



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 04:06 AM UTC

PDB ID : 7AS9 / pdb_00007as9
EMDB ID : EMD-11890
Title : Bacillus subtilis ribosome-associated quality control complex state A. Ribosomal 50S subunit with peptidyl tRNA in the A/P position and RqcH.
Authors : Crowe-McAuliffe, C.; Wilson, D.N.
Deposited on : 2020-10-27
Resolution : 3.50 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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

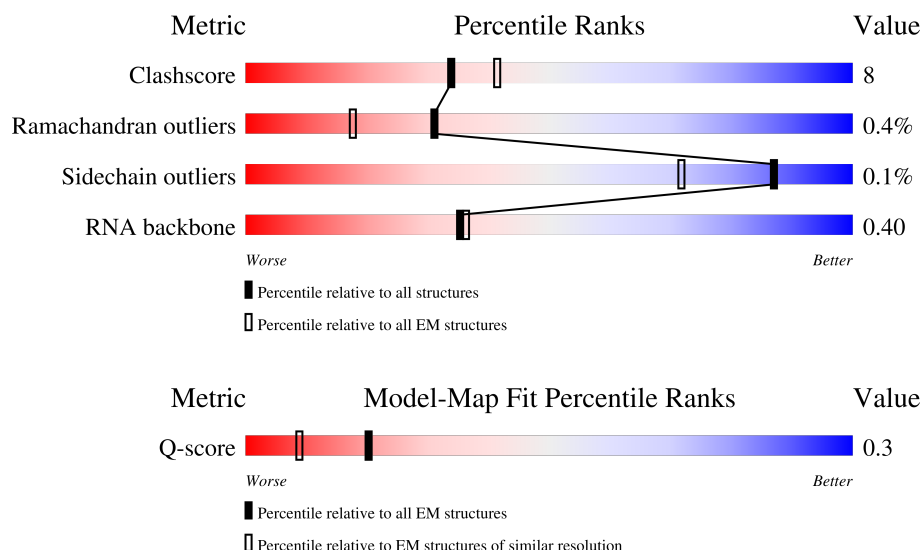
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13950 (3.00 - 4.00)

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

Mol	Chain	Length	Quality of chain
1	0	597	
2	2	76	
3	A	2926	

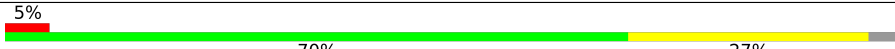
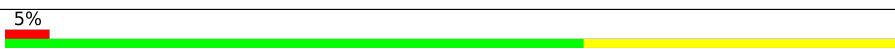
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Mol	Chain	Length	Quality of chain
4	B	119	
5	E	277	
6	F	209	
7	G	207	
8	H	179	
9	I	179	
10	K	141	
11	L	166	
12	N	145	
13	O	122	
14	P	146	
15	Q	144	
16	R	120	
17	S	120	
18	T	115	
19	U	119	
20	V	102	
21	W	113	
22	X	95	
23	Y	103	
24	a	94	
25	b	62	
26	c	66	
27	d	59	
28	f	59	

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Mol	Chain	Length	Quality of chain
29	g	49	
30	h	44	
31	i	66	
32	j	37	

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 93137 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 Rqc2 homolog RqcH.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	535	Total	C	N	O	S	0	0
			3987	2517	712	748	10		

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	571	GLY	-	expression tag	UNP O34693
0	572	SER	-	expression tag	UNP O34693
0	573	GLY	-	expression tag	UNP O34693
0	574	GLY	-	expression tag	UNP O34693
0	575	ASP	-	expression tag	UNP O34693
0	576	TYR	-	expression tag	UNP O34693
0	577	LYS	-	expression tag	UNP O34693
0	578	ASP	-	expression tag	UNP O34693
0	579	HIS	-	expression tag	UNP O34693
0	580	ASP	-	expression tag	UNP O34693
0	581	GLY	-	expression tag	UNP O34693
0	582	ASP	-	expression tag	UNP O34693
0	583	TYR	-	expression tag	UNP O34693
0	584	LYS	-	expression tag	UNP O34693
0	585	ASP	-	expression tag	UNP O34693
0	586	HIS	-	expression tag	UNP O34693
0	587	ASP	-	expression tag	UNP O34693
0	588	ILE	-	expression tag	UNP O34693
0	589	ASP	-	expression tag	UNP O34693
0	590	TYR	-	expression tag	UNP O34693
0	591	LYS	-	expression tag	UNP O34693
0	592	ASP	-	expression tag	UNP O34693
0	593	ASP	-	expression tag	UNP O34693
0	594	ASP	-	expression tag	UNP O34693
0	595	ASP	-	expression tag	UNP O34693
0	596	LYS	-	expression tag	UNP O34693
0	597	GLY	-	expression tag	UNP O34693

- Molecule 2 is a RNA chain called tRNA-Ala-1-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	75	Total	C	N	O	P	0	0
			1603	713	288	527	75		

- Molecule 3 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	2812	Total	C	N	O	P	0	0
			60389	26942	11160	19477	2810		

- Molecule 4 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	112	Total	C	N	O	P	0	0
			2392	1068	435	778	111		

- Molecule 5 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	272	Total	C	N	O	S	0	0
			2083	1296	408	373	6		

- Molecule 6 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	206	Total	C	N	O	S	0	0
			1569	985	289	290	5		

- Molecule 7 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	205	Total	C	N	O	S	0	0
			1561	980	289	290	2		

- Molecule 8 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	164	Total	C	N	O	S	0	0
			1284	813	228	236	7		

- Molecule 9 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	175	Total	C	N	O	S	0	0
			1342	835	248	257	2		

- Molecule 10 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	132	Total	C	N	O	S	0	0
			974	612	172	184	6		

- Molecule 11 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	113	Total	C	N	O	S	0	0
			886	559	152	174	1		

- Molecule 12 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	142	Total	C	N	O	S	0	0
			1123	710	206	202	5		

- Molecule 13 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	122	Total	C	N	O	S	0	0
			920	571	173	172	4		

- Molecule 14 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	146	Total	C	N	O	S	0	0
			1081	671	207	201	2		

- Molecule 15 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	135	Total	C	N	O	S	0	0
			1076	690	205	176	5		

- Molecule 16 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	119	Total	C	N	O	S	0	0
			953	583	186	180	4		

- Molecule 17 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	120	Total	C	N	O	S	0	0
			912	564	176	171	1		

- Molecule 18 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	115	Total	C	N	O	S	0	0
			944	600	185	158	1		

- Molecule 19 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	117	Total	C	N	O	S	0	0
			940	591	189	156	4		

- Molecule 20 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	V	100	Total	C	N	O	0	0
			781	498	138	145		

- Molecule 21 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	109	Total	C	N	O	S	0	0
			842	525	164	150	3		

- Molecule 22 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	90	Total	C	N	O	S	0	0
			725	452	134	136	3		

- Molecule 23 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	101	Total	C	N	O	S	0	0
			762	478	142	138	4		

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	75	Total	C	N	O		0	0
			585	363	114	108			

- Molecule 25 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	58	Total	C	N	O	S	0	0
			444	275	92	75	2		

- Molecule 26 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	65	Total	C	N	O	S	0	0
			530	328	102	98	2		

- Molecule 27 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	d	58	Total	C	N	O	S	0	0
			455	281	89	84	1		

- Molecule 28 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	f	53	Total	C	N	O	S	0	0
			418	258	84	69	7		

- Molecule 29 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	g	48	Total	C	N	O	S	0	0
			401	244	80	73	4		

- Molecule 30 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	h	44	Total	C	N	O	S	0	0
			367	222	89	54	2		

- Molecule 31 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	i	64	Total	C	N	O	S	0	0
			512	321	107	82	2		

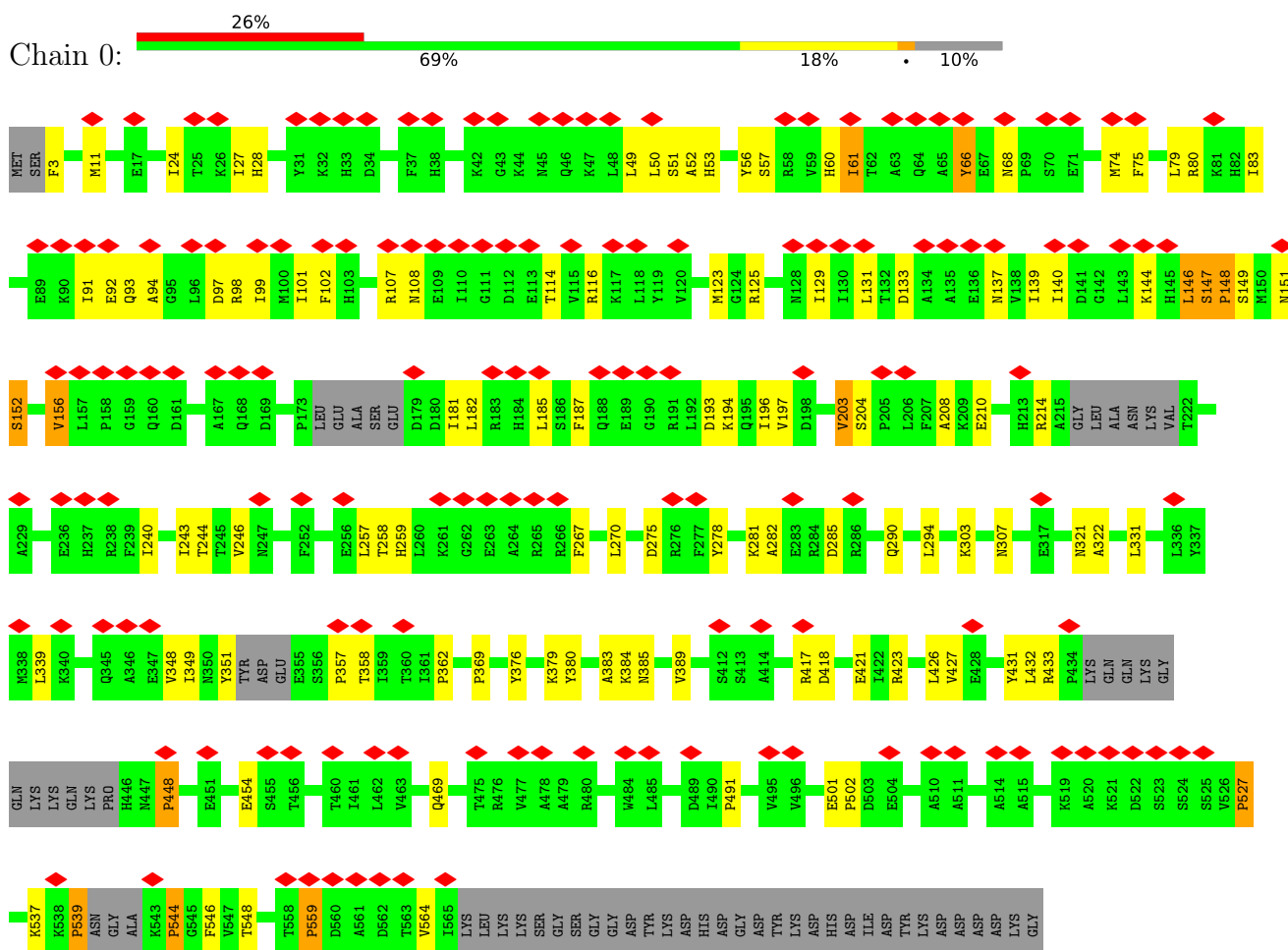
- Molecule 32 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	j	37	Total	C	N	O	S	0	0
			296	186	60	45	5		

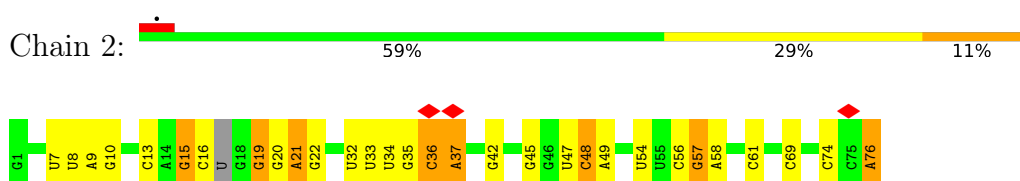
3 Residue-property plots

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

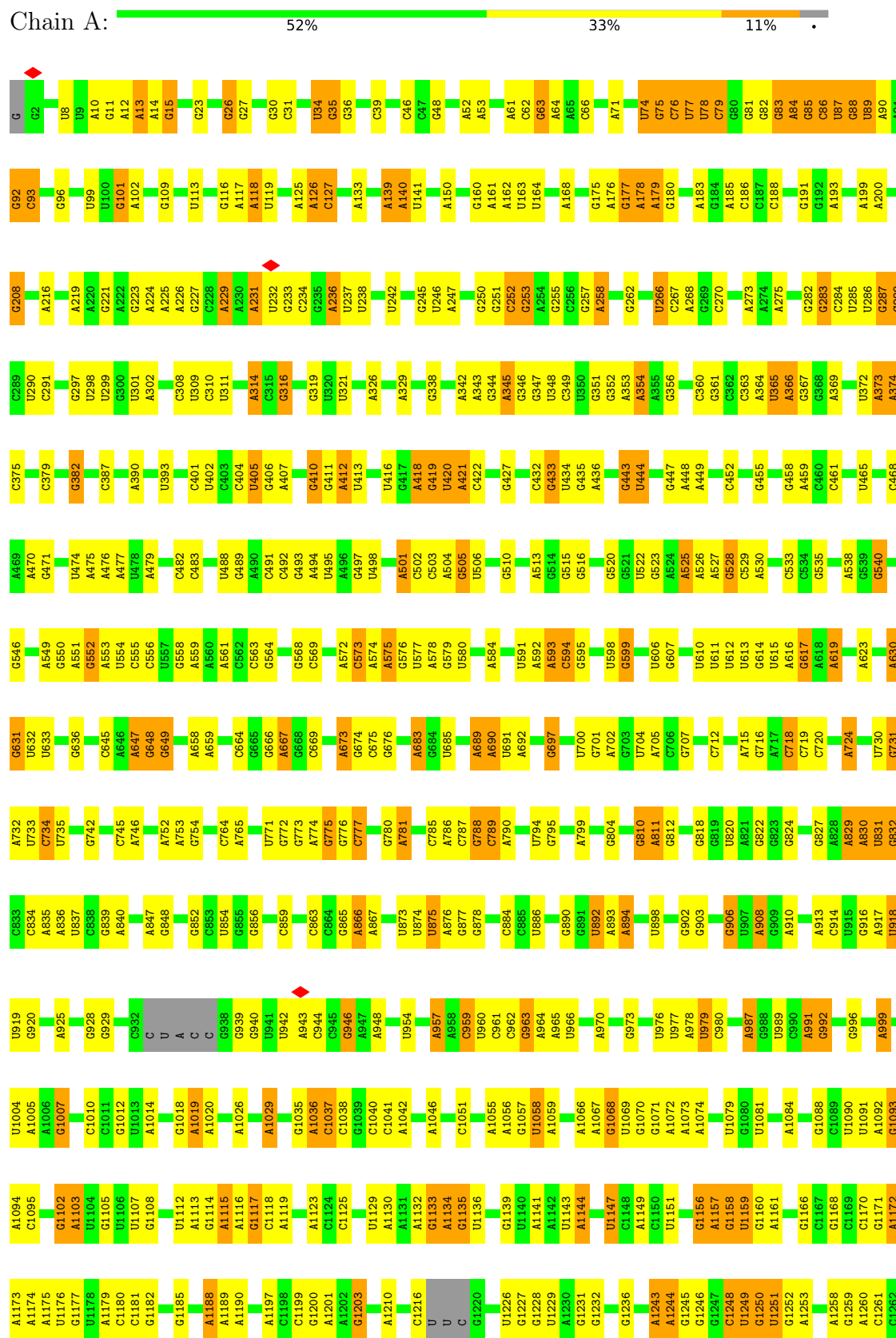
• Molecule 1: Rqc2 homolog RqcH



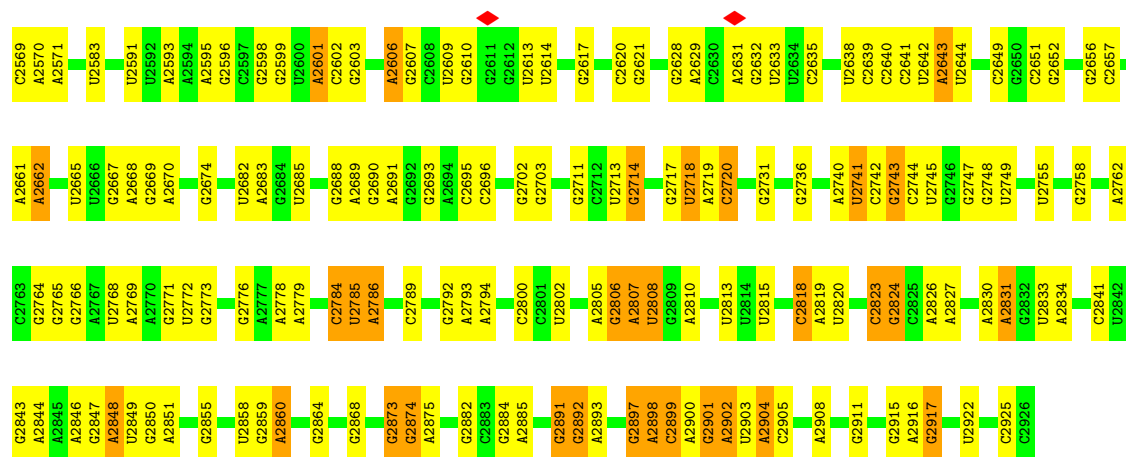
• Molecule 2: tRNA-Ala-1-1



• Molecule 3: 23S rRNA

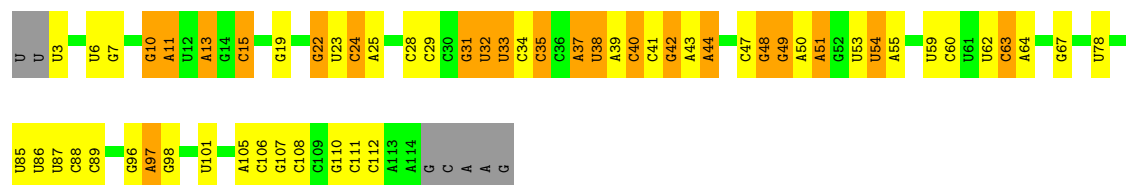


C2474	C2384	G	C2065	A1768	G1600	G1525	A1432	A1347	G1263
G2475	C2385	C	A2066	A1769	A1601	G1526	U1433	A1351	G1264
G2476	U2386	G	G	U1790	G1602	U1527	U1434	U1352	A1265
A2477	C2387	G	U2070	G1791	U1603	U1528	A1435	C1353	G1266
U2478	C2388	A	C2071	G1792	C1604	G1529	U1436	G1267	G1268
A2479	U2392	U	C2072	G1793	A1708	G1530	A1442	A1357	A1269
G2484	C2393	C	A2080	A1802	A1710	G1531	A1447	G1358	G1276
U2491	C2394	C	G2081	G1810	A1711	A1532	C1448	G1359	A1277
C2492	A2316	U	G2085	A1811	A1713	A1536	U1449	G1362	G1278
A2497	A2317	G	G2088	A1812	G1718	C1539	C1450	G1363	C1279
A2498	G2318	G	G2089	A1813	G1719	A1540	U1456	G1364	G1280
C2499	A2227	A	G2090	A1814	C1720	A1541	U1457	U1365	
	A2228	A	A2089	A1815	A1721	U1542	U1458	C1366	
	C2231	A	A2090	A1816	A1727	U1543	U1459	G1367	U1283
	C2232	C	C2092	A1817	A1733	C1544	G1460	C1368	A1284
	C2233	C	G	A1818	U1737	U1545		U1369	
	U2331	G	U2097	A1819	G1738	G1546		C1370	G1288
	U2332	G	G2098	A1820	U1739			C1371	U1289
	U2333	G	A2099	G1821	C1739	C1550	A1464	C1372	G1290
	U2334	G	A2100	A1828	U1740	C1551	U1465	A1291	
	U2335	C	A2106	C1829	G1743	C1552	U1466	G1292	G1293
	G2245	C	C2107	A1831	U1744	U	G1467	G1376	A1294
	G2246	C	A1930	A1832	A1745	A1553	G1468	G1377	U1295
	G2249	A	G1933	G1841	G1748	A1555	G1470	G1378	C1297
	A2252	U	C1934	G1844	U1647	G1558	G1471	U1380	
	A2253	U	G1935	A1845	A1648	C1559	A1472	C1384	G1304
	A2254	C	G1936	A1846	C1649	U1560	C1474	G1304	
	C2255	G	C1937	A1845	G1651	G1561	G1475	G1306	
	U2344	G	U1940	G1846	C1652	A1562	C1476		
	U2345	G	A	U1849	A1653	U1565	G1481	G1311	
	G2259	U	A	U1849	A1654	U1566	A1485	A1312	
	G2263	G	C	G1853	A1655	U1567		A1313	
	G2267	C	U	G1854	C1656	G1568		A1314	
	G2268	C	A	C1855	A1661	A1569	U1489	G1315	
	G2275	U	A	A1858	G1664	U1570	A1490	A1316	
	A2276	U	C1949	C1872	G1671	G1571	C1493	G1317	
	A2277	C	A	U1873	A1672	C1577	G1494	G1318	
	C2277	C	C1953	G1862	A1679	G	A1499	U1321	
	G2278	G	C1953	G1863	U1679	A	U1500	G1322	
	G2279	G	A1956	G1864	A1679	A	U1501	A1323	
	G2280	U	A1957	C1865	C1770	A	G1502	G1324	
	G2281	G	G1958	C1866	U1694	U	U1507	A1325	
	G2282	G	G1959	C1867	A1685	A	G1502	A1326	
	A2287	A	U1960	C1872	G1690	U	U1506	U1327	
	U2291	U	G1964	U1873	A1691	A	A1506	U1418	
	C2292	C	A1965	A1876	A1691	G	U1507	G1419	
	C2293	C	A1966	A1877	G1692	U	C1508	A1424	
	U2294	U	A1967	A1877	C1693	A	C1509	A1339	
	U2295	A	U1968	G1882	G1694		U1513	A1340	
	A2296	C	U1969	A1883	A1696		U1516	A1426	
	A2297	C	U1970	A1884	A1697		A1516	U1427	
	A2297	C	C1971	A1885	G1698		A1516	G1428	
	A2302	G	U1972	G1886	A1699		U1523	C1343	
					G1785		A1524	G1431	



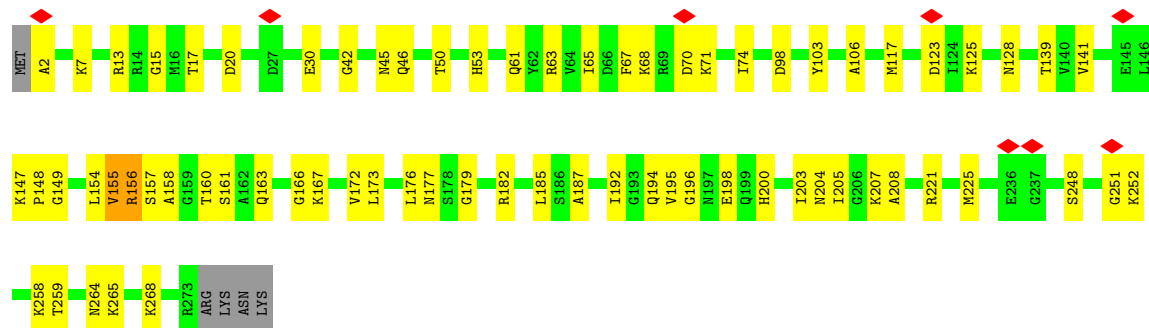
• Molecule 4: 5S rRNA

Chain B: 45% 31% 18% 6%



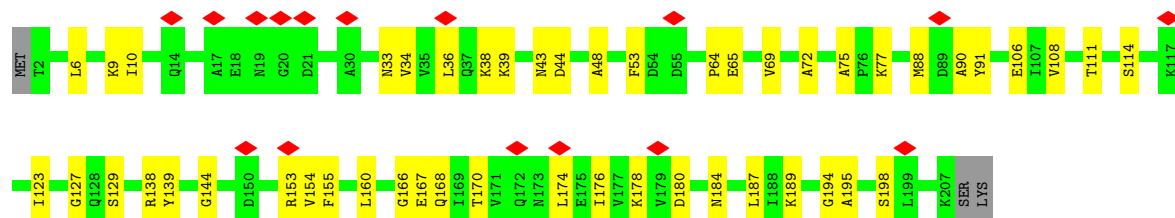
• Molecule 5: 50S ribosomal protein L2

Chain E: 73% 25% ..

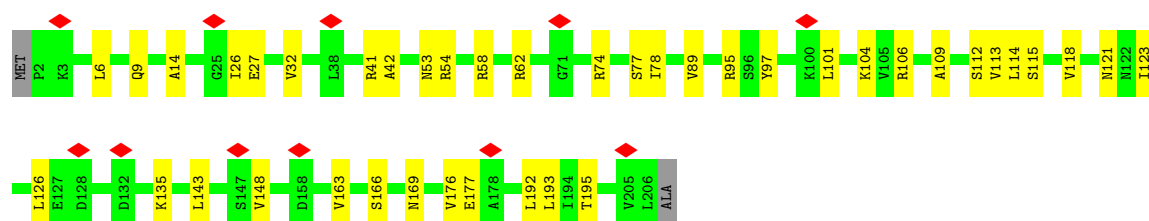
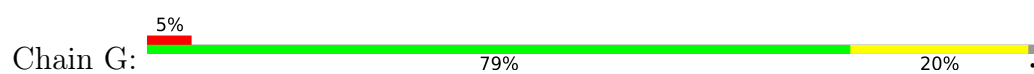


• Molecule 6: 50S ribosomal protein L3

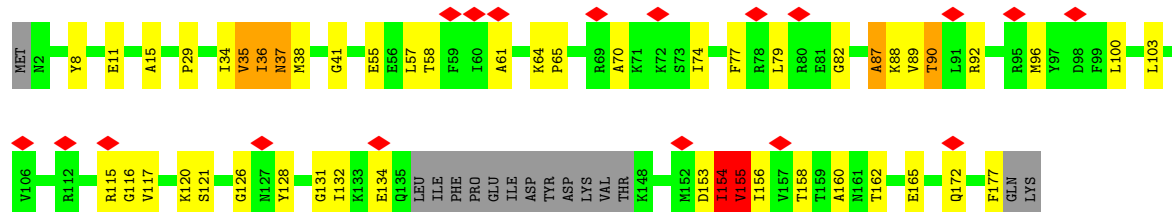
Chain F: 8% 75% 23%



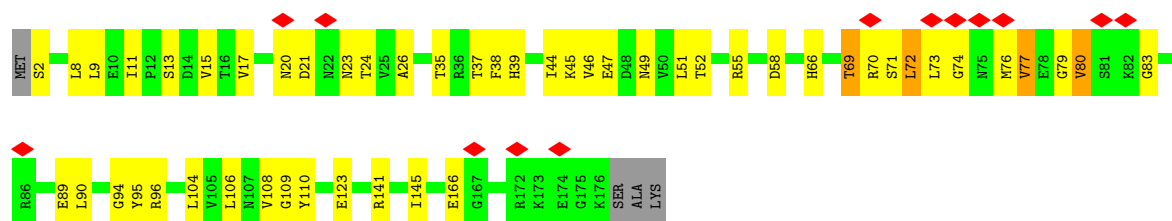
• Molecule 7: 50S ribosomal protein L4



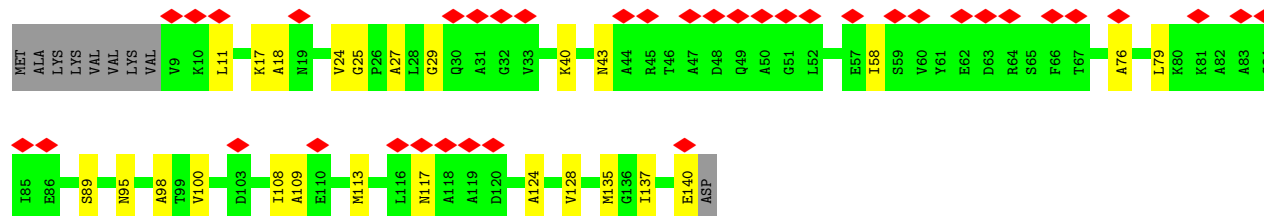
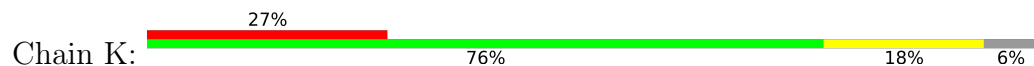
• Molecule 8: 50S ribosomal protein L5



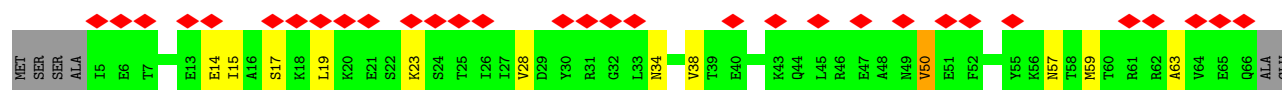
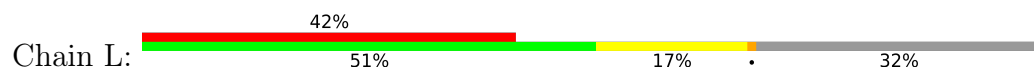
• Molecule 9: 50S ribosomal protein L6

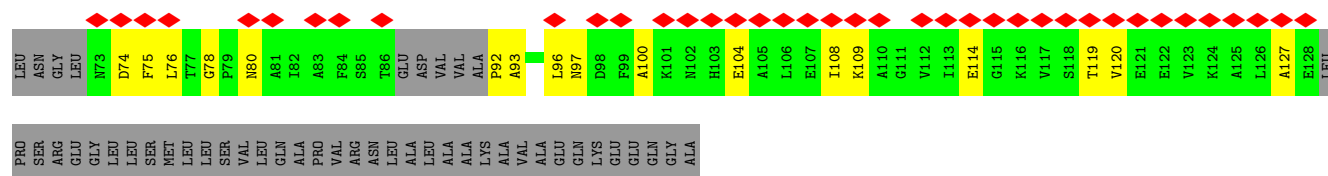


• Molecule 10: 50S ribosomal protein L11



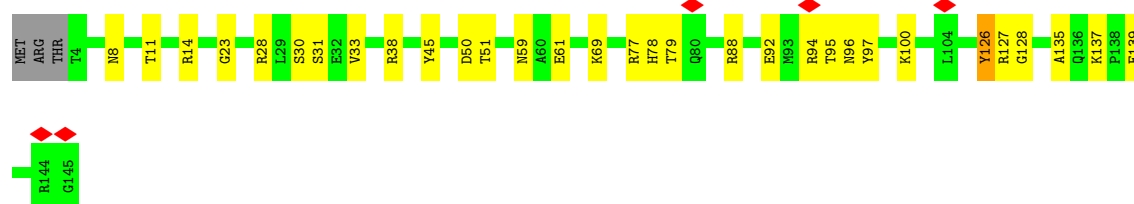
• Molecule 11: 50S ribosomal protein L10





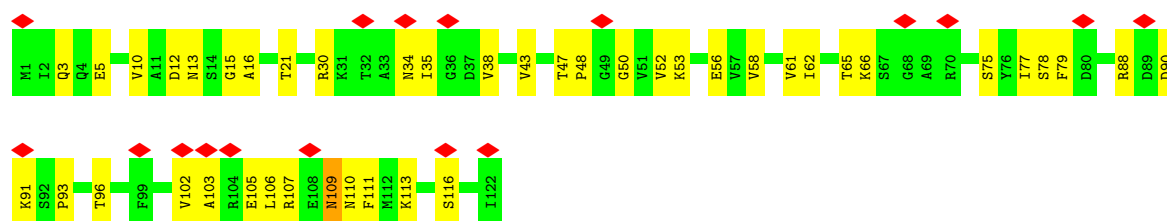
• Molecule 12: 50S ribosomal protein L13

Chain N: 77% 21% ..



• Molecule 13: 50S ribosomal protein L14

Chain O: 14% 65% 34% .



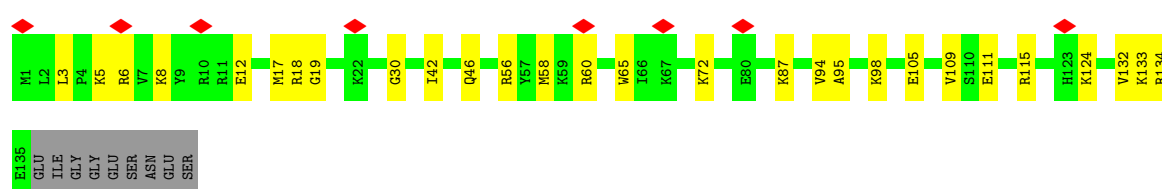
• Molecule 14: 50S ribosomal protein L15

Chain P: 10% 75% 25%



• Molecule 15: 50S ribosomal protein L16

Chain Q: 6% 74% 19% 6%



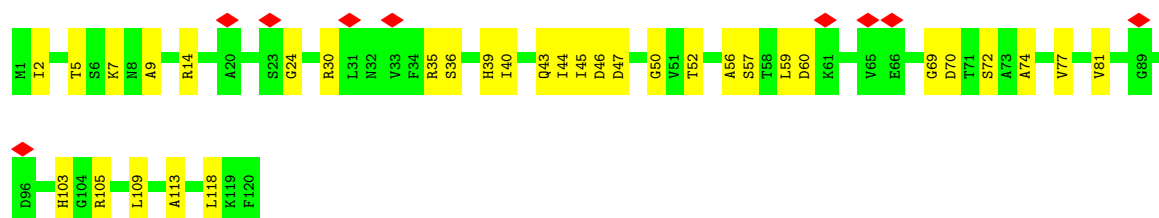
- Molecule 16: 50S ribosomal protein L17

Chain R:  76% 23%



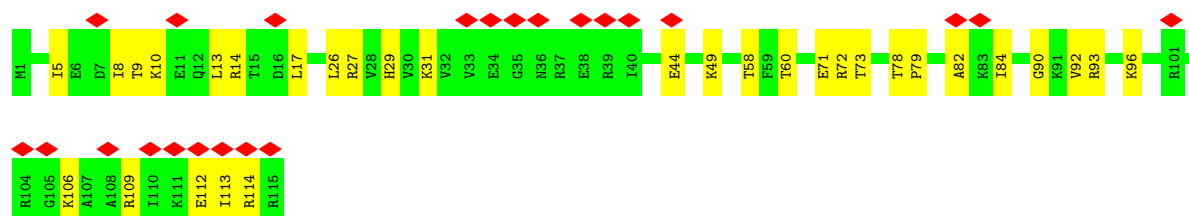
- Molecule 17: 50S ribosomal protein L18

Chain S:  8% 72% 28%



- Molecule 18: 50S ribosomal protein L19

Chain T:  20% 73% 27%



- Molecule 19: 50S ribosomal protein L20

Chain U:  79% 18%



- Molecule 20: 50S ribosomal protein L21

Chain V:  7% 74% 25%

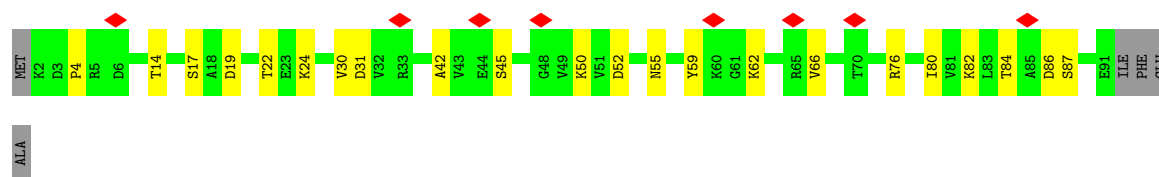


- Molecule 21: 50S ribosomal protein L22

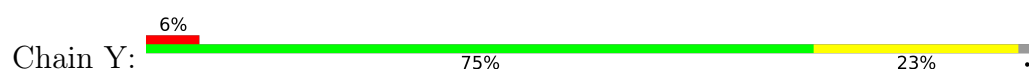
Chain W:  83% 13%



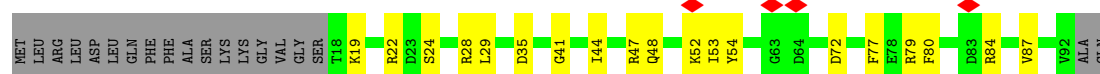
- Molecule 22: 50S ribosomal protein L23



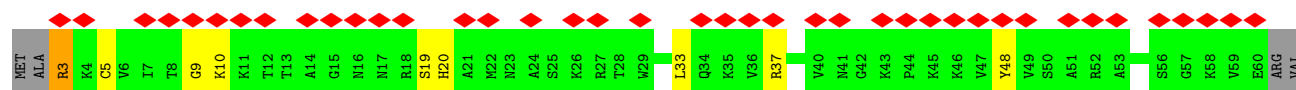
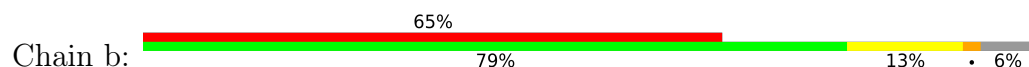
- Molecule 23: 50S ribosomal protein L24



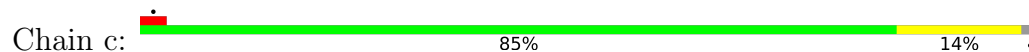
- Molecule 24: 50S ribosomal protein L27



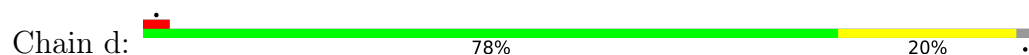
- Molecule 25: 50S ribosomal protein L28



- Molecule 26: 50S ribosomal protein L29

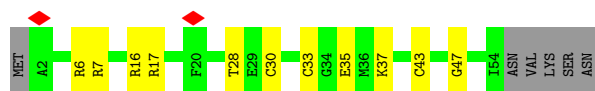


- Molecule 27: 50S ribosomal protein L30

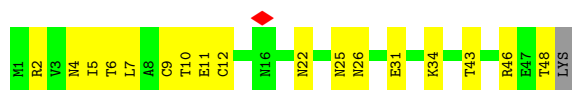




- Molecule 28: 50S ribosomal protein L32



- Molecule 29: 50S ribosomal protein L33 1



- Molecule 30: 50S ribosomal protein L34



- Molecule 31: 50S ribosomal protein L35



- Molecule 32: 50S ribosomal protein L36



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10703	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	29	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.032	Depositor
Minimum map value	-0.012	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.007	Depositor
Map size (Å)	344.4, 344.4, 344.4	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.31	0/4052	0.73	11/5477 (0.2%)
2	2	0.28	0/1790	0.43	0/2788
3	A	0.37	0/67640	0.46	0/105516
4	B	0.32	0/2675	0.45	0/4170
5	E	0.38	0/2120	0.61	0/2845
6	F	0.39	0/1591	0.57	0/2132
7	G	0.41	0/1580	0.60	0/2132
8	H	0.59	1/1299 (0.1%)	0.81	5/1740 (0.3%)
9	I	0.47	0/1360	0.95	9/1832 (0.5%)
10	K	0.29	0/988	0.54	0/1336
11	L	0.27	0/892	0.55	0/1196
12	N	0.42	0/1146	0.62	0/1542
13	O	0.39	0/927	0.63	0/1245
14	P	0.37	0/1093	0.61	0/1457
15	Q	0.43	0/1099	0.62	0/1468
16	R	0.42	0/960	0.61	0/1284
17	S	0.34	0/921	0.63	0/1236
18	T	0.37	0/957	0.63	0/1279
19	U	0.49	0/952	0.67	0/1266
20	V	0.42	0/792	0.64	0/1063
21	W	0.43	0/851	0.60	0/1146
22	X	0.37	0/731	0.58	0/974
23	Y	0.37	0/772	0.67	2/1032 (0.2%)
24	a	0.39	0/593	0.63	0/789
25	b	0.35	0/448	0.70	0/596
26	c	0.40	0/531	0.61	0/707
27	d	0.38	0/457	0.58	0/613
28	f	0.39	0/425	0.57	0/563
29	g	0.37	0/406	0.55	0/540
30	h	0.49	0/370	0.58	0/483
31	i	0.44	0/519	0.56	0/680
32	j	0.47	0/299	0.64	0/393
All	All	0.37	1/101236 (0.0%)	0.52	27/151520 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	6
8	H	0	4
9	I	0	3
11	L	0	1
12	N	0	2
13	O	0	2
14	P	0	2
15	Q	0	3
19	U	0	1
20	V	0	2
21	W	0	1
25	b	0	1
30	h	0	1
All	All	0	29

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	155	VAL	C-N	10.61	1.46	1.33

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	72	LEU	CA-CB-CG	11.88	157.86	116.30
9	I	80	VAL	N-CA-CB	8.25	119.28	110.62
9	I	69	THR	N-CA-C	8.15	122.06	112.93
1	0	544	PRO	N-CA-CB	7.92	111.56	103.25
1	0	491	PRO	N-CA-CB	7.41	111.03	103.25
1	0	559	PRO	N-CA-CB	7.33	110.94	103.25
1	0	539	PRO	N-CA-CB	7.26	110.98	103.00
1	0	204	SER	N-CA-C	-7.18	99.89	108.14
9	I	80	VAL	CB-CA-C	-7.10	102.61	111.70
1	0	527	PRO	N-CA-CB	6.88	110.47	103.25
8	H	35	VAL	CG1-CB-CG2	-6.84	95.75	110.80
1	0	448	PRO	N-CA-CB	6.66	110.24	103.25
9	I	38	PHE	CA-C-N	6.48	130.53	120.68
9	I	38	PHE	C-N-CA	6.48	130.53	120.68
1	0	502	PRO	N-CA-CB	6.38	109.94	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	77	VAL	CG1-CB-CG2	-6.01	97.57	110.80
1	0	147	SER	C-N-CD	-5.97	107.47	120.60
8	H	35	VAL	CA-CB-CG1	5.94	120.50	110.40
23	Y	50	ALA	CA-C-N	5.86	136.09	121.80
23	Y	50	ALA	C-N-CA	5.86	136.09	121.80
9	I	72	LEU	CB-CA-C	-5.83	101.57	112.00
9	I	79	GLY	N-CA-C	5.64	126.56	113.18
1	0	147	SER	CA-C-N	5.56	140.35	127.00
1	0	147	SER	C-N-CA	5.56	140.35	127.00
8	H	36	ILE	N-CA-C	5.47	120.72	109.34
8	H	154	ILE	CA-C-N	5.19	131.31	121.97
8	H	154	ILE	C-N-CA	5.19	131.31	121.97

There are no chirality outliers.

All (29) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	146	LEU	Peptide
1	0	152	SER	Peptide
1	0	156	VAL	Peptide
1	0	203	VAL	Peptide
1	0	61	ILE	Peptide
1	0	66	TYR	Peptide
8	H	120	LYS	Peptide
8	H	131	GLY	Peptide
8	H	87	ALA	Peptide
8	H	90	THR	Peptide
9	I	8	LEU	Peptide
9	I	83	GLY	Peptide
9	I	9	LEU	Peptide
11	L	50	VAL	Peptide
12	N	126	TYR	Peptide
12	N	23	GLY	Peptide
13	O	109	ASN	Peptide
13	O	58	VAL	Peptide
14	P	2	LYS	Peptide
14	P	59	GLN	Peptide
15	Q	124	LYS	Peptide
15	Q	3	LEU	Peptide
15	Q	60	ARG	Peptide
19	U	8	THR	Peptide
20	V	5	ILE	Peptide

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Mol	Chain	Res	Type	Group
20	V	50	ASN	Peptide
21	W	21	MET	Peptide
25	b	3	ARG	Peptide
30	h	36	ARG	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	3987	0	3684	72	0
2	2	1603	0	813	14	0
3	A	60389	0	30397	595	0
4	B	2392	0	1213	40	0
5	E	2083	0	2168	50	0
6	F	1569	0	1637	36	0
7	G	1561	0	1647	28	0
8	H	1284	0	1344	50	0
9	I	1342	0	1388	42	0
10	K	974	0	1011	18	0
11	L	886	0	920	17	0
12	N	1123	0	1162	23	0
13	O	920	0	977	29	0
14	P	1081	0	1132	28	0
15	Q	1076	0	1145	20	0
16	R	953	0	983	18	0
17	S	912	0	947	26	0
18	T	944	0	1020	22	0
19	U	940	0	1005	19	0
20	V	781	0	821	19	0
21	W	842	0	899	11	0
22	X	725	0	770	16	0
23	Y	762	0	821	16	0
24	a	585	0	593	15	0
25	b	444	0	487	7	0
26	c	530	0	568	6	0
27	d	455	0	491	9	0
28	f	418	0	435	8	0
29	g	401	0	413	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	h	367	0	410	11	0
31	i	512	0	564	20	0
32	j	296	0	342	10	0
All	All	93137	0	62207	1118	0

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

All (1118) 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)
3:A:1757:G:O6	3:A:1776:A:N6	2.02	0.92
3:A:421:A:N7	3:A:447:G:N2	2.18	0.91
3:A:2498:A:O2'	15:Q:56:ARG:NH1	2.13	0.81
3:A:2841:C:O2	3:A:2908:A:O2'	1.98	0.81
2:2:8:U:O2'	2:2:21:A:N1	2.14	0.81
3:A:1485:A:N6	3:A:1600:G:O2'	2.14	0.81
20:V:27:ALA:HB3	20:V:62:VAL:HG21	1.62	0.81
8:H:38:MET:N	8:H:154:ILE:O	2.14	0.81
1:0:281:LYS:O	1:0:285:ASP:N	2.13	0.81
3:A:2670:A:OP1	12:N:77:ARG:NH2	2.14	0.80
3:A:776:G:O4'	5:E:207:LYS:NZ	2.15	0.80
3:A:2714:G:OP2	18:T:49:LYS:NZ	2.15	0.80
13:O:107:ARG:O	13:O:110:ASN:ND2	2.15	0.80
2:2:54:U:O2	2:2:58:A:N7	2.15	0.79
3:A:1058:U:O4	12:N:31:SER:OG	2.00	0.79
4:B:29:C:O2	4:B:51:A:N6	2.15	0.79
29:g:9:CYS:SG	29:g:10:THR:N	2.55	0.79
3:A:1081:U:O2	3:A:1166:G:O6	2.01	0.79
3:A:1290:G:OP2	14:P:21:ARG:NH1	2.16	0.79
1:0:278:TYR:O	1:0:282:ALA:N	2.16	0.79
16:R:46:LYS:O	16:R:49:THR:OG1	2.00	0.79
3:A:1553:A:O3'	3:A:1555:A:OP1	2.01	0.79
3:A:1380:U:OP1	3:A:1647:U:O2'	2.01	0.78
3:A:2382:G:O2'	24:a:41:GLY:O	2.01	0.78
3:A:2394:G:O6	31:i:43:LYS:NZ	2.16	0.78
3:A:282:G:O2'	3:A:283:G:O4'	2.02	0.78
3:A:326:A:N1	3:A:401:C:O2'	2.16	0.78
3:A:420:U:O2	3:A:448:A:N6	2.14	0.78
3:A:746:A:H62	3:A:780:G:H21	1.28	0.78
3:A:610:U:OP1	20:V:81:ASN:ND2	2.17	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:35:VAL:O	8:H:156:ILE:HA	1.83	0.78
3:A:959:C:OP1	15:Q:8:LYS:NZ	2.16	0.78
4:B:11:A:O2'	4:B:13:A:O5'	2.02	0.78
8:H:126:GLY:O	8:H:158:THR:OG1	2.02	0.78
3:A:227:G:OP2	3:A:455:G:N2	2.16	0.77
3:A:2287:C:O2'	3:A:2456:C:OP2	2.01	0.77
3:A:247:A:OP2	31:i:8:ARG:NH1	2.18	0.77
3:A:2668:A:O2'	12:N:100:LYS:NZ	2.17	0.77
15:Q:12:GLU:O	15:Q:87:LYS:NZ	2.17	0.77
16:R:9:THR:OG1	16:R:12:GLN:OE1	2.03	0.77
3:A:250:G:OP2	3:A:252:C:N4	2.18	0.77
3:A:515:G:O2'	7:G:62:ARG:NH1	2.18	0.77
3:A:1983:G:O2'	3:A:1985:U:O4	2.02	0.77
3:A:1036:A:O2'	3:A:1038:C:OP2	2.03	0.77
3:A:1159:U:OP1	9:I:2:SER:OG	2.03	0.77
18:T:14:ARG:NH1	18:T:78:THR:O	2.17	0.77
3:A:343:A:OP2	23:Y:80:ARG:NH2	2.17	0.77
3:A:573:C:N4	3:A:2808:U:OP2	2.17	0.77
3:A:2824:G:O2'	3:A:2827:A:N6	2.18	0.77
8:H:70:ALA:N	8:H:82:GLY:O	2.18	0.77
7:G:109:ALA:O	7:G:112:SER:OG	2.01	0.76
3:A:611:U:O3'	14:P:36:LYS:NZ	2.18	0.76
3:A:2072:C:OP1	3:A:2806:G:O2'	2.02	0.76
3:A:2468:A:O2'	3:A:2629:A:OP1	2.02	0.76
3:A:1055:A:O4'	19:U:59:LYS:NZ	2.17	0.76
4:B:3:U:O2'	4:B:24:C:N4	2.17	0.76
3:A:1114:G:N2	3:A:1141:A:O2'	2.19	0.76
3:A:1664:G:N3	30:h:1:MET:N	2.34	0.75
4:B:40:C:O2	8:H:90:THR:OG1	2.04	0.75
22:X:84:THR:OG1	22:X:87:SER:OG	2.03	0.75
3:A:1867:C:O2	3:A:1930:A:N6	2.20	0.75
3:A:1291:A:OP1	19:U:10:THR:OG1	2.02	0.75
3:A:1523:U:O2	3:A:1562:A:N6	2.16	0.75
3:A:1754:U:O2	3:A:2884:G:N2	2.18	0.75
3:A:1783:C:N4	3:A:2745:U:O2'	2.17	0.75
32:j:5:PRO:O	32:j:36:GLN:NE2	2.19	0.75
3:A:262:G:N3	3:A:667:A:O2'	2.19	0.75
8:H:37:ASN:HA	8:H:154:ILE:O	1.87	0.75
3:A:1513:U:HO2'	3:A:1594:G:HO2'	1.26	0.75
3:A:1790:U:O2'	3:A:1791:A:O4'	2.04	0.75
6:F:9:LYS:NZ	6:F:194:GLY:O	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:575:A:N6	3:A:2070:U:O2	2.20	0.75
22:X:24:LYS:NZ	22:X:84:THR:O	2.19	0.75
1:O:426:LEU:O	1:O:431:TYR:N	2.20	0.74
3:A:613:U:O2	3:A:1029:A:N6	2.19	0.74
3:A:1135:G:N2	3:A:1147:U:O4	2.20	0.74
3:A:1493:C:O2	3:A:1593:A:O2'	2.05	0.74
3:A:1055:A:O2'	3:A:1056:A:O4'	2.02	0.74
3:A:1509:C:HO2'	3:A:2731:G:HO2'	1.34	0.74
3:A:1253:A:OP2	3:A:1276:G:N2	2.20	0.74
4:B:15:C:N4	4:B:106:C:O2	2.19	0.74
3:A:2601:A:OP1	3:A:2603:G:O2'	2.05	0.74
3:A:1733:U:O2'	3:A:1745:A:N7	2.21	0.74
3:A:2875:A:N7	3:A:2893:A:O2'	2.19	0.74
3:A:1664:G:N2	30:h:1:MET:O	2.18	0.74
3:A:840:A:OP2	3:A:2100:A:O2'	2.06	0.73
3:A:1884:G:O2'	3:A:1885:A:OP1	2.05	0.73
3:A:252:C:O2	14:P:63:LYS:NZ	2.21	0.73
3:A:790:A:O2'	3:A:1704:U:OP1	2.05	0.73
31:i:32:LEU:O	31:i:36:LYS:NZ	2.22	0.73
3:A:2532:A:O2'	3:A:2534:G:OP2	2.05	0.73
6:F:114:SER:OG	6:F:166:GLY:N	2.21	0.73
13:O:113:LYS:O	13:O:116:SER:OG	2.06	0.73
3:A:26:G:O2'	3:A:27:G:O4'	2.02	0.73
3:A:697:G:OP1	31:i:19:SER:OG	2.05	0.73
3:A:914:C:N3	3:A:959:C:O2'	2.20	0.73
12:N:61:GLU:O	12:N:94:ARG:NE	2.21	0.73
3:A:2558:G:N7	32:j:31:LYS:NZ	2.36	0.73
3:A:775:G:O2'	3:A:777:C:O4'	2.06	0.73
3:A:1710:A:O5'	13:O:66:LYS:NZ	2.22	0.73
1:O:114:THR:O	1:O:116:ARG:NH2	2.22	0.72
3:A:645:C:O2'	3:A:649:G:OP1	2.06	0.72
3:A:1248:C:O2'	3:A:1249:U:O4'	2.05	0.72
3:A:1829:C:O2	3:A:1846:G:N2	2.21	0.72
16:R:94:ARG:NH1	16:R:120:VAL:O	2.22	0.72
3:A:87:U:OP2	23:Y:29:LYS:NZ	2.21	0.72
3:A:2688:G:O2'	3:A:2690:G:N7	2.21	0.72
3:A:2802:U:OP1	6:F:168:GLN:NE2	2.22	0.72
28:f:43:CYS:O	28:f:47:GLY:N	2.22	0.72
3:A:2127:U:O2'	3:A:2128:U:OP1	2.08	0.72
3:A:584:A:H62	3:A:599:G:H21	1.38	0.72
3:A:2089:A:O2'	3:A:2090:G:OP2	2.07	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:T:106:LYS:O	18:T:109:ARG:NE	2.23	0.72
3:A:75:G:O2'	3:A:76:C:OP2	2.03	0.72
3:A:633:U:O3'	7:G:95:ARG:NH2	2.22	0.72
3:A:1347:A:H62	3:A:1651:G:N2	1.87	0.72
8:H:115:ARG:NH1	8:H:116:GLY:O	2.22	0.72
1:O:93:GLN:NE2	1:O:97:ASP:O	2.23	0.72
3:A:92:G:O2'	3:A:93:C:OP1	2.08	0.72
3:A:1347:A:H62	3:A:1651:G:H21	1.35	0.72
3:A:314:A:O2'	3:A:316:G:O6	2.03	0.72
3:A:878:G:O2'	14:P:38:GLN:OE1	2.08	0.71
25:b:5:CYS:O	25:b:9:GLY:N	2.23	0.71
3:A:675:C:O2	3:A:685:U:O2'	2.07	0.71
3:A:1895:A:N6	3:A:1904:G:O2'	2.23	0.71
3:A:2060:A:N3	3:A:2484:G:O2'	2.23	0.71
3:A:246:U:OP2	31:i:8:ARG:NH2	2.23	0.71
6:F:69:VAL:O	6:F:72:ALA:N	2.23	0.71
3:A:353:A:N3	3:A:373:A:O2'	2.23	0.71
3:A:2640:C:OP1	6:F:138:ARG:NH1	2.24	0.71
3:A:1467:G:H21	3:A:1541:A:H61	1.36	0.71
3:A:1649:C:O2'	3:A:1655:A:N6	2.23	0.71
3:A:619:A:OP2	3:A:2528:C:O2'	2.07	0.71
3:A:712:C:O2	31:i:60:GLN:NE2	2.23	0.71
3:A:31:C:O2'	3:A:1278:G:OP1	2.08	0.71
3:A:1070:G:O2'	3:A:1190:A:O2'	2.09	0.71
3:A:364:A:O2'	3:A:366:A:OP2	2.09	0.70
8:H:57:LEU:O	8:H:61:ALA:N	2.24	0.70
3:A:372:U:O2'	23:Y:67:ASN:OD1	2.07	0.70
3:A:513:A:OP1	30:h:34:ARG:NH2	2.24	0.70
3:A:718:C:OP1	14:P:43:GLY:N	2.24	0.70
3:A:1102:G:O2'	3:A:1149:A:N6	2.24	0.70
4:B:38:U:O2'	4:B:43:A:N6	2.18	0.70
12:N:14:ARG:NH2	12:N:50:ASP:O	2.24	0.70
3:A:160:G:N2	3:A:168:A:OP2	2.24	0.70
3:A:1130:A:N3	3:A:1151:U:O2'	2.19	0.70
3:A:1315:G:OP2	3:A:1690:G:O2'	2.03	0.70
15:Q:30:GLY:O	15:Q:134:ARG:NH2	2.24	0.70
3:A:569:C:O2	3:A:598:U:O2'	2.07	0.70
3:A:1499:A:O2'	3:A:1500:U:O5'	2.07	0.70
3:A:1699:A:O2'	3:A:1700:A:O4'	2.08	0.70
15:Q:30:GLY:N	15:Q:105:GLU:OE1	2.25	0.70
3:A:2662:A:O2'	6:F:65:GLU:OE2	2.08	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:867:A:N3	3:A:989:U:O2'	2.25	0.70
3:A:1042:A:OP2	19:U:93:LYS:NZ	2.24	0.70
3:A:1093:G:O2'	3:A:1157:A:N6	2.25	0.70
3:A:2106:A:N3	3:A:2463:A:O2'	2.24	0.70
3:A:2688:G:N2	3:A:2691:A:OP2	2.24	0.70
3:A:1284:A:OP1	14:P:7:LYS:NZ	2.25	0.70
3:A:2844:A:O2'	3:A:2846:A:N7	2.23	0.70
3:A:1469:G:O2'	3:A:1545:C:O2'	2.09	0.70
3:A:1876:A:O2'	3:A:1877:A:N7	2.25	0.70
3:A:730:U:O3'	30:h:21:ARG:NH2	2.24	0.69
3:A:1359:G:OP2	3:A:1359:G:N2	2.20	0.69
3:A:2569:C:O2'	3:A:2769:A:N3	2.24	0.69
13:O:78:SER:OG	18:T:71:GLU:OE2	2.10	0.69
3:A:432:C:O2'	3:A:435:G:N2	2.25	0.69
3:A:1036:A:O2'	3:A:1037:C:OP1	2.06	0.69
3:A:1058:U:O2	12:N:28:ARG:NH1	2.24	0.69
3:A:1849:U:OP1	5:E:177:ASN:ND2	2.26	0.69
3:A:2741:U:O2'	3:A:2744:C:OP1	2.09	0.69
22:X:14:THR:O	22:X:17:SER:OG	2.07	0.69
17:S:69:GLY:O	17:S:105:ARG:NH1	2.26	0.69
3:A:1263:G:OP2	20:V:89:ARG:NH2	2.26	0.69
3:A:13:A:O4'	3:A:572:A:N6	2.25	0.69
1:O:92:GLU:O	1:O:101:ILE:N	2.26	0.69
3:A:2819:A:O2'	3:A:2917:G:O2'	2.07	0.69
3:A:689:A:O2'	3:A:690:A:O5'	2.11	0.68
3:A:2372:U:O2'	3:A:2402:A:O2'	2.10	0.68
4:B:22:G:O6	4:B:54:U:O2'	2.07	0.68
3:A:731:G:O3'	3:A:835:A:N6	2.26	0.68
10:K:18:ALA:HB2	10:K:43:ASN:OD1	1.94	0.68
3:A:1283:U:O2'	14:P:6:LEU:O	2.11	0.68
3:A:1403:G:N2	3:A:1406:A:OP2	2.18	0.68
2:2:19:G:O4'	2:2:57:G:N2	2.26	0.68
3:A:342:A:N3	3:A:363:C:O2'	2.26	0.68
3:A:2540:U:O3'	6:F:129:SER:OG	2.10	0.68
3:A:34:U:O2'	3:A:35:G:O5'	2.09	0.68
23:Y:27:PHE:O	23:Y:31:ASP:N	2.26	0.68
3:A:250:G:O2'	3:A:253:G:O6	2.11	0.68
3:A:2497:A:O5'	3:A:2505:A:N6	2.27	0.68
23:Y:13:SER:OG	23:Y:67:ASN:O	2.05	0.68
29:g:9:CYS:SG	29:g:11:GLU:N	2.67	0.68
3:A:344:G:O2'	3:A:345:A:O5'	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:647:A:O5'	3:A:702:A:N6	2.27	0.68
22:X:42:ALA:O	22:X:45:SER:OG	2.11	0.68
3:A:1530:G:O2'	3:A:1531:G:OP1	2.11	0.68
20:V:27:ALA:HB1	20:V:31:GLU:HB2	1.75	0.67
1:O:362:PRO:O	1:O:376:TYR:OH	2.10	0.67
5:E:194:GLN:NE2	5:E:198:GLU:OE1	2.27	0.67
6:F:38:LYS:NZ	6:F:91:TYR:O	2.21	0.67
8:H:37:ASN:CA	8:H:154:ILE:O	2.42	0.67
1:O:423:ARG:NH2	1:O:433:ARG:O	2.27	0.67
3:A:753:A:OP1	5:E:7:LYS:NZ	2.27	0.67
3:A:1757:G:O6	3:A:1776:A:C6	2.47	0.67
3:A:525:A:N6	3:A:546:G:O2'	2.27	0.67
3:A:617:G:N2	3:A:2060:A:OP1	2.25	0.67
3:A:876:A:N7	3:A:2276:A:O2'	2.27	0.67
3:A:1713:A:H61	3:A:1721:A:H61	1.42	0.67
3:A:2394:G:N7	31:i:39:LYS:NZ	2.38	0.67
3:A:1175:A:O2'	3:A:2544:C:O2	2.06	0.67
3:A:373:A:N1	23:Y:15:LYS:NZ	2.43	0.67
28:f:30:CYS:N	28:f:35:GLU:O	2.26	0.67
3:A:1306:G:OP2	28:f:17:ARG:NH2	2.28	0.67
3:A:510:G:N2	3:A:513:A:OP2	2.28	0.67
3:A:724:A:O2'	3:A:2099:G:O2'	2.10	0.67
1:O:147:SER:OG	1:O:149:SER:N	2.28	0.67
3:A:139:A:O2'	3:A:1449:C:O5'	2.13	0.67
16:R:8:ARG:O	16:R:13:ARG:NH2	2.28	0.67
1:O:66:TYR:OH	1:O:275:ASP:OD1	2.13	0.66
14:P:51:GLU:OE2	31:i:57:ARG:NH2	2.28	0.66
3:A:1980:U:O2'	3:A:1982:A:N7	2.22	0.66
3:A:2860:A:N6	3:A:2904:A:O5'	2.27	0.66
18:T:60:THR:HG23	18:T:73:THR:HG22	1.78	0.66
3:A:1250:G:OP1	3:A:1251:U:O2'	2.11	0.66
27:d:39:ASP:OD1	27:d:44:ARG:NH2	2.28	0.66
3:A:2048:U:OP1	28:f:7:ARG:NH1	2.28	0.66
3:A:268:A:N1	3:A:474:U:O2'	2.22	0.66
4:B:64:A:O4'	4:B:106:C:N4	2.29	0.66
6:F:39:LYS:N	6:F:48:ALA:O	2.28	0.66
6:F:180:ASP:O	6:F:184:ASN:N	2.29	0.66
29:g:34:LYS:O	29:g:43:THR:N	2.29	0.66
24:a:80:PHE:N	24:a:84:ARG:O	2.29	0.65
28:f:28:THR:O	28:f:37:LYS:N	2.28	0.65
3:A:1456:A:O2'	3:A:1631:A:N6	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1873:U:O3'	5:E:258:LYS:NZ	2.30	0.65
5:E:248:SER:OG	5:E:251:GLY:N	2.28	0.65
3:A:1199:C:OP1	19:U:92:ARG:NH2	2.30	0.65
9:I:47:GLU:OE2	9:I:52:THR:OG1	2.14	0.65
3:A:11:G:O2'	3:A:12:A:O4'	2.10	0.65
3:A:1265:A:OP1	20:V:70:LYS:NZ	2.29	0.65
3:A:1362:G:OP1	21:W:98:LYS:NZ	2.29	0.65
9:I:166:GLU:OE1	9:I:166:GLU:N	2.30	0.65
3:A:2420:G:OP2	31:i:35:ASN:ND2	2.29	0.65
3:A:13:A:O2'	3:A:15:G:N7	2.23	0.65
3:A:866:A:OP2	3:A:1228:G:N2	2.29	0.65
3:A:1010:C:O2'	3:A:2302:A:N3	2.29	0.65
9:I:70:ARG:N	9:I:77:VAL:O	2.30	0.65
3:A:1695:A:O2'	3:A:1696:G:O5'	2.15	0.65
27:d:15:ARG:O	27:d:20:ARG:NH2	2.30	0.65
3:A:140:A:O2'	3:A:1447:C:O2'	2.13	0.64
3:A:186:C:O2'	3:A:479:A:N3	2.27	0.64
3:A:419:G:N2	3:A:448:A:OP2	2.29	0.64
3:A:2901:G:O2'	3:A:2902:A:O5'	2.09	0.64
3:A:928:G:O6	3:A:942:U:O2	2.16	0.64
9:I:73:LEU:N	9:I:77:VAL:HG23	2.11	0.64
11:L:76:LEU:O	11:L:80:ASN:ND2	2.30	0.64
3:A:2326:C:N4	3:A:2348:C:OP1	2.31	0.64
10:K:79:LEU:HD22	10:K:100:VAL:HG11	1.78	0.64
12:N:92:GLU:O	12:N:95:THR:OG1	2.12	0.64
3:A:2009:G:O2'	3:A:2011:U:OP2	2.09	0.64
3:A:2080:A:O2'	3:A:2643:A:N6	2.30	0.64
5:E:61:GLN:O	5:E:63:ARG:NH2	2.31	0.64
3:A:645:C:O2'	7:G:104:LYS:NZ	2.30	0.64
8:H:35:VAL:O	8:H:156:ILE:HD13	1.98	0.64
3:A:623:A:O2'	3:A:2048:U:OP1	2.16	0.64
2:2:15:G:O6	2:2:48:C:O2	2.15	0.64
2:2:32:U:O2'	2:2:33:U:O4'	2.11	0.64
3:A:79:C:O2'	3:A:390:A:N3	2.27	0.64
3:A:1171:G:OP2	3:A:1172:A:O2'	2.11	0.63
3:A:2315:A:OP1	29:g:25:ASN:ND2	2.30	0.63
3:A:2922:U:O2'	12:N:137:LYS:NZ	2.32	0.63
19:U:90:VAL:HG23	19:U:91:ASN:H	1.62	0.63
22:X:19:ASP:O	22:X:22:THR:OG1	2.16	0.63
3:A:867:A:OP2	3:A:1019:A:N6	2.19	0.63
3:A:925:A:N6	3:A:946:G:O2'	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:27:ILE:HD13	1:0:79:LEU:HB3	1.79	0.63
1:0:133:ASP:O	1:0:137:ASN:N	2.31	0.63
3:A:1157:A:O2'	3:A:1158:G:O4'	2.16	0.63
3:A:1379:U:OP2	22:X:59:TYR:OH	2.15	0.63
3:A:908:A:H62	3:A:963:G:H21	1.47	0.63
5:E:157:SER:O	5:E:160:THR:OG1	2.13	0.63
9:I:72:LEU:HD12	9:I:80:VAL:HG22	1.79	0.63
20:V:16:GLU:OE2	20:V:99:LYS:N	2.32	0.63
3:A:179:A:O2'	3:A:180:G:O4'	2.17	0.63
3:A:2656:G:O2'	3:A:2810:A:N1	2.26	0.63
10:K:100:VAL:O	10:K:140:GLU:N	2.33	0.62
3:A:619:A:O2'	3:A:2530:C:OP1	2.17	0.62
3:A:1263:G:N2	3:A:1266:A:OP2	2.24	0.62
29:g:6:THR:HG1	29:g:48:THR:HG1	1.36	0.62
3:A:1068:G:O6	12:N:69:LYS:NZ	2.29	0.62
10:K:89:SER:OG	10:K:95:ASN:O	2.14	0.62
16:R:18:ARG:O	16:R:21:THR:OG1	2.15	0.62
3:A:1866:C:O2'	3:A:1956:A:N3	2.24	0.62
8:H:8:TYR:OH	8:H:29:PRO:O	2.17	0.62
3:A:584:A:H62	3:A:599:G:N2	1.96	0.62
5:E:123:ASP:OD2	5:E:125:LYS:NZ	2.30	0.62
24:a:19:LYS:O	24:a:22:ARG:NH1	2.33	0.62
3:A:707:G:O2'	14:P:13:ARG:NH1	2.32	0.62
3:A:917:A:OP1	15:Q:6:ARG:NH2	2.33	0.62
3:A:1264:G:OP2	20:V:67:ARG:NH1	2.33	0.62
3:A:1968:U:OP1	3:A:2633:U:O2'	2.13	0.62
8:H:34:ILE:HD13	8:H:96:MET:HB3	1.81	0.62
3:A:1417:A:O2'	3:A:1419:G:OP2	2.17	0.62
3:A:494:A:O2'	3:A:520:G:N7	2.25	0.62
18:T:5:ILE:O	18:T:9:THR:OG1	2.15	0.62
18:T:60:THR:CG2	18:T:73:THR:HG22	2.30	0.62
3:A:732:A:O2'	3:A:820:U:O4	2.13	0.62
3:A:1081:U:C2	3:A:1166:G:O6	2.53	0.62
3:A:2529:U:O2'	3:A:2533:U:OP1	2.17	0.62
3:A:177:G:O2'	3:A:178:A:O5'	2.18	0.61
3:A:1264:G:O2'	3:A:1265:A:O5'	2.17	0.61
3:A:1359:G:N1	3:A:1369:C:OP2	2.33	0.61
30:h:20:SER:O	30:h:23:SER:OG	2.12	0.61
3:A:754:G:O6	3:A:772:G:N2	2.33	0.61
12:N:30:SER:HA	12:N:33:VAL:HG22	1.81	0.61
20:V:41:VAL:HG22	20:V:47:LYS:H	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:928:G:O6	3:A:942:U:C2	2.52	0.61
3:A:1035:G:OP2	27:d:11:SER:OG	2.10	0.61
3:A:1347:A:N6	3:A:1651:G:H21	1.99	0.61
18:T:26:LEU:HD21	18:T:84:ILE:HG23	1.83	0.61
3:A:1090:U:O2'	3:A:1157:A:N1	2.33	0.61
3:A:2758:G:O3'	6:F:189:LYS:NZ	2.30	0.61
3:A:11:G:N2	3:A:2657:C:OP1	2.34	0.61
3:A:1474:C:N4	3:A:1618:A:OP2	2.34	0.61
3:A:515:G:N7	30:h:39:ARG:NH2	2.48	0.60
7:G:32:VAL:HG12	7:G:109:ALA:HB2	1.83	0.60
9:I:72:LEU:C	9:I:77:VAL:HG23	2.26	0.60
9:I:90:LEU:HD13	9:I:95:TYR:HB2	1.83	0.60
27:d:17:GLU:N	27:d:17:GLU:OE1	2.34	0.60
3:A:2294:U:OP2	3:A:2295:A:O2'	2.18	0.60
3:A:2702:G:O2'	13:O:30:ARG:NH2	2.34	0.60
5:E:166:GLY:O	5:E:173:LEU:N	2.35	0.60
3:A:594:C:OP2	20:V:64:LYS:NZ	2.31	0.60
3:A:613:U:OP1	3:A:991:A:O2'	2.13	0.60
3:A:1888:A:N6	3:A:1912:G:O2'	2.34	0.60
3:A:2311:G:O2'	3:A:2419:U:O4	2.12	0.60
1:O:537:LYS:N	1:O:548:THR:O	2.34	0.60
3:A:2741:U:OP1	3:A:2743:G:O2'	2.17	0.60
20:V:68:ALA:O	20:V:89:ARG:NE	2.32	0.60
5:E:123:ASP:OD1	5:E:128:ASN:ND2	2.35	0.60
19:U:24:TYR:O	19:U:29:HIS:ND1	2.35	0.60
3:A:1069:U:OP2	3:A:1071:G:O2'	2.19	0.60
3:A:1103:A:N6	3:A:1133:G:OP1	2.35	0.60
3:A:1757:G:O2'	3:A:1758:U:O5'	2.20	0.60
3:A:2520:U:O2'	3:A:2599:G:OP1	2.20	0.60
3:A:1788:A:O4'	3:A:2743:G:N2	2.30	0.59
23:Y:94:ALA:N	23:Y:99:GLN:O	2.33	0.59
14:P:125:ALA:O	14:P:146:ILE:N	2.34	0.59
3:A:1197:A:O2'	19:U:77:SER:O	2.20	0.59
3:A:2446:C:OP1	14:P:64:ARG:NH1	2.33	0.59
13:O:65:THR:O	13:O:79:PHE:N	2.34	0.59
3:A:2364:A:O2'	3:A:2365:A:O5'	2.20	0.59
3:A:2819:A:HO2'	3:A:2917:G:HO2'	1.47	0.59
3:A:1123:A:O2'	3:A:1134:A:N6	2.35	0.59
3:A:746:A:H62	3:A:780:G:N2	1.98	0.59
3:A:2874:G:O3'	3:A:2891:G:N2	2.35	0.59
4:B:34:C:N4	4:B:47:C:O2	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:N:78:HIS:ND1	12:N:79:THR:O	2.32	0.59
3:A:1695:A:HO2'	3:A:1696:G:C5'	2.15	0.59
9:I:20:ASN:N	9:I:24:THR:O	2.35	0.59
1:O:11:MET:HE1	1:O:270:LEU:HD22	1.85	0.59
3:A:139:A:N6	3:A:1640:G:O2'	2.36	0.59
3:A:647:A:N6	3:A:702:A:O4'	2.36	0.59
3:A:1244:A:O2'	14:P:3:LEU:HD12	2.03	0.59
3:A:1290:G:O6	14:P:18:ARG:NH2	2.35	0.59
3:A:2784:C:O2'	3:A:2785:U:O5'	2.21	0.59
5:E:154:LEU:O	5:E:156:ARG:N	2.35	0.59
3:A:689:A:N1	3:A:2398:A:O2'	2.33	0.58
15:Q:18:ARG:O	15:Q:98:LYS:NZ	2.23	0.58
3:A:898:U:OP1	27:d:49:LYS:NZ	2.36	0.58
4:B:63:C:O2'	4:B:106:C:N4	2.22	0.58
17:S:24:GLY:N	17:S:47:ASP:OD2	2.36	0.58
1:O:321:ASN:O	1:O:379:LYS:NZ	2.22	0.58
3:A:745:C:O2'	3:A:781:A:N6	2.36	0.58
3:A:1965:A:OP2	3:A:1991:C:N4	2.36	0.58
10:K:25:GLY:O	10:K:29:GLY:HA3	2.03	0.58
8:H:36:ILE:H	8:H:154:ILE:HB	1.69	0.58
22:X:52:ASP:N	22:X:82:LYS:O	2.37	0.58
1:O:384:LYS:NZ	3:A:1113:A:OP2	2.36	0.58
3:A:648:G:O2'	3:A:649:G:OP2	2.22	0.58
3:A:1821:G:P	5:E:205:ILE:HD12	2.43	0.58
1:O:125:ARG:NE	2:2:32:U:O2'	2.35	0.58
3:A:1365:U:O2'	3:A:1366:C:O5'	2.22	0.57
8:H:65:PRO:HA	8:H:89:VAL:HG13	1.85	0.57
1:O:243:ILE:HD12	1:O:267:PHE:CE2	2.39	0.57
3:A:77:U:O2'	3:A:78:U:O5'	2.20	0.57
3:A:1933:G:O2'	3:A:1957:A:N1	2.29	0.57
3:A:2040:U:OP2	21:W:16:LYS:NZ	2.28	0.57
3:A:920:G:O2'	15:Q:65:TRP:NE1	2.37	0.57
8:H:162:THR:N	8:H:165:GLU:OE2	2.37	0.57
29:g:6:THR:OG1	29:g:48:THR:OG1	2.11	0.57
3:A:2421:A:OP1	31:i:31:HIS:NE2	2.38	0.57
3:A:2815:U:O2'	6:F:64:PRO:O	2.16	0.57
4:B:35:C:O2	17:S:103:HIS:NE2	2.36	0.57
3:A:734:C:H42	3:A:834:C:H4'	1.69	0.57
3:A:2331:U:N3	3:A:2344:U:O2	2.37	0.57
7:G:112:SER:O	7:G:115:SER:OG	2.17	0.57
3:A:273:A:OP2	3:A:297:G:N1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1105:G:O4'	10:K:117:ASN:ND2	2.38	0.57
3:A:1697:A:O2'	3:A:2847:G:N2	2.38	0.57
3:A:314:A:N6	3:A:405:U:OP2	2.37	0.57
3:A:612:U:O5'	3:A:991:A:N6	2.38	0.56
3:A:1509:C:O2'	3:A:2731:G:O2'	2.08	0.56
3:A:2054:C:OP2	6:F:153:ARG:NE	2.38	0.56
3:A:2667:G:N2	3:A:2807:A:H62	2.02	0.56
11:L:14:GLU:O	11:L:17:SER:OG	2.15	0.56
3:A:2433:C:O3'	14:P:68:ASN:ND2	2.38	0.56
3:A:673:A:N6	3:A:683:A:O5'	2.38	0.56
8:H:165:GLU:OE1	8:H:165:GLU:N	2.38	0.56
30:h:34:ARG:HG2	30:h:42:LEU:HD12	1.88	0.56
3:A:84:A:N6	3:A:101:G:O2'	2.37	0.56
3:A:2667:G:N2	3:A:2807:A:N6	2.53	0.56
13:O:5:GLU:N	13:O:21:THR:OG1	2.39	0.56
3:A:1026:A:N3	3:A:2066:A:O2'	2.29	0.56
5:E:2:ALA:N	5:E:20:ASP:OD2	2.38	0.56
8:H:162:THR:OG1	8:H:165:GLU:OE1	2.16	0.56
18:T:112:GLU:O	18:T:114:ARG:NH1	2.38	0.56
4:B:10:G:OP1	4:B:13:A:N6	2.22	0.56
3:A:461:C:O2	3:A:1893:U:O2'	2.14	0.56
5:E:42:GLY:O	5:E:50:THR:OG1	2.15	0.56
3:A:647:A:O4'	3:A:702:A:N6	2.39	0.56
3:A:2314:C:OP2	29:g:22:ASN:ND2	2.36	0.56
3:A:2713:U:OP1	18:T:58:THR:HG21	2.05	0.56
3:A:2344:U:OP1	17:S:2:ILE:HD13	2.05	0.56
3:A:2830:A:O2'	3:A:2831:A:OP2	2.23	0.56
21:W:66:ALA:HA	21:W:69:LEU:HD12	1.88	0.56
3:A:584:A:N6	3:A:599:G:H21	2.04	0.56
3:A:2823:C:O2'	3:A:2824:G:O5'	2.24	0.56
19:U:39:VAL:O	19:U:42:SER:OG	2.20	0.55
3:A:82:G:N1	3:A:102:A:OP2	2.39	0.55
3:A:505:G:O2'	3:A:516:G:O6	2.24	0.55
3:A:854:U:O2'	3:A:2089:A:N1	2.38	0.55
3:A:632:U:O5'	14:P:16:ARG:NH2	2.38	0.55
10:K:135:MET:HE2	10:K:137:ILE:HD11	1.87	0.55
16:R:94:ARG:O	16:R:98:TYR:OH	2.20	0.55
3:A:957:A:N3	3:A:2293:C:O2'	2.36	0.55
13:O:88:ARG:NE	13:O:93:PRO:O	2.40	0.55
29:g:9:CYS:SG	29:g:12:CYS:N	2.79	0.55
3:A:2610:G:OP2	3:A:2610:G:N2	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:15:G:C6	2:2:48:C:O2	2.60	0.55
3:A:1377:G:O2'	3:A:1432:A:N1	2.37	0.55
25:b:33:LEU:HD13	25:b:48:TYR:CG	2.42	0.55
1:0:303:LYS:O	1:0:307:ASN:ND2	2.40	0.55
3:A:1855:C:O2'	3:A:2000:A:OP2	2.24	0.55
4:B:64:A:O2'	4:B:105:A:N6	2.39	0.55
3:A:2291:U:OP2	24:a:24:SER:OG	2.13	0.55
17:S:30:ARG:HE	17:S:45:ILE:HD13	1.72	0.55
31:i:18:GLY:O	31:i:19:SER:OG	2.23	0.55
4:B:32:U:O2	4:B:34:C:N4	2.36	0.54
3:A:160:G:O2'	3:A:168:A:N6	2.36	0.54
3:A:1727:A:OP2	3:A:1744:G:N2	2.40	0.54
16:R:29:ARG:NE	16:R:118:GLU:OE2	2.41	0.54
1:0:3:PHE:O	1:0:98:ARG:NH2	2.41	0.54
3:A:2813:U:O2'	6:F:44:ASP:OD1	2.21	0.54
4:B:96:G:O2'	4:B:97:A:O4'	2.25	0.54
15:Q:58:MET:HE3	15:Q:109:VAL:HG11	1.90	0.54
3:A:351:G:H1'	3:A:374:A:H61	1.71	0.54
4:B:41:C:H42	8:H:92:ARG:CZ	2.20	0.54
3:A:530:A:C4	23:Y:56:ILE:HD11	2.43	0.54
3:A:1007:G:H22	3:A:2059:A:P	2.31	0.54
3:A:1429:U:O2	3:A:1434:A:N7	2.41	0.54
3:A:2898:A:O2'	3:A:2899:C:OP1	2.18	0.54
8:H:70:ALA:HB1	8:H:79:LEU:HD21	1.89	0.54
12:N:139:GLU:OE1	12:N:139:GLU:N	2.41	0.54
3:A:1474:C:O2'	3:A:1617:A:OP2	2.19	0.54
3:A:2717:G:N1	3:A:2749:U:OP2	2.38	0.54
5:E:17:THR:OG1	5:E:204:ASN:N	2.40	0.54
5:E:176:LEU:O	5:E:179:GLY:N	2.38	0.54
14:P:132:ALA:O	14:P:136:VAL:HG23	2.08	0.54
16:R:107:ARG:HB2	16:R:114:MET:HE2	1.89	0.54
27:d:2:ALA:O	27:d:39:ASP:N	2.39	0.54
3:A:139:A:H61	3:A:1640:G:H1'	1.73	0.53
3:A:443:G:OP1	25:b:10:LYS:NZ	2.39	0.53
3:A:774:A:O2'	5:E:13:ARG:NH2	2.41	0.53
3:A:1170:C:O2'	32:j:37:GLY:O	2.24	0.53
3:A:2333:G:N2	3:A:2341:U:O4	2.28	0.53
17:S:113:ALA:HB1	17:S:118:LEU:HD12	1.89	0.53
3:A:250:G:O2'	3:A:433:G:N1	2.40	0.53
3:A:365:U:OP1	7:G:135:LYS:NZ	2.42	0.53
3:A:1325:A:O2'	3:A:1327:U:OP2	2.17	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1972:U:O2'	3:A:1973:U:OP2	2.26	0.53
18:T:29:HIS:O	18:T:82:ALA:N	2.41	0.53
3:A:1460:G:O2'	3:A:1631:A:N6	2.39	0.53
3:A:2226:U:O2'	3:A:2227:A:O5'	2.25	0.53
6:F:195:ALA:O	6:F:198:SER:OG	2.23	0.53
7:G:101:LEU:O	7:G:106:ARG:NH2	2.41	0.53
8:H:100:LEU:HD23	8:H:103:LEU:HD12	1.90	0.53
18:T:14:ARG:HB2	18:T:17:LEU:HD11	1.90	0.53
5:E:68:LYS:NZ	5:E:149:GLY:O	2.35	0.53
1:O:197:VAL:HG22	1:O:203:VAL:HG13	1.90	0.53
3:A:505:G:O6	7:G:58:ARG:NE	2.30	0.53
3:A:2233:C:O2'	5:E:148:PRO:O	2.21	0.53
3:A:2651:C:O2'	3:A:2850:G:N7	2.41	0.53
9:I:17:VAL:HG11	9:I:46:VAL:HG21	1.91	0.53
11:L:50:VAL:HG21	11:L:92:PRO:HB3	1.90	0.53
11:L:57:ASN:OD1	11:L:80:ASN:ND2	2.41	0.53
24:a:77:PHE:CE1	24:a:87:VAL:HG12	2.44	0.53
32:j:11:CYS:SG	32:j:14:CYS:N	2.79	0.53
3:A:831:U:O2'	3:A:832:G:O5'	2.25	0.53
3:A:2474:G:OP1	7:G:74:ARG:NH2	2.42	0.53
3:A:831:U:O4	3:A:840:A:N6	2.42	0.53
3:A:1516:A:OP2	3:A:1569:A:N6	2.41	0.53
3:A:1919:A:N1	3:A:2263:G:O2'	2.41	0.53
3:A:2384:C:O4'	24:a:44:ILE:HD11	2.09	0.53
3:A:1757:G:O2'	3:A:1758:U:O3'	2.26	0.53
3:A:2874:G:OP1	18:T:93:ARG:NE	2.42	0.53
5:E:15:GLY:O	5:E:204:ASN:ND2	2.42	0.53
9:I:71:SER:OG	9:I:80:VAL:N	2.37	0.53
6:F:75:ALA:HB3	6:F:77:LYS:HE3	1.91	0.53
1:O:28:HIS:ND1	1:O:68:ASN:OD1	2.43	0.52
3:A:26:G:N3	3:A:561:A:N6	2.56	0.52
3:A:675:C:O2'	3:A:685:U:O2	2.27	0.52
3:A:1867:C:N4	3:A:1928:A:O4'	2.42	0.52
10:K:79:LEU:HD21	10:K:108:ILE:HD11	1.91	0.52
3:A:1759:U:HO2'	3:A:1760:A:P	2.33	0.52
3:A:2667:G:H21	3:A:2807:A:N6	2.07	0.52
3:A:2703:G:H4'	13:O:30:ARG:HE	1.73	0.52
3:A:2452:U:O2	3:A:2454:A:O2'	2.19	0.52
3:A:2502:U:OP1	3:A:2558:G:N2	2.38	0.52
4:B:33:U:O2'	4:B:34:C:O4'	2.27	0.52
3:A:906:G:O2'	3:A:963:G:O6	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1970:C:N4	3:A:1994:C:O4'	2.43	0.52
3:A:2278:U:N3	3:A:2282:G:OP2	2.39	0.52
3:A:2388:C:O2'	31:i:54:ASP:OD2	2.27	0.52
7:G:192:LEU:C	7:G:193:LEU:HD12	2.34	0.52
3:A:918:U:OP1	15:Q:5:LYS:N	2.43	0.52
3:A:1365:U:O2'	3:A:1366:C:O4'	2.28	0.52
4:B:41:C:O2'	4:B:42:G:O5'	2.27	0.52
10:K:76:ALA:HA	10:K:135:MET:HE1	1.90	0.52
14:P:96:LEU:O	14:P:99:THR:OG1	2.24	0.52
16:R:50:LEU:HD22	16:R:58:ALA:HB1	1.92	0.52
12:N:59:ASN:N	12:N:128:GLY:O	2.42	0.52
1:0:24:ILE:HD13	1:0:83:ILE:HG22	1.91	0.52
3:A:2742:C:O2'	3:A:2744:C:OP2	2.10	0.52
13:O:34:ASN:O	13:O:62:ILE:HG21	2.09	0.52
3:A:2314:C:OP2	29:g:2:ARG:NH2	2.43	0.52
4:B:47:C:OP2	17:S:35:ARG:NH2	2.41	0.52
9:I:74:GLY:N	9:I:76:MET:SD	2.82	0.52
13:O:50:GLY:O	13:O:53:LYS:NZ	2.27	0.52
23:Y:58:ASN:OD1	23:Y:59:GLN:N	2.42	0.52
3:A:418:A:N6	3:A:449:A:OP2	2.29	0.52
12:N:38:ARG:NE	12:N:45:TYR:OH	2.40	0.52
13:O:75:SER:OG	18:T:72:ARG:NH2	2.43	0.52
1:0:144:LYS:NZ	2:2:37:A:N3	2.58	0.51
3:A:1788:A:C4'	3:A:2743:G:H21	2.23	0.51
3:A:2348:C:OP2	3:A:2350:G:N1	2.44	0.51
8:H:36:ILE:O	8:H:156:ILE:N	2.42	0.51
3:A:63:G:N2	22:X:66:VAL:HG22	2.25	0.51
11:L:80:ASN:OD1	11:L:109:LYS:NZ	2.27	0.51
1:0:539:PRO:O	1:0:546:PHE:N	2.42	0.51
4:B:42:G:C4'	4:B:44:A:H62	2.23	0.51
5:E:155:VAL:O	5:E:160:THR:OG1	2.29	0.51
6:F:6:LEU:HD11	6:F:53:PHE:HB3	1.93	0.51
8:H:36:ILE:HB	8:H:154:ILE:H	1.75	0.51
31:i:51:SER:OG	31:i:54:ASP:OD2	2.29	0.51
17:S:44:ILE:HD12	17:S:81:VAL:CG2	2.41	0.51
2:2:35:G:N2	2:2:35:G:OP2	2.43	0.51
3:A:354:A:O2'	3:A:356:G:N7	2.36	0.51
3:A:892:U:O2	3:A:894:A:N6	2.44	0.51
3:A:2043:A:O2'	3:A:2044:A:O4'	2.09	0.51
1:0:107:ARG:NH2	1:0:108:ASN:O	2.42	0.51
3:A:2860:A:H61	3:A:2904:A:C5'	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:33:LEU:HD22	25:b:48:TYR:HB3	1.91	0.51
3:A:74:U:OP1	26:c:47:ARG:NE	2.44	0.51
3:A:1325:A:O2'	3:A:1326:A:O5'	2.29	0.51
3:A:2035:C:O2'	3:A:2848:A:N3	2.44	0.51
3:A:2379:C:OP1	31:i:46:LYS:NZ	2.33	0.51
11:L:34:ASN:O	11:L:38:VAL:HG23	2.10	0.51
12:N:96:ASN:O	12:N:127:ARG:NH2	2.43	0.51
13:O:15:GLY:O	13:O:47:THR:OG1	2.23	0.51
3:A:540:G:N2	21:W:57:ASN:OD1	2.35	0.51
3:A:1998:A:H2'	3:A:2001:G:H21	1.76	0.51
3:A:2525:C:O2'	3:A:2526:A:O5'	2.21	0.51
3:A:2718:U:OP2	3:A:2897:G:N1	2.39	0.51
8:H:89:VAL:HG12	8:H:90:THR:H	1.75	0.51
3:A:884:C:N3	3:A:987:A:N6	2.59	0.50
3:A:992:G:O6	3:A:1018:G:N2	2.43	0.50
3:A:1829:C:OP1	5:E:182:ARG:NH2	2.43	0.50
9:I:72:LEU:CG	9:I:80:VAL:HG22	2.41	0.50
6:F:139:TYR:OH	6:F:144:GLY:N	2.44	0.50
3:A:863:C:OP1	3:A:1226:U:O2'	2.27	0.50
3:A:1542:A:O2'	3:A:1544:C:N4	2.35	0.50
3:A:1969:U:O2'	3:A:1970:C:OP2	2.27	0.50
4:B:11:A:N1	4:B:67:G:O2'	2.30	0.50
16:R:93:GLU:O	16:R:95:GLN:NE2	2.42	0.50
22:X:4:PRO:HB3	22:X:42:ALA:HB1	1.93	0.50
3:A:875:U:O2'	3:A:876:A:O4'	2.28	0.50
3:A:2041:G:OP1	21:W:11:ARG:NH2	2.42	0.50
3:A:2392:U:OP1	31:i:40:GLN:NE2	2.45	0.50
4:B:112:C:O2	17:S:43:GLN:NE2	2.44	0.50
5:E:155:VAL:HG11	5:E:161:SER:CA	2.42	0.50
9:I:66:HIS:O	9:I:69:THR:OG1	2.13	0.50
1:0:421:GLU:OE2	1:0:469:GLN:N	2.44	0.50
1:0:427:VAL:HG22	1:0:432:LEU:O	2.11	0.50
3:A:1081:U:O2	3:A:1166:G:C6	2.64	0.50
10:K:79:LEU:HD22	10:K:100:VAL:CG1	2.41	0.50
1:0:290:GLN:O	1:0:294:LEU:HD23	2.11	0.50
3:A:1095:C:H41	3:A:1156:G:N2	2.09	0.50
3:A:1832:A:O2'	5:E:259:THR:HG21	2.12	0.50
32:j:14:CYS:SG	32:j:32:HIS:ND1	2.85	0.50
9:I:46:VAL:HG22	9:I:51:LEU:HD23	1.94	0.50
13:O:106:LEU:O	13:O:111:PHE:N	2.45	0.50
1:0:27:ILE:HD12	1:0:80:ARG:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2479:A:N6	3:A:2530:C:C4	2.80	0.50
1:0:131:LEU:HD23	1:0:140:ILE:CG2	2.42	0.50
1:0:193:ASP:OD1	1:0:194:LYS:N	2.42	0.50
3:A:2332:G:O2'	8:H:121:SER:O	2.28	0.50
3:A:2874:G:O2'	3:A:2891:G:N2	2.39	0.50
8:H:35:VAL:HG13	8:H:154:ILE:HG22	1.94	0.50
8:H:154:ILE:O	8:H:155:VAL:HG23	2.11	0.50
18:T:8:ILE:HG23	18:T:9:THR:HG23	1.94	0.50
24:a:41:GLY:N	24:a:72:ASP:OD1	2.42	0.50
1:0:49:LEU:C	1:0:50:LEU:HD12	2.37	0.49
3:A:505:G:N7	7:G:58:ARG:NH2	2.60	0.49
3:A:1818:A:OP1	5:E:221:ARG:NE	2.41	0.49
5:E:155:VAL:O	5:E:155:VAL:HG12	2.12	0.49
9:I:26:ALA:HB1	9:I:35:THR:HG22	1.94	0.49
12:N:38:ARG:O	12:N:51:THR:OG1	2.27	0.49
16:R:85:SER:O	16:R:89:THR:HG23	2.12	0.49
1:0:322:ALA:HB2	1:0:383:ALA:HB3	1.94	0.49
3:A:82:G:O2'	3:A:83:G:O4'	2.30	0.49
3:A:2771:G:OP1	32:j:35:LYS:NZ	2.40	0.49
4:B:10:G:O4'	24:a:79:ARG:NH2	2.45	0.49
4:B:37:A:H2	4:B:44:A:H61	1.59	0.49
9:I:72:LEU:N	9:I:80:VAL:HG23	2.27	0.49
9:I:123:GLU:N	9:I:123:GLU:OE1	2.45	0.49
11:L:23:LYS:O	11:L:114:GLU:N	2.45	0.49
7:G:114:LEU:O	7:G:118:VAL:HG23	2.12	0.49
3:A:2336:G:O6	8:H:41:GLY:N	2.45	0.49
9:I:72:LEU:HD13	9:I:76:MET:HB2	1.94	0.49
15:Q:111:GLU:OE2	15:Q:115:ARG:NE	2.45	0.49
3:A:1012:G:O4'	3:A:2296:A:N6	2.45	0.49
3:A:2324:C:OP1	17:S:14:ARG:NH2	2.39	0.49
5:E:248:SER:N	5:E:252:LYS:O	2.44	0.49
12:N:88:ARG:NH1	12:N:97:TYR:OH	2.43	0.49
13:O:53:LYS:N	13:O:56:GLU:OE1	2.45	0.49
1:0:196:ILE:HB	1:0:208:ALA:HB1	1.93	0.49
3:A:1546:G:N2	5:E:98:ASP:O	2.39	0.49
3:A:2353:U:O2	3:A:2414:C:N4	2.45	0.49
5:E:139:THR:N	5:E:163:GLN:OE1	2.45	0.49
13:O:109:ASN:O	13:O:111:PHE:N	2.45	0.49
1:0:94:ALA:HB3	1:0:99:ILE:HB	1.94	0.49
13:O:48:PRO:O	13:O:50:GLY:N	2.46	0.49
15:Q:42:ILE:O	15:Q:95:ALA:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:U:94:MET:HE1	20:V:13:LYS:N	2.27	0.49
20:V:67:ARG:O	20:V:89:ARG:NH1	2.45	0.49
23:Y:72:ASP:N	23:Y:77:GLU:O	2.38	0.49
9:I:45:LYS:O	9:I:51:LEU:HD22	2.13	0.49
1:O:357:PRO:O	1:O:358:THR:OG1	2.22	0.49
2:2:76:A:N1	3:A:2479:A:O2'	2.37	0.49
18:T:31:LYS:NZ	18:T:79:PRO:O	2.34	0.49
23:Y:41:VAL:CG1	23:Y:61:ALA:HB2	2.43	0.49
1:O:182:LEU:HD21	1:O:187:PHE:CE1	2.48	0.48
3:A:1306:G:O2'	3:A:2041:G:O6	2.30	0.48
3:A:2609:U:OP1	6:F:138:ARG:NH1	2.46	0.48
16:R:56:LEU:HD21	16:R:60:ARG:NE	2.27	0.48
3:A:523:G:N1	3:A:526:A:OP2	2.45	0.48
3:A:636:G:H21	31:i:4:MET:CE	2.25	0.48
3:A:1036:A:HO2'	3:A:1037:C:P	2.31	0.48
3:A:1231:G:OP1	14:P:30:THR:OG1	2.27	0.48
3:A:2667:G:C2	3:A:2807:A:N6	2.81	0.48
15:Q:12:GLU:OE1	15:Q:72:LYS:NZ	2.42	0.48
8:H:37:ASN:C	8:H:154:ILE:O	2.55	0.48
1:O:131:LEU:HD23	1:O:140:ILE:HG21	1.94	0.48
3:A:497:G:N1	3:A:501:A:OP2	2.45	0.48
3:A:2106:A:OP1	3:A:2267:G:N1	2.40	0.48
3:A:2806:G:OP2	3:A:2810:A:O2'	2.24	0.48
17:S:46:ASP:O	17:S:50:GLY:N	2.46	0.48
3:A:610:U:O2'	3:A:856:G:OP2	2.29	0.48
5:E:30:GLU:N	5:E:103:TYR:OH	2.47	0.48
7:G:163:VAL:O	7:G:166:SER:OG	2.15	0.48
23:Y:46:LYS:HB3	23:Y:48:THR:HG23	1.95	0.48
2:2:33:U:C2'	2:2:37:A:H61	2.27	0.48
3:A:221:G:H22	3:A:238:U:H4'	1.78	0.48
3:A:1964:G:H2'	3:A:1991:C:H42	1.77	0.48
3:A:630:A:H5'	7:G:89:VAL:HG21	1.95	0.48
3:A:866:A:HO2'	3:A:884:C:HO2'	1.51	0.48
3:A:2875:A:P	3:A:2891:G:H22	2.37	0.48
9:I:72:LEU:CD1	9:I:80:VAL:HG22	2.42	0.48
3:A:116:G:OP2	3:A:118:A:O2'	2.32	0.48
6:F:43:ASN:OD1	6:F:44:ASP:N	2.46	0.48
1:O:24:ILE:HD13	1:O:83:ILE:CG2	2.44	0.48
3:A:1117:G:N3	3:A:1135:G:O2'	2.46	0.48
3:A:2514:G:OP1	15:Q:46:GLN:NE2	2.45	0.48
4:B:89:C:OP1	15:Q:19:GLY:N	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:417:ARG:NH2	1:0:418:ASP:OD1	2.47	0.48
3:A:1132:A:H1'	3:A:1149:A:H62	1.77	0.48
3:A:2518:G:H21	3:A:2520:U:H5	1.60	0.48
3:A:2559:U:OP2	3:A:2564:G:N2	2.47	0.48
22:X:59:TYR:N	22:X:76:ARG:O	2.47	0.48
3:A:827:G:H21	3:A:830:A:H62	1.62	0.47
3:A:1102:G:H1'	3:A:1149:A:H61	1.79	0.47
17:S:35:ARG:HG3	17:S:40:ILE:HD12	1.96	0.47
3:A:1040:C:OP2	19:U:54:LYS:NZ	2.45	0.47
3:A:594:C:OP2	20:V:92:TYR:OH	2.32	0.47
3:A:1759:U:O2'	3:A:1760:A:O5'	2.31	0.47
3:A:1333:C:O2'	16:R:69:GLU:OE2	2.27	0.47
3:A:1605:C:OP2	3:A:1606:A:O2'	2.13	0.47
5:E:264:ASN:OD1	5:E:265:LYS:N	2.44	0.47
1:0:98:ARG:NH2	1:0:123:MET:SD	2.88	0.47
4:B:38:U:O2	4:B:41:C:O2'	2.31	0.47
7:G:26:ILE:HD12	7:G:27:GLU:N	2.30	0.47
10:K:11:LEU:HD13	10:K:58:ILE:HD12	1.97	0.47
13:O:16:ALA:HB2	13:O:52:VAL:HG23	1.97	0.47
1:0:151:ASN:OD1	1:0:152:SER:N	2.48	0.47
3:A:1485:A:H2	3:A:1600:G:H21	1.61	0.47
3:A:1829:C:C2	3:A:1846:G:N2	2.76	0.47
9:I:44:ILE:CG2	9:I:51:LEU:HD21	2.44	0.47
11:L:28:VAL:HG11	11:L:96:LEU:HD11	1.95	0.47
13:O:38:VAL:HG22	13:O:61:VAL:HG22	1.95	0.47
14:P:99:THR:OG1	14:P:101:VAL:HG23	2.15	0.47
20:V:36:GLU:OE1	20:V:36:GLU:N	2.48	0.47
1:0:210:GLU:HB3	1:0:258:THR:HG21	1.96	0.47
3:A:448:A:O2'	3:A:449:A:O4'	2.20	0.47
3:A:810:G:O2'	3:A:811:A:O5'	2.29	0.47
3:A:1377:G:N7	22:X:62:LYS:NZ	2.62	0.47
3:A:2549:C:H41	3:A:2571:A:H61	1.61	0.47
5:E:141:VAL:HG22	5:E:192:ILE:HA	1.95	0.47
8:H:132:ILE:HG22	8:H:134:GLU:H	1.79	0.47
9:I:26:ALA:CB	9:I:35:THR:HG22	2.45	0.47
22:X:55:ASN:N	22:X:80:ILE:O	2.46	0.47
25:b:3:ARG:HE	25:b:10:LYS:HB2	1.80	0.47
3:A:865:G:N1	3:A:1229:U:OP2	2.40	0.47
3:A:2340:A:HO2'	3:A:2341:U:P	2.37	0.47
5:E:167:LYS:HG2	5:E:172:VAL:HG13	1.97	0.47
9:I:24:THR:HG22	9:I:37:THR:CG2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1070:G:OP2	3:A:1071:G:O2'	2.33	0.47
3:A:2089:A:HO2'	3:A:2090:G:P	2.33	0.47
4:B:28:C:OP1	17:S:7:LYS:NZ	2.34	0.47
12:N:8:ASN:ND2	12:N:11:THR:OG1	2.40	0.47
30:h:31:LEU:HA	30:h:42:LEU:HD11	1.96	0.47
1:0:60:HIS:NE2	1:0:270:LEU:O	2.44	0.47
3:A:886:U:O2'	3:A:1232:G:N3	2.48	0.47
3:A:1046:A:OP2	3:A:1200:G:N1	2.41	0.47
3:A:2092:C:H42	3:A:2479:A:H61	1.63	0.47
3:A:2785:U:OP2	32:j:19:ARG:NH2	2.47	0.47
21:W:5:ALA:CB	21:W:54:ALA:HB2	2.45	0.47
24:a:48:GLN:OE1	24:a:52:LYS:N	2.42	0.47
1:0:258:THR:HG22	1:0:259:HIS:ND1	2.30	0.46
3:A:443:G:O2'	3:A:444:U:OP1	2.31	0.46
3:A:535:G:N2	3:A:538:A:OP2	2.37	0.46
3:A:1853:G:OP2	5:E:53:HIS:ND1	2.48	0.46
3:A:2048:U:OP2	28:f:6:ARG:NH2	2.49	0.46
3:A:2238:C:OP2	3:A:2239:U:O2'	2.21	0.46
3:A:2421:A:OP2	3:A:2451:C:N4	2.48	0.46
10:K:98:ALA:HB3	10:K:137:ILE:HG12	1.96	0.46
1:0:243:ILE:HD12	1:0:267:PHE:HE2	1.80	0.46
3:A:2054:C:OP1	6:F:153:ARG:NH1	2.48	0.46
3:A:2649:C:O4'	6:F:160:LEU:HD12	2.15	0.46
13:O:103:ALA:HB1	13:O:105:GLU:OE1	2.16	0.46
3:A:162:A:OP2	3:A:163:U:O2'	2.29	0.46
3:A:2233:C:OP1	5:E:147:LYS:NZ	2.47	0.46
1:0:322:ALA:HB1	1:0:380:TYR:CD1	2.50	0.46
3:A:2874:G:N2	3:A:2892:G:OP2	2.49	0.46
4:B:31:G:O2'	4:B:32:U:OP1	2.22	0.46
9:I:108:VAL:HG13	9:I:109:GLY:N	2.31	0.46
12:N:45:TYR:O	19:U:64:ARG:NH2	2.41	0.46
17:S:39:HIS:CD2	17:S:59:LEU:HD12	2.51	0.46
29:g:22:ASN:O	29:g:26:ASN:N	2.47	0.46
3:A:53:A:H62	3:A:116:G:H21	1.64	0.46
14:P:55:MET:O	14:P:60:ARG:NH2	2.49	0.46
14:P:123:VAL:N	14:P:142:THR:OG1	2.47	0.46
17:S:56:ALA:HB1	17:S:77:VAL:CG2	2.46	0.46
23:Y:85:VAL:HG13	23:Y:88:GLY:O	2.15	0.46
3:A:2771:G:O6	3:A:2792:G:N2	2.48	0.46
3:A:448:A:H61	3:A:470:A:H2	1.62	0.46
3:A:752:A:OP2	3:A:773:G:N2	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1243:A:O4'	7:G:41:ARG:NH2	2.48	0.46
11:L:93:ALA:HB1	11:L:127:ALA:HB2	1.97	0.46
19:U:51:ARG:O	19:U:55:ARG:NE	2.48	0.46
29:g:31:GLU:OE1	29:g:46:ARG:NH2	2.45	0.46
3:A:2882:G:N2	3:A:2885:A:OP2	2.39	0.46
21:W:50:VAL:HG12	21:W:105:ILE:HD12	1.97	0.46
29:g:6:THR:C	29:g:7:LEU:HD12	2.41	0.46
2:2:54:U:C2	2:2:58:A:N7	2.84	0.46
3:A:2227:A:O2'	3:A:2228:A:O5'	2.34	0.46
5:E:45:ASN:OD1	5:E:46:GLN:N	2.48	0.46
18:T:10:LYS:HA	18:T:13:LEU:HD12	1.97	0.46
3:A:88:G:O2'	3:A:89:U:OP1	2.33	0.46
3:A:299:U:O4	3:A:416:U:O2'	2.21	0.46
3:A:892:U:O4	3:A:893:A:N6	2.49	0.46
3:A:1158:G:HO2'	3:A:1159:U:P	2.39	0.46
1:0:214:ARG:CG	1:0:258:THR:HG23	2.45	0.45
3:A:410:G:H22	3:A:412:A:H61	1.64	0.45
3:A:1524:A:N6	3:A:1561:G:O2'	2.49	0.45
3:A:1546:G:H21	5:E:98:ASP:C	2.23	0.45
3:A:1004:U:O4	15:Q:17:MET:HE2	2.16	0.45
5:E:74:ILE:N	5:E:117:MET:SD	2.89	0.45
8:H:74:ILE:HG21	8:H:77:PHE:CD2	2.51	0.45
3:A:999:A:OP1	15:Q:18:ARG:NH1	2.46	0.45
9:I:104:LEU:HD21	9:I:106:LEU:HD21	1.98	0.45
11:L:100:ALA:O	11:L:104:GLU:N	2.49	0.45
13:O:34:ASN:OD1	13:O:35:ILE:N	2.46	0.45
1:0:116:ARG:HG3	1:0:131:LEU:HD11	1.98	0.45
6:F:108:VAL:N	6:F:174:LEU:O	2.49	0.45
9:I:72:LEU:HG	9:I:80:VAL:HG22	1.99	0.45
11:L:57:ASN:ND2	11:L:78:GLY:O	2.49	0.45
1:0:139:ILE:HG21	1:0:156:VAL:O	2.16	0.45
3:A:139:A:O2'	3:A:1449:C:O4'	2.33	0.45
3:A:752:A:H62	3:A:773:G:H1'	1.82	0.45
3:A:2864:G:O6	3:A:2903:U:N3	2.49	0.45
7:G:143:LEU:HD22	7:G:148:VAL:HG11	1.99	0.45
3:A:252:C:OP2	3:A:2423:C:O2'	2.31	0.45
3:A:580:U:O2'	19:U:49:ASP:OD2	2.28	0.45
3:A:593:A:O2'	3:A:594:C:O5'	2.35	0.45
3:A:1057:G:OP2	19:U:66:ASN:ND2	2.50	0.45
3:A:1467:G:H21	3:A:1541:A:N6	2.08	0.45
3:A:2652:G:OP1	3:A:2851:A:O2'	2.26	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2669:G:OP1	12:N:88:ARG:NH1	2.50	0.45
6:F:38:LYS:NZ	6:F:88:MET:O	2.42	0.45
9:I:21:ASP:OD1	9:I:24:THR:N	2.41	0.45
13:O:102:VAL:HG12	13:O:103:ALA:N	2.31	0.45
21:W:16:LYS:O	21:W:20:VAL:HG23	2.16	0.45
3:A:1718:G:N2	3:A:1720:C:O4'	2.50	0.45
3:A:2776:G:H21	3:A:2786:A:H62	1.65	0.45
7:G:42:ALA:HB1	7:G:97:TYR:O	2.17	0.45
8:H:35:VAL:HG12	8:H:155:VAL:HB	1.99	0.45
8:H:117:VAL:HG12	8:H:177:PHE:HA	1.97	0.45
9:I:23:ASN:ND2	9:I:39:HIS:O	2.49	0.45
3:A:287:G:N3	3:A:288:C:N4	2.65	0.45
3:A:898:U:O2	27:d:42:ALA:HB1	2.16	0.45
3:A:2873:G:O2'	3:A:2874:G:O5'	2.32	0.45
3:A:2922:U:O2	12:N:135:ALA:HB1	2.16	0.45
4:B:63:C:HO2'	4:B:106:C:H41	1.55	0.45
9:I:21:ASP:N	9:I:24:THR:OG1	2.49	0.45
17:S:74:ALA:HB1	17:S:109:LEU:HB2	1.98	0.45
28:f:28:THR:N	28:f:37:LYS:O	2.47	0.45
30:h:25:LYS:HA	30:h:28:ARG:HE	1.82	0.45
3:A:1886:G:O2'	3:A:1914:A:N6	2.49	0.45
3:A:2606:A:O4'	3:A:2641:C:N4	2.49	0.45
7:G:9:GLN:HA	7:G:126:LEU:HD21	1.98	0.45
13:O:43:VAL:HG21	13:O:53:LYS:O	2.17	0.45
1:O:146:LEU:HD13	1:O:148:PRO:HA	1.99	0.45
3:A:829:A:C6	5:E:225:MET:HE2	2.51	0.45
3:A:957:A:H62	15:Q:12:GLU:HA	1.82	0.45
3:A:1819:C:O2'	5:E:208:ALA:HB2	2.17	0.45
7:G:176:VAL:HG22	7:G:177:GLU:H	1.81	0.45
8:H:34:ILE:C	8:H:35:VAL:HG23	2.42	0.45
23:Y:41:VAL:HG12	23:Y:61:ALA:HB2	1.99	0.45
3:A:2372:U:HO2'	3:A:2402:A:HO2'	1.48	0.44
3:A:2834:A:OP2	3:A:2915:G:N2	2.45	0.44
5:E:158:ALA:HA	5:E:195:VAL:HG11	1.99	0.44
11:L:97:ASN:OD1	11:L:127:ALA:HB1	2.18	0.44
3:A:64:A:H1'	22:X:66:VAL:HG21	1.99	0.44
3:A:1258:A:OP1	19:U:19:LYS:NZ	2.41	0.44
3:A:1327:U:P	3:A:1328:C:H41	2.41	0.44
8:H:15:ALA:HB3	8:H:172:GLN:NE2	2.33	0.44
3:A:85:G:O2'	3:A:86:C:OP2	2.28	0.44
3:A:1378:G:N1	3:A:1379:U:O4	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1882:A:O2'	3:A:1883:A:OP1	2.32	0.44
7:G:126:LEU:O	7:G:195:THR:HG22	2.17	0.44
10:K:117:ASN:OD1	10:K:117:ASN:N	2.50	0.44
32:j:17:ILE:HD11	32:j:24:MET:SD	2.58	0.44
3:A:1035:G:OP1	3:A:1203:G:O2'	2.25	0.44
3:A:1321:U:C2	3:A:1325:A:N6	2.85	0.44
3:A:2695:C:H41	9:I:110:TYR:HA	1.83	0.44
7:G:77:SER:OG	7:G:78:ILE:N	2.51	0.44
11:L:108:ILE:HG22	11:L:108:ILE:O	2.17	0.44
1:0:349:ILE:HG22	1:0:351:TYR:H	1.83	0.44
3:A:2378:G:OP1	31:i:45:ARG:NH1	2.46	0.44
8:H:36:ILE:HA	8:H:156:ILE:HG12	2.00	0.44
16:R:18:ARG:NE	16:R:65:TYR:O	2.51	0.44
1:0:454:GLU:N	1:0:564:VAL:O	2.47	0.44
3:A:492:C:H2'	3:A:493:G:O4'	2.18	0.44
3:A:612:U:N3	3:A:615:U:OP2	2.43	0.44
3:A:2122:G:N3	3:A:2227:A:N6	2.66	0.44
4:B:40:C:O2'	4:B:41:C:O4'	2.35	0.44
7:G:6:LEU:HD22	7:G:14:ALA:HB3	2.00	0.44
9:I:66:HIS:HA	9:I:69:THR:HG23	2.00	0.44
14:P:1:MET:HE1	14:P:7:LYS:O	2.18	0.44
20:V:11:GLN:O	20:V:12:ILE:HD13	2.17	0.44
26:c:52:ARG:O	26:c:56:VAL:HG23	2.18	0.44
3:A:223:G:N2	3:A:475:A:OP2	2.51	0.44
3:A:631:G:OP2	14:P:21:ARG:NH2	2.50	0.44
20:V:12:ILE:HG22	20:V:13:LYS:C	2.43	0.44
3:A:996:G:O6	3:A:1014:A:N6	2.51	0.44
3:A:2772:U:P	3:A:2784:C:H42	2.41	0.44
25:b:19:SER:OG	25:b:20:HIS:N	2.50	0.44
1:0:181:ILE:HG21	1:0:187:PHE:HB3	1.99	0.44
3:A:266:U:O2'	3:A:477:A:N3	2.39	0.44
3:A:1757:G:C6	3:A:1776:A:N6	2.83	0.44
6:F:6:LEU:HD23	6:F:33:ASN:ND2	2.33	0.44
8:H:96:MET:SD	8:H:96:MET:N	2.91	0.44
1:0:244:THR:HG21	1:0:257:LEU:HD13	2.00	0.43
3:A:81:G:HO2'	3:A:338:G:HO2'	1.63	0.43
3:A:160:G:O2'	3:A:168:A:N7	2.51	0.43
3:A:2129:G:N2	3:A:2218:U:O2	2.50	0.43
3:A:2348:C:N4	3:A:2363:C:OP2	2.50	0.43
3:A:2778:A:OP2	3:A:2779:A:O2'	2.25	0.43
4:B:40:C:H5'	8:H:64:LYS:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:65:ILE:HG21	5:E:67:PHE:CZ	2.53	0.43
26:c:38:GLU:O	26:c:40:THR:N	2.48	0.43
3:A:753:A:H61	3:A:772:G:H1'	1.83	0.43
3:A:2785:U:OP2	32:j:19:ARG:NE	2.48	0.43
1:0:240:ILE:HG23	1:0:240:ILE:O	2.18	0.43
3:A:126:A:O2'	3:A:127:C:OP1	2.32	0.43
17:S:5:THR:HB	17:S:9:ALA:HB3	1.99	0.43
3:A:631:G:H22	14:P:33:LYS:NZ	2.17	0.43
3:A:829:A:C2	5:E:225:MET:HE2	2.52	0.43
3:A:1737:U:O2'	3:A:1740:G:O6	2.34	0.43
3:A:2308:G:O6	24:a:22:ARG:NE	2.52	0.43
3:A:2758:G:O2'	6:F:189:LYS:NZ	2.51	0.43
10:K:24:VAL:O	10:K:27:ALA:N	2.51	0.43
3:A:2386:U:OP1	24:a:28:ARG:NH2	2.51	0.43
4:B:29:C:O2'	4:B:51:A:N1	2.49	0.43
6:F:123:ILE:O	6:F:127:GLY:N	2.47	0.43
7:G:112:SER:OG	7:G:113:VAL:N	2.50	0.43
19:U:90:VAL:O	20:V:11:GLN:NE2	2.52	0.43
3:A:614:G:O4'	3:A:1029:A:N6	2.51	0.43
3:A:1971:C:OP2	3:A:1972:U:O2'	2.36	0.43
6:F:90:ALA:HB3	6:F:91:TYR:CD2	2.54	0.43
11:L:15:ILE:HD12	11:L:59:MET:HE1	1.99	0.43
3:A:223:G:H22	3:A:474:U:H3'	1.84	0.43
5:E:106:ALA:O	5:E:196:GLY:N	2.43	0.43
22:X:50:LYS:NZ	22:X:86:ASP:O	2.45	0.43
23:Y:69:MET:HE3	23:Y:80:ARG:HG2	2.00	0.43
27:d:10:ARG:HB3	27:d:53:LEU:HD13	1.99	0.43
1:0:53:HIS:N	1:0:56:TYR:O	2.51	0.43
3:A:193:A:OP2	3:A:208:G:N2	2.50	0.43
3:A:2434:G:H1'	3:A:2441:A:H61	1.84	0.43
8:H:38:MET:HG3	8:H:87:ALA:HB3	2.01	0.43
26:c:9:LEU:C	26:c:14:ILE:HD12	2.43	0.43
3:A:311:U:C2	3:A:406:G:N1	2.87	0.43
3:A:1392:A:OP2	3:A:1416:G:N1	2.43	0.43
3:A:1473:A:N6	3:A:1619:A:OP2	2.38	0.43
8:H:55:GLU:O	8:H:58:THR:OG1	2.25	0.43
8:H:88:LYS:HD3	8:H:155:VAL:HG21	2.01	0.43
9:I:21:ASP:OD1	9:I:24:THR:HG23	2.18	0.43
10:K:124:ALA:O	10:K:128:VAL:HG23	2.19	0.43
12:N:59:ASN:N	12:N:126:TYR:O	2.52	0.43
32:j:27:CYS:SG	32:j:28:GLU:N	2.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2352:G:H2'	3:A:2353:U:O4'	2.19	0.43
14:P:86:ALA:O	14:P:121:LEU:HD23	2.18	0.43
3:A:364:A:O2'	7:G:169:ASN:OD1	2.34	0.42
3:A:704:U:O4	3:A:705:A:N6	2.52	0.42
3:A:2824:G:N2	3:A:2827:A:C8	2.81	0.42
3:A:1460:G:N2	3:A:1631:A:OP2	2.44	0.42
3:A:1543:U:O2'	3:A:1544:C:O5'	2.18	0.42
3:A:1831:A:H2	3:A:1844:A:H62	1.65	0.42
5:E:248:SER:OG	5:E:252:LYS:N	2.48	0.42
10:K:18:ALA:HB3	10:K:40:LYS:HE2	2.01	0.42
17:S:39:HIS:CG	17:S:59:LEU:HD12	2.54	0.42
22:X:30:VAL:HG12	22:X:31:ASP:N	2.33	0.42
30:h:15:VAL:O	30:h:20:SER:OG	2.21	0.42
3:A:227:G:P	3:A:455:G:H21	2.41	0.42
3:A:965:A:N3	4:B:78:U:O2'	2.50	0.42
4:B:22:G:O2'	4:B:25:A:N6	2.52	0.42
6:F:111:THR:OG1	6:F:170:THR:HG22	2.20	0.42
16:R:107:ARG:CB	16:R:114:MET:HE2	2.49	0.42
19:U:69:ALA:O	19:U:74:LEU:N	2.51	0.42
1:0:539:PRO:N	1:0:546:PHE:O	2.52	0.42
3:A:894:A:H62	3:A:979:U:H3	1.67	0.42
3:A:1068:G:H22	3:A:1188:A:H2	1.68	0.42
3:A:1380:U:OP1	3:A:1436:U:N3	2.52	0.42
8:H:35:VAL:O	8:H:156:ILE:CA	2.61	0.42
13:O:10:VAL:HG12	13:O:12:ASP:H	1.85	0.42
13:O:90:ASP:OD1	13:O:91:LYS:N	2.48	0.42
23:Y:39:ASN:ND2	23:Y:62:PRO:O	2.52	0.42
1:0:75:PHE:O	1:0:79:LEU:HD13	2.19	0.42
3:A:1158:G:O2'	3:A:1159:U:O5'	2.35	0.42
5:E:185:LEU:HD23	5:E:187:ALA:N	2.34	0.42
9:I:89:GLU:OE1	9:I:89:GLU:N	2.52	0.42
13:O:10:VAL:HG21	13:O:16:ALA:C	2.45	0.42
15:Q:72:LYS:O	15:Q:94:VAL:N	2.52	0.42
20:V:57:THR:O	20:V:101:ASN:N	2.53	0.42
2:2:10:G:OP1	2:2:45:G:O2'	2.20	0.42
3:A:528:G:H1'	3:A:552:G:H21	1.84	0.42
3:A:1093:G:N2	3:A:1156:G:O2'	2.53	0.42
3:A:2378:G:OP1	31:i:45:ARG:NH2	2.51	0.42
4:B:6:U:O2'	17:S:30:ARG:NH2	2.51	0.42
10:K:109:ALA:O	10:K:113:MET:N	2.48	0.42
11:L:74:ASP:OD1	11:L:75:PHE:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:119:THR:HG22	11:L:120:VAL:N	2.34	0.42
14:P:102:ILE:HG22	14:P:104:LYS:H	1.84	0.42
3:A:229:A:O2'	3:A:231:A:N6	2.52	0.42
3:A:799:A:OP1	30:h:3:ARG:NH1	2.47	0.42
3:A:2340:A:O2'	3:A:2341:U:O5'	2.29	0.42
6:F:36:LEU:HA	6:F:72:ALA:HB2	2.01	0.42
6:F:114:SER:OG	6:F:167:GLU:N	2.49	0.42
8:H:11:GLU:OE1	8:H:11:GLU:N	2.53	0.42
9:I:55:ARG:HE	9:I:58:ASP:HA	1.84	0.42
19:U:76:TYR:OH	19:U:92:ARG:NE	2.50	0.42
3:A:1248:C:HO2'	3:A:1249:U:H6	1.67	0.42
3:A:2748:G:OP1	18:T:96:LYS:NZ	2.52	0.42
9:I:11:ILE:N	9:I:49:ASN:O	2.50	0.42
13:O:13:ASN:ND2	13:O:96:THR:OG1	2.43	0.42
3:A:771:U:H2'	3:A:772:G:O4'	2.20	0.42
3:A:1494:G:O2'	3:A:1592:A:N3	2.46	0.42
3:A:1516:A:H5''	3:A:1569:A:H61	1.85	0.42
3:A:2682:U:OP2	3:A:2683:A:O2'	2.34	0.42
1:O:74:MET:SD	1:O:74:MET:N	2.92	0.42
3:A:236:A:H61	3:A:476:A:N6	2.17	0.42
3:A:353:A:N7	3:A:374:A:N6	2.67	0.42
3:A:563:C:O2'	21:W:18:ARG:NH2	2.48	0.42
4:B:48:G:O2'	4:B:49:G:OP1	2.37	0.42
8:H:35:VAL:HG12	8:H:155:VAL:O	2.19	0.42
14:P:85:PHE:HB3	14:P:121:LEU:HD21	2.02	0.42
19:U:93:LYS:HE3	19:U:94:MET:HE3	2.01	0.42
26:c:13:GLU:OE1	26:c:13:GLU:N	2.48	0.42
1:O:339:LEU:HD13	1:O:369:PRO:CB	2.49	0.41
3:A:902:G:O2'	24:a:35:ASP:OD2	2.37	0.41
3:A:2561:G:N2	3:A:2693:G:O4'	2.50	0.41
8:H:37:ASN:C	8:H:153:ASP:HB3	2.44	0.41
9:I:51:LEU:HD22	9:I:52:THR:H	1.85	0.41
1:O:51:SER:O	1:O:57:SER:OG	2.35	0.41
6:F:34:VAL:HG12	6:F:77:LYS:NZ	2.35	0.41
6:F:178:LYS:CB	6:F:187:LEU:HD12	2.50	0.41
8:H:38:MET:HB2	8:H:154:ILE:HA	2.02	0.41
8:H:160:ALA:HB1	8:H:165:GLU:OE2	2.20	0.41
3:A:77:U:HO2'	3:A:78:U:P	2.43	0.41
3:A:1398:A:H62	3:A:1411:U:H3	1.68	0.41
3:A:2874:G:N7	3:A:2892:G:N2	2.56	0.41
8:H:128:TYR:O	8:H:156:ILE:HB	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:24:THR:HG22	9:I:37:THR:HG23	2.02	0.41
13:O:77:ILE:HD12	18:T:72:ARG:HD3	2.02	0.41
14:P:79:LEU:HD11	14:P:135:ALA:HB3	2.01	0.41
20:V:34:THR:HG22	20:V:59:THR:HG22	2.01	0.41
22:X:59:TYR:O	22:X:76:ARG:N	2.48	0.41
24:a:29:LEU:HD23	24:a:47:ARG:HB3	2.01	0.41
24:a:53:ILE:HG22	24:a:54:TYR:O	2.19	0.41
3:A:369:A:N6	3:A:382:G:N3	2.68	0.41
3:A:676:G:OP1	31:i:23:LYS:NZ	2.51	0.41
3:A:1243:A:O2'	3:A:1244:A:OP1	2.24	0.41
3:A:2922:U:O3'	12:N:137:LYS:NZ	2.49	0.41
4:B:42:G:O4'	4:B:44:A:N6	2.52	0.41
8:H:37:ASN:HA	8:H:155:VAL:HA	2.00	0.41
15:Q:132:VAL:HG12	15:Q:133:LYS:N	2.36	0.41
18:T:27:ARG:NH2	18:T:44:GLU:OE2	2.53	0.41
1:O:52:ALA:HB2	1:O:129:ILE:HD12	2.01	0.41
3:A:1464:A:O2'	3:A:1465:A:OP2	2.35	0.41
7:G:121:ASN:HA	7:G:123:ILE:HG22	2.02	0.41
2:2:36:C:O2'	2:2:37:A:OP2	2.33	0.41
3:A:66:C:O4'	3:A:503:C:N4	2.54	0.41
3:A:1139:G:O2'	3:A:1144:A:N6	2.48	0.41
3:A:1542:A:N3	3:A:1625:C:O2'	2.39	0.41
9:I:74:GLY:O	9:I:77:VAL:HB	2.21	0.41
3:A:75:G:OP1	26:c:44:ARG:NH2	2.54	0.41
3:A:1351:U:H1'	3:A:1353:C:H41	1.85	0.41
3:A:1506:A:H2'	3:A:1507:U:H5'	2.02	0.41
3:A:1711:G:N3	13:O:3:GLN:NE2	2.69	0.41
3:A:1886:G:H8	3:A:1914:A:H62	1.69	0.41
3:A:2549:C:H41	3:A:2571:A:N6	2.18	0.41
1:O:244:THR:HG21	1:O:257:LEU:HD22	2.02	0.41
1:O:339:LEU:HD13	1:O:369:PRO:HB3	2.02	0.41
3:A:866:A:N7	3:A:1229:U:O4	2.54	0.41
3:A:910:A:O3'	4:B:98:G:N2	2.54	0.41
3:A:1304:G:OP1	28:f:16:ARG:NH1	2.47	0.41
3:A:1500:U:O2'	3:A:1501:U:O5'	2.33	0.41
3:A:2231:C:O2'	3:A:2233:C:OP1	2.37	0.41
6:F:154:VAL:HG12	6:F:155:PHE:O	2.20	0.41
16:R:83:LEU:HA	16:R:87:ILE:HD12	2.02	0.41
17:S:57:SER:N	17:S:60:ASP:OD2	2.46	0.41
17:S:109:LEU:HD23	17:S:109:LEU:O	2.19	0.41
29:g:4:ASN:O	29:g:5:ILE:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:245:G:O2'	3:A:257:G:O6	2.37	0.41
3:A:772:G:H2'	3:A:773:G:C1'	2.50	0.41
3:A:1508:C:H2'	3:A:1509:C:C6	2.55	0.41
3:A:1539:C:O2'	3:A:1540:A:OP1	2.36	0.41
3:A:1699:A:N6	3:A:2035:C:O4'	2.54	0.41
9:I:13:SER:O	9:I:15:VAL:HG23	2.21	0.41
10:K:17:LYS:O	10:K:43:ASN:ND2	2.51	0.41
17:S:70:ASP:CG	17:S:72:SER:HG	2.27	0.41
18:T:92:VAL:HG12	18:T:93:ARG:N	2.36	0.41
27:d:5:GLU:OE1	27:d:5:GLU:N	2.52	0.41
1:0:246:VAL:O	1:0:246:VAL:HG13	2.21	0.41
3:A:245:G:N2	3:A:258:A:OP2	2.53	0.41
3:A:2119:A:N6	3:A:2259:G:O6	2.54	0.41
3:A:2315:A:H4'	3:A:2316:A:O4'	2.21	0.41
3:A:2620:C:N4	3:A:2621:G:O6	2.54	0.41
4:B:111:C:O2'	17:S:52:THR:OG1	2.11	0.41
6:F:10:ILE:HD12	6:F:10:ILE:H	1.86	0.41
7:G:53:ASN:OD1	7:G:54:ARG:N	2.54	0.41
8:H:29:PRO:HB2	8:H:160:ALA:HB2	2.03	0.41
8:H:37:ASN:N	8:H:154:ILE:C	2.79	0.41
16:R:17:LEU:O	16:R:21:THR:HG23	2.20	0.41
17:S:44:ILE:HD12	17:S:81:VAL:HG21	2.03	0.41
1:0:331:LEU:HD13	1:0:348:VAL:HG22	2.02	0.40
3:A:785:C:O2'	3:A:786:A:O5'	2.39	0.40
3:A:1841:G:H21	5:E:50:THR:HG21	1.86	0.40
3:A:2108:U:H2'	3:A:2109:G:O4'	2.21	0.40
4:B:33:U:HO2'	4:B:34:C:C4'	2.33	0.40
5:E:70:ASP:OD1	5:E:71:LYS:N	2.54	0.40
9:I:94:GLY:O	9:I:96:ARG:NH1	2.52	0.40
1:0:61:ILE:CG1	1:0:270:LEU:HD11	2.51	0.40
1:0:91:ILE:HG23	1:0:102:PHE:CE1	2.56	0.40
1:0:181:ILE:O	1:0:185:LEU:C	2.64	0.40
3:A:223:G:O4'	3:A:237:U:O2'	2.38	0.40
3:A:1713:A:N6	3:A:1721:A:H61	2.14	0.40
3:A:2246:G:O3'	25:b:37:ARG:NH2	2.54	0.40
16:R:50:LEU:HD22	16:R:58:ALA:CB	2.51	0.40
3:A:229:A:N1	3:A:465:U:O2'	2.51	0.40
3:A:344:G:O2'	3:A:345:A:O3'	2.39	0.40
3:A:788:G:H2'	3:A:789:C:O4'	2.21	0.40
6:F:106:GLU:HB2	6:F:176:ILE:HD12	2.04	0.40
24:a:77:PHE:CD1	24:a:87:VAL:HG12	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:52:A:OP2	3:A:116:G:N1	2.48	0.40
3:A:1471:G:N2	3:A:1622:C:N3	2.69	0.40
3:A:1543:U:HO2'	3:A:1544:C:C5'	2.27	0.40
3:A:1625:C:H2'	3:A:1626:U:C1'	2.51	0.40
3:A:2042:A:OP1	21:W:97:ASN:N	2.53	0.40
3:A:2718:U:OP1	3:A:2720:C:N4	2.54	0.40
3:A:2818:C:O2'	3:A:2917:G:N2	2.54	0.40
5:E:200:HIS:O	5:E:203:ILE:HD12	2.21	0.40
17:S:44:ILE:C	17:S:45:ILE:HD12	2.47	0.40
18:T:90:GLY:N	18:T:113:ILE:HG22	2.36	0.40
21:W:46:ILE:H	21:W:46:ILE:HD12	1.86	0.40
31:i:54:ASP:OD1	31:i:57:ARG:NH1	2.51	0.40
1:0:385:ASN:O	1:0:389:VAL:HG23	2.21	0.40
3:A:75:G:HO2'	3:A:76:C:P	2.31	0.40
3:A:236:A:H61	3:A:476:A:H61	1.67	0.40
3:A:593:A:O2'	3:A:593:A:N3	2.51	0.40
3:A:1112:U:N3	3:A:1115:A:OP2	2.46	0.40
3:A:1565:U:HO2'	3:A:1566:G:P	2.41	0.40
3:A:1758:U:O2'	3:A:1759:U:OP1	2.30	0.40
9:I:141:ARG:O	9:I:145:ILE:HD12	2.22	0.40
11:L:19:LEU:HD21	11:L:63:ALA:HB2	2.04	0.40
17:S:36:SER:N	17:S:39:HIS:O	2.54	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	523/597 (88%)	439 (84%)	78 (15%)	6 (1%)	11	43
5	E	270/277 (98%)	245 (91%)	23 (8%)	2 (1%)	18	51
6	F	204/209 (98%)	181 (89%)	23 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	203/207 (98%)	176 (87%)	27 (13%)	0	100	100
8	H	160/179 (89%)	128 (80%)	29 (18%)	3 (2%)	6	33
9	I	173/179 (97%)	137 (79%)	36 (21%)	0	100	100
10	K	130/141 (92%)	115 (88%)	15 (12%)	0	100	100
11	L	107/166 (64%)	103 (96%)	4 (4%)	0	100	100
12	N	140/145 (97%)	130 (93%)	10 (7%)	0	100	100
13	O	120/122 (98%)	99 (82%)	21 (18%)	0	100	100
14	P	144/146 (99%)	122 (85%)	22 (15%)	0	100	100
15	Q	133/144 (92%)	120 (90%)	13 (10%)	0	100	100
16	R	117/120 (98%)	102 (87%)	15 (13%)	0	100	100
17	S	118/120 (98%)	105 (89%)	13 (11%)	0	100	100
18	T	113/115 (98%)	98 (87%)	15 (13%)	0	100	100
19	U	115/119 (97%)	104 (90%)	10 (9%)	1 (1%)	14	47
20	V	98/102 (96%)	80 (82%)	17 (17%)	1 (1%)	12	44
21	W	107/113 (95%)	89 (83%)	18 (17%)	0	100	100
22	X	88/95 (93%)	80 (91%)	8 (9%)	0	100	100
23	Y	99/103 (96%)	84 (85%)	15 (15%)	0	100	100
24	a	73/94 (78%)	65 (89%)	8 (11%)	0	100	100
25	b	56/62 (90%)	42 (75%)	14 (25%)	0	100	100
26	c	63/66 (96%)	57 (90%)	6 (10%)	0	100	100
27	d	56/59 (95%)	49 (88%)	7 (12%)	0	100	100
28	f	51/59 (86%)	46 (90%)	5 (10%)	0	100	100
29	g	46/49 (94%)	36 (78%)	10 (22%)	0	100	100
30	h	42/44 (96%)	39 (93%)	3 (7%)	0	100	100
31	i	62/66 (94%)	56 (90%)	6 (10%)	0	100	100
32	j	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
All	All	3646/3935 (93%)	3158 (87%)	475 (13%)	13 (0%)	31	62

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	448	PRO
1	0	544	PRO

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Mol	Chain	Res	Type
1	0	559	PRO
5	E	156	ARG
8	H	37	ASN
5	E	155	VAL
8	H	154	ILE
1	0	501	GLU
1	0	527	PRO
8	H	155	VAL
19	U	90	VAL
20	V	51	PRO
1	0	148	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	371/527 (70%)	371 (100%)	0	100	100
5	E	220/225 (98%)	219 (100%)	1 (0%)	81	80
6	F	167/170 (98%)	167 (100%)	0	100	100
7	G	169/170 (99%)	169 (100%)	0	100	100
8	H	139/154 (90%)	139 (100%)	0	100	100
9	I	148/151 (98%)	148 (100%)	0	100	100
10	K	102/110 (93%)	102 (100%)	0	100	100
11	L	98/138 (71%)	98 (100%)	0	100	100
12	N	120/123 (98%)	120 (100%)	0	100	100
13	O	101/101 (100%)	101 (100%)	0	100	100
14	P	110/110 (100%)	110 (100%)	0	100	100
15	Q	109/116 (94%)	109 (100%)	0	100	100
16	R	99/100 (99%)	99 (100%)	0	100	100
17	S	93/93 (100%)	93 (100%)	0	100	100
18	T	100/100 (100%)	100 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	U	96/98 (98%)	96 (100%)	0	100	100
20	V	83/84 (99%)	83 (100%)	0	100	100
21	W	90/93 (97%)	90 (100%)	0	100	100
22	X	81/85 (95%)	81 (100%)	0	100	100
23	Y	85/87 (98%)	85 (100%)	0	100	100
24	a	59/74 (80%)	59 (100%)	0	100	100
25	b	47/50 (94%)	47 (100%)	0	100	100
26	c	56/57 (98%)	56 (100%)	0	100	100
27	d	52/53 (98%)	52 (100%)	0	100	100
28	f	47/53 (89%)	46 (98%)	1 (2%)	47	66
29	g	46/47 (98%)	46 (100%)	0	100	100
30	h	39/39 (100%)	39 (100%)	0	100	100
31	i	54/56 (96%)	54 (100%)	0	100	100
32	j	35/35 (100%)	35 (100%)	0	100	100
All	All	3016/3299 (91%)	3014 (100%)	2 (0%)	87	87

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	268	LYS
28	f	33	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	33	HIS
1	0	145	HIS
1	0	406	GLN
5	E	86	ASN
9	I	75	ASN
11	L	103	HIS
12	N	136	GLN
13	O	109	ASN
15	Q	123	HIS
16	R	57	HIS
16	R	61	GLN

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Mol	Chain	Res	Type
27	d	32	ASN
31	i	35	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	2	74/76 (97%)	22 (29%)	1 (1%)
3	A	2806/2926 (95%)	815 (29%)	65 (2%)
4	B	111/119 (93%)	38 (34%)	3 (2%)
All	All	2991/3121 (95%)	875 (29%)	69 (2%)

All (875) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	2	7	U
2	2	9	A
2	2	13	C
2	2	15	G
2	2	16	C
2	2	19	G
2	2	20	G
2	2	21	A
2	2	22	G
2	2	34	U
2	2	36	C
2	2	37	A
2	2	42	G
2	2	47	U
2	2	48	C
2	2	49	A
2	2	56	C
2	2	57	G
2	2	61	C
2	2	69	C
2	2	74	C
2	2	76	A
3	A	8	U
3	A	10	A
3	A	13	A
3	A	14	A
3	A	15	G

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Mol	Chain	Res	Type
3	A	23	G
3	A	26	G
3	A	30	G
3	A	34	U
3	A	35	G
3	A	36	G
3	A	39	C
3	A	46	C
3	A	48	G
3	A	61	A
3	A	62	C
3	A	63	G
3	A	71	A
3	A	74	U
3	A	75	G
3	A	76	C
3	A	77	U
3	A	78	U
3	A	79	C
3	A	83	G
3	A	84	A
3	A	85	G
3	A	86	C
3	A	87	U
3	A	89	U
3	A	90	A
3	A	93	C
3	A	96	G
3	A	99	U
3	A	101	G
3	A	109	G
3	A	113	U
3	A	117	A
3	A	118	A
3	A	119	U
3	A	125	A
3	A	126	A
3	A	127	C
3	A	133	A
3	A	139	A
3	A	140	A
3	A	141	U

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Mol	Chain	Res	Type
3	A	150	A
3	A	161	A
3	A	164	U
3	A	175	G
3	A	176	A
3	A	177	G
3	A	178	A
3	A	179	A
3	A	183	A
3	A	185	A
3	A	188	C
3	A	191	G
3	A	199	A
3	A	200	A
3	A	208	G
3	A	216	A
3	A	219	A
3	A	224	A
3	A	225	A
3	A	226	A
3	A	229	A
3	A	231	A
3	A	232	U
3	A	233	G
3	A	234	C
3	A	236	A
3	A	242	U
3	A	251	G
3	A	252	C
3	A	253	G
3	A	255	G
3	A	258	A
3	A	266	U
3	A	267	C
3	A	270	C
3	A	275	A
3	A	283	G
3	A	284	C
3	A	285	U
3	A	286	U
3	A	287	G
3	A	288	C

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Mol	Chain	Res	Type
3	A	290	U
3	A	291	C
3	A	298	U
3	A	301	U
3	A	302	A
3	A	308	C
3	A	309	U
3	A	310	C
3	A	314	A
3	A	316	G
3	A	319	G
3	A	321	U
3	A	329	A
3	A	345	A
3	A	346	G
3	A	348	U
3	A	349	C
3	A	352	G
3	A	354	A
3	A	360	C
3	A	361	G
3	A	365	U
3	A	366	A
3	A	367	G
3	A	373	A
3	A	374	A
3	A	375	C
3	A	379	C
3	A	382	G
3	A	387	C
3	A	393	U
3	A	402	U
3	A	404	C
3	A	405	U
3	A	407	A
3	A	410	G
3	A	411	G
3	A	412	A
3	A	413	U
3	A	418	A
3	A	419	G
3	A	420	U

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Mol	Chain	Res	Type
3	A	421	A
3	A	422	C
3	A	427	G
3	A	433	G
3	A	434	U
3	A	436	A
3	A	444	U
3	A	452	C
3	A	458	G
3	A	459	A
3	A	468	C
3	A	471	G
3	A	482	C
3	A	483	C
3	A	488	U
3	A	489	G
3	A	491	C
3	A	495	U
3	A	498	U
3	A	501	A
3	A	502	C
3	A	504	A
3	A	505	G
3	A	506	U
3	A	522	U
3	A	525	A
3	A	527	A
3	A	528	G
3	A	529	C
3	A	533	C
3	A	540	G
3	A	550	G
3	A	551	A
3	A	552	G
3	A	553	A
3	A	554	U
3	A	555	C
3	A	556	C
3	A	559	A
3	A	564	G
3	A	568	G
3	A	573	C

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Mol	Chain	Res	Type
3	A	574	A
3	A	575	A
3	A	576	G
3	A	577	U
3	A	578	A
3	A	579	G
3	A	591	U
3	A	592	A
3	A	593	A
3	A	594	C
3	A	595	G
3	A	599	G
3	A	606	U
3	A	607	G
3	A	616	A
3	A	617	G
3	A	619	A
3	A	630	A
3	A	631	G
3	A	647	A
3	A	648	G
3	A	649	G
3	A	658	A
3	A	659	A
3	A	664	C
3	A	666	G
3	A	667	A
3	A	669	C
3	A	673	A
3	A	674	G
3	A	683	A
3	A	689	A
3	A	690	A
3	A	691	U
3	A	692	A
3	A	697	G
3	A	700	U
3	A	701	G
3	A	715	A
3	A	716	G
3	A	718	C
3	A	719	C

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Mol	Chain	Res	Type
3	A	720	C
3	A	724	A
3	A	731	G
3	A	733	U
3	A	734	C
3	A	735	U
3	A	742	G
3	A	764	C
3	A	765	A
3	A	775	G
3	A	777	C
3	A	781	A
3	A	787	C
3	A	788	G
3	A	789	C
3	A	794	U
3	A	795	G
3	A	804	G
3	A	810	G
3	A	811	A
3	A	812	G
3	A	818	G
3	A	822	G
3	A	824	G
3	A	829	A
3	A	830	A
3	A	831	U
3	A	832	G
3	A	836	A
3	A	837	U
3	A	839	G
3	A	847	A
3	A	848	G
3	A	852	G
3	A	859	C
3	A	866	A
3	A	873	U
3	A	874	U
3	A	875	U
3	A	877	G
3	A	890	G
3	A	892	U

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Mol	Chain	Res	Type
3	A	894	A
3	A	903	G
3	A	906	G
3	A	908	A
3	A	913	A
3	A	916	G
3	A	918	U
3	A	919	U
3	A	929	G
3	A	939	G
3	A	940	G
3	A	943	A
3	A	944	C
3	A	946	G
3	A	948	A
3	A	954	U
3	A	957	A
3	A	959	C
3	A	960	U
3	A	961	C
3	A	962	C
3	A	963	G
3	A	964	A
3	A	966	U
3	A	970	A
3	A	973	G
3	A	977	U
3	A	978	A
3	A	979	U
3	A	980	C
3	A	987	A
3	A	991	A
3	A	992	G
3	A	999	A
3	A	1005	A
3	A	1007	G
3	A	1019	A
3	A	1020	A
3	A	1029	A
3	A	1036	A
3	A	1037	C
3	A	1041	C

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Mol	Chain	Res	Type
3	A	1051	C
3	A	1058	U
3	A	1059	A
3	A	1066	A
3	A	1067	A
3	A	1068	G
3	A	1072	A
3	A	1073	A
3	A	1074	A
3	A	1079	U
3	A	1084	A
3	A	1088	G
3	A	1091	U
3	A	1092	A
3	A	1093	G
3	A	1094	A
3	A	1102	G
3	A	1103	A
3	A	1107	U
3	A	1108	G
3	A	1115	A
3	A	1116	A
3	A	1117	G
3	A	1118	C
3	A	1119	A
3	A	1125	C
3	A	1129	U
3	A	1133	G
3	A	1134	A
3	A	1135	G
3	A	1136	U
3	A	1143	U
3	A	1144	A
3	A	1147	U
3	A	1156	G
3	A	1157	A
3	A	1158	G
3	A	1159	U
3	A	1160	G
3	A	1161	A
3	A	1168	G
3	A	1173	A

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Mol	Chain	Res	Type
3	A	1174	A
3	A	1176	U
3	A	1177	G
3	A	1179	A
3	A	1180	C
3	A	1181	C
3	A	1182	G
3	A	1185	G
3	A	1188	A
3	A	1189	A
3	A	1201	A
3	A	1203	G
3	A	1210	A
3	A	1216	C
3	A	1227	G
3	A	1236	G
3	A	1244	A
3	A	1245	G
3	A	1246	G
3	A	1248	C
3	A	1249	U
3	A	1250	G
3	A	1251	U
3	A	1252	G
3	A	1259	G
3	A	1260	A
3	A	1261	C
3	A	1265	A
3	A	1267	G
3	A	1269	A
3	A	1278	G
3	A	1280	G
3	A	1288	G
3	A	1289	U
3	A	1290	G
3	A	1293	A
3	A	1295	U
3	A	1296	G
3	A	1297	C
3	A	1305	A
3	A	1306	G
3	A	1311	G

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Mol	Chain	Res	Type
3	A	1312	A
3	A	1313	A
3	A	1314	A
3	A	1315	G
3	A	1317	G
3	A	1319	G
3	A	1323	A
3	A	1326	A
3	A	1333	C
3	A	1339	A
3	A	1340	A
3	A	1341	U
3	A	1343	C
3	A	1346	A
3	A	1351	U
3	A	1352	U
3	A	1357	A
3	A	1363	G
3	A	1364	C
3	A	1365	U
3	A	1366	C
3	A	1368	U
3	A	1370	C
3	A	1371	G
3	A	1372	C
3	A	1375	A
3	A	1376	G
3	A	1380	U
3	A	1384	C
3	A	1388	A
3	A	1389	C
3	A	1398	A
3	A	1404	A
3	A	1407	G
3	A	1417	A
3	A	1418	U
3	A	1424	A
3	A	1425	C
3	A	1426	A
3	A	1427	G
3	A	1431	G
3	A	1434	A

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Mol	Chain	Res	Type
3	A	1435	U
3	A	1436	U
3	A	1442	A
3	A	1448	U
3	A	1449	C
3	A	1450	C
3	A	1457	U
3	A	1459	U
3	A	1460	G
3	A	1465	A
3	A	1472	G
3	A	1473	A
3	A	1474	C
3	A	1475	G
3	A	1476	C
3	A	1481	G
3	A	1489	U
3	A	1490	A
3	A	1499	A
3	A	1500	U
3	A	1501	U
3	A	1502	G
3	A	1505	U
3	A	1506	A
3	A	1507	U
3	A	1508	C
3	A	1516	A
3	A	1525	G
3	A	1526	G
3	A	1527	C
3	A	1528	U
3	A	1529	G
3	A	1530	G
3	A	1531	G
3	A	1532	A
3	A	1536	A
3	A	1539	C
3	A	1540	A
3	A	1542	A
3	A	1543	U
3	A	1544	C
3	A	1545	C

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Mol	Chain	Res	Type
3	A	1550	C
3	A	1551	C
3	A	1552	C
3	A	1553	A
3	A	1555	A
3	A	1558	G
3	A	1559	C
3	A	1560	U
3	A	1561	G
3	A	1566	G
3	A	1568	G
3	A	1569	A
3	A	1570	U
3	A	1571	G
3	A	1577	C
3	A	1595	U
3	A	1601	A
3	A	1602	U
3	A	1603	U
3	A	1608	A
3	A	1614	A
3	A	1617	A
3	A	1626	U
3	A	1631	A
3	A	1632	G
3	A	1647	U
3	A	1652	C
3	A	1653	A
3	A	1655	A
3	A	1656	C
3	A	1661	A
3	A	1672	A
3	A	1679	A
3	A	1684	U
3	A	1685	A
3	A	1692	U
3	A	1693	C
3	A	1694	G
3	A	1696	G
3	A	1697	A
3	A	1699	A
3	A	1705	C

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Mol	Chain	Res	Type
3	A	1708	U
3	A	1710	A
3	A	1719	G
3	A	1720	C
3	A	1738	U
3	A	1743	A
3	A	1744	G
3	A	1745	A
3	A	1748	G
3	A	1756	U
3	A	1757	G
3	A	1758	U
3	A	1759	U
3	A	1760	A
3	A	1762	G
3	A	1766	C
3	A	1767	A
3	A	1768	A
3	A	1770	C
3	A	1771	C
3	A	1772	C
3	A	1776	A
3	A	1777	G
3	A	1778	A
3	A	1779	G
3	A	1780	C
3	A	1782	G
3	A	1783	C
3	A	1784	A
3	A	1785	G
3	A	1792	G
3	A	1793	G
3	A	1802	A
3	A	1810	G
3	A	1811	C
3	A	1812	A
3	A	1814	A
3	A	1815	A
3	A	1816	A
3	A	1817	C
3	A	1820	A
3	A	1829	C

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Mol	Chain	Res	Type
3	A	1830	G
3	A	1845	A
3	A	1846	G
3	A	1858	A
3	A	1862	C
3	A	1864	G
3	A	1865	C
3	A	1872	C
3	A	1877	A
3	A	1882	A
3	A	1883	A
3	A	1884	G
3	A	1885	A
3	A	1886	G
3	A	1887	G
3	A	1889	G
3	A	1891	G
3	A	1898	G
3	A	1899	U
3	A	1904	G
3	A	1905	A
3	A	1930	A
3	A	1935	G
3	A	1937	C
3	A	1953	C
3	A	1956	A
3	A	1958	G
3	A	1959	G
3	A	1960	U
3	A	1965	A
3	A	1967	A
3	A	1968	U
3	A	1969	U
3	A	1970	C
3	A	1972	U
3	A	1973	U
3	A	1974	G
3	A	1981	A
3	A	1984	U
3	A	1989	A
3	A	1993	G
3	A	1996	C

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Mol	Chain	Res	Type
3	A	1999	A
3	A	2000	A
3	A	2001	G
3	A	2002	G
3	A	2020	U
3	A	2021	G
3	A	2022	U
3	A	2025	C
3	A	2026	A
3	A	2033	G
3	A	2049	A
3	A	2051	U
3	A	2052	A
3	A	2054	C
3	A	2059	A
3	A	2060	A
3	A	2061	G
3	A	2062	A
3	A	2064	G
3	A	2065	C
3	A	2072	C
3	A	2080	A
3	A	2081	G
3	A	2084	C
3	A	2085	G
3	A	2089	A
3	A	2090	G
3	A	2097	U
3	A	2098	G
3	A	2109	G
3	A	2119	A
3	A	2121	U
3	A	2123	A
3	A	2125	U
3	A	2128	U
3	A	2129	G
3	A	2219	G
3	A	2227	A
3	A	2228	A
3	A	2232	G
3	A	2233	C
3	A	2240	U

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Mol	Chain	Res	Type
3	A	2241	A
3	A	2245	G
3	A	2246	G
3	A	2249	G
3	A	2252	A
3	A	2254	A
3	A	2255	C
3	A	2267	G
3	A	2268	G
3	A	2275	G
3	A	2280	G
3	A	2296	A
3	A	2297	A
3	A	2307	A
3	A	2308	G
3	A	2311	G
3	A	2312	C
3	A	2314	C
3	A	2315	A
3	A	2316	A
3	A	2317	A
3	A	2319	G
3	A	2325	U
3	A	2333	G
3	A	2334	U
3	A	2335	U
3	A	2336	G
3	A	2337	G
3	A	2338	A
3	A	2340	A
3	A	2341	U
3	A	2342	C
3	A	2343	A
3	A	2345	U
3	A	2347	G
3	A	2349	A
3	A	2350	G
3	A	2351	A
3	A	2354	G
3	A	2356	A
3	A	2360	G
3	A	2363	C

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Mol	Chain	Res	Type
3	A	2364	A
3	A	2374	G
3	A	2379	C
3	A	2383	A
3	A	2387	A
3	A	2400	G
3	A	2401	G
3	A	2412	G
3	A	2414	C
3	A	2415	U
3	A	2417	A
3	A	2420	G
3	A	2421	A
3	A	2425	G
3	A	2430	U
3	A	2431	U
3	A	2435	C
3	A	2445	C
3	A	2451	C
3	A	2452	U
3	A	2453	C
3	A	2454	A
3	A	2455	A
3	A	2457	G
3	A	2458	G
3	A	2459	A
3	A	2463	A
3	A	2464	A
3	A	2468	A
3	A	2469	C
3	A	2470	C
3	A	2474	G
3	A	2476	G
3	A	2477	A
3	A	2479	A
3	A	2499	G
3	A	2505	A
3	A	2507	A
3	A	2509	C
3	A	2516	G
3	A	2520	U
3	A	2526	A

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Mol	Chain	Res	Type
3	A	2527	C
3	A	2530	C
3	A	2531	G
3	A	2532	A
3	A	2533	U
3	A	2534	G
3	A	2542	A
3	A	2547	A
3	A	2549	C
3	A	2558	G
3	A	2560	A
3	A	2564	G
3	A	2570	A
3	A	2583	U
3	A	2591	U
3	A	2593	A
3	A	2595	A
3	A	2596	G
3	A	2598	G
3	A	2601	A
3	A	2602	C
3	A	2606	A
3	A	2607	G
3	A	2613	U
3	A	2614	U
3	A	2617	G
3	A	2628	G
3	A	2631	A
3	A	2632	G
3	A	2635	C
3	A	2638	U
3	A	2639	C
3	A	2642	U
3	A	2643	A
3	A	2644	U
3	A	2661	A
3	A	2662	A
3	A	2665	U
3	A	2674	G
3	A	2685	U
3	A	2689	A
3	A	2696	C

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Mol	Chain	Res	Type
3	A	2711	G
3	A	2714	G
3	A	2718	U
3	A	2719	A
3	A	2720	C
3	A	2736	G
3	A	2741	U
3	A	2743	G
3	A	2747	G
3	A	2755	U
3	A	2762	A
3	A	2764	G
3	A	2765	G
3	A	2766	G
3	A	2768	U
3	A	2773	G
3	A	2784	C
3	A	2785	U
3	A	2786	A
3	A	2789	C
3	A	2793	A
3	A	2794	A
3	A	2800	C
3	A	2806	G
3	A	2807	A
3	A	2808	U
3	A	2818	C
3	A	2820	U
3	A	2823	C
3	A	2824	G
3	A	2826	A
3	A	2831	A
3	A	2833	U
3	A	2843	G
3	A	2849	U
3	A	2855	G
3	A	2858	U
3	A	2859	G
3	A	2860	A
3	A	2868	G
3	A	2873	G
3	A	2874	G

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Mol	Chain	Res	Type
3	A	2891	G
3	A	2892	G
3	A	2897	G
3	A	2899	C
3	A	2900	A
3	A	2901	G
3	A	2902	A
3	A	2905	C
3	A	2911	G
3	A	2916	A
3	A	2917	G
3	A	2925	C
4	B	7	G
4	B	10	G
4	B	11	A
4	B	13	A
4	B	15	C
4	B	19	G
4	B	22	G
4	B	23	U
4	B	24	C
4	B	32	U
4	B	33	U
4	B	35	C
4	B	37	A
4	B	38	U
4	B	39	A
4	B	40	C
4	B	42	G
4	B	44	A
4	B	48	G
4	B	49	G
4	B	50	A
4	B	51	A
4	B	53	U
4	B	54	U
4	B	55	A
4	B	59	U
4	B	60	C
4	B	62	U
4	B	63	C
4	B	85	U

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Mol	Chain	Res	Type
4	B	86	U
4	B	87	U
4	B	88	C
4	B	97	A
4	B	101	U
4	B	107	G
4	B	108	C
4	B	110	G

All (69) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	2	36	C
3	A	13	A
3	A	62	C
3	A	88	G
3	A	92	G
3	A	125	A
3	A	175	G
3	A	224	A
3	A	252	C
3	A	347	G
3	A	410	G
3	A	411	G
3	A	443	G
3	A	528	G
3	A	549	A
3	A	554	U
3	A	558	G
3	A	689	A
3	A	831	U
3	A	976	U
3	A	1036	A
3	A	1066	A
3	A	1172	A
3	A	1243	A
3	A	1250	G
3	A	1305	A
3	A	1339	A
3	A	1351	U
3	A	1397	G
3	A	1406	A

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Mol	Chain	Res	Type
3	A	1448	U
3	A	1464	A
3	A	1507	U
3	A	1525	G
3	A	1530	G
3	A	1565	U
3	A	1570	U
3	A	1631	A
3	A	1671	G
3	A	1691	A
3	A	1757	G
3	A	1758	U
3	A	1784	A
3	A	1813	A
3	A	1828	G
3	A	1882	A
3	A	1883	A
3	A	1884	G
3	A	1886	G
3	A	2127	U
3	A	2226	U
3	A	2254	A
3	A	2295	A
3	A	2316	A
3	A	2337	G
3	A	2420	G
3	A	2452	U
3	A	2454	A
3	A	2468	A
3	A	2631	A
3	A	2740	A
3	A	2784	C
3	A	2805	A
3	A	2848	A
3	A	2898	A
3	A	2904	A
4	B	31	G
4	B	48	G
4	B	49	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

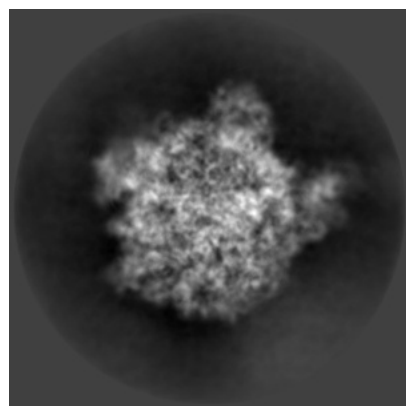
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11890. These allow visual inspection of the internal detail of the map and identification of artifacts.

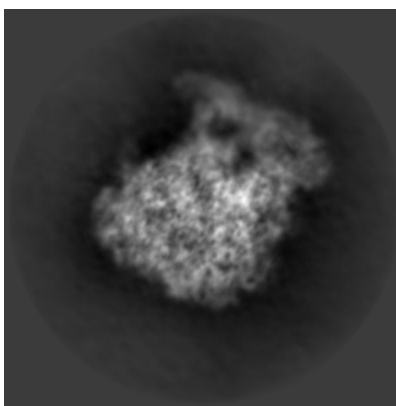
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

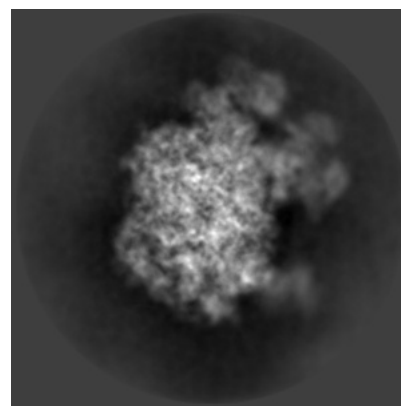
6.1.1 Primary map



X

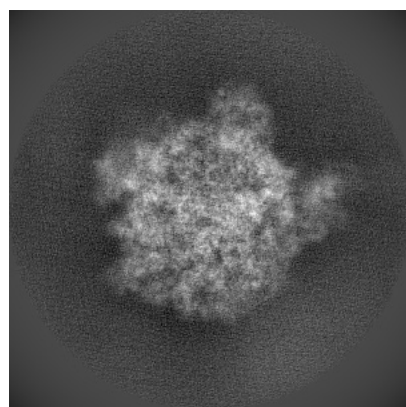


Y

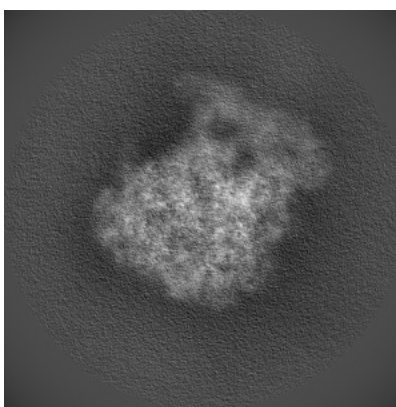


Z

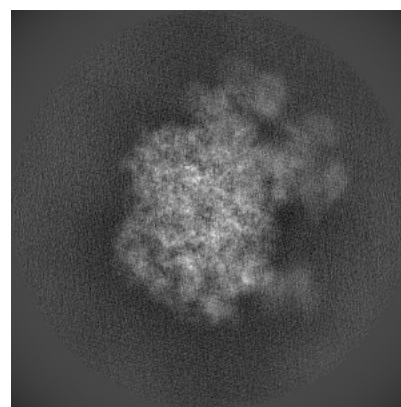
6.1.2 Raw map



X



Y

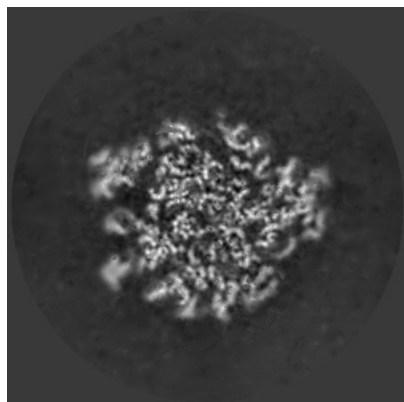


Z

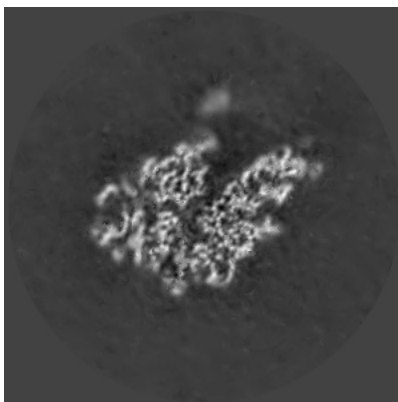
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

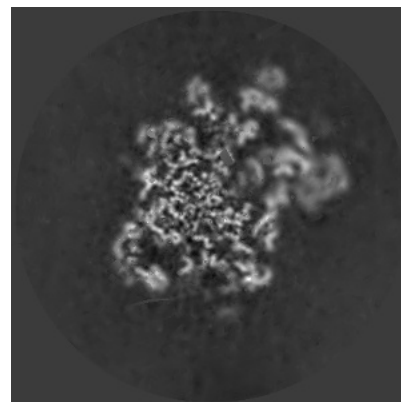
6.2.1 Primary map



X Index: 210

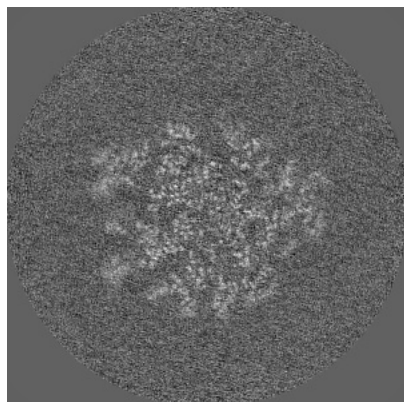


Y Index: 210

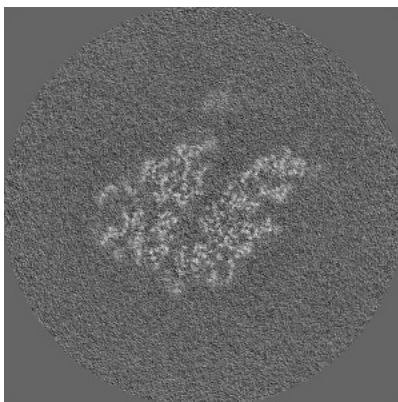


Z Index: 210

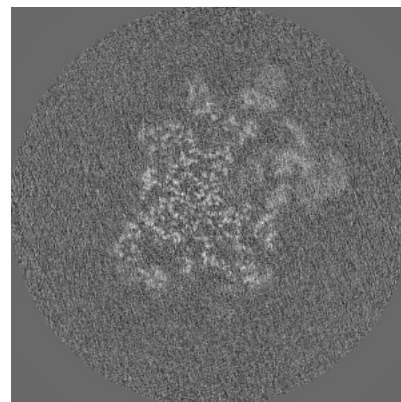
6.2.2 Raw map



X Index: 210



Y Index: 210

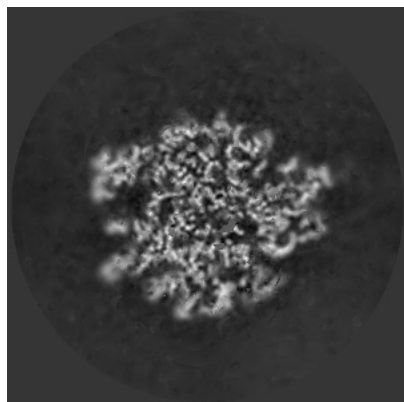


Z Index: 210

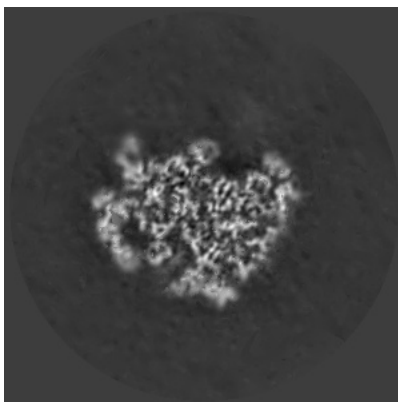
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

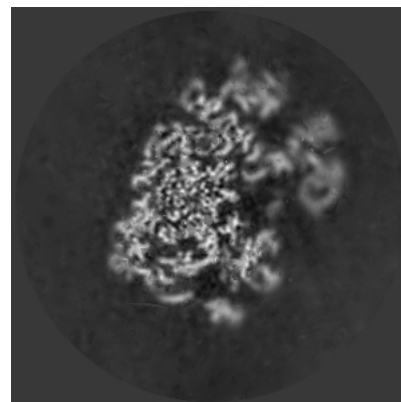
6.3.1 Primary map



X Index: 215

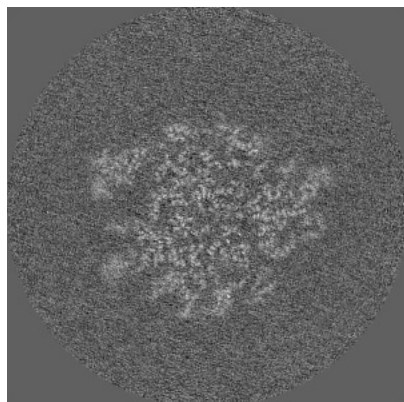


Y Index: 185

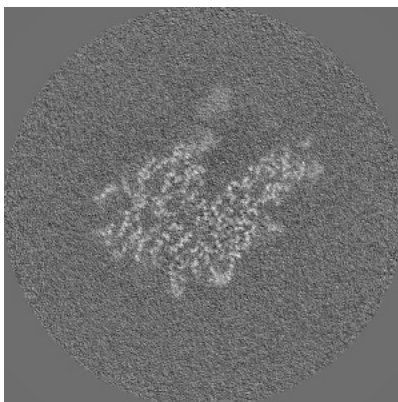


Z Index: 222

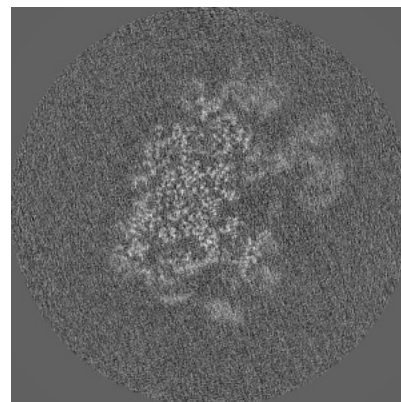
6.3.2 Raw map



X Index: 213



Y Index: 213

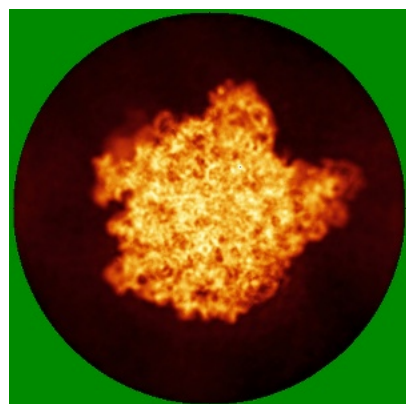


Z Index: 222

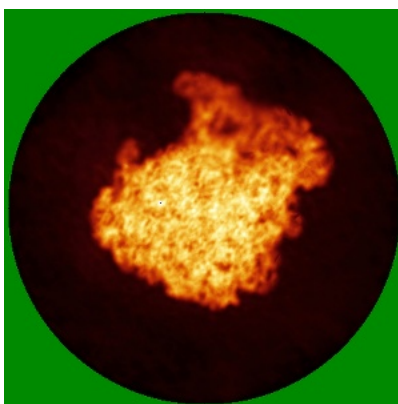
The images above show the largest variance slices of the map in three orthogonal directions.

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

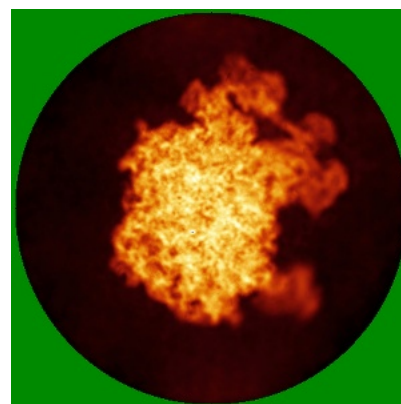
6.4.1 Primary map



X

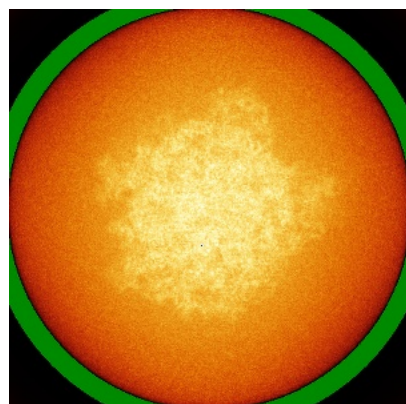


Y

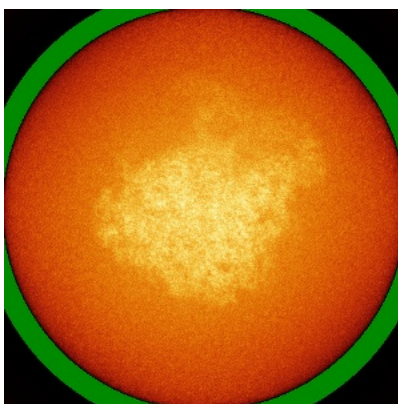


Z

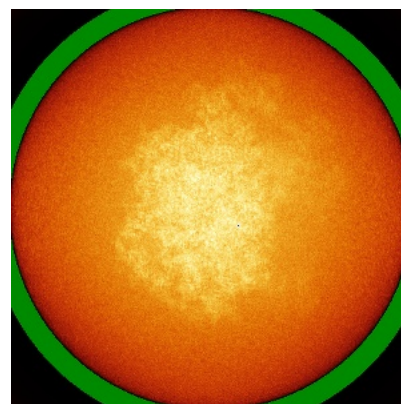
6.4.2 Raw map



X



Y

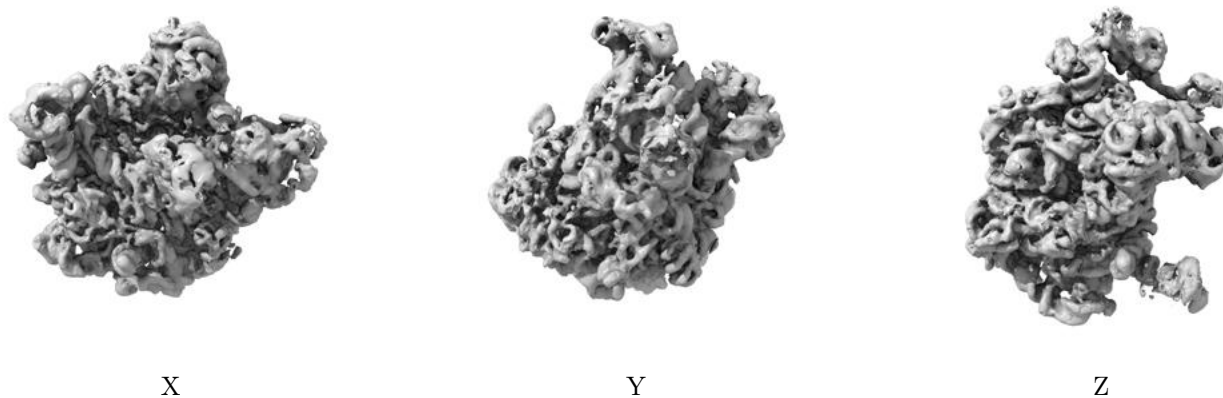


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

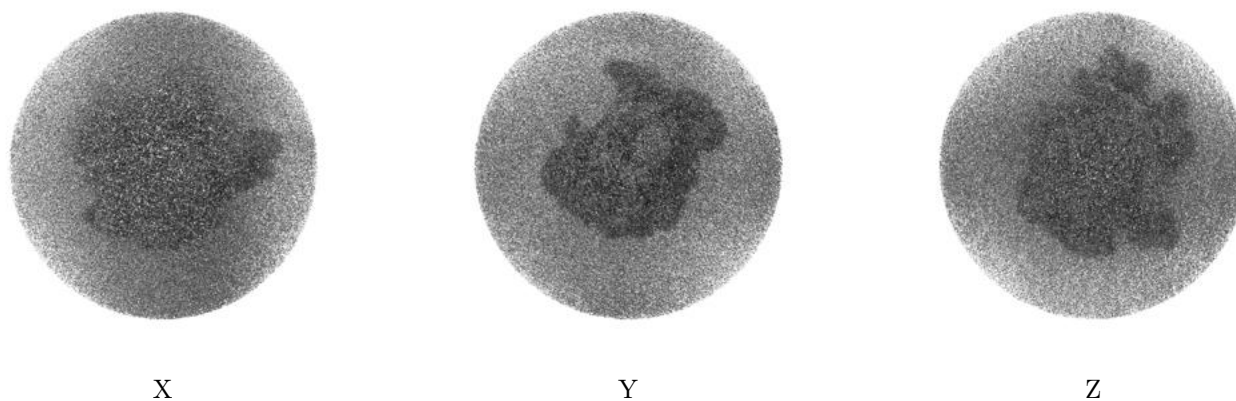
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.007. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

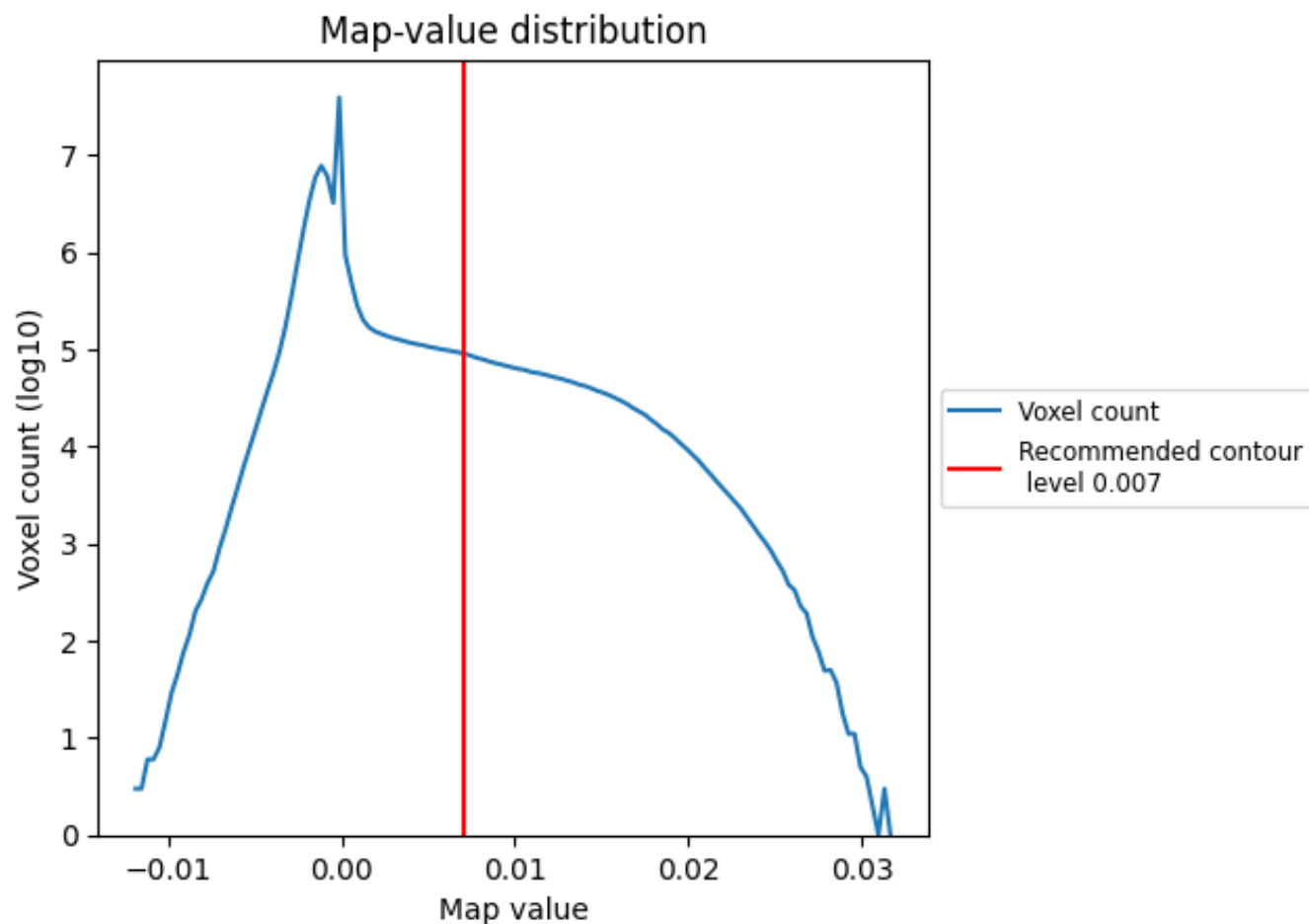
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

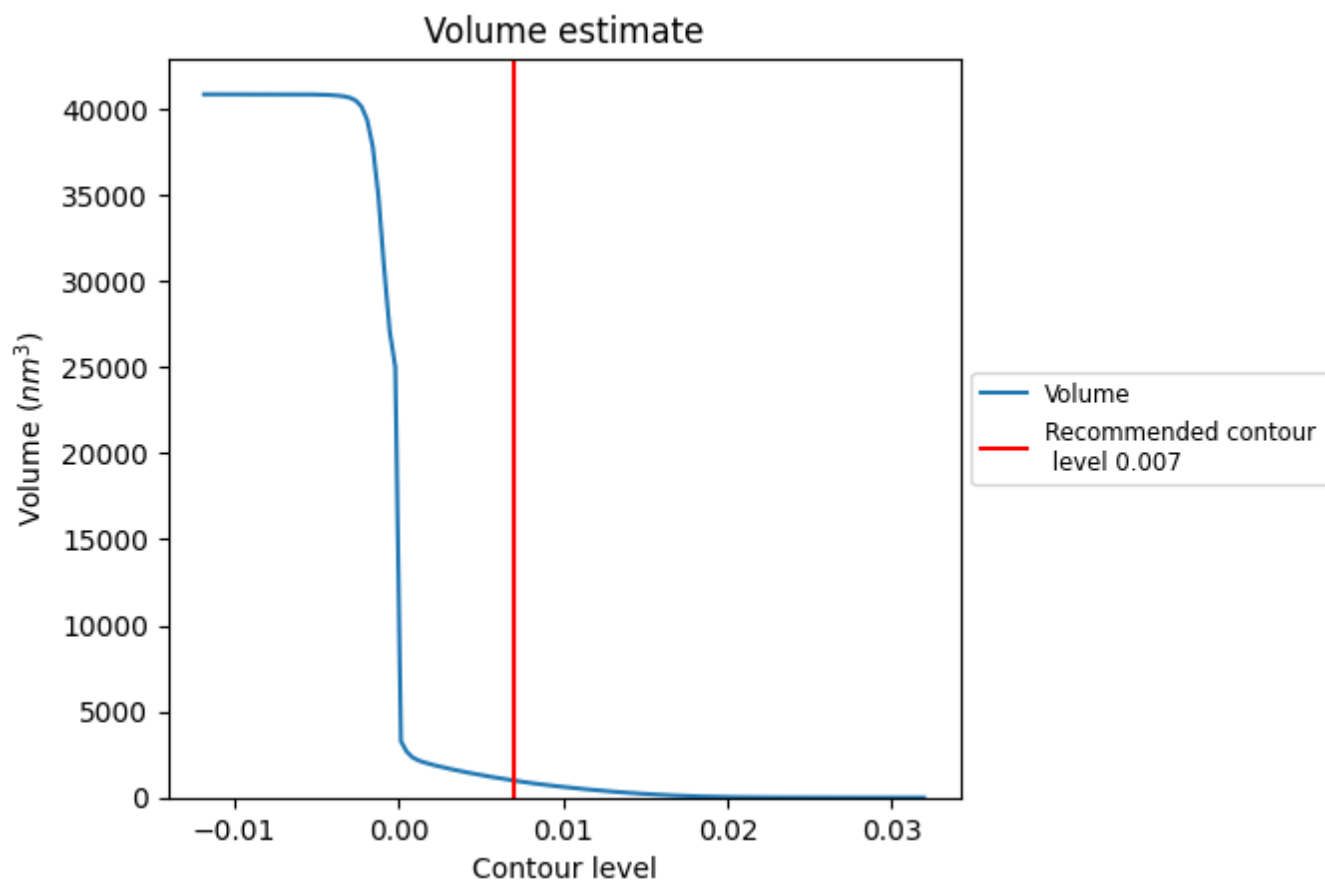
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

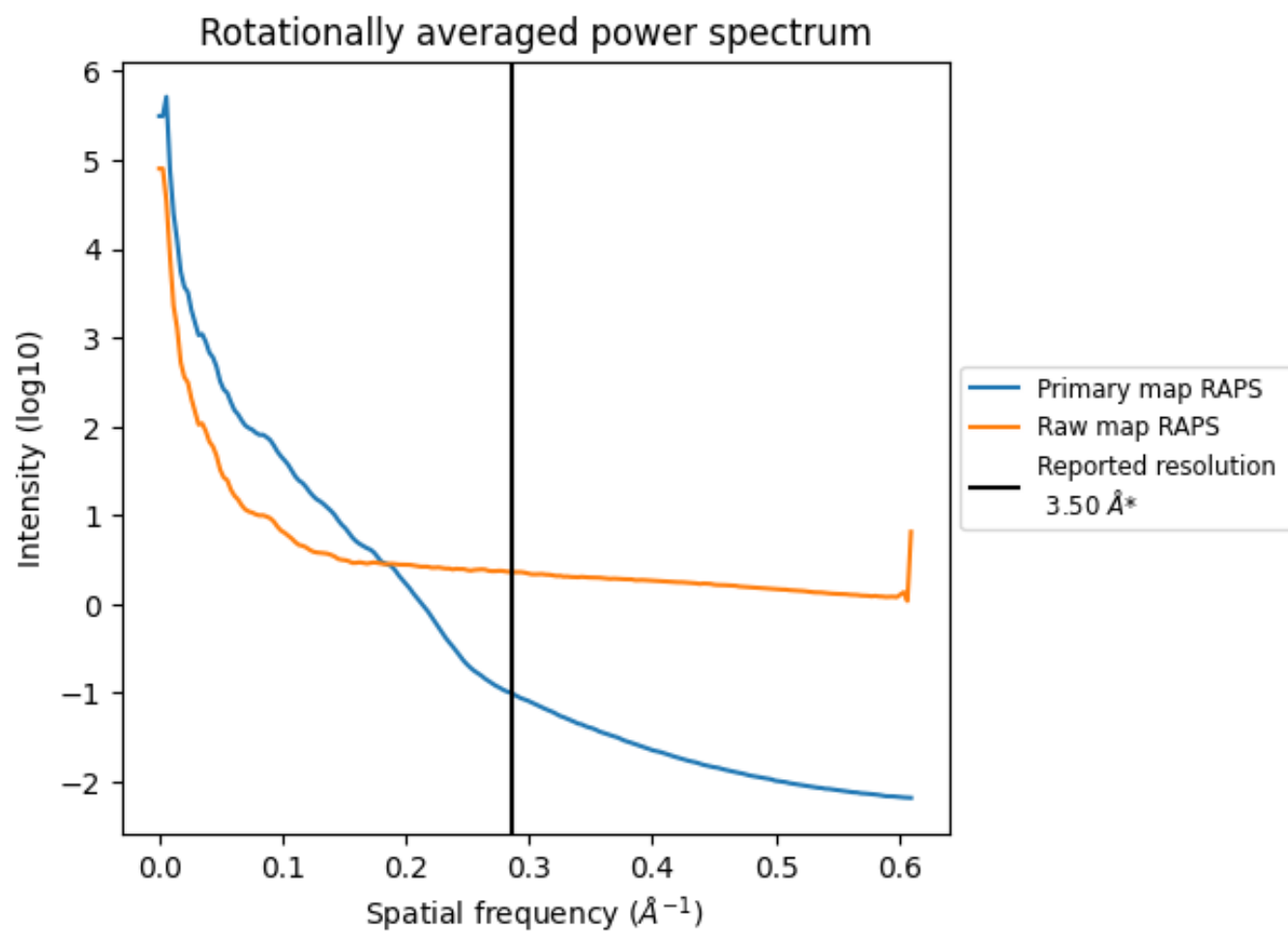
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 990 nm^3 ; this corresponds to an approximate mass of 894 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

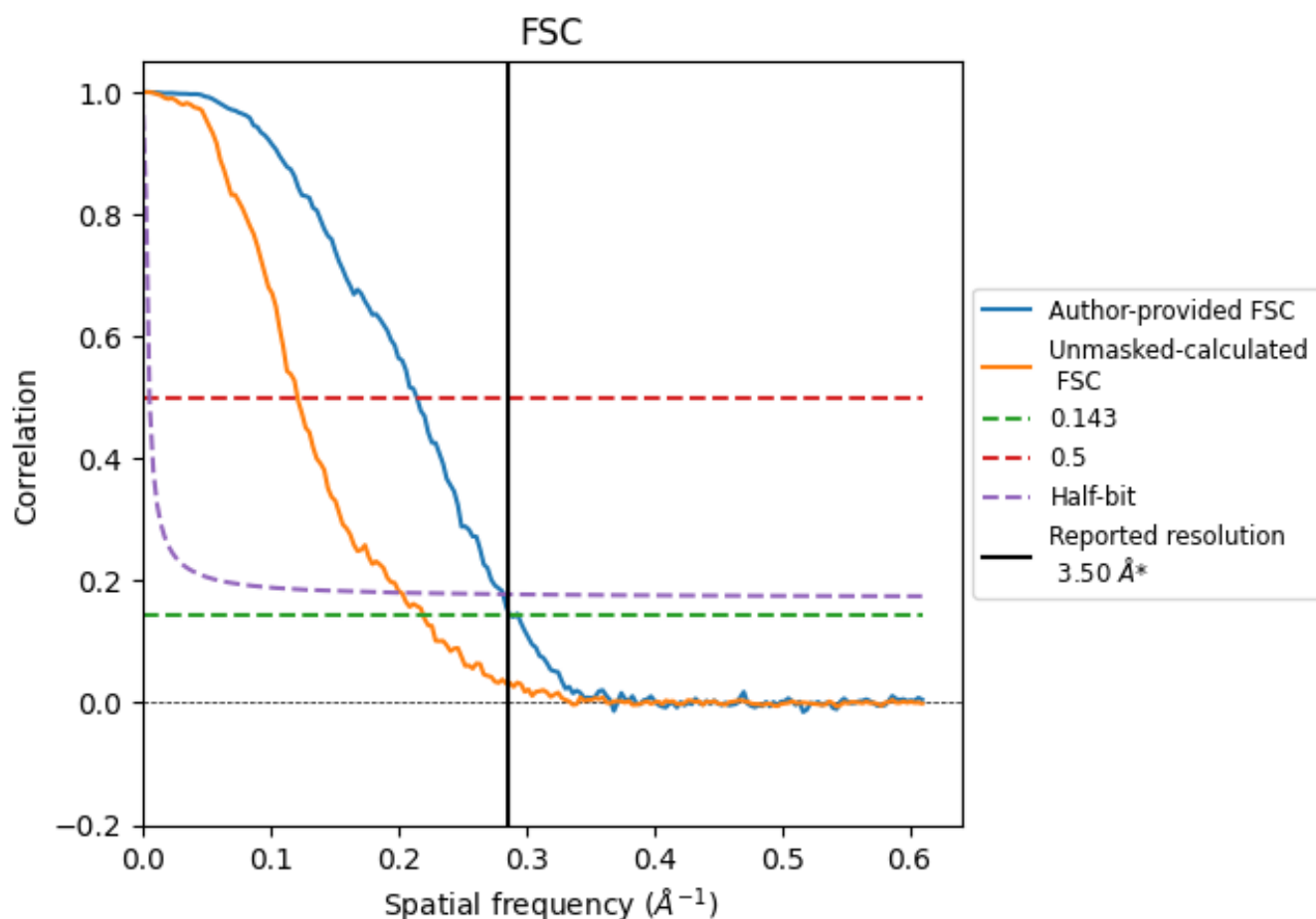


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

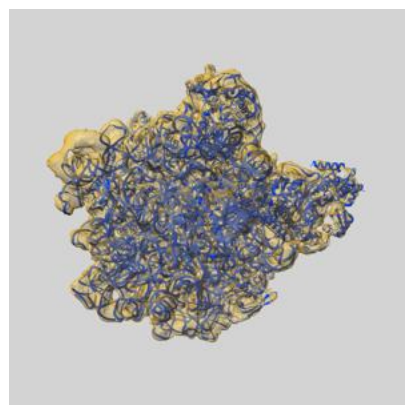
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.48	4.66	3.54
Unmasked-calculated*	4.55	8.24	4.94

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.55 differs from the reported value 3.5 by more than 10 %

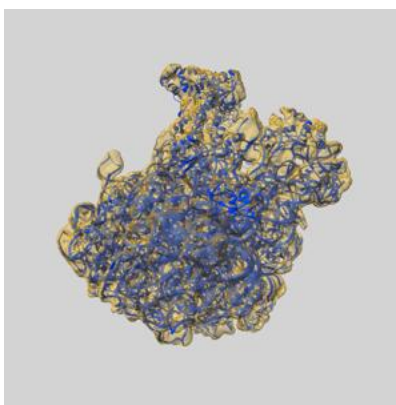
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11890 and PDB model 7AS9. Per-residue inclusion information can be found in section [3](#) on page [11](#).

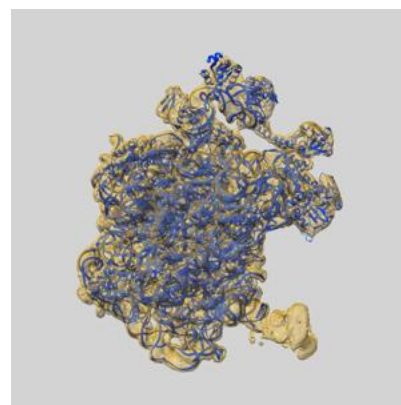
9.1 Map-model overlay [i](#)



X



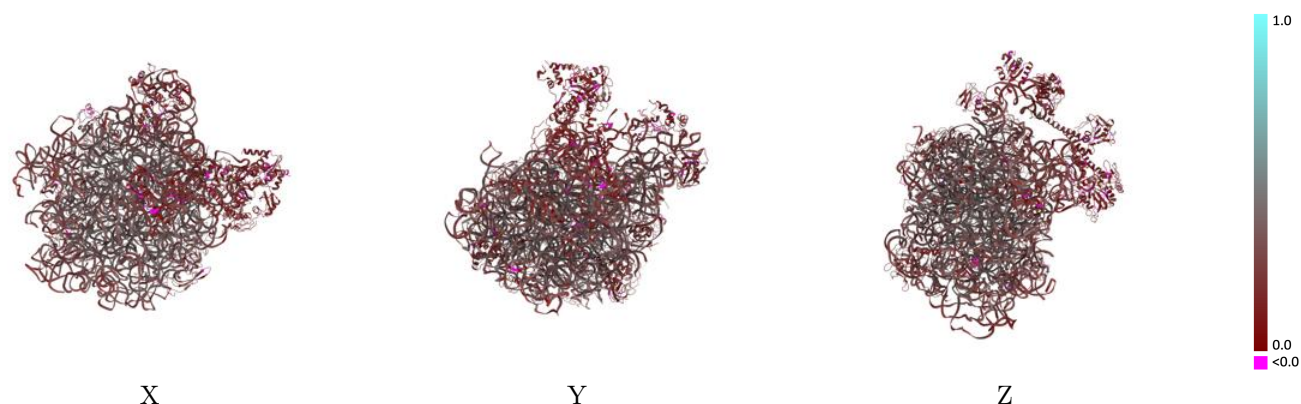
Y



Z

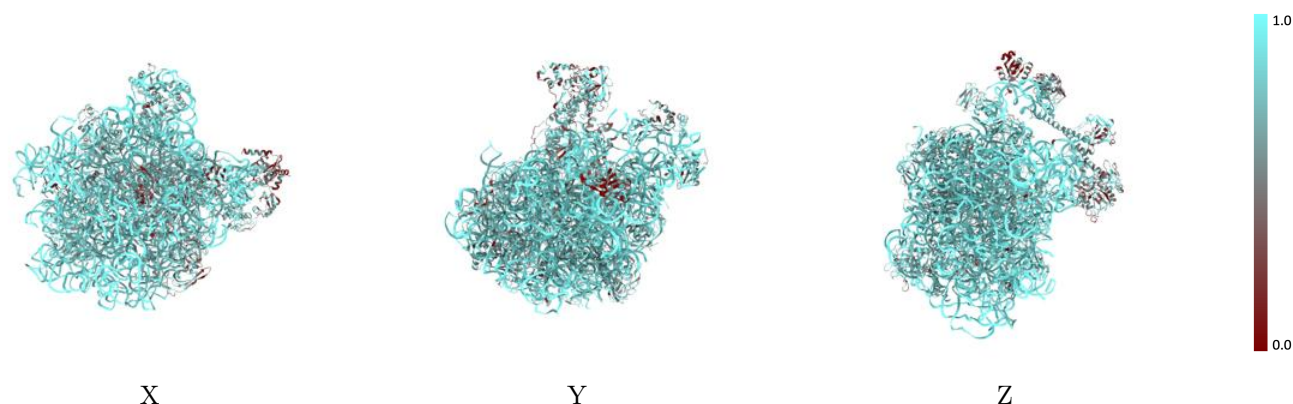
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



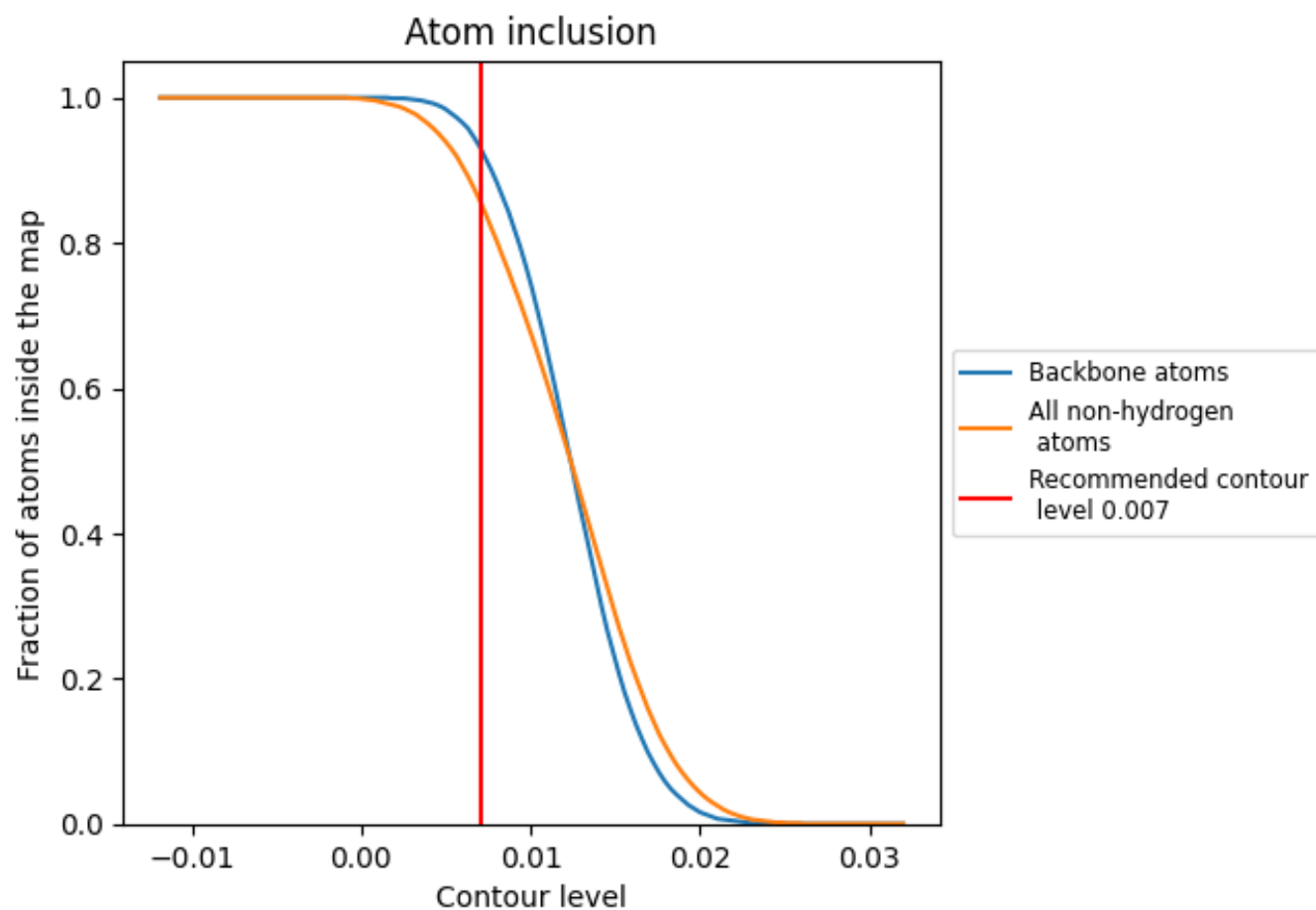
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.007).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 86% 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 (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8580	 0.3000
0	 0.5820	 0.1600
2	 0.8500	 0.2330
A	 0.9460	 0.3290
B	 0.9630	 0.2840
E	 0.7590	 0.2980
F	 0.6640	 0.2830
G	 0.6970	 0.2730
H	 0.6790	 0.1650
I	 0.7280	 0.1940
K	 0.5450	 0.1620
L	 0.2930	 0.1650
N	 0.7420	 0.2910
O	 0.6300	 0.2690
P	 0.6870	 0.2870
Q	 0.6930	 0.2730
R	 0.7090	 0.2540
S	 0.7060	 0.1930
T	 0.5920	 0.2520
U	 0.7460	 0.2940
V	 0.7060	 0.2790
W	 0.7290	 0.3070
X	 0.6720	 0.2840
Y	 0.7140	 0.2330
a	 0.7500	 0.3100
b	 0.2760	 0.2300
c	 0.6650	 0.2000
d	 0.7330	 0.2600
f	 0.7480	 0.3210
g	 0.7440	 0.2510
h	 0.6990	 0.3550
i	 0.7030	 0.3580
j	 0.6930	 0.2950

