Full wwPDB EM Validation Report ⓘ

Dec 11, 2022 – 01:49 am GMT

PDB ID	:	4V19
EMDB ID	:	EMD-2787
Title	:	Structure of the large subunit of the mammalian mitoribosome, part 1 of 2
Authors	:	Greber, B.J.; Boehringer, D.; Leibundgut, M.; Bieri, P.; Leitner, A.; Schmitz, N.; Aebersold, R.; Ban, N.
Deposited on	:	2014-09-25
Resolution	:	3.40 Å(reported)

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

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

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

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

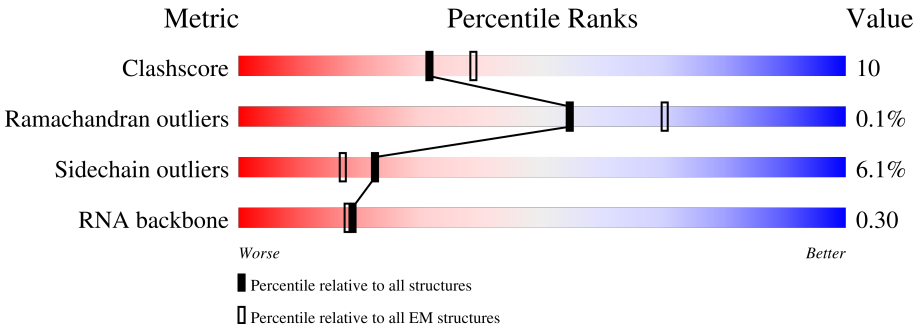
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance

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

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	0	148	56% 20% • 23%
2	1	256	7% 73% 21% • 5%
3	2	252	58% 13% 29%
4	3	161	57% 16% • 27%
5	4	126	13% 21% 14% 64%
6	5	188	43% 15% 41%
7	6	65	72% 35% 35% • 26%

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Mol	Chain	Length	Quality of chain
8	7	95	36% 9% 52%
9	8	188	36% 12% 49%
10	9	100	24% 13% 62%
11	A	1570	38% 37% 20%
12	B	62	31% 11% 39% 50%
13	C	3	33% 33% 33%
13	Z	3	33% 100%
14	D	306	52% 25% 22%
15	E	348	64% 22% 12%
16	F	294	59% 25% 15%
17	I	268	10% 25% 12% 63%
18	J	262	29% 40% 24% 36%
19	K	192	60% 48% 23% 26%
20	N	178	81% 17%
21	O	145	54% 23% 21%
22	P	296	67% 29%
23	Q	251	72% 14% 12%
24	R	169	63% 25% 9%
25	S	180	50% 28% 21%
26	T	292	5% 55% 21% 23%
27	U	149	5% 67% 25% 6%
28	V	209	52% 20% 26%
29	W	210	63% 14% 21%
30	X	150	10% 61% 25% 11%
31	Y	216	36% 66% 25% 6%

2 Entry composition (i)

There are 34 unique types of molecules in this entry. The entry contains 69409 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called MITORIBOSOMAL PROTEIN BL27M, MRPL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	114	878	564	160	151	3	0	0

- Molecule 2 is a protein called MITORIBOSOMAL PROTEIN BL28M, MRPL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	244	2036	1315	363	353	5	0	0

- Molecule 3 is a protein called MITORIBOSOMAL PROTEIN UL29M, MRPL47.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	178	1544	990	289	259	6	0	0

- Molecule 4 is a protein called MITORIBOSOMAL PROTEIN UL30M, MRPL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	118	968	622	178	165	3	0	0

- Molecule 5 is a protein called MITORIBOSOMAL PROTEIN BL31M, MRPL55.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	45	381	239	77	62	3	0	0

- Molecule 6 is a protein called MITORIBOSOMAL PROTEIN BL32M, MRPL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	5	110	902	553	181	162	6	0	0

- Molecule 7 is a protein called MITORIBOSOMAL PROTEIN BL33M, MRPL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	48	Total	C	N	O	S	0	0
			391	253	70	66	2		

- Molecule 8 is a protein called MITORIBOSOMAL PROTEIN BL34M, MRPL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	46	Total	C	N	O	S	0	0
			387	239	89	58	1		

- Molecule 9 is a protein called MITORIBOSOMAL PROTEIN BL35M, MRPL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	8	95	Total	C	N	O	S	0	0
			833	539	163	129	2		

- Molecule 10 is a protein called MITORIBOSOMAL PROTEIN BL36M, MRPL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	9	38	Total	C	N	O	S	0	0
			335	214	70	47	4		

- Molecule 11 is a RNA chain called MITORIBOSOMAL 16S RRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A	1515	Total	C	N	O	P	0	0
			32233	14473	5860	10385	1515		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	127A	G	-	insertion	GB 4220565

- Molecule 12 is a RNA chain called MITORIBOSOMAL CP TRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	B	62	Total	C	N	O	P	0	0
			1225	594	196	373	62		

- Molecule 13 is a RNA chain called TRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	C	3	Total	C	N	O	P	0	0
			62	28	11	20	3		
13	Z	3	Total	C	N	O	P	0	0
			62	28	11	20	3		

- Molecule 14 is a protein called MITORIBOSOMAL PROTEIN UL2M, MRPL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	D	240	Total	C	N	O	S	0	0
			1860	1160	371	319	10		

- Molecule 15 is a protein called MITORIBOSOMAL PROTEIN UL3M, MRPL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	E	307	Total	C	N	O	S	0	0
			2420	1554	426	430	10		

- Molecule 16 is a protein called MITORIBOSOMAL PROTEIN UL4M, MRPL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	F	250	Total	C	N	O	S	0	0
			2011	1294	367	344	6		

- Molecule 17 is a protein called MITORIBOSOMAL PROTEIN BL9M, MRPL9.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	I	98	Total	C	N	O	0	0
			805	509	155	141		

- Molecule 18 is a protein called MITORIBOSOMAL PROTEIN UL10M, MRPL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	J	168	Total	C	N	O	S	0	0
			1361	879	248	226	8		

- Molecule 19 is a protein called MITORIBOSOMAL PROTEIN UL11M, MRPL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	K	142	Total	C	N	O	S	0	0
			1081	690	197	192	2		

- Molecule 20 is a protein called MITORIBOSOMAL PROTEIN UL13M, MRPL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	177	Total	C	N	O	S	0	0
			1444	926	258	253	7		

- Molecule 21 is a protein called MITORIBOSOMAL PROTEIN UL14M, MRPL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O	115	Total	C	N	O	S	0	0
			896	562	176	154	4		

- Molecule 22 is a protein called MITORIBOSOMAL PROTEIN UL15M, MRPL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P	288	Total	C	N	O	S	0	0
			2312	1473	430	403	6		

- Molecule 23 is a protein called MITORIBOSOMAL PROTEIN UL16M, MRPL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Q	221	Total	C	N	O	S	0	0
			1792	1147	330	305	10		

- Molecule 24 is a protein called MITORIBOSOMAL PROTEIN BL17M, MRPL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R	153	Total	C	N	O	S	0	0
			1240	777	236	222	5		

- Molecule 25 is a protein called MITORIBOSOMAL PROTEIN UL18M, MRPL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	S	143	Total	C	N	O	S	0	0
			1168	733	227	204	4		

- Molecule 26 is a protein called MITORIBOSOMAL PROTEIN BL19M, MRPL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	T	224	Total	C	N	O	S	0	0
			1860	1189	324	338	9		

- Molecule 27 is a protein called MITORIBOSOMAL PROTEIN BL20M, MRPL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U	140	Total	C	N	O	S	0	0
			1159	732	239	185	3		

- Molecule 28 is a protein called MITORIBOSOMAL PROTEIN BL21M, MRPL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	V	155	Total	C	N	O	S	0	0
			1231	789	219	219	4		

- Molecule 29 is a protein called MITORIBOSOMAL PROTEIN UL22M, MRPL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	W	166	Total	C	N	O	S	0	0
			1374	876	258	234	6		

- Molecule 30 is a protein called MITORIBOSOMAL PROTEIN UL23M, MRPL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	X	134	Total	C	N	O	S	0	0
			1120	715	217	186	2		

- Molecule 31 is a protein called MITORIBOSOMAL PROTEIN UL24M, MRPL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Y	204	Total	C	N	O	S	0	0
			1663	1047	305	306	5		

- Molecule 32 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
32	5	1	Total	Zn	0
			1	1	
32	9	1	Total	Zn	0
			1	1	

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
33	A	163	Total	Mg	0
			163	163	
33	D	2	Total	Mg	0
			2	2	

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Mol	Chain	Residues	Atoms	AltConf
33	P	2	Total Mg 2 2	0
33	Q	1	Total Mg 1 1	0
33	R	1	Total Mg 1 1	0

- Molecule 34 is water.

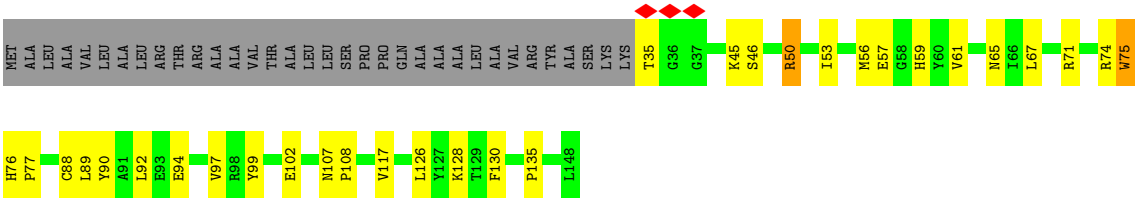
Mol	Chain	Residues	Atoms	AltConf
34	A	192	Total O 192 192	0
34	D	6	Total O 6 6	0
34	P	6	Total O 6 6	0

3 Residue-property plots (i)

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

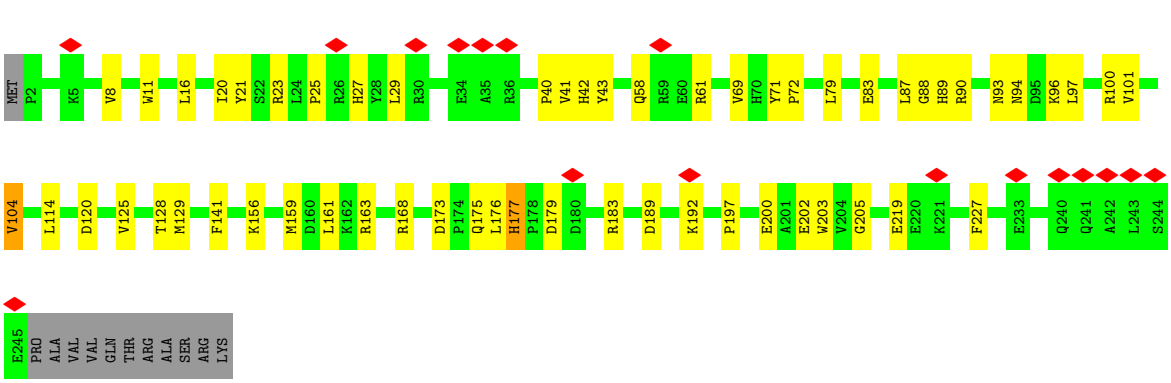
• Molecule 1: MITORIBOSOMAL PROTEIN BL27M, MRPL27

Chain 0:



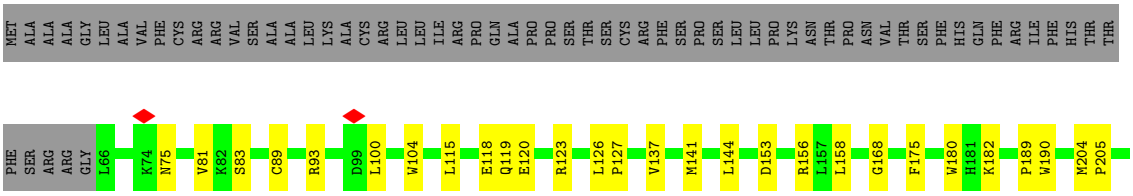
• Molecule 2: MITORIBOSOMAL PROTEIN BL28M, MRPL28

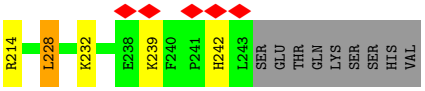
Chain 1:



• Molecule 3: MITORIBOSOMAL PROTEIN UL29M, MRPL47

Chain 2:



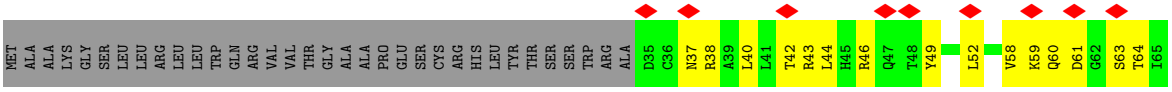


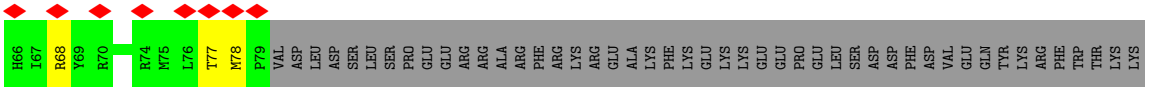
• Molecule 4: MITORIBOSOMAL PROTEIN UL30M, MRPL30

Chain 3:

• Molecule 5: MITORIBOSOMAL PROTEIN BL31M, MRPL55

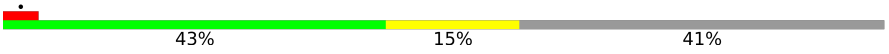
Chain 4:

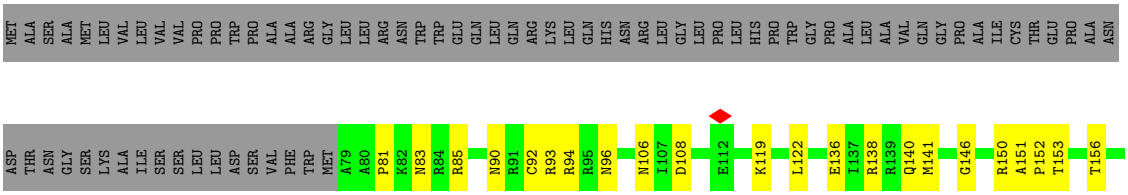


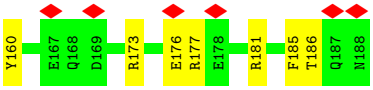


• Molecule 6: MITORIBOSOMAL PROTEIN BL32M, MRPL32

Chain 5:

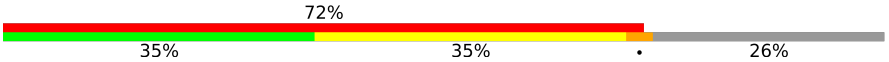


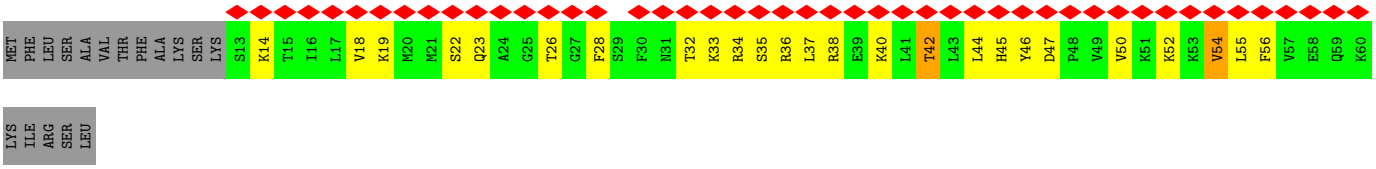




• Molecule 7: MITORIBOSOMAL PROTEIN BL33M, MRPL33

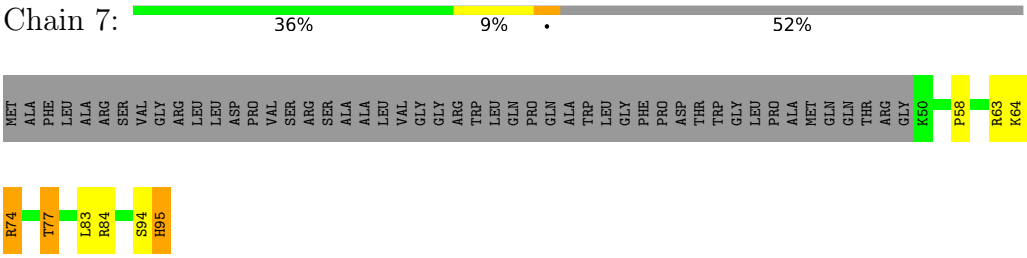
Chain 6:





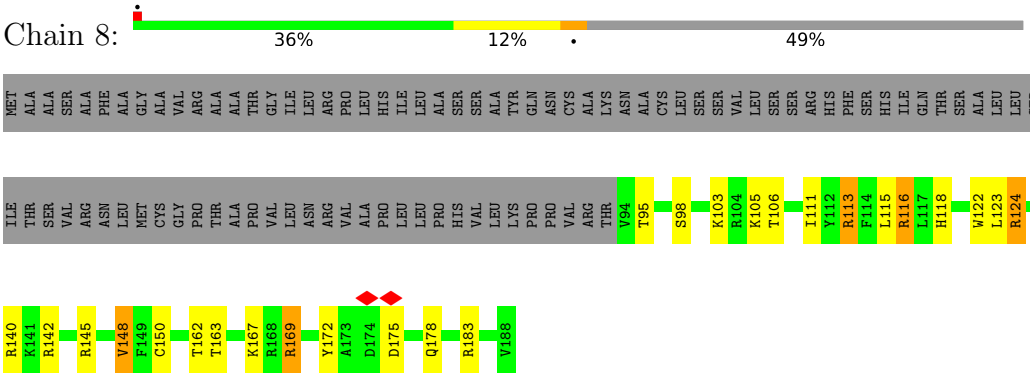
• Molecule 8: MITORIBOSOMAL PROTEIN BL34M, MRPL34

Chain 7:



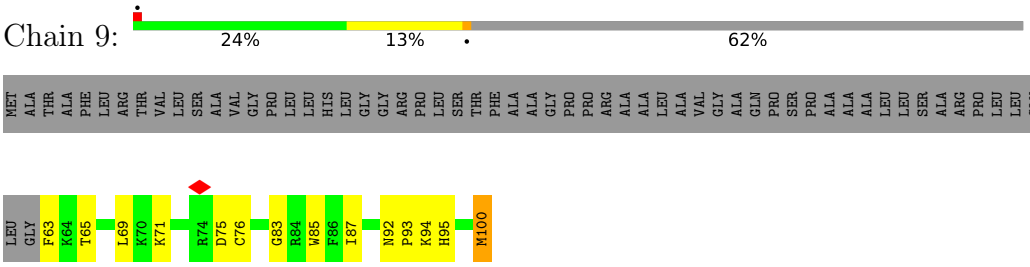
• Molecule 9: MITORIBOSOMAL PROTEIN BL35M, MRPL35

Chain 8:



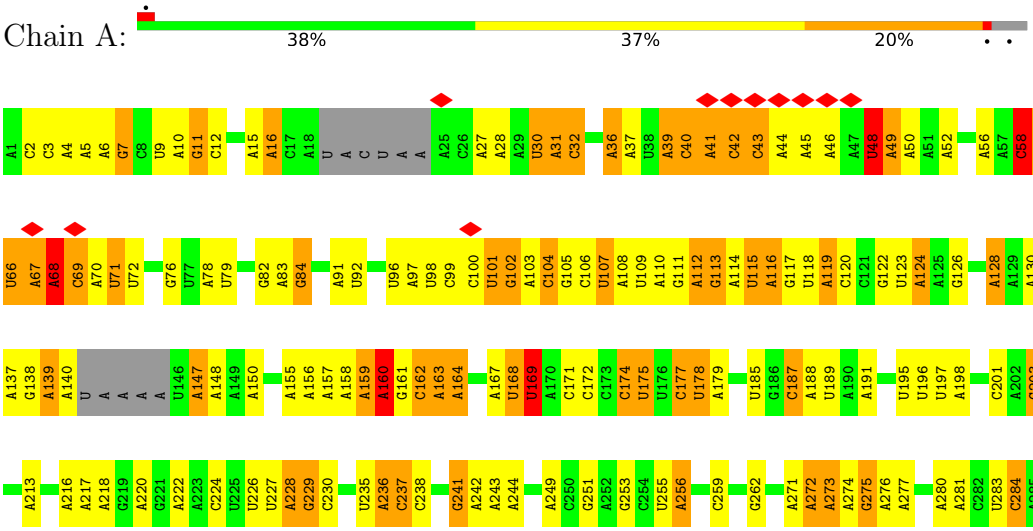
• Molecule 10: MITORIBOSOMAL PROTEIN BL36M, MRPL36

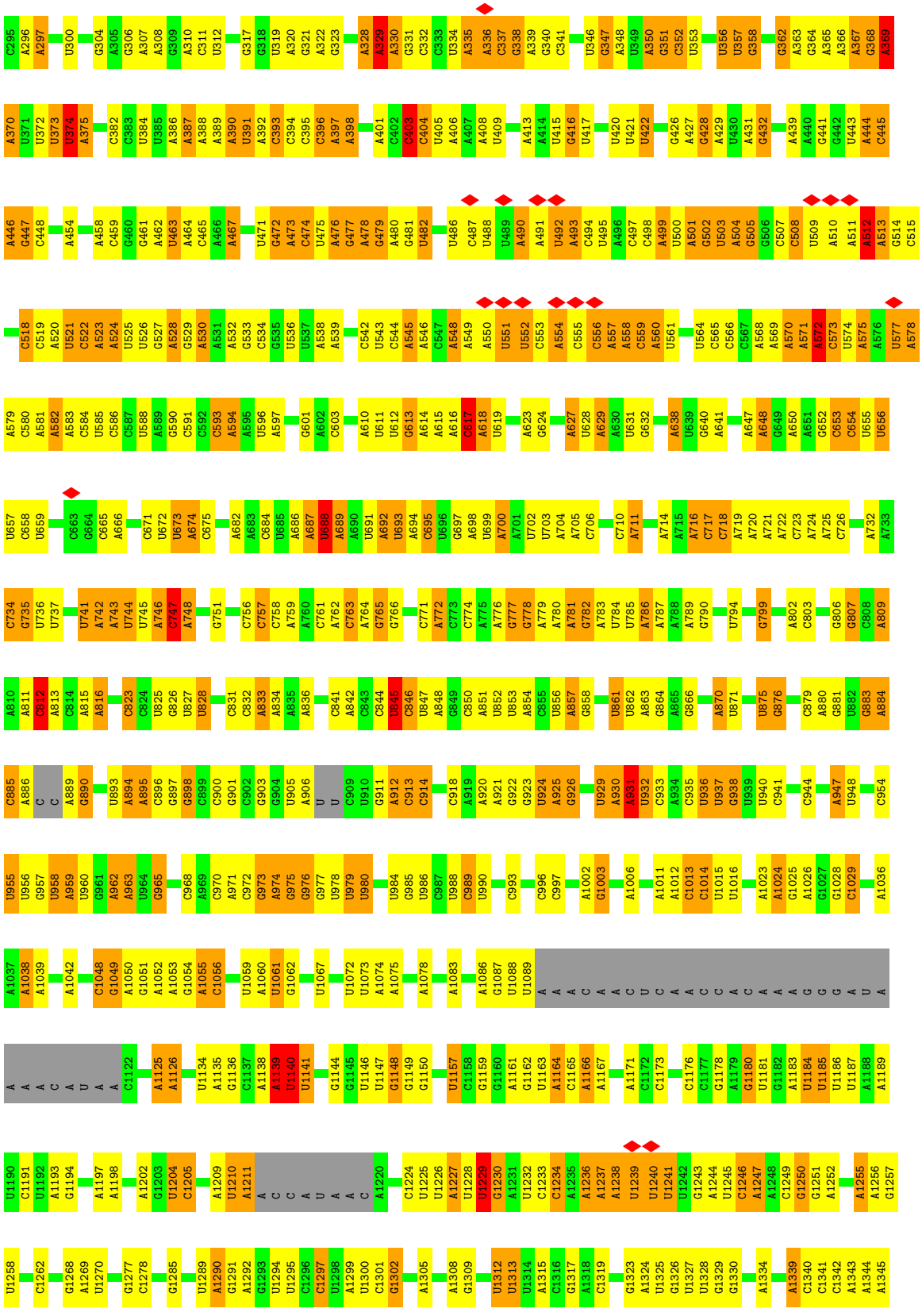
Chain 9:

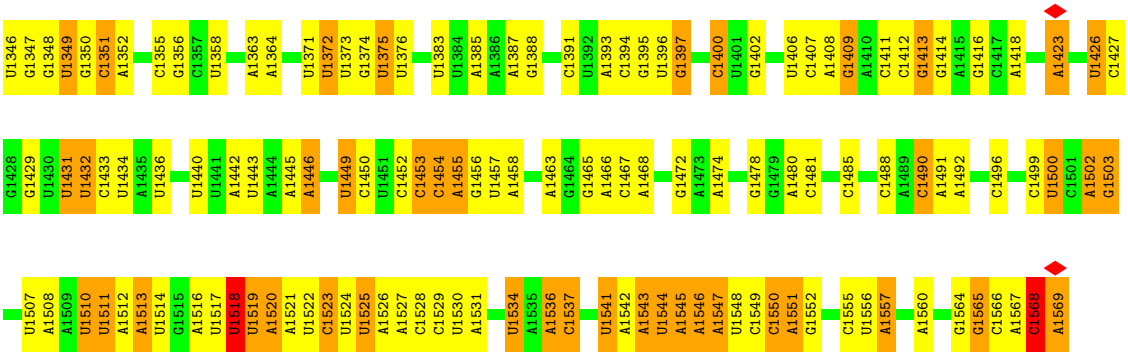


• Molecule 11: MITORIBOSOMAL 16S RRNA

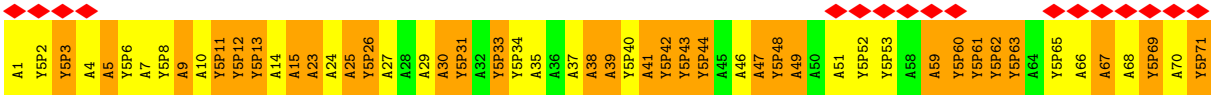
Chain A:



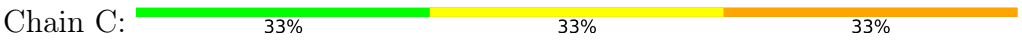




• Molecule 12: MITORIBOSOMAL CP TRNA

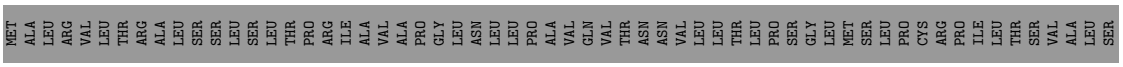


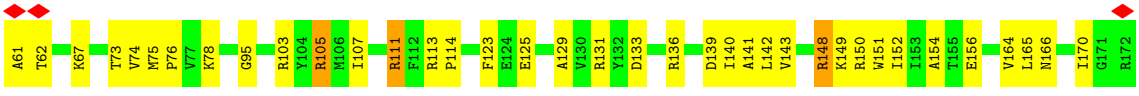
• Molecule 13: TRNA



• Molecule 13: TRNA

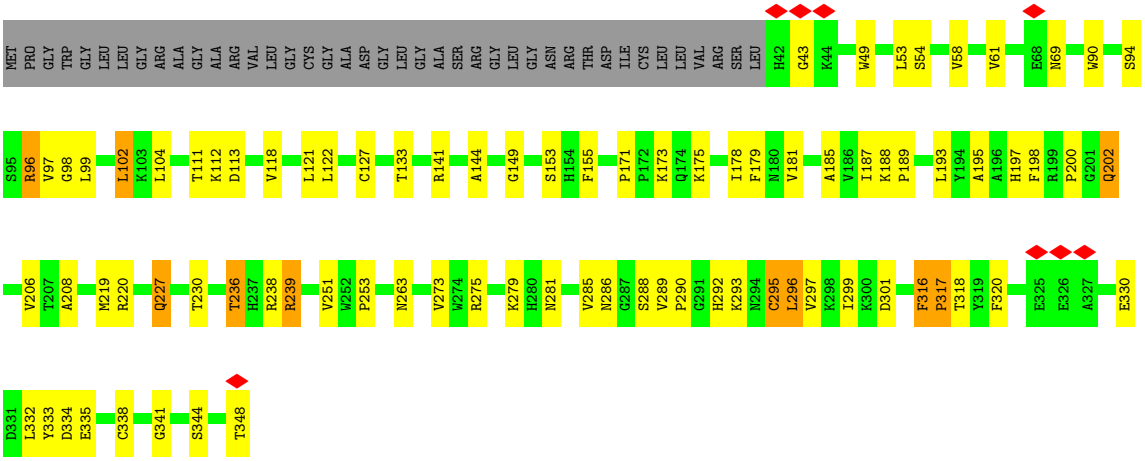
• Molecule 14: MITORIBOSOMAL PROTEIN UL2M, MRPL2





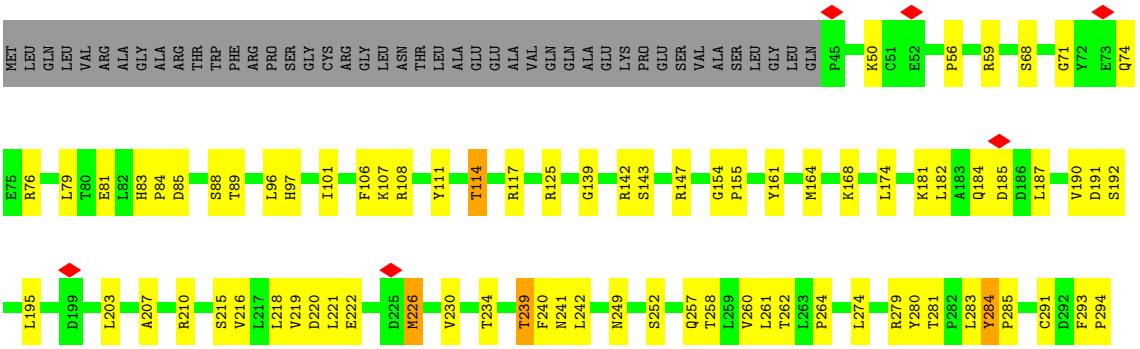
• Molecule 15: MITORIBOSOMAL PROTEIN UL3M, MRPL3

Chain E:



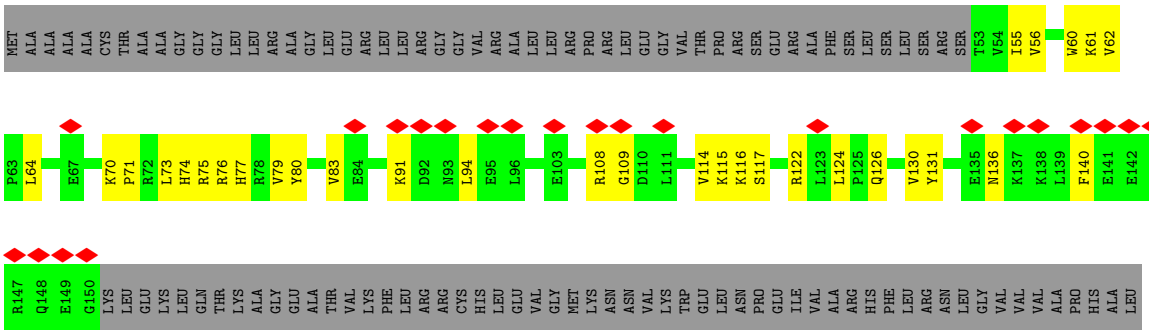
• Molecule 16: MITORIBOSOMAL PROTEIN UL4M, MRPL4

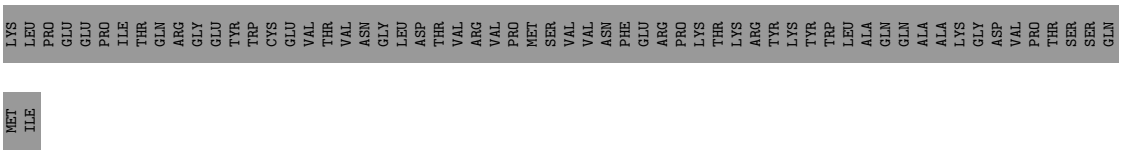
Chain F:



• Molecule 17: MITORIBOSOMAL PROTEIN BL9M, MRPL9

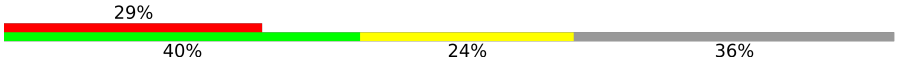
Chain I:

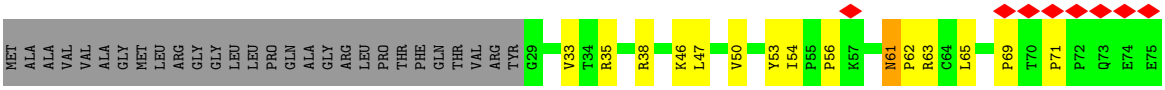


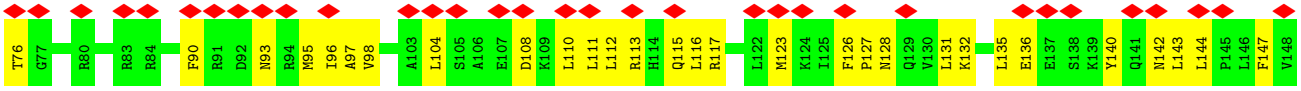


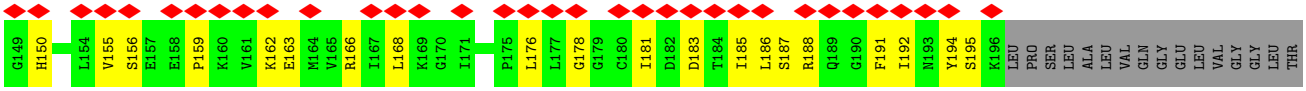
• Molecule 18: MITORIBOSOMAL PROTEIN UL10M, MRPL10

Chain J:



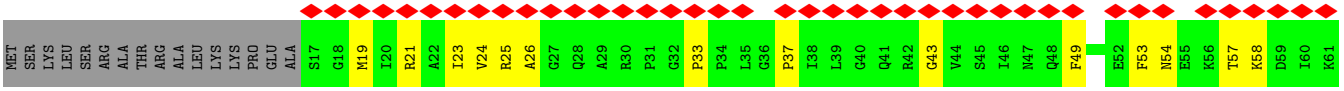


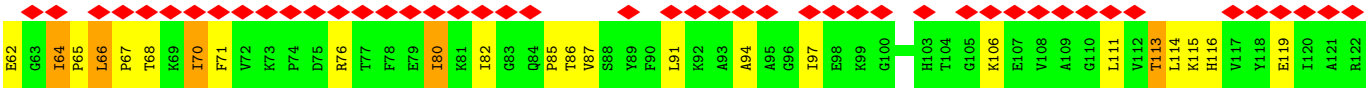


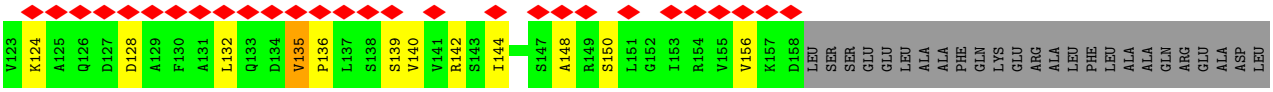


• Molecule 19: MITORIBOSOMAL PROTEIN UL11M, MRPL11

Chain K:

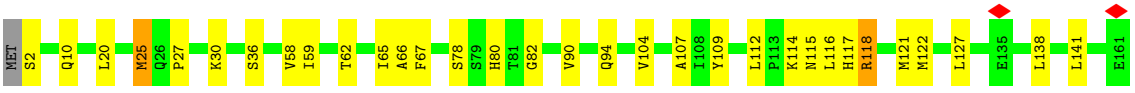






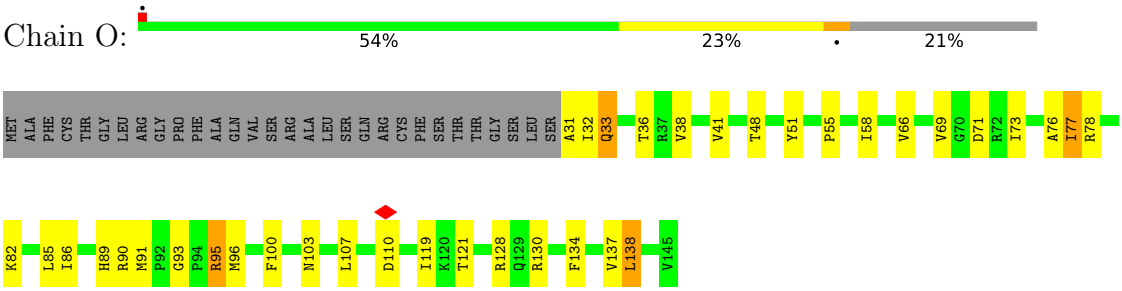
• Molecule 20: MITORIBOSOMAL PROTEIN UL13M, MRPL13

Chain N:



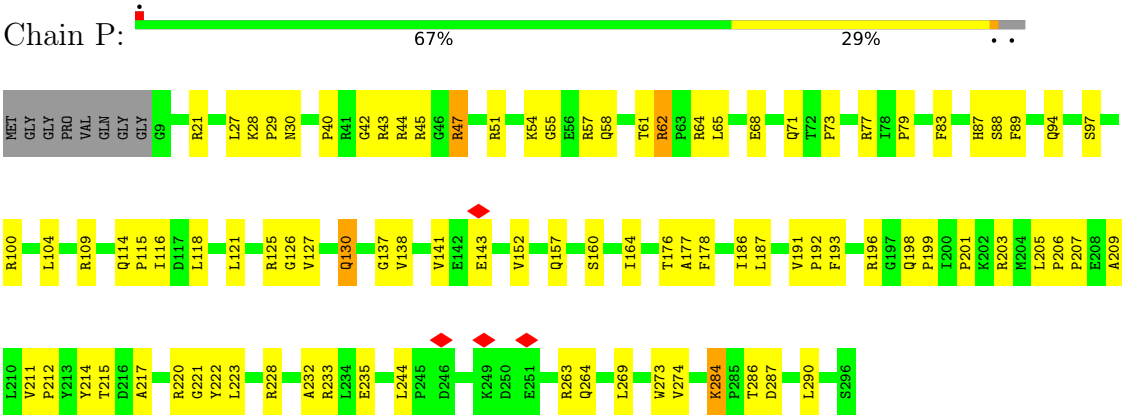
• Molecule 21: MITORIBOSOMAL PROTEIN UL14M, MRPL14

Chain O:



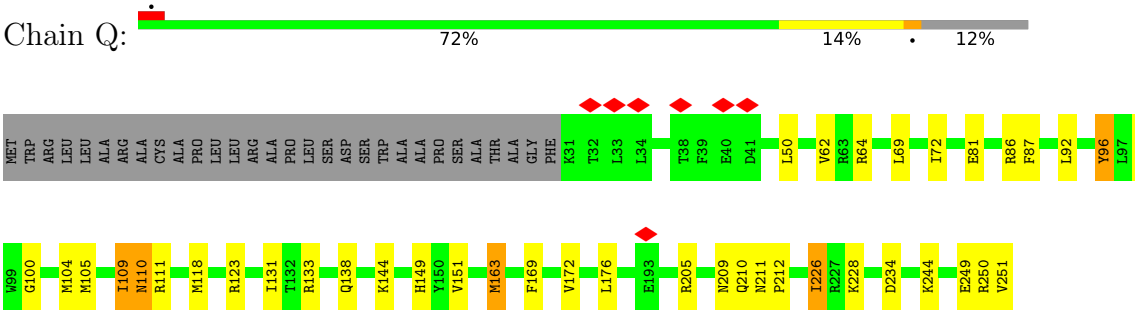
• Molecule 22: MITORIBOSOMAL PROTEIN UL15M, MRPL15

Chain P:



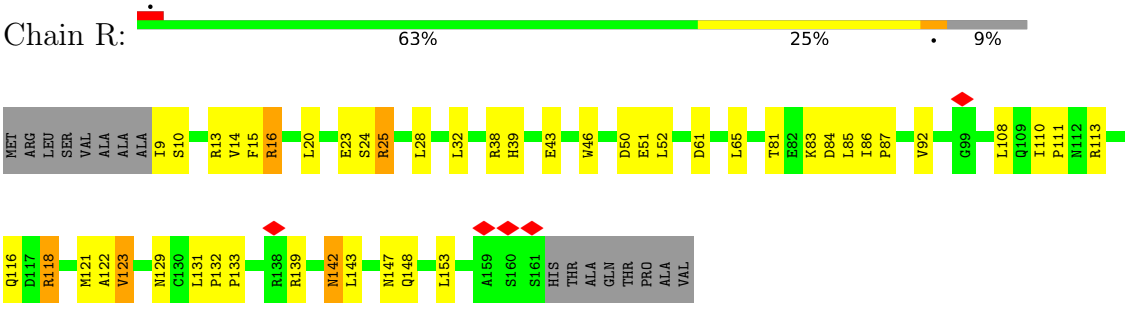
• Molecule 23: MITORIBOSOMAL PROTEIN UL16M, MRPL16

Chain Q:

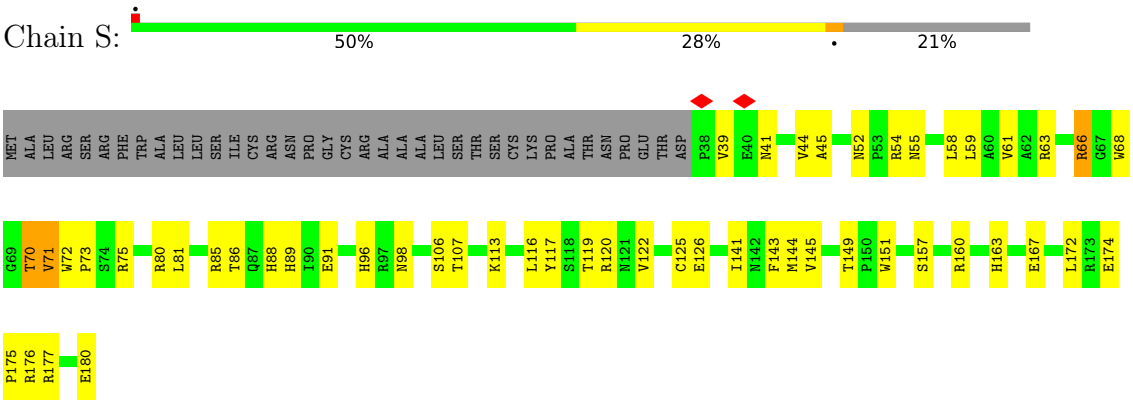


• Molecule 24: MITORIBOSOMAL PROTEIN BL17M, MRPL17

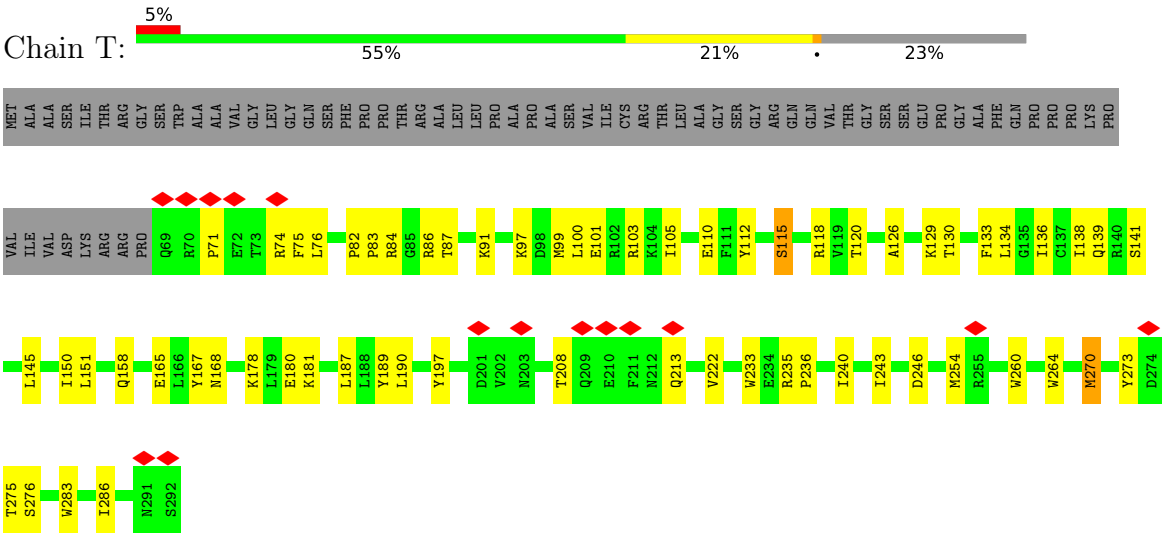
Chain R:



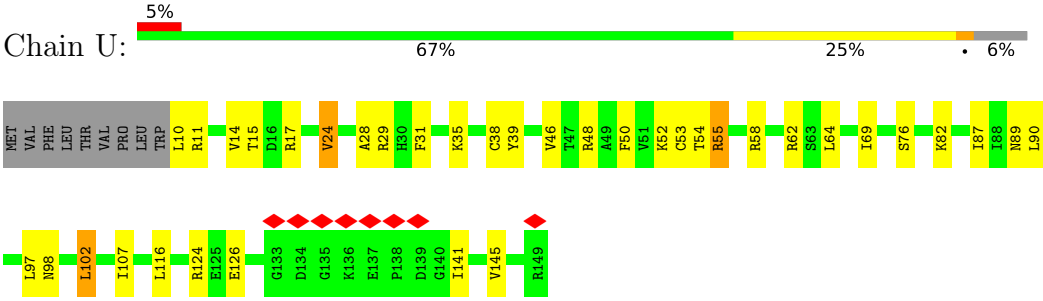
• Molecule 25: MITORIBOSOMAL PROTEIN UL18M, MRPL18



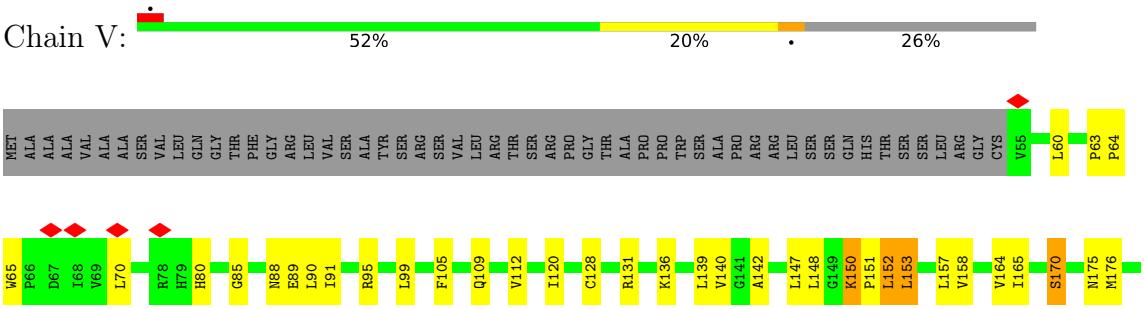
• Molecule 26: MITORIBOSOMAL PROTEIN BL19M, MRPL19

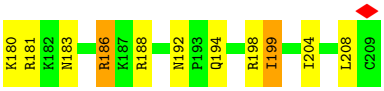


• Molecule 27: MITORIBOSOMAL PROTEIN BL20M, MRPL20



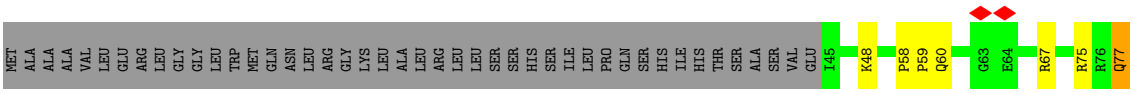
• Molecule 28: MITORIBOSOMAL PROTEIN BL21M, MRPL21





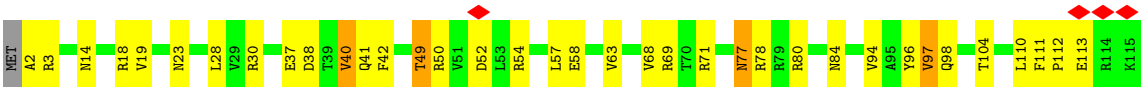
• Molecule 29: MITORIBOSOMAL PROTEIN UL22M, MRPL22

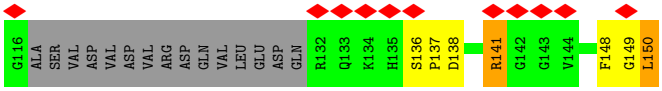
Chain W:



• Molecule 30: MITORIBOSOMAL PROTEIN UL23M, MRPL23

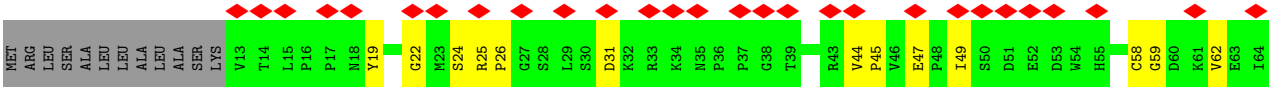
Chain X:

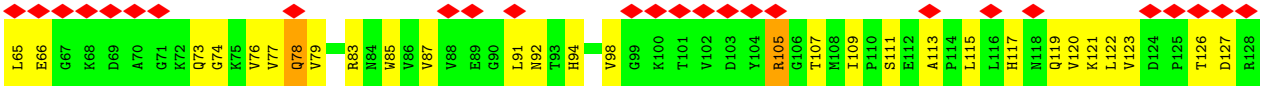


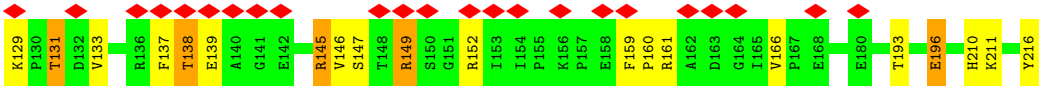


• Molecule 31: MITORIBOSOMAL PROTEIN UL24M, MRPL24

Chain Y:







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	141675	Depositor
Resolution determination method	Not provided	
CTF correction method	PER DETECTOR FRAME	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	100000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.560	Depositor
Minimum map value	-0.257	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	302.4, 302.4, 302.4	wwPDB
Map dimensions	216, 216, 216	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, P5P, ZN, Y5P

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	0	0.43	0/901	0.59	0/1217
2	1	0.35	0/2093	0.51	0/2835
3	2	0.36	0/1582	0.52	0/2118
4	3	0.41	0/993	0.59	0/1341
5	4	0.29	0/388	0.57	0/523
6	5	0.38	0/917	0.53	0/1227
7	6	0.35	0/396	0.54	0/526
8	7	0.45	0/395	0.55	0/524
9	8	0.48	0/853	0.60	0/1136
10	9	0.47	0/342	0.57	0/450
11	A	0.62	2/36094 (0.0%)	1.06	72/56186 (0.1%)
13	C	0.50	0/68	1.01	0/103
13	Z	0.32	0/68	0.86	0/103
14	D	0.38	0/1898	0.58	0/2555
15	E	0.38	0/2493	0.61	0/3387
16	F	0.42	0/2069	0.58	0/2816
17	I	0.35	0/819	0.52	0/1101
18	J	0.35	0/1392	0.55	0/1881
19	K	0.35	0/1099	0.49	0/1480
20	N	0.40	0/1487	0.57	0/2017
21	O	0.36	0/912	0.56	0/1231
22	P	0.40	0/2368	0.60	0/3198
23	Q	0.39	0/1838	0.57	0/2475
24	R	0.39	0/1262	0.57	0/1700
25	S	0.36	0/1197	0.55	0/1624
26	T	0.35	0/1903	0.54	0/2567
27	U	0.46	0/1179	0.61	0/1578
28	V	0.40	0/1256	0.58	0/1706
29	W	0.42	0/1407	0.57	0/1891
30	X	0.37	0/1149	0.59	0/1554
31	Y	0.35	0/1704	0.54	0/2310
All	All	0.52	2/72522 (0.0%)	0.87	72/105360 (0.1%)

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
15	E	0	2
28	V	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1255	A	N9-C4	-6.05	1.34	1.37
11	A	490	A	C8-N7	5.63	1.35	1.31

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	374	U	N1-C2-O2	8.42	128.70	122.80
11	A	374	U	N3-C2-O2	-8.24	116.43	122.20
11	A	48	U	N3-C2-O2	-7.50	116.95	122.20
11	A	593	C	C6-N1-C2	-7.38	117.35	120.30
11	A	1413	G	C4-N9-C1'	7.14	135.78	126.50
11	A	490	A	C2-N3-C4	7.01	114.11	110.60
11	A	353	U	O5'-P-OP1	-6.83	99.55	105.70
11	A	104	C	C2-N1-C1'	6.64	126.10	118.80
11	A	845	U	C5-C6-N1	6.43	125.92	122.70
11	A	559	C	N1-C2-O2	6.43	122.76	118.90
11	A	104	C	N1-C2-O2	6.42	122.75	118.90
11	A	1255	A	C5-N7-C8	-6.39	100.70	103.90
11	A	169	U	N3-C2-O2	-6.37	117.74	122.20
11	A	1433	C	C2-N1-C1'	6.35	125.79	118.80
11	A	237	C	O4'-C1'-N1	6.34	113.27	108.20
11	A	284	C	C6-N1-C2	-6.30	117.78	120.30
11	A	518	C	C2-N1-C1'	6.17	125.59	118.80
11	A	812	C	N1-C2-O2	6.15	122.59	118.90
11	A	572	A	C2-N3-C4	6.08	113.64	110.60
11	A	374	U	C2-N1-C1'	6.05	124.97	117.70
11	A	1205	C	C6-N1-C2	-6.03	117.89	120.30
11	A	60	U	N3-C2-O2	-6.01	117.99	122.20
11	A	160	A	P-O3'-C3'	6.00	126.91	119.70
11	A	931	A	P-O3'-C3'	5.97	126.86	119.70
11	A	512	A	P-O3'-C3'	5.91	126.79	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	1413	G	N3-C4-C5	-5.90	125.65	128.60
11	A	1433	C	C6-N1-C2	-5.88	117.95	120.30
11	A	329	A	C8-N9-C4	-5.85	103.46	105.80
11	A	474	C	C6-N1-C2	-5.85	117.96	120.30
11	A	369	A	C8-N9-C4	-5.82	103.47	105.80
11	A	48	U	N1-C2-O2	5.81	126.87	122.80
11	A	58	C	N3-C2-O2	-5.80	117.84	121.90
11	A	1413	G	N3-C4-N9	5.79	129.47	126.00
11	A	688	U	C2-N1-C1'	5.78	124.63	117.70
11	A	373	U	N1-C2-O2	5.77	126.84	122.80
11	A	1140	U	P-O3'-C3'	5.73	126.58	119.70
11	A	898	G	C4-N9-C1'	5.71	133.92	126.50
11	A	1255	A	C4-C5-N7	5.66	113.53	110.70
11	A	1413	G	C8-N9-C1'	-5.65	119.65	127.00
11	A	881	G	C4-N9-C1'	5.63	133.83	126.50
11	A	931	A	OP1-P-O3'	5.58	117.48	105.20
11	A	104	C	C5-C6-N1	5.57	123.78	121.00
11	A	68	A	O4'-C1'-N9	5.55	112.64	108.20
11	A	823	C	C2-N1-C1'	5.55	124.90	118.80
11	A	1139	A	C8-N9-C4	-5.53	103.59	105.80
11	A	1229	U	C5-C6-N1	5.52	125.46	122.70
11	A	373	U	C2-N1-C1'	5.50	124.30	117.70
11	A	58	C	N1-C2-O2	5.48	122.19	118.90
11	A	823	C	N3-C2-O2	-5.42	118.11	121.90
11	A	799	G	C4-N9-C1'	-5.41	119.47	126.50
11	A	593	C	N3-C2-O2	-5.39	118.13	121.90
11	A	1013	C	P-O3'-C3'	5.36	126.14	119.70
11	A	823	C	N1-C2-O2	5.36	122.12	118.90
11	A	174	C	C2-N1-C1'	5.36	124.69	118.80
11	A	1568	C	N1-C2-O2	5.35	122.11	118.90
11	A	174	C	C6-N1-C2	-5.34	118.16	120.30
11	A	66	U	C2-N1-C1'	5.34	124.11	117.70
11	A	1166	A	P-O3'-C3'	5.31	126.08	119.70
11	A	1518	U	P-O3'-C3'	5.30	126.07	119.70
11	A	617	C	P-O3'-C3'	5.30	126.06	119.70
11	A	765	G	P-O3'-C3'	5.30	126.06	119.70
11	A	467	A	O4'-C1'-N9	5.26	112.41	108.20
11	A	559	C	N3-C2-O2	-5.25	118.23	121.90
11	A	201	C	C2-N1-C1'	-5.22	113.06	118.80
11	A	1234	C	C5-C6-N1	5.18	123.59	121.00
11	A	593	C	C2-N1-C1'	5.15	124.47	118.80
11	A	747	C	O4'-C1'-N1	5.07	112.26	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	1523	C	N1-C2-O2	5.07	121.94	118.90
11	A	572	A	C3'-C2'-C1'	5.05	105.54	101.50
11	A	403	C	C2-N1-C1'	5.03	124.33	118.80
11	A	812	C	N3-C2-O2	-5.01	118.39	121.90
11	A	306	G	P-O3'-C3'	5.00	125.71	119.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	E	316	PHE	Peptide
15	E	43	GLY	Peptide
28	V	150	LYS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	878	0	896	20	0
2	1	2036	0	2058	36	0
3	2	1544	0	1580	26	0
4	3	968	0	1018	23	0
5	4	381	0	400	9	0
6	5	902	0	916	22	0
7	6	391	0	429	18	0
8	7	387	0	413	10	0
9	8	833	0	883	17	0
10	9	335	0	359	11	0
11	A	32233	0	16310	440	0
12	B	1225	0	675	29	0
13	C	62	0	34	1	0
13	Z	62	0	34	0	0
14	D	1860	0	1923	58	0
15	E	2420	0	2418	63	0
16	F	2011	0	2049	50	0
17	I	805	0	845	21	0
18	J	1361	0	1449	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	K	1081	0	1146	36	0
20	N	1444	0	1437	22	0
21	O	896	0	946	25	0
22	P	2312	0	2373	63	0
23	Q	1792	0	1832	31	0
24	R	1240	0	1260	40	0
25	S	1168	0	1159	46	0
26	T	1860	0	1875	45	0
27	U	1159	0	1228	35	0
28	V	1231	0	1278	35	0
29	W	1374	0	1405	20	0
30	X	1120	0	1133	27	0
31	Y	1663	0	1665	50	0
32	5	1	0	0	0	0
32	9	1	0	0	0	0
33	A	163	0	0	0	0
33	D	2	0	0	0	0
33	P	2	0	0	0	0
33	Q	1	0	0	0	0
33	R	1	0	0	0	0
34	A	192	0	0	5	0
34	D	6	0	0	0	0
34	P	6	0	0	4	0
All	All	69409	0	53426	1171	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 10.

All (1171) 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)
11:A:346:U:H4'	11:A:347:G:H5'	1.53	0.91
27:U:54:THR:HG21	28:V:176:MET:H	1.38	0.88
14:D:111:ARG:HH11	14:D:182:ALA:HB2	1.40	0.86
16:F:262:THR:HG22	16:F:264:PRO:HD2	1.59	0.85
18:J:156:SER:HB3	18:J:159:PRO:HB3	1.59	0.84
22:P:137:GLY:HA3	22:P:157:GLN:HG3	1.60	0.84
31:Y:122:LEU:HD23	31:Y:133:VAL:HG21	1.61	0.83
2:1:96:LYS:O	11:A:60:U:O2'	1.98	0.82
11:A:1230:G:O2'	11:A:1246:C:N4	2.13	0.81
11:A:68:A:O2'	11:A:69:C:O4'	1.97	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:D:186:GLY:HA3	14:D:239:GLU:HG3	1.63	0.81
11:A:845:U:H6	11:A:845:U:H5'	1.46	0.80
5:4:61:ASP:HB3	5:4:63:SER:H	1.46	0.79
11:A:177:C:H1'	27:U:55:ARG:HH22	1.47	0.79
15:E:206:VAL:HG22	15:E:299:ILE:HD13	1.64	0.79
25:S:86:THR:HG22	25:S:88:HIS:H	1.47	0.79
31:Y:127:ASP:H	31:Y:152:ARG:HH12	1.29	0.77
3:2:182:LYS:NZ	11:A:28:A:OP2	2.16	0.77
19:K:70:ILE:HG12	19:K:80:ILE:HD12	1.67	0.76
11:A:136:A:OP1	31:Y:83:ARG:NH2	2.18	0.76
11:A:512:A:H4'	11:A:513:A:H5"	1.65	0.76
1:0:56:MET:H	1:0:59:HIS:HD2	1.32	0.76
11:A:993:C:H5"	24:R:13:ARG:HH22	1.49	0.76
8:7:74:ARG:NH2	11:A:31:A:O2'	2.19	0.75
11:A:746:A:O2'	11:A:747:C:O5'	2.04	0.75
11:A:893:U:OP1	14:D:285:ARG:NH2	2.20	0.75
11:A:572:A:N3	11:A:572:A:H2'	2.02	0.75
18:J:142:ASN:HB2	18:J:185:ILE:HG21	1.70	0.73
11:A:163:A:OP1	27:U:52:LYS:NZ	2.21	0.73
30:X:40:VAL:HG23	30:X:97:VAL:HG23	1.70	0.73
9:8:142:ARG:NH1	11:A:1191:C:OP2	2.20	0.73
11:A:786:A:H3'	24:R:10:SER:HB2	1.71	0.73
11:A:1250:G:N3	22:P:77:ARG:NH2	2.37	0.73
11:A:1312:U:H5'	11:A:1391:C:H5"	1.69	0.73
3:2:175:PHE:O	3:2:214:ARG:NH2	2.22	0.72
3:2:120:GLU:HG2	30:X:110:LEU:HD12	1.70	0.72
25:S:85:ARG:HB3	25:S:120:ARG:HH12	1.55	0.72
14:D:195:ASN:HD22	14:D:248:VAL:HG22	1.53	0.71
15:E:317:PRO:HG2	15:E:320:PHE:HE1	1.54	0.71
22:P:97:SER:HB2	22:P:143:GLU:HB2	1.72	0.71
22:P:94:GLN:OE1	34:P:5543:HOH:O	2.08	0.71
4:3:126:GLN:HE22	4:3:146:VAL:HG13	1.55	0.71
16:F:85:ASP:HB3	16:F:274:LEU:HD21	1.73	0.71
31:Y:105:ARG:H	31:Y:105:ARG:HD3	1.55	0.71
7:6:47:ASP:HB2	7:6:54:VAL:HG21	1.72	0.71
11:A:947:A:N3	11:A:1372:U:H5"	2.06	0.70
11:A:1440:U:H5"	15:E:253:PRO:HA	1.73	0.70
18:J:93:ASN:HB2	18:J:96:ILE:HG12	1.74	0.70
19:K:43:GLY:HA3	19:K:76:ARG:HH11	1.56	0.70
15:E:96:ARG:NH2	15:E:197:HIS:O	2.21	0.70
11:A:1184:U:O2'	11:A:1185:U:O4'	2.10	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:P:205:LEU:HG	22:P:263:ARG:HH21	1.56	0.70
15:E:181:VAL:HG13	15:E:185:ALA:HB3	1.73	0.70
11:A:370:A:O2'	22:P:71:GLN:NE2	2.26	0.69
22:P:104:LEU:HD11	22:P:126:GLY:HA3	1.74	0.69
5:4:52:LEU:HG	5:4:68:ARG:HB3	1.75	0.69
11:A:1048:C:H2'	11:A:1325:U:H4'	1.74	0.69
24:R:43:GLU:HB2	24:R:123:VAL:HG23	1.74	0.69
11:A:462:A:H3'	11:A:463:U:H5'	1.75	0.69
11:A:69:C:O2'	11:A:70:A:O5'	2.08	0.69
11:A:747:C:O2'	11:A:748:A:H5"	1.92	0.69
23:Q:131:ILE:HB	23:Q:149:HIS:HB3	1.75	0.69
4:3:75:THR:HG22	4:3:86:ILE:HD13	1.73	0.68
30:X:49:THR:HG23	30:X:52:ASP:HB2	1.76	0.68
25:S:126:GLU:HG2	25:S:160:ARG:HB3	1.74	0.68
11:A:9:U:O4	11:A:107:U:O2'	2.11	0.68
6:5:140:GLN:NE2	6:5:176:GLU:O	2.23	0.68
15:E:187:ILE:HG22	15:E:188:LYS:H	1.58	0.68
25:S:39:VAL:HG12	25:S:41:ASN:H	1.59	0.68
11:A:185:U:O4'	11:A:432:G:O2'	2.12	0.68
25:S:116:LEU:HG	25:S:117:TYR:H	1.58	0.68
31:Y:129:LYS:HD3	31:Y:149:ARG:HH21	1.59	0.68
11:A:403:C:H2'	11:A:404:C:H5'	1.77	0.67
15:E:227:GLN:HG3	15:E:236:THR:O	1.93	0.67
16:F:226:MET:HE1	16:F:242:LEU:HD11	1.74	0.67
21:O:128:ARG:HA	21:O:138:LEU:HD21	1.76	0.67
30:X:68:VAL:HG22	30:X:97:VAL:HG12	1.77	0.67
8:7:63:ARG:HH21	8:7:64:LYS:HE2	1.59	0.67
2:1:16:LEU:HD12	2:1:21:TYR:HB3	1.77	0.67
22:P:186:ILE:HD13	22:P:201:PRO:HG3	1.77	0.67
5:4:59:LYS:HA	5:4:78:MET:HB2	1.77	0.67
11:A:504:A:OP2	19:K:21:ARG:NH1	2.28	0.67
2:1:156:LYS:NZ	2:1:205:GLY:O	2.28	0.66
11:A:794:U:H4'	26:T:260:TRP:HZ3	1.59	0.66
5:4:37:ASN:HD22	5:4:40:LEU:HD12	1.59	0.66
26:T:165:GLU:HB2	26:T:168:ASN:HB2	1.77	0.66
11:A:1148:G:OP2	11:A:1173:C:O2'	2.07	0.66
11:A:428:G:OP1	22:P:62:ARG:NH2	2.29	0.66
11:A:1344:A:HO2'	11:A:1534:U:HO2'	1.43	0.66
22:P:264:GLN:NE2	22:P:269:LEU:O	2.29	0.66
14:D:219:ARG:HE	14:D:226:ILE:HD12	1.61	0.65
31:Y:131:THR:HG21	31:Y:147:SER:HB3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:8:172:TYR:HB2	9:8:175:ASP:HB2	1.77	0.65
4:3:74:SER:HB2	11:A:471:U:H5"	1.78	0.65
11:A:931:A:O2'	11:A:932:U:OP1	2.14	0.65
18:J:33:VAL:HB	23:Q:69:LEU:HB3	1.78	0.65
11:A:111:G:H2'	11:A:112:A:H5"	1.78	0.65
11:A:1454:C:H2'	11:A:1455:A:H2'	1.78	0.65
24:R:38:ARG:HG2	24:R:39:HIS:CD2	2.31	0.64
18:J:186:LEU:HD13	18:J:194:TYR:CE2	2.33	0.64
23:Q:118:MET:HB3	23:Q:163:MET:HE1	1.80	0.64
16:F:257:GLN:HB3	22:P:21:ARG:HH11	1.62	0.64
31:Y:19:TYR:OH	31:Y:31:ASP:OD2	2.16	0.64
29:W:77:GLN:H	29:W:171:HIS:CD2	2.16	0.64
11:A:476:A:O2'	28:V:192:ASN:ND2	2.30	0.64
12:B:9:P5P:H5'2	12:B:47:P5P:H1'	1.79	0.64
16:F:283:LEU:HB2	22:P:125:ARG:HH12	1.63	0.64
21:O:130:ARG:HD2	21:O:134:PHE:HE2	1.63	0.64
29:W:77:GLN:H	29:W:171:HIS:HD2	1.45	0.64
11:A:1550:C:H5'	11:A:1551:A:OP1	1.97	0.64
9:8:116:ARG:HG3	9:8:122:TRP:CE2	2.33	0.64
11:A:1209:A:P	25:S:176:ARG:HH22	2.20	0.64
11:A:1510:U:H2'	11:A:1511:U:H5"	1.79	0.64
11:A:228:A:H4'	11:A:229:G:H5'	1.80	0.63
14:D:236:GLN:HB3	14:D:295:SER:HA	1.80	0.63
11:A:178:U:O2'	11:A:188:A:O4'	2.14	0.63
15:E:341:GLY:HA2	26:T:105:ILE:HD11	1.80	0.63
18:J:104:LEU:HB3	18:J:108:ASP:HB2	1.79	0.63
11:A:1512:A:H2'	11:A:1513:A:H5"	1.81	0.63
23:Q:81:GLU:O	23:Q:123:ARG:NH2	2.31	0.63
19:K:57:THR:HG23	19:K:66:LEU:HD21	1.80	0.63
14:D:107:ILE:HD11	14:D:140:ILE:HD13	1.81	0.63
3:2:89:CYS:HB3	3:2:93:ARG:HE	1.64	0.63
3:2:189:PRO:HA	31:Y:216:TYR:OH	1.99	0.63
11:A:785:U:OP1	24:R:16:ARG:NH1	2.32	0.63
11:A:391:U:H2'	11:A:392:A:C8	2.34	0.62
11:A:572:A:O2'	11:A:573:C:O2	2.17	0.62
19:K:19:MET:HG2	19:K:71:PHE:HD1	1.64	0.62
25:S:174:GLU:HG3	25:S:175:PRO:HD2	1.80	0.62
4:3:36:PHE:CE1	23:Q:228:LYS:HA	2.33	0.62
16:F:220:ASP:OD1	16:F:221:LEU:N	2.32	0.62
18:J:54:ILE:HD12	23:Q:211:ASN:HB3	1.79	0.62
19:K:94:ALA:HB1	19:K:116:HIS:HD2	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:P:116:ILE:HD12	22:P:152:VAL:HG13	1.81	0.62
21:O:32:ILE:HD11	21:O:38:VAL:HG12	1.82	0.62
11:A:335:A:H4'	11:A:336:A:OP2	2.00	0.62
11:A:1343:A:H4'	11:A:1449:U:OP1	2.00	0.62
16:F:83:HIS:HD2	16:F:85:ASP:H	1.47	0.62
11:A:911:G:H21	11:A:912:A:N6	1.97	0.62
11:A:1546:A:H5'	11:A:1547:A:OP2	2.00	0.62
14:D:123:PHE:HB2	14:D:166:ASN:HB2	1.81	0.62
11:A:809:A:H1'	15:E:230:THR:HG23	1.83	0.61
14:D:198:GLU:OE2	14:D:202:GLY:N	2.33	0.61
6:5:90:ASN:OD1	6:5:93:ARG:NH2	2.33	0.61
27:U:97:LEU:HA	28:V:109:GLN:HE22	1.64	0.61
31:Y:133:VAL:HG13	31:Y:145:ARG:HB3	1.82	0.61
17:I:94:LEU:HB3	17:I:114:VAL:HG23	1.82	0.61
24:R:110:ILE:HD11	24:R:123:VAL:HB	1.81	0.61
11:A:163:A:HO2'	11:A:1014:C:H5	1.49	0.61
11:A:330:A:O2'	11:A:338:G:N7	2.33	0.61
11:A:747:C:O2	30:X:54:ARG:NH1	2.30	0.61
26:T:74:ARG:HB3	26:T:283:TRP:CZ2	2.35	0.61
10:9:93:PRO:HG2	11:A:1349:U:OP1	2.00	0.61
12:B:23:P5P:OP2	25:S:113:LYS:NZ	2.32	0.61
16:F:56:PRO:HG2	16:F:59:ARG:HB3	1.81	0.61
1:0:61:VAL:HG21	1:0:97:VAL:HG23	1.81	0.61
11:A:220:A:N7	16:F:281:THR:OG1	2.34	0.61
6:5:136:GLU:HG2	6:5:177:ARG:NH2	2.14	0.61
3:2:126:LEU:HD12	3:2:127:PRO:HD2	1.83	0.60
5:4:44:LEU:HD22	5:4:49:TYR:CG	2.36	0.60
11:A:875:U:O2'	11:A:876:G:OP2	2.17	0.60
2:1:177:HIS:CD2	2:1:183:ARG:HD2	2.36	0.60
15:E:285:VAL:HG12	15:E:286:ASN:H	1.65	0.60
14:D:179:GLU:HA	14:D:245:VAL:O	2.00	0.60
11:A:68:A:O2'	11:A:69:C:O5'	2.18	0.60
1:0:76:HIS:HD2	25:S:70:THR:HG21	1.67	0.60
16:F:74:GLN:O	16:F:210:ARG:NH2	2.35	0.60
18:J:56:PRO:HA	23:Q:210:GLN:HE21	1.66	0.60
21:O:110:ASP:OD1	21:O:110:ASP:N	2.34	0.60
24:R:129:ASN:HD22	24:R:131:LEU:HD12	1.66	0.60
31:Y:131:THR:HG23	31:Y:149:ARG:HB3	1.84	0.60
11:A:895:A:H2'	11:A:896:C:H6	1.67	0.60
22:P:54:LYS:N	22:P:58:GLN:OE1	2.31	0.60
11:A:58:C:H2'	11:A:59:A:H5"	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:627:A:O2'	11:A:629:A:OP1	2.20	0.59
18:J:163:GLU:HG3	18:J:166:ARG:CZ	2.31	0.59
1:0:56:MET:H	1:0:59:HIS:CD2	2.19	0.59
30:X:37:GLU:HB3	30:X:104:THR:HG23	1.84	0.59
11:A:503:U:H4'	11:A:504:A:H5'	1.85	0.59
11:A:689:A:OP2	34:A:5366:HOH:O	2.16	0.59
18:J:110:LEU:HB3	19:K:132:LEU:HD13	1.85	0.59
18:J:111:LEU:O	18:J:115:GLN:HG2	2.01	0.59
26:T:120:THR:HG23	26:T:130:THR:HG23	1.83	0.59
11:A:816:A:OP1	11:A:816:A:H4'	2.00	0.59
11:A:1408:A:H5'	11:A:1409:G:OP2	2.01	0.59
11:A:404:C:H2'	11:A:405:U:O4'	2.01	0.59
12:B:60:Y5P:H4A	12:B:61:Y5P:H4	1.85	0.59
18:J:128:ASN:ND2	18:J:147:PHE:O	2.28	0.59
25:S:54:ARG:NH2	25:S:141:ILE:HG22	2.18	0.59
18:J:98:VAL:N	18:J:178:GLY:O	2.35	0.59
19:K:26:ALA:HA	19:K:57:THR:HG22	1.84	0.59
30:X:50:ARG:NH1	30:X:69:ARG:HA	2.18	0.59
11:A:319:U:OP1	14:D:61:ALA:N	2.35	0.59
18:J:95:MET:HB3	18:J:156:SER:HB2	1.83	0.59
23:Q:50:LEU:H	23:Q:110:ASN:HD21	1.50	0.59
15:E:98:GLY:HA3	15:E:179:PHE:CE1	2.38	0.59
22:P:130:GLN:NE2	34:P:5540:HOH:O	2.36	0.59
15:E:99:LEU:HD21	15:E:193:LEU:HB3	1.85	0.58
24:R:118:ARG:HG2	29:W:108:ASP:OD1	2.02	0.58
3:2:123:ARG:NH1	30:X:30:ARG:O	2.35	0.58
5:4:58:VAL:HG22	5:4:64:THR:HG22	1.84	0.58
11:A:694:A:H3'	11:A:695:C:H5"	1.84	0.58
12:B:41:P5P:C6	12:B:42:Y5P:H4	2.32	0.58
11:A:744:U:H4'	11:A:744:U:OP1	2.02	0.58
5:4:44:LEU:HD21	5:4:46:ARG:HB2	1.86	0.58
11:A:65:C:OP1	11:A:67:A:N6	2.37	0.58
11:A:445:C:H1'	11:A:1278:C:O2'	2.02	0.58
11:A:1250:G:N7	34:A:5125:HOH:O	2.31	0.58
20:N:27:PRO:HG2	20:N:30:LYS:HB2	1.85	0.58
11:A:163:A:OP2	27:U:48:ARG:HD2	2.03	0.58
19:K:87:VAL:HG22	19:K:124:LYS:HD3	1.85	0.58
15:E:334:ASP:OD1	15:E:335:GLU:N	2.37	0.58
7:6:34:ARG:HG3	7:6:36:ARG:HG2	1.86	0.58
9:8:132:LYS:HE3	11:A:1230:G:H3'	1.86	0.58
11:A:1228:U:H5'	11:A:1229:U:OP1	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:958:U:O2'	11:A:959:A:OP2	2.20	0.57
16:F:85:ASP:O	16:F:89:THR:OG1	2.22	0.57
23:Q:172:VAL:HG12	23:Q:176:LEU:HG	1.86	0.57
1:0:74:ARG:HD3	1:0:75:TRP:CZ2	2.38	0.57
11:A:1481:C:H5'	15:E:290:PRO:HA	1.86	0.57
28:V:186:ARG:HH21	28:V:188:ARG:NH2	2.02	0.57
11:A:79:U:O2'	17:I:61:LYS:NZ	2.36	0.57
11:A:988:U:H3'	11:A:989:C:H2'	1.85	0.57
11:A:174:C:H5'	20:N:115:ASN:HB3	1.85	0.57
24:R:32:LEU:HB3	24:R:52:LEU:HD22	1.86	0.57
14:D:156:GLU:HA	14:D:249:SER:HA	1.87	0.57
30:X:149:GLY:O	30:X:150:LEU:HB2	2.05	0.57
10:9:92:ASN:HD22	10:9:95:HIS:CE1	2.23	0.57
11:A:884:A:H2'	11:A:885:C:O4'	2.04	0.57
16:F:182:LEU:HD13	16:F:187:LEU:HD23	1.85	0.57
22:P:100:ARG:HH21	22:P:126:GLY:HA2	1.70	0.57
7:6:37:LEU:HD11	7:6:40:LYS:HA	1.86	0.57
11:A:1002:A:H2'	11:A:1003:G:H5"	1.87	0.57
21:O:93:GLY:O	21:O:95:ARG:NH1	2.38	0.57
16:F:226:MET:HE2	16:F:242:LEU:HD21	1.87	0.57
3:2:190:TRP:HB3	31:Y:216:TYR:CE1	2.40	0.57
11:A:638:A:OP1	29:W:147:ARG:NH1	2.38	0.57
11:A:743:A:H5'	11:A:744:U:H5"	1.85	0.57
6:5:85:ARG:NH1	11:A:640:G:OP1	2.38	0.56
3:2:232:LYS:NZ	11:A:10:A:OP1	2.36	0.56
6:5:151:ALA:N	24:R:84:ASP:OD2	2.36	0.56
16:F:215:SER:HA	16:F:239:THR:HG22	1.86	0.56
2:1:87:LEU:HD23	2:1:104:VAL:HB	1.88	0.56
11:A:503:U:C2	11:A:505:G:H5"	2.40	0.56
16:F:83:HIS:CD2	16:F:85:ASP:H	2.22	0.56
22:P:217:ALA:HB2	22:P:228:ARG:HB2	1.87	0.56
30:X:2:ALA:HB2	30:X:19:VAL:HG11	1.87	0.56
16:F:249:ASN:ND2	16:F:252:SER:H	2.03	0.56
11:A:686:A:H3'	11:A:687:A:H4'	1.88	0.56
11:A:975:G:H5'	11:A:976:G:OP2	2.05	0.56
18:J:168:LEU:HD13	18:J:176:LEU:HB2	1.88	0.56
11:A:39:A:H4'	11:A:40:C:OP1	2.06	0.56
15:E:122:LEU:HD13	15:E:299:ILE:HD11	1.86	0.56
30:X:71:ARG:NH1	30:X:96:TYR:OH	2.39	0.56
1:0:76:HIS:CD2	25:S:70:THR:HG21	2.41	0.56
16:F:207:ALA:HB2	16:F:240:PHE:HZ	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:I:56:VAL:CG1	17:I:80:TYR:HB3	2.35	0.56
24:R:143:LEU:HA	24:R:148:GLN:HE21	1.69	0.56
11:A:911:G:H21	11:A:912:A:H62	1.54	0.56
4:3:76:LYS:HZ1	11:A:472:G:H8	1.54	0.56
7:6:23:GLN:NE2	7:6:55:LEU:HB3	2.21	0.56
11:A:687:A:N1	29:W:155:ARG:HG3	2.21	0.56
16:F:257:GLN:HB3	22:P:21:ARG:NH1	2.21	0.56
18:J:97:ALA:HB1	18:J:176:LEU:HD11	1.88	0.56
19:K:25:ARG:HA	19:K:65:PRO:HB3	1.87	0.56
11:A:241:G:OP1	16:F:117:ARG:NH2	2.37	0.55
11:A:794:U:H4'	26:T:260:TRP:CZ3	2.40	0.55
22:P:287:ASP:HB3	22:P:290:LEU:HB2	1.87	0.55
11:A:716:A:H5'	11:A:717:C:OP2	2.06	0.55
18:J:162:LYS:O	18:J:166:ARG:HG3	2.07	0.55
27:U:141:ILE:HG21	28:V:80:HIS:CE1	2.41	0.55
11:A:551:U:H2'	11:A:552:U:H5"	1.89	0.55
20:N:62:THR:O	20:N:65:ILE:HG13	2.06	0.55
3:2:228:LEU:HD11	11:A:11:G:H5"	1.88	0.55
6:5:90:ASN:O	6:5:94:ARG:HG2	2.06	0.55
11:A:174:C:H5'	20:N:115:ASN:CB	2.36	0.55
14:D:76:PRO:HB2	14:D:103:ARG:HD3	1.88	0.55
11:A:1002:A:N6	34:A:5048:HOH:O	2.39	0.55
11:A:1125:A:H2'	11:A:1126:A:C8	2.41	0.55
15:E:200:PRO:HG3	15:E:332:LEU:HB3	1.87	0.55
11:A:395:C:H5'	11:A:396:C:OP1	2.06	0.55
11:A:1074:A:H2'	11:A:1075:A:C8	2.42	0.55
11:A:366:A:O2'	11:A:367:A:OP2	2.18	0.55
26:T:246:ASP:OD1	26:T:246:ASP:N	2.40	0.55
10:9:65:THR:HG23	10:9:100:MET:HB3	1.88	0.55
16:F:219:VAL:HB	16:F:261:LEU:HD23	1.89	0.55
16:F:284:TYR:HB2	16:F:285:PRO:HD2	1.89	0.55
19:K:140:VAL:O	19:K:144:ILE:HG12	2.06	0.55
15:E:53:LEU:HA	24:R:147:ASN:HD21	1.71	0.55
17:I:122:ARG:O	17:I:126:GLN:HG2	2.07	0.55
1:0:76:HIS:HE1	1:0:128:LYS:HD2	1.72	0.54
11:A:60:U:C5	11:A:61:U:H1'	2.41	0.54
14:D:111:ARG:HE	14:D:152:ILE:HD12	1.71	0.54
16:F:83:HIS:CG	16:F:274:LEU:HD11	2.42	0.54
11:A:718:C:H5'	14:D:75:MET:HG2	1.90	0.54
11:A:889:A:H3'	11:A:890:G:C8	2.43	0.54
11:A:979:U:H5'	11:A:980:U:OP2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:1290:A:H4'	23:Q:111:ARG:CZ	2.37	0.54
27:U:54:THR:CG2	28:V:176:MET:H	2.18	0.54
11:A:78:A:OP1	22:P:87:HIS:HE1	1.91	0.54
11:A:428:G:H5'	22:P:57:ARG:HD3	1.88	0.54
11:A:368:G:H2'	11:A:369:A:H5"	1.89	0.54
11:A:530:A:N6	19:K:150:SER:HB3	2.21	0.54
16:F:249:ASN:HD21	16:F:252:SER:H	1.55	0.54
27:U:28:ALA:HA	27:U:31:PHE:CE1	2.42	0.54
31:Y:49:ILE:HD11	31:Y:117:HIS:CE1	2.42	0.54
2:1:41:VAL:HG11	2:1:83:GLU:HB3	1.89	0.54
8:7:95:HIS:CD2	11:A:124:A:H5"	2.41	0.54
11:A:446:A:H5'	11:A:447:G:OP2	2.07	0.54
11:A:857:A:H5"	14:D:67:LYS:HE2	1.90	0.54
31:Y:78:GLN:HE21	31:Y:87:VAL:HG21	1.73	0.54
11:A:658:C:O3'	24:R:81:THR:HG21	2.08	0.54
17:I:109:GLY:HA2	17:I:140:PHE:CE2	2.43	0.54
19:K:49:PHE:CE1	19:K:80:ILE:HD13	2.42	0.54
26:T:233:TRP:HB3	26:T:240:ILE:HD12	1.89	0.54
10:9:85:TRP:CZ2	11:A:492:U:O2'	2.61	0.54
11:A:1431:U:H4'	11:A:1432:U:H5'	1.89	0.54
2:1:20:ILE:HA	2:1:23:ARG:HD2	1.90	0.53
11:A:585:U:H2'	11:A:586:C:H6	1.71	0.53
11:A:924:U:O2'	11:A:925:A:H8	1.91	0.53
14:D:73:THR:HG22	14:D:75:MET:H	1.72	0.53
15:E:295:CYS:SG	15:E:296:LEU:N	2.82	0.53
11:A:577:U:O2'	11:A:578:A:OP2	2.20	0.53
11:A:1300:U:OP1	11:A:1358:U:O2'	2.17	0.53
16:F:83:HIS:CD2	16:F:274:LEU:HD11	2.43	0.53
1:0:135:PRO:HB3	25:S:63:ARG:NH1	2.23	0.53
14:D:178:ARG:HG2	14:D:179:GLU:H	1.73	0.53
22:P:273:TRP:CD1	22:P:284:LYS:HB3	2.44	0.53
28:V:99:LEU:HD23	28:V:142:ALA:HB2	1.90	0.53
11:A:297:A:C2	11:A:335:A:H2'	2.42	0.53
11:A:362:G:H8	11:A:362:G:H5'	1.72	0.53
11:A:444:A:H2	23:Q:244:LYS:HD2	1.74	0.53
11:A:975:G:N7	34:A:5239:HOH:O	2.34	0.53
25:S:66:ARG:HH11	25:S:180:GLU:HG2	1.73	0.53
15:E:133:THR:HB	15:E:144:ALA:HB3	1.91	0.53
22:P:130:GLN:NE2	34:P:5544:HOH:O	2.38	0.53
15:E:104:LEU:HB2	15:E:121:LEU:HB2	1.90	0.53
21:O:100:PHE:HB3	26:T:158:GLN:HE21	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:239:LYS:NZ	31:Y:45:PRO:HG3	2.23	0.53
11:A:272:A:O2'	11:A:273:A:H5"	2.09	0.53
22:P:130:GLN:NE2	34:P:5541:HOH:O	2.41	0.53
25:S:89:HIS:CD2	25:S:119:THR:HG21	2.44	0.53
11:A:403:C:C2'	11:A:404:C:H5'	2.38	0.53
16:F:108:ARG:HG2	16:F:161:TYR:CD1	2.44	0.53
22:P:199:PRO:HA	22:P:274:VAL:HG22	1.91	0.53
26:T:110:GLU:OE1	26:T:110:GLU:N	2.40	0.53
11:A:69:C:HO2'	11:A:70:A:P	2.30	0.53
12:B:59:P5P:C6	12:B:60:Y5P:H4	2.39	0.53
25:S:107:THR:HG21	25:S:119:THR:HG23	1.90	0.53
4:3:148:ARG:HH21	4:3:151:LEU:HD13	1.74	0.53
11:A:352:C:OP1	11:A:375:A:O2'	2.23	0.53
11:A:617:C:H4'	11:A:618:A:OP1	2.09	0.53
19:K:62:GLU:HB2	19:K:64:ILE:HD11	1.91	0.53
24:R:84:ASP:O	24:R:87:PRO:HD2	2.08	0.53
4:3:72:ILE:HD11	4:3:118:ARG:HD2	1.90	0.52
11:A:653:C:H3'	11:A:654:C:C6	2.44	0.52
11:A:1234:C:H6	11:A:1234:C:O5'	1.93	0.52
18:J:93:ASN:ND2	18:J:155:VAL:HG22	2.24	0.52
22:P:196:ARG:HB3	22:P:198:GLN:HG3	1.91	0.52
28:V:147:LEU:HD13	28:V:157:LEU:HD21	1.90	0.52
7:6:44:LEU:HA	7:6:54:VAL:O	2.09	0.52
14:D:114:PRO:HA	14:D:123:PHE:CZ	2.44	0.52
15:E:202:GLN:NE2	15:E:301:ASP:OD1	2.41	0.52
18:J:90:PHE:CZ	18:J:135:LEU:HD21	2.44	0.52
20:N:112:LEU:HD13	20:N:121:MET:HG3	1.91	0.52
29:W:150:TYR:CE2	29:W:168:VAL:HG13	2.45	0.52
2:1:168:ARG:HH21	2:1:175:GLN:HG3	1.74	0.52
7:6:33:LYS:HE3	7:6:37:LEU:HD13	1.91	0.52
11:A:658:C:H4'	24:R:81:THR:HG21	1.91	0.52
21:O:71:ASP:HB3	21:O:86:ILE:HD12	1.91	0.52
7:6:38:ARG:HE	11:A:1184:U:H5'	1.73	0.52
11:A:30:U:H5'	11:A:31:A:OP1	2.10	0.52
11:A:128:A:OP1	16:F:142:ARG:NH2	2.41	0.52
11:A:1564:G:H2'	11:A:1565:G:H5"	1.92	0.52
22:P:176:THR:HG22	22:P:214:TYR:HE1	1.74	0.52
11:A:334:U:OP1	11:A:337:C:N4	2.36	0.52
11:A:494:C:C5	11:A:554:A:H2	2.28	0.52
11:A:1255:A:C8	11:A:1255:A:H3'	2.44	0.52
15:E:316:PHE:CG	15:E:316:PHE:O	2.63	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:I:62:VAL:HG22	17:I:77:HIS:CD2	2.45	0.52
21:O:51:TYR:CE2	21:O:78:ARG:HA	2.45	0.52
11:A:67:A:H2'	11:A:68:A:O4'	2.09	0.52
15:E:99:LEU:HD12	15:E:198:PHE:HE1	1.73	0.52
28:V:165:ILE:HD11	28:V:198:ARG:HB2	1.91	0.52
31:Y:78:GLN:NE2	31:Y:87:VAL:HG21	2.24	0.52
6:5:153:THR:O	24:R:92:VAL:HG22	2.10	0.52
25:S:89:HIS:HA	25:S:119:THR:HG21	1.91	0.52
26:T:189:TYR:CD1	26:T:243:ILE:HD11	2.44	0.52
7:6:42:THR:HG22	7:6:55:LEU:HD11	1.92	0.52
11:A:513:A:OP1	11:A:513:A:H4'	2.10	0.52
11:A:521:U:O2'	11:A:522:C:O5'	2.26	0.52
11:A:575:A:OP1	27:U:82:LYS:NZ	2.34	0.52
11:A:1255:A:H3'	11:A:1255:A:H8	1.73	0.52
2:1:114:LEU:HD13	2:1:141:PHE:CE1	2.45	0.52
11:A:185:U:OP1	11:A:431:A:O2'	2.28	0.52
12:B:42:Y5P:OP2	25:S:85:ARG:NH2	2.43	0.52
15:E:69:ASN:OD1	15:E:171:PRO:HB3	2.10	0.52
2:1:8:VAL:O	2:1:11:TRP:HB2	2.09	0.52
11:A:164:A:H5'	27:U:31:PHE:CD2	2.45	0.52
11:A:1290:A:O5'	23:Q:111:ARG:NH2	2.41	0.52
11:A:1499:C:H2'	11:A:1500:U:C6	2.45	0.52
12:B:68:P5P:C6	12:B:69:Y5P:H4	2.39	0.52
2:1:197:PRO:HG2	2:1:200:GLU:HG3	1.91	0.51
6:5:185:PHE:CD2	24:R:132:PRO:HA	2.44	0.51
11:A:1138:A:C2'	11:A:1139:A:H5"	2.40	0.51
11:A:351:G:H5'	11:A:352:C:C5	2.45	0.51
17:I:74:HIS:CG	17:I:75:ARG:N	2.78	0.51
15:E:292:HIS:O	15:E:295:CYS:HB3	2.10	0.51
16:F:216:VAL:HG22	16:F:258:THR:HB	1.92	0.51
23:Q:64:ARG:HH11	23:Q:144:LYS:HB3	1.76	0.51
30:X:38:ASP:O	30:X:98:GLN:HA	2.10	0.51
30:X:41:GLN:HE21	30:X:94:VAL:HG11	1.75	0.51
11:A:861:U:C2	14:D:254:ASN:HB2	2.46	0.51
1:0:61:VAL:HG13	1:0:65:ASN:HD22	1.75	0.51
15:E:317:PRO:HG2	15:E:320:PHE:CE1	2.42	0.51
18:J:53:TYR:HB2	23:Q:251:VAL:HG23	1.92	0.51
19:K:33:PRO:HA	19:K:37:PRO:HD2	1.91	0.51
11:A:178:U:C4	11:A:1029:C:H1'	2.46	0.51
11:A:557:A:H2'	11:A:558:A:C2	2.45	0.51
11:A:443:U:H4'	23:Q:133:ARG:NH1	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:F:97:HIS:CE1	16:F:101:ILE:HD11	2.45	0.51
27:U:94:GLN:NE2	27:U:145:VAL:HG13	2.26	0.51
27:U:141:ILE:HG21	28:V:80:HIS:HE1	1.76	0.51
11:A:548:A:H5'	18:J:127:PRO:HA	1.92	0.51
31:Y:58:CYS:HA	31:Y:76:VAL:HG12	1.93	0.51
12:B:33:Y5P:H6	12:B:33:Y5P:O5'	2.10	0.51
18:J:126:PHE:HB2	18:J:131:LEU:HD22	1.91	0.51
11:A:391:U:H2'	11:A:392:A:H8	1.76	0.51
11:A:973:G:H3'	11:A:974:A:H5"	1.92	0.51
21:O:55:PRO:HB3	21:O:77:ILE:HG23	1.92	0.51
23:Q:250:ARG:O	23:Q:251:VAL:HB	2.11	0.51
11:A:48:U:O2'	11:A:49:A:H4'	2.11	0.50
11:A:397:A:H2'	11:A:398:A:H5'	1.93	0.50
11:A:1568:C:H3'	11:A:1569:A:H3'	1.93	0.50
16:F:280:TYR:OH	22:P:109:ARG:HD3	2.11	0.50
17:I:74:HIS:CG	17:I:75:ARG:H	2.29	0.50
28:V:112:VAL:HG13	28:V:199:ILE:HG21	1.93	0.50
11:A:861:U:O2	14:D:254:ASN:HB2	2.12	0.50
14:D:227:ILE:HG12	14:D:235:MET:HB3	1.92	0.50
15:E:197:HIS:NE2	15:E:318:THR:HG22	2.26	0.50
25:S:54:ARG:HH22	25:S:141:ILE:HG22	1.74	0.50
25:S:176:ARG:HG2	25:S:177:ARG:H	1.76	0.50
4:3:126:GLN:NE2	4:3:146:VAL:HG13	2.25	0.50
10:9:83:GLY:H	11:A:1525:U:H5'	1.77	0.50
11:A:195:U:O2'	11:A:1012:A:OP1	2.26	0.50
25:S:122:VAL:HG12	25:S:160:ARG:HD2	1.92	0.50
4:3:68:ILE:HD11	4:3:122:LEU:HD13	1.94	0.50
11:A:1520:A:H2'	11:A:1521:A:O4'	2.11	0.50
19:K:33:PRO:HB3	19:K:37:PRO:HG2	1.93	0.50
27:U:54:THR:HG21	28:V:176:MET:N	2.16	0.50
2:1:100:ARG:HH22	17:I:75:ARG:NE	2.08	0.50
11:A:229:G:H2'	11:A:230:C:C6	2.46	0.50
11:A:1048:C:H2'	11:A:1325:U:C4'	2.41	0.50
16:F:50:LYS:HD2	16:F:81:GLU:OE1	2.12	0.50
6:5:138:ARG:HA	6:5:141:MET:HG2	1.94	0.50
11:A:691:U:H1'	11:A:692:A:H5'	1.92	0.50
14:D:114:PRO:HA	14:D:123:PHE:CE2	2.46	0.50
11:A:936:U:H4'	11:A:937:U:H3'	1.93	0.50
11:A:1291:G:O6	11:A:1297:C:O2'	2.26	0.50
19:K:54:ASN:HB3	19:K:58:LYS:HE3	1.93	0.50
21:O:95:ARG:O	21:O:96:MET:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:26:THR:HB	11:A:1239:U:H3'	1.92	0.50
11:A:656:U:H2'	11:A:657:U:C6	2.47	0.50
11:A:771:C:H2'	11:A:772:A:H5"	1.94	0.50
18:J:181:ILE:HD11	18:J:191:PHE:CE2	2.47	0.50
19:K:115:LYS:O	19:K:119:GLU:HG3	2.12	0.50
2:1:163:ARG:HD3	2:1:205:GLY:H	1.77	0.49
11:A:187:C:H3'	28:V:181:ARG:NH2	2.27	0.49
11:A:390:A:O2'	11:A:391:U:O4'	2.29	0.49
11:A:894:A:H5'	11:A:963:A:H5"	1.94	0.49
11:A:1512:A:C2'	11:A:1513:A:H5"	2.42	0.49
18:J:163:GLU:OE1	18:J:163:GLU:N	2.45	0.49
25:S:52:ASN:OD1	25:S:55:ASN:HB2	2.12	0.49
2:1:177:HIS:NE2	2:1:183:ARG:HD2	2.26	0.49
11:A:653:C:H3'	11:A:654:C:H6	1.77	0.49
11:A:693:U:H5"	11:A:693:U:H6	1.77	0.49
12:B:62:Y5P:H4A	12:B:63:Y5P:H4	1.94	0.49
19:K:49:PHE:HE1	19:K:80:ILE:HD13	1.77	0.49
19:K:66:LEU:HD13	19:K:82:ILE:HG23	1.94	0.49
21:O:85:LEU:HD23	21:O:137:VAL:HG11	1.94	0.49
22:P:177:ALA:HA	22:P:222:TYR:CD1	2.46	0.49
24:R:20:LEU:HB2	24:R:24:SER:OG	2.12	0.49
26:T:71:PRO:O	26:T:213:GLN:HG2	2.12	0.49
30:X:138:ASP:HB3	30:X:141:ARG:HB2	1.94	0.49
31:Y:126:THR:HB	31:Y:152:ARG:CZ	2.42	0.49
3:2:137:VAL:O	3:2:141:MET:HG3	2.12	0.49
11:A:115:U:H3'	11:A:116:A:H5"	1.94	0.49
11:A:329:A:N3	11:A:330:A:H5"	2.26	0.49
11:A:499:A:N6	11:A:544:C:OP2	2.45	0.49
16:F:218:LEU:HD23	16:F:260:VAL:HB	1.94	0.49
11:A:159:A:H5'	11:A:160:A:OP2	2.12	0.49
11:A:415:U:H2'	11:A:416:G:C8	2.47	0.49
11:A:734:C:OP1	14:D:78:LYS:HD2	2.11	0.49
23:Q:87:PHE:CD1	23:Q:169:PHE:HD1	2.30	0.49
3:2:104:TRP:HE3	3:2:144:LEU:HD23	1.77	0.49
11:A:686:A:C3'	11:A:687:A:H4'	2.42	0.49
11:A:1555:C:H4'	26:T:86:ARG:HH12	1.76	0.49
15:E:53:LEU:HD21	15:E:61:VAL:HG21	1.95	0.49
25:S:149:THR:HG21	25:S:151:TRP:CZ2	2.47	0.49
1:0:90:TYR:HE2	1:0:92:LEU:HD21	1.77	0.49
7:6:14:LYS:H	7:6:35:SER:HB2	1.77	0.49
11:A:15:A:H2'	11:A:16:A:H8	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:674:A:H5'	11:A:675:C:OP2	2.13	0.49
11:A:688:U:H1'	11:A:1003:G:H21	1.78	0.49
11:A:870:A:H5"	11:A:871:U:OP2	2.13	0.49
19:K:67:PRO:HD2	19:K:85:PRO:HA	1.95	0.49
3:2:242:HIS:NE2	31:Y:47:GLU:OE1	2.41	0.49
11:A:841:C:OP1	14:D:264:ASN:ND2	2.43	0.49
11:A:1519:U:C5	20:N:177:ARG:HG3	2.47	0.49
7:6:45:HIS:CG	7:6:46:TYR:H	2.31	0.49
11:A:351:G:H5'	11:A:352:C:H5	1.78	0.49
15:E:206:VAL:HG13	15:E:297:VAL:HG13	1.95	0.49
25:S:72:TRP:CD1	25:S:73:PRO:HA	2.48	0.49
11:A:1028:G:H5'	11:A:1029:C:H5	1.78	0.49
22:P:186:ILE:HG12	22:P:193:PHE:CD1	2.47	0.49
26:T:75:PHE:CD2	26:T:110:GLU:HG3	2.48	0.49
31:Y:92:ASN:HD22	31:Y:115:LEU:HD21	1.77	0.49
11:A:63:A:N3	11:A:63:A:H2'	2.28	0.49
11:A:1543:A:H5'	11:A:1544:U:OP2	2.12	0.49
25:S:107:THR:HG21	25:S:119:THR:CG2	2.42	0.49
31:Y:59:GLY:N	31:Y:76:VAL:O	2.46	0.49
2:1:58:GLN:HG3	22:P:89:PHE:CZ	2.48	0.48
3:2:115:LEU:O	3:2:118:GLU:HB3	2.12	0.48
11:A:741:U:H3'	11:A:742:A:H5"	1.93	0.48
11:A:1517:U:OP2	11:A:1518:U:O2'	2.30	0.48
6:5:136:GLU:HG2	6:5:177:ARG:HH22	1.77	0.48
7:6:36:ARG:HD3	11:A:1183:A:OP1	2.14	0.48
11:A:70:A:H3'	11:A:71:U:C6	2.48	0.48
11:A:844:C:C2'	11:A:845:U:H5"	2.43	0.48
15:E:208:ALA:HB3	15:E:290:PRO:O	2.13	0.48
21:O:69:VAL:HG23	21:O:89:HIS:CE1	2.48	0.48
15:E:175:LYS:HD2	15:E:296:LEU:HB3	1.94	0.48
20:N:114:LYS:HA	20:N:118:ARG:NH1	2.27	0.48
11:A:115:U:H3'	11:A:116:A:C5'	2.44	0.48
11:A:340:G:H2'	11:A:341:C:C6	2.49	0.48
11:A:924:U:O2'	11:A:925:A:C8	2.65	0.48
25:S:145:VAL:HG22	25:S:174:GLU:HB2	1.94	0.48
11:A:70:A:H5'	11:A:71:U:OP2	2.13	0.48
11:A:1349:U:H2'	11:A:1351:C:H5"	1.95	0.48
11:A:1418:A:H4'	14:D:278:ARG:HH12	1.78	0.48
24:R:110:ILE:HG23	24:R:111:PRO:HD2	1.95	0.48
26:T:75:PHE:HD2	26:T:110:GLU:HG3	1.78	0.48
11:A:520:A:OP1	19:K:106:LYS:HE3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:925:A:H2'	11:A:926:G:O4'	2.13	0.48
11:A:1329:G:HO2'	11:A:1375:U:HO2'	1.60	0.48
14:D:198:GLU:OE2	14:D:203:ARG:N	2.46	0.48
31:Y:159:PHE:CG	31:Y:160:PRO:HD2	2.47	0.48
9:8:113:ARG:NH2	11:A:84:G:OP2	2.46	0.48
11:A:479:G:N2	11:A:480:A:H1'	2.29	0.48
11:A:1536:A:H3'	11:A:1537:C:H6	1.78	0.48
12:B:25:P5P:H5'1	12:B:25:P5P:H8	1.96	0.48
26:T:87:THR:HG21	26:T:91:LYS:HD3	1.95	0.48
26:T:139:GLN:HE21	26:T:150:ILE:HD12	1.78	0.48
28:V:140:VAL:HG21	28:V:158:VAL:HG21	1.95	0.48
2:1:25:PRO:HB2	2:1:27:HIS:CE1	2.49	0.48
11:A:1423:A:H5'	13:C:75:C:OP1	2.14	0.48
15:E:102:LEU:HD23	15:E:296:LEU:HD13	1.96	0.48
15:E:275:ARG:HD2	15:E:333:TYR:CE1	2.49	0.48
22:P:127:VAL:HG11	22:P:138:VAL:HG22	1.96	0.48
31:Y:138:THR:HG22	31:Y:139:GLU:H	1.79	0.48
11:A:1236:A:H5'	11:A:1237:A:OP2	2.14	0.48
17:I:109:GLY:HA2	17:I:140:PHE:HE2	1.78	0.48
17:I:124:LEU:HD13	17:I:131:TYR:CZ	2.48	0.48
24:R:23:GLU:HG3	26:T:264:TRP:CZ3	2.49	0.48
31:Y:94:HIS:ND1	31:Y:113:ALA:HB2	2.29	0.48
1:0:50:ARG:NH1	11:A:1198:A:OP1	2.47	0.48
22:P:233:ARG:HE	22:P:244:LEU:HD11	1.79	0.48
24:R:38:ARG:HB2	24:R:85:LEU:HD11	1.96	0.48
30:X:14:ASN:ND2	31:Y:210:HIS:HA	2.29	0.48
6:5:81:PRO:HA	11:A:1436:U:C2	2.49	0.47
14:D:291:PRO:HA	14:D:292:PRO:HD3	1.74	0.47
15:E:58:VAL:HG21	24:R:139:ARG:HH21	1.78	0.47
18:J:136:GLU:HG2	18:J:144:LEU:HD11	1.96	0.47
19:K:94:ALA:HB1	19:K:116:HIS:CD2	2.46	0.47
25:S:91:GLU:HG3	25:S:106:SER:HB3	1.96	0.47
9:8:124:ARG:NH2	11:A:1202:A:OP1	2.47	0.47
11:A:358:G:H5'	22:P:42:GLY:HA2	1.96	0.47
18:J:95:MET:HG3	18:J:181:ILE:HG12	1.96	0.47
28:V:153:LEU:HD12	28:V:153:LEU:HA	1.70	0.47
6:5:146:GLY:HA3	6:5:150:ARG:NH2	2.28	0.47
11:A:329:A:H8	11:A:828:U:O2'	1.97	0.47
18:J:187:SER:O	18:J:191:PHE:HD1	1.97	0.47
27:U:98:ASN:O	27:U:102:LEU:HB2	2.14	0.47
11:A:1024:A:C6	11:A:1319:C:H1'	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:84:ASP:O	4:3:88:MET:HG2	2.14	0.47
11:A:1397:G:O2'	11:A:1400:C:OP2	2.30	0.47
11:A:1445:A:H5"	11:A:1446:A:OP1	2.15	0.47
27:U:24:VAL:HG11	27:U:39:TYR:CE1	2.48	0.47
31:Y:126:THR:HB	31:Y:152:ARG:NH1	2.30	0.47
3:2:204:MET:HB3	3:2:205:PRO:HD2	1.97	0.47
5:4:52:LEU:CG	5:4:68:ARG:HB3	2.43	0.47
11:A:618:A:HO2'	11:A:619:U:H6	1.61	0.47
11:A:845:U:H5'	11:A:845:U:C6	2.38	0.47
14:D:142:LEU:HB2	14:D:151:TRP:CZ3	2.50	0.47
3:2:239:LYS:HZ1	31:Y:45:PRO:HG3	1.79	0.47
6:5:83:ASN:ND2	11:A:1013:C:H41	2.12	0.47
11:A:2:C:OP1	29:W:48:LYS:N	2.47	0.47
11:A:397:A:C3'	11:A:398:A:H5'	2.45	0.47
11:A:697:G:H2'	11:A:698:A:C8	2.49	0.47
11:A:1290:A:N6	11:A:1302:G:O2'	2.47	0.47
11:A:1519:U:H3'	11:A:1520:A:H5'	1.96	0.47
14:D:148:ARG:HD3	14:D:150:ARG:HD2	1.97	0.47
24:R:15:PHE:HD1	24:R:25:ARG:HH22	1.62	0.47
30:X:28:LEU:HD13	30:X:42:PHE:CE1	2.49	0.47
31:Y:74:GLY:HA3	31:Y:91:LEU:HD11	1.96	0.47
3:2:190:TRP:HB3	31:Y:216:TYR:CZ	2.49	0.47
11:A:16:A:H1'	11:A:101:U:H5	1.80	0.47
11:A:580:C:H5"	27:U:69:ILE:HD13	1.97	0.47
12:B:13:Y5P:N3	12:B:23:P5P:N1	2.63	0.47
19:K:23:ILE:HG12	19:K:67:PRO:HB3	1.96	0.47
21:O:82:LYS:HD2	21:O:82:LYS:HA	1.75	0.47
22:P:114:GLN:HB3	22:P:115:PRO:HD2	1.96	0.47
11:A:62:C:OP1	17:I:76:ARG:NH1	2.48	0.47
11:A:522:C:H5	11:A:530:A:H5"	1.80	0.47
11:A:613:G:H1'	11:A:617:C:O2	2.15	0.47
11:A:1541:U:OP2	15:E:141:ARG:HD2	2.15	0.47
20:N:116:LEU:HD23	20:N:116:LEU:HA	1.76	0.47
28:V:136:LYS:HB3	28:V:152:LEU:HD21	1.97	0.47
31:Y:44:VAL:HG11	31:Y:83:ARG:NE	2.30	0.47
3:2:228:LEU:HD23	3:2:228:LEU:HA	1.70	0.47
10:9:83:GLY:N	11:A:1525:U:H5'	2.30	0.47
18:J:117:ARG:HA	18:J:117:ARG:HD3	1.71	0.47
30:X:80:ARG:HD2	30:X:84:ASN:OD1	2.15	0.47
11:A:1371:U:C2'	11:A:1372:U:H5'	2.45	0.46
22:P:232:ALA:O	22:P:235:GLU:HB3	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:72:ILE:HD11	4:3:118:ARG:HB2	1.96	0.46
11:A:363:A:O2'	11:A:384:U:H5"	2.14	0.46
11:A:386:A:H3'	11:A:387:A:H5"	1.97	0.46
11:A:481:G:H2'	11:A:482:U:O4'	2.14	0.46
11:A:528:A:O2'	11:A:545:A:N1	2.48	0.46
11:A:806:G:H2'	11:A:807:G:H5"	1.97	0.46
11:A:1485:C:OP1	26:T:141:SER:HB3	2.15	0.46
11:A:374:U:H2'	11:A:374:U:O2	2.14	0.46
11:A:478:A:N1	29:W:208:HIS:HA	2.31	0.46
11:A:883:G:H3'	11:A:884:A:H8	1.80	0.46
21:O:77:ILE:HG22	21:O:78:ARG:HG3	1.97	0.46
11:A:1510:U:C2'	11:A:1511:U:H5"	2.45	0.46
17:I:91:LYS:HE2	17:I:116:LYS:HB2	1.98	0.46
20:N:25:MET:HE2	20:N:25:MET:HB3	1.89	0.46
7:6:23:GLN:HE21	7:6:55:LEU:HB3	1.79	0.46
25:S:81:LEU:HB2	25:S:144:MET:SD	2.55	0.46
28:V:90:LEU:HD22	28:V:95:ARG:HD2	1.98	0.46
11:A:196:U:H2'	11:A:197:U:C6	2.50	0.46
11:A:718:C:OP2	14:D:149:LYS:NZ	2.39	0.46
11:A:895:A:H2'	11:A:896:C:C6	2.49	0.46
21:O:41:VAL:HG12	21:O:119:ILE:HG23	1.97	0.46
24:R:25:ARG:NH2	24:R:51:GLU:OE2	2.49	0.46
11:A:1502:A:H4'	11:A:1503:G:OP1	2.15	0.46
18:J:143:LEU:HB3	18:J:147:PHE:HE2	1.81	0.46
24:R:46:TRP:HD1	24:R:122:ALA:HB2	1.80	0.46
28:V:180:LYS:O	28:V:181:ARG:HG2	2.15	0.46
2:1:83:GLU:OE2	2:1:128:THR:HG21	2.16	0.46
11:A:177:C:O2'	27:U:55:ARG:NH1	2.49	0.46
11:A:1139:A:H2'	11:A:1140:U:C6	2.50	0.46
11:A:1140:U:H2'	11:A:1141:U:C6	2.51	0.46
14:D:141:ALA:HB2	14:D:154:ALA:HB2	1.97	0.46
19:K:91:LEU:HD13	19:K:148:ALA:HA	1.98	0.46
20:N:59:ILE:HB	20:N:127:LEU:HD23	1.98	0.46
23:Q:96:TYR:HB3	23:Q:151:VAL:HG11	1.97	0.46
6:5:122:LEU:HD21	24:R:108:LEU:HD13	1.98	0.46
11:A:275:G:N7	14:D:260:LYS:HB2	2.30	0.46
11:A:833:A:H5"	11:A:1429:G:H4'	1.98	0.46
11:A:935:C:H3'	11:A:936:U:H2'	1.98	0.46
14:D:217:LEU:HD11	14:D:225:ALA:HB1	1.98	0.46
15:E:49:TRP:CD1	15:E:155:PHE:HB3	2.50	0.46
21:O:90:ARG:H	21:O:103:ASN:ND2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:P:207:PRO:O	22:P:211:VAL:HG23	2.15	0.46
26:T:76:LEU:HD13	26:T:283:TRP:CE3	2.51	0.46
27:U:116:LEU:HD21	28:V:148:LEU:HD11	1.97	0.46
1:0:53:ILE:HD11	1:0:99:TYR:OH	2.16	0.46
2:1:40:PRO:HB3	2:1:43:TYR:CZ	2.51	0.46
11:A:937:U:H4'	11:A:938:G:OP2	2.16	0.46
11:A:940:U:H2'	11:A:941:C:C6	2.51	0.46
11:A:1139:A:H5'	11:A:1139:A:H8	1.80	0.46
16:F:181:LYS:HA	16:F:181:LYS:HD3	1.70	0.46
6:5:185:PHE:CE2	24:R:132:PRO:HA	2.51	0.45
11:A:624:G:O4'	16:F:154:GLY:HA2	2.15	0.45
20:N:20:LEU:HB2	20:N:141:LEU:HD13	1.98	0.45
2:1:58:GLN:HG3	22:P:89:PHE:CE1	2.52	0.45
11:A:962:A:O2'	11:A:965:G:N3	2.39	0.45
11:A:1527:A:H5'	11:A:1528:C:OP2	2.17	0.45
12:B:38:P5P:H2'	12:B:39:P5P:H8	1.98	0.45
17:I:74:HIS:HB3	17:I:77:HIS:CE1	2.51	0.45
25:S:59:LEU:HB3	25:S:61:VAL:HG23	1.97	0.45
11:A:1519:U:H5	20:N:177:ARG:HG3	1.79	0.45
18:J:143:LEU:HB3	18:J:147:PHE:CE2	2.52	0.45
29:W:194:ALA:O	29:W:198:ILE:HG12	2.16	0.45
1:0:102:GLU:HB2	1:0:130:PHE:CE2	2.51	0.45
2:1:227:PHE:HB2	3:2:158:LEU:O	2.17	0.45
4:3:38:ARG:HB2	11:A:409:U:OP1	2.16	0.45
11:A:786:A:N6	34:A:5158:HOH:O	2.46	0.45
14:D:197:VAL:HG11	14:D:227:ILE:HD13	1.98	0.45
14:D:198:GLU:HG3	14:D:204:GLY:O	2.16	0.45
15:E:111:THR:HG23	15:E:113:ASP:H	1.82	0.45
25:S:72:TRP:CG	25:S:73:PRO:HA	2.51	0.45
30:X:58:GLU:HG2	30:X:63:VAL:O	2.16	0.45
6:5:152:PRO:HG3	6:5:173:ARG:NH1	2.31	0.45
11:A:549:A:P	18:J:128:ASN:HB2	2.56	0.45
11:A:617:C:O3'	11:A:618:A:H8	2.00	0.45
11:A:1312:U:C5'	11:A:1391:C:H5"	2.42	0.45
11:A:1519:U:O2'	20:N:177:ARG:NH2	2.49	0.45
14:D:95:GLY:HA2	14:D:270:ARG:HB2	1.98	0.45
14:D:164:VAL:HG13	14:D:180:GLY:O	2.16	0.45
15:E:197:HIS:CD2	15:E:318:THR:HG22	2.52	0.45
18:J:181:ILE:HB	18:J:186:LEU:HD12	1.98	0.45
19:K:68:THR:OG1	19:K:80:ILE:HD11	2.16	0.45
25:S:71:VAL:HG12	25:S:72:TRP:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:Y:98:VAL:HB	31:Y:107:THR:HB	1.98	0.45
4:3:88:MET:CE	11:A:416:G:H21	2.29	0.45
11:A:58:C:C2’	11:A:59:A:H5”	2.46	0.45
11:A:581:A:H5’	11:A:582:A:OP1	2.16	0.45
11:A:789:A:O3’	15:E:238:ARG:HB2	2.16	0.45
16:F:283:LEU:HB2	22:P:125:ARG:NH1	2.31	0.45
18:J:156:SER:HB3	18:J:159:PRO:CB	2.37	0.45
21:O:31:ALA:HA	21:O:66:VAL:HG13	1.99	0.45
22:P:40:PRO:HA	22:P:45:ARG:HB3	1.98	0.45
27:U:89:ASN:ND2	27:U:124:ARG:HB2	2.32	0.45
28:V:139:LEU:HD12	28:V:147:LEU:O	2.16	0.45
29:W:155:ARG:HD2	29:W:165:MET:SD	2.57	0.45
11:A:41:A:H2’	11:A:42:C:H4’	1.97	0.45
11:A:875:U:HO2’	11:A:876:G:P	2.37	0.45
11:A:1373:U:C2	11:A:1375:U:H5”	2.51	0.45
15:E:97:VAL:HG21	15:E:187:ILE:HD11	1.98	0.45
31:Y:129:LYS:HD3	31:Y:149:ARG:NH2	2.29	0.45
2:1:128:THR:HG22	2:1:129:MET:H	1.81	0.45
5:4:58:VAL:HB	5:4:77:THR:HG23	1.99	0.45
6:5:106:ASN:O	6:5:119:LYS:HG3	2.17	0.45
11:A:993:C:C5’	24:R:13:ARG:HH22	2.25	0.45
15:E:90:TRP:HD1	15:E:316:PHE:CD2	2.35	0.45
16:F:106:PHE:CE1	16:F:107:LYS:HG3	2.52	0.45
28:V:112:VAL:CG1	28:V:199:ILE:HG12	2.46	0.45
1:0:67:LEU:N	1:0:89:LEU:O	2.37	0.45
6:5:138:ARG:HB3	11:A:653:C:O2	2.16	0.45
11:A:102:G:O2’	11:A:103:A:H5’	2.17	0.45
11:A:1518:U:H6	11:A:1518:U:O5’	2.00	0.45
15:E:348:THR:HA	26:T:129:LYS:HE3	1.98	0.45
18:J:135:LEU:HD22	18:J:140:TYR:HB2	1.99	0.45
23:Q:250:ARG:HD2	23:Q:250:ARG:HA	1.77	0.45
27:U:54:THR:HG22	28:V:175:ASN:HA	1.98	0.45
2:1:189:ASP:O	2:1:192:LYS:HB2	2.17	0.45
11:A:203:G:N3	11:A:203:G:H2’	2.31	0.45
11:A:235:U:H5’	11:A:236:A:OP2	2.17	0.45
11:A:524:A:O2’	19:K:135:VAL:HG21	2.16	0.45
11:A:732:A:OP2	14:D:105:ARG:NH2	2.50	0.45
11:A:1055:A:H5”	11:A:1056:C:OP2	2.16	0.45
11:A:1159:G:H4’	11:A:1227:A:H5’	1.99	0.45
22:P:191:VAL:HB	22:P:192:PRO:HD3	1.98	0.45
30:X:14:ASN:HD21	31:Y:211:LYS:H	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:Y:127:ASP:OD1	31:Y:152:ARG:NH1	2.50	0.45
31:Y:133:VAL:CG1	31:Y:145:ARG:HB3	2.47	0.45
11:A:163:A:O2'	11:A:1014:C:H5	1.99	0.44
11:A:502:G:H2'	11:A:503:U:C6	2.52	0.44
11:A:530:A:H2'	11:A:530:A:N3	2.32	0.44
11:A:556:C:O2'	11:A:557:A:OP1	2.32	0.44
11:A:1164:A:N6	11:A:1171:A:OP2	2.43	0.44
16:F:96:LEU:HD23	16:F:96:LEU:HA	1.82	0.44
22:P:54:LYS:HB3	22:P:55:GLY:H	1.50	0.44
27:U:64:LEU:HA	27:U:64:LEU:HD23	1.66	0.44
31:Y:25:ARG:HA	31:Y:26:PRO:HD2	1.82	0.44
9:8:116:ARG:HH11	9:8:167:LYS:HG2	1.82	0.44
11:A:32:C:O2'	11:A:36:A:N6	2.50	0.44
11:A:196:U:H2'	11:A:197:U:H6	1.81	0.44
11:A:476:A:C3'	11:A:477:G:H5"	2.47	0.44
12:B:71:Y5P:H4A	12:B:72:Y5P:H4	1.98	0.44
16:F:114:THR:HB	16:F:155:PRO:HD2	1.99	0.44
17:I:130:VAL:HB	17:I:136:ASN:HD21	1.82	0.44
28:V:60:LEU:HA	28:V:60:LEU:HD23	1.70	0.44
29:W:79:LYS:HA	29:W:79:LYS:HD2	1.86	0.44
31:Y:62:VAL:HB	31:Y:120:VAL:HG13	1.98	0.44
11:A:42:C:H5'	11:A:43:C:OP2	2.17	0.44
11:A:420:U:H2'	11:A:421:U:C6	2.53	0.44
11:A:1028:G:H5'	11:A:1029:C:C5	2.52	0.44
16:F:168:LYS:HE3	16:F:279:ARG:HE	1.82	0.44
16:F:191:ASP:O	16:F:192:SER:OG	2.28	0.44
16:F:293:PHE:HA	16:F:294:PRO:HD3	1.85	0.44
19:K:113:THR:HG22	19:K:114:LEU:H	1.82	0.44
26:T:99:MET:O	26:T:103:ARG:HG2	2.16	0.44
31:Y:196:GLU:H	31:Y:196:GLU:HG2	1.47	0.44
8:7:95:HIS:HD2	11:A:124:A:H5"	1.82	0.44
11:A:6:A:H5'	11:A:7:G:OP2	2.18	0.44
11:A:393:C:H5'	11:A:394:C:OP2	2.17	0.44
17:I:60:TRP:CG	17:I:76:ARG:HG3	2.52	0.44
11:A:473:A:N6	11:A:594:A:C6	2.85	0.44
11:A:1138:A:H2'	11:A:1139:A:H5"	2.00	0.44
20:N:109:TYR:HA	20:N:122:MET:HE1	2.00	0.44
24:R:86:ILE:HB	24:R:87:PRO:HD3	2.00	0.44
27:U:14:VAL:HB	27:U:17:ARG:HH21	1.82	0.44
2:1:42:HIS:CE1	2:1:83:GLU:HB2	2.53	0.44
11:A:816:A:H5"	11:A:816:A:H8	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:913:C:H2'	11:A:914:C:H5'	1.99	0.44
11:A:1374:G:H8	11:A:1374:G:OP1	2.01	0.44
15:E:193:LEU:HD23	15:E:193:LEU:HA	1.76	0.44
22:P:220:ARG:NH2	22:P:233:ARG:HA	2.32	0.44
2:1:42:HIS:O	17:I:55:ILE:HA	2.18	0.44
11:A:549:A:OP1	18:J:128:ASN:HB2	2.17	0.44
11:A:711:A:H4'	11:A:711:A:OP1	2.18	0.44
12:B:25:P5P:C6	12:B:26:Y5P:H4	2.47	0.44
12:B:38:P5P:H2'	12:B:39:P5P:C8	2.48	0.44
15:E:219:MET:SD	15:E:238:ARG:HD3	2.58	0.44
17:I:130:VAL:HB	17:I:136:ASN:ND2	2.33	0.44
19:K:66:LEU:HA	19:K:85:PRO:HA	1.98	0.44
29:W:151:LEU:HB2	29:W:167:LYS:HB2	2.00	0.44
11:A:1485:C:H1'	21:O:95:ARG:NH2	2.32	0.44
11:A:1557:A:H4'	15:E:263:ASN:ND2	2.33	0.44
15:E:112:LYS:HA	15:E:338:CYS:SG	2.58	0.44
30:X:77:ASN:HD22	30:X:77:ASN:HA	1.59	0.44
1:0:90:TYR:CE2	1:0:92:LEU:HD21	2.53	0.44
2:1:97:LEU:HD23	2:1:97:LEU:HA	1.79	0.44
4:3:128:LEU:HA	4:3:129:PRO:HD3	1.89	0.44
11:A:577:U:HO2'	11:A:578:A:P	2.38	0.44
15:E:193:LEU:HD21	15:E:318:THR:HG21	2.00	0.44
16:F:71:GLY:HA3	16:F:74:GLN:HG2	2.00	0.44
23:Q:109:ILE:HD11	23:Q:176:LEU:HD21	2.00	0.44
26:T:197:TYR:CE2	26:T:222:VAL:HG13	2.53	0.44
6:5:108:ASP:OD2	6:5:119:LYS:HE2	2.17	0.43
8:7:77:THR:HG21	11:A:249:A:H5'	1.99	0.43
11:A:572:A:O2'	11:A:573:C:O5'	2.36	0.43
11:A:954:C:C2'	11:A:955:U:H5'	2.47	0.43
15:E:187:ILE:HG22	15:E:188:LYS:N	2.29	0.43
24:R:113:ARG:HD3	24:R:121:MET:SD	2.58	0.43
28:V:88:ASN:ND2	28:V:208:LEU:O	2.51	0.43
11:A:1139:A:O2'	11:A:1140:U:OP1	2.35	0.43
12:B:25:P5P:O5'	25:S:86:THR:HG21	2.18	0.43
15:E:208:ALA:HB2	15:E:297:VAL:HG22	2.00	0.43
16:F:191:ASP:C	16:F:192:SER:HG	2.21	0.43
21:O:128:ARG:NH1	26:T:126:ALA:HA	2.33	0.43
26:T:178:LYS:HB2	26:T:178:LYS:HE3	1.82	0.43
28:V:105:PHE:CE2	28:V:120:ILE:HD13	2.52	0.43
28:V:152:LEU:HD23	28:V:152:LEU:HA	1.84	0.43
10:9:63:PHE:HD2	11:A:1347:G:HO2'	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:9:94:LYS:HE2	11:A:1299:A:H5'	2.00	0.43
14:D:185:LEU:HA	14:D:185:LEU:HD23	1.76	0.43
18:J:95:MET:O	18:J:156:SER:HB2	2.18	0.43
20:N:80:HIS:CD2	20:N:82:GLY:H	2.37	0.43
25:S:126:GLU:CG	25:S:160:ARG:HB3	2.47	0.43
31:Y:98:VAL:HG21	31:Y:109:ILE:HD12	2.01	0.43
31:Y:159:PHE:CD1	31:Y:160:PRO:HD2	2.53	0.43
2:1:168:ARG:NH2	2:1:176:LEU:HA	2.33	0.43
3:2:126:LEU:HD23	30:X:111:PHE:CD1	2.53	0.43
11:A:275:G:C5	14:D:260:LYS:HB2	2.54	0.43
11:A:476:A:H8	11:A:476:A:H5"	1.84	0.43
11:A:570:A:OP1	20:N:107:ALA:HA	2.18	0.43
11:A:1197:A:H2'	11:A:1198:A:O4'	2.19	0.43
15:E:296:LEU:HD12	15:E:296:LEU:HA	1.74	0.43
22:P:178:PHE:CE2	22:P:206:PRO:HA	2.54	0.43
26:T:100:LEU:HD23	26:T:100:LEU:HA	1.88	0.43
26:T:197:TYR:CD2	26:T:222:VAL:HG13	2.53	0.43
27:U:107:ILE:HD13	29:W:206:ILE:HG21	2.00	0.43
4:3:133:ASP:HB3	4:3:147:VAL:HG22	2.01	0.43
11:A:68:A:N3	11:A:69:C:H5'	2.33	0.43
11:A:959:A:H8	11:A:959:A:OP1	2.02	0.43
11:A:1568:C:H5"	11:A:1569:A:H2'	2.00	0.43
18:J:162:LYS:HE3	18:J:195:SER:O	2.17	0.43
22:P:177:ALA:HB1	22:P:203:ARG:NH2	2.33	0.43
25:S:68:TRP:CD1	25:S:75:ARG:HB2	2.54	0.43
27:U:87:ILE:O	27:U:91:ILE:HG13	2.18	0.43
2:1:161:LEU:HD12	2:1:161:LEU:HA	1.76	0.43
9:8:115:LEU:HB2	22:P:83:PHE:CD1	2.53	0.43
9:8:175:ASP:HB3	9:8:178:GLN:HB2	2.01	0.43
11:A:809:A:N3	15:E:230:THR:HG21	2.33	0.43
12:B:30:P5P:H3'	12:B:31:Y5P:H6	2.00	0.43
18:J:108:ASP:O	18:J:112:LEU:HB2	2.18	0.43
22:P:47:ARG:HD2	28:V:183:ASN:ND2	2.33	0.43
25:S:143:PHE:CD1	25:S:175:PRO:HD3	2.53	0.43
4:3:101:LYS:HE3	11:A:416:G:OP1	2.18	0.43
8:7:58:PRO:HG2	11:A:758:C:H5'	2.01	0.43
11:A:421:U:H2'	11:A:422:U:C6	2.53	0.43
11:A:428:G:C5'	22:P:57:ARG:HD3	2.47	0.43
11:A:502:G:C6	11:A:523:A:C2	3.07	0.43
11:A:931:A:H1'	11:A:1426:U:O2'	2.19	0.43
11:A:1157:U:H1'	11:A:1249:C:H2'	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:D:170:ILE:HG21	14:D:239:GLU:OE2	2.18	0.43
18:J:47:LEU:HD22	23:Q:226:ILE:HG13	2.01	0.43
19:K:24:VAL:HB	19:K:53:PHE:CZ	2.54	0.43
23:Q:211:ASN:HA	23:Q:212:PRO:HD3	1.80	0.43
1:0:92:LEU:HB3	25:S:66:ARG:HE	1.84	0.43
11:A:328:A:C2	14:D:275:LEU:HD13	2.52	0.43
11:A:772:A:H8	11:A:772:A:C5'	2.31	0.43
16:F:168:LYS:HE3	16:F:279:ARG:HH21	1.83	0.43
22:P:68:GLU:CG	22:P:73:PRO:HA	2.48	0.43
22:P:121:LEU:HD23	22:P:121:LEU:HA	1.83	0.43
25:S:58:LEU:HD23	25:S:58:LEU:HA	1.77	0.43
26:T:99:MET:HB2	26:T:167:TYR:CE1	2.54	0.43
26:T:233:TRP:CE3	26:T:240:ILE:HD11	2.54	0.43
27:U:50:PHE:O	27:U:54:THR:HG23	2.19	0.43
30:X:112:PRO:O	30:X:113:GLU:HB2	2.18	0.43
11:A:501:A:H1'	11:A:524:A:C2	2.53	0.43
11:A:1255:A:C8	11:A:1255:A:C3'	3.02	0.43
12:B:43:Y5P:H2'	12:B:44:Y5P:HB2	2.01	0.43
14:D:111:ARG:HD2	14:D:182:ALA:HB2	2.01	0.43
22:P:118:LEU:HD23	22:P:187:LEU:HD23	2.01	0.43
23:Q:205:ARG:NH1	23:Q:249:GLU:HA	2.34	0.43
2:1:93:ASN:O	2:1:94:ASN:HB2	2.19	0.43
7:6:38:ARG:NE	11:A:1184:U:H5'	2.33	0.43
8:7:84:ARG:NH1	11:A:126:G:OP1	2.52	0.43
11:A:101:U:O2'	11:A:102:G:O4'	2.30	0.43
11:A:624:G:C5	27:U:11:ARG:HB2	2.53	0.43
11:A:913:C:C2'	11:A:914:C:H5'	2.48	0.43
11:A:936:U:H4'	11:A:937:U:OP1	2.18	0.43
12:B:4:P5P:O5'	12:B:4:P5P:H8	2.19	0.43
14:D:133:ASP:OD2	14:D:136:ARG:HG2	2.18	0.43
23:Q:98:HIS:HD2	23:Q:100:GLY:H	1.67	0.43
31:Y:73:GLN:OE1	31:Y:123:VAL:HG21	2.19	0.43
3:2:119:GLN:NE2	11:A:700:A:OP1	2.50	0.42
11:A:759:A:N1	11:A:763:C:H2'	2.33	0.42
16:F:84:PRO:O	16:F:88:SER:HB3	2.18	0.42
27:U:87:ILE:HD13	27:U:87:ILE:HA	1.69	0.42
31:Y:19:TYR:OH	31:Y:26:PRO:HA	2.19	0.42
10:9:69:LEU:HD11	10:9:85:TRP:O	2.18	0.42
11:A:70:A:H3'	11:A:71:U:H6	1.84	0.42
11:A:571:A:H5"	11:A:572:A:OP2	2.19	0.42
16:F:221:LEU:HG	16:F:222:GLU:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:K:139:SER:HA	19:K:142:ARG:HD2	2.02	0.42
23:Q:205:ARG:HH12	23:Q:249:GLU:HA	1.84	0.42
25:S:163:HIS:O	25:S:167:GLU:HG2	2.19	0.42
27:U:29:ARG:HD3	27:U:29:ARG:HA	1.87	0.42
29:W:92:ILE:HD12	29:W:140:VAL:HG21	2.00	0.42
30:X:136:SER:HA	30:X:137:PRO:HD3	1.88	0.42
11:A:162:C:H5	11:A:1011:A:H61	1.66	0.42
11:A:704:A:OP1	30:X:50:ARG:NH2	2.26	0.42
11:A:718:C:H6	11:A:718:C:OP1	2.02	0.42
11:A:1393:A:OP2	11:A:1393:A:H8	2.02	0.42
11:A:1544:U:H5"	11:A:1545:A:OP2	2.19	0.42
25:S:125:CYS:SG	25:S:157:SER:HB2	2.59	0.42
31:Y:65:LEU:HD11	31:Y:121:LYS:HG3	2.01	0.42
2:1:16:LEU:HD11	2:1:29:LEU:HD22	2.01	0.42
11:A:150:A:O5'	11:A:150:A:H8	2.02	0.42
11:A:397:A:C2'	11:A:398:A:H5'	2.50	0.42
11:A:799:G:H4'	21:O:36:THR:HG22	2.01	0.42
11:A:863:A:H2'	11:A:864:G:H8	1.84	0.42
15:E:149:GLY:O	15:E:173:LYS:HD2	2.19	0.42
19:K:135:VAL:HG12	19:K:136:PRO:HD2	2.01	0.42
20:N:117:HIS:O	20:N:121:MET:HG2	2.19	0.42
25:S:144:MET:O	25:S:172:LEU:HA	2.19	0.42
26:T:118:ARG:HA	26:T:133:PHE:O	2.19	0.42
31:Y:66:GLU:HB3	31:Y:119:GLN:HB3	2.01	0.42
12:B:69:Y5P:H2'	12:B:70:P5P:O4'	2.20	0.42
22:P:28:LYS:HA	22:P:29:PRO:HD2	1.91	0.42
23:Q:105:MET:O	23:Q:109:ILE:HB	2.19	0.42
26:T:82:PRO:HA	26:T:83:PRO:HD3	1.77	0.42
1:0:35:THR:HG21	23:Q:138:GLN:OE1	2.20	0.42
11:A:255:U:H2'	11:A:256:A:H5'	2.01	0.42
23:Q:72:ILE:HD11	23:Q:96:TYR:CZ	2.55	0.42
26:T:76:LEU:HD13	26:T:283:TRP:CZ3	2.55	0.42
26:T:84:ARG:HG3	26:T:273:TYR:HE1	1.85	0.42
26:T:97:LYS:O	26:T:101:GLU:HG2	2.19	0.42
26:T:190:LEU:HD23	26:T:190:LEU:HA	1.86	0.42
28:V:165:ILE:CD1	28:V:198:ARG:HB2	2.49	0.42
28:V:176:MET:HE2	28:V:176:MET:HB3	1.76	0.42
4:3:73:LYS:HB3	4:3:73:LYS:HE2	1.43	0.42
7:6:50:VAL:HB	7:6:52:LYS:HG2	2.01	0.42
9:8:95:THR:HB	9:8:105:LYS:HB2	2.00	0.42
11:A:91:A:C8	11:A:92:U:C6	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:890:G:O5'	11:A:890:G:H8	2.02	0.42
11:A:1547:A:N6	11:A:1548:U:O4	2.53	0.42
12:B:3:Y5P:N3	12:B:67:P5P:N1	2.68	0.42
14:D:175:VAL:HG11	14:D:183:HIS:CE1	2.54	0.42
15:E:195:ALA:H	15:E:281:ASN:ND2	2.18	0.42
16:F:184:GLN:O	16:F:185:ASP:HB2	2.19	0.42
22:P:160:SER:O	22:P:164:ILE:HG13	2.20	0.42
23:Q:226:ILE:HD13	23:Q:226:ILE:HA	1.74	0.42
25:S:96:HIS:HD2	25:S:98:ASN:HB2	1.84	0.42
28:V:85:GLY:O	28:V:89:GLU:HG2	2.20	0.42
28:V:91:ILE:HD12	28:V:204:ILE:HD13	2.02	0.42
30:X:3:ARG:H	30:X:23:ASN:HB3	1.85	0.42
31:Y:22:GLY:C	31:Y:24:SER:H	2.21	0.42
3:2:75:ASN:OD1	3:2:81:VAL:HG11	2.20	0.42
11:A:163:A:H3'	27:U:35:LYS:HZ2	1.84	0.42
11:A:673:U:H4'	11:A:674:A:H5"	2.01	0.42
11:A:929:U:C3'	11:A:930:A:H5'	2.50	0.42
11:A:993:C:H5"	24:R:13:ARG:NH2	2.27	0.42
11:A:1339:A:N3	11:A:1339:A:H2'	2.34	0.42
14:D:189:PRO:HD2	14:D:192:THR:HG21	2.01	0.42
22:P:209:ALA:O	22:P:212:PRO:HD2	2.19	0.42
24:R:83:LYS:HA	24:R:83:LYS:HD2	1.81	0.42
25:S:89:HIS:HA	25:S:119:THR:CG2	2.49	0.42
28:V:150:LYS:HA	28:V:151:PRO:HA	1.85	0.42
30:X:141:ARG:HA	30:X:141:ARG:HD2	1.66	0.42
1:0:53:ILE:HD11	1:0:99:TYR:CZ	2.54	0.42
2:1:202:GLU:HG3	2:1:203:TRP:CD1	2.55	0.42
4:3:88:MET:HG2	4:3:88:MET:H	1.56	0.42
11:A:136:A:H5"	31:Y:85:TRP:CH2	2.55	0.42
11:A:671:C:O2'	11:A:757:C:H5"	2.20	0.42
11:A:735:G:H2'	11:A:736:U:C6	2.55	0.42
11:A:777:G:H5'	11:A:778:G:OP2	2.20	0.42
11:A:954:C:H2'	11:A:955:U:H5'	2.02	0.42
11:A:1209:A:OP2	25:S:176:ARG:NH2	2.49	0.42
11:A:1452:C:H2'	11:A:1453:C:O4'	2.20	0.42
14:D:74:VAL:HG13	14:D:151:TRP:NE1	2.35	0.42
22:P:27:LEU:HD23	22:P:27:LEU:HA	1.88	0.42
1:0:77:PRO:HD2	25:S:70:THR:OG1	2.20	0.42
10:9:71:LYS:HB3	10:9:76:CYS:HB2	2.02	0.42
11:A:1048:C:O5'	11:A:1049:G:H5"	2.20	0.42
11:A:1060:A:H3'	11:A:1061:U:H5"	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:1194:G:H8	11:A:1194:G:O5'	2.03	0.42
12:B:61:Y5P:H2'	12:B:62:Y5P:H6	2.01	0.42
15:E:99:LEU:HD12	15:E:198:PHE:CE1	2.53	0.42
18:J:61:ASN:CG	18:J:62:PRO:HD2	2.40	0.42
26:T:100:LEU:HD11	26:T:286:ILE:HG12	2.01	0.42
26:T:112:TYR:O	26:T:115:SER:HB3	2.19	0.42
29:W:78:ILE:HG22	29:W:80:TYR:H	1.84	0.42
31:Y:127:ASP:HB3	31:Y:152:ARG:HH22	1.85	0.42
4:3:108:ALA:O	4:3:111:LYS:HB2	2.19	0.41
11:A:812:C:O2	11:A:812:C:H2'	2.20	0.41
14:D:125:GLU:HB3	14:D:143:VAL:HG13	2.02	0.41
18:J:69:PRO:O	18:J:71:PRO:HD3	2.20	0.41
22:P:176:THR:HB	22:P:221:GLY:HA2	2.01	0.41
3:2:168:GLY:HA3	3:2:180:TRP:CZ2	2.55	0.41
9:8:142:ARG:HA	9:8:145:ARG:NH1	2.35	0.41
10:9:69:LEU:HD13	10:9:87:ILE:HG12	2.02	0.41
11:A:52:A:H4'	11:A:244:A:H2	1.85	0.41
11:A:356:U:H5"	11:A:357:U:OP1	2.20	0.41
11:A:691:U:O2'	11:A:692:A:P	2.79	0.41
17:I:115:LYS:HE3	17:I:117:SER:HB2	2.02	0.41
26:T:115:SER:HB2	26:T:180:GLU:H	1.85	0.41
27:U:90:LEU:HD12	27:U:90:LEU:HA	1.72	0.41
31:Y:105:ARG:HD3	31:Y:105:ARG:N	2.28	0.41
2:1:156:LYS:HD2	2:1:156:LYS:HA	1.85	0.41
9:8:140:ARG:HD2	11:A:1204:U:OP1	2.21	0.41
11:A:119:A:H3'	11:A:120:C:H6	1.86	0.41
11:A:530:A:H61	19:K:150:SER:HB3	1.85	0.41
20:N:20:LEU:HD12	20:N:58:VAL:O	2.19	0.41
21:O:33:GLN:H	21:O:36:THR:HG21	1.86	0.41
21:O:107:LEU:HD23	21:O:107:LEU:HA	1.75	0.41
22:P:51:ARG:HD3	22:P:51:ARG:HA	1.86	0.41
24:R:132:PRO:HA	24:R:133:PRO:HD3	1.96	0.41
25:S:149:THR:HG21	25:S:151:TRP:CH2	2.56	0.41
4:3:91:LEU:HD23	4:3:91:LEU:HA	1.75	0.41
9:8:127:ALA:HA	22:P:79:PRO:HD3	2.02	0.41
11:A:174:C:H3'	11:A:175:U:C6	2.55	0.41
11:A:226:U:O2'	11:A:229:G:H4'	2.21	0.41
11:A:648:A:O2'	11:A:782:G:H5"	2.20	0.41
11:A:741:U:C3'	11:A:742:A:H5"	2.51	0.41
11:A:1180:G:O2'	11:A:1247:A:N6	2.53	0.41
16:F:274:LEU:HD23	16:F:274:LEU:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:O:89:HIS:HA	21:O:103:ASN:HD22	1.85	0.41
22:P:223:LEU:HD23	22:P:223:LEU:HA	1.80	0.41
8:7:66:LYS:O	8:7:71:ARG:HG2	2.21	0.41
8:7:74:ARG:HD3	8:7:74:ARG:HA	1.54	0.41
9:8:123:LEU:HD12	9:8:148:VAL:O	2.20	0.41
11:A:251:G:N1	11:A:320:A:C2	2.88	0.41
11:A:772:A:H8	11:A:772:A:H5'	1.85	0.41
11:A:781:A:C2	24:R:20:LEU:HG	2.55	0.41
11:A:1395:G:H2'	11:A:1396:U:O4'	2.20	0.41
12:B:4:P5P:H2'	12:B:5:P5P:C8	2.50	0.41
12:B:14:P5P:H5'2	12:B:15:P5P:OP2	2.20	0.41
24:R:65:LEU:HD23	24:R:65:LEU:HA	1.91	0.41
28:V:63:PRO:HA	28:V:64:PRO:HD3	1.69	0.41
1:0:107:ASN:OD1	1:0:108:PRO:HD2	2.20	0.41
4:3:110:LEU:HD23	4:3:110:LEU:HA	1.88	0.41
6:5:96:ASN:ND2	11:A:1039:A:O4'	2.52	0.41
6:5:96:ASN:HD21	11:A:1038:A:H2'	1.85	0.41
11:A:255:U:C2'	11:A:256:A:H5'	2.50	0.41
11:A:511:A:H61	11:A:512:A:N6	2.18	0.41
11:A:1418:A:H5'	14:D:278:ARG:NH2	2.36	0.41
21:O:51:TYR:CZ	21:O:78:ARG:HA	2.55	0.41
24:R:153:LEU:HA	24:R:153:LEU:HD23	1.68	0.41
27:U:58:ARG:HG2	27:U:62:ARG:NH2	2.36	0.41
2:1:88:GLY:C	2:1:89:HIS:HD2	2.24	0.41
11:A:386:A:C3'	11:A:387:A:H5"	2.50	0.41
11:A:1240:U:O2'	11:A:1241:U:OP2	2.34	0.41
12:B:23:P5P:H2'	12:B:24:P5P:O4'	2.20	0.41
14:D:113:ARG:HB3	14:D:148:ARG:HH22	1.85	0.41
15:E:239:ARG:H	15:E:239:ARG:HG3	1.59	0.41
16:F:71:GLY:H	16:F:74:GLN:HE21	1.69	0.41
16:F:195:LEU:HG	16:F:230:VAL:HG22	2.03	0.41
17:I:70:LYS:HA	17:I:71:PRO:HD3	1.82	0.41
17:I:73:LEU:HA	17:I:73:LEU:HD23	1.84	0.41
22:P:269:LEU:HD23	22:P:269:LEU:HA	1.91	0.41
26:T:136:ILE:O	26:T:151:LEU:HA	2.21	0.41
3:2:100:LEU:HD22	3:2:144:LEU:CD1	2.51	0.41
7:6:47:ASP:HB2	7:6:54:VAL:CG2	2.45	0.41
11:A:196:U:O3'	27:U:38:CYS:HB3	2.20	0.41
11:A:275:G:H5"	14:D:260:LYS:HD3	2.02	0.41
11:A:507:C:H2'	11:A:508:C:O4'	2.21	0.41
12:B:9:P5P:H5'2	12:B:47:P5P:C1'	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:D:129:ALA:HB1	14:D:131:ARG:HE	1.85	0.41
15:E:195:ALA:HB3	15:E:281:ASN:HD22	1.86	0.41
15:E:206:VAL:HG11	15:E:289:VAL:HG13	2.03	0.41
15:E:279:LYS:HB2	15:E:330:GLU:OE1	2.20	0.41
20:N:27:PRO:HA	20:N:66:ALA:O	2.20	0.41
26:T:145:LEU:HD12	26:T:145:LEU:HA	1.84	0.41
2:1:71:TYR:HA	2:1:72:PRO:HD2	1.94	0.41
9:8:103:LYS:NZ	11:A:76:G:OP2	2.53	0.41
11:A:70:A:N3	11:A:70:A:H2'	2.36	0.41
11:A:118:U:H2'	11:A:119:A:H5"	2.03	0.41
11:A:137:A:C2	11:A:139:A:C4	3.09	0.41
11:A:429:A:OP2	22:P:57:ARG:HD2	2.20	0.41
11:A:522:C:C5	11:A:530:A:H5"	2.54	0.41
11:A:1074:A:H2'	11:A:1075:A:H8	1.82	0.41
11:A:1312:U:HO2'	11:A:1313:U:H6	1.69	0.41
11:A:1545:A:N7	15:E:178:ILE:HD12	2.36	0.41
12:B:48:Y5P:HA	12:B:49:P5P:O5'	2.20	0.41
12:B:63:Y5P:O5'	12:B:63:Y5P:H6	2.21	0.41
15:E:54:SER:O	15:E:58:VAL:HG23	2.21	0.41
18:J:132:LYS:O	18:J:136:GLU:HG3	2.21	0.41
18:J:188:ARG:O	18:J:192:ILE:HG13	2.20	0.41
22:P:127:VAL:HG11	22:P:138:VAL:CG2	2.51	0.41
25:S:126:GLU:OE2	25:S:160:ARG:HD3	2.20	0.41
26:T:235:ARG:HA	26:T:236:PRO:HD3	1.78	0.41
27:U:116:LEU:HD23	27:U:116:LEU:HA	1.75	0.41
27:U:126:GLU:OE2	28:V:70:LEU:HD21	2.21	0.41
29:W:58:PRO:HA	29:W:59:PRO:HD3	1.88	0.41
31:Y:58:CYS:HB2	31:Y:77:VAL:O	2.20	0.41
4:3:73:LYS:HA	11:A:471:U:OP1	2.20	0.41
7:6:22:SER:HB3	7:6:56:PHE:CZ	2.56	0.41
9:8:118:HIS:CD2	9:8:169:ARG:HH11	2.39	0.41
11:A:3:C:OP1	29:W:171:HIS:HE1	2.04	0.41
11:A:844:C:C3'	11:A:845:U:H5"	2.51	0.41
11:A:1490:C:N3	24:R:15:PHE:HD2	2.19	0.41
15:E:285:VAL:HG12	15:E:286:ASN:N	2.33	0.41
22:P:68:GLU:HG3	22:P:73:PRO:HA	2.02	0.41
24:R:142:ASN:O	24:R:148:GLN:NE2	2.54	0.41
27:U:94:GLN:HE22	27:U:145:VAL:HG13	1.85	0.41
29:W:157:HIS:HB2	29:W:161:ARG:O	2.21	0.41
31:Y:146:VAL:HA	31:Y:152:ARG:O	2.21	0.41
2:1:128:THR:HG22	2:1:129:MET:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:160:TYR:CD2	6:5:181:ARG:HB2	2.56	0.40
7:6:19:LYS:HE3	7:6:28:PHE:CD1	2.56	0.40
11:A:113:G:N2	11:A:116:A:O2'	2.54	0.40
11:A:168:U:H5"	11:A:169:U:OP2	2.21	0.40
11:A:492:U:H2'	11:A:493:A:H5"	2.02	0.40
11:A:1210:U:H5'	11:A:1211:A:OP2	2.21	0.40
23:Q:92:LEU:HA	23:Q:92:LEU:HD23	1.75	0.40
3:2:100:LEU:HD23	3:2:100:LEU:HA	1.89	0.40
8:7:83:LEU:HD23	8:7:83:LEU:HA	1.87	0.40
11:A:147:A:H8	11:A:147:A:OP2	2.04	0.40
11:A:241:G:H5'	16:F:139:GLY:N	2.35	0.40
11:A:476:A:H3'	11:A:477:G:H5"	2.03	0.40
18:J:46:LYS:O	18:J:50:VAL:HG23	2.21	0.40
19:K:54:ASN:HB3	19:K:58:LYS:CE	2.52	0.40
20:N:90:VAL:CG1	20:N:94:GLN:HB2	2.51	0.40
24:R:28:LEU:HD23	24:R:28:LEU:HA	1.94	0.40
24:R:131:LEU:HD23	24:R:131:LEU:HA	1.94	0.40
4:3:88:MET:HE3	11:A:416:G:H21	1.86	0.40
9:8:118:HIS:CG	9:8:169:ARG:HD3	2.56	0.40
11:A:197:U:H2'	11:A:198:A:C8	2.56	0.40
11:A:350:A:H5'	11:A:351:G:OP2	2.20	0.40
11:A:560:A:H3'	11:A:560:A:N3	2.36	0.40
14:D:123:PHE:O	14:D:165:LEU:HD12	2.20	0.40
14:D:139:ASP:OD2	14:D:250:ASN:HB2	2.20	0.40
15:E:341:GLY:CA	26:T:105:ILE:HD11	2.47	0.40
20:N:10:GLN:HE21	29:W:202:ARG:HA	1.86	0.40
25:S:86:THR:O	25:S:120:ARG:NH1	2.53	0.40
26:T:74:ARG:HD3	26:T:283:TRP:NE1	2.36	0.40
2:1:79:LEU:HG	2:1:125:VAL:HG11	2.03	0.40
11:A:504:A:H1'	11:A:513:A:C8	2.57	0.40
11:A:520:A:H5"	11:A:521:U:OP2	2.21	0.40
11:A:845:U:H2'	11:A:846:C:O4'	2.21	0.40
11:A:936:U:C4'	11:A:937:U:H3'	2.52	0.40
14:D:290:LEU:HD12	14:D:291:PRO:HD2	2.02	0.40
15:E:293:LYS:HE2	15:E:293:LYS:HB3	1.72	0.40
18:J:113:ARG:HG2	18:J:123:MET:SD	2.62	0.40
23:Q:172:VAL:H	23:Q:172:VAL:HG23	1.68	0.40
2:1:23:ARG:HD3	2:1:219:GLU:OE2	2.20	0.40
11:A:420:U:H2'	11:A:421:U:H6	1.86	0.40
11:A:503:U:H5"	19:K:86:THR:HG23	2.03	0.40
11:A:673:U:H5"	30:X:78:ARG:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:1238:A:O2'	11:A:1239:U:OP2	2.36	0.40
12:B:11:Y5P:H4A	12:B:12:Y5P:H4	2.04	0.40
14:D:247:ARG:NH1	14:D:251:VAL:HG11	2.36	0.40
14:D:258:ILE:HG23	14:D:263:ARG:CB	2.51	0.40
18:J:176:LEU:HB3	18:J:188:ARG:HH11	1.87	0.40
19:K:111:LEU:HD11	19:K:156:VAL:HG23	2.03	0.40
20:N:138:LEU:HD23	20:N:138:LEU:HA	1.89	0.40
21:O:58:ILE:HD11	21:O:76:ALA:HB2	2.02	0.40
26:T:112:TYR:CE2	26:T:181:LYS:HE2	2.57	0.40
26:T:240:ILE:HG21	26:T:243:ILE:HG12	2.02	0.40
28:V:170:SER:HB2	28:V:194:GLN:CD	2.42	0.40
29:W:96:SER:HB3	29:W:181:PRO:HG3	2.03	0.40
31:Y:98:VAL:CG2	31:Y:109:ILE:HD12	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	112/148 (76%)	110 (98%)	2 (2%)	0	100	100
2	1	242/256 (94%)	235 (97%)	7 (3%)	0	100	100
3	2	176/252 (70%)	167 (95%)	9 (5%)	0	100	100
4	3	116/161 (72%)	113 (97%)	3 (3%)	0	100	100
5	4	43/126 (34%)	42 (98%)	1 (2%)	0	100	100
6	5	108/188 (57%)	107 (99%)	1 (1%)	0	100	100
7	6	46/65 (71%)	44 (96%)	2 (4%)	0	100	100
8	7	44/95 (46%)	44 (100%)	0	0	100	100
9	8	93/188 (50%)	91 (98%)	2 (2%)	0	100	100
10	9	36/100 (36%)	36 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	D	238/306 (78%)	230 (97%)	8 (3%)	0	100	100
15	E	305/348 (88%)	279 (92%)	24 (8%)	2 (1%)	22	55
16	F	248/294 (84%)	237 (96%)	10 (4%)	1 (0%)	34	67
17	I	96/268 (36%)	87 (91%)	9 (9%)	0	100	100
18	J	166/262 (63%)	158 (95%)	8 (5%)	0	100	100
19	K	140/192 (73%)	133 (95%)	7 (5%)	0	100	100
20	N	175/178 (98%)	171 (98%)	4 (2%)	0	100	100
21	O	113/145 (78%)	109 (96%)	4 (4%)	0	100	100
22	P	286/296 (97%)	275 (96%)	11 (4%)	0	100	100
23	Q	219/251 (87%)	217 (99%)	2 (1%)	0	100	100
24	R	151/169 (89%)	148 (98%)	3 (2%)	0	100	100
25	S	141/180 (78%)	128 (91%)	12 (8%)	1 (1%)	22	55
26	T	222/292 (76%)	215 (97%)	6 (3%)	1 (0%)	29	61
27	U	138/149 (93%)	136 (99%)	2 (1%)	0	100	100
28	V	153/209 (73%)	148 (97%)	5 (3%)	0	100	100
29	W	164/210 (78%)	159 (97%)	5 (3%)	0	100	100
30	X	130/150 (87%)	125 (96%)	5 (4%)	0	100	100
31	Y	202/216 (94%)	191 (95%)	11 (5%)	0	100	100
All	All	4303/5694 (76%)	4135 (96%)	163 (4%)	5 (0%)	54	82

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	E	202	GLN
15	E	317	PRO
26	T	270	MET
16	F	291	CYS
25	S	45	ALA

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	92/115 (80%)	82 (89%)	10 (11%)	6	23
2	1	219/229 (96%)	209 (95%)	10 (5%)	27	57
3	2	164/228 (72%)	160 (98%)	4 (2%)	49	74
4	3	110/147 (75%)	107 (97%)	3 (3%)	44	70
5	4	42/114 (37%)	38 (90%)	4 (10%)	8	29
6	5	99/163 (61%)	96 (97%)	3 (3%)	41	68
7	6	45/60 (75%)	41 (91%)	4 (9%)	9	33
8	7	41/78 (53%)	36 (88%)	5 (12%)	5	18
9	8	87/162 (54%)	75 (86%)	12 (14%)	3	14
10	9	36/77 (47%)	34 (94%)	2 (6%)	21	51
14	D	193/248 (78%)	186 (96%)	7 (4%)	35	63
15	E	263/290 (91%)	246 (94%)	17 (6%)	17	46
16	F	217/251 (86%)	200 (92%)	17 (8%)	12	39
17	I	88/228 (39%)	84 (96%)	4 (4%)	27	58
18	J	154/230 (67%)	145 (94%)	9 (6%)	20	50
19	K	115/151 (76%)	107 (93%)	8 (7%)	15	44
20	N	156/157 (99%)	148 (95%)	8 (5%)	24	54
21	O	99/123 (80%)	91 (92%)	8 (8%)	11	38
22	P	245/249 (98%)	231 (94%)	14 (6%)	20	50
23	Q	189/210 (90%)	179 (95%)	10 (5%)	22	52
24	R	132/143 (92%)	122 (92%)	10 (8%)	13	41
25	S	123/153 (80%)	118 (96%)	5 (4%)	30	59
26	T	206/258 (80%)	197 (96%)	9 (4%)	28	58
27	U	118/127 (93%)	109 (92%)	9 (8%)	13	41
28	V	136/178 (76%)	127 (93%)	9 (7%)	16	46
29	W	144/180 (80%)	135 (94%)	9 (6%)	18	47
30	X	119/134 (89%)	110 (92%)	9 (8%)	13	41
31	Y	183/192 (95%)	170 (93%)	13 (7%)	14	44
All	All	3815/4875 (78%)	3583 (94%)	232 (6%)	22	48

All (232) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	45	LYS
1	0	46	SER
1	0	50	ARG
1	0	57	GLU
1	0	71	ARG
1	0	75	TRP
1	0	88	CYS
1	0	94	GLU
1	0	117	VAL
1	0	126	LEU
2	1	61	ARG
2	1	69	VAL
2	1	90	ARG
2	1	101	VAL
2	1	104	VAL
2	1	120	ASP
2	1	159	MET
2	1	173	ASP
2	1	177	HIS
2	1	179	ASP
3	2	83	SER
3	2	153	ASP
3	2	156	ARG
3	2	228	LEU
4	3	40	ARG
4	3	88	MET
4	3	147	VAL
5	4	38	ARG
5	4	42	THR
5	4	43	ARG
5	4	60	GLN
6	5	92	CYS
6	5	156	THR
6	5	186	THR
7	6	18	VAL
7	6	32	THR
7	6	42	THR
7	6	54	VAL
8	7	65	HIS
8	7	74	ARG
8	7	77	THR
8	7	94	SER
8	7	95	HIS

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Mol	Chain	Res	Type
9	8	98	SER
9	8	106	THR
9	8	111	ILE
9	8	113	ARG
9	8	116	ARG
9	8	124	ARG
9	8	148	VAL
9	8	150	CYS
9	8	162	THR
9	8	163	THR
9	8	169	ARG
9	8	183	ARG
10	9	75	ASP
10	9	100	MET
14	D	62	THR
14	D	105	ARG
14	D	111	ARG
14	D	148	ARG
14	D	179	GLU
14	D	256	ARG
14	D	278	ARG
15	E	94	SER
15	E	96	ARG
15	E	102	LEU
15	E	118	VAL
15	E	127	CYS
15	E	153	SER
15	E	189	PRO
15	E	220	ARG
15	E	227	GLN
15	E	236	THR
15	E	239	ARG
15	E	251	VAL
15	E	273	VAL
15	E	288	SER
15	E	295	CYS
15	E	296	LEU
15	E	344	SER
16	F	68	SER
16	F	76	ARG
16	F	79	LEU
16	F	111	TYR

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Mol	Chain	Res	Type
16	F	114	THR
16	F	125	ARG
16	F	143	SER
16	F	147	ARG
16	F	164	MET
16	F	174	LEU
16	F	190	VAL
16	F	203	LEU
16	F	226	MET
16	F	234	THR
16	F	239	THR
16	F	241	ASN
16	F	284	TYR
17	I	64	LEU
17	I	79	VAL
17	I	83	VAL
17	I	108	ARG
18	J	35	ARG
18	J	38	ARG
18	J	61	ASN
18	J	63	ARG
18	J	65	LEU
18	J	76	THR
18	J	116	LEU
18	J	150	HIS
18	J	183	ASP
19	K	64	ILE
19	K	66	LEU
19	K	70	ILE
19	K	80	ILE
19	K	97	ILE
19	K	113	THR
19	K	128	ASP
19	K	135	VAL
20	N	2	SER
20	N	25	MET
20	N	36	SER
20	N	67	PHE
20	N	78	SER
20	N	104	VAL
20	N	118	ARG
20	N	177	ARG

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Mol	Chain	Res	Type
21	O	33	GLN
21	O	48	THR
21	O	73	ILE
21	O	77	ILE
21	O	91	MET
21	O	95	ARG
21	O	121	THR
21	O	138	LEU
22	P	30	ASN
22	P	43	ARG
22	P	44	ARG
22	P	47	ARG
22	P	61	THR
22	P	62	ARG
22	P	64	ARG
22	P	65	LEU
22	P	88	SER
22	P	130	GLN
22	P	141	VAL
22	P	215	THR
22	P	284	LYS
22	P	286	THR
23	Q	62	VAL
23	Q	86	ARG
23	Q	96	TYR
23	Q	104	MET
23	Q	109	ILE
23	Q	110	ASN
23	Q	163	MET
23	Q	209	ASN
23	Q	226	ILE
23	Q	234	ASP
24	R	9	ILE
24	R	14	VAL
24	R	16	ARG
24	R	25	ARG
24	R	50	ASP
24	R	61	ASP
24	R	116	GLN
24	R	118	ARG
24	R	123	VAL
24	R	142	ASN

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Mol	Chain	Res	Type
25	S	44	VAL
25	S	66	ARG
25	S	70	THR
25	S	71	VAL
25	S	80	ARG
26	T	115	SER
26	T	134	LEU
26	T	138	ILE
26	T	187	LEU
26	T	208	THR
26	T	254	MET
26	T	270	MET
26	T	275	THR
26	T	276	SER
27	U	10	LEU
27	U	15	THR
27	U	24	VAL
27	U	46	VAL
27	U	53	CYS
27	U	55	ARG
27	U	76	SER
27	U	93	CYS
27	U	102	LEU
28	V	65	TRP
28	V	128	CYS
28	V	131	ARG
28	V	152	LEU
28	V	153	LEU
28	V	164	VAL
28	V	170	SER
28	V	186	ARG
28	V	199	ILE
29	W	60	GLN
29	W	67	ARG
29	W	75	ARG
29	W	77	GLN
29	W	80	TYR
29	W	144	THR
29	W	151	LEU
29	W	199	GLN
29	W	207	THR
30	X	18	ARG

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Mol	Chain	Res	Type
30	X	40	VAL
30	X	49	THR
30	X	57	LEU
30	X	77	ASN
30	X	97	VAL
30	X	141	ARG
30	X	148	PHE
30	X	150	LEU
31	Y	78	GLN
31	Y	79	VAL
31	Y	105	ARG
31	Y	111	SER
31	Y	131	THR
31	Y	137	PHE
31	Y	138	THR
31	Y	145	ARG
31	Y	149	ARG
31	Y	161	ARG
31	Y	166	VAL
31	Y	193	THR
31	Y	196	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	41	ASN
1	0	59	HIS
1	0	65	ASN
1	0	76	HIS
2	1	27	HIS
2	1	42	HIS
3	2	97	ASN
3	2	197	ASN
4	3	67	HIS
5	4	37	ASN
6	5	83	ASN
6	5	170	GLN
7	6	23	GLN
8	7	95	HIS
9	8	118	HIS
10	9	92	ASN
14	D	116	HIS

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Mol	Chain	Res	Type
14	D	183	HIS
14	D	195	ASN
14	D	196	ASN
14	D	272	ASN
15	E	128	HIS
15	E	281	ASN
15	E	292	HIS
16	F	74	GLN
16	F	83	HIS
16	F	103	GLN
16	F	105	ASN
16	F	153	HIS
16	F	241	ASN
16	F	249	ASN
16	F	276	HIS
17	I	93	ASN
17	I	136	ASN
18	J	41	HIS
19	K	103	HIS
19	K	126	GLN
21	O	89	HIS
21	O	103	ASN
22	P	53	HIS
22	P	71	GLN
22	P	84	ASN
22	P	87	HIS
22	P	91	HIS
22	P	130	GLN
22	P	170	ASN
23	Q	98	HIS
23	Q	110	ASN
23	Q	209	ASN
23	Q	210	GLN
24	R	39	HIS
24	R	112	ASN
24	R	142	ASN
24	R	147	ASN
24	R	148	GLN
25	S	96	HIS
26	T	132	GLN
26	T	139	GLN
26	T	158	GLN

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Mol	Chain	Res	Type
27	U	89	ASN
27	U	94	GLN
28	V	80	HIS
28	V	104	HIS
28	V	109	GLN
29	W	130	HIS
29	W	171	HIS
29	W	199	GLN
29	W	203	ASN
30	X	14	ASN
30	X	41	GLN
30	X	73	GLN
30	X	77	ASN
30	X	135	HIS
31	Y	78	GLN
31	Y	117	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	A	1508/1570 (96%)	726 (48%)	29 (1%)
12	B	0/62	-	-
13	C	2/3 (66%)	2 (100%)	0
13	Z	2/3 (66%)	0	0
All	All	1512/1638 (92%)	728 (48%)	29 (1%)

All (728) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	A	4	A
11	A	5	A
11	A	7	G
11	A	11	G
11	A	12	C
11	A	16	A
11	A	27	A
11	A	30	U
11	A	31	A
11	A	32	C
11	A	36	A
11	A	37	A

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Mol	Chain	Res	Type
11	A	39	A
11	A	40	C
11	A	41	A
11	A	42	C
11	A	43	C
11	A	44	A
11	A	45	A
11	A	46	A
11	A	49	A
11	A	50	A
11	A	56	A
11	A	58	C
11	A	59	A
11	A	60	U
11	A	63	A
11	A	64	C
11	A	66	U
11	A	67	A
11	A	68	A
11	A	69	C
11	A	71	U
11	A	72	U
11	A	82	G
11	A	83	A
11	A	84	G
11	A	96	U
11	A	97	A
11	A	98	U
11	A	99	C
11	A	100	C
11	A	101	U
11	A	102	G
11	A	104	C
11	A	105	G
11	A	106	C
11	A	107	U
11	A	108	A
11	A	109	U
11	A	110	A
11	A	112	A
11	A	113	G
11	A	114	A

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Mol	Chain	Res	Type
11	A	115	U
11	A	116	A
11	A	117	G
11	A	119	A
11	A	122	G
11	A	123	U
11	A	124	A
11	A	128	A
11	A	130	A
11	A	131	G
11	A	132	A
11	A	135	A
11	A	136	A
11	A	138	G
11	A	139	A
11	A	140	A
11	A	147	A
11	A	148	A
11	A	155	A
11	A	156	A
11	A	157	A
11	A	158	A
11	A	159	A
11	A	160	A
11	A	161	G
11	A	162	C
11	A	163	A
11	A	164	A
11	A	167	A
11	A	168	U
11	A	169	U
11	A	171	C
11	A	172	C
11	A	175	U
11	A	177	C
11	A	178	U
11	A	179	A
11	A	187	C
11	A	189	U
11	A	191	A
11	A	203	G
11	A	204	A

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Mol	Chain	Res	Type
11	A	206	A
11	A	207	A
11	A	213	A
11	A	216	A
11	A	217	A
11	A	218	A
11	A	222	A
11	A	224	C
11	A	227	U
11	A	228	A
11	A	229	G
11	A	236	A
11	A	237	C
11	A	238	C
11	A	241	G
11	A	242	A
11	A	243	A
11	A	253	G
11	A	256	A
11	A	259	C
11	A	262	G
11	A	271	A
11	A	272	A
11	A	273	A
11	A	274	A
11	A	275	G
11	A	276	A
11	A	277	A
11	A	280	A
11	A	281	A
11	A	283	U
11	A	284	C
11	A	286	U
11	A	293	G
11	A	294	G
11	A	296	A
11	A	297	A
11	A	300	U
11	A	304	G
11	A	307	A
11	A	308	A
11	A	310	A

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Mol	Chain	Res	Type
11	A	311	C
11	A	312	U
11	A	317	G
11	A	321	G
11	A	322	A
11	A	323	G
11	A	328	A
11	A	329	A
11	A	330	A
11	A	331	G
11	A	332	C
11	A	335	A
11	A	336	A
11	A	337	C
11	A	338	G
11	A	339	A
11	A	347	G
11	A	348	A
11	A	351	G
11	A	352	C
11	A	356	U
11	A	357	U
11	A	358	G
11	A	362	G
11	A	364	G
11	A	365	A
11	A	367	A
11	A	368	G
11	A	369	A
11	A	370	A
11	A	372	U
11	A	373	U
11	A	375	A
11	A	382	C
11	A	387	A
11	A	388	A
11	A	389	A
11	A	390	A
11	A	391	U
11	A	393	C
11	A	396	C
11	A	397	A

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Mol	Chain	Res	Type
11	A	398	A
11	A	401	A
11	A	403	C
11	A	404	C
11	A	406	A
11	A	408	A
11	A	413	A
11	A	416	G
11	A	417	U
11	A	422	U
11	A	426	G
11	A	427	A
11	A	428	G
11	A	432	G
11	A	439	A
11	A	441	G
11	A	444	A
11	A	445	C
11	A	447	G
11	A	448	C
11	A	454	A
11	A	458	A
11	A	459	C
11	A	461	G
11	A	463	U
11	A	464	A
11	A	465	C
11	A	467	A
11	A	472	G
11	A	473	A
11	A	474	C
11	A	475	U
11	A	476	A
11	A	477	G
11	A	478	A
11	A	479	G
11	A	482	U
11	A	486	U
11	A	487	C
11	A	488	U
11	A	490	A
11	A	491	A

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Mol	Chain	Res	Type
11	A	492	U
11	A	493	A
11	A	495	U
11	A	497	C
11	A	498	C
11	A	499	A
11	A	500	U
11	A	501	A
11	A	502	G
11	A	503	U
11	A	504	A
11	A	505	G
11	A	508	C
11	A	509	U
11	A	510	A
11	A	513	A
11	A	514	G
11	A	515	C
11	A	518	C
11	A	519	C
11	A	521	U
11	A	522	C
11	A	523	A
11	A	524	A
11	A	525	U
11	A	526	U
11	A	527	G
11	A	528	A
11	A	529	G
11	A	530	A
11	A	532	A
11	A	533	G
11	A	534	C
11	A	536	U
11	A	538	A
11	A	539	A
11	A	542	C
11	A	543	U
11	A	545	A
11	A	546	A
11	A	548	A
11	A	550	A

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Mol	Chain	Res	Type
11	A	551	U
11	A	552	U
11	A	553	C
11	A	554	A
11	A	555	C
11	A	556	C
11	A	557	A
11	A	558	A
11	A	559	C
11	A	560	A
11	A	561	U
11	A	564	U
11	A	565	C
11	A	566	C
11	A	568	A
11	A	570	A
11	A	571	A
11	A	572	A
11	A	573	C
11	A	574	U
11	A	575	A
11	A	577	U
11	A	578	A
11	A	579	A
11	A	582	A
11	A	583	A
11	A	584	C
11	A	588	U
11	A	590	G
11	A	591	C
11	A	593	C
11	A	594	A
11	A	596	U
11	A	597	A
11	A	601	G
11	A	603	C
11	A	610	A
11	A	611	U
11	A	612	U
11	A	613	G
11	A	614	A
11	A	615	A

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Mol	Chain	Res	Type
11	A	616	A
11	A	617	C
11	A	618	A
11	A	623	A
11	A	627	A
11	A	628	U
11	A	629	A
11	A	631	U
11	A	632	G
11	A	638	A
11	A	641	A
11	A	647	A
11	A	648	A
11	A	650	A
11	A	652	G
11	A	653	C
11	A	654	C
11	A	655	U
11	A	656	U
11	A	659	U
11	A	665	C
11	A	666	A
11	A	672	U
11	A	673	U
11	A	674	A
11	A	682	A
11	A	684	C
11	A	687	A
11	A	688	U
11	A	689	A
11	A	692	A
11	A	693	U
11	A	695	C
11	A	699	U
11	A	700	A
11	A	702	U
11	A	703	U
11	A	705	A
11	A	706	C
11	A	710	C
11	A	711	A
11	A	714	A

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Mol	Chain	Res	Type
11	A	716	A
11	A	717	C
11	A	718	C
11	A	719	A
11	A	720	A
11	A	721	A
11	A	722	A
11	A	723	C
11	A	724	A
11	A	725	A
11	A	726	C
11	A	734	C
11	A	735	G
11	A	737	U
11	A	741	U
11	A	742	A
11	A	743	A
11	A	744	U
11	A	745	U
11	A	746	A
11	A	747	C
11	A	748	A
11	A	751	G
11	A	756	C
11	A	757	C
11	A	761	C
11	A	762	A
11	A	763	C
11	A	764	A
11	A	765	G
11	A	766	G
11	A	772	A
11	A	774	C
11	A	776	A
11	A	777	G
11	A	778	G
11	A	779	A
11	A	780	A
11	A	781	A
11	A	782	G
11	A	783	A
11	A	784	U

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Mol	Chain	Res	Type
11	A	786	A
11	A	787	A
11	A	790	G
11	A	802	A
11	A	803	C
11	A	807	G
11	A	809	A
11	A	811	A
11	A	812	C
11	A	813	A
11	A	815	A
11	A	816	A
11	A	823	C
11	A	825	U
11	A	826	G
11	A	827	U
11	A	828	U
11	A	831	C
11	A	832	C
11	A	833	A
11	A	834	A
11	A	836	A
11	A	842	A
11	A	845	U
11	A	846	C
11	A	847	U
11	A	848	A
11	A	850	C
11	A	851	A
11	A	852	U
11	A	853	U
11	A	854	A
11	A	856	U
11	A	857	A
11	A	858	G
11	A	861	U
11	A	862	U
11	A	866	G
11	A	870	A
11	A	876	G
11	A	879	C
11	A	880	A

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Mol	Chain	Res	Type
11	A	883	G
11	A	884	A
11	A	885	C
11	A	886	A
11	A	890	G
11	A	894	A
11	A	895	A
11	A	897	G
11	A	898	G
11	A	900	C
11	A	901	G
11	A	903	G
11	A	905	U
11	A	906	A
11	A	912	A
11	A	913	C
11	A	914	C
11	A	918	C
11	A	920	A
11	A	921	A
11	A	922	G
11	A	923	G
11	A	924	U
11	A	925	A
11	A	926	G
11	A	929	U
11	A	930	A
11	A	931	A
11	A	932	U
11	A	933	C
11	A	936	U
11	A	937	U
11	A	938	G
11	A	944	C
11	A	947	A
11	A	948	U
11	A	955	U
11	A	956	U
11	A	957	G
11	A	958	U
11	A	959	A
11	A	960	U

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Mol	Chain	Res	Type
11	A	962	A
11	A	963	A
11	A	965	G
11	A	968	C
11	A	970	C
11	A	971	A
11	A	972	C
11	A	973	G
11	A	974	A
11	A	975	G
11	A	976	G
11	A	977	G
11	A	978	U
11	A	979	U
11	A	980	U
11	A	984	U
11	A	985	G
11	A	986	U
11	A	989	C
11	A	990	U
11	A	996	C
11	A	997	C
11	A	1003	G
11	A	1006	A
11	A	1014	C
11	A	1015	U
11	A	1016	U
11	A	1023	A
11	A	1024	A
11	A	1025	G
11	A	1026	A
11	A	1029	C
11	A	1036	A
11	A	1038	A
11	A	1042	A
11	A	1048	C
11	A	1049	G
11	A	1050	A
11	A	1051	G
11	A	1052	A
11	A	1053	A
11	A	1054	G

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Mol	Chain	Res	Type
11	A	1055	A
11	A	1056	C
11	A	1059	U
11	A	1061	U
11	A	1062	G
11	A	1067	U
11	A	1072	U
11	A	1073	U
11	A	1078	A
11	A	1083	A
11	A	1086	A
11	A	1087	G
11	A	1088	U
11	A	1089	U
11	A	1125	A
11	A	1126	A
11	A	1134	U
11	A	1135	A
11	A	1136	G
11	A	1139	A
11	A	1140	U
11	A	1141	U
11	A	1144	G
11	A	1146	U
11	A	1147	U
11	A	1148	G
11	A	1149	G
11	A	1150	G
11	A	1157	U
11	A	1161	A
11	A	1162	G
11	A	1163	U
11	A	1164	A
11	A	1165	C
11	A	1166	A
11	A	1167	A
11	A	1176	C
11	A	1178	G
11	A	1180	G
11	A	1181	U
11	A	1184	U
11	A	1185	U

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Mol	Chain	Res	Type
11	A	1186	U
11	A	1187	U
11	A	1189	A
11	A	1193	A
11	A	1204	U
11	A	1205	C
11	A	1210	U
11	A	1211	A
11	A	1224	C
11	A	1225	U
11	A	1226	U
11	A	1227	A
11	A	1229	U
11	A	1230	G
11	A	1232	U
11	A	1233	C
11	A	1236	A
11	A	1237	A
11	A	1238	A
11	A	1239	U
11	A	1240	U
11	A	1241	U
11	A	1243	G
11	A	1244	A
11	A	1245	U
11	A	1246	C
11	A	1247	A
11	A	1250	G
11	A	1251	G
11	A	1252	A
11	A	1256	A
11	A	1257	G
11	A	1258	U
11	A	1262	C
11	A	1268	G
11	A	1269	A
11	A	1270	U
11	A	1277	G
11	A	1285	G
11	A	1289	U
11	A	1290	A
11	A	1292	A

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Mol	Chain	Res	Type
11	A	1294	U
11	A	1295	U
11	A	1297	C
11	A	1301	C
11	A	1302	G
11	A	1305	A
11	A	1308	A
11	A	1309	G
11	A	1312	U
11	A	1313	U
11	A	1315	A
11	A	1317	G
11	A	1323	G
11	A	1324	A
11	A	1326	G
11	A	1327	U
11	A	1328	U
11	A	1330	G
11	A	1334	A
11	A	1339	A
11	A	1340	C
11	A	1341	C
11	A	1342	C
11	A	1345	A
11	A	1346	U
11	A	1348	G
11	A	1349	U
11	A	1350	G
11	A	1351	C
11	A	1352	A
11	A	1355	C
11	A	1356	G
11	A	1363	A
11	A	1364	A
11	A	1372	U
11	A	1375	U
11	A	1376	U
11	A	1383	U
11	A	1385	A
11	A	1387	A
11	A	1388	G
11	A	1394	C

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Mol	Chain	Res	Type
11	A	1397	G
11	A	1400	C
11	A	1402	G
11	A	1406	U
11	A	1407	C
11	A	1409	G
11	A	1411	C
11	A	1412	C
11	A	1413	G
11	A	1414	G
11	A	1416	G
11	A	1423	A
11	A	1426	U
11	A	1427	C
11	A	1431	U
11	A	1432	U
11	A	1434	U
11	A	1442	A
11	A	1443	U
11	A	1446	A
11	A	1449	U
11	A	1450	C
11	A	1453	C
11	A	1454	C
11	A	1455	A
11	A	1456	G
11	A	1457	U
11	A	1458	A
11	A	1463	A
11	A	1465	G
11	A	1466	A
11	A	1468	A
11	A	1472	G
11	A	1474	A
11	A	1478	G
11	A	1480	A
11	A	1488	C
11	A	1490	C
11	A	1491	A
11	A	1492	A
11	A	1496	C
11	A	1500	U

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Mol	Chain	Res	Type
11	A	1502	A
11	A	1503	G
11	A	1507	U
11	A	1508	A
11	A	1510	U
11	A	1511	U
11	A	1513	A
11	A	1514	U
11	A	1516	A
11	A	1518	U
11	A	1519	U
11	A	1520	A
11	A	1522	U
11	A	1523	C
11	A	1524	U
11	A	1525	U
11	A	1526	A
11	A	1529	C
11	A	1530	U
11	A	1531	A
11	A	1534	U
11	A	1536	A
11	A	1537	C
11	A	1541	U
11	A	1542	A
11	A	1543	A
11	A	1544	U
11	A	1545	A
11	A	1546	A
11	A	1547	A
11	A	1549	C
11	A	1550	C
11	A	1551	A
11	A	1552	G
11	A	1556	U
11	A	1557	A
11	A	1560	A
11	A	1565	G
11	A	1566	C
11	A	1567	A
11	A	1568	C
11	A	1569	A

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Mol	Chain	Res	Type
13	C	75	C
13	C	76	A

All (29) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	A	39	A
11	A	48	U
11	A	160	A
11	A	204	A
11	A	335	A
11	A	347	G
11	A	350	A
11	A	374	U
11	A	446	A
11	A	512	A
11	A	521	U
11	A	555	C
11	A	556	C
11	A	569	A
11	A	572	A
11	A	573	C
11	A	583	A
11	A	617	C
11	A	762	A
11	A	875	U
11	A	912	A
11	A	931	A
11	A	936	U
11	A	937	U
11	A	1139	A
11	A	1140	U
11	A	1431	U
11	A	1467	C
11	A	1518	U

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	P5P	B	37	12	16,23,24	0.80	0	14,33,36	0.81	1 (7%)
12	P5P	B	50	12	16,23,24	0.83	0	14,33,36	0.81	0
12	Y5P	B	42	12	14,19,20	3.60	1 (7%)	18,26,29	0.85	1 (5%)
12	P5P	B	51	12	16,23,24	1.40	3 (18%)	14,33,36	2.02	2 (14%)
12	Y5P	B	11	12	14,19,20	3.67	1 (7%)	18,26,29	0.80	1 (5%)
12	Y5P	B	48	12	14,19,20	2.32	1 (7%)	18,26,29	0.96	1 (5%)
12	P5P	B	73	12	16,23,24	0.81	1 (6%)	14,33,36	0.63	0
12	P5P	B	64	12	16,23,24	0.79	0	14,33,36	0.81	0
12	Y5P	B	72	12	14,19,20	3.61	2 (14%)	18,26,29	0.81	1 (5%)
12	P5P	B	14	12	16,23,24	0.81	0	14,33,36	0.80	0
12	P5P	B	10	12	16,23,24	1.31	3 (18%)	14,33,36	1.95	2 (14%)
12	Y5P	B	61	12	14,19,20	2.26	1 (7%)	18,26,29	1.05	1 (5%)
12	Y5P	B	6	12	14,19,20	2.27	1 (7%)	18,26,29	0.98	1 (5%)
12	Y5P	B	65	12	14,19,20	2.28	1 (7%)	18,26,29	1.03	1 (5%)
12	P5P	B	28	12	16,23,24	0.87	0	14,33,36	0.72	0
12	P5P	B	45	12	16,23,24	0.80	0	14,33,36	0.75	0
12	P5P	B	47	12	16,23,24	0.78	1 (6%)	14,33,36	0.81	1 (7%)
12	P5P	B	27	12	16,23,24	0.79	1 (6%)	14,33,36	0.91	1 (7%)
12	Y5P	B	26	12	14,19,20	3.57	1 (7%)	18,26,29	0.85	2 (11%)
12	Y5P	B	63	12	14,19,20	3.61	1 (7%)	18,26,29	0.85	2 (11%)
12	P5P	B	29	12	16,23,24	1.37	3 (18%)	14,33,36	2.15	2 (14%)
12	Y5P	B	8	12	14,19,20	2.18	1 (7%)	18,26,29	1.18	1 (5%)
12	P5P	B	41	12	16,23,24	1.32	3 (18%)	14,33,36	1.84	2 (14%)
12	P5P	B	7	12	16,23,24	1.41	3 (18%)	14,33,36	2.10	2 (14%)
12	P5P	B	46	12	16,23,24	1.33	3 (18%)	14,33,36	1.95	2 (14%)
12	Y5P	B	12	12	14,19,20	2.22	1 (7%)	18,26,29	0.97	1 (5%)
12	Y5P	B	62	12	14,19,20	2.26	1 (7%)	18,26,29	0.99	1 (5%)
12	P5P	B	39	12	16,23,24	0.78	0	14,33,36	0.84	1 (7%)
12	P5P	B	24	12	16,23,24	0.83	0	14,33,36	0.76	0
12	Y5P	B	31	12	14,19,20	3.75	1 (7%)	18,26,29	0.82	1 (5%)
12	P5P	B	68	12	16,23,24	0.80	0	14,33,36	0.80	0
12	P5P	B	15	12	16,23,24	0.81	0	14,33,36	0.82	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	Y5P	B	13	12	14,19,20	2.36	1 (7%)	18,26,29	1.16	1 (5%)
12	P5P	B	25	12	16,23,24	1.37	3 (18%)	14,33,36	2.04	3 (21%)
12	P5P	B	36	12	16,23,24	0.83	0	14,33,36	0.85	0
12	P5P	B	1	12	20,24,24	1.37	3 (15%)	21,36,36	1.72	2 (9%)
12	P5P	B	49	12	16,23,24	1.43	3 (18%)	14,33,36	2.06	2 (14%)
12	Y5P	B	3	12	14,19,20	2.30	1 (7%)	18,26,29	1.07	1 (5%)
12	Y5P	B	33	12	14,19,20	3.71	1 (7%)	18,26,29	0.80	1 (5%)
12	P5P	B	4	12	16,23,24	0.80	0	14,33,36	0.74	0
12	Y5P	B	43	12	14,19,20	3.77	1 (7%)	18,26,29	0.76	1 (5%)
12	Y5P	B	44	12	14,19,20	2.22	1 (7%)	18,26,29	0.98	1 (5%)
12	Y5P	B	40	12	14,19,20	2.37	1 (7%)	18,26,29	1.05	1 (5%)
12	P5P	B	59	12	16,23,24	1.43	3 (18%)	14,33,36	2.02	2 (14%)
12	P5P	B	66	12	16,23,24	0.82	1 (6%)	14,33,36	0.73	0
12	P5P	B	32	12	16,23,24	0.77	0	14,33,36	0.83	0
12	P5P	B	70	12	16,23,24	0.80	0	14,33,36	0.75	0
12	Y5P	B	60	12	14,19,20	3.52	1 (7%)	18,26,29	0.90	2 (11%)
12	Y5P	B	2	12	14,19,20	2.27	1 (7%)	18,26,29	0.94	1 (5%)
12	P5P	B	35	12	16,23,24	1.52	3 (18%)	14,33,36	1.87	2 (14%)
12	Y5P	B	71	12	14,19,20	3.59	2 (14%)	18,26,29	0.83	1 (5%)
12	Y5P	B	52	12	14,19,20	3.58	1 (7%)	18,26,29	0.83	1 (5%)
12	P5P	B	67	12	16,23,24	0.81	0	14,33,36	0.83	1 (7%)
12	P5P	B	30	12	16,23,24	1.36	2 (12%)	14,33,36	1.94	2 (14%)
12	P5P	B	58	12	16,23,24	0.80	0	14,33,36	0.76	0
12	Y5P	B	69	12	14,19,20	3.55	1 (7%)	18,26,29	0.92	1 (5%)
12	P5P	B	38	12	16,23,24	0.79	0	14,33,36	0.89	1 (7%)
12	P5P	B	9	12	16,23,24	0.83	0	14,33,36	0.78	1 (7%)
12	P5P	B	5	12	16,23,24	0.80	0	14,33,36	0.81	1 (7%)
12	Y5P	B	34	12	14,19,20	2.26	1 (7%)	18,26,29	1.05	1 (5%)
12	P5P	B	23	12	16,23,24	0.86	1 (6%)	14,33,36	0.80	0
12	Y5P	B	53	12	14,19,20	3.62	2 (14%)	18,26,29	0.82	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	P5P	B	37	12	-	0/3/25/26	0/3/3/3
12	P5P	B	50	12	-	0/3/25/26	0/3/3/3
12	Y5P	B	42	12	-	1/7/33/34	0/2/2/2
12	P5P	B	51	12	-	0/3/25/26	0/3/3/3
12	Y5P	B	11	12	-	1/7/33/34	0/2/2/2
12	Y5P	B	48	12	-	1/7/33/34	0/2/2/2
12	P5P	B	73	12	-	0/3/25/26	0/3/3/3
12	P5P	B	64	12	-	0/3/25/26	0/3/3/3
12	Y5P	B	72	12	-	1/7/33/34	0/2/2/2
12	P5P	B	14	12	-	1/3/25/26	0/3/3/3
12	P5P	B	10	12	-	0/3/25/26	0/3/3/3
12	Y5P	B	61	12	-	1/7/33/34	0/2/2/2
12	Y5P	B	6	12	-	2/7/33/34	0/2/2/2
12	Y5P	B	65	12	-	1/7/33/34	0/2/2/2
12	P5P	B	28	12	-	2/3/25/26	0/3/3/3
12	P5P	B	45	12	-	0/3/25/26	0/3/3/3
12	P5P	B	47	12	-	0/3/25/26	0/3/3/3
12	P5P	B	27	12	-	1/3/25/26	0/3/3/3
12	Y5P	B	26	12	-	3/7/33/34	0/2/2/2
12	Y5P	B	63	12	-	1/7/33/34	0/2/2/2
12	P5P	B	29	12	-	0/3/25/26	0/3/3/3
12	Y5P	B	8	12	-	2/7/33/34	0/2/2/2
12	P5P	B	41	12	-	2/3/25/26	0/3/3/3
12	P5P	B	7	12	-	1/3/25/26	0/3/3/3
12	P5P	B	46	12	-	3/3/25/26	0/3/3/3
12	Y5P	B	12	12	-	3/7/33/34	0/2/2/2
12	Y5P	B	62	12	-	1/7/33/34	0/2/2/2
12	P5P	B	39	12	-	1/3/25/26	0/3/3/3
12	P5P	B	24	12	-	0/3/25/26	0/3/3/3
12	Y5P	B	31	12	-	1/7/33/34	0/2/2/2
12	P5P	B	68	12	-	0/3/25/26	0/3/3/3
12	P5P	B	15	12	-	3/3/25/26	0/3/3/3
12	Y5P	B	13	12	-	1/7/33/34	0/2/2/2
12	P5P	B	25	12	-	2/3/25/26	0/3/3/3
12	P5P	B	36	12	-	1/3/25/26	0/3/3/3
12	P5P	B	1	12	-	3/6/26/26	0/3/3/3
12	P5P	B	49	12	-	2/3/25/26	0/3/3/3
12	Y5P	B	3	12	-	2/7/33/34	0/2/2/2
12	Y5P	B	33	12	-	3/7/33/34	0/2/2/2
12	P5P	B	4	12	-	0/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	Y5P	B	43	12	-	3/7/33/34	0/2/2/2
12	Y5P	B	44	12	-	3/7/33/34	0/2/2/2
12	Y5P	B	40	12	-	3/7/33/34	0/2/2/2
12	P5P	B	59	12	-	0/3/25/26	0/3/3/3
12	P5P	B	66	12	-	2/3/25/26	0/3/3/3
12	P5P	B	32	12	-	2/3/25/26	0/3/3/3
12	P5P	B	70	12	-	2/3/25/26	0/3/3/3
12	Y5P	B	60	12	-	1/7/33/34	0/2/2/2
12	Y5P	B	2	12	-	3/7/33/34	0/2/2/2
12	P5P	B	35	12	-	2/3/25/26	0/3/3/3
12	Y5P	B	71	12	-	1/7/33/34	0/2/2/2
12	Y5P	B	52	12	-	1/7/33/34	0/2/2/2
12	P5P	B	67	12	-	3/3/25/26	0/3/3/3
12	P5P	B	30	12	-	3/3/25/26	0/3/3/3
12	P5P	B	58	12	-	0/3/25/26	0/3/3/3
12	Y5P	B	69	12	-	1/7/33/34	0/2/2/2
12	P5P	B	38	12	-	0/3/25/26	0/3/3/3
12	P5P	B	9	12	-	3/3/25/26	0/3/3/3
12	P5P	B	5	12	-	3/3/25/26	0/3/3/3
12	Y5P	B	34	12	-	3/7/33/34	0/2/2/2
12	P5P	B	23	12	-	3/3/25/26	0/3/3/3
12	Y5P	B	53	12	-	1/7/33/34	0/2/2/2

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	43	Y5P	C4-N3	-13.89	1.33	1.46
12	B	31	Y5P	C4-N3	-13.84	1.33	1.46
12	B	33	Y5P	C4-N3	-13.74	1.33	1.46
12	B	11	Y5P	C4-N3	-13.54	1.33	1.46
12	B	63	Y5P	C4-N3	-13.32	1.34	1.46
12	B	42	Y5P	C4-N3	-13.30	1.34	1.46
12	B	53	Y5P	C4-N3	-13.30	1.34	1.46
12	B	72	Y5P	C4-N3	-13.27	1.34	1.46
12	B	71	Y5P	C4-N3	-13.19	1.34	1.46
12	B	26	Y5P	C4-N3	-13.16	1.34	1.46
12	B	52	Y5P	C4-N3	-13.14	1.34	1.46
12	B	69	Y5P	C4-N3	-13.04	1.34	1.46
12	B	60	Y5P	C4-N3	-12.91	1.34	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	40	Y5P	C4-N3	-8.73	1.38	1.46
12	B	13	Y5P	C4-N3	-8.70	1.38	1.46
12	B	48	Y5P	C4-N3	-8.42	1.38	1.46
12	B	3	Y5P	C4-N3	-8.40	1.38	1.46
12	B	65	Y5P	C4-N3	-8.32	1.38	1.46
12	B	6	Y5P	C4-N3	-8.29	1.38	1.46
12	B	2	Y5P	C4-N3	-8.24	1.38	1.46
12	B	62	Y5P	C4-N3	-8.23	1.38	1.46
12	B	34	Y5P	C4-N3	-8.21	1.38	1.46
12	B	61	Y5P	C4-N3	-8.18	1.38	1.46
12	B	12	Y5P	C4-N3	-8.11	1.38	1.46
12	B	44	Y5P	C4-N3	-8.00	1.38	1.46
12	B	8	Y5P	C4-N3	-7.90	1.39	1.46
12	B	35	P5P	C6-N1	4.70	1.40	1.32
12	B	1	P5P	C6-N1	4.48	1.40	1.32
12	B	49	P5P	C6-N1	4.46	1.40	1.32
12	B	7	P5P	C6-N1	4.42	1.40	1.32
12	B	59	P5P	C6-N1	4.41	1.40	1.32
12	B	51	P5P	C6-N1	4.35	1.40	1.32
12	B	29	P5P	C6-N1	4.32	1.40	1.32
12	B	41	P5P	C6-N1	4.12	1.39	1.32
12	B	46	P5P	C6-N1	4.03	1.39	1.32
12	B	30	P5P	C6-N1	4.01	1.39	1.32
12	B	10	P5P	C6-N1	3.98	1.39	1.32
12	B	25	P5P	C6-N1	3.91	1.39	1.32
12	B	25	P5P	C8-N7	-2.48	1.30	1.34
12	B	35	P5P	C2-N1	2.48	1.38	1.33
12	B	1	P5P	C2-N1	2.48	1.38	1.33
12	B	49	P5P	C2-N1	2.46	1.38	1.33
12	B	30	P5P	C8-N7	-2.42	1.30	1.34
12	B	51	P5P	C2-N1	2.35	1.38	1.33
12	B	46	P5P	C8-N7	-2.30	1.30	1.34
12	B	7	P5P	C2-N1	2.28	1.38	1.33
12	B	10	P5P	C8-N7	-2.28	1.30	1.34
12	B	59	P5P	C2-N1	2.27	1.38	1.33
12	B	73	P5P	C6-N1	2.20	1.36	1.32
12	B	29	P5P	C2-N1	2.18	1.37	1.33
12	B	41	P5P	C2-N1	2.17	1.37	1.33
12	B	59	P5P	C8-N7	-2.15	1.30	1.34
12	B	25	P5P	C2-N1	2.14	1.37	1.33
12	B	23	P5P	C8-N7	-2.14	1.30	1.34
12	B	35	P5P	C8-N7	-2.14	1.30	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	66	P5P	C6-N1	2.12	1.36	1.32
12	B	10	P5P	C2-N1	2.11	1.37	1.33
12	B	1	P5P	C8-N7	-2.10	1.31	1.34
12	B	49	P5P	C8-N7	-2.06	1.31	1.34
12	B	51	P5P	C8-N7	-2.05	1.31	1.34
12	B	46	P5P	C2-N1	2.04	1.37	1.33
12	B	71	Y5P	C2-N1	2.03	1.41	1.36
12	B	72	Y5P	C2-N1	2.03	1.41	1.36
12	B	27	P5P	C8-N7	-2.03	1.31	1.34
12	B	7	P5P	C8-N7	-2.03	1.31	1.34
12	B	47	P5P	C6-N1	2.02	1.36	1.32
12	B	53	Y5P	C2-N1	2.01	1.41	1.36
12	B	41	P5P	C8-N7	-2.01	1.31	1.34
12	B	29	P5P	C8-N7	-2.01	1.31	1.34

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	B	7	P5P	C6-N1-C2	6.87	125.68	115.84
12	B	29	P5P	C6-N1-C2	6.75	125.51	115.84
12	B	49	P5P	C6-N1-C2	6.65	125.36	115.84
12	B	51	P5P	C6-N1-C2	6.59	125.29	115.84
12	B	59	P5P	C6-N1-C2	6.59	125.29	115.84
12	B	1	P5P	C6-N1-C2	6.58	125.27	115.84
12	B	46	P5P	C6-N1-C2	6.51	125.17	115.84
12	B	10	P5P	C6-N1-C2	6.39	124.99	115.84
12	B	25	P5P	C6-N1-C2	6.33	124.91	115.84
12	B	41	P5P	C6-N1-C2	6.20	124.72	115.84
12	B	30	P5P	C6-N1-C2	6.17	124.68	115.84
12	B	35	P5P	C6-N1-C2	6.04	124.49	115.84
12	B	8	Y5P	N1-C2-N3	-3.91	113.87	125.33
12	B	13	Y5P	N1-C2-N3	-3.90	113.89	125.33
12	B	3	Y5P	N1-C2-N3	-3.87	114.00	125.33
12	B	6	Y5P	N1-C2-N3	-3.60	114.76	125.33
12	B	65	Y5P	N1-C2-N3	-3.58	114.82	125.33
12	B	62	Y5P	N1-C2-N3	-3.57	114.85	125.33
12	B	29	P5P	N1-C2-N3	-3.50	123.17	127.65
12	B	2	Y5P	N1-C2-N3	-3.49	115.10	125.33
12	B	12	Y5P	N1-C2-N3	-3.48	115.11	125.33
12	B	40	Y5P	N1-C2-N3	-3.48	115.14	125.33
12	B	61	Y5P	N1-C2-N3	-3.45	115.22	125.33
12	B	34	Y5P	N1-C2-N3	-3.42	115.30	125.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	B	48	Y5P	N1-C2-N3	-3.41	115.32	125.33
12	B	44	Y5P	N1-C2-N3	-3.35	115.51	125.33
12	B	59	P5P	N1-C2-N3	-3.28	123.45	127.65
12	B	7	P5P	N1-C2-N3	-3.25	123.50	127.65
12	B	49	P5P	N1-C2-N3	-3.22	123.54	127.65
12	B	51	P5P	N1-C2-N3	-3.16	123.61	127.65
12	B	1	P5P	N1-C2-N3	-3.14	123.63	127.65
12	B	30	P5P	N1-C2-N3	-3.02	123.78	127.65
12	B	35	P5P	N1-C2-N3	-2.99	123.82	127.65
12	B	46	P5P	N1-C2-N3	-2.94	123.89	127.65
12	B	25	P5P	N1-C2-N3	-2.75	124.13	127.65
12	B	25	P5P	C1'-N9-C4	2.68	131.34	126.64
12	B	10	P5P	N1-C2-N3	-2.67	124.23	127.65
12	B	41	P5P	N1-C2-N3	-2.52	124.42	127.65
12	B	26	Y5P	N1-C2-N3	-2.32	118.54	125.33
12	B	5	P5P	C6-N1-C2	2.29	119.11	115.84
12	B	15	P5P	C6-N1-C2	2.27	119.08	115.84
12	B	39	P5P	C6-N1-C2	2.25	119.07	115.84
12	B	52	Y5P	N1-C2-N3	-2.24	118.77	125.33
12	B	53	Y5P	N1-C2-N3	-2.23	118.80	125.33
12	B	67	P5P	C6-N1-C2	2.22	119.01	115.84
12	B	60	Y5P	N1-C2-N3	-2.19	118.90	125.33
12	B	47	P5P	C6-N1-C2	2.16	118.94	115.84
12	B	42	Y5P	N1-C2-N3	-2.16	118.98	125.33
12	B	63	Y5P	N1-C2-N3	-2.15	119.03	125.33
12	B	71	Y5P	N1-C2-N3	-2.13	119.08	125.33
12	B	38	P5P	C6-N1-C2	2.09	118.84	115.84
12	B	72	Y5P	N1-C2-N3	-2.09	119.21	125.33
12	B	11	Y5P	N1-C2-N3	-2.08	119.24	125.33
12	B	37	P5P	C6-N1-C2	2.06	118.79	115.84
12	B	33	Y5P	N1-C2-N3	-2.04	119.34	125.33
12	B	26	Y5P	C4-C5-C6	-2.04	116.99	122.78
12	B	31	Y5P	N1-C2-N3	-2.02	119.41	125.33
12	B	60	Y5P	C4-C5-C6	-2.02	117.05	122.78
12	B	69	Y5P	N1-C2-N3	-2.01	119.42	125.33
12	B	9	P5P	C6-N1-C2	2.01	118.72	115.84
12	B	27	P5P	C1'-N9-C4	2.01	130.17	126.64
12	B	43	Y5P	N1-C2-N3	-2.01	119.44	125.33
12	B	63	Y5P	C4-C5-C6	-2.00	117.09	122.78

There are no chirality outliers.

All (90) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	B	1	P5P	C5'-O5'-P-OP1
12	B	1	P5P	C5'-O5'-P-OP2
12	B	1	P5P	C5'-O5'-P-OP3
12	B	5	P5P	C3'-C4'-C5'-O5'
12	B	5	P5P	O4'-C4'-C5'-O5'
12	B	15	P5P	C3'-C4'-C5'-O5'
12	B	15	P5P	O4'-C4'-C5'-O5'
12	B	23	P5P	C3'-C4'-C5'-O5'
12	B	23	P5P	C4'-C5'-O5'-P
12	B	25	P5P	C3'-C4'-C5'-O5'
12	B	28	P5P	C3'-C4'-C5'-O5'
12	B	30	P5P	C3'-C4'-C5'-O5'
12	B	30	P5P	O4'-C4'-C5'-O5'
12	B	35	P5P	C3'-C4'-C5'-O5'
12	B	35	P5P	O4'-C4'-C5'-O5'
12	B	49	P5P	O4'-C4'-C5'-O5'
12	B	66	P5P	C3'-C4'-C5'-O5'
12	B	66	P5P	O4'-C4'-C5'-O5'
12	B	2	Y5P	O4'-C4'-C5'-O5'
12	B	2	Y5P	C3'-C4'-C5'-O5'
12	B	26	Y5P	O4'-C4'-C5'-O5'
12	B	26	Y5P	C3'-C4'-C5'-O5'
12	B	33	Y5P	O4'-C1'-N1-C2
12	B	40	Y5P	O4'-C1'-N1-C2
12	B	42	Y5P	O4'-C1'-N1-C2
12	B	43	Y5P	O4'-C4'-C5'-O5'
12	B	43	Y5P	C3'-C4'-C5'-O5'
12	B	61	Y5P	O4'-C1'-N1-C2
12	B	65	Y5P	O4'-C1'-N1-C2
12	B	71	Y5P	O4'-C1'-N1-C2
12	B	72	Y5P	O4'-C1'-N1-C2
12	B	2	Y5P	O4'-C1'-N1-C2
12	B	3	Y5P	O4'-C1'-N1-C2
12	B	6	Y5P	O4'-C1'-N1-C2
12	B	8	Y5P	O4'-C1'-N1-C2
12	B	11	Y5P	O4'-C1'-N1-C2
12	B	12	Y5P	O4'-C1'-N1-C2
12	B	13	Y5P	O4'-C1'-N1-C2
12	B	26	Y5P	O4'-C1'-N1-C2
12	B	31	Y5P	O4'-C1'-N1-C2
12	B	43	Y5P	O4'-C1'-N1-C2
12	B	44	Y5P	O4'-C1'-N1-C2
12	B	52	Y5P	O4'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
12	B	53	Y5P	O4'-C1'-N1-C2
12	B	60	Y5P	O4'-C1'-N1-C2
12	B	62	Y5P	O4'-C1'-N1-C2
12	B	63	Y5P	O4'-C1'-N1-C2
12	B	69	Y5P	O4'-C1'-N1-C2
12	B	28	P5P	O4'-C4'-C5'-O5'
12	B	67	P5P	C3'-C4'-C5'-O5'
12	B	70	P5P	C3'-C4'-C5'-O5'
12	B	33	Y5P	O4'-C4'-C5'-O5'
12	B	44	Y5P	O4'-C4'-C5'-O5'
12	B	44	Y5P	C3'-C4'-C5'-O5'
12	B	34	Y5P	O4'-C1'-N1-C2
12	B	23	P5P	O4'-C4'-C5'-O5'
12	B	25	P5P	O4'-C4'-C5'-O5'
12	B	32	P5P	O4'-C4'-C5'-O5'
12	B	46	P5P	C3'-C4'-C5'-O5'
12	B	46	P5P	O4'-C4'-C5'-O5'
12	B	49	P5P	C3'-C4'-C5'-O5'
12	B	67	P5P	O4'-C4'-C5'-O5'
12	B	33	Y5P	C3'-C4'-C5'-O5'
12	B	48	Y5P	O4'-C1'-N1-C2
12	B	32	P5P	C3'-C4'-C5'-O5'
12	B	40	Y5P	C3'-C4'-C5'-O5'
12	B	46	P5P	C4'-C5'-O5'-P
12	B	9	P5P	O4'-C4'-C5'-O5'
12	B	70	P5P	O4'-C4'-C5'-O5'
12	B	12	Y5P	C3'-C4'-C5'-O5'
12	B	34	Y5P	O4'-C4'-C5'-O5'
12	B	40	Y5P	O4'-C4'-C5'-O5'
12	B	9	P5P	C3'-C4'-C5'-O5'
12	B	34	Y5P	C3'-C4'-C5'-O5'
12	B	12	Y5P	O4'-C4'-C5'-O5'
12	B	15	P5P	C4'-C5'-O5'-P
12	B	67	P5P	C4'-C5'-O5'-P
12	B	27	P5P	C3'-C4'-C5'-O5'
12	B	5	P5P	C4'-C5'-O5'-P
12	B	7	P5P	C4'-C5'-O5'-P
12	B	14	P5P	C4'-C5'-O5'-P
12	B	41	P5P	O4'-C4'-C5'-O5'
12	B	30	P5P	C4'-C5'-O5'-P
12	B	8	Y5P	C4'-C5'-O5'-P
12	B	36	P5P	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
12	B	6	Y5P	C4'-C5'-O5'-P
12	B	39	P5P	O4'-C4'-C5'-O5'
12	B	9	P5P	C4'-C5'-O5'-P
12	B	41	P5P	C3'-C4'-C5'-O5'
12	B	3	Y5P	C4'-C5'-O5'-P

There are no ring outliers.

36 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	42	Y5P	2	0
12	B	11	Y5P	1	0
12	B	48	Y5P	1	0
12	B	72	Y5P	1	0
12	B	14	P5P	1	0
12	B	61	Y5P	2	0
12	B	47	P5P	2	0
12	B	26	Y5P	1	0
12	B	63	Y5P	2	0
12	B	41	P5P	1	0
12	B	12	Y5P	1	0
12	B	62	Y5P	2	0
12	B	39	P5P	2	0
12	B	24	P5P	1	0
12	B	31	Y5P	1	0
12	B	68	P5P	1	0
12	B	15	P5P	1	0
12	B	13	Y5P	1	0
12	B	25	P5P	3	0
12	B	49	P5P	1	0
12	B	3	Y5P	1	0
12	B	33	Y5P	1	0
12	B	4	P5P	2	0
12	B	43	Y5P	1	0
12	B	44	Y5P	1	0
12	B	59	P5P	1	0
12	B	70	P5P	1	0
12	B	60	Y5P	2	0
12	B	71	Y5P	1	0
12	B	67	P5P	1	0
12	B	30	P5P	1	0
12	B	69	Y5P	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	38	P5P	2	0
12	B	9	P5P	2	0
12	B	5	P5P	1	0
12	B	23	P5P	3	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 171 ligands modelled in this entry, 171 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
12	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	53:Y5P	O3'	58:P5P	P	17.46
1	B	15:P5P	O3'	23:P5P	P	12.62

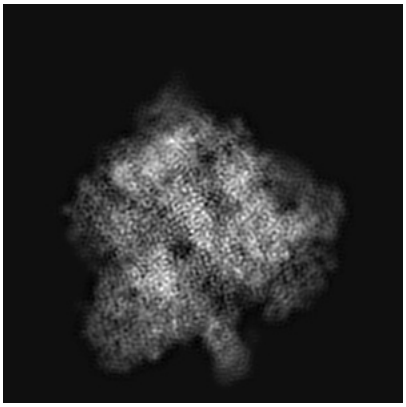
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-2787. These allow visual inspection of the internal detail of the map and identification of artifacts.

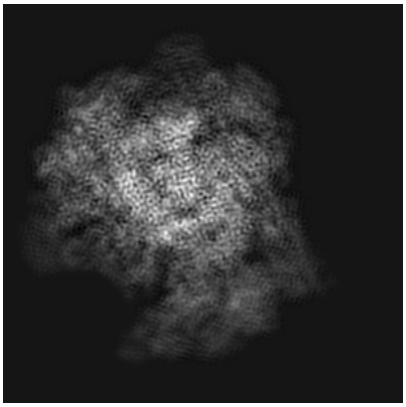
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

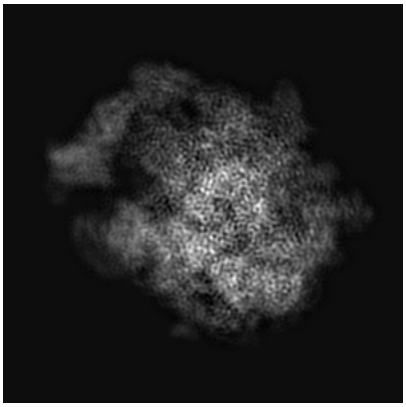
6.1.1 Primary map



X



Y

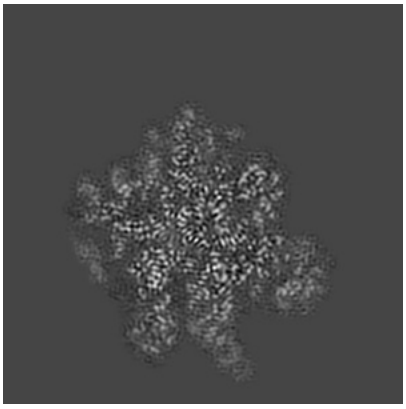


Z

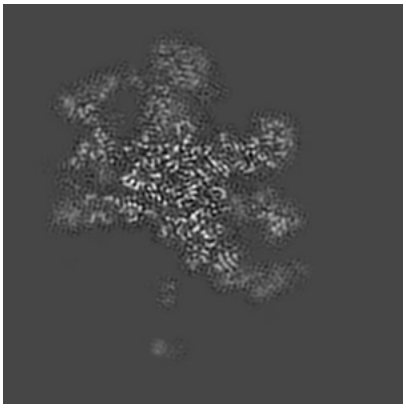
The images above show the map projected in three orthogonal directions.

6.2 Central slices

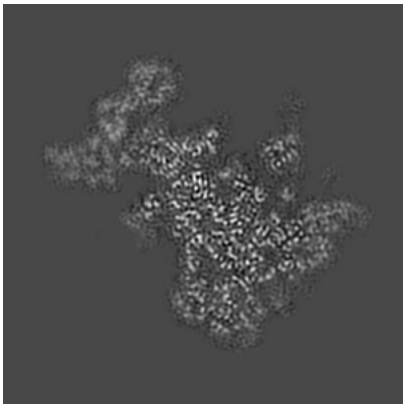
6.2.1 Primary map



X Index: 108



Y Index: 108

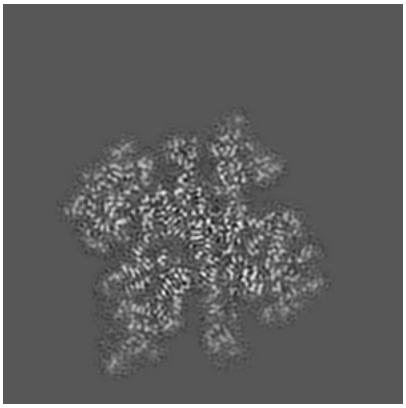


Z Index: 108

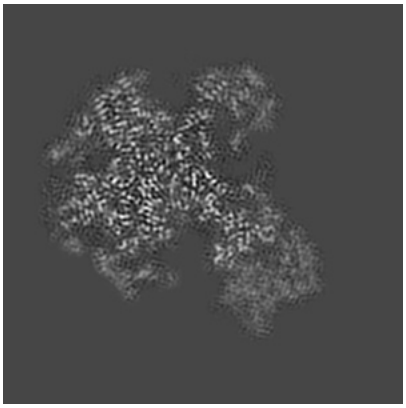
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

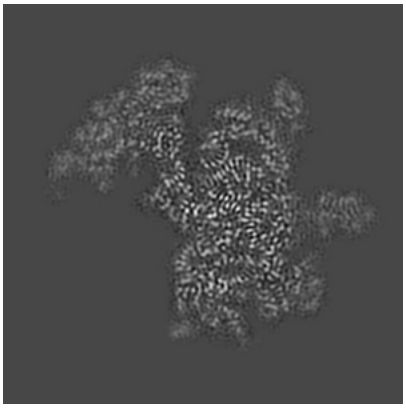
6.3.1 Primary map



X Index: 120



Y Index: 86

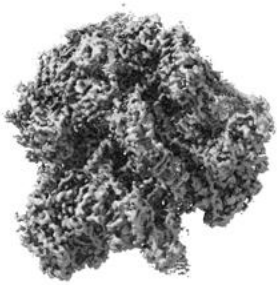


Z Index: 98

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

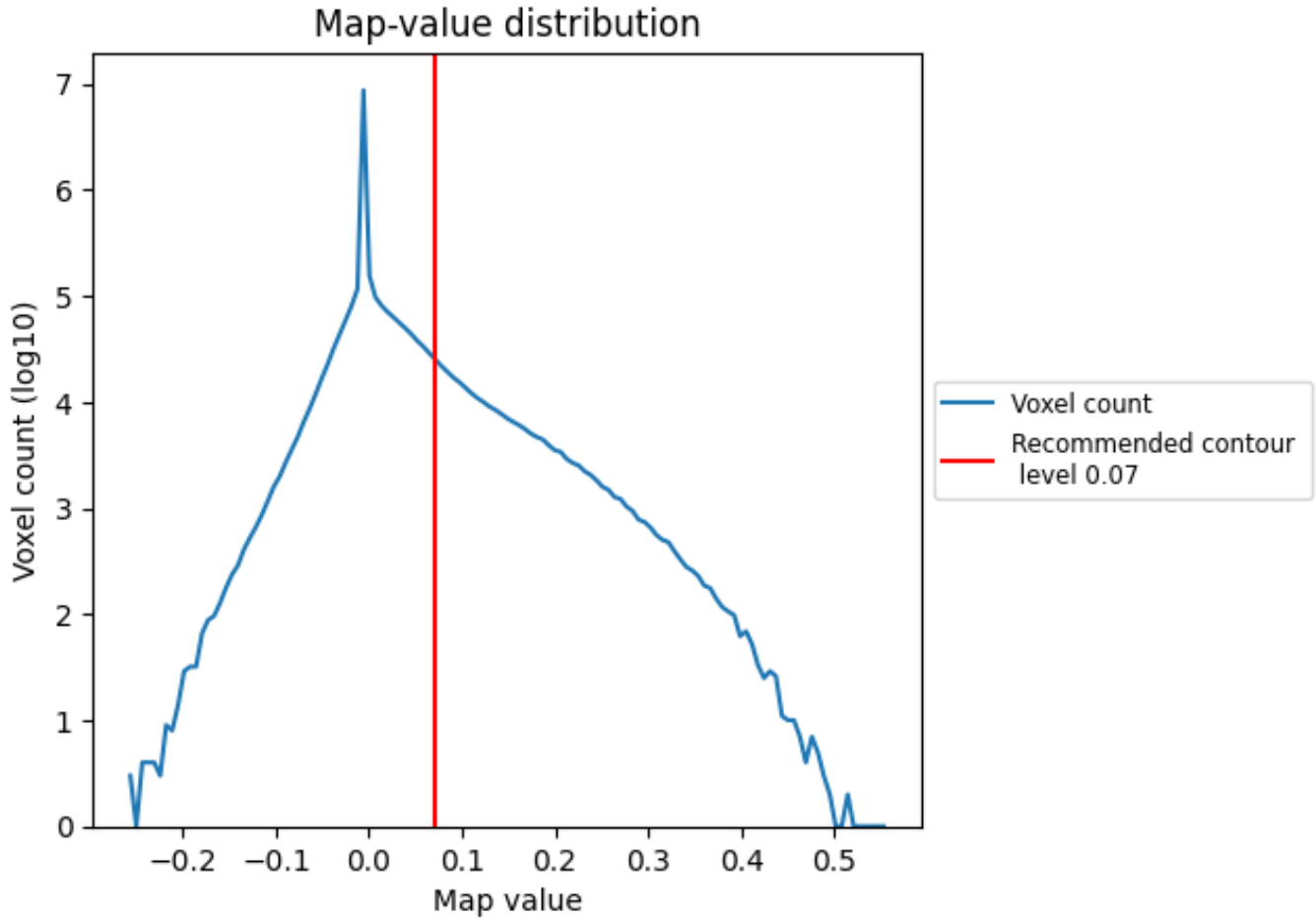
6.5 Mask visualisation (i)

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

7 Map analysis

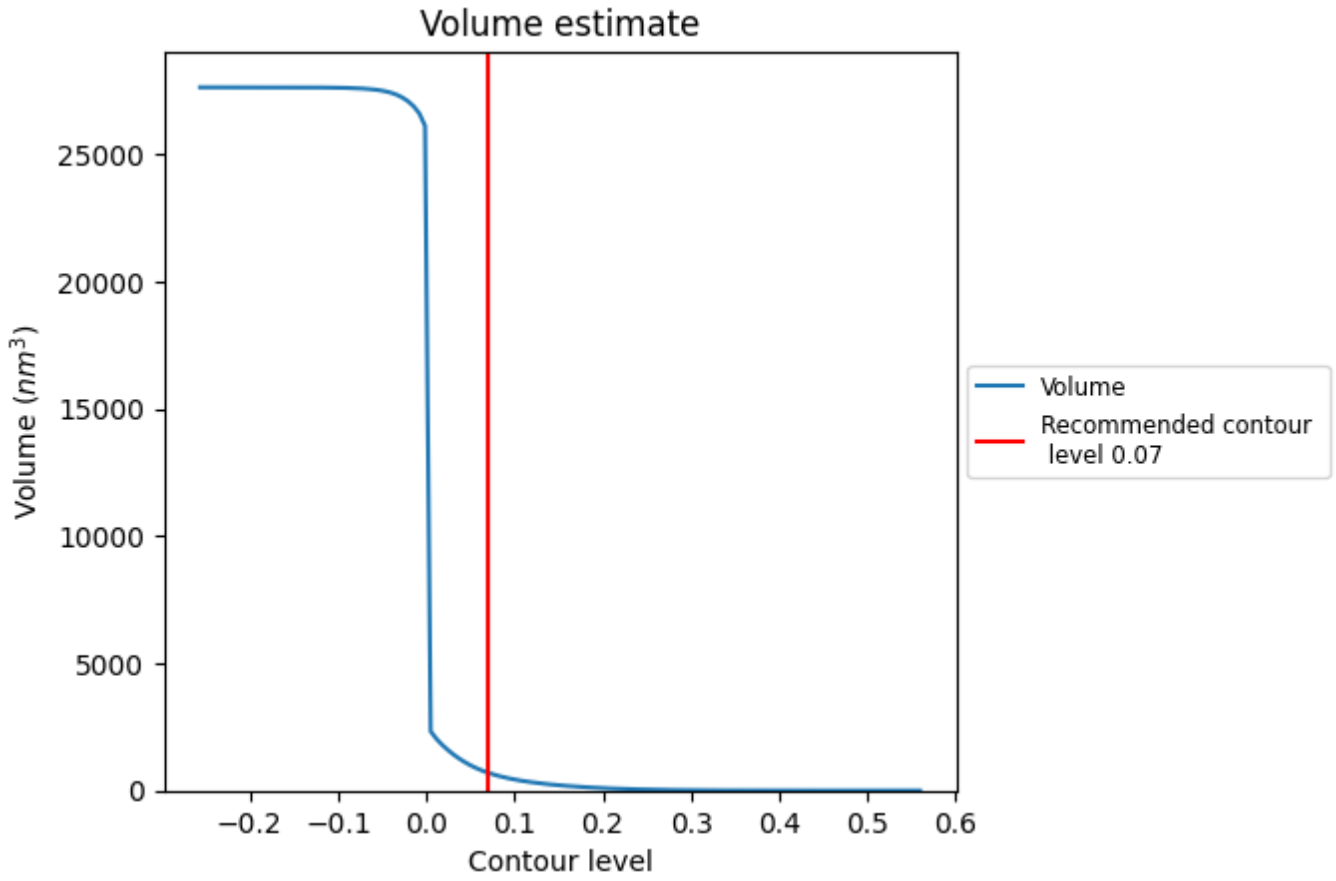
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

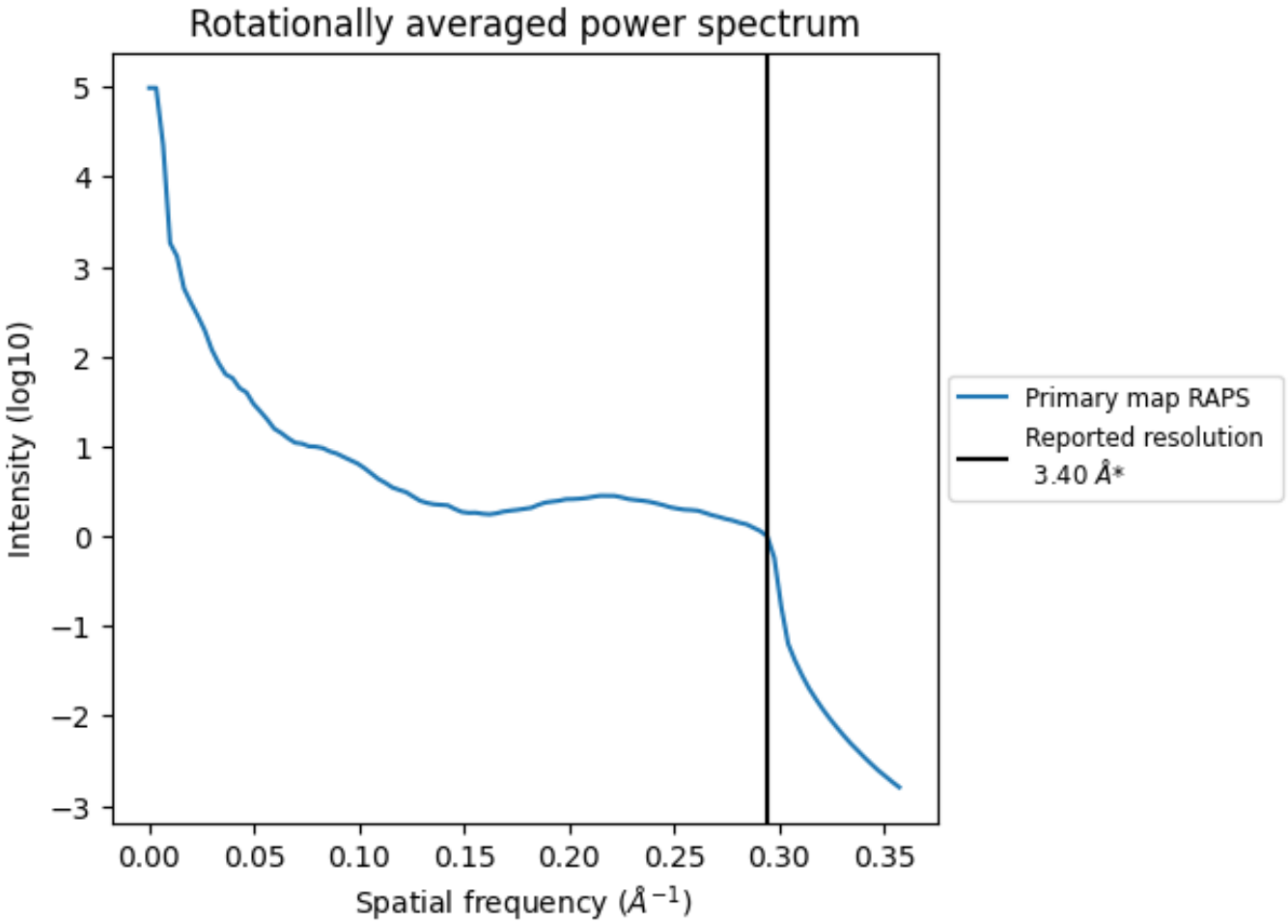
7.2 Volume estimate



The volume at the recommended contour level is 700 nm^3; this corresponds to an approximate mass of 632 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

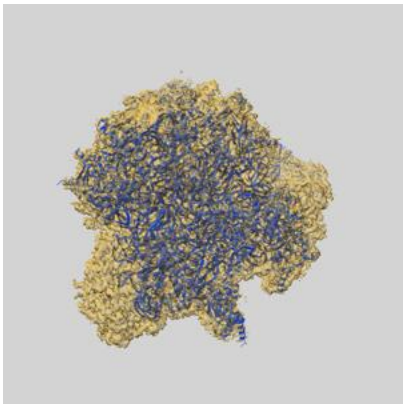
8 Fourier-Shell correlation (i)

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

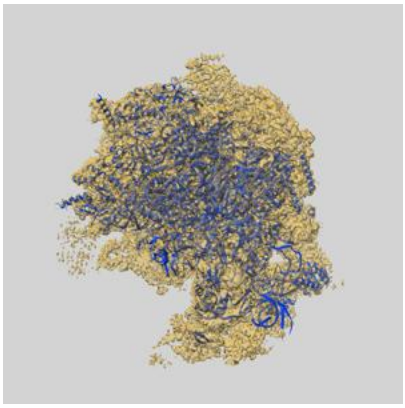
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-2787 and PDB model 4V19. Per-residue inclusion information can be found in section 3 on page 10.

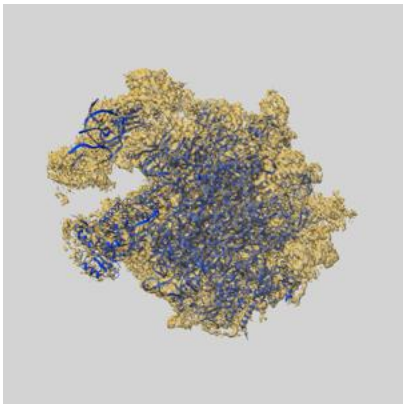
9.1 Map-model overlay



X



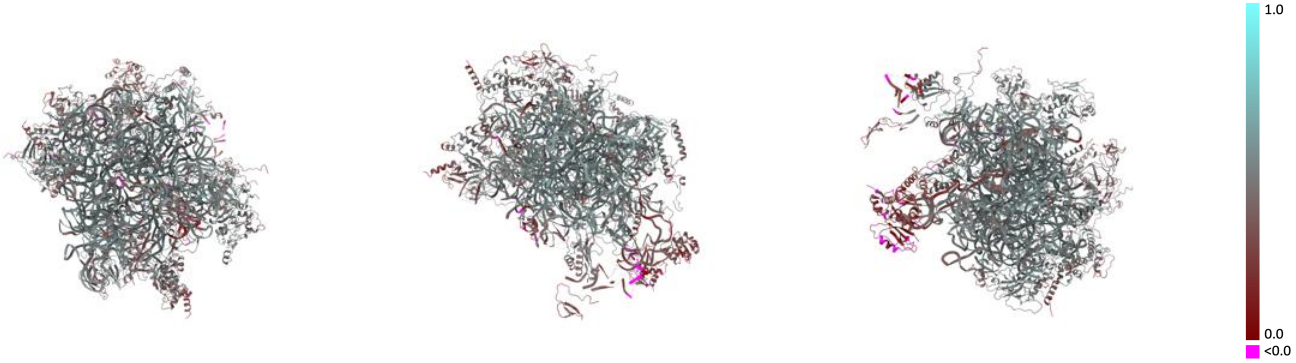
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

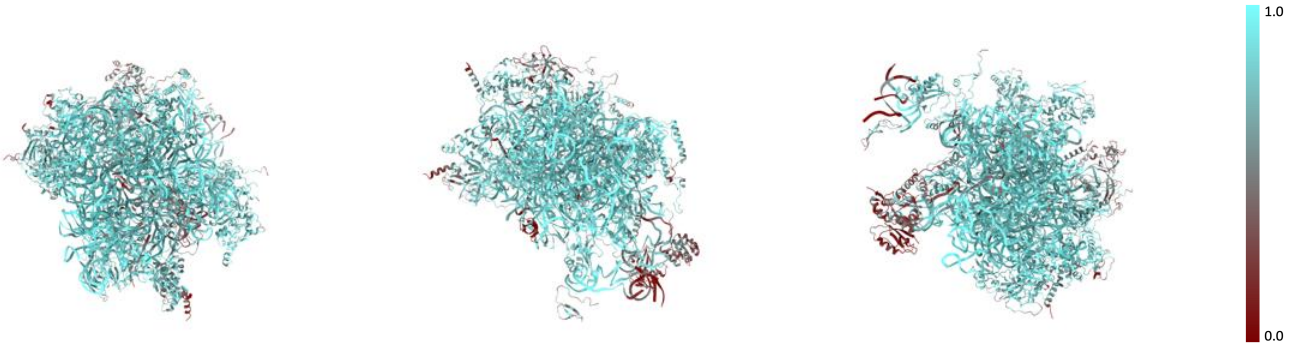
9.2 Q-score mapped to coordinate model



X Y Z

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

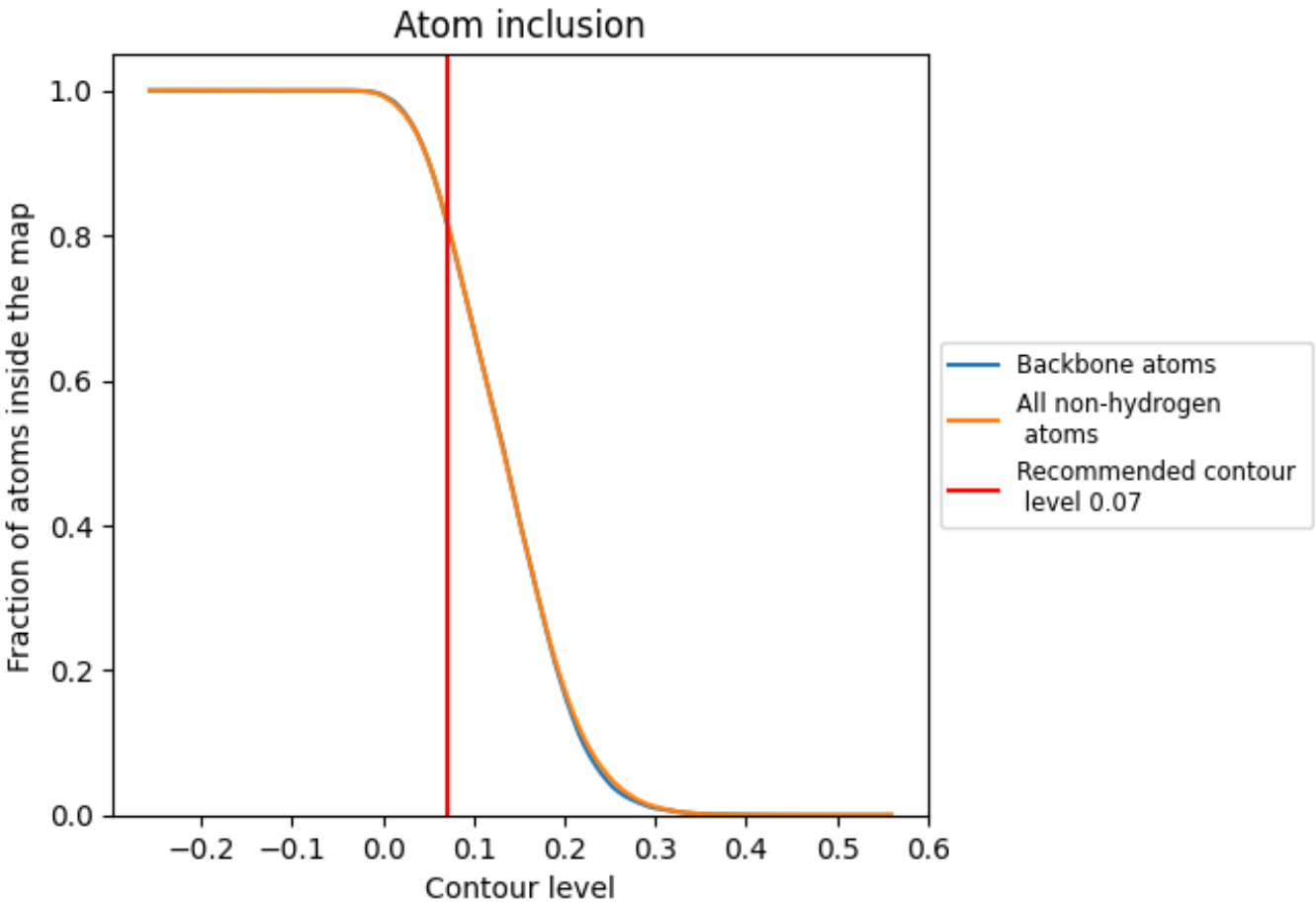
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.07).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 82% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8204	0.4730
0	0.8422	0.5140
1	0.7336	0.4400
2	0.7977	0.4680
3	0.8230	0.4960
4	0.5193	0.2340
5	0.7715	0.4430
6	0.0547	0.1590
7	0.8943	0.5470
8	0.8733	0.5350
9	0.8879	0.5290
A	0.9151	0.5020
B	0.5992	0.2180
C	0.6613	0.4510
D	0.8074	0.4880
E	0.8255	0.4920
F	0.8479	0.5070
I	0.5956	0.3810
J	0.4684	0.3080
K	0.2134	0.1500
N	0.8526	0.5130
O	0.8149	0.5010
P	0.8400	0.4890
Q	0.8161	0.4850
R	0.8110	0.4910
S	0.7806	0.4340
T	0.7534	0.4680
U	0.8284	0.5000
V	0.7968	0.4890
W	0.7953	0.5080
X	0.7886	0.4770
Y	0.4882	0.3760
Z	0.3871	0.4190