092	26	0
8	i	990	0	1035	15	0
9	j	800	0	846	18	0
10	k	863	0	882	23	0
11	l	1065	0	1133	33	0
12	m	870	0	918	30	0
13	n	492	0	509	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	o	741	0	756	19	0
15	p	708	0	746	11	0
16	q	681	0	719	18	0
17	r	537	0	572	11	0
18	s	634	0	649	17	0
19	t	617	0	648	13	0
20	A	58793	0	29547	419	0
21	B	2480	0	1249	41	0
22	C	2115	0	2202	31	0
23	D	1579	0	1661	32	0
24	E	1574	0	1621	29	0
25	F	1392	0	1454	52	0
26	G	1345	0	1375	36	0
27	K	1130	0	1169	15	0
28	L	922	0	985	17	0
29	M	1095	0	1149	16	0
30	N	1118	0	1180	27	0
31	O	991	0	1028	23	0
32	P	899	0	932	27	0
33	Q	924	0	979	16	0
34	R	950	0	1009	11	0
35	S	784	0	826	12	0
36	T	849	0	906	13	0
37	U	720	0	772	14	0
38	V	763	0	824	16	0
39	X	572	0	580	9	0
40	Y	425	0	460	4	0
41	Z	504	0	538	5	0
42	0	435	0	472	7	0
43	2	429	0	444	3	0
44	3	419	0	435	9	0
45	4	374	0	424	8	0
46	5	522	0	576	5	0
47	6	304	0	337	6	0
48	2	1	0	0	0	0
48	3	1	0	0	0	0
48	6	1	0	0	0	0
48	n	1	0	0	0	0
All	All	133554	0	88700	1428	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (1428) 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)
1:a:1019:G:C2	1:a:1052:A:N6	2.20	1.09
1:a:1019:G:N2	1:a:1052:A:N6	2.03	1.07
20:A:1571:G:N2	20:A:1591:A:H62	1.58	1.01
20:A:275:A:H62	20:A:296:G:N2	1.67	0.93
1:a:858:U:O2	1:a:860:C:N4	2.03	0.92
20:A:1571:G:H22	20:A:1591:A:H62	0.94	0.92
1:a:1019:G:N2	1:a:1051:G:N7	2.18	0.91
1:a:1019:G:N2	1:a:1052:A:C6	2.38	0.91
20:A:1871:G:N2	20:A:1899:A:H62	1.69	0.91
20:A:1871:G:H21	20:A:1899:A:H62	0.92	0.90
20:A:2280:A:H62	20:A:2287:A:H2	1.19	0.86
20:A:1571:G:H22	20:A:1591:A:N6	1.73	0.85
1:a:353:A:P	28:L:97:ARG:HH12	1.99	0.85
6:g:153:HIS:NE2	10:k:94:GLU:OE2	2.09	0.85
20:A:1178:G:H21	27:K:109:MET:HE3	1.40	0.85
30:N:51:ARG:HG3	30:N:66:ILE:HD11	1.59	0.85
20:A:1004:C:HO2'	20:A:2287:A:H8	0.89	0.85
20:A:1871:G:H21	20:A:1899:A:N6	1.75	0.84
18:s:22:GLN:HE22	18:s:28:LYS:H	1.24	0.84
20:A:2704:A:N6	31:O:39:GLU:OE1	2.11	0.83
1:a:360:C:OP2	33:Q:37:ARG:NH1	2.11	0.82
4:e:61:ARG:NH1	4:e:65:GLU:OE2	2.12	0.82
22:C:16:MET:HG2	22:C:206:GLY:HA3	1.62	0.81
20:A:2406:A:H2	20:A:2438:C:H42	1.25	0.81
20:A:162:A:O2'	20:A:169:A:N6	2.14	0.81
1:a:966:U:O4	12:m:103:LYS:NZ	2.14	0.81
20:A:500:A:H62	20:A:509:G:H8	1.28	0.81
1:a:976:U:O2	1:a:1237:G:O2'	1.99	0.81
32:P:6:ASP:OD1	32:P:6:ASP:N	2.09	0.81
26:G:44:ASN:ND2	26:G:51:THR:O	2.14	0.80
38:V:94:SER:OG	38:V:95:LYS:O	1.99	0.79
1:a:1480:G:OP2	33:Q:109:ARG:NH2	2.15	0.79
6:g:111:ARG:HB3	6:g:119:ARG:HD3	1.64	0.78
20:A:1868:A:H62	20:A:1902:G:H8	1.30	0.78
1:a:151:G:H22	1:a:183:G:H1	1.31	0.78
20:A:1004:C:O2'	20:A:2287:A:H8	1.67	0.78
26:G:54:ARG:NH1	26:G:56:ASN:OD1	2.17	0.78
20:A:904:A:HO2'	20:A:905:G:H8	1.31	0.77
22:C:179:GLY:O	22:C:274:ARG:NH1	2.17	0.77
20:A:347:A:O2'	20:A:348:A:H2'	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:j:85:ASP:OD1	9:j:85:ASP:N	2.18	0.77
1:a:428:G:O2'	1:a:443:G:N2	2.18	0.76
20:A:1578:A:H2'	20:A:1579:U:C6	2.20	0.76
31:O:96:ARG:HH21	31:O:126:VAL:HG23	1.50	0.76
1:a:1181:G:N1	1:a:1184:A:OP2	2.17	0.76
20:A:1151:A:H8	20:A:1152:G:H1'	1.49	0.76
16:q:8:ARG:NH1	16:q:67:THR:O	2.18	0.76
25:F:40:VAL:HG12	25:F:42:ASP:H	1.49	0.76
20:A:85:A:O2'	20:A:100:A:N6	2.16	0.76
20:A:2454:C:O2'	20:A:2455:C:O5'	2.02	0.76
20:A:1488:G:O6	20:A:1508:G:O6	2.04	0.76
4:e:161:VAL:HG13	4:e:162:GLU:HG2	1.66	0.75
26:G:164:TYR:HB2	26:G:167:GLU:HG3	1.68	0.75
1:a:27:C:H5	1:a:568:G:H1	1.32	0.75
1:a:361:G:OP1	33:Q:39:ARG:NH2	2.19	0.75
20:A:1832:U:O2'	22:C:154:LEU:O	2.03	0.75
20:A:653:G:N1	20:A:655:G:OP2	2.19	0.74
20:A:287:G:N2	20:A:289:U:OP1	2.21	0.74
2:c:110:LEU:HD11	2:c:145:ALA:HB2	1.69	0.74
6:g:146:ASP:O	6:g:149:ARG:NH2	2.21	0.73
20:A:2348:G:O2'	32:P:20:ASN:ND2	2.21	0.73
20:A:84:G:H21	20:A:103:A:H2	1.34	0.73
25:F:36:ILE:HB	25:F:89:VAL:HG12	1.68	0.73
18:s:6:LYS:HD3	18:s:6:LYS:H	1.53	0.73
27:K:131:HIS:HD2	27:K:133:HIS:H	1.35	0.73
35:S:15:GLU:OE1	35:S:18:GLN:NE2	2.22	0.73
20:A:275:A:H62	20:A:296:G:H21	1.34	0.72
21:B:76:A:H62	21:B:96:G:H8	1.34	0.72
20:A:1861:A:HO2'	20:A:1862:A:H8	1.36	0.72
1:a:1422:C:O2'	20:A:1926:A:N1	2.23	0.72
20:A:2673:G:OP2	26:G:158:LYS:NZ	2.22	0.72
20:A:2811:U:H4'	20:A:2812:A:O5'	1.89	0.72
20:A:568:A:H2	20:A:2055:U:H3	1.37	0.72
1:a:1024:C:O2	1:a:1038:C:N4	2.23	0.72
20:A:716:A:H8	20:A:2083:G:H21	1.35	0.72
1:a:182:C:H2'	1:a:183:G:C8	2.25	0.72
20:A:509:G:H1	45:4:37:LYS:HZ3	1.34	0.71
32:P:56:ALA:HB3	32:P:79:VAL:HG22	1.71	0.71
24:E:2:PRO:HD3	24:E:21:GLU:HG3	1.73	0.71
25:F:52:LYS:NZ	25:F:147:ASP:OD2	2.24	0.71
21:B:29:C:OP1	32:P:4:LYS:NZ	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:1:U:H3	21:B:115:G:H1	1.38	0.71
13:n:23:ARG:NH1	13:n:28:GLY:O	2.24	0.71
26:G:124:GLU:HB2	26:G:132:ILE:HB	1.71	0.71
1:a:1054:A:H2'	1:a:1055:A:C8	2.26	0.71
18:s:80:TYR:OH	18:s:81:ARG:NH1	2.24	0.71
20:A:951:A:O2'	20:A:952:A:N7	2.23	0.71
20:A:885:U:H2'	20:A:886:U:H4'	1.72	0.70
10:k:75:MET:HE1	10:k:104:GLY:HA3	1.73	0.70
27:K:7:ALA:H	27:K:46:THR:HG21	1.55	0.70
1:a:1206:A:H5''	2:c:4:LYS:HE3	1.72	0.70
16:q:67:THR:HG22	16:q:68:ARG:HG2	1.72	0.70
1:a:1316:U:O2'	1:a:1317:U:H5'	1.91	0.70
20:A:2329:U:H2'	20:A:2330:U:C6	2.26	0.70
20:A:2318:G:H22	20:A:2326:U:H3	1.38	0.70
33:Q:17:ILE:HD13	33:Q:76:LEU:HD22	1.72	0.70
1:a:477:U:H2'	1:a:478:A:C8	2.27	0.69
20:A:899:G:OP2	39:X:86:LYS:NZ	2.24	0.69
20:A:2636:C:O2'	20:A:2836:G:N2	2.25	0.69
35:S:88:HIS:HE1	35:S:90:GLN:HG2	1.56	0.69
1:a:1450:G:H2'	1:a:1451:U:C6	2.28	0.69
3:d:191:ASP:OD1	3:d:193:ALA:N	2.25	0.69
20:A:2856:A:H62	20:A:2882:G:H21	1.38	0.69
20:A:275:A:N6	20:A:296:G:H21	1.90	0.69
20:A:1756:U:O2'	20:A:1760:G:N2	2.25	0.69
1:a:151:G:N2	1:a:183:G:H22	1.91	0.69
1:a:1019:G:H3'	1:a:1042:C:H42	1.56	0.69
1:a:727:A:H2'	1:a:728:G:C8	2.29	0.69
23:D:123:ILE:HD12	23:D:141:ARG:HG3	1.75	0.69
21:B:78:U:H2'	21:B:79:G:H21	1.57	0.68
1:a:1054:A:H2'	1:a:1055:A:H8	1.59	0.68
20:A:1629:A:H3'	20:A:1630:G:H5''	1.75	0.68
36:T:48:SER:HA	36:T:51:ILE:HD12	1.76	0.68
1:a:688:G:H2'	1:a:689:G:C8	2.28	0.68
1:a:1058:U:H2'	1:a:1059:G:C8	2.28	0.68
1:a:1473:G:OP1	19:t:34:LYS:NZ	2.23	0.68
23:D:125:ARG:HG3	23:D:164:MET:HG3	1.76	0.68
24:E:10:ASP:OD1	24:E:10:ASP:N	2.23	0.68
1:a:672:U:H3	1:a:764:A:H62	1.42	0.68
1:a:1432:G:O2'	1:a:1499:A:N6	2.27	0.68
21:B:97:A:O2'	21:B:98:G:OP1	2.10	0.68
25:F:130:LEU:HD13	25:F:131:GLY:H	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:F:170:LEU:HD22	25:F:175:MET:HG3	1.76	0.67
20:A:1504:G:O2'	20:A:1505:C:OP2	2.12	0.67
21:B:70:G:H8	21:B:102:A:H62	1.41	0.67
11:l:102:ASP:OD1	11:l:103:LEU:N	2.28	0.67
20:A:337:A:OP2	38:V:95:LYS:NZ	2.28	0.67
22:C:108:LYS:HG3	22:C:196:GLY:HA2	1.76	0.67
20:A:13:U:O2'	20:A:14:A:OP1	2.10	0.67
20:A:232:U:O2'	20:A:233:U:O5'	2.13	0.67
37:U:23:LYS:NZ	37:U:84:GLU:HA	2.10	0.67
6:g:70:MET:HB3	6:g:96:ARG:HG2	1.75	0.67
1:a:26:A:O2'	1:a:27:C:O2	2.11	0.67
10:k:20:VAL:HG22	10:k:83:ASP:HB2	1.75	0.67
1:a:360:C:O2	1:a:361:G:N1	2.27	0.67
1:a:477:U:H2'	1:a:478:A:H8	1.59	0.67
1:a:1292:C:HO2'	1:a:1294:A:H8	1.41	0.67
37:U:29:VAL:HG21	37:U:38:VAL:HG22	1.78	0.66
44:3:31:GLU:HG2	44:3:46:ARG:HG2	1.77	0.66
17:r:20:ASN:OD1	17:r:20:ASN:N	2.27	0.66
16:q:21:ASP:OD1	16:q:21:ASP:N	2.19	0.66
20:A:1216:G:OP2	20:A:1217:G:N2	2.29	0.66
3:d:15:LEU:HB3	3:d:56:LYS:HD3	1.77	0.66
4:e:6:PRO:HB2	4:e:8:HIS:CD2	2.30	0.66
24:E:78:ILE:HG22	24:E:79:ARG:HD2	1.76	0.66
11:l:26:LYS:HD3	11:l:72:ASN:HB3	1.76	0.66
25:F:6:GLU:O	25:F:10:LYS:HB2	1.95	0.66
4:e:94:ILE:HD11	4:e:136:VAL:HG13	1.78	0.66
7:h:77:LEU:HD13	7:h:131:VAL:HB	1.77	0.66
16:q:71:SER:HB2	16:q:74:LYS:HG2	1.75	0.66
9:j:6:ILE:HG23	9:j:76:ILE:HB	1.78	0.66
20:A:2328:A:H2'	20:A:2329:U:C6	2.30	0.66
1:a:483:C:O2'	1:a:484:U:O4'	2.14	0.66
1:a:1427:C:H2'	1:a:1428:A:C8	2.31	0.66
20:A:533:G:H4'	36:T:11:THR:HG23	1.78	0.65
28:L:73:ASP:OD1	28:L:73:ASP:N	2.27	0.65
13:n:16:HIS:HB2	13:n:19:GLN:HG3	1.78	0.65
14:o:29:ILE:HD13	14:o:67:LEU:HD11	1.78	0.65
39:X:81:LYS:HB2	39:X:87:GLN:HG3	1.78	0.65
11:l:10:LYS:O	11:l:10:LYS:NZ	2.21	0.65
20:A:654:A:H1'	20:A:655:G:H2'	1.76	0.65
10:k:17:GLU:HA	10:k:79:LEU:HA	1.78	0.65
20:A:1585:U:H2'	20:A:1586:A:C8	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:1576:A:N1	20:A:1578:A:N6	2.44	0.65
25:F:38:MET:HE3	25:F:150:ARG:HH11	1.62	0.65
47:6:17:ILE:HG22	47:6:18:ARG:H	1.61	0.65
20:A:1630:G:H1'	20:A:1631:A:C5	2.32	0.65
39:X:55:TYR:HE1	39:X:85:LYS:HD3	1.61	0.65
20:A:1167:A:C8	20:A:2532:A:H5''	2.33	0.64
20:A:2342:A:H2'	20:A:2343:A:C8	2.32	0.64
1:a:560:C:H5''	3:d:65:GLU:HG3	1.77	0.64
1:a:1056:A:H2'	1:a:1057:G:C8	2.33	0.64
24:E:8:LYS:HD3	24:E:14:ASN:HD22	1.63	0.64
1:a:101:A:H2'	1:a:102:G:C8	2.33	0.64
4:e:32:ARG:HD3	4:e:52:LYS:HD3	1.80	0.64
11:l:36:THR:O	11:l:36:THR:OG1	2.16	0.64
20:A:2453:A:H4'	20:A:2454:C:H3'	1.78	0.64
20:A:2520:U:H3	20:A:2597:G:H1	1.46	0.64
29:M:85:PHE:O	29:M:119:LYS:NZ	2.31	0.64
20:A:1216:G:H3'	20:A:1217:G:H5''	1.78	0.64
1:a:1164:C:OP2	8:i:11:ARG:NH2	2.30	0.64
1:a:1201:G:N2	13:n:61:TRP:O	2.27	0.64
1:a:1508:A:O2'	1:a:1509:A:O5'	2.14	0.64
18:s:55:ARG:HD2	18:s:56:LYS:HG3	1.78	0.64
20:A:904:A:O2'	20:A:905:G:H8	1.80	0.64
20:A:623:A:H62	20:A:1288:A:H2	1.46	0.64
27:K:4:THR:HG21	34:R:61:TRP:HE1	1.62	0.64
1:a:1277:G:H2'	1:a:1278:A:C8	2.32	0.64
10:k:94:GLU:HG3	10:k:98:ARG:HH12	1.63	0.64
8:i:112:GLU:OE2	8:i:115:LYS:NZ	2.30	0.63
20:A:508:G:H2'	20:A:509:G:H5'	1.80	0.63
20:A:1535:U:O2'	20:A:1536:A:OP1	2.14	0.63
20:A:1074:G:O4'	47:6:18:ARG:NH1	2.31	0.63
1:a:991:A:H4'	1:a:992:G:H5''	1.80	0.63
38:V:97:THR:OG1	38:V:99:GLU:OE2	2.16	0.63
20:A:853:U:H2'	20:A:854:C:C6	2.34	0.63
1:a:467:A:H62	1:a:495:U:H3	1.47	0.63
20:A:1860:G:H2'	20:A:1861:A:C8	2.34	0.63
46:5:10:LEU:HB3	46:5:62:LEU:HD21	1.81	0.63
20:A:359:A:OP1	24:E:168:ARG:NH1	2.32	0.62
24:E:59:GLY:HA3	24:E:79:ARG:HD3	1.79	0.62
1:a:965:A:P	12:m:105:ASN:HD22	2.22	0.62
1:a:763:A:H1'	1:a:764:A:H2	1.62	0.62
5:f:36:ASN:N	5:f:36:ASN:OD1	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:S:24:LYS:HA	35:S:93:THR:HG23	1.81	0.62
20:A:2333:A:H4'	20:A:2334:A:H5'	1.82	0.62
39:X:49:GLN:HE22	39:X:54:ILE:H	1.45	0.62
20:A:1570:G:H22	20:A:1592:G:H1	1.47	0.62
21:B:70:G:H8	21:B:102:A:N6	1.96	0.62
25:F:12:VAL:HG22	25:F:172:GLN:HG2	1.81	0.62
20:A:500:A:N6	20:A:509:G:H8	1.95	0.62
21:B:57:G:O2'	32:P:6:ASP:OD2	2.18	0.62
1:a:354:C:OP2	28:L:97:ARG:HD2	2.00	0.62
1:a:1508:A:H2'	1:a:1509:A:C8	2.34	0.62
4:e:88:VAL:HG22	4:e:93:ARG:HG2	1.81	0.62
10:k:29:ASN:OD1	10:k:30:THR:N	2.30	0.62
26:G:25:THR:HB	26:G:34:THR:HG22	1.82	0.62
30:N:43:THR:HG22	30:N:94:VAL:HG12	1.82	0.61
20:A:285:U:O2'	20:A:287:G:OP1	2.17	0.61
22:C:133:GLU:HG3	22:C:186:ALA:HB1	1.82	0.61
36:T:5:ILE:HD11	36:T:67:PHE:CG	2.35	0.61
1:a:1038:C:O2'	1:a:1039:U:O5'	2.18	0.61
14:o:89:ARG:HH21	14:o:89:ARG:C	2.09	0.61
20:A:539:G:N1	20:A:542:A:OP2	2.30	0.61
20:A:2280:A:N6	20:A:2287:A:H2	1.95	0.61
20:A:2329:U:H2'	20:A:2330:U:H6	1.65	0.61
20:A:2207:C:H2'	20:A:2208:C:O4'	2.00	0.61
1:a:108:U:OP1	19:t:12:ARG:NH1	2.34	0.61
1:a:360:C:H5'	33:Q:39:ARG:NE	2.16	0.61
11:l:32:LYS:O	11:l:33:LYS:NZ	2.24	0.61
20:A:2517:A:O2'	20:A:2519:G:OP2	2.18	0.61
22:C:158:ALA:HB1	22:C:197:ASN:O	2.01	0.61
20:A:891:A:O2'	42:O:22:THR:HG22	2.00	0.61
20:A:1310:A:O2'	20:A:1689:A:N6	2.34	0.61
30:N:19:GLY:HA2	30:N:98:LYS:HD2	1.81	0.61
1:a:201:C:O2'	16:q:77:ARG:NH2	2.34	0.61
31:O:55:ASP:OD1	31:O:55:ASP:N	2.31	0.61
2:c:152:VAL:HG23	2:c:197:VAL:HG22	1.82	0.61
3:d:97:ASN:OD1	3:d:108:ARG:NH1	2.34	0.61
14:o:89:ARG:HE	20:A:754:U:H5''	1.66	0.61
20:A:1194:G:OP2	34:R:58:ARG:NH1	2.34	0.61
4:e:7:LYS:HD3	4:e:68:LYS:HB3	1.82	0.60
1:a:487:A:N1	1:a:488:C:N4	2.48	0.60
2:c:14:ILE:HG22	2:c:15:ILE:HG23	1.83	0.60
20:A:626:U:H2'	20:A:627:A:H8	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:76:A:N6	21:B:96:G:H8	1.98	0.60
1:a:1063:G:H5''	13:n:4:LYS:HD3	1.81	0.60
10:k:14:LYS:HE3	10:k:16:ILE:HD11	1.82	0.60
20:A:1994:G:O2'	20:A:1996:U:OP2	2.19	0.60
20:A:2514:U:O2	20:A:2518:U:N3	2.35	0.60
20:A:2771:A:N1	26:G:67:THR:HG21	2.15	0.60
1:a:1330:U:HO2'	1:a:1375:A:H8	1.49	0.60
20:A:1724:G:H21	20:A:1776:A:H3'	1.67	0.60
20:A:1756:U:O4	20:A:1758:C:H5''	2.01	0.60
1:a:1017:U:C5	1:a:1018:U:H1'	2.37	0.60
7:h:98:LEU:HD22	7:h:132:TRP:HB2	1.83	0.60
20:A:1814:C:H3'	22:C:146:MET:HE1	1.83	0.60
1:a:722:U:H2'	1:a:723:A:H8	1.66	0.60
7:h:29:ALA:H	7:h:58:GLY:HA2	1.66	0.60
20:A:626:U:H2'	20:A:627:A:C8	2.37	0.60
23:D:55:ASP:OD1	23:D:77:LYS:NZ	2.26	0.60
28:L:24:VAL:HG13	28:L:33:ALA:HB2	1.83	0.60
32:P:40:ILE:HD11	32:P:72:ALA:HA	1.82	0.60
34:R:97:ASP:OD1	34:R:101:ASN:ND2	2.35	0.60
1:a:225:U:O2'	1:a:228:G:N7	2.20	0.60
7:h:76:ASN:HB3	7:h:132:TRP:CZ2	2.37	0.60
3:d:83:HIS:O	3:d:83:HIS:ND1	2.35	0.60
7:h:39:ILE:HG12	7:h:42:ARG:NH2	2.16	0.60
15:p:88:ASN:OD1	15:p:88:ASN:N	2.35	0.60
20:A:1494:G:H1	20:A:1504:G:H21	1.50	0.60
25:F:166:SER:O	25:F:170:LEU:HB2	2.01	0.60
26:G:58:SER:O	26:G:61:MET:HG2	2.02	0.60
20:A:285:U:H2'	20:A:287:G:H8	1.66	0.59
27:K:63:VAL:HG21	27:K:102:ILE:HD11	1.83	0.59
20:A:262:G:H21	20:A:660:A:H8	1.51	0.59
20:A:2328:A:H2'	20:A:2329:U:H6	1.65	0.59
29:M:1:MET:HE2	29:M:6:LEU:HA	1.84	0.59
20:A:225:A:H62	20:A:235:G:H8	1.49	0.59
20:A:1323:A:H8	31:O:113:ARG:HD3	1.67	0.59
20:A:2341:A:H2'	20:A:2342:A:C8	2.36	0.59
30:N:41:TRP:HZ3	30:N:74:TYR:CE1	2.21	0.59
36:T:17:THR:HG22	36:T:47:LYS:HE3	1.84	0.59
1:a:100:A:H2'	1:a:101:A:H8	1.67	0.59
41:Z:51:ALA:O	41:Z:55:THR:HG22	2.03	0.59
1:a:856:U:H3	1:a:859:C:HO2'	1.50	0.59
8:i:130:ARG:HH11	8:i:130:ARG:HB3	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:92:A:H2'	20:A:93:G:H5'	1.82	0.59
1:a:1056:A:H2'	1:a:1057:G:H8	1.65	0.59
1:a:29:A:H2'	1:a:30:A:C8	2.38	0.59
1:a:427:A:H4'	1:a:428:G:O5'	2.03	0.59
1:a:1021:C:N4	1:a:1041:U:OP2	2.35	0.59
20:A:585:A:H4'	20:A:586:A:H5'	1.84	0.59
20:A:2810:U:C2	20:A:2811:U:H5	2.20	0.59
20:A:2758:G:N2	26:G:143:GLU:OE2	2.36	0.59
1:a:1021:C:O5'	1:a:1040:U:H2'	2.03	0.58
20:A:2361:C:OP1	44:3:34:LYS:NZ	2.34	0.58
20:A:2738:U:OP1	23:D:124:LYS:NZ	2.30	0.58
11:l:27:GLY:HA3	11:l:35:GLN:H	1.68	0.58
20:A:2461:G:N2	20:A:2464:A:OP2	2.35	0.58
20:A:2856:A:H62	20:A:2882:G:N2	2.01	0.58
39:X:73:ASP:OD1	39:X:73:ASP:N	2.34	0.58
42:0:50:ILE:HG23	42:0:53:LEU:HD12	1.85	0.58
11:l:26:LYS:HE3	11:l:70:LEU:HD12	1.85	0.58
20:A:77:C:O2'	41:Z:55:THR:HG21	2.04	0.58
1:a:31:C:HO2'	1:a:32:G:H8	1.46	0.58
10:k:14:LYS:HG2	10:k:16:ILE:HG12	1.85	0.58
20:A:154:U:HO2'	20:A:155:U:H6	1.51	0.58
20:A:1376:U:OP1	37:U:15:LYS:NZ	2.37	0.58
11:l:68:VAL:HG11	11:l:95:LEU:HD11	1.85	0.58
14:o:25:PRO:O	14:o:29:ILE:HG23	2.03	0.58
20:A:1408:U:HO2'	20:A:2226:A:H8	1.49	0.58
1:a:1149:A:N6	1:a:1157:G:O6	2.37	0.58
7:h:47:ARG:HG3	7:h:65:LYS:HB2	1.85	0.58
20:A:1208:C:H2'	20:A:1209:A:C8	2.39	0.58
32:P:15:HIS:HE1	32:P:94:ASP:OD2	1.87	0.58
1:a:1277:G:H2'	1:a:1278:A:H8	1.68	0.58
27:K:145:ASN:OD1	27:K:145:ASN:N	2.36	0.58
20:A:586:A:O2'	20:A:587:U:H5''	2.04	0.58
22:C:118:SER:O	22:C:118:SER:OG	2.20	0.58
25:F:53:ALA:HB2	25:F:150:ARG:HH12	1.68	0.58
26:G:4:ILE:O	26:G:69:ARG:HD3	2.04	0.58
44:3:29:ARG:NH1	44:3:49:LYS:HB2	2.19	0.58
14:o:24:SER:O	14:o:26:GLU:N	2.37	0.57
25:F:42:ASP:O	25:F:49:ASN:ND2	2.37	0.57
1:a:861:G:O2'	1:a:862:C:OP1	2.22	0.57
18:s:44:PHE:HB3	18:s:62:ILE:HD12	1.86	0.57
39:X:55:TYR:CE1	39:X:85:LYS:HD3	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:P:100:TYR:OH	32:P:112:ARG:NH2	2.37	0.57
20:A:1490:A:C2'	20:A:1491:U:H5'	2.34	0.57
20:A:1861:A:O2'	20:A:1862:A:H8	1.87	0.57
1:a:1292:C:O2'	1:a:1294:A:H8	1.87	0.57
20:A:607:G:H2'	20:A:2044:A:C2	2.40	0.57
17:r:26:ASP:O	17:r:28:LYS:N	2.37	0.57
32:P:40:ILE:H	32:P:58:ALA:HB2	1.69	0.57
14:o:5:GLN:O	14:o:9:ASN:ND2	2.36	0.57
23:D:9:LYS:HB2	23:D:200:ILE:HD11	1.86	0.57
25:F:46:ASN:O	25:F:49:ASN:ND2	2.37	0.57
45:4:34:ARG:NH1	45:4:41:VAL:O	2.37	0.57
14:o:7:ARG:O	14:o:11:ILE:HG23	2.05	0.57
20:A:1458:G:H1	20:A:1628:G:H21	1.53	0.57
29:M:101:ILE:HG22	29:M:102:VAL:HG23	1.85	0.57
1:a:506:A:H2'	1:a:507:A:C8	2.40	0.56
20:A:1086:A:H2'	20:A:1086:A:N3	2.19	0.56
20:A:1585:U:H2'	20:A:1586:A:H8	1.69	0.56
35:S:50:ALA:O	35:S:52:THR:N	2.37	0.56
1:a:427:A:O5'	1:a:427:A:H8	1.88	0.56
20:A:1633:A:O2'	20:A:1634:A:H5''	2.05	0.56
6:g:150:ALA:O	10:k:98:ARG:NH2	2.38	0.56
11:l:127:ARG:HB3	11:l:132:THR:HB	1.87	0.56
20:A:1793:U:H5	20:A:1798:A:N7	2.03	0.56
1:a:965:A:OP2	12:m:105:ASN:HB2	2.05	0.56
1:a:1508:A:O2'	1:a:1509:A:O4'	2.23	0.56
4:e:148:LYS:HE2	7:h:75:THR:HG21	1.88	0.56
20:A:2219:A:H2'	20:A:2220:C:C6	2.41	0.56
2:c:94:THR:HB	2:c:96:LYS:HD2	1.88	0.56
22:C:108:LYS:HE2	22:C:198:GLU:HG2	1.88	0.56
30:N:41:TRP:HZ3	30:N:74:TYR:HE1	1.53	0.56
14:o:8:LYS:O	14:o:12:ILE:HG23	2.06	0.56
20:A:951:A:O2'	20:A:952:A:C8	2.56	0.56
8:i:10:GLY:HA2	8:i:81:HIS:HD2	1.71	0.56
1:a:1317:U:OP2	12:m:21:TYR:OH	2.22	0.56
20:A:905:G:H21	20:A:907:A:N6	2.03	0.56
1:a:1019:G:N2	1:a:1052:A:C5	2.73	0.56
20:A:160:U:H2'	20:A:161:G:O4'	2.06	0.56
20:A:2204:A:H2'	20:A:2205:A:C8	2.41	0.56
30:N:42:ILE:HD12	30:N:97:VAL:HG21	1.87	0.56
20:A:2085:A:H2'	20:A:2086:G:C8	2.41	0.56
25:F:138:PHE:HB2	25:F:141:VAL:HG23	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:L:63:VAL:HG11	28:L:102:VAL:HG22	1.88	0.56
12:m:106:ALA:O	12:m:110:LYS:N	2.38	0.55
20:A:344:G:H8	20:A:367:A:H61	1.53	0.55
20:A:916:A:H2'	20:A:917:C:O4'	2.07	0.55
20:A:1422:C:H2'	20:A:1423:A:C8	2.41	0.55
20:A:1571:G:N2	20:A:1591:A:N6	2.41	0.55
24:E:67:GLN:HG3	24:E:68:LYS:HG3	1.88	0.55
24:E:158:ASN:O	24:E:160:ASN:N	2.33	0.55
26:G:95:ARG:HB3	26:G:128:ASN:HB3	1.87	0.55
1:a:647:G:H4'	1:a:648:U:H5	1.71	0.55
1:a:1196:G:O2'	1:a:1197:G:N7	2.37	0.55
20:A:1490:A:N1	20:A:1506:A:N1	2.54	0.55
6:g:151:PHE:O	6:g:155:ARG:NH1	2.40	0.55
22:C:76:ALA:HB1	22:C:94:VAL:HG13	1.86	0.55
25:F:129:THR:HG22	25:F:155:VAL:HG22	1.88	0.55
35:S:5:ILE:HD11	35:S:58:VAL:HG21	1.88	0.55
1:a:578:A:N3	11:l:12:ARG:NH1	2.54	0.55
7:h:34:ARG:O	7:h:38:GLU:HG2	2.06	0.55
9:j:55:THR:HG22	13:n:42:ILE:HD12	1.89	0.55
12:m:7:VAL:HG22	12:m:8:ASP:HB2	1.89	0.55
15:p:37:VAL:HG11	15:p:56:VAL:HG22	1.89	0.55
17:r:25:ILE:HD13	17:r:62:ALA:HB2	1.88	0.55
20:A:391:C:O2'	20:A:392:A:O5'	2.24	0.55
1:a:974:A:O2'	1:a:975:A:OP1	2.24	0.55
9:j:59:LYS:HE2	9:j:62:ARG:HH21	1.70	0.55
20:A:162:A:HO2'	20:A:169:A:H61	1.48	0.55
1:a:1044:C:H2'	1:a:1045:U:C2	2.41	0.55
1:a:1106:U:H2'	1:a:1107:U:C6	2.41	0.55
9:j:54:ALA:O	13:n:41:ARG:NH1	2.39	0.55
20:A:234:C:O2'	20:A:235:G:O4'	2.24	0.55
20:A:1583:A:N3	20:A:1583:A:H2'	2.20	0.55
25:F:60:ILE:HG22	25:F:61:THR:HG23	1.89	0.55
37:U:64:ARG:HG3	37:U:69:ALA:HB2	1.88	0.55
2:c:21:LYS:HG3	2:c:57:GLU:HG2	1.89	0.55
7:h:11:LEU:HG	7:h:77:LEU:HG	1.87	0.55
12:m:81:MET:HG3	12:m:82:GLU:HG3	1.89	0.55
1:a:100:A:H2'	1:a:101:A:C8	2.42	0.55
1:a:1549:C:O2	1:a:1550:A:N6	2.39	0.55
16:q:18:ASP:OD1	16:q:18:ASP:N	2.40	0.55
20:A:151:A:H61	20:A:179:A:H2	1.54	0.55
20:A:311:A:O2'	20:A:399:A:N1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:1931:U:H2'	20:A:1932:A:O4'	2.07	0.55
26:G:26:VAL:HG12	26:G:79:VAL:HG11	1.88	0.55
1:a:993:A:H2'	1:a:994:A:H5''	1.89	0.55
1:a:1031:G:OP2	1:a:1031:G:H8	1.90	0.55
1:a:1412:C:OP2	4:e:29:ARG:NH2	2.39	0.55
1:a:1534:A:H2'	1:a:1535:A:C8	2.41	0.55
20:A:1394:G:H8	20:A:1409:A:H62	1.54	0.55
20:A:275:A:N6	20:A:296:G:N2	2.44	0.54
20:A:1208:C:H2'	20:A:1209:A:H8	1.72	0.54
23:D:89:GLY:O	23:D:91:TYR:N	2.40	0.54
20:A:2673:G:P	26:G:158:LYS:HZ2	2.28	0.54
1:a:487:A:C6	1:a:488:C:N4	2.76	0.54
6:g:150:ALA:O	6:g:153:HIS:ND1	2.40	0.54
21:B:68:C:H5	21:B:104:G:H22	1.56	0.54
1:a:1427:C:H2'	1:a:1428:A:H8	1.73	0.54
20:A:2860:G:OP1	33:Q:93:ARG:NH1	2.40	0.54
21:B:39:G:OP1	21:B:41:C:N4	2.40	0.54
44:3:3:VAL:HG12	44:3:4:ASN:O	2.07	0.54
1:a:360:C:H1'	1:a:361:G:C2	2.43	0.54
1:a:709:A:OP1	10:k:55:SER:OG	2.25	0.54
2:c:44:THR:HG23	2:c:45:LYS:H	1.72	0.54
3:d:20:SER:O	3:d:20:SER:OG	2.20	0.54
10:k:23:ILE:HB	10:k:86:VAL:HG13	1.90	0.54
20:A:883:A:H2'	20:A:884:A:C8	2.43	0.54
20:A:1151:A:C8	20:A:1152:G:H1'	2.37	0.54
30:N:85:LYS:HG2	39:X:18:SER:N	2.22	0.54
20:A:950:A:H2'	20:A:953:C:C5	2.42	0.54
1:a:511:G:H21	1:a:512:A:H5''	1.73	0.54
6:g:7:VAL:HG22	6:g:8:ALA:H	1.71	0.54
20:A:508:G:C2'	20:A:509:G:H5'	2.38	0.54
25:F:119:LYS:HB3	25:F:167:ARG:NH2	2.23	0.54
29:M:122:THR:O	29:M:122:THR:OG1	2.25	0.54
38:V:84:LYS:HB2	38:V:93:VAL:HG21	1.88	0.54
20:A:313:A:H2'	20:A:314:U:O4'	2.08	0.54
31:O:100:ARG:HG3	31:O:101:GLN:O	2.08	0.54
1:a:137:C:O2'	1:a:277:A:H8	1.91	0.54
7:h:12:THR:HG22	7:h:15:ARG:HH21	1.72	0.54
20:A:1310:A:HO2'	20:A:1689:A:N6	2.06	0.54
25:F:5:LYS:HE3	25:F:97:TYR:HE2	1.73	0.54
1:a:475:G:H1	1:a:488:C:N4	2.06	0.53
4:e:161:VAL:C	4:e:163:GLU:H	2.15	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:r:26:ASP:C	17:r:28:LYS:H	2.16	0.53
18:s:16:MET:HA	18:s:19:VAL:HG12	1.89	0.53
28:L:102:VAL:HG13	28:L:106:LEU:HD12	1.90	0.53
1:a:18:G:H2'	1:a:19:G:C8	2.43	0.53
20:A:1081:U:H2'	20:A:1082:G:H8	1.73	0.53
20:A:285:U:H2'	20:A:287:G:C8	2.43	0.53
20:A:1754:A:H2'	20:A:1755:C:O4'	2.08	0.53
32:P:75:VAL:O	32:P:79:VAL:HG23	2.09	0.53
6:g:72:VAL:HG12	6:g:142:HIS:CE1	2.42	0.53
20:A:904:A:H2'	30:N:22:LYS:HE3	1.89	0.53
20:A:1591:A:H2'	20:A:1592:G:C8	2.43	0.53
21:B:68:C:H5	21:B:104:G:H1	1.55	0.53
22:C:272:ARG:HD3	22:C:274:ARG:HE	1.73	0.53
42:O:37:LYS:HB3	42:O:43:ILE:HD13	1.89	0.53
1:a:1505:G:H2'	1:a:1506:U:C6	2.43	0.53
20:A:1202:G:O3'	35:S:24:LYS:NZ	2.42	0.53
20:A:2712:U:H2'	20:A:2713:U:C6	2.43	0.53
29:M:84:ARG:HH21	29:M:101:ILE:HD11	1.74	0.53
42:O:18:ASN:O	42:O:22:THR:HG23	2.09	0.53
1:a:31:C:O2'	1:a:32:G:H8	1.91	0.53
1:a:795:A:H5''	10:k:125:LYS:HD2	1.91	0.53
8:i:130:ARG:HB3	8:i:130:ARG:NH1	2.23	0.53
20:A:1631:A:C4	20:A:1632:A:H2	2.27	0.53
1:a:352:G:H2'	1:a:353:A:C8	2.44	0.53
1:a:1164:C:P	8:i:11:ARG:HH21	2.32	0.53
1:a:1475:C:OP1	19:t:26:ASN:ND2	2.39	0.53
4:e:160:SER:OG	4:e:161:VAL:O	2.27	0.53
20:A:118:A:OP2	20:A:119:A:H5''	2.09	0.53
22:C:69:ARG:NH2	22:C:127:GLY:O	2.41	0.53
22:C:108:LYS:HE3	22:C:195:VAL:O	2.08	0.53
23:D:120:GLN:HG2	23:D:164:MET:HE3	1.90	0.53
36:T:16:ARG:NH1	36:T:103:LYS:HD3	2.23	0.53
38:V:87:ASP:O	38:V:89:LYS:N	2.36	0.53
3:d:140:ILE:O	3:d:140:ILE:HG13	2.09	0.53
3:d:152:ILE:O	3:d:156:VAL:HG23	2.09	0.53
20:A:292:U:H2'	20:A:293:U:C6	2.44	0.53
36:T:16:ARG:HH11	36:T:103:LYS:HD3	1.74	0.53
2:c:18:TRP:O	2:c:21:LYS:NZ	2.40	0.53
9:j:19:ASP:OD1	9:j:20:GLN:N	2.42	0.53
23:D:13:THR:OG1	23:D:14:GLN:N	2.42	0.53
37:U:23:LYS:HZ1	37:U:84:GLU:HA	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1078:U:H2'	1:a:1079:C:C6	2.43	0.52
19:t:58:ASP:OD1	19:t:75:LYS:HD3	2.08	0.52
20:A:2836:G:O5'	20:A:2836:G:H8	1.91	0.52
21:B:40:C:C5	25:F:66:LEU:HG	2.44	0.52
42:0:7:THR:HB	42:0:34:THR:HG22	1.90	0.52
45:4:8:ASN:HD22	45:4:11:LYS:H	1.57	0.52
1:a:35:G:H8	1:a:35:G:OP1	1.92	0.52
1:a:1344:A:OP1	12:m:29:THR:OG1	2.19	0.52
20:A:2111:G:H2'	20:A:2112:U:C6	2.44	0.52
32:P:69:THR:HG22	32:P:103:ARG:HB3	1.91	0.52
13:n:41:ARG:HD2	13:n:42:ILE:HG23	1.91	0.52
20:A:899:G:N3	20:A:2282:A:H2'	2.24	0.52
20:A:2323:A:OP1	20:A:2323:A:H8	1.92	0.52
32:P:8:ASN:O	32:P:12:GLN:HG2	2.08	0.52
1:a:1020:A:H1'	1:a:1052:A:C6	2.45	0.52
18:s:32:LYS:HD2	18:s:57:HIS:CD2	2.44	0.52
21:B:86:U:H4'	21:B:87:U:H5	1.74	0.52
1:a:897:G:P	11:l:9:ARG:HH22	2.32	0.52
5:f:14:ARG:N	5:f:89:ASP:O	2.42	0.52
22:C:168:GLU:OE1	22:C:169:GLY:N	2.43	0.52
28:L:28:SER:O	28:L:28:SER:OG	2.24	0.52
1:a:699:U:H1'	10:k:40:ASN:HA	1.91	0.52
1:a:1226:U:O2'	1:a:1227:U:OP2	2.25	0.52
5:f:42:GLU:HB3	5:f:67:ASN:HB2	1.91	0.52
7:h:13:ARG:HD2	7:h:27:VAL:HG13	1.92	0.52
19:t:50:TYR:CE2	19:t:83:LYS:HD2	2.45	0.52
20:A:65:A:C5	37:U:65:MET:HE2	2.44	0.52
20:A:181:G:H2'	20:A:182:U:O4'	2.10	0.52
20:A:498:G:O6	24:E:58:ARG:HD3	2.08	0.52
20:A:1758:C:H2'	20:A:1759:G:C8	2.45	0.52
20:A:1872:G:H1'	20:A:1898:A:N6	2.23	0.52
21:B:48:A:OP1	32:P:69:THR:N	2.42	0.52
3:d:159:THR:O	3:d:159:THR:OG1	2.27	0.52
4:e:83:HIS:CD2	4:e:147:LEU:HD12	2.45	0.52
20:A:943:U:H2'	20:A:944:U:C6	2.45	0.52
20:A:945:C:H2'	20:A:946:A:O4'	2.10	0.52
25:F:40:VAL:HB	25:F:85:ILE:O	2.10	0.52
1:a:880:A:H2'	1:a:881:A:C8	2.45	0.52
1:a:1127:A:N1	2:c:176:THR:HG22	2.25	0.52
1:a:1146:A:C5	1:a:1147:U:H5	2.28	0.52
5:f:29:PHE:HA	5:f:32:ILE:HG12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Q:60:THR:HB	33:Q:73:THR:HG22	1.92	0.52
1:a:1480:G:P	33:Q:109:ARG:HH22	2.32	0.52
3:d:15:LEU:HD13	3:d:56:LYS:HA	1.92	0.52
4:e:82:PRO:HD2	4:e:147:LEU:HG	1.92	0.52
14:o:21:ASP:OD1	14:o:24:SER:OG	2.24	0.52
20:A:1451:U:O2'	20:A:1452:G:OP2	2.27	0.52
23:D:107:VAL:HG23	23:D:173:ASN:HA	1.92	0.52
1:a:711:A:H2'	1:a:712:U:H6	1.74	0.52
4:e:60:ILE:O	4:e:64:ILE:HG13	2.10	0.52
7:h:10:PHE:CE1	7:h:27:VAL:HG21	2.45	0.52
30:N:32:TRP:CZ3	30:N:133:LYS:HG2	2.45	0.52
31:O:40:VAL:O	31:O:44:VAL:HG23	2.10	0.52
1:a:1447:G:OP1	33:Q:105:GLY:HA3	2.10	0.51
11:l:26:LYS:NZ	11:l:70:LEU:HB2	2.25	0.51
12:m:4:ILE:HG12	12:m:9:ILE:HG13	1.93	0.51
20:A:678:U:H2'	20:A:679:C:C6	2.45	0.51
20:A:1212:A:HO2'	20:A:1213:U:H6	1.53	0.51
20:A:1591:A:H3'	20:A:1591:A:N3	2.25	0.51
1:a:445:A:OP1	3:d:9:TRP:HB3	2.11	0.51
3:d:45:SER:O	3:d:49:MET:HG2	2.11	0.51
20:A:203:U:H4'	40:Y:22:MET:HB3	1.92	0.51
47:6:36:ARG:O	47:6:36:ARG:HG3	2.10	0.51
1:a:1113:C:H2'	1:a:1114:C:H6	1.75	0.51
11:l:33:LYS:NZ	11:l:33:LYS:HA	2.26	0.51
20:A:1330:C:H5'	31:O:69:GLU:O	2.09	0.51
26:G:103:LEU:HB2	26:G:123:PHE:CE2	2.46	0.51
37:U:58:VAL:HB	37:U:75:ARG:HB2	1.91	0.51
10:k:67:ALA:O	10:k:71:THR:HG23	2.11	0.51
11:l:52:THR:OG1	11:l:62:LEU:HB3	2.10	0.51
20:A:282:A:H2'	20:A:283:G:H8	1.74	0.51
20:A:1301:G:OP1	43:2:16:ARG:NH2	2.28	0.51
20:A:1867:A:H2'	20:A:1868:A:C8	2.46	0.51
26:G:10:VAL:HG22	26:G:49:GLU:HG3	1.93	0.51
2:c:46:LEU:HD13	2:c:51:VAL:HG22	1.93	0.51
15:p:20:ILE:HB	15:p:37:VAL:O	2.10	0.51
21:B:50:A:C6	32:P:38:LYS:HE2	2.45	0.51
11:l:26:LYS:HZ1	11:l:70:LEU:HB2	1.75	0.51
20:A:1491:U:O2'	20:A:1492:G:C8	2.59	0.51
2:c:69:THR:OG1	2:c:70:ALA:N	2.42	0.51
20:A:92:A:C2'	20:A:93:G:H5'	2.41	0.51
20:A:154:U:O2'	20:A:155:U:H6	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:D:108:VAL:HG22	23:D:203:LYS:O	2.11	0.51
24:E:75:GLN:NE2	24:E:83:TRP:HE1	2.08	0.51
30:N:7:VAL:HG11	30:N:93:TRP:HH2	1.76	0.51
1:a:562:A:OP2	3:d:2:SER:OG	2.19	0.51
12:m:3:ARG:HB3	12:m:9:ILE:H	1.76	0.51
20:A:288:C:HO2'	20:A:289:U:H5	1.59	0.51
20:A:2444:A:HO2'	20:A:2445:U:H6	1.59	0.51
20:A:2481:C:H2'	20:A:2482:A:O4'	2.08	0.51
20:A:1572:A:H62	20:A:1589:G:H8	1.58	0.51
20:A:1593:U:H2'	20:A:1594:U:C6	2.46	0.51
20:A:2035:G:H2'	20:A:2035:G:N3	2.26	0.51
1:a:628:C:OP1	3:d:77:LYS:HE3	2.11	0.50
6:g:149:ARG:HA	6:g:152:ALA:HB3	1.93	0.50
20:A:306:C:H2'	20:A:307:U:C6	2.45	0.50
20:A:2637:G:O5'	20:A:2836:G:N2	2.44	0.50
23:D:34:VAL:HG11	23:D:74:THR:HG21	1.93	0.50
30:N:109:VAL:HG13	30:N:113:VAL:HB	1.93	0.50
38:V:70:VAL:HG11	38:V:92:ARG:HH12	1.76	0.50
1:a:33:C:H2'	1:a:34:U:O4'	2.11	0.50
1:a:101:A:H2'	1:a:102:G:H8	1.74	0.50
1:a:1019:G:N2	1:a:1052:A:H62	1.88	0.50
3:d:46:GLU:O	3:d:50:GLN:NE2	2.44	0.50
3:d:143:ARG:O	3:d:145:LYS:N	2.44	0.50
6:g:115:THR:O	6:g:119:ARG:HG3	2.12	0.50
20:A:179:A:O3'	20:A:180:G:H8	1.94	0.50
20:A:1872:G:H1'	20:A:1898:A:H61	1.75	0.50
47:6:17:ILE:HD12	47:6:26:ILE:HD12	1.94	0.50
1:a:1362:G:O2'	1:a:1388:G:O6	2.26	0.50
3:d:82:LYS:O	3:d:86:ASN:ND2	2.45	0.50
6:g:145:ALA:C	6:g:147:ALA:H	2.17	0.50
20:A:991:C:H2'	20:A:992:G:H5'	1.92	0.50
20:A:1206:U:H2'	20:A:1207:A:C8	2.46	0.50
21:B:39:G:P	21:B:41:C:H41	2.33	0.50
26:G:18:LYS:HB2	26:G:25:THR:HG23	1.93	0.50
14:o:89:ARG:NH1	20:A:753:G:H3'	2.27	0.50
17:r:21:HIS:N	17:r:21:HIS:CD2	2.78	0.50
1:a:294:A:H5''	1:a:295:C:H3'	1.92	0.50
1:a:1055:A:H2'	1:a:1056:A:H8	1.76	0.50
4:e:22:THR:HG22	4:e:31:LEU:HD23	1.92	0.50
16:q:12:GLN:HG2	16:q:63:LYS:HD2	1.94	0.50
20:A:769:G:N2	22:C:209:GLY:N	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:1167:A:H8	20:A:2532:A:H5''	1.76	0.50
1:a:894:U:H5''	7:h:83:PRO:O	2.12	0.50
1:a:1057:G:O2'	1:a:1058:U:H5'	2.11	0.50
12:m:104:ASN:OD1	12:m:105:ASN:N	2.44	0.50
20:A:650:G:N2	20:A:654:A:H5'	2.27	0.50
20:A:1816:A:H2'	20:A:1817:A:C8	2.46	0.50
20:A:2044:A:C8	20:A:2513:C:H5''	2.47	0.50
21:B:72:U:C2'	21:B:73:U:H5'	2.42	0.50
4:e:6:PRO:HB2	4:e:8:HIS:HD2	1.75	0.50
9:j:63:GLU:OE2	13:n:58:LYS:HE3	2.12	0.50
11:l:49:ARG:HG2	11:l:67:ARG:HB2	1.93	0.50
20:A:161:G:H2'	20:A:162:A:N3	2.26	0.50
20:A:454:C:H2'	20:A:455:A:C8	2.47	0.50
41:Z:14:MET:HG3	41:Z:57:LEU:HD21	1.94	0.50
3:d:76:SER:HB2	3:d:83:HIS:NE2	2.26	0.50
7:h:69:ASN:OD1	7:h:69:ASN:N	2.41	0.50
20:A:897:G:H2'	20:A:898:A:C8	2.47	0.50
37:U:51:ALA:O	37:U:81:THR:HB	2.12	0.50
1:a:974:A:C6	18:s:55:ARG:HB2	2.46	0.49
20:A:1207:A:H2'	20:A:1208:C:C6	2.47	0.49
20:A:2475:C:H2'	20:A:2476:U:C6	2.46	0.49
11:l:26:LYS:HB2	11:l:43:LYS:HE3	1.94	0.49
12:m:104:ASN:O	12:m:106:ALA:N	2.38	0.49
20:A:1399:C:O2'	20:A:1823:A:N3	2.40	0.49
1:a:722:U:H2'	1:a:723:A:C8	2.46	0.49
1:a:1055:A:H2'	1:a:1056:A:C8	2.47	0.49
1:a:1397:C:O2'	6:g:79:ARG:NH1	2.46	0.49
1:a:1512:C:H2'	1:a:1513:G:O4'	2.12	0.49
6:g:111:ARG:HD2	6:g:119:ARG:HA	1.93	0.49
12:m:84:GLY:H	12:m:85:SER:HB2	1.78	0.49
30:N:59:LYS:O	30:N:60:ARG:HB2	2.13	0.49
31:O:17:LEU:O	31:O:21:THR:HG23	2.12	0.49
1:a:515:G:H2'	1:a:516:C:C6	2.48	0.49
3:d:163:PRO:HD2	3:d:166:VAL:HB	1.94	0.49
20:A:653:G:H2'	20:A:654:A:H5''	1.93	0.49
20:A:943:U:H2'	20:A:944:U:H6	1.77	0.49
20:A:1537:A:N3	20:A:1624:U:O2'	2.43	0.49
20:A:1624:U:OP2	20:A:1624:U:H6	1.96	0.49
20:A:1872:G:O2'	20:A:1898:A:N6	2.46	0.49
30:N:36:ALA:HB2	30:N:103:MET:SD	2.53	0.49
47:6:22:ARG:HH11	47:6:36:ARG:HD3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:F:8:TYR:CE1	25:F:173:LEU:HD21	2.47	0.49
34:R:29:HIS:CD2	34:R:30:THR:HG23	2.48	0.49
1:a:977:U:C2	1:a:999:A:C2	3.01	0.49
1:a:1330:U:O2'	1:a:1375:A:H8	1.95	0.49
5:f:27:GLU:O	5:f:31:THR:HG23	2.13	0.49
20:A:1757:U:H4'	20:A:1757:U:OP2	2.13	0.49
38:V:73:PRO:HD3	38:V:101:LEU:HD22	1.95	0.49
3:d:165:PHE:CD2	3:d:181:PRO:HB3	2.48	0.49
9:j:59:LYS:HE2	9:j:62:ARG:NH2	2.28	0.49
20:A:161:G:N2	20:A:168:U:H5	2.11	0.49
20:A:1206:U:H2'	20:A:1207:A:H8	1.77	0.49
20:A:1315:A:H2'	20:A:1316:G:O4'	2.13	0.49
20:A:2551:U:H2'	20:A:2552:C:C6	2.48	0.49
1:a:977:U:N3	1:a:999:A:N1	2.60	0.49
1:a:1156:U:O2'	1:a:1157:G:H8	1.96	0.49
3:d:17:ILE:HB	3:d:56:LYS:HD2	1.95	0.49
3:d:191:ASP:OD2	3:d:195:VAL:HG23	2.13	0.49
10:k:64:GLN:HG2	10:k:99:SER:OG	2.13	0.49
20:A:1502:G:H5''	20:A:1503:U:H3'	1.95	0.49
21:B:84:G:C2	21:B:85:U:C2	3.01	0.49
1:a:216:A:OP1	19:t:59:MET:HG2	2.13	0.49
1:a:1009:G:O2'	1:a:1011:C:N4	2.46	0.49
1:a:1104:G:H21	1:a:1182:A:H61	1.61	0.49
2:c:126:ARG:HH11	2:c:190:THR:HG21	1.78	0.49
23:D:109:ASP:OD2	23:D:206:VAL:HG23	2.13	0.49
1:a:29:A:H2'	1:a:30:A:H8	1.77	0.49
5:f:81:ASP:O	5:f:85:LYS:HG2	2.12	0.49
20:A:509:G:H22	45:4:37:LYS:NZ	2.10	0.49
20:A:2011:A:OP2	23:D:130:ARG:HD3	2.13	0.49
20:A:2674:A:OP1	26:G:176:THR:HB	2.13	0.49
27:K:100:ARG:O	27:K:104:THR:HG23	2.13	0.49
36:T:14:THR:HG22	36:T:105:THR:HG21	1.95	0.49
1:a:1160:C:H4'	1:a:1161:A:H5'	1.94	0.48
1:a:1423:A:H2'	1:a:1424:C:C6	2.49	0.48
3:d:191:ASP:CG	3:d:192:GLU:N	2.71	0.48
6:g:89:VAL:HG13	6:g:90:GLU:O	2.13	0.48
7:h:65:LYS:HD3	7:h:73:VAL:HG11	1.94	0.48
21:B:46:A:OP1	32:P:35:ARG:NH2	2.44	0.48
21:B:78:U:H2'	21:B:79:G:N2	2.27	0.48
1:a:14:U:H2'	1:a:15:C:C6	2.48	0.48
1:a:483:C:O2'	1:a:484:U:O5'	2.24	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:82:GLU:HA	2:c:85:ASN:ND2	2.28	0.48
3:d:54:LYS:NZ	3:d:65:GLU:OE2	2.33	0.48
9:j:12:ALA:HB3	9:j:18:LEU:HG	1.94	0.48
12:m:15:VAL:HG12	12:m:34:LEU:HD21	1.96	0.48
18:s:32:LYS:HA	18:s:50:ALA:HB3	1.95	0.48
20:A:950:A:H2'	20:A:953:C:H5	1.77	0.48
1:a:861:G:HO2'	1:a:862:C:P	2.36	0.48
17:r:20:ASN:HB2	17:r:22:ILE:HG22	1.95	0.48
20:A:1886:G:O2'	20:A:1887:G:OP2	2.24	0.48
2:c:189:ASP:OD1	2:c:190:THR:N	2.46	0.48
20:A:1408:U:O2'	20:A:2226:A:H8	1.97	0.48
23:D:92:GLU:HG2	23:D:95:LYS:HE3	1.96	0.48
26:G:118:PRO:HD2	26:G:144:LEU:HD11	1.95	0.48
29:M:92:THR:H	29:M:95:VAL:HG12	1.78	0.48
32:P:29:PRO:HG2	32:P:91:VAL:HG12	1.94	0.48
1:a:1291:G:H2'	1:a:1292:C:O4'	2.11	0.48
7:h:108:THR:HB	7:h:123:ILE:HD12	1.96	0.48
20:A:273:A:OP2	20:A:297:G:N1	2.44	0.48
20:A:1453:U:C6	20:A:1628:G:H2'	2.48	0.48
20:A:2044:A:H8	20:A:2513:C:H5''	1.79	0.48
24:E:6:LEU:HG	24:E:17:ILE:HG13	1.95	0.48
31:O:68:ASN:O	31:O:70:VAL:N	2.40	0.48
6:g:29:ARG:HG2	6:g:105:VAL:HG21	1.96	0.48
1:a:196:U:H2'	1:a:197:G:C8	2.48	0.48
1:a:524:A:N3	1:a:558:G:O2'	2.42	0.48
2:c:12:VAL:HA	2:c:16:ARG:HG3	1.96	0.48
19:t:33:LYS:HE2	19:t:37:GLU:HG3	1.95	0.48
20:A:912:U:OP1	30:N:5:LYS:N	2.44	0.48
20:A:1166:A:H8	20:A:1166:A:OP1	1.96	0.48
1:a:1020:A:H5''	1:a:1042:C:N4	2.29	0.48
1:a:1294:A:N3	1:a:1294:A:H2'	2.28	0.48
1:a:1342:G:H2'	1:a:1343:C:C6	2.48	0.48
20:A:1256:G:OP1	34:R:22:LYS:NZ	2.47	0.48
25:F:70:ALA:HB3	25:F:82:GLY:H	1.78	0.48
36:T:87:MET:HB2	36:T:103:LYS:HB2	1.95	0.48
38:V:1:MET:SD	38:V:65:VAL:HG21	2.54	0.48
1:a:936:U:H2'	1:a:937:U:C6	2.49	0.48
4:e:162:GLU:HA	4:e:165:ILE:HD11	1.96	0.48
9:j:51:VAL:HG22	13:n:41:ARG:HG2	1.96	0.48
20:A:194:A:H2'	20:A:195:C:C6	2.49	0.48
31:O:45:GLU:O	31:O:49:THR:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:293:C:OP2	16:q:46:LYS:NZ	2.47	0.48
1:a:1059:G:H2'	1:a:1060:A:C8	2.48	0.48
3:d:12:SER:OG	3:d:25:GLU:HG3	2.14	0.48
4:e:41:ASP:OD1	4:e:41:ASP:N	2.46	0.48
5:f:9:ILE:HG23	5:f:95:ILE:HG12	1.96	0.48
7:h:24:THR:HG22	7:h:25:LEU:H	1.79	0.48
20:A:509:G:H1	45:4:37:LYS:NZ	2.06	0.48
20:A:1009:G:H2'	20:A:1010:U:C6	2.49	0.48
20:A:1532:A:H8	22:C:98:ASP:HA	1.77	0.48
9:j:83:THR:O	9:j:87:LEU:HB2	2.14	0.47
14:o:11:ILE:HD11	14:o:31:VAL:HA	1.96	0.47
14:o:81:LEU:O	14:o:84:ARG:N	2.46	0.47
16:q:70:LEU:O	16:q:71:SER:OG	2.29	0.47
20:A:290:U:H2'	20:A:291:G:O4'	2.14	0.47
25:F:164:GLU:HA	25:F:167:ARG:HG3	1.96	0.47
26:G:159:GLY:O	26:G:163:ARG:NH2	2.47	0.47
1:a:482:A:H2'	1:a:483:C:C6	2.49	0.47
1:a:1465:U:H3'	1:a:1466:U:C5	2.49	0.47
16:q:32:LYS:HA	16:q:32:LYS:HE3	1.96	0.47
45:4:31:LEU:HD22	45:4:42:ILE:HD12	1.96	0.47
1:a:1172:A:C2	1:a:1196:G:C4	3.02	0.47
1:a:1243:C:H2'	1:a:1244:A:H8	1.79	0.47
3:d:13:ARG:HA	3:d:26:LEU:HD21	1.96	0.47
20:A:4:U:H2'	20:A:5:U:C6	2.49	0.47
20:A:519:A:N3	20:A:521:G:H5''	2.29	0.47
21:B:58:C:H2'	21:B:59:U:C6	2.49	0.47
25:F:3:ARG:O	25:F:7:LYS:HG3	2.14	0.47
1:a:1311:C:P	12:m:44:ARG:HH21	2.37	0.47
4:e:108:GLY:O	4:e:112:ARG:HB3	2.15	0.47
6:g:86:GLN:HG3	6:g:148:ASN:HD22	1.79	0.47
20:A:392:A:H2'	20:A:393:A:C8	2.50	0.47
26:G:59:LYS:HG3	26:G:60:GLU:HG3	1.97	0.47
31:O:24:LEU:HB2	31:O:30:ILE:HD12	1.96	0.47
32:P:89:LYS:HG2	32:P:115:GLY:O	2.15	0.47
35:S:25:LEU:O	35:S:26:ASN:HB2	2.13	0.47
1:a:833:G:O2'	1:a:835:U:OP2	2.22	0.47
1:a:1113:C:H2'	1:a:1114:C:C6	2.49	0.47
7:h:96:LYS:HG3	7:h:119:ARG:NH2	2.30	0.47
12:m:90:ARG:HH11	12:m:95:LEU:HD13	1.80	0.47
20:A:1535:U:HO2'	20:A:1536:A:P	2.33	0.47
20:A:2343:A:H2'	20:A:2344:G:C8	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:85:U:O4	21:B:86:U:N3	2.47	0.47
36:T:85:PRO:O	36:T:105:THR:OG1	2.31	0.47
37:U:2:GLU:CD	37:U:2:GLU:N	2.72	0.47
2:c:43:ALA:HA	2:c:46:LEU:HB3	1.96	0.47
5:f:89:ASP:OD1	5:f:89:ASP:N	2.36	0.47
10:k:37:THR:O	10:k:37:THR:OG1	2.32	0.47
20:A:900:G:O2'	20:A:901:U:OP2	2.32	0.47
21:B:59:U:H2'	21:B:60:U:C6	2.50	0.47
23:D:100:ASP:OD1	23:D:100:ASP:N	2.36	0.47
27:K:131:HIS:CD2	27:K:133:HIS:H	2.24	0.47
1:a:105:G:H2'	1:a:106:A:C8	2.50	0.47
1:a:1142:U:O4	9:j:9:ARG:NH1	2.48	0.47
1:a:1251:A:H2'	1:a:1252:C:C6	2.50	0.47
8:i:101:ALA:O	8:i:103:LEU:HG	2.14	0.47
11:l:93:VAL:HG22	11:l:94:LEU:H	1.79	0.47
14:o:33:THR:HA	14:o:36:ILE:HG12	1.96	0.47
20:A:727:C:H1'	45:4:4:THR:HG22	1.95	0.47
20:A:1178:G:H21	27:K:109:MET:CE	2.19	0.47
20:A:1591:A:N3	20:A:1591:A:O5'	2.48	0.47
23:D:2:THR:OG1	23:D:3:LYS:N	2.47	0.47
26:G:48:ASN:O	26:G:49:GLU:HB2	2.14	0.47
35:S:19:ALA:HB1	35:S:94:LYS:HD3	1.96	0.47
37:U:8:LYS:HB2	37:U:28:GLU:O	2.14	0.47
2:c:45:LYS:HB3	2:c:45:LYS:NZ	2.30	0.47
3:d:143:ARG:C	3:d:145:LYS:H	2.23	0.47
20:A:11:A:H2'	20:A:12:A:C8	2.50	0.47
20:A:282:A:H2'	20:A:283:G:C8	2.49	0.47
20:A:2851:U:H5''	31:O:49:THR:HG21	1.96	0.47
1:a:1273:G:H2'	1:a:1274:C:H6	1.80	0.47
3:d:57:LEU:HD12	3:d:57:LEU:HA	1.72	0.47
7:h:50:GLU:HG2	7:h:61:ARG:HB3	1.96	0.47
20:A:1085:C:O2'	20:A:1086:A:OP1	2.29	0.47
20:A:1868:A:N6	20:A:1902:G:H8	2.06	0.47
20:A:1885:C:H41	20:A:1886:G:H21	1.62	0.47
21:B:32:U:O2'	21:B:33:U:O5'	2.32	0.47
23:D:19:SER:O	33:Q:80:ARG:NH2	2.36	0.47
25:F:70:ALA:HB3	25:F:82:GLY:N	2.30	0.47
30:N:54:MET:HE1	30:N:104:PHE:CD1	2.50	0.47
1:a:995:C:O2	13:n:19:GLN:NE2	2.47	0.47
6:g:11:ASP:N	6:g:11:ASP:OD1	2.45	0.47
8:i:63:VAL:HG11	8:i:83:ILE:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:i:119:LYS:HB3	8:i:123:LYS:HD3	1.96	0.47
17:r:59:LEU:O	17:r:63:ILE:HG23	2.14	0.47
20:A:526:C:O2'	36:T:65:ASN:ND2	2.48	0.47
22:C:173:LEU:HD23	22:C:182:ARG:O	2.14	0.47
1:a:228:G:H3'	1:a:229:G:O4'	2.14	0.46
12:m:14:ARG:H	12:m:14:ARG:HG2	1.47	0.46
18:s:6:LYS:HD3	18:s:6:LYS:N	2.26	0.46
18:s:6:LYS:HG2	18:s:7:LYS:HE3	1.97	0.46
20:A:1457:A:N1	20:A:1630:G:H4'	2.30	0.46
1:a:314:G:H2'	1:a:315:A:C8	2.50	0.46
6:g:75:VAL:HA	6:g:88:PRO:HA	1.97	0.46
28:L:111:PHE:O	28:L:115:VAL:HG23	2.14	0.46
11:l:103:LEU:HD22	11:l:104:PRO:HD2	1.97	0.46
20:A:998:U:OP2	30:N:14:ARG:NH1	2.47	0.46
20:A:1834:U:C2	22:C:201:GLU:HB2	2.49	0.46
21:B:89:C:OP1	30:N:99:ARG:NH2	2.34	0.46
25:F:13:THR:O	25:F:17:VAL:HB	2.14	0.46
29:M:33:ARG:NH1	29:M:41:ARG:O	2.49	0.46
29:M:133:GLN:HG3	29:M:143:ILE:HG12	1.98	0.46
35:S:21:TYR:CE2	35:S:94:LYS:HG3	2.51	0.46
36:T:63:ALA:O	36:T:68:ASP:N	2.44	0.46
1:a:1270:G:H2'	1:a:1294:A:H61	1.81	0.46
23:D:13:THR:HG23	23:D:25:VAL:HG12	1.97	0.46
24:E:41:ARG:HG2	24:E:41:ARG:HH11	1.80	0.46
1:a:35:G:O4'	1:a:35:G:P	2.73	0.46
2:c:83:VAL:HG13	2:c:100:ILE:HG13	1.96	0.46
2:c:119:ILE:HG21	2:c:136:ALA:HB2	1.98	0.46
20:A:654:A:H4'	20:A:655:G:C8	2.50	0.46
20:A:1490:A:H2'	20:A:1491:U:H5'	1.97	0.46
6:g:28:ASN:HD21	6:g:36:ARG:NH1	2.13	0.46
23:D:5:ILE:HG13	23:D:102:PHE:HE2	1.79	0.46
25:F:135:GLN:O	25:F:141:VAL:HG21	2.16	0.46
26:G:63:THR:O	26:G:67:THR:HG23	2.16	0.46
27:K:3:THR:O	27:K:3:THR:OG1	2.32	0.46
33:Q:32:VAL:HG21	33:Q:41:GLN:HE21	1.81	0.46
35:S:65:HIS:ND1	35:S:93:THR:HG22	2.31	0.46
41:Z:10:THR:O	41:Z:14:MET:HG2	2.15	0.46
1:a:31:C:O2'	1:a:32:G:C8	2.67	0.46
1:a:1155:U:O2'	1:a:1156:U:H5'	2.15	0.46
15:p:15:SER:O	15:p:15:SER:OG	2.28	0.46
16:q:23:THR:OG1	16:q:74:LYS:HE3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:61:G:OP1	41:Z:47:ARG:NH2	2.48	0.46
20:A:1088:A:H2'	20:A:1088:A:N3	2.31	0.46
20:A:1631:A:N3	20:A:1631:A:H2'	2.31	0.46
2:c:72:PRO:HD3	2:c:104:GLU:OE2	2.16	0.46
3:d:149:ILE:HD12	3:d:152:ILE:HD11	1.97	0.46
11:l:8:VAL:HG22	16:q:34:HIS:CD2	2.51	0.46
20:A:2855:A:H2'	20:A:2856:A:C8	2.50	0.46
26:G:5:GLY:HA3	26:G:65:HIS:CD2	2.50	0.46
28:L:23:LYS:O	28:L:39:ILE:HG13	2.15	0.46
44:3:32:LYS:HA	44:3:32:LYS:HD3	1.74	0.46
1:a:593:A:O2'	1:a:743:A:N3	2.43	0.46
8:i:96:SER:O	8:i:100:ARG:HG2	2.16	0.46
20:A:492:G:C8	24:E:58:ARG:HD2	2.51	0.46
20:A:1492:G:N2	20:A:1504:G:H22	2.14	0.46
20:A:1692:G:O2'	31:O:116:ASP:OD1	2.32	0.46
32:P:35:ARG:HA	32:P:40:ILE:HG22	1.97	0.46
1:a:426:A:H61	1:a:445:A:H62	1.62	0.46
1:a:590:G:O2'	1:a:836:G:OP2	2.28	0.46
11:l:120:VAL:HG13	11:l:130:TYR:HB3	1.97	0.46
20:A:1474:G:H2'	20:A:1475:U:C6	2.50	0.46
25:F:83:MET:O	25:F:85:ILE:HG13	2.16	0.46
31:O:47:MET:HE2	31:O:65:PHE:HB3	1.98	0.46
38:V:47:PRO:HB3	38:V:52:PRO:O	2.15	0.46
1:a:1030:A:H2	1:a:1234:U:H1'	1.81	0.45
5:f:14:ARG:HH21	5:f:89:ASP:HB3	1.80	0.45
20:A:782:U:H2'	20:A:783:A:C8	2.51	0.45
20:A:903:G:O6	20:A:956:C:N3	2.50	0.45
20:A:1833:A:H5''	22:C:157:SER:OG	2.15	0.45
20:A:2314:A:H2'	20:A:2315:A:C8	2.51	0.45
25:F:4:LEU:HD22	25:F:7:LYS:HD2	1.98	0.45
25:F:55:GLU:O	25:F:59:LEU:HG	2.16	0.45
25:F:104:VAL:HG22	25:F:175:MET:H	1.80	0.45
1:a:1030:A:C2	1:a:1234:U:H1'	2.50	0.45
1:a:1201:G:H21	13:n:61:TRP:C	2.18	0.45
2:c:62:ARG:HD2	2:c:97:ARG:NH2	2.31	0.45
20:A:1447:U:H2'	20:A:1448:U:O4'	2.16	0.45
1:a:1088:G:H2'	1:a:1089:U:C6	2.51	0.45
12:m:66:GLU:OE1	12:m:67:GLY:N	2.42	0.45
20:A:469:A:H2'	20:A:470:A:C8	2.52	0.45
20:A:2763:A:H4'	26:G:62:LYS:HB2	1.97	0.45
44:3:41:LYS:HD3	44:3:41:LYS:HA	1.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:506:A:H2'	1:a:507:A:H8	1.81	0.45
1:a:542:G:O2'	1:a:550:A:N1	2.45	0.45
20:A:1167:A:N3	20:A:1167:A:H2'	2.31	0.45
20:A:2809:U:OP2	20:A:2810:U:N3	2.49	0.45
23:D:146:MET:HA	23:D:158:LYS:HE2	1.97	0.45
25:F:66:LEU:HD23	25:F:66:LEU:HA	1.73	0.45
35:S:88:HIS:CE1	35:S:90:GLN:HG2	2.44	0.45
1:a:962:A:H2'	1:a:963:G:C8	2.51	0.45
2:c:133:GLN:O	2:c:137:ILE:HG23	2.16	0.45
14:o:89:ARG:C	14:o:89:ARG:HD3	2.41	0.45
19:t:45:ASN:O	19:t:45:ASN:ND2	2.48	0.45
20:A:251:G:O5'	20:A:252:C:H5''	2.17	0.45
20:A:900:G:O2'	20:A:957:G:O6	2.27	0.45
20:A:1804:C:H2'	20:A:1805:A:C5	2.51	0.45
20:A:1861:A:H8	20:A:1861:A:OP2	1.99	0.45
20:A:2439:A:H5''	20:A:2441:C:O4'	2.17	0.45
20:A:2908:U:H2'	20:A:2909:A:O4'	2.15	0.45
23:D:88:LEU:O	23:D:89:GLY:C	2.59	0.45
25:F:117:VAL:HG12	25:F:118:SER:O	2.16	0.45
31:O:22:THR:HG21	31:O:67:ARG:HB2	1.99	0.45
16:q:51:ASP:OD1	16:q:78:LEU:HD22	2.17	0.45
25:F:68:THR:N	25:F:86:GLY:O	2.42	0.45
1:a:897:G:OP2	11:l:9:ARG:NH2	2.46	0.45
1:a:1038:C:O2'	1:a:1039:U:H6	1.99	0.45
18:s:7:LYS:HA	18:s:7:LYS:HD3	1.50	0.45
19:t:71:ALA:O	19:t:75:LYS:HG3	2.17	0.45
20:A:523:A:H5''	38:V:46:LYS:HG2	1.98	0.45
20:A:697:U:H2'	20:A:698:A:C8	2.52	0.45
20:A:2812:A:O2'	20:A:2813:A:OP1	2.20	0.45
22:C:107:PRO:HG2	22:C:110:LEU:HG	1.99	0.45
24:E:158:ASN:C	24:E:160:ASN:H	2.23	0.45
31:O:96:ARG:HH21	31:O:126:VAL:CG2	2.25	0.45
35:S:69:LYS:HB3	35:S:69:LYS:HE2	1.67	0.45
46:5:32:ARG:H	46:5:32:ARG:HG3	1.24	0.45
3:d:54:LYS:HD3	3:d:198:TYR:CE1	2.51	0.45
3:d:187:TYR:C	3:d:189:GLU:H	2.25	0.45
5:f:14:ARG:HG2	5:f:15:PRO:HD2	1.99	0.45
20:A:324:U:H2'	20:A:325:U:O4'	2.17	0.45
20:A:613:U:H2'	20:A:614:G:C8	2.52	0.45
20:A:1390:A:H2'	20:A:1391:G:O4'	2.17	0.45
20:A:2264:G:N2	30:N:84:GLY:HA2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:2359:G:N3	20:A:2395:C:H2'	2.31	0.45
25:F:152:MET:HE3	25:F:152:MET:HB2	1.70	0.45
29:M:83:ASN:O	29:M:119:LYS:NZ	2.47	0.45
37:U:19:ALA:HB1	37:U:24:LYS:HB2	1.99	0.45
12:m:80:LEU:HA	12:m:80:LEU:HD12	1.68	0.45
15:p:9:ARG:CZ	15:p:16:PRO:HB3	2.47	0.45
20:A:1052:U:OP2	34:R:70:ARG:NH2	2.44	0.45
20:A:1453:U:H4'	20:A:1454:U:C6	2.52	0.45
22:C:119:GLY:O	22:C:130:LEU:HG	2.17	0.45
25:F:117:VAL:HB	25:F:177:PHE:HD1	1.81	0.45
26:G:154:PRO:HA	26:G:160:LYS:O	2.17	0.45
29:M:2:LYS:HD3	29:M:4:HIS:CE1	2.52	0.45
1:a:555:G:H21	3:d:35:GLN:NE2	2.14	0.45
1:a:1057:G:H2'	1:a:1058:U:O4'	2.16	0.45
1:a:1227:U:H4'	1:a:1228:A:C8	2.51	0.45
5:f:10:MET:HE2	5:f:63:TYR:CD2	2.52	0.45
7:h:29:ALA:O	7:h:57:GLN:NE2	2.50	0.45
20:A:1328:G:H2'	20:A:1329:U:C6	2.52	0.45
20:A:1833:A:H61	22:C:276:LYS:HZ2	1.63	0.45
20:A:2458:G:OP2	24:E:68:LYS:NZ	2.38	0.45
38:V:41:VAL:O	38:V:58:GLU:HA	2.17	0.45
1:a:1532:G:H2'	1:a:1534:A:OP2	2.17	0.44
15:p:68:ASP:OD1	15:p:68:ASP:N	2.39	0.44
17:r:26:ASP:C	17:r:28:LYS:N	2.75	0.44
20:A:1451:U:P	20:A:1630:G:H22	2.40	0.44
20:A:2342:A:H2'	20:A:2343:A:H8	1.82	0.44
24:E:12:THR:O	24:E:14:ASN:N	2.50	0.44
26:G:10:VAL:HG13	26:G:48:ASN:O	2.17	0.44
32:P:40:ILE:O	32:P:58:ALA:HB2	2.18	0.44
43:2:23:THR:HG21	43:2:25:LYS:HE3	1.99	0.44
1:a:1502:G:H2'	1:a:1503:G:C8	2.52	0.44
20:A:1499:G:H22	20:A:2716:G:H22	1.66	0.44
31:O:38:LYS:O	31:O:41:ARG:HG2	2.18	0.44
1:a:352:G:H2'	1:a:353:A:H8	1.83	0.44
1:a:1059:G:O2'	1:a:1060:A:O5'	2.34	0.44
1:a:1233:C:H2'	1:a:1234:U:C6	2.53	0.44
1:a:1466:U:C4	1:a:1467:U:C2	3.05	0.44
10:k:64:GLN:O	10:k:68:GLU:HG3	2.17	0.44
11:l:56:LYS:HG2	11:l:57:LYS:H	1.82	0.44
11:l:120:VAL:CG2	11:l:123:ARG:HG3	2.46	0.44
16:q:14:ARG:NH1	16:q:29:GLU:OE2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:885:U:N3	20:A:886:U:H1'	2.32	0.44
20:A:1960:U:H2'	20:A:1961:C:C6	2.52	0.44
20:A:2078:C:H2'	20:A:2079:C:C6	2.53	0.44
20:A:2595:G:H2'	20:A:2595:G:N3	2.32	0.44
38:V:24:LEU:HD23	38:V:24:LEU:HA	1.66	0.44
1:a:136:A:N3	1:a:278:A:O2'	2.44	0.44
1:a:991:A:H8	1:a:991:A:H5'	1.83	0.44
18:s:52:TYR:HA	18:s:56:LYS:O	2.18	0.44
19:t:50:TYR:O	19:t:54:VAL:HG23	2.17	0.44
20:A:900:G:N2	20:A:958:A:OP2	2.30	0.44
20:A:2494:C:H2'	20:A:2495:G:H5'	2.00	0.44
24:E:6:LEU:HD23	24:E:6:LEU:HA	1.74	0.44
3:d:143:ARG:C	3:d:145:LYS:N	2.75	0.44
12:m:103:LYS:HG3	12:m:104:ASN:N	2.27	0.44
20:A:1489:C:H3'	20:A:1490:A:C8	2.53	0.44
20:A:1584:G:H1'	20:A:1585:U:OP2	2.18	0.44
20:A:2605:C:H2'	20:A:2606:G:C8	2.52	0.44
24:E:28:PRO:HA	24:E:112:SER:HB2	1.98	0.44
25:F:69:LYS:HA	25:F:84:PRO:HA	1.98	0.44
26:G:90:ILE:HG22	26:G:91:GLY:H	1.82	0.44
1:a:668:U:N3	7:h:56:LYS:HB3	2.32	0.44
1:a:980:A:N3	1:a:985:A:O2'	2.39	0.44
5:f:10:MET:HE2	5:f:63:TYR:HD2	1.82	0.44
6:g:88:PRO:HD2	6:g:152:ALA:CB	2.47	0.44
11:l:25:ASN:OD1	11:l:25:ASN:N	2.50	0.44
20:A:2299:C:OP2	44:3:2:ARG:NH1	2.50	0.44
23:D:6:LEU:HD11	23:D:81:LYS:HB2	2.00	0.44
28:L:61:VAL:HG21	28:L:111:PHE:CE2	2.53	0.44
32:P:27:GLU:OE1	32:P:90:LYS:NZ	2.35	0.44
1:a:135:A:H4'	1:a:136:A:H5''	1.98	0.44
1:a:1044:C:H2'	1:a:1045:U:O2	2.17	0.44
5:f:4:ASP:OD1	5:f:4:ASP:N	2.49	0.44
9:j:21:SER:O	9:j:25:ILE:HG12	2.18	0.44
9:j:42:LEU:HB2	9:j:71:LYS:HB2	1.99	0.44
20:A:1240:A:H2'	20:A:1241:A:C8	2.53	0.44
21:B:73:U:O2'	21:B:74:G:H8	2.00	0.44
23:D:33:ASN:N	23:D:33:ASN:HD22	2.16	0.44
25:F:14:PRO:O	25:F:17:VAL:HG12	2.18	0.44
1:a:1057:G:C5	1:a:1058:U:N3	2.86	0.44
3:d:24:LYS:HB3	3:d:27:ALA:HB2	2.00	0.44
3:d:60:MET:HE3	3:d:60:MET:HB3	1.69	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:71:LEU:HD13	3:d:91:LEU:HD12	2.00	0.44
4:e:160:SER:O	4:e:163:GLU:HB2	2.17	0.44
20:A:283:G:N2	20:A:288:C:O2	2.37	0.44
20:A:1802:C:H5'	22:C:224:VAL:HG11	2.00	0.44
21:B:27:A:H2'	21:B:28:C:C6	2.53	0.44
23:D:31:THR:HG22	23:D:184:ASN:HD22	1.83	0.44
26:G:45:ILE:HG22	26:G:46:GLU:H	1.82	0.44
1:a:140:A:H1'	1:a:340:A:C5	2.53	0.44
1:a:972:U:O2	1:a:976:U:H5	2.01	0.44
1:a:1505:G:H2'	1:a:1506:U:H6	1.83	0.44
6:g:71:PRO:HG3	6:g:103:TRP:CH2	2.53	0.44
12:m:2:ALA:HA	12:m:3:ARG:HA	1.75	0.44
12:m:98:ARG:NH2	12:m:99:GLY:O	2.51	0.44
20:A:162:A:N6	20:A:166:C:OP2	2.47	0.44
20:A:339:G:H2'	20:A:340:A:C8	2.53	0.44
20:A:516:G:N1	20:A:519:A:OP2	2.51	0.44
20:A:1823:A:H2'	20:A:1824:A:C8	2.52	0.44
20:A:2393:G:H2'	20:A:2394:U:C6	2.53	0.44
1:a:939:A:O2'	1:a:1414:C:OP2	2.35	0.43
1:a:1392:A:C5	6:g:7:VAL:HG11	2.53	0.43
1:a:1533:G:C5	20:A:1934:C:H5'	2.52	0.43
4:e:11:LEU:HD23	4:e:41:ASP:HB3	2.00	0.43
11:l:49:ARG:HD3	11:l:67:ARG:HD3	2.00	0.43
18:s:32:LYS:HD2	18:s:57:HIS:CG	2.53	0.43
25:F:119:LYS:HB3	25:F:167:ARG:HH21	1.83	0.43
30:N:133:LYS:H	30:N:133:LYS:HG3	1.73	0.43
1:a:1314:A:N3	1:a:1314:A:H2'	2.33	0.43
1:a:1338:G:H2'	1:a:1339:C:C6	2.53	0.43
2:c:72:PRO:O	2:c:76:ILE:HG23	2.17	0.43
20:A:276:C:C2'	20:A:277:C:H5'	2.49	0.43
20:A:1068:A:N6	20:A:1165:G:H2'	2.32	0.43
25:F:102:LYS:O	25:F:107:SER:OG	2.24	0.43
26:G:7:LYS:HE3	26:G:7:LYS:HB2	1.85	0.43
33:Q:92:VAL:HG11	33:Q:97:LEU:HD21	2.01	0.43
38:V:1:MET:O	38:V:2:PHE:HD1	2.01	0.43
1:a:32:G:H2'	1:a:33:C:C6	2.53	0.43
1:a:226:U:H2'	1:a:227:C:C5	2.54	0.43
1:a:1191:A:H2'	1:a:1192:G:C8	2.53	0.43
5:f:91:ILE:O	5:f:92:ARG:HG2	2.18	0.43
7:h:74:ILE:O	7:h:74:ILE:HG13	2.18	0.43
16:q:27:VAL:HG22	16:q:46:LYS:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:s:22:GLN:NE2	18:s:28:LYS:H	2.04	0.43
20:A:1393:C:H2'	20:A:1394:G:O4'	2.17	0.43
21:B:46:A:P	32:P:35:ARG:HH22	2.41	0.43
27:K:2:ARG:HD2	27:K:3:THR:HG23	1.99	0.43
1:a:100:A:O5'	1:a:100:A:H8	2.02	0.43
1:a:856:U:C4	1:a:857:U:H1'	2.53	0.43
1:a:977:U:N3	1:a:999:A:C6	2.86	0.43
1:a:1386:G:O3'	8:i:71:GLY:HA3	2.18	0.43
1:a:1490:G:H2'	1:a:1491:G:O4'	2.18	0.43
7:h:12:THR:HG22	7:h:15:ARG:NH2	2.33	0.43
20:A:499:U:H5''	45:4:40:LYS:HD3	2.00	0.43
20:A:1035:C:O2	27:K:4:THR:HG23	2.19	0.43
20:A:2571:G:H2'	20:A:2572:C:C6	2.53	0.43
1:a:151:G:N2	1:a:183:G:N2	2.64	0.43
1:a:700:G:H5''	1:a:701:U:OP1	2.17	0.43
3:d:162:ARG:HA	3:d:163:PRO:HD3	1.83	0.43
5:f:28:ARG:O	5:f:31:THR:OG1	2.33	0.43
1:a:711:A:H2'	1:a:712:U:C6	2.53	0.43
1:a:858:U:C2'	1:a:860:C:H41	2.32	0.43
1:a:1371:G:O2'	1:a:1372:A:C8	2.69	0.43
4:e:5:ASP:OD2	4:e:45:HIS:ND1	2.47	0.43
12:m:89:ILE:HD13	12:m:89:ILE:HA	1.90	0.43
19:t:2:PRO:HG2	19:t:8:ILE:HG12	2.01	0.43
20:A:573:U:O2'	34:R:49:ASP:OD2	2.28	0.43
20:A:1088:A:N1	20:A:1152:G:O2'	2.47	0.43
20:A:1167:A:O2'	20:A:1168:A:H5''	2.19	0.43
30:N:30:GLY:O	30:N:134:ARG:NH1	2.51	0.43
1:a:1370:G:O2'	1:a:1371:G:H5'	2.19	0.43
8:i:80:ARG:HH11	8:i:103:LEU:HD23	1.83	0.43
20:A:872:G:H2'	20:A:873:C:C6	2.53	0.43
24:E:135:LYS:HE2	24:E:135:LYS:HB2	1.79	0.43
36:T:74:LEU:HD23	36:T:114:GLU:HA	2.01	0.43
1:a:278:A:H2'	1:a:279:C:C5	2.54	0.43
1:a:1329:C:H2'	1:a:1330:U:C6	2.54	0.43
1:a:1532:G:N2	1:a:1535:A:OP2	2.52	0.43
7:h:13:ARG:HB3	7:h:25:LEU:HD11	2.00	0.43
21:B:10:G:OP2	39:X:80:ARG:NH1	2.52	0.43
23:D:4:GLY:HA2	23:D:202:ILE:O	2.19	0.43
24:E:200:THR:O	24:E:204:GLU:HG3	2.19	0.43
26:G:149:ARG:O	26:G:149:ARG:HG2	2.18	0.43
29:M:73:ASP:OD1	29:M:73:ASP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:202:A:H62	16:q:67:THR:HG23	1.82	0.43
1:a:1053:C:H2'	1:a:1054:A:C8	2.54	0.43
1:a:1135:U:H2'	1:a:1136:G:H8	1.84	0.43
3:d:54:LYS:HE2	3:d:54:LYS:HB3	1.81	0.43
5:f:78:ASN:H	5:f:78:ASN:ND2	2.17	0.43
6:g:150:ALA:HA	10:k:98:ARG:HE	1.84	0.43
23:D:107:VAL:HA	23:D:174:LEU:O	2.18	0.43
33:Q:43:PHE:HE2	33:Q:61:VAL:HB	1.84	0.43
1:a:397:A:H2'	1:a:398:A:C8	2.54	0.43
1:a:1275:U:O2'	1:a:1276:A:OP2	2.29	0.43
14:o:53:TYR:O	14:o:57:MET:HG2	2.18	0.43
18:s:71:LEU:HD23	18:s:71:LEU:HA	1.83	0.43
20:A:1525:U:O2	20:A:1552:A:N6	2.52	0.43
20:A:1725:A:H2'	20:A:1726:C:C6	2.53	0.43
21:B:1:U:O2	21:B:115:G:N2	2.39	0.43
23:D:111:THR:HG22	23:D:170:THR:HB	2.01	0.43
30:N:28:ALA:C	30:N:134:ARG:HH21	2.27	0.43
36:T:29:ILE:HD11	36:T:41:LEU:HG	1.99	0.43
37:U:29:VAL:HG21	37:U:38:VAL:CG2	2.47	0.43
1:a:859:C:H5''	1:a:860:C:H5	1.84	0.42
2:c:121:ARG:HA	2:c:121:ARG:HD3	1.74	0.42
20:A:345:G:H2'	20:A:346:A:C8	2.53	0.42
20:A:357:A:N3	24:E:169:ASN:ND2	2.66	0.42
20:A:854:C:H1'	20:A:1262:G:N2	2.34	0.42
20:A:2106:U:H4'	20:A:2107:G:H5''	2.00	0.42
20:A:2295:C:O2'	20:A:2296:G:H5'	2.19	0.42
20:A:2454:C:O2'	20:A:2455:C:O4'	2.37	0.42
23:D:123:ILE:HD13	23:D:130:ARG:HG3	2.01	0.42
23:D:159:ARG:HE	23:D:159:ARG:HB2	1.67	0.42
29:M:84:ARG:NH2	29:M:101:ILE:HD11	2.33	0.42
44:3:5:ILE:HG22	44:3:19:THR:HG23	2.01	0.42
46:5:54:ASP:O	46:5:58:ILE:HB	2.19	0.42
1:a:635:C:H1'	3:d:129:ILE:HD11	2.00	0.42
1:a:858:U:H2'	1:a:860:C:H5	1.83	0.42
2:c:86:LEU:HD23	2:c:86:LEU:HA	1.84	0.42
20:A:505:G:H2'	20:A:506:A:C8	2.54	0.42
20:A:1212:A:O2'	20:A:1213:U:H6	2.01	0.42
20:A:1216:G:N3	20:A:1216:G:H2'	2.34	0.42
20:A:1834:U:O2	22:C:201:GLU:HB2	2.20	0.42
22:C:272:ARG:HD3	22:C:274:ARG:NE	2.34	0.42
25:F:15:SER:O	25:F:19:LYS:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1273:G:H2'	1:a:1274:C:C6	2.54	0.42
1:a:1465:U:H5''	1:a:1466:U:C5	2.54	0.42
3:d:7:PRO:O	3:d:9:TRP:N	2.53	0.42
15:p:70:VAL:O	15:p:74:LEU:HB2	2.19	0.42
20:A:339:G:H2'	20:A:340:A:H8	1.85	0.42
20:A:1872:G:HO2'	20:A:1873:A:H8	1.65	0.42
20:A:2052:G:H2'	20:A:2053:G:O4'	2.19	0.42
20:A:2085:A:H2'	20:A:2086:G:H8	1.80	0.42
20:A:2855:A:H2'	20:A:2856:A:H8	1.84	0.42
25:F:74:ILE:O	25:F:79:LEU:HB2	2.18	0.42
1:a:441:U:H4'	3:d:34:GLY:O	2.19	0.42
10:k:56:LYS:H	10:k:56:LYS:HG2	1.39	0.42
11:l:80:ILE:O	11:l:80:ILE:HG13	2.20	0.42
20:A:1447:U:N3	20:A:1448:U:C4	2.87	0.42
20:A:1489:C:H2'	20:A:1490:A:C8	2.54	0.42
20:A:1755:C:H2'	20:A:1756:U:H4'	2.01	0.42
20:A:2079:C:H2'	20:A:2080:C:H6	1.84	0.42
20:A:2099:U:H2'	20:A:2100:U:C6	2.54	0.42
32:P:67:THR:O	32:P:67:THR:OG1	2.32	0.42
34:R:119:LYS:HA	34:R:119:LYS:HD3	1.85	0.42
43:2:15:LYS:O	43:2:18:THR:HG23	2.19	0.42
4:e:58:GLU:O	4:e:62:LYS:HG3	2.19	0.42
6:g:71:PRO:HG3	6:g:103:TRP:CZ3	2.54	0.42
10:k:126:ARG:N	10:k:126:ARG:HD2	2.34	0.42
12:m:3:ARG:HH12	12:m:11:ARG:HG2	1.84	0.42
20:A:1093:U:H2'	20:A:1094:A:O4'	2.20	0.42
20:A:1172:U:H5'	27:K:85:LEU:HD11	2.01	0.42
20:A:2317:G:O2'	25:F:121:ALA:HA	2.19	0.42
21:B:50:A:N6	32:P:38:LYS:HG2	2.35	0.42
21:B:97:A:HO2'	21:B:98:G:P	2.37	0.42
44:3:19:THR:OG1	44:3:20:ASN:N	2.53	0.42
1:a:524:A:O2'	1:a:525:A:OP1	2.34	0.42
1:a:668:U:C4	7:h:56:LYS:HB3	2.55	0.42
1:a:1020:A:C8	1:a:1041:U:H4'	2.54	0.42
1:a:1167:G:OP1	9:j:70:HIS:ND1	2.46	0.42
11:l:27:GLY:H	11:l:72:ASN:HD22	1.68	0.42
20:A:131:A:H2'	20:A:132:A:C8	2.55	0.42
20:A:572:G:H2'	20:A:573:U:C6	2.54	0.42
20:A:672:A:H5''	20:A:673:G:OP2	2.19	0.42
20:A:1757:U:H2'	20:A:1758:C:C2	2.54	0.42
28:L:66:LYS:HE3	28:L:66:LYS:HB3	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:X:75:VAL:O	39:X:90:VAL:HA	2.20	0.42
40:Y:40:ILE:HD11	40:Y:45:LYS:HB2	2.01	0.42
3:d:190:ILE:H	3:d:190:ILE:HG12	1.44	0.42
6:g:146:ASP:OD1	6:g:146:ASP:N	2.50	0.42
20:A:156:U:H2'	20:A:157:C:C6	2.54	0.42
20:A:987:A:H2'	20:A:988:C:C6	2.54	0.42
20:A:1409:A:H5'	20:A:2226:A:O4'	2.20	0.42
20:A:2219:A:H2'	20:A:2220:C:H6	1.83	0.42
21:B:89:C:P	30:N:99:ARG:HH22	2.42	0.42
23:D:2:THR:OG1	23:D:204:SER:OG	2.37	0.42
24:E:2:PRO:HD2	24:E:19:LEU:O	2.20	0.42
24:E:59:GLY:HA2	24:E:79:ARG:HH11	1.84	0.42
30:N:64:VAL:HG22	30:N:106:ILE:HG12	2.02	0.42
34:R:48:ARG:HE	34:R:48:ARG:HB3	1.66	0.42
1:a:418:C:H5''	3:d:130:PRO:HD2	2.01	0.42
1:a:964:C:H5''	12:m:105:ASN:ND2	2.35	0.42
1:a:1404:C:H2'	1:a:1405:U:O4'	2.20	0.42
11:l:115:LEU:HD23	11:l:115:LEU:HA	1.86	0.42
14:o:67:LEU:HD12	14:o:67:LEU:HA	1.80	0.42
20:A:2319:U:N3	25:F:151:GLY:O	2.44	0.42
23:D:16:PHE:CE1	23:D:22:LEU:HG	2.55	0.42
30:N:66:ILE:HG12	30:N:104:PHE:CE1	2.55	0.42
1:a:1406:U:H2'	1:a:1407:G:C8	2.55	0.42
7:h:88:TYR:CE1	7:h:126:GLU:HG3	2.55	0.42
8:i:56:GLU:CD	8:i:61:TYR:HE2	2.27	0.42
20:A:454:C:H2'	20:A:455:A:H8	1.85	0.42
20:A:1699:C:H2'	20:A:1700:U:H6	1.85	0.42
28:L:91:LYS:HB3	28:L:111:PHE:CD2	2.55	0.42
32:P:57:SER:HB2	32:P:60:ASP:HB2	2.00	0.42
38:V:81:VAL:HG13	38:V:92:ARG:HB3	2.01	0.42
1:a:517:C:OP1	11:l:128:SER:HB3	2.20	0.42
1:a:1020:A:H5''	1:a:1042:C:C4	2.55	0.42
1:a:1425:A:H2'	1:a:1426:C:C6	2.54	0.42
2:c:200:TRP:CD1	2:c:200:TRP:N	2.88	0.42
4:e:52:LYS:HB3	4:e:52:LYS:HE3	1.87	0.42
20:A:288:C:H1'	20:A:289:U:H5	1.85	0.42
20:A:1394:G:N1	20:A:1407:G:N7	2.68	0.42
20:A:2911:C:H6	20:A:2911:C:O5'	2.02	0.42
21:B:70:G:N3	21:B:70:G:O4'	2.52	0.42
21:B:72:U:H2'	21:B:73:U:H5'	2.02	0.42
22:C:195:VAL:HG12	22:C:196:GLY:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:O:18:ARG:HD3	31:O:65:PHE:HA	2.01	0.42
1:a:1506:U:H2'	1:a:1507:G:O4'	2.20	0.41
9:j:80:THR:OG1	9:j:82:LYS:NZ	2.42	0.41
15:p:18:TYR:HE2	15:p:42:PRO:HG3	1.85	0.41
20:A:891:A:HO2'	42:O:22:THR:HG22	1.84	0.41
20:A:2429:G:H2'	20:A:2430:C:C6	2.55	0.41
20:A:2454:C:HO2'	20:A:2455:C:P	2.42	0.41
25:F:42:ASP:C	25:F:49:ASN:HD22	2.27	0.41
1:a:125:A:H8	1:a:125:A:H2'	1.60	0.41
1:a:590:G:O2'	1:a:836:G:H5'	2.20	0.41
1:a:1020:A:H2'	1:a:1021:C:H5	1.85	0.41
12:m:14:ARG:HD2	12:m:43:VAL:O	2.20	0.41
20:A:312:U:O5'	20:A:312:U:H6	2.02	0.41
20:A:697:U:H2'	20:A:698:A:H8	1.85	0.41
20:A:1323:A:C8	31:O:113:ARG:HD3	2.51	0.41
20:A:1355:G:O2'	20:A:1356:G:H5'	2.20	0.41
20:A:1461:A:N3	20:A:1461:A:H2'	2.36	0.41
20:A:1808:U:H2'	20:A:1809:C:C6	2.55	0.41
20:A:2453:A:H4'	20:A:2454:C:C3'	2.47	0.41
22:C:2:ALA:HA	22:C:199:GLN:HE22	1.86	0.41
22:C:214:MET:H	22:C:214:MET:HG3	1.58	0.41
25:F:32:ASP:OD2	32:P:2:ILE:HD12	2.21	0.41
27:K:76:TYR:CE1	27:K:87:SER:HB3	2.55	0.41
1:a:1417:C:H2'	1:a:1418:C:O4'	2.20	0.41
1:a:1450:G:H2'	1:a:1451:U:H6	1.83	0.41
3:d:102:LEU:HG	3:d:168:PHE:CD1	2.55	0.41
4:e:101:GLU:H	4:e:101:GLU:HG2	1.54	0.41
11:l:72:ASN:O	11:l:72:ASN:CG	2.63	0.41
12:m:106:ALA:HB3	12:m:110:LYS:HE2	2.02	0.41
20:A:154:U:O2'	20:A:155:U:H5'	2.20	0.41
20:A:1181:U:H4'	20:A:1182:A:O4'	2.20	0.41
20:A:2088:U:H2'	20:A:2089:U:C6	2.55	0.41
20:A:2420:C:C4	29:M:69:ILE:HD12	2.55	0.41
24:E:158:ASN:HB3	24:E:159:GLY:H	1.74	0.41
25:F:104:VAL:CG2	25:F:175:MET:H	2.33	0.41
26:G:18:LYS:HB2	26:G:25:THR:CG2	2.50	0.41
34:R:88:ILE:HD11	34:R:112:GLN:OE1	2.20	0.41
1:a:967:G:C6	1:a:1246:G:C6	3.08	0.41
1:a:1020:A:H1'	1:a:1052:A:N1	2.34	0.41
3:d:56:LYS:HG2	3:d:190:ILE:HG21	2.02	0.41
6:g:50:ILE:HD11	6:g:124:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:911:U:H5''	30:N:6:ARG:O	2.20	0.41
20:A:2419:G:O2'	20:A:2420:C:OP2	2.34	0.41
21:B:50:A:N1	32:P:38:LYS:HE2	2.35	0.41
24:E:157:GLU:H	24:E:157:GLU:HG3	1.56	0.41
25:F:163:ASP:O	25:F:167:ARG:HG3	2.21	0.41
26:G:107:VAL:O	26:G:109:TYR:N	2.54	0.41
31:O:68:ASN:C	31:O:70:VAL:H	2.25	0.41
32:P:63:ILE:HD11	32:P:78:LEU:HD12	2.01	0.41
34:R:70:ARG:HA	34:R:74:LEU:O	2.20	0.41
1:a:1243:C:H2'	1:a:1244:A:C8	2.56	0.41
3:d:77:LYS:HB3	3:d:77:LYS:HE2	1.86	0.41
3:d:183:ARG:HH11	3:d:188:PRO:HA	1.85	0.41
20:A:11:A:H2'	20:A:12:A:H8	1.86	0.41
20:A:1489:C:H3'	20:A:1490:A:H8	1.85	0.41
20:A:2482:A:HO2'	20:A:2483:A:H8	1.69	0.41
26:G:73:ASN:O	26:G:77:VAL:HG23	2.21	0.41
26:G:101:ASN:O	26:G:116:THR:HA	2.20	0.41
1:a:501:U:H2'	1:a:502:A:C8	2.56	0.41
2:c:21:LYS:HB3	2:c:21:LYS:HZ3	1.86	0.41
6:g:13:LEU:HD23	6:g:14:PRO:HD2	2.02	0.41
20:A:591:U:H2'	20:A:592:G:O4'	2.21	0.41
20:A:1492:G:H22	20:A:1504:G:N2	2.19	0.41
21:B:113:A:H2'	21:B:114:C:C6	2.55	0.41
24:E:40:GLN:OE1	24:E:184:LEU:HB2	2.20	0.41
30:N:32:TRP:CZ2	30:N:111:GLU:HG2	2.54	0.41
38:V:81:VAL:CG1	38:V:92:ARG:HB3	2.50	0.41
42:O:5:LYS:HB3	42:O:5:LYS:HE3	1.86	0.41
1:a:354:C:P	28:L:97:ARG:HD2	2.60	0.41
1:a:683:A:O2'	14:o:46:HIS:HD2	2.03	0.41
8:i:66:ASN:C	8:i:66:ASN:HD22	2.27	0.41
12:m:19:LEU:HD23	12:m:19:LEU:HA	1.85	0.41
15:p:81:LYS:O	15:p:85:GLU:HG3	2.19	0.41
17:r:25:ILE:H	17:r:25:ILE:HG13	1.65	0.41
17:r:25:ILE:HD12	17:r:26:ASP:N	2.36	0.41
18:s:40:ILE:HG12	18:s:69:HIS:O	2.20	0.41
20:A:441:A:H2'	20:A:442:A:C8	2.56	0.41
20:A:853:U:H2'	20:A:854:C:H6	1.82	0.41
20:A:1518:U:O2'	20:A:1519:G:C8	2.73	0.41
20:A:1600:C:H6	20:A:1600:C:H2'	1.57	0.41
20:A:1699:C:H2'	20:A:1700:U:C6	2.56	0.41
25:F:40:VAL:HG22	25:F:150:ARG:NH1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:F:164:GLU:HA	25:F:167:ARG:CG	2.50	0.41
30:N:63:LYS:HD2	30:N:65:TRP:CZ2	2.56	0.41
37:U:23:LYS:HZ3	37:U:84:GLU:HA	1.84	0.41
2:c:191:THR:HG23	2:c:192:TYR:CD2	2.56	0.41
3:d:95:LEU:HD21	3:d:120:ILE:HD11	2.03	0.41
4:e:104:GLY:O	4:e:122:ASP:HA	2.21	0.41
6:g:115:THR:HB	6:g:117:GLU:HG2	2.03	0.41
8:i:57:THR:HA	8:i:58:LYS:HA	1.70	0.41
15:p:37:VAL:CG1	15:p:56:VAL:HG22	2.50	0.41
20:A:84:G:N2	20:A:103:A:H2	2.10	0.41
20:A:91:A:OP1	20:A:91:A:H8	2.04	0.41
26:G:163:ARG:HG3	26:G:164:TYR:O	2.21	0.41
27:K:15:LYS:O	27:K:53:ASP:HB3	2.20	0.41
29:M:130:LYS:HB2	29:M:130:LYS:HE2	1.88	0.41
47:6:11:CYS:SG	47:6:12:GLU:N	2.94	0.41
1:a:488:C:O2'	1:a:489:G:H8	2.03	0.41
1:a:532:G:N2	1:a:545:G:OP1	2.51	0.41
1:a:539:G:H2'	1:a:540:C:C6	2.56	0.41
1:a:586:U:H5	1:a:881:A:N1	2.19	0.41
1:a:1122:G:H2'	1:a:1123:C:H6	1.85	0.41
1:a:1134:U:H1'	1:a:1194:A:C5	2.56	0.41
2:c:174:LEU:HA	2:c:174:LEU:HD12	1.87	0.41
5:f:94:MET:HB2	17:r:69:MET:HE3	2.02	0.41
6:g:77:ALA:HA	6:g:86:GLN:HA	2.03	0.41
11:l:80:ILE:HG12	11:l:85:HIS:CD2	2.56	0.41
12:m:25:ILE:HG12	12:m:65:VAL:HG21	2.02	0.41
16:q:42:LYS:H	16:q:42:LYS:HG2	1.59	0.41
16:q:57:LYS:HE2	16:q:57:LYS:HB3	1.88	0.41
20:A:234:C:O2'	20:A:235:G:N3	2.46	0.41
20:A:716:A:H2	20:A:842:A:H61	1.69	0.41
20:A:1237:U:H2'	20:A:1238:C:C6	2.55	0.41
20:A:1518:U:O2'	20:A:1519:G:OP2	2.30	0.41
20:A:1538:A:H5''	20:A:1539:U:OP1	2.20	0.41
20:A:2379:G:N7	46:5:39:LYS:NZ	2.68	0.41
20:A:2575:A:O2'	28:L:23:LYS:HG3	2.20	0.41
20:A:2806:U:H2'	20:A:2807:U:C6	2.56	0.41
20:A:2809:U:O2	20:A:2809:U:H2'	2.20	0.41
23:D:5:ILE:HD11	23:D:101:VAL:HB	2.02	0.41
24:E:196:GLN:O	24:E:200:THR:HG23	2.21	0.41
29:M:27:ASN:O	29:M:31:ALA:HA	2.21	0.41
31:O:113:ARG:HD2	31:O:116:ASP:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:O:116:ASP:HB3	31:O:118:ALA:H	1.85	0.41
40:Y:6:TYR:CD2	40:Y:47:VAL:HG21	2.55	0.41
40:Y:19:SER:O	40:Y:19:SER:OG	2.33	0.41
1:a:151:G:H21	1:a:183:G:H22	1.67	0.41
1:a:1059:G:H2'	1:a:1060:A:H8	1.85	0.41
1:a:1402:G:H2'	1:a:1403:C:C6	2.55	0.41
2:c:25:GLU:C	2:c:27:GLU:H	2.30	0.41
9:j:6:ILE:CG2	9:j:76:ILE:HB	2.49	0.41
20:A:807:U:O2'	20:A:808:G:OP2	2.38	0.41
20:A:2300:A:H4'	20:A:2301:A:O4'	2.20	0.41
21:B:23:A:H2'	21:B:24:U:C6	2.56	0.41
21:B:32:U:HO2'	21:B:33:U:P	2.44	0.41
22:C:72:ASP:O	22:C:74:VAL:HG23	2.20	0.41
22:C:183:MET:HE3	22:C:269:LEU:HD23	2.03	0.41
1:a:447:A:H3'	1:a:448:A:H8	1.86	0.40
1:a:545:G:O2'	1:a:546:U:OP2	2.37	0.40
1:a:1022:C:H3'	1:a:1023:A:H8	1.86	0.40
2:c:72:PRO:O	2:c:75:VAL:HG12	2.21	0.40
4:e:79:SER:HB2	4:e:121:ALA:HB3	2.02	0.40
19:t:12:ARG:H	19:t:12:ARG:HG2	1.66	0.40
19:t:58:ASP:OD1	19:t:58:ASP:N	2.54	0.40
20:A:176:U:H2'	20:A:177:A:C8	2.57	0.40
20:A:297:G:H5''	20:A:305:A:OP1	2.21	0.40
20:A:1802:C:C5'	22:C:224:VAL:HG11	2.51	0.40
20:A:1824:A:H8	20:A:1824:A:O5'	2.04	0.40
20:A:1969:U:C4	20:A:2566:U:H1'	2.57	0.40
20:A:2318:G:O2'	25:F:153:ASP:OD1	2.33	0.40
20:A:2319:U:H3	25:F:151:GLY:C	2.28	0.40
33:Q:34:GLU:CD	33:Q:39:ARG:HH21	2.29	0.40
5:f:29:PHE:CD2	5:f:32:ILE:HD11	2.56	0.40
6:g:151:PHE:CD2	10:k:60:PRO:HG2	2.56	0.40
14:o:32:LEU:O	14:o:36:ILE:HG23	2.21	0.40
14:o:58:LYS:HB3	14:o:58:LYS:HE3	1.82	0.40
20:A:53:A:H2'	20:A:54:A:C8	2.56	0.40
20:A:713:C:H4'	24:E:82:GLN:HE22	1.85	0.40
20:A:1631:A:N9	20:A:1632:A:H2	2.19	0.40
24:E:12:THR:O	24:E:13:GLN:C	2.65	0.40
28:L:64:ARG:O	28:L:82:ASN:HA	2.21	0.40
31:O:4:ARG:HB2	31:O:39:GLU:OE2	2.21	0.40
1:a:271:U:H2'	1:a:272:G:O4'	2.20	0.40
1:a:709:A:H2'	1:a:710:A:O4'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1056:A:C2	1:a:1057:G:C5	3.09	0.40
1:a:1058:U:H2'	1:a:1059:G:N9	2.37	0.40
1:a:1114:C:C2	1:a:1115:G:C8	3.09	0.40
9:j:18:LEU:HD23	9:j:18:LEU:HA	1.84	0.40
20:A:288:C:H1'	20:A:289:U:C5	2.56	0.40
20:A:887:G:H5''	20:A:888:A:OP1	2.22	0.40
20:A:1213:U:H2'	20:A:1214:U:O4'	2.21	0.40
20:A:1492:G:N2	20:A:1504:G:N2	2.69	0.40
21:B:110:G:H2'	21:B:111:C:H6	1.87	0.40
28:L:63:VAL:HG22	28:L:106:LEU:HD11	2.03	0.40
28:L:105:GLU:H	28:L:105:GLU:HG2	1.64	0.40
1:a:1397:C:H1'	6:g:79:ARG:HD2	2.03	0.40
1:a:1400:G:H2'	1:a:1401:G:H8	1.87	0.40
6:g:72:VAL:HG12	6:g:142:HIS:NE2	2.36	0.40
10:k:17:GLU:O	10:k:81:THR:OG1	2.40	0.40
10:k:36:ASP:C	10:k:38:HIS:H	2.28	0.40
11:l:2:PRO:HD2	11:l:12:ARG:HH21	1.86	0.40
12:m:57:ARG:HE	12:m:57:ARG:HB2	1.54	0.40
15:p:81:LYS:HE2	15:p:81:LYS:HB2	1.77	0.40
20:A:897:G:H2'	20:A:898:A:H8	1.85	0.40
20:A:1960:U:H2'	20:A:1961:C:H6	1.86	0.40
20:A:2454:C:H6	20:A:2454:C:H2'	1.70	0.40
26:G:78:GLY:HA2	26:G:82:GLY:H	1.87	0.40
29:M:87:ASP:OD1	29:M:119:LYS:HA	2.22	0.40
33:Q:72:ARG:HD3	33:Q:74:PHE:CZ	2.57	0.40
38:V:100:VAL:C	38:V:101:LEU:HD23	2.47	0.40
1:a:427:A:O5'	1:a:427:A:C8	2.72	0.40
1:a:483:C:O2'	1:a:484:U:H6	2.04	0.40
1:a:1046:U:H5''	1:a:1047:C:C5	2.56	0.40
2:c:148:ILE:HG13	2:c:201:ILE:HG22	2.03	0.40
20:A:573:U:H2'	20:A:574:C:C6	2.56	0.40
25:F:30:LYS:O	25:F:158:THR:HB	2.22	0.40
33:Q:82:ALA:O	33:Q:83:GLN:HG2	2.21	0.40
37:U:23:LYS:HE2	37:U:85:ASP:H	1.87	0.40
46:5:14:VAL:HG13	46:5:22:LEU:HD22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	c	202/204 (99%)	174 (86%)	28 (14%)	0	100	100
3	d	199/201 (99%)	168 (84%)	29 (15%)	2 (1%)	12	39
4	e	161/163 (99%)	146 (91%)	15 (9%)	0	100	100
5	f	95/97 (98%)	82 (86%)	13 (14%)	0	100	100
6	g	152/154 (99%)	138 (91%)	14 (9%)	0	100	100
7	h	129/131 (98%)	115 (89%)	14 (11%)	0	100	100
8	i	126/128 (98%)	105 (83%)	21 (17%)	0	100	100
9	j	97/99 (98%)	79 (81%)	18 (19%)	0	100	100
10	k	115/117 (98%)	94 (82%)	21 (18%)	0	100	100
11	l	134/136 (98%)	110 (82%)	24 (18%)	0	100	100
12	m	108/112 (96%)	85 (79%)	23 (21%)	0	100	100
13	n	58/60 (97%)	49 (84%)	9 (16%)	0	100	100
14	o	86/88 (98%)	74 (86%)	11 (13%)	1 (1%)	10	34
15	p	87/89 (98%)	75 (86%)	12 (14%)	0	100	100
16	q	81/83 (98%)	69 (85%)	12 (15%)	0	100	100
17	r	64/66 (97%)	52 (81%)	11 (17%)	1 (2%)	7	27
18	s	76/78 (97%)	62 (82%)	13 (17%)	1 (1%)	9	32
19	t	80/82 (98%)	76 (95%)	3 (4%)	1 (1%)	9	32
22	C	273/275 (99%)	247 (90%)	25 (9%)	1 (0%)	30	59
23	D	205/207 (99%)	188 (92%)	16 (8%)	1 (0%)	24	54
24	E	204/206 (99%)	181 (89%)	21 (10%)	2 (1%)	12	39
25	F	175/177 (99%)	148 (85%)	27 (15%)	0	100	100
26	G	174/176 (99%)	145 (83%)	27 (16%)	2 (1%)	11	36
27	K	143/145 (99%)	133 (93%)	10 (7%)	0	100	100
28	L	120/122 (98%)	104 (87%)	15 (12%)	1 (1%)	16	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	M	144/146 (99%)	118 (82%)	25 (17%)	1 (1%)	18	48
30	N	139/141 (99%)	119 (86%)	20 (14%)	0	100	100
31	O	122/124 (98%)	102 (84%)	20 (16%)	0	100	100
32	P	115/117 (98%)	105 (91%)	10 (9%)	0	100	100
33	Q	112/114 (98%)	104 (93%)	8 (7%)	0	100	100
34	R	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
35	S	100/102 (98%)	91 (91%)	8 (8%)	1 (1%)	12	39
36	T	110/112 (98%)	103 (94%)	7 (6%)	0	100	100
37	U	87/89 (98%)	73 (84%)	14 (16%)	0	100	100
38	V	99/101 (98%)	81 (82%)	18 (18%)	0	100	100
39	X	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
40	Y	52/54 (96%)	43 (83%)	8 (15%)	1 (2%)	6	23
41	Z	59/61 (97%)	57 (97%)	2 (3%)	0	100	100
42	0	56/58 (97%)	54 (96%)	2 (4%)	0	100	100
43	2	54/56 (96%)	46 (85%)	8 (15%)	0	100	100
44	3	47/49 (96%)	43 (92%)	4 (8%)	0	100	100
45	4	42/44 (96%)	42 (100%)	0	0	100	100
46	5	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
47	6	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
All	All	4970/5060 (98%)	4354 (88%)	600 (12%)	16 (0%)	37	65

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
23	D	90	GLU
19	t	67	HIS
3	d	144	GLU
29	M	16	ARG
24	E	13	GLN
28	L	25	LEU
3	d	4	TYR
14	o	25	PRO
17	r	27	TYR
18	s	6	LYS
40	Y	20	HIS

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Mol	Chain	Res	Type
22	C	197	ASN
26	G	47	GLY
24	E	159	GLY
26	G	108	GLY
35	S	51	PRO

5.3.2 Protein sidechains ⓘ

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	
2	c	162/162 (100%)	138 (85%)	24 (15%)	3	10
3	d	175/175 (100%)	139 (79%)	36 (21%)	1	4
4	e	126/126 (100%)	104 (82%)	22 (18%)	2	6
5	f	86/86 (100%)	71 (83%)	15 (17%)	2	7
6	g	131/131 (100%)	111 (85%)	20 (15%)	3	9
7	h	112/112 (100%)	89 (80%)	23 (20%)	1	4
8	i	101/101 (100%)	91 (90%)	10 (10%)	7	24
9	j	90/90 (100%)	75 (83%)	15 (17%)	2	7
10	k	91/91 (100%)	76 (84%)	15 (16%)	2	8
11	l	118/118 (100%)	91 (77%)	27 (23%)	1	3
12	m	93/95 (98%)	77 (83%)	16 (17%)	2	7
13	n	51/51 (100%)	48 (94%)	3 (6%)	18	48
14	o	78/78 (100%)	67 (86%)	11 (14%)	3	11
15	p	79/79 (100%)	68 (86%)	11 (14%)	3	11
16	q	76/76 (100%)	59 (78%)	17 (22%)	1	3
17	r	57/57 (100%)	52 (91%)	5 (9%)	9	29
18	s	68/68 (100%)	53 (78%)	15 (22%)	1	3
19	t	63/63 (100%)	52 (82%)	11 (18%)	2	6
22	C	225/225 (100%)	200 (89%)	25 (11%)	6	20
23	D	170/170 (100%)	140 (82%)	30 (18%)	2	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	E	172/172 (100%)	139 (81%)	33 (19%)	1	5
25	F	154/154 (100%)	122 (79%)	32 (21%)	1	4
26	G	146/146 (100%)	121 (83%)	25 (17%)	2	7
27	K	122/122 (100%)	103 (84%)	19 (16%)	2	9
28	L	98/98 (100%)	81 (83%)	17 (17%)	2	7
29	M	112/112 (100%)	95 (85%)	17 (15%)	3	9
30	N	112/112 (100%)	96 (86%)	16 (14%)	3	11
31	O	106/106 (100%)	91 (86%)	15 (14%)	3	11
32	P	91/91 (100%)	76 (84%)	15 (16%)	2	8
33	Q	97/97 (100%)	82 (84%)	15 (16%)	2	9
34	R	94/94 (100%)	86 (92%)	8 (8%)	10	31
35	S	83/83 (100%)	67 (81%)	16 (19%)	1	5
36	T	95/95 (100%)	83 (87%)	12 (13%)	4	14
37	U	80/80 (100%)	60 (75%)	20 (25%)	0	2
38	V	85/85 (100%)	67 (79%)	18 (21%)	1	4
39	X	61/61 (100%)	46 (75%)	15 (25%)	1	2
40	Y	47/47 (100%)	39 (83%)	8 (17%)	2	7
41	Z	55/55 (100%)	44 (80%)	11 (20%)	1	4
42	0	49/49 (100%)	44 (90%)	5 (10%)	7	23
43	2	46/46 (100%)	40 (87%)	6 (13%)	4	13
44	3	49/49 (100%)	44 (90%)	5 (10%)	7	23
45	4	39/39 (100%)	33 (85%)	6 (15%)	2	9
46	5	51/51 (100%)	42 (82%)	9 (18%)	2	6
47	6	35/35 (100%)	30 (86%)	5 (14%)	3	11
All	All	4231/4233 (100%)	3532 (84%)	699 (16%)	4	8

All (699) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	c	21	LYS
2	c	25	GLU
2	c	39	ARG
2	c	40	LYS
2	c	42	ILE

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Mol	Chain	Res	Type
2	c	44	THR
2	c	45	LYS
2	c	46	LEU
2	c	51	VAL
2	c	55	GLU
2	c	56	ILE
2	c	67	ILE
2	c	69	THR
2	c	78	LYS
2	c	81	SER
2	c	98	VAL
2	c	100	ILE
2	c	103	VAL
2	c	171	THR
2	c	172	VAL
2	c	174	LEU
2	c	191	THR
2	c	199	VAL
2	c	200	TRP
3	d	9	TRP
3	d	14	ARG
3	d	17	ILE
3	d	22	THR
3	d	24	LYS
3	d	25	GLU
3	d	28	ARG
3	d	29	ARG
3	d	50	GLN
3	d	53	GLU
3	d	56	LYS
3	d	57	LEU
3	d	58	ARG
3	d	63	MET
3	d	65	GLU
3	d	71	LEU
3	d	74	LYS
3	d	91	LEU
3	d	102	LEU
3	d	104	LEU
3	d	114	LEU
3	d	122	VAL
3	d	123	ASP

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Mol	Chain	Res	Type
3	d	135	GLU
3	d	139	VAL
3	d	140	ILE
3	d	142	VAL
3	d	143	ARG
3	d	152	ILE
3	d	159	THR
3	d	186	LEU
3	d	189	GLU
3	d	190	ILE
3	d	192	GLU
3	d	201	GLN
3	d	202	LYS
4	e	22	THR
4	e	24	VAL
4	e	39	VAL
4	e	42	LYS
4	e	43	ASN
4	e	50	THR
4	e	71	LEU
4	e	76	MET
4	e	95	LEU
4	e	100	VAL
4	e	101	GLU
4	e	105	VAL
4	e	111	VAL
4	e	112	ARG
4	e	117	LEU
4	e	123	ILE
4	e	126	LYS
4	e	128	LEU
4	e	144	LEU
4	e	147	LEU
4	e	160	SER
4	e	165	ILE
5	f	3	GLN
5	f	4	ASP
5	f	5	THR
5	f	33	LEU
5	f	36	ASN
5	f	41	ILE
5	f	45	ASP

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Mol	Chain	Res	Type
5	f	65	ILE
5	f	66	VAL
5	f	68	VAL
5	f	77	ILE
5	f	78	ASN
5	f	88	ASP
5	f	96	VAL
5	f	99	GLU
6	g	9	LYS
6	g	10	ARG
6	g	12	VAL
6	g	13	LEU
6	g	22	LEU
6	g	43	ILE
6	g	52	GLU
6	g	56	ASN
6	g	64	GLN
6	g	72	VAL
6	g	75	VAL
6	g	85	TYR
6	g	91	VAL
6	g	94	GLU
6	g	115	THR
6	g	120	LEU
6	g	131	THR
6	g	141	THR
6	g	151	PHE
6	g	155	ARG
7	h	2	VAL
7	h	11	LEU
7	h	25	LEU
7	h	27	VAL
7	h	40	LEU
7	h	49	VAL
7	h	52	ILE
7	h	54	ASP
7	h	57	GLN
7	h	65	LYS
7	h	69	ASN
7	h	73	VAL
7	h	74	ILE
7	h	75	THR

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Mol	Chain	Res	Type
7	h	79	ARG
7	h	89	VAL
7	h	92	ASP
7	h	97	VAL
7	h	101	LEU
7	h	113	ILE
7	h	114	THR
7	h	126	GLU
7	h	131	VAL
8	i	16	VAL
8	i	28	ILE
8	i	29	THR
8	i	30	VAL
8	i	35	VAL
8	i	47	VAL
8	i	65	VAL
8	i	83	ILE
8	i	99	LYS
8	i	130	ARG
9	j	4	GLN
9	j	8	ILE
9	j	18	LEU
9	j	25	ILE
9	j	27	GLU
9	j	32	THR
9	j	48	LEU
9	j	51	VAL
9	j	63	GLU
9	j	67	MET
9	j	72	ARG
9	j	85	ASP
9	j	87	LEU
9	j	89	LYS
9	j	91	ASP
10	k	23	ILE
10	k	30	THR
10	k	32	VAL
10	k	35	THR
10	k	37	THR
10	k	40	ASN
10	k	45	SER
10	k	55	SER

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Mol	Chain	Res	Type
10	k	56	LYS
10	k	65	MET
10	k	81	THR
10	k	82	VAL
10	k	85	THR
10	k	86	VAL
10	k	113	VAL
11	l	8	VAL
11	l	10	LYS
11	l	18	LYS
11	l	20	ASP
11	l	24	LEU
11	l	25	ASN
11	l	32	LYS
11	l	33	LYS
11	l	35	GLN
11	l	36	THR
11	l	37	ASN
11	l	42	GLN
11	l	54	THR
11	l	63	ARG
11	l	64	LYS
11	l	72	ASN
11	l	77	THR
11	l	80	ILE
11	l	92	VAL
11	l	102	ASP
11	l	106	VAL
11	l	110	ILE
11	l	111	VAL
11	l	117	THR
11	l	120	VAL
11	l	122	ASP
11	l	129	LYS
12	m	14	ARG
12	m	22	ILE
12	m	28	THR
12	m	29	THR
12	m	34	LEU
12	m	41	GLU
12	m	66	GLU
12	m	72	GLU

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Mol	Chain	Res	Type
12	m	80	LEU
12	m	83	ILE
12	m	91	HIS
12	m	98	ARG
12	m	100	GLN
12	m	102	THR
12	m	103	LYS
12	m	109	ARG
13	n	6	MET
13	n	17	SER
13	n	33	VAL
14	o	7	ARG
14	o	12	ILE
14	o	22	THR
14	o	29	ILE
14	o	54	ARG
14	o	56	LEU
14	o	67	LEU
14	o	75	ILE
14	o	81	LEU
14	o	87	LEU
14	o	89	ARG
15	p	21	VAL
15	p	22	VAL
15	p	32	ARG
15	p	36	THR
15	p	39	THR
15	p	44	LYS
15	p	54	ASP
15	p	56	VAL
15	p	73	ILE
15	p	74	LEU
15	p	88	ASN
16	q	4	GLU
16	q	10	VAL
16	q	14	ARG
16	q	16	VAL
16	q	18	ASP
16	q	21	ASP
16	q	28	VAL
16	q	30	THR
16	q	32	LYS

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Mol	Chain	Res	Type
16	q	40	ARG
16	q	42	LYS
16	q	55	THR
16	q	62	VAL
16	q	63	LYS
16	q	79	LEU
16	q	81	VAL
16	q	86	VAL
17	r	20	ASN
17	r	22	ILE
17	r	25	ILE
17	r	28	LYS
17	r	63	ILE
18	s	6	LYS
18	s	7	LYS
18	s	11	VAL
18	s	14	HIS
18	s	17	LYS
18	s	22	GLN
18	s	26	GLU
18	s	27	LYS
18	s	36	ARG
18	s	39	THR
18	s	45	VAL
18	s	70	LYS
18	s	73	GLU
18	s	78	ARG
18	s	81	ARG
19	t	12	ARG
19	t	13	THR
19	t	20	LYS
19	t	33	LYS
19	t	36	GLU
19	t	39	VAL
19	t	44	ASP
19	t	47	ASP
19	t	49	LEU
19	t	62	THR
19	t	81	LEU
22	C	23	GLU
22	C	28	THR
22	C	30	GLU

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Mol	Chain	Res	Type
22	C	38	LYS
22	C	77	VAL
22	C	91	ILE
22	C	93	LEU
22	C	94	VAL
22	C	104	ILE
22	C	110	LEU
22	C	124	ILE
22	C	130	LEU
22	C	139	THR
22	C	141	ILE
22	C	167	LYS
22	C	168	GLU
22	C	177	ASN
22	C	182	ARG
22	C	191	THR
22	C	198	GLU
22	C	216	LYS
22	C	219	THR
22	C	260	ARG
22	C	261	ASN
22	C	275	THR
23	D	15	ILE
23	D	21	GLU
23	D	23	ILE
23	D	25	VAL
23	D	43	THR
23	D	49	ILE
23	D	50	GLN
23	D	58	GLU
23	D	59	VAL
23	D	62	ASN
23	D	69	VAL
23	D	71	LYS
23	D	86	VAL
23	D	90	GLU
23	D	103	GLN
23	D	107	VAL
23	D	108	VAL
23	D	111	THR
23	D	120	GLN
23	D	145	SER

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Mol	Chain	Res	Type
23	D	158	LYS
23	D	164	MET
23	D	167	ASP
23	D	168	ARG
23	D	170	THR
23	D	175	GLU
23	D	186	ILE
23	D	191	ASN
23	D	199	LEU
23	D	201	THR
24	E	6	LEU
24	E	8	LYS
24	E	17	ILE
24	E	18	THR
24	E	21	GLU
24	E	31	SER
24	E	45	ARG
24	E	49	HIS
24	E	65	TRP
24	E	77	SER
24	E	78	ILE
24	E	79	ARG
24	E	80	SER
24	E	82	GLN
24	E	89	VAL
24	E	93	THR
24	E	105	VAL
24	E	113	VAL
24	E	136	THR
24	E	142	VAL
24	E	152	VAL
24	E	153	LEU
24	E	157	GLU
24	E	160	ASN
24	E	165	LEU
24	E	168	ARG
24	E	176	VAL
24	E	184	LEU
24	E	190	ASN
24	E	193	LEU
24	E	195	THR
24	E	200	THR

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Mol	Chain	Res	Type
24	E	205	VAL
25	F	6	GLU
25	F	15	SER
25	F	17	VAL
25	F	31	VAL
25	F	32	ASP
25	F	36	ILE
25	F	44	VAL
25	F	57	LEU
25	F	61	THR
25	F	66	LEU
25	F	67	ILE
25	F	77	PHE
25	F	81	GLU
25	F	88	LYS
25	F	89	VAL
25	F	110	ARG
25	F	114	PHE
25	F	127	ASN
25	F	130	LEU
25	F	133	LYS
25	F	136	LEU
25	F	137	ILE
25	F	141	VAL
25	F	142	ASP
25	F	143	TYR
25	F	149	VAL
25	F	152	MET
25	F	154	ILE
25	F	162	THR
25	F	169	LEU
25	F	170	LEU
25	F	172	GLN
26	G	8	VAL
26	G	9	VAL
26	G	11	LEU
26	G	25	THR
26	G	32	GLU
26	G	35	ARG
26	G	44	ASN
26	G	45	ILE
26	G	46	GLU

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Mol	Chain	Res	Type
26	G	63	THR
26	G	67	THR
26	G	79	VAL
26	G	84	GLN
26	G	90	ILE
26	G	101	ASN
26	G	103	LEU
26	G	107	VAL
26	G	121	VAL
26	G	122	THR
26	G	133	VAL
26	G	136	ILE
26	G	143	GLU
26	G	144	LEU
26	G	165	VAL
26	G	171	ARG
27	K	2	ARG
27	K	14	ARG
27	K	22	THR
27	K	26	LEU
27	K	29	LEU
27	K	30	SER
27	K	46	THR
27	K	58	ILE
27	K	77	ARG
27	K	80	MET
27	K	85	LEU
27	K	94	ARG
27	K	101	LEU
27	K	113	ASN
27	K	114	THR
27	K	115	LEU
27	K	118	LYS
27	K	123	LEU
27	K	145	ASN
28	L	1	MET
28	L	2	ILE
28	L	5	GLU
28	L	18	GLU
28	L	19	ILE
28	L	21	THR
28	L	39	ILE

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Mol	Chain	Res	Type
28	L	42	THR
28	L	53	LYS
28	L	54	LYS
28	L	63	VAL
28	L	73	ASP
28	L	87	ILE
28	L	90	ASP
28	L	102	VAL
28	L	105	GLU
28	L	110	ASN
29	M	3	LEU
29	M	16	ARG
29	M	39	LYS
29	M	42	SER
29	M	60	ARG
29	M	67	THR
29	M	76	VAL
29	M	77	VAL
29	M	79	LEU
29	M	81	THR
29	M	84	ARG
29	M	87	ASP
29	M	98	GLU
29	M	120	LYS
29	M	122	THR
29	M	131	SER
29	M	143	ILE
30	N	5	LYS
30	N	10	ARG
30	N	11	ARG
30	N	25	LYS
30	N	26	GLU
30	N	34	LEU
30	N	37	THR
30	N	51	ARG
30	N	74	TYR
30	N	76	SER
30	N	85	LYS
30	N	103	MET
30	N	109	VAL
30	N	111	GLU
30	N	127	VAL

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Mol	Chain	Res	Type
30	N	133	LYS
31	O	23	ASP
31	O	24	LEU
31	O	47	MET
31	O	48	ILE
31	O	49	THR
31	O	55	ASP
31	O	56	LEU
31	O	61	GLN
31	O	70	VAL
31	O	84	SER
31	O	89	LEU
31	O	106	ARG
31	O	108	LEU
31	O	121	VAL
31	O	124	GLU
32	P	2	ILE
32	P	6	ASP
32	P	13	LYS
32	P	22	ILE
32	P	31	LEU
32	P	35	ARG
32	P	40	ILE
32	P	46	ASP
32	P	51	VAL
32	P	57	SER
32	P	63	ILE
32	P	67	THR
32	P	79	VAL
32	P	95	ARG
32	P	104	VAL
33	Q	2	ASN
33	Q	4	LEU
33	Q	10	GLN
33	Q	11	GLU
33	Q	36	THR
33	Q	49	LYS
33	Q	55	ILE
33	Q	60	THR
33	Q	72	ARG
33	Q	76	LEU
33	Q	78	THR

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Mol	Chain	Res	Type
33	Q	80	ARG
33	Q	109	ARG
33	Q	113	ILE
33	Q	114	ARG
34	R	9	VAL
34	R	10	THR
34	R	30	THR
34	R	38	GLN
34	R	60	LEU
34	R	79	LEU
34	R	90	ILE
34	R	92	ARG
35	S	1	MET
35	S	2	TYR
35	S	10	LYS
35	S	12	VAL
35	S	14	VAL
35	S	20	ILE
35	S	22	VAL
35	S	24	LYS
35	S	33	VAL
35	S	61	THR
35	S	67	LYS
35	S	73	THR
35	S	75	GLN
35	S	90	GLN
35	S	94	LYS
35	S	101	ASN
36	T	4	GLN
36	T	11	THR
36	T	14	THR
36	T	26	ILE
36	T	29	ILE
36	T	70	ASP
36	T	75	VAL
36	T	88	LYS
36	T	93	ARG
36	T	105	THR
36	T	109	THR
36	T	115	LYS
37	U	2	GLU
37	U	3	LEU

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Mol	Chain	Res	Type
37	U	14	GLU
37	U	16	SER
37	U	23	LYS
37	U	26	THR
37	U	29	VAL
37	U	37	LEU
37	U	42	VAL
37	U	47	ASP
37	U	49	LYS
37	U	52	ASN
37	U	55	ILE
37	U	56	LEU
37	U	65	MET
37	U	75	ARG
37	U	76	ARG
37	U	84	GLU
37	U	87	LYS
37	U	89	ILE
38	V	1	MET
38	V	2	PHE
38	V	3	VAL
38	V	5	LYS
38	V	9	VAL
38	V	13	THR
38	V	17	LYS
38	V	29	LYS
38	V	33	VAL
38	V	41	VAL
38	V	46	LYS
38	V	58	GLU
38	V	59	VAL
38	V	68	VAL
38	V	69	MET
38	V	91	VAL
38	V	94	SER
38	V	99	GLU
39	X	18	SER
39	X	19	THR
39	X	20	SER
39	X	23	ARG
39	X	39	THR
39	X	40	VAL

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Mol	Chain	Res	Type
39	X	53	LYS
39	X	58	VAL
39	X	62	ILE
39	X	67	THR
39	X	73	ASP
39	X	79	GLU
39	X	85	LYS
39	X	88	VAL
39	X	93	VAL
40	Y	12	THR
40	Y	22	MET
40	Y	24	SER
40	Y	27	ARG
40	Y	28	THR
40	Y	34	GLN
40	Y	36	VAL
40	Y	40	ILE
41	Z	3	VAL
41	Z	4	LYS
41	Z	5	GLU
41	Z	10	THR
41	Z	15	LEU
41	Z	17	LYS
41	Z	24	GLU
41	Z	32	LEU
41	Z	37	LEU
41	Z	38	GLU
41	Z	55	THR
42	0	8	LEU
42	0	35	VAL
42	0	54	VAL
42	0	55	ASP
42	0	59	VAL
43	2	3	VAL
43	2	8	THR
43	2	18	THR
43	2	23	THR
43	2	35	GLU
43	2	56	SER
44	3	5	ILE
44	3	8	GLU
44	3	10	THR

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Mol	Chain	Res	Type
44	3	11	SER
44	3	44	LEU
45	4	1	MET
45	4	10	ARG
45	4	14	LYS
45	4	20	LYS
45	4	24	THR
45	4	43	SER
46	5	14	VAL
46	5	31	HIS
46	5	32	ARG
46	5	41	ARG
46	5	46	LYS
46	5	57	ARG
46	5	58	ILE
46	5	60	GLN
46	5	65	MET
47	6	4	ARG
47	6	11	CYS
47	6	15	LYS
47	6	26	ILE
47	6	36	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
2	c	64	ASN
2	c	85	ASN
2	c	122	GLN
2	c	125	ASN
2	c	138	GLN
3	d	35	GLN
3	d	50	GLN
3	d	59	HIS
3	d	93	GLN
3	d	113	GLN
3	d	119	HIS
3	d	201	GLN
5	f	78	ASN
6	g	28	ASN
6	g	56	ASN
6	g	64	GLN

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Mol	Chain	Res	Type
6	g	86	GLN
7	h	22	HIS
7	h	57	GLN
7	h	99	ASN
8	i	66	ASN
8	i	81	HIS
8	i	89	GLN
10	k	22	HIS
11	l	5	ASN
11	l	39	ASN
11	l	90	HIS
11	l	125	GLN
12	m	105	ASN
14	o	37	ASN
14	o	42	HIS
14	o	46	HIS
14	o	83	GLN
15	p	41	ASN
15	p	72	ASN
16	q	34	HIS
16	q	53	ASN
18	s	22	GLN
18	s	57	HIS
19	t	24	GLN
19	t	45	ASN
22	C	90	ASN
22	C	95	HIS
22	C	142	HIS
22	C	143	ASN
22	C	163	GLN
22	C	199	GLN
22	C	200	HIS
23	D	37	GLN
23	D	68	HIS
23	D	120	GLN
23	D	184	ASN
24	E	13	GLN
24	E	14	ASN
24	E	46	GLN
24	E	49	HIS
24	E	75	GLN
24	E	82	GLN

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Mol	Chain	Res	Type
24	E	196	GLN
25	F	27	GLN
25	F	46	ASN
25	F	49	ASN
27	K	59	ASN
27	K	113	ASN
27	K	131	HIS
29	M	4	HIS
29	M	38	GLN
29	M	133	GLN
31	O	57	HIS
32	P	12	GLN
32	P	15	HIS
32	P	20	ASN
32	P	114	ASN
33	Q	41	GLN
34	R	101	ASN
35	S	11	GLN
35	S	86	GLN
35	S	88	HIS
36	T	4	GLN
36	T	46	ASN
36	T	65	ASN
39	X	49	GLN
39	X	87	GLN
40	Y	32	ASN
40	Y	34	GLN
41	Z	36	GLN
41	Z	48	GLN
43	2	28	ASN
45	4	8	ASN
46	5	31	HIS
47	6	35	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1521/1548 (98%)	308 (20%)	0
20	A	2733/2908 (93%)	536 (19%)	28 (1%)
21	B	115/116 (99%)	32 (27%)	3 (2%)
All	All	4369/4572 (95%)	876 (20%)	31 (0%)

All (876) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	4	G
1	a	5	A
1	a	6	G
1	a	13	A
1	a	19	G
1	a	27	C
1	a	29	A
1	a	30	A
1	a	32	G
1	a	35	G
1	a	36	G
1	a	38	G
1	a	41	G
1	a	44	C
1	a	45	C
1	a	48	A
1	a	52	A
1	a	70	U
1	a	71	U
1	a	101	A
1	a	103	A
1	a	106	A
1	a	113	G
1	a	114	A
1	a	122	G
1	a	125	A
1	a	126	C
1	a	137	C
1	a	147	A
1	a	165	G
1	a	167	A
1	a	169	C
1	a	171	G
1	a	172	G
1	a	183	G
1	a	188	A
1	a	189	C
1	a	202	A
1	a	210	A
1	a	211	G
1	a	212	A
1	a	213	G

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Mol	Chain	Res	Type
1	a	214	U
1	a	215	G
1	a	216	A
1	a	218	A
1	a	225	U
1	a	226	U
1	a	228	G
1	a	229	G
1	a	230	G
1	a	235	G
1	a	246	G
1	a	254	G
1	a	255	U
1	a	256	G
1	a	258	A
1	a	259	U
1	a	260	U
1	a	262	G
1	a	266	G
1	a	281	G
1	a	282	C
1	a	295	C
1	a	298	U
1	a	304	G
1	a	321	A
1	a	332	U
1	a	336	A
1	a	337	C
1	a	342	A
1	a	343	C
1	a	344	A
1	a	360	C
1	a	362	G
1	a	367	C
1	a	369	G
1	a	371	A
1	a	382	U
1	a	387	C
1	a	388	A
1	a	390	U
1	a	399	G
1	a	412	A

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Mol	Chain	Res	Type
1	a	421	G
1	a	426	A
1	a	427	A
1	a	428	G
1	a	429	A
1	a	431	G
1	a	444	U
1	a	447	A
1	a	463	A
1	a	464	A
1	a	468	C
1	a	473	A
1	a	474	C
1	a	478	A
1	a	480	U
1	a	484	U
1	a	485	G
1	a	488	C
1	a	489	G
1	a	490	U
1	a	495	U
1	a	498	C
1	a	499	G
1	a	500	G
1	a	516	C
1	a	524	A
1	a	525	A
1	a	526	C
1	a	532	G
1	a	533	C
1	a	539	G
1	a	542	G
1	a	546	U
1	a	548	A
1	a	551	C
1	a	560	C
1	a	562	A
1	a	574	A
1	a	576	U
1	a	577	U
1	a	584	C
1	a	585	G

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Mol	Chain	Res	Type
1	a	587	A
1	a	588	A
1	a	590	G
1	a	591	C
1	a	592	G
1	a	593	A
1	a	594	G
1	a	596	G
1	a	602	G
1	a	608	U
1	a	637	A
1	a	643	G
1	a	648	U
1	a	668	U
1	a	671	G
1	a	680	A
1	a	701	U
1	a	702	A
1	a	710	A
1	a	716	U
1	a	717	A
1	a	718	G
1	a	726	G
1	a	738	U
1	a	744	A
1	a	755	U
1	a	764	A
1	a	770	G
1	a	777	C
1	a	780	G
1	a	792	A
1	a	793	G
1	a	802	A
1	a	809	A
1	a	817	A
1	a	830	A
1	a	832	C
1	a	835	U
1	a	836	G
1	a	842	U
1	a	843	A
1	a	857	U

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Mol	Chain	Res	Type
1	a	858	U
1	a	859	C
1	a	860	C
1	a	861	G
1	a	862	C
1	a	876	A
1	a	883	G
1	a	888	A
1	a	893	C
1	a	930	A
1	a	940	C
1	a	942	G
1	a	943	G
1	a	947	C
1	a	948	C
1	a	950	C
1	a	951	A
1	a	962	A
1	a	963	G
1	a	974	A
1	a	975	A
1	a	976	U
1	a	977	U
1	a	982	G
1	a	985	A
1	a	987	G
1	a	988	C
1	a	991	A
1	a	992	G
1	a	993	A
1	a	999	A
1	a	1003	G
1	a	1008	U
1	a	1009	G
1	a	1015	C
1	a	1018	U
1	a	1020	A
1	a	1022	C
1	a	1031	G
1	a	1039	U
1	a	1040	U
1	a	1041	U

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Mol	Chain	Res	Type
1	a	1042	C
1	a	1044	C
1	a	1045	U
1	a	1046	U
1	a	1047	C
1	a	1048	G
1	a	1049	G
1	a	1057	G
1	a	1058	U
1	a	1060	A
1	a	1061	C
1	a	1062	A
1	a	1069	G
1	a	1080	G
1	a	1081	U
1	a	1096	A
1	a	1110	G
1	a	1111	U
1	a	1117	A
1	a	1140	G
1	a	1142	U
1	a	1144	C
1	a	1146	A
1	a	1149	A
1	a	1154	G
1	a	1155	U
1	a	1156	U
1	a	1157	G
1	a	1172	A
1	a	1174	U
1	a	1183	C
1	a	1196	G
1	a	1199	G
1	a	1202	G
1	a	1211	A
1	a	1212	A
1	a	1215	C
1	a	1219	A
1	a	1227	U
1	a	1229	U
1	a	1240	A
1	a	1242	A

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Mol	Chain	Res	Type
1	a	1248	G
1	a	1253	A
1	a	1263	A
1	a	1272	C
1	a	1275	U
1	a	1276	A
1	a	1294	A
1	a	1295	A
1	a	1301	U
1	a	1302	A
1	a	1310	U
1	a	1312	U
1	a	1314	A
1	a	1317	U
1	a	1320	G
1	a	1334	A
1	a	1335	C
1	a	1353	G
1	a	1368	G
1	a	1372	A
1	a	1374	C
1	a	1378	A
1	a	1379	C
1	a	1383	G
1	a	1392	A
1	a	1393	C
1	a	1409	A
1	a	1412	C
1	a	1416	G
1	a	1438	G
1	a	1455	U
1	a	1457	A
1	a	1461	A
1	a	1466	U
1	a	1467	U
1	a	1468	U
1	a	1469	U
1	a	1470	G
1	a	1479	C
1	a	1483	U
1	a	1498	G
1	a	1503	G

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Mol	Chain	Res	Type
1	a	1508	A
1	a	1509	A
1	a	1518	A
1	a	1519	A
1	a	1520	G
1	a	1522	U
1	a	1523	A
1	a	1524	G
1	a	1533	G
1	a	1542	G
1	a	1545	G
1	a	1546	G
1	a	1547	A
1	a	1550	A
20	A	13	U
20	A	14	A
20	A	28	G
20	A	35	U
20	A	42	A
20	A	52	G
20	A	68	A
20	A	71	G
20	A	72	A
20	A	75	U
20	A	76	G
20	A	92	A
20	A	93	G
20	A	97	G
20	A	102	G
20	A	110	G
20	A	118	A
20	A	119	A
20	A	120	U
20	A	131	A
20	A	148	A
20	A	155	U
20	A	156	U
20	A	158	A
20	A	165	A
20	A	166	C
20	A	168	U
20	A	169	A

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Mol	Chain	Res	Type
20	A	177	A
20	A	180	G
20	A	182	U
20	A	185	A
20	A	199	A
20	A	202	A
20	A	218	G
20	A	219	A
20	A	220	A
20	A	225	A
20	A	231	A
20	A	232	U
20	A	233	U
20	A	235	G
20	A	236	A
20	A	251	G
20	A	255	G
20	A	265	A
20	A	268	A
20	A	277	C
20	A	279	A
20	A	284	C
20	A	285	U
20	A	286	U
20	A	287	G
20	A	288	C
20	A	289	U
20	A	296	G
20	A	297	G
20	A	298	U
20	A	300	G
20	A	302	A
20	A	309	C
20	A	313	A
20	A	315	G
20	A	316	G
20	A	318	A
20	A	321	C
20	A	322	U
20	A	325	U
20	A	327	G
20	A	332	G

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Mol	Chain	Res	Type
20	A	347	A
20	A	352	C
20	A	367	A
20	A	383	A
20	A	392	A
20	A	393	A
20	A	396	C
20	A	399	A
20	A	404	G
20	A	420	G
20	A	426	G
20	A	429	A
20	A	439	G
20	A	446	G
20	A	451	G
20	A	452	A
20	A	491	U
20	A	496	C
20	A	507	G
20	A	517	A
20	A	520	A
20	A	521	G
20	A	524	C
20	A	542	A
20	A	543	U
20	A	544	A
20	A	547	U
20	A	548	C
20	A	551	G
20	A	560	U
20	A	561	G
20	A	569	C
20	A	570	A
20	A	571	A
20	A	572	G
20	A	577	A
20	A	581	C
20	A	586	A
20	A	587	U
20	A	588	G
20	A	596	G
20	A	600	G

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Mol	Chain	Res	Type
20	A	609	A
20	A	610	G
20	A	611	A
20	A	612	A
20	A	613	U
20	A	614	G
20	A	624	G
20	A	631	U
20	A	640	A
20	A	652	A
20	A	654	A
20	A	655	G
20	A	656	A
20	A	660	A
20	A	673	G
20	A	676	A
20	A	677	G
20	A	684	U
20	A	685	A
20	A	692	A
20	A	695	A
20	A	704	U
20	A	722	G
20	A	726	U
20	A	752	G
20	A	753	G
20	A	755	A
20	A	757	A
20	A	759	C
20	A	764	U
20	A	770	A
20	A	778	C
20	A	779	A
20	A	784	C
20	A	787	U
20	A	804	A
20	A	805	G
20	A	808	G
20	A	810	G
20	A	815	G
20	A	817	G
20	A	822	A

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Mol	Chain	Res	Type
20	A	824	U
20	A	832	G
20	A	833	A
20	A	845	G
20	A	852	C
20	A	867	U
20	A	868	U
20	A	878	C
20	A	886	U
20	A	887	G
20	A	889	G
20	A	890	A
20	A	891	A
20	A	900	G
20	A	903	G
20	A	905	G
20	A	909	U
20	A	910	G
20	A	917	C
20	A	919	A
20	A	920	G
20	A	947	G
20	A	948	A
20	A	950	A
20	A	951	A
20	A	956	C
20	A	958	A
20	A	965	U
20	A	966	U
20	A	967	C
20	A	981	A
20	A	985	A
20	A	986	G
20	A	990	G
20	A	992	G
20	A	993	A
20	A	999	A
20	A	1001	G
20	A	1014	A
20	A	1023	A
20	A	1029	G
20	A	1036	A

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Mol	Chain	Res	Type
20	A	1045	C
20	A	1049	A
20	A	1052	U
20	A	1053	A
20	A	1057	G
20	A	1062	G
20	A	1066	A
20	A	1070	G
20	A	1073	U
20	A	1075	U
20	A	1086	A
20	A	1087	G
20	A	1088	A
20	A	1092	C
20	A	1093	U
20	A	1149	C
20	A	1150	G
20	A	1151	A
20	A	1152	G
20	A	1167	A
20	A	1168	A
20	A	1170	U
20	A	1172	U
20	A	1173	A
20	A	1174	C
20	A	1175	C
20	A	1179	G
20	A	1182	A
20	A	1188	A
20	A	1209	A
20	A	1210	C
20	A	1212	A
20	A	1215	A
20	A	1217	G
20	A	1224	G
20	A	1257	A
20	A	1275	G
20	A	1284	A
20	A	1285	G
20	A	1287	G
20	A	1290	A
20	A	1293	G

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Mol	Chain	Res	Type
20	A	1299	A
20	A	1305	A
20	A	1308	G
20	A	1309	A
20	A	1310	A
20	A	1317	G
20	A	1320	A
20	A	1336	U
20	A	1337	A
20	A	1350	C
20	A	1365	U
20	A	1373	G
20	A	1380	U
20	A	1388	U
20	A	1397	G
20	A	1398	C
20	A	1399	C
20	A	1401	A
20	A	1404	G
20	A	1406	C
20	A	1409	A
20	A	1411	G
20	A	1415	U
20	A	1420	A
20	A	1428	G
20	A	1429	A
20	A	1431	A
20	A	1432	U
20	A	1446	G
20	A	1447	U
20	A	1452	G
20	A	1453	U
20	A	1454	U
20	A	1455	U
20	A	1456	G
20	A	1457	A
20	A	1460	A
20	A	1461	A
20	A	1462	U
20	A	1469	A
20	A	1470	C
20	A	1471	G

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Mol	Chain	Res	Type
20	A	1475	U
20	A	1487	U
20	A	1489	C
20	A	1491	U
20	A	1492	G
20	A	1493	C
20	A	1494	G
20	A	1495	A
20	A	1497	U
20	A	1501	A
20	A	1502	G
20	A	1503	U
20	A	1504	G
20	A	1505	C
20	A	1510	C
20	A	1519	G
20	A	1521	G
20	A	1525	U
20	A	1527	A
20	A	1528	G
20	A	1532	A
20	A	1535	U
20	A	1536	A
20	A	1539	U
20	A	1548	C
20	A	1551	U
20	A	1552	A
20	A	1559	A
20	A	1560	G
20	A	1567	C
20	A	1568	G
20	A	1573	G
20	A	1577	A
20	A	1578	A
20	A	1584	G
20	A	1585	U
20	A	1586	A
20	A	1591	A
20	A	1593	U
20	A	1601	G
20	A	1605	C
20	A	1606	A

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Mol	Chain	Res	Type
20	A	1612	A
20	A	1615	A
20	A	1624	U
20	A	1629	A
20	A	1630	G
20	A	1631	A
20	A	1632	A
20	A	1634	A
20	A	1635	C
20	A	1637	A
20	A	1638	C
20	A	1651	A
20	A	1653	A
20	A	1674	G
20	A	1686	G
20	A	1689	A
20	A	1690	G
20	A	1691	C
20	A	1717	G
20	A	1730	G
20	A	1734	C
20	A	1746	G
20	A	1756	U
20	A	1757	U
20	A	1758	C
20	A	1759	G
20	A	1762	C
20	A	1770	G
20	A	1777	G
20	A	1778	G
20	A	1787	A
20	A	1790	G
20	A	1796	C
20	A	1798	A
20	A	1814	C
20	A	1815	A
20	A	1824	A
20	A	1826	A
20	A	1830	A
20	A	1837	G
20	A	1843	A
20	A	1853	G

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Mol	Chain	Res	Type
20	A	1856	G
20	A	1861	A
20	A	1862	A
20	A	1864	G
20	A	1874	U
20	A	1876	G
20	A	1877	G
20	A	1884	U
20	A	1886	G
20	A	1887	G
20	A	1890	A
20	A	1894	U
20	A	1896	A
20	A	1910	A
20	A	1920	G
20	A	1927	A
20	A	1928	C
20	A	1930	A
20	A	1934	C
20	A	1936	G
20	A	1943	G
20	A	1944	G
20	A	1950	A
20	A	1969	U
20	A	1970	U
20	A	1977	C
20	A	1981	C
20	A	1984	A
20	A	1985	A
20	A	1986	G
20	A	1996	U
20	A	2001	G
20	A	2005	U
20	A	2007	U
20	A	2035	G
20	A	2037	A
20	A	2044	A
20	A	2045	A
20	A	2046	G
20	A	2047	A
20	A	2050	C
20	A	2057	C

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Mol	Chain	Res	Type
20	A	2065	A
20	A	2069	C
20	A	2070	G
20	A	2074	A
20	A	2075	G
20	A	2076	A
20	A	2080	C
20	A	2083	G
20	A	2107	G
20	A	2109	G
20	A	2112	U
20	A	2113	U
20	A	2208	C
20	A	2211	U
20	A	2212	A
20	A	2213	A
20	A	2216	C
20	A	2217	G
20	A	2218	C
20	A	2238	G
20	A	2239	A
20	A	2252	G
20	A	2253	G
20	A	2267	G
20	A	2277	C
20	A	2283	A
20	A	2293	G
20	A	2296	G
20	A	2297	C
20	A	2301	A
20	A	2302	A
20	A	2303	G
20	A	2317	G
20	A	2319	U
20	A	2323	A
20	A	2331	C
20	A	2333	A
20	A	2334	A
20	A	2335	G
20	A	2336	A
20	A	2339	G
20	A	2340	U

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Mol	Chain	Res	Type
20	A	2343	A
20	A	2348	G
20	A	2349	A
20	A	2361	C
20	A	2364	C
20	A	2393	G
20	A	2397	G
20	A	2399	C
20	A	2402	A
20	A	2404	U
20	A	2405	G
20	A	2416	U
20	A	2417	C
20	A	2418	C
20	A	2420	C
20	A	2436	C
20	A	2437	U
20	A	2439	A
20	A	2443	G
20	A	2445	U
20	A	2449	A
20	A	2455	C
20	A	2462	A
20	A	2473	A
20	A	2488	C
20	A	2492	A
20	A	2505	U
20	A	2512	C
20	A	2517	A
20	A	2518	U
20	A	2519	G
20	A	2521	C
20	A	2522	G
20	A	2532	A
20	A	2534	C
20	A	2542	U
20	A	2543	G
20	A	2548	C
20	A	2570	C
20	A	2580	A
20	A	2581	G
20	A	2587	C

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Mol	Chain	Res	Type
20	A	2597	G
20	A	2599	U
20	A	2600	C
20	A	2616	A
20	A	2624	C
20	A	2627	U
20	A	2629	U
20	A	2650	U
20	A	2677	G
20	A	2699	G
20	A	2703	U
20	A	2719	A
20	A	2728	G
20	A	2740	U
20	A	2747	A
20	A	2749	G
20	A	2758	G
20	A	2762	A
20	A	2766	C
20	A	2773	G
20	A	2779	A
20	A	2780	G
20	A	2789	A
20	A	2792	A
20	A	2793	U
20	A	2794	G
20	A	2795	A
20	A	2804	A
20	A	2805	U
20	A	2809	U
20	A	2810	U
20	A	2812	A
20	A	2813	A
20	A	2815	A
20	A	2831	G
20	A	2836	G
20	A	2844	A
20	A	2846	A
20	A	2847	U
20	A	2870	G
20	A	2871	A
20	A	2878	G

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Mol	Chain	Res	Type
20	A	2883	G
20	A	2891	C
20	A	2897	G
20	A	2904	G
21	B	7	G
21	B	10	G
21	B	11	A
21	B	13	A
21	B	20	A
21	B	23	A
21	B	24	U
21	B	27	A
21	B	33	U
21	B	35	C
21	B	54	U
21	B	55	A
21	B	57	G
21	B	67	G
21	B	70	G
21	B	73	U
21	B	74	G
21	B	75	U
21	B	78	U
21	B	79	G
21	B	83	G
21	B	85	U
21	B	86	U
21	B	87	U
21	B	91	U
21	B	97	A
21	B	98	G
21	B	99	A
21	B	101	U
21	B	106	C
21	B	107	G
21	B	114	C

All (31) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
20	A	13	U
20	A	29	A

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Mol	Chain	Res	Type
20	A	179	A
20	A	427	A
20	A	519	A
20	A	545	G
20	A	655	G
20	A	725	A
20	A	890	A
20	A	947	G
20	A	949	U
20	A	974	A
20	A	1022	C
20	A	1167	A
20	A	1431	A
20	A	1486	A
20	A	1584	G
20	A	1585	U
20	A	1590	A
20	A	1600	C
20	A	1604	A
20	A	1605	C
20	A	1861	A
20	A	2419	G
20	A	2444	A
20	A	2532	A
20	A	2811	U
20	A	2812	A
21	B	32	U
21	B	90	C
21	B	97	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
29	M	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	60:ARG	C	61:LEU	N	1.18

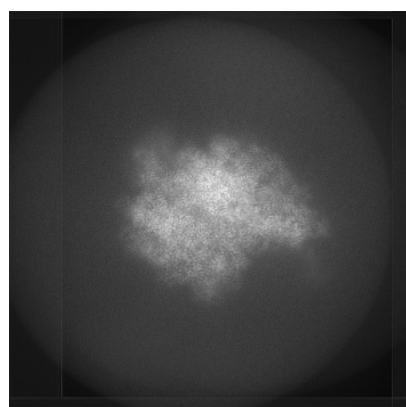
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21562. These allow visual inspection of the internal detail of the map and identification of artifacts.

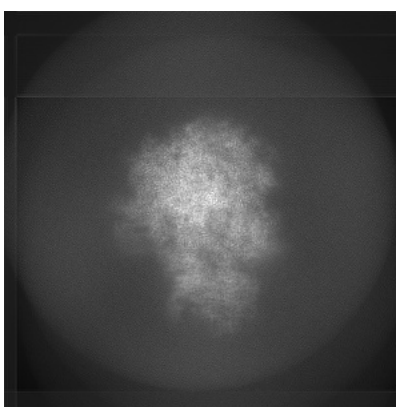
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

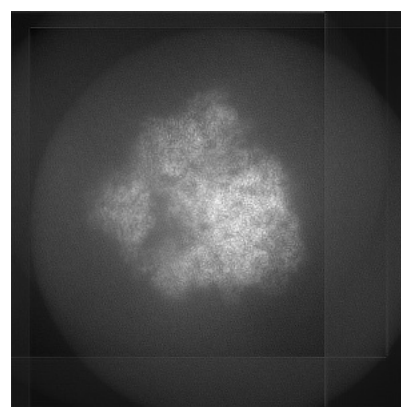
6.1.1 Primary map



X



Y

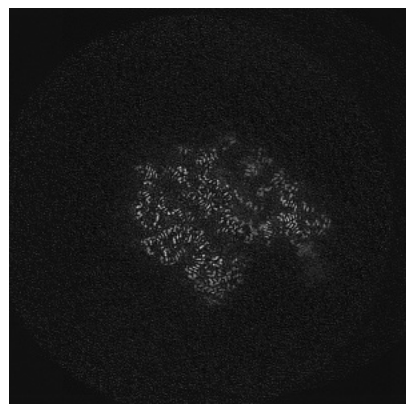


Z

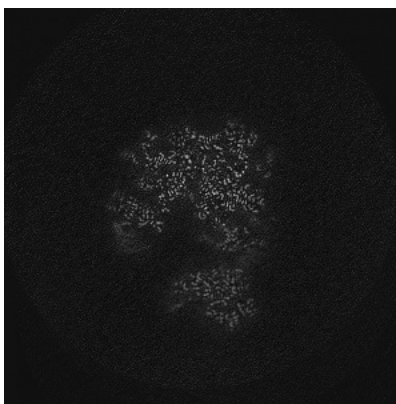
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

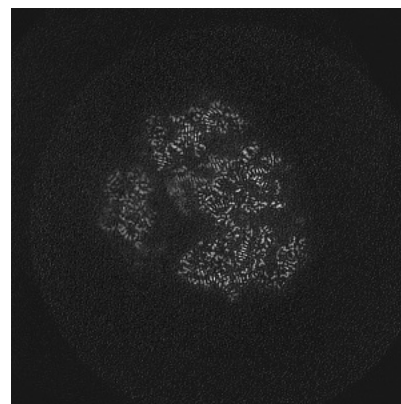
6.2.1 Primary map



X Index: 220



Y Index: 220

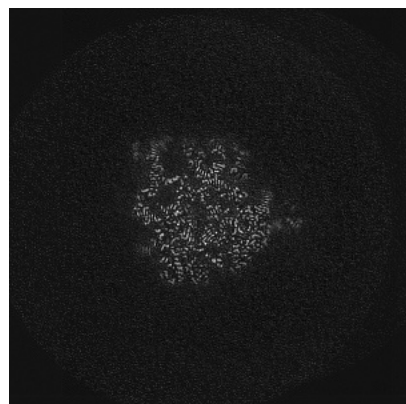


Z Index: 220

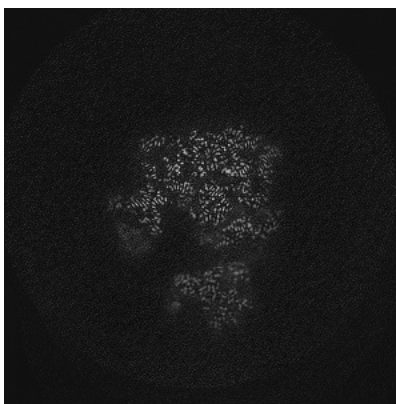
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

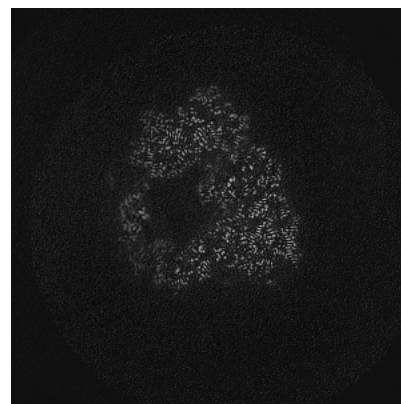
6.3.1 Primary map



X Index: 258



Y Index: 228

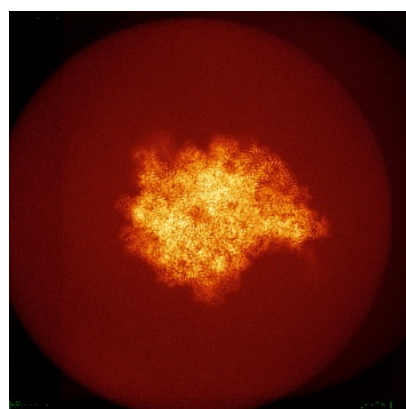


Z Index: 205

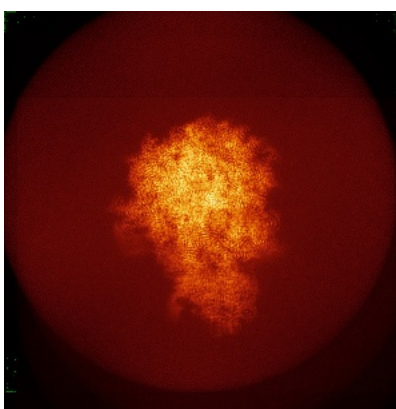
The images above show the largest variance slices of the map in three orthogonal directions.

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

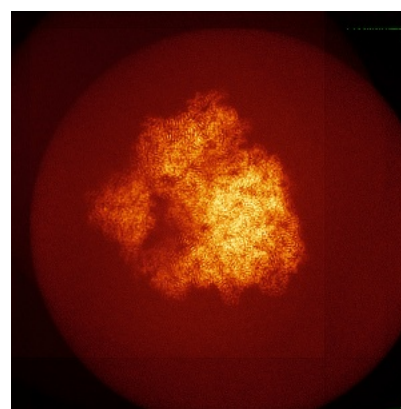
6.4.1 Primary map



X



Y

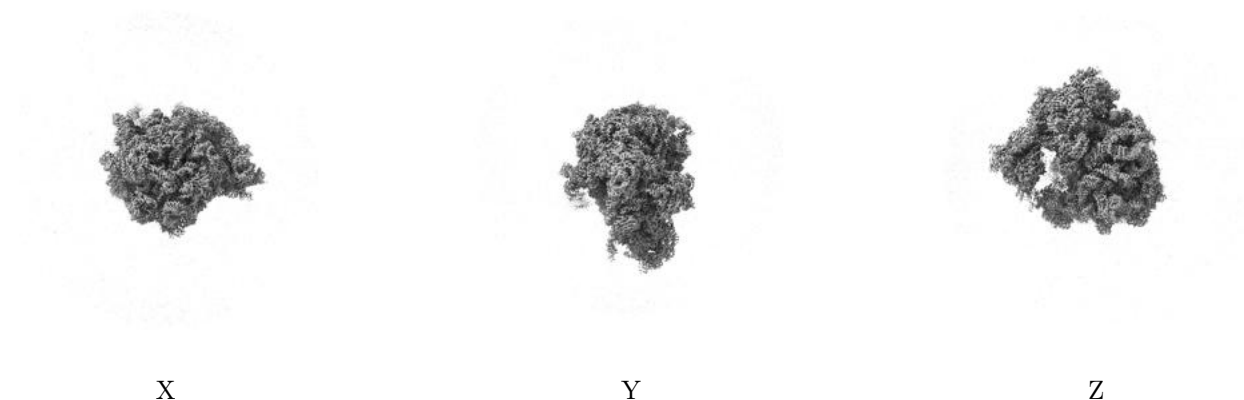


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

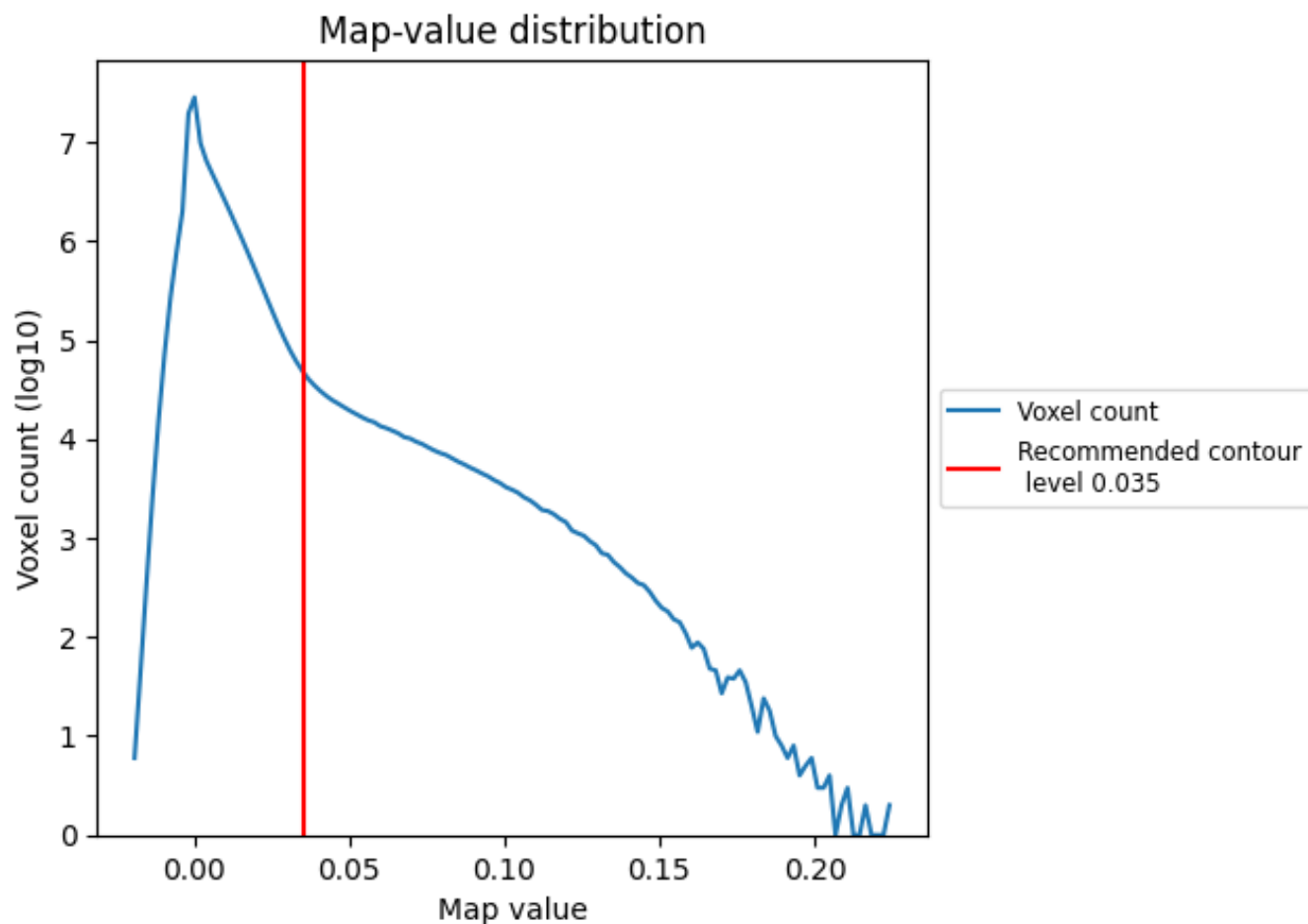
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

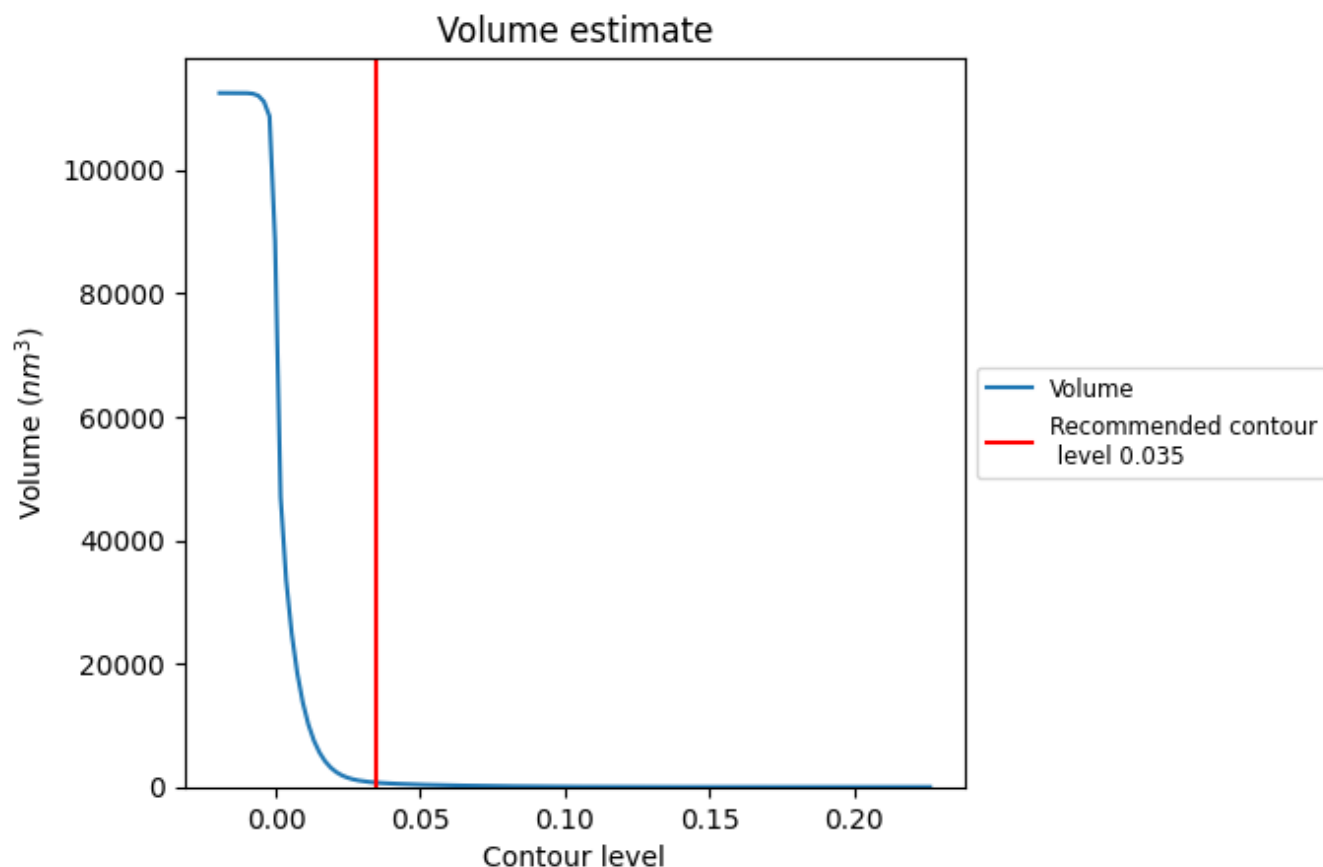
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

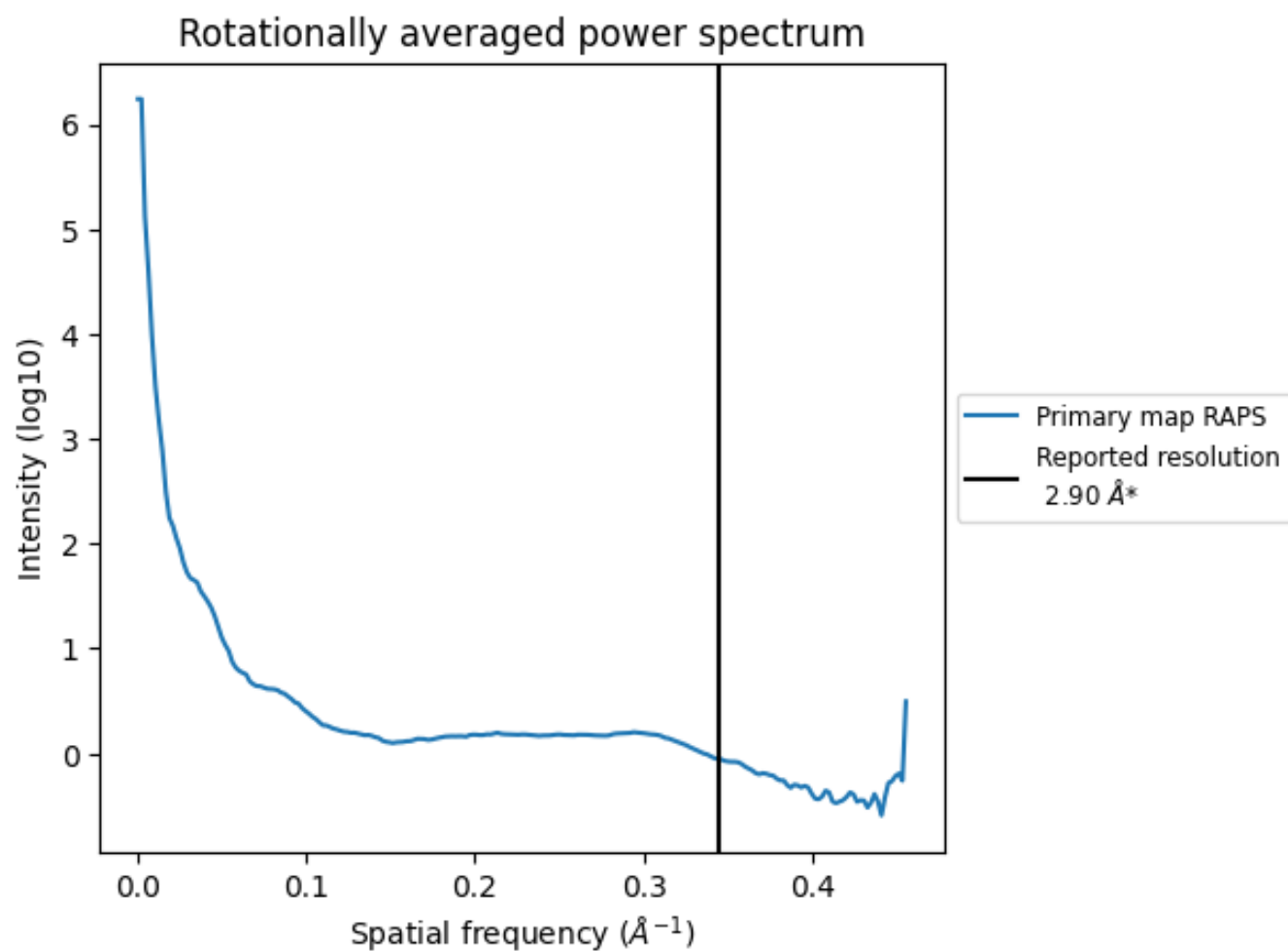
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 697 nm^3 ; this corresponds to an approximate mass of 629 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

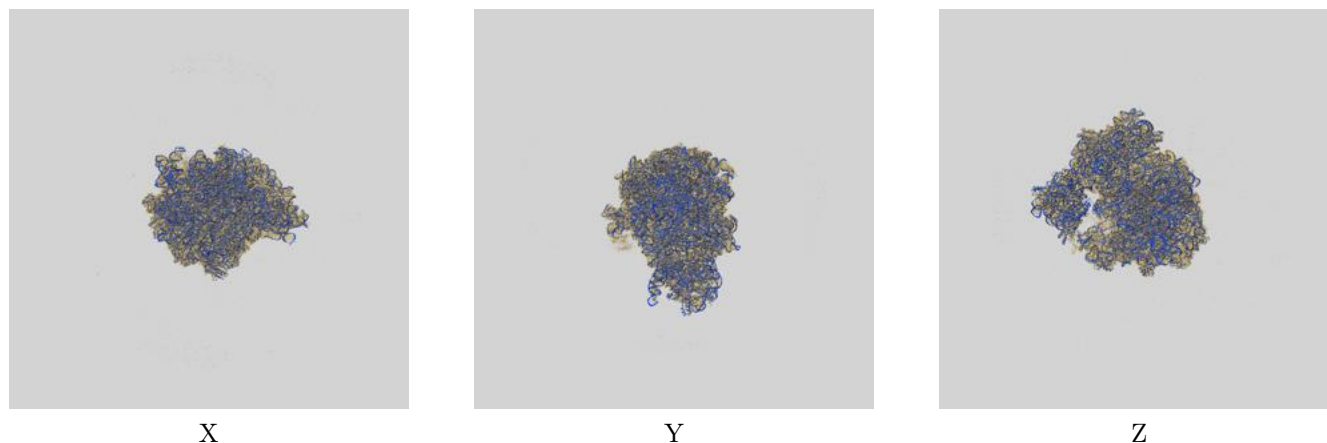
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

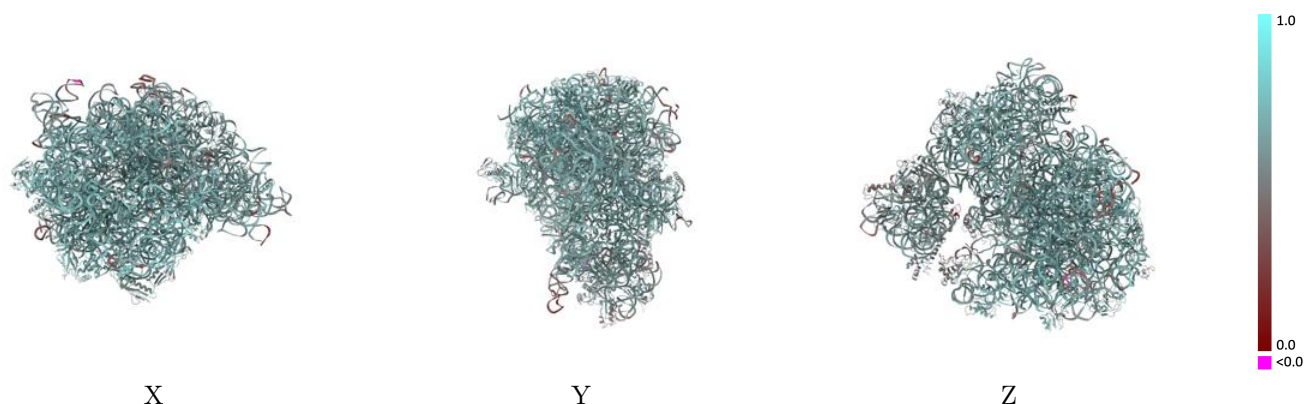
This section contains information regarding the fit between EMDB map EMD-21562 and PDB model 6W6P. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



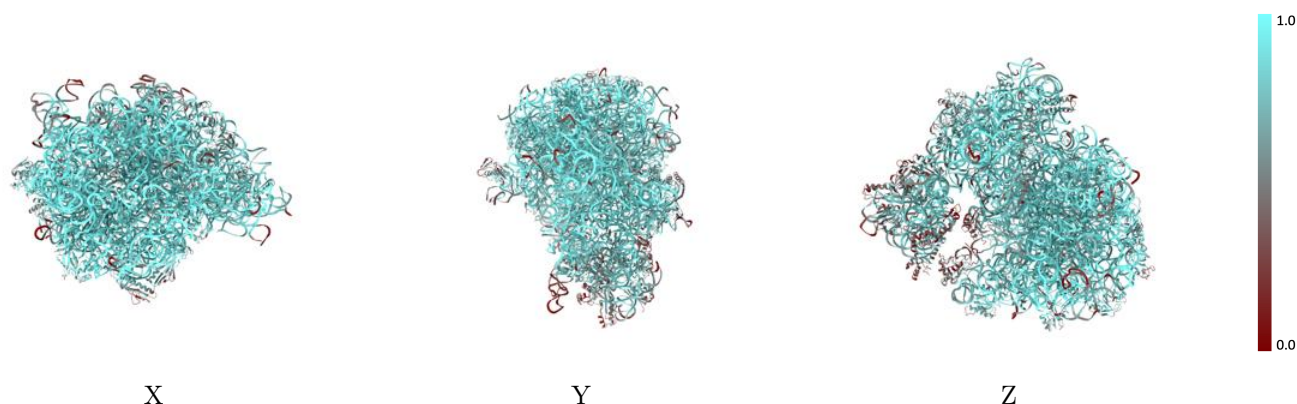
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



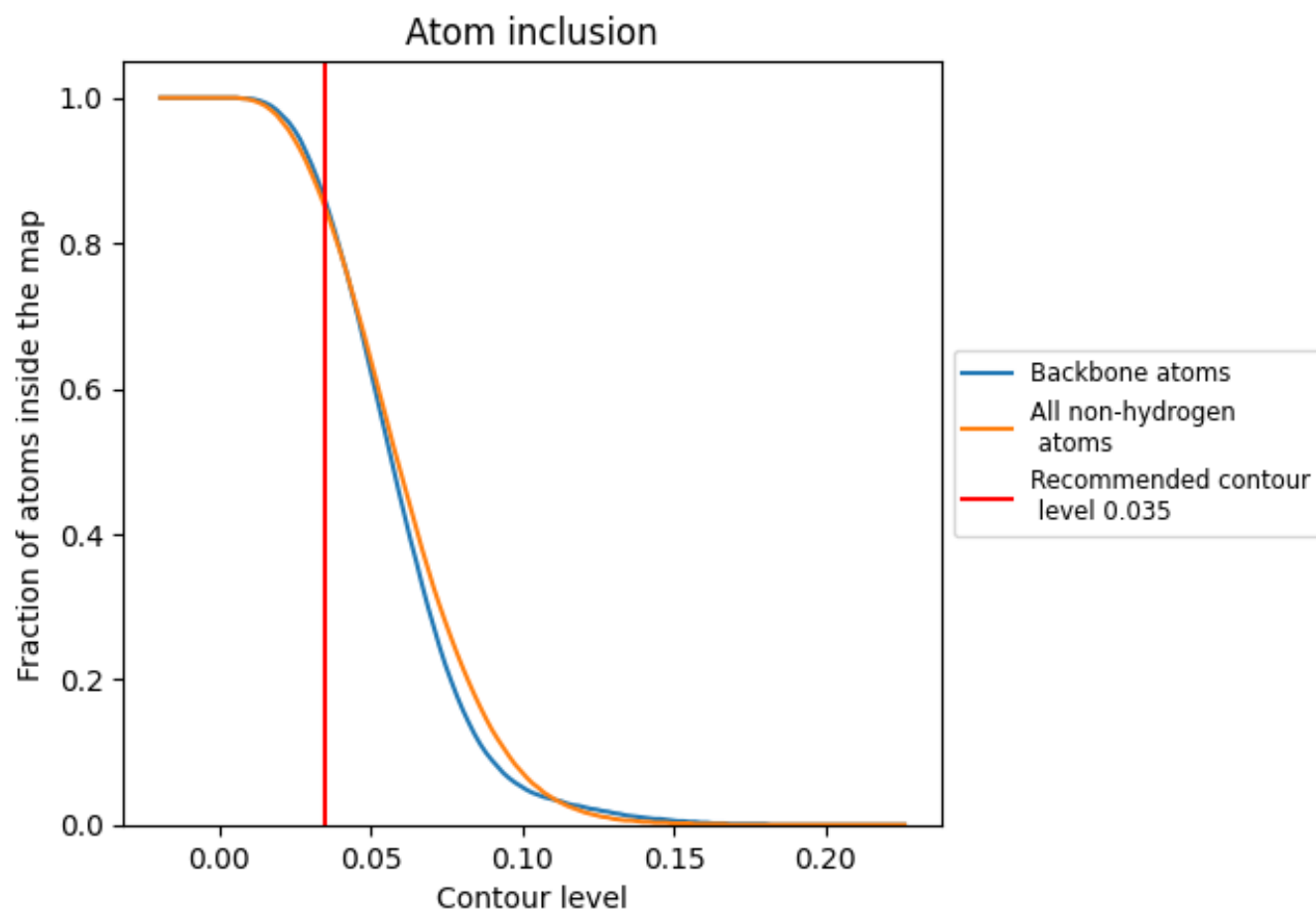
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.035).

9.4 Atom inclusion ⓘ



At the recommended contour level, 86% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8490	 0.6270
0	 0.8300	 0.6450
2	 0.8980	 0.6810
3	 0.7400	 0.6580
4	 0.9570	 0.7020
5	 0.9360	 0.6980
6	 0.9220	 0.6660
A	 0.9220	 0.6510
B	 0.8040	 0.5900
C	 0.9160	 0.6770
D	 0.9010	 0.6830
E	 0.8460	 0.6580
F	 0.3600	 0.4980
G	 0.5630	 0.5650
K	 0.9060	 0.6680
L	 0.8810	 0.6610
M	 0.8050	 0.6510
N	 0.7920	 0.6310
O	 0.8680	 0.6490
P	 0.7200	 0.6140
Q	 0.8730	 0.6590
R	 0.9240	 0.6850
S	 0.8120	 0.6500
T	 0.8780	 0.6690
U	 0.8260	 0.6440
V	 0.6280	 0.5900
X	 0.9100	 0.6840
Y	 0.7650	 0.6380
Z	 0.7110	 0.6210
a	 0.8680	 0.6050
c	 0.5060	 0.5560
d	 0.6650	 0.5800
e	 0.6690	 0.5920
f	 0.5440	 0.5670
g	 0.3160	 0.5080



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Chain	Atom inclusion	Q-score
h	 0.7450	 0.6190
i	 0.5730	 0.5630
j	 0.5120	 0.5310
k	 0.4870	 0.5420
l	 0.7490	 0.5950
m	 0.4850	 0.5230
n	 0.7920	 0.6020
o	 0.7140	 0.5900
p	 0.8050	 0.6280
q	 0.6860	 0.6100
r	 0.6710	 0.5980
s	 0.6560	 0.5550
t	 0.7440	 0.6140