



Full wwPDB EM Validation Report ⓘ

Jun 23, 2026 – 03:09 PM JST

PDB ID : 8J1Z / pdb_00008j1z
EMDB ID : EMD-35939
Title : The global structure of pre50S related to DbpA in state3
Authors : Yu, T.; Zeng, F.
Deposited on : 2023-04-13
Resolution : 2.60 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

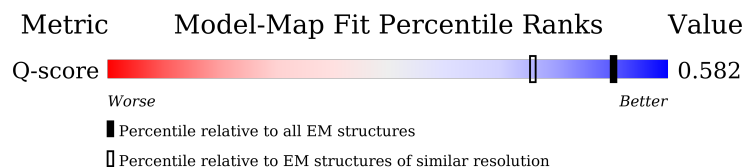
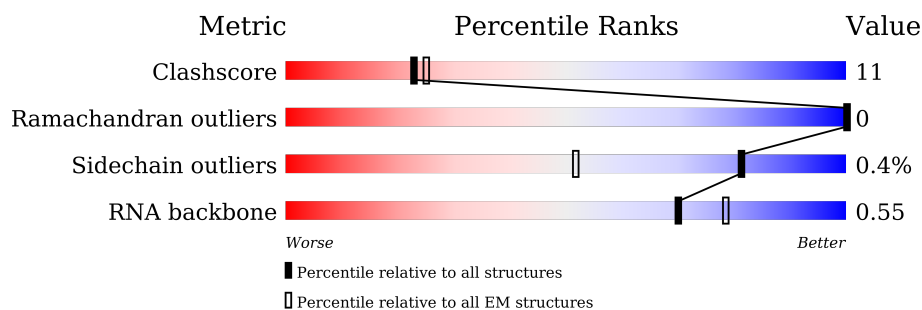
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

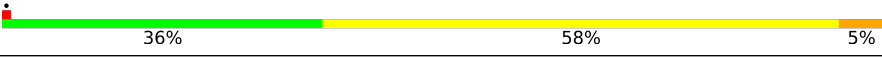
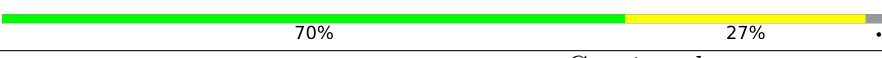
The reported resolution of this entry is 2.60 Å.

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.



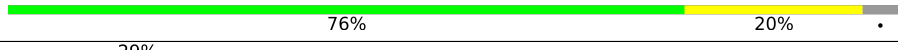
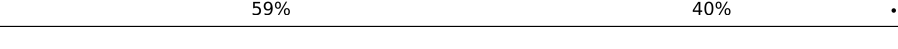
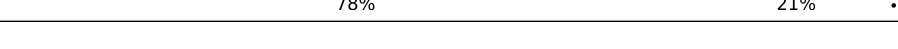
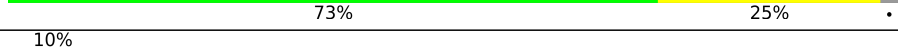
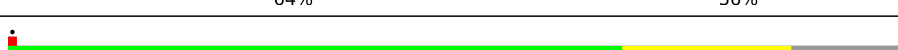
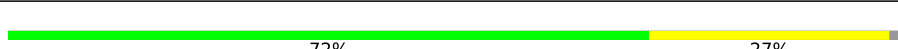
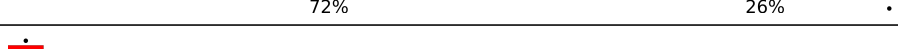
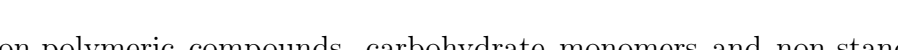
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	8728 (2.10 - 3.10)

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

Mol	Chain	Length	Quality of chain
1	a	2904	
2	b	120	
3	c	273	

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Mol	Chain	Length	Quality of chain
4	d	209	
5	e	201	
6	f	179	
7	i	142	
8	j	123	
9	k	144	
10	m	127	
11	n	117	
12	o	115	
13	p	118	
14	q	103	
15	r	110	
16	s	100	
17	t	104	
18	u	94	
19	v	85	
20	w	78	
21	x	63	
22	y	59	
23	z	57	
24	0	55	
25	1	46	
26	2	65	
27	h	149	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	G7M	a	2069	X	-	-	-

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 79520 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	2513	Total	C	N	O	P	0	0
			54003	24093	9979	17418	2513		

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	119	Total	C	N	O	P	0	0
			2549	1135	466	829	119		

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	265	Total	C	N	O	S	0	0
			2035	1260	413	355	7		

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	186	Total	C	N	O	S	0	0
			1397	882	253	258	4		

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	193	Total	C	N	O	S	0	0
			1483	932	266	280	5		

- Molecule 6 is a protein called 50S ribosomal protein L5.

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

- Molecule 7 is a protein called 50S ribosomal protein L13.

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

- Molecule 8 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	j	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 9 is a protein called 50S ribosomal protein L15.

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

- Molecule 10 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	m	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 11 is a protein called 50S ribosomal protein L18.

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

- Molecule 12 is a protein called 50S ribosomal protein L19.

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

- Molecule 13 is a protein called 50S ribosomal protein L20.

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

- Molecule 14 is a protein called 50S ribosomal protein L21.

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

- Molecule 15 is a protein called 50S ribosomal protein L22.

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

- Molecule 16 is a protein called 50S ribosomal protein L23.

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

- Molecule 17 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	t	102	Total	C	N	O	S	0	0
			779	492	146	141			

- Molecule 18 is a protein called 50S ribosomal protein L25.

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

- Molecule 19 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	v	75	Total	C	N	O	S	0	0
			569	353	113	102	1		

- Molecule 20 is a protein called 50S ribosomal protein L28.

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

- Molecule 21 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	x	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 22 is a protein called 50S ribosomal protein L30.

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

- Molecule 23 is a protein called 50S ribosomal protein L32.

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

- Molecule 24 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	0	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 25 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 26 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 27 is a protein called 50S ribosomal protein L9.

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

- Molecule 28 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
28	a	202	Total 202	Mg 202	0
28	b	5	Total 5	Mg 5	0
28	c	1	Total 1	Mg 1	0
28	p	1	Total 1	Mg 1	0
28	z	1	Total 1	Mg 1	0

- Molecule 29 is water.

Mol	Chain	Residues	Atoms		AltConf
29	a	137	Total 137	O 137	0
29	b	117	Total 117	O 117	0
29	c	63	Total 63	O 63	0
29	d	17	Total 17	O 17	0
29	e	22	Total 22	O 22	0
29	f	22	Total 22	O 22	0
29	i	13	Total 13	O 13	0
29	j	14	Total 14	O 14	0
29	k	28	Total 28	O 28	0
29	m	28	Total 28	O 28	0
29	n	34	Total 34	O 34	0
29	o	9	Total 9	O 9	0
29	p	22	Total 22	O 22	0
29	q	17	Total 17	O 17	0
29	r	15	Total 15	O 15	0

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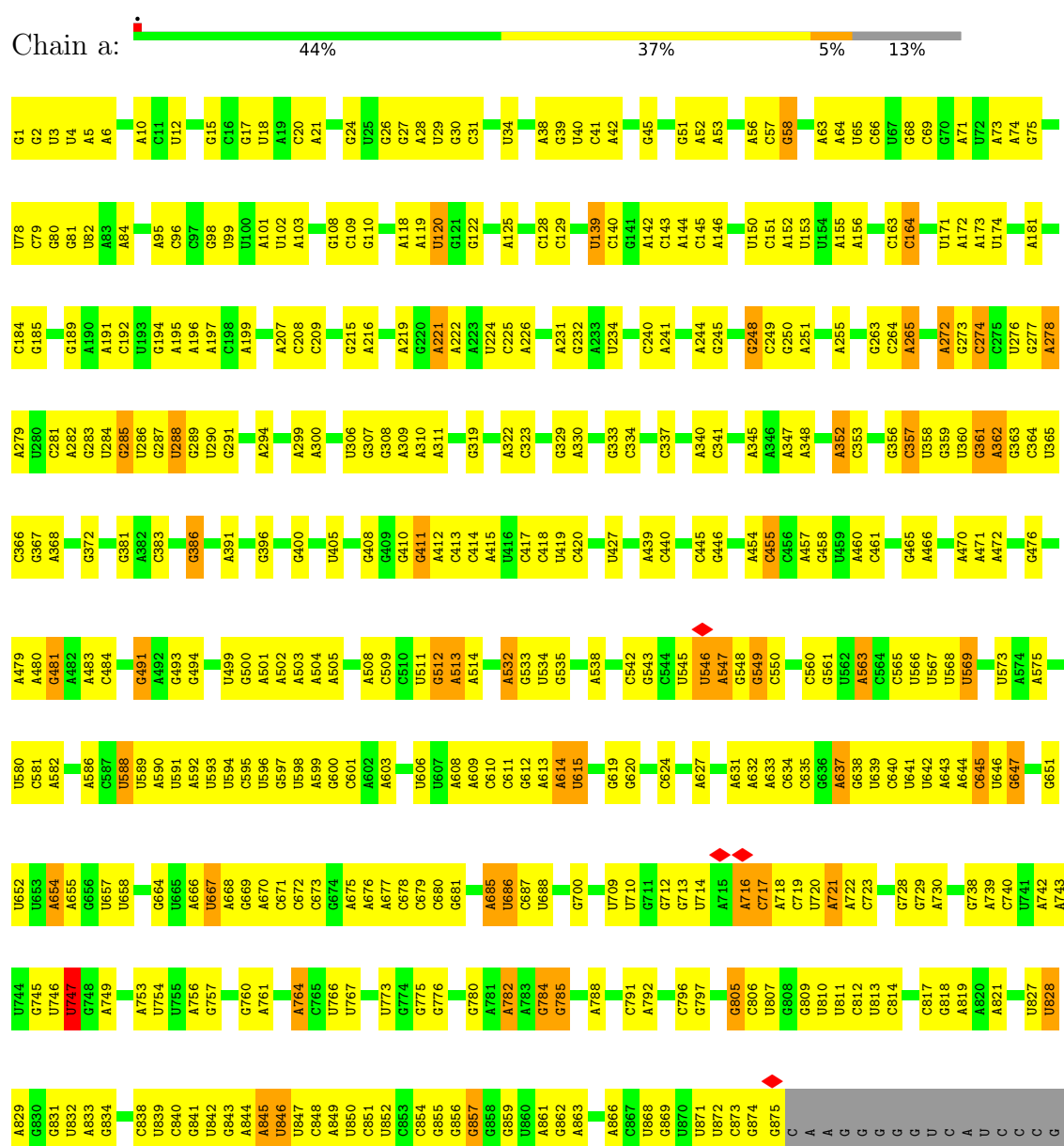
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Mol	Chain	Residues	Atoms		AltConf
29	s	6	Total 6	O 6	0
29	t	2	Total 2	O 2	0
29	u	2	Total 2	O 2	0
29	v	12	Total 12	O 12	0
29	w	15	Total 15	O 15	0
29	y	6	Total 6	O 6	0
29	z	17	Total 17	O 17	0
29	0	6	Total 6	O 6	0
29	1	25	Total 25	O 25	0
29	2	15	Total 15	O 15	0

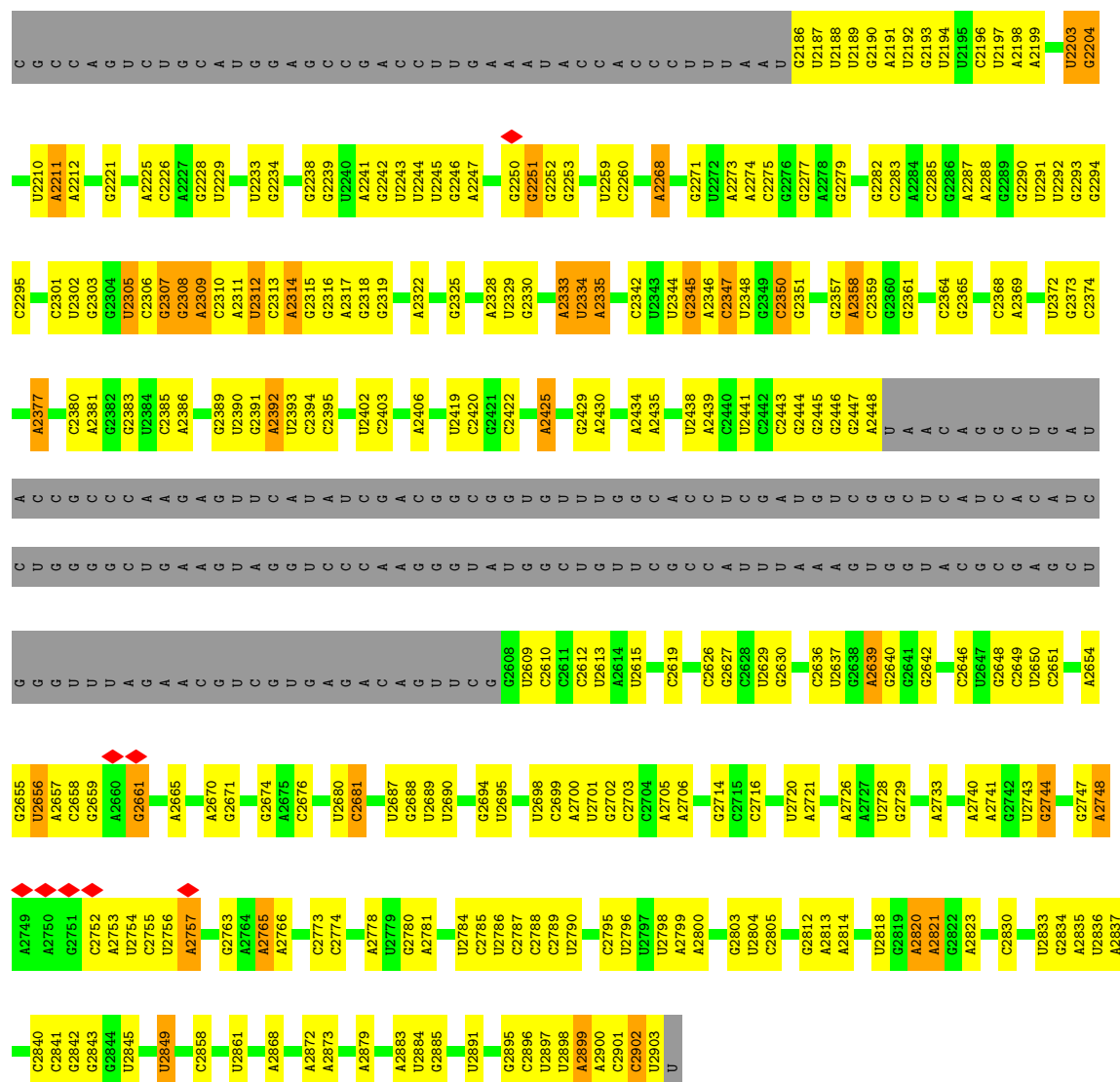
3 Residue-property plots [i](#)

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

• Molecule 1: 23S rRNA

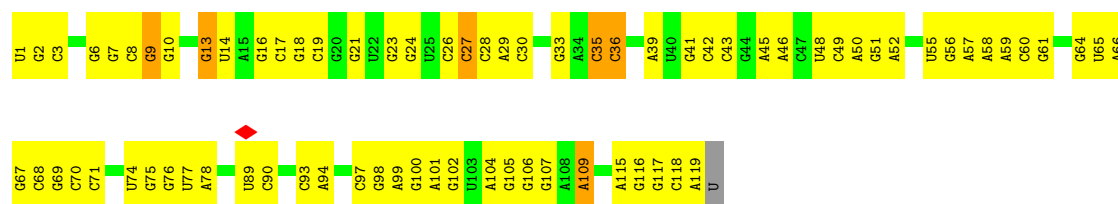


U2081	A2005	C1925	G1840	U1758	G1659	U1484	A1387	C1290	G1190	C	C	G986	A
A2082	C2006	U1926	U1841	A1759	A1664	U1485	A1392	C1291	G1191	U	C	U967	C
G2083	G2012	A1927	G1842	C1760	A1664	U1486	A1393	G1292	G	G	A	C988	U
U2086	A2013	A1928	G1847	G1761	G1667	U1487	A1394	C1293	G1197	U	G	A972	A
G2087	A2014	G1929	A1846	G1762	A1668	C1483	A1395	U1294	U	C	A	A973	C
A2088	A2015	U1931	G1847	G1763	A1668	A1494	U1396	G1296	U1199	C	A	C974	C
C2091	U2016	A1932	G1850	C1764	C1574	A1495	U1396	G1296	G	A	G	A	A
U2092	U2017	G1933	U1851	G1674	C1575	A1496	A1403	G1300	A1205	G	C	A983	A
G2093	A2020	C1934	U1852	C1675	C1577	A1496	C1404	A1301	G1212	U	C	A984	A
A2095	C2023	A	U1855	A1676	A1578	A1505	U1405	C1306	G1216	G	G	C987	C
C2096	G2024	A	U1856	A1677	A1579	U1506	U1406	C1306	G1216	G	G	A988	A
A2097	U2026	U1857	U1680	A1678	A1579	C1507	G1407	C1315	G1223	C	A	G989	A
U2098	C2025	G1858	G1681	U1679	U1584	A1508	G1408	U1316	G1223	U	G	C992	C
U2099	U2026	A1859	G1682	A1679	C1585	U1509	U1409	U1317	U1224	U	G	G993	C
G2100	G2030	C	U1860	U1683	G1587	G1511	U1411	U1318	G1225	G	U	C994	C
A2101	A2031	U	G1861	C1685	U1589	C1512	G1416	C1320	G1227	U	G	A909	C
G	G2032	U	A1789	C1685	U1590	U1513	G1417	A1321	U1231	U	C	A911	C
C	A2033	G	C1790	U1688	A1591	G1514	G1418	A1328	U1232	U	C	C912	C
C	C	U	G1791	A1689	C1592	U1515	A1419	U1329	G1233	U	U	U913	C
U	A2037	C	G1792	A1690	U1593	G1519	A1420	C1330	G1235	U	U	G914	C
U	G2038	G	A1794	G1697	U1594	U1520	G1421	C1330	U1236	U	A	C915	C
G	U2039	G	U1795	G1697	C1595	G1527	A1427	G1338	G1236	U	G	G916	C
A	G2040	U	U1796	U1700	C1599	A1528	G1428	U1339	G1236	U	A	A917	C
C	C2043	U	U1797	A1700	C1600	U1529	G1429	G1340	G1239	U	A	A918	C
G	C	A	U1798	G1710	U1599	G1530	G1430	U1340	G1239	U	G	C1006	C
U	U	A	G1799	G1710	C1600	U1530	A1431	C1348	U1240	C	A	C1007	C
U	G2046	G	C1800	G1715	A1603	G1531	A1432	C1349	C1241	C	C	A1008	C
U	C2047	U	U1801	G1715	C1604	C1532	G1433	C1350	U1242	U	G	A1009	C
A	U1880	U	A1802	U1720	C1607	U1534	A1434	C1351	C1243	U	C	U0112	C
U	U1881	C	A1803	G1721	A1608	A1535	G1435	U1352	G1248	U	C	C1013	C
U	U1882	C	A1804	G1721	A1609	C1536	G1436	U1353	U1249	U	U	A1014	C
G	A2054	G	A1805	U1725	U1610	G1537	G1437	A1354	G1250	U	C	U0115	C
G	C2055	U	A1808	C1726	G1613	U1539	G1441	C1357	G1253	U	A	G1016	C
U	G2056	C	A1809	U1729	A1614	U1540	U1442	G1358	A1254	U	U	U019	C
C	C2057	U	G1810	U1729	U1618	G1541	U1443	A1359	U1255	U	U	A1020	C
U	A2058	G	U1811	C1730	A1618	U1542	G1444	G1360	G1256	A	A	A1021	C
G	A	C	G1812	G1731	A1632	U1543	G1445	G1361	G1257	A	A	U1023	C
G	G2061	A1966	G1813	C1732	G1633	A1544	C1446	C1362	G1266	A	A	G1026	C
C	A2062	C1967	C1816	G1733	A1634	A1545	C1447	C1363	U1269	G	A	A1027	C
A	C2063	U	G1816	A1735	A1635	G1546	G1448	G1364	A1269	A	A	A1028	C
G	C2064	A1970	G1824	G1738	U1636	C1547	G1452	A1365	C1270	A	A	A1029	C
G	C2065	U1971	G1825	A1739	A1637	A1549	A1453	A1367	G1271	U	A	G	C
C	C2066	G1972	U1827	G1740	A1641	U1554	U1460	C1370	A1272	U	C	A1032	C
U	G2069	G1980	G1828	G1743	G1642	U1554	U1469	G1371	G1177	G	G	U1033	C
U	A2070	A1981	A1829	A1744	U1647	C1558	A1470	U1372	C1178	U	U	G1034	C
U	A2071	U1982	C1830	G1745	U1647	U1559	A1470	A1378	U1278	A	A	U1035	C
G	C2072	G1989	G1831	A1746	U1647	G1560	U1379	U1378	G1279	U	U	G1036	C
A	C2073	C1832	C1833	A1746	U1647	U1561	U1379	U1378	U1282	A	A	G	C
G	U2074	U1990	G1834	U1747	G1649	U1562	U1379	U1378	U1283	A	A	A	C
U	U2075	U1991	G1835	C1748	A1655	U1563	U1383	A1384	G1288	U	U	A	C
C	U2076	G1992	G1836	U1748	C1656	U1564	U1481	A1385	U188	C	C	G	C
U	A2077	U1993	C1837	A1754	C1657	C1565	G1482	U1385	G1289	U	U	C	C
U	C2078	C2000	U1923	A1757	C1658	U1566	G1483	C1386					
G	U2079												
A	A2080												



• Molecule 2: 5S rRNA

Chain b: 36% 58% 5%



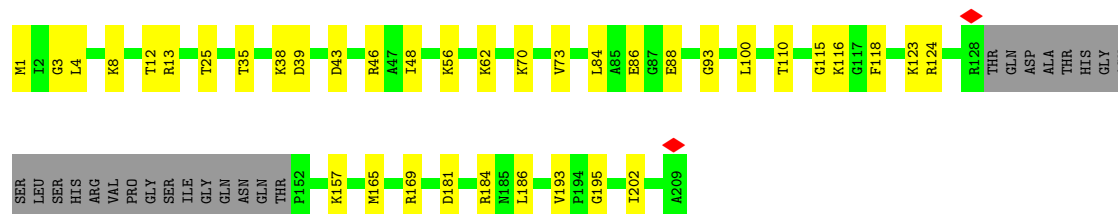
• Molecule 3: 50S ribosomal protein L2

Chain c: 70% 27%

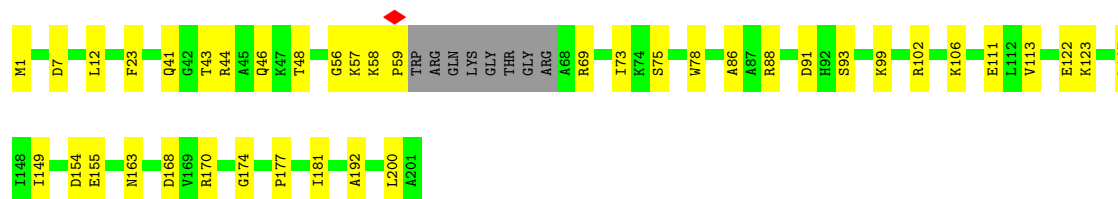
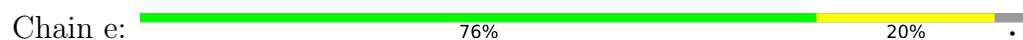




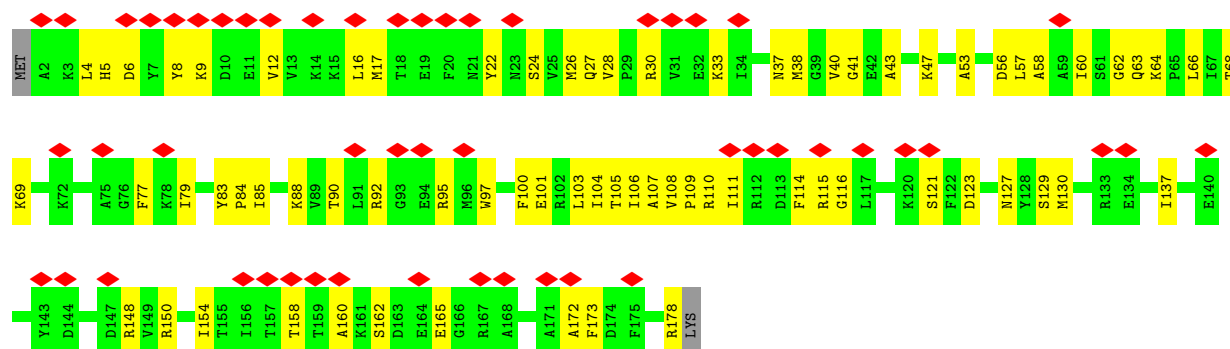
• Molecule 4: 50S ribosomal protein L3



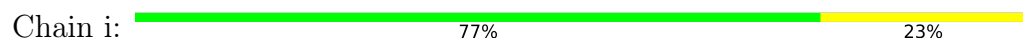
• Molecule 5: 50S ribosomal protein L4



• Molecule 6: 50S ribosomal protein L5

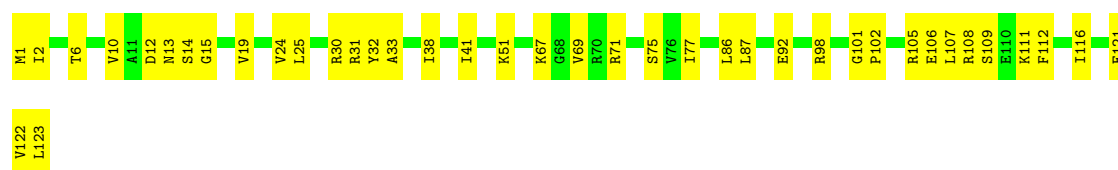


• Molecule 7: 50S ribosomal protein L13



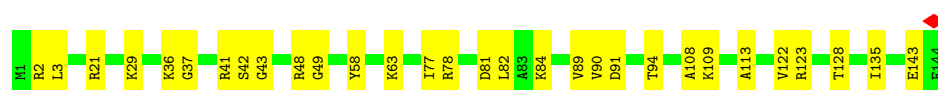
- Molecule 8: 50S ribosomal protein L14

Chain j:  67% 33%



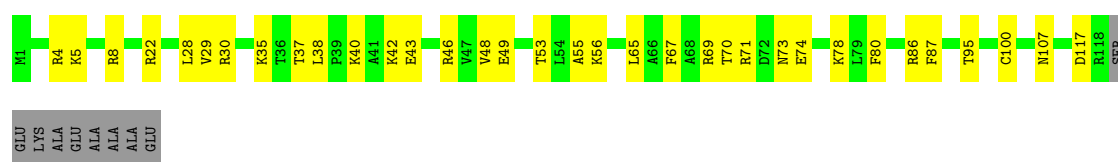
- Molecule 9: 50S ribosomal protein L15

Chain k:  79% 21%



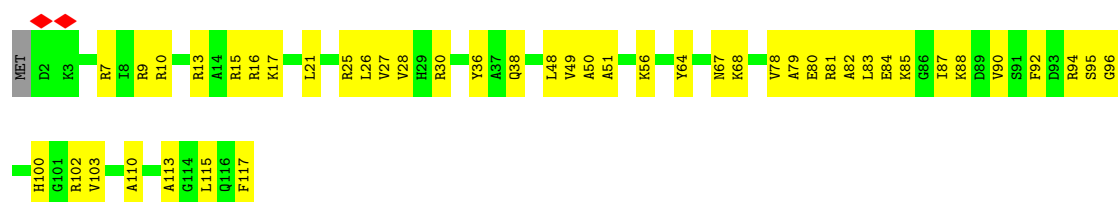
- Molecule 10: 50S ribosomal protein L17

Chain m:  66% 27% 7%



- Molecule 11: 50S ribosomal protein L18

Chain n:  60% 39%



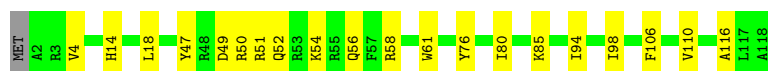
- Molecule 12: 50S ribosomal protein L19

Chain o:  78% 21%



- Molecule 13: 50S ribosomal protein L20

Chain p:  82% 17%



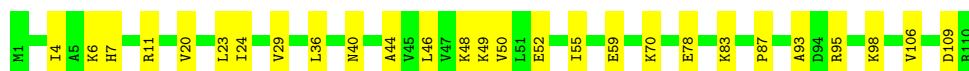
- Molecule 14: 50S ribosomal protein L21

Chain q: 85% 15%



- Molecule 15: 50S ribosomal protein L22

Chain r: 75% 25%



- Molecule 16: 50S ribosomal protein L23

Chain s: 75% 18% 7%



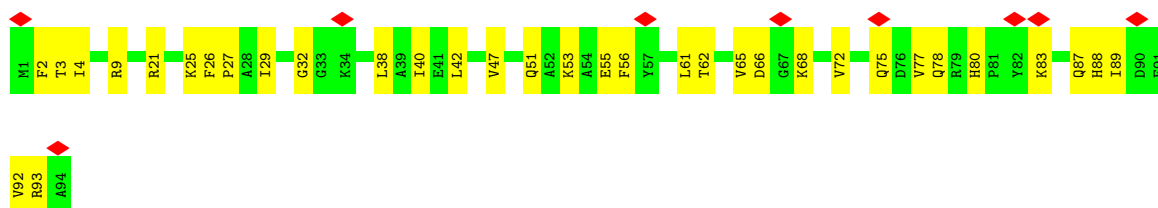
- Molecule 17: 50S ribosomal protein L24

Chain t: 73% 25%



- Molecule 18: 50S ribosomal protein L25

Chain u: 10% 64% 36%



- Molecule 19: 50S ribosomal protein L27

Chain v: 69% 19% 12%



- Molecule 20: 50S ribosomal protein L28

Chain w:  72% 27%



- Molecule 21: 50S ribosomal protein L29

Chain x:  73% 25%



- Molecule 22: 50S ribosomal protein L30

Chain y:  76% 22%



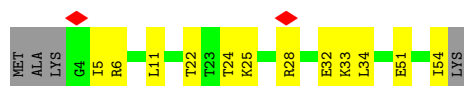
- Molecule 23: 50S ribosomal protein L32

Chain z:  72% 26%



- Molecule 24: 50S ribosomal protein L33

Chain 0:  71% 22% 7%



- Molecule 25: 50S ribosomal protein L34

Chain 1:  80% 17%

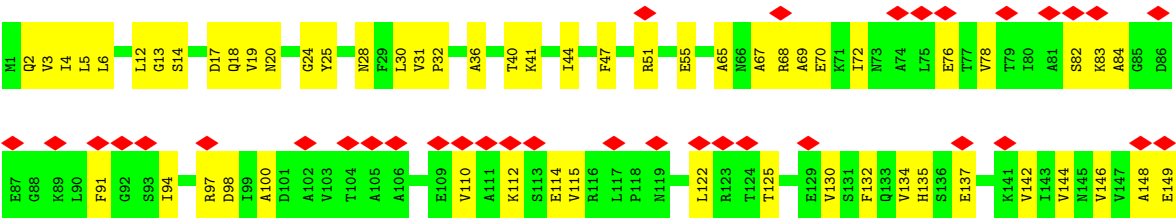


- Molecule 26: 50S ribosomal protein L35

Chain 2:  6% 63% 32%



• Molecule 27: 50S ribosomal protein L9



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55280	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 ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.088	Depositor
Minimum map value	-0.035	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.005	Depositor
Map size ($\text{\AA}$)	403.19998, 403.19998, 403.19998	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.05, 1.05, 1.05	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 1MG, 6MZ, G7M, MG, PSU, OMG, 5MU, 2MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	a	0.61	1/60188 (0.0%)	0.38	0/93883
2	b	0.32	0/2850	0.32	1/4444 (0.0%)
3	c	0.56	0/2072	0.55	0/2786
4	d	0.58	0/1414	0.49	0/1897
5	e	0.53	0/1499	0.57	0/2016
6	f	0.25	0/1434	0.56	0/1926
7	i	0.57	0/1152	0.49	0/1551
8	j	0.49	0/955	0.53	0/1279
9	k	0.53	0/1062	0.55	0/1413
10	m	0.63	0/958	0.58	0/1281
11	n	0.32	0/902	0.55	0/1209
12	o	0.53	0/929	0.51	0/1242
13	p	0.66	0/960	0.52	0/1278
14	q	0.56	0/829	0.48	0/1107
15	r	0.61	0/864	0.52	0/1156
16	s	0.53	0/744	0.55	0/994
17	t	0.53	0/787	0.63	0/1051
18	u	0.24	0/766	0.46	0/1025
19	v	0.43	0/576	0.44	0/762
20	w	0.59	0/635	0.56	0/848
21	x	0.47	0/502	0.56	0/667
22	y	0.49	0/453	0.53	0/605
23	z	0.62	0/450	0.53	0/599
24	0	0.29	0/424	0.43	0/565
25	1	0.67	0/380	0.56	0/498
26	2	0.34	0/513	0.43	0/676
27	h	0.32	0/1122	0.56	0/1515
All	All	0.58	1/85420 (0.0%)	0.42	1/128273 (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	a	3	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	2069	G7M	O3'-P	5.64	1.61	1.56

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	17	C	C2'-C3'-O3'	-5.19	105.92	113.70

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	a	2069	G7M	C2',C4',C3'

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	54003	0	27172	884	0
2	b	2549	0	1291	88	0
3	c	2035	0	2113	70	0
4	d	1397	0	1461	28	0
5	e	1483	0	1548	29	0
6	f	1410	0	1444	67	0
7	i	1129	0	1162	25	0
8	j	946	0	1023	30	0
9	k	1053	0	1129	27	0
10	m	945	0	989	21	0
11	n	892	0	923	44	0
12	o	917	0	962	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	p	947	0	1019	13	0
14	q	816	0	839	11	0
15	r	857	0	922	22	0
16	s	738	0	807	12	0
17	t	779	0	831	18	0
18	u	753	0	780	28	0
19	v	569	0	581	14	0
20	w	625	0	652	17	0
21	x	501	0	531	11	0
22	y	449	0	488	10	0
23	z	444	0	458	17	0
24	0	417	0	451	9	0
25	1	377	0	418	9	0
26	2	504	0	572	22	0
27	h	1111	0	1148	42	0
28	a	202	0	0	0	0
28	b	5	0	0	0	0
28	c	1	0	0	0	0
28	p	1	0	0	0	0
28	z	1	0	0	0	0
29	0	6	0	0	0	0
29	1	25	0	0	2	0
29	2	15	0	0	1	0
29	a	137	0	0	7	0
29	b	117	0	0	25	0
29	c	63	0	0	6	0
29	d	17	0	0	1	0
29	e	22	0	0	0	0
29	f	22	0	0	0	0
29	i	13	0	0	0	0
29	j	14	0	0	1	0
29	k	28	0	0	1	0
29	m	28	0	0	3	0
29	n	34	0	0	3	0
29	o	9	0	0	3	0
29	p	22	0	0	0	0
29	q	17	0	0	1	0
29	r	15	0	0	0	0
29	s	6	0	0	0	0
29	t	2	0	0	0	0
29	u	2	0	0	0	0
29	v	12	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	w	15	0	0	0	0
29	y	6	0	0	2	0
29	z	17	0	0	2	0
All	All	79520	0	51714	1427	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 11.

All (1427) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:2796:U:H3	1:a:2799:A:H61	1.02	0.96
1:a:353:C:H5''	1:a:353:C:H6	1.41	0.84
9:k:77:ILE:HD11	9:k:108:ALA:HB1	1.60	0.83
3:c:24:LEU:HD23	3:c:83:TYR:HB2	1.59	0.83
1:a:2054:A:H2'	23:z:5:GLN:HE22	1.43	0.82
1:a:353:C:H5''	1:a:353:C:C6	2.13	0.82
5:e:58:LYS:HB2	5:e:59:PRO:HD3	1.61	0.82
1:a:2313:C:H2'	1:a:2314:A:H8	1.45	0.82
27:h:84:ALA:HA	27:h:91:PHE:H	1.43	0.82
2:b:55:U:H1'	6:f:26:MET:HE1	1.60	0.81
27:h:70:GLU:HB3	27:h:134:VAL:HG11	1.63	0.80
5:e:56:GLY:HA2	5:e:73:ILE:HG22	1.62	0.79
1:a:2054:A:H2'	23:z:5:GLN:NE2	1.96	0.79
1:a:2313:C:H2'	1:a:2314:A:C8	2.19	0.78
3:c:21:ASN:HB3	3:c:24:LEU:HD13	1.67	0.76
1:a:2365:G:N7	26:2:39:LYS:NZ	2.33	0.76
7:i:125:TYR:HH	7:i:132:HIS:HE2	1.28	0.76
3:c:165:VAL:HG21	3:c:181:MET:HE1	1.67	0.75
9:k:81:ASP:HA	9:k:84:LYS:HZ3	1.50	0.75
6:f:123:ASP:OD2	6:f:127:ASN:ND2	2.20	0.75
1:a:2656:U:C2	1:a:2665:A:N7	2.55	0.74
1:a:2796:U:H3	1:a:2799:A:N6	1.82	0.73
1:a:2656:U:O2	1:a:2665:A:N7	2.22	0.73
1:a:721:A:H3'	1:a:722:A:H8	1.54	0.73
1:a:845:A:H3'	1:a:845:A:N3	2.03	0.73
2:b:26:C:N3	29:b:308:HOH:O	2.22	0.72
2:b:33:G:N7	29:b:310:HOH:O	2.23	0.72
2:b:52:A:N1	29:b:307:HOH:O	2.22	0.72
1:a:483:A:OP1	17:t:47:LYS:NZ	2.22	0.72
10:m:46:ARG:NH2	29:m:201:HOH:O	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1434:A:H2'	1:a:1435:G:C8	2.25	0.72
1:a:2656:U:N3	1:a:2665:A:C8	2.58	0.71
2:b:101:A:N6	29:b:303:HOH:O	2.24	0.71
1:a:2012:G:OP1	15:r:11:ARG:NH2	2.23	0.70
1:a:2204:G:O6	1:a:2221:G:C6	2.44	0.70
1:a:717:C:H4'	1:a:717:C:OP1	1.90	0.70
1:a:1315:C:O2'	1:a:1392:A:N3	2.23	0.70
1:a:2314:A:H2'	1:a:2315:G:H8	1.56	0.70
6:f:104:ILE:HG13	6:f:105:THR:HG23	1.73	0.70
2:b:76:G:N2	29:b:313:HOH:O	2.24	0.70
1:a:2246:G:H2'	1:a:2247:A:C8	2.27	0.70
24:0:25:LYS:NZ	24:0:51:GLU:OE1	2.25	0.70
3:c:29:PRO:HA	3:c:82:GLU:OE1	1.92	0.70
4:d:12:THR:HG22	4:d:13:ARG:H	1.57	0.70
11:n:7:ARG:NH1	11:n:95:SER:O	2.24	0.70
1:a:639:U:H2'	1:a:640:C:C6	2.27	0.70
1:a:1434:A:H2'	1:a:1435:G:H8	1.57	0.69
27:h:5:LEU:HD22	27:h:13:GLY:HA3	1.73	0.69
1:a:2204:G:C6	1:a:2221:G:C2	2.80	0.69
2:b:48:U:OP2	11:n:30:ARG:NH2	2.24	0.69
7:i:13:ARG:NH1	7:i:49:ASP:O	2.26	0.69
6:f:38:MET:HE1	6:f:57:LEU:HD11	1.74	0.69
26:2:62:LEU:HB3	26:2:65:ALA:HB2	1.75	0.69
1:a:2086:U:H2'	1:a:2087:G:C8	2.28	0.69
1:a:2740:A:OP2	1:a:2763:G:N1	2.26	0.69
2:b:21:G:N7	29:b:318:HOH:O	2.26	0.69
1:a:1811:G:N3	29:a:6310:HOH:O	2.25	0.68
11:n:50:ALA:O	11:n:81:ARG:NH2	2.25	0.68
1:a:645:C:H2'	1:a:647:G:C8	2.29	0.68
26:2:28:ASN:O	26:2:36:LYS:NZ	2.21	0.68
1:a:829:A:N7	1:a:2247:A:O2'	2.25	0.68
27:h:12:LEU:HD12	27:h:19:VAL:HG11	1.74	0.68
1:a:1469:A:H2'	1:a:1470:A:C8	2.29	0.67
6:f:68:THR:HG22	6:f:88:LYS:HG2	1.77	0.67
2:b:102:G:N2	29:b:323:HOH:O	2.28	0.66
2:b:6:G:N7	29:b:325:HOH:O	2.28	0.66
1:a:2328:A:H2'	1:a:2329:U:C6	2.30	0.66
2:b:7:G:N7	29:b:321:HOH:O	2.27	0.66
6:f:110:ARG:HD2	6:f:137:ILE:HA	1.76	0.66
18:u:26:PHE:HE2	18:u:89:ILE:HG12	1.61	0.66
21:x:10:SER:N	21:x:13:GLU:OE2	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:2204:G:C5	1:a:2221:G:C2	2.84	0.66
10:m:56:LYS:NZ	10:m:87:PHE:O	2.24	0.66
13:p:52:GLN:O	13:p:56:GLN:HG3	1.96	0.66
1:a:2246:G:H2'	1:a:2247:A:H8	1.60	0.65
8:j:1:MET:SD	8:j:67:LYS:NZ	2.69	0.65
19:v:24:LYS:NZ	29:v:104:HOH:O	2.29	0.65
1:a:2187:U:H2'	1:a:2188:U:C6	2.31	0.65
17:t:97:LYS:O	17:t:98:SER:OG	2.15	0.65
1:a:2190:G:H2'	1:a:2191:A:C8	2.32	0.65
1:a:1190:G:N7	29:a:6317:HOH:O	2.30	0.65
1:a:1794:A:H2'	1:a:1795:C:C6	2.32	0.65
1:a:2097:A:H2'	1:a:2098:U:C6	2.31	0.65
3:c:2:ALA:N	3:c:20:VAL:O	2.30	0.65
2:b:115:A:N7	29:b:326:HOH:O	2.29	0.65
11:n:68:LYS:NZ	29:n:204:HOH:O	2.28	0.65
1:a:84:A:N1	1:a:98:G:O2'	2.29	0.65
22:y:11:ARG:NH1	29:y:101:HOH:O	2.30	0.65
1:a:1910:G:H1	1:a:1920:C:H42	1.45	0.64
1:a:2803:G:H2'	1:a:2804:U:C6	2.32	0.64
8:j:92:GLU:O	8:j:111:LYS:NZ	2.31	0.64
12:o:93:ARG:NH1	29:o:202:HOH:O	2.28	0.64
22:y:41:THR:HG22	22:y:43:ALA:H	1.62	0.64
27:h:83:LYS:HA	27:h:149:GLU:HB3	1.78	0.64
1:a:1548:A:H2'	1:a:1549:A:C8	2.31	0.64
1:a:12:U:O2	1:a:2626:C:H4'	1.98	0.64
1:a:717:C:H3'	1:a:718:A:H8	1.62	0.64
1:a:2313:C:O3'	6:f:88:LYS:NZ	2.30	0.64
1:a:2333:A:OP2	19:v:77:ARG:NH2	2.23	0.64
11:n:87:ILE:HG13	11:n:88:LYS:H	1.62	0.64
18:u:42:LEU:HB3	18:u:47:VAL:HG21	1.79	0.64
1:a:721:A:H3'	1:a:722:A:C8	2.32	0.64
2:b:42:C:H4'	6:f:64:LYS:HG3	1.79	0.64
15:r:11:ARG:HH21	15:r:98:LYS:HE3	1.63	0.64
1:a:2000:C:OP1	10:m:5:LYS:NZ	2.26	0.64
17:t:49:VAL:HG13	17:t:52:LEU:O	1.97	0.64
1:a:500:G:N1	1:a:503:A:OP2	2.31	0.64
1:a:813:U:H2'	1:a:814:C:C6	2.32	0.64
7:i:60:ASP:OD1	7:i:60:ASP:N	2.31	0.64
1:a:728:G:H4'	3:c:13:ARG:HD3	1.80	0.64
27:h:97:ARG:HG3	27:h:112:LYS:HD2	1.80	0.64
1:a:2091:C:H4'	20:w:56:MET:HE1	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:z:2:ALA:N	29:z:203:HOH:O	2.31	0.63
1:a:1796:U:H2'	1:a:1797:G:H8	1.62	0.63
1:a:494:G:H4'	15:r:6:LYS:HB2	1.79	0.63
1:a:1796:U:H2'	1:a:1797:G:C8	2.34	0.63
1:a:1802:A:H2'	1:a:1803:A:C8	2.33	0.63
15:r:4:ILE:HG12	15:r:106:VAL:HG22	1.79	0.63
1:a:594:U:H2'	1:a:595:C:C6	2.34	0.63
1:a:873:C:H2'	1:a:874:G:H8	1.64	0.63
3:c:25:HIS:HB3	3:c:82:GLU:HG2	1.81	0.63
11:n:7:ARG:NH2	29:n:206:HOH:O	2.32	0.63
1:a:631:A:OP2	26:2:23:LYS:NZ	2.32	0.62
1:a:2313:C:O4'	6:f:37:ASN:ND2	2.32	0.62
1:a:288:U:H2'	1:a:289:G:H8	1.63	0.62
1:a:924:G:H2'	1:a:925:A:H8	1.64	0.62
1:a:2313:C:H5''	6:f:88:LYS:HD3	1.81	0.62
1:a:2741:A:N6	1:a:2763:G:O2'	2.33	0.62
1:a:1168:G:H2'	1:a:1169:A:C8	2.34	0.62
24:0:6:ARG:HG2	24:0:24:THR:HB	1.81	0.62
1:a:1177:G:H2'	1:a:1178:C:C6	2.34	0.62
10:m:73:ASN:ND2	29:m:204:HOH:O	2.32	0.62
10:m:28:LEU:HD23	10:m:48:VAL:HG21	1.82	0.62
17:t:38:GLY:N	17:t:62:GLU:OE1	2.24	0.62
1:a:873:C:H2'	1:a:874:G:C8	2.35	0.61
1:a:1364:G:N2	1:a:1367:A:OP2	2.28	0.61
1:a:1668:A:O2'	1:a:1674:G:N7	2.27	0.61
1:a:1007:C:OP1	7:i:37:ARG:NH2	2.32	0.61
1:a:1538:G:H2'	1:a:1539:U:C6	2.35	0.61
1:a:1746:A:H2'	1:a:1747:U:C6	2.35	0.61
1:a:2314:A:H2'	1:a:2315:G:C8	2.34	0.61
1:a:2845:U:H5''	12:o:52:ASN:O	2.00	0.61
6:f:47:LYS:NZ	6:f:83:TYR:OH	2.22	0.61
1:a:993:G:OP2	13:p:51:ARG:NH2	2.33	0.61
1:a:1275:A:N1	1:a:1295:C:O2'	2.28	0.61
1:a:1532:A:H2'	1:a:1533:C:C6	2.36	0.61
1:a:1534:U:H2'	1:a:1536:C:C6	2.35	0.61
5:e:168:ASP:OD2	5:e:170:ARG:NH2	2.33	0.61
1:a:1405:U:H2'	1:a:1406:U:C6	2.35	0.61
11:n:82:ALA:HB1	11:n:87:ILE:HD11	1.82	0.61
1:a:2:G:H2'	1:a:3:U:C6	2.35	0.61
2:b:100:G:N7	29:b:329:HOH:O	2.31	0.61
1:a:282:A:H2'	1:a:283:G:C8	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:51:G:N7	29:b:327:HOH:O	2.30	0.61
1:a:2294:G:P	11:n:94:ARG:HH12	2.23	0.61
2:b:66:A:H8	2:b:68:C:H41	1.49	0.61
2:b:61:G:N7	29:b:331:HOH:O	2.31	0.60
1:a:2273:A:H2'	1:a:2274:A:C8	2.35	0.60
10:m:22:ARG:HG3	10:m:70:THR:HA	1.83	0.60
6:f:40:VAL:HG12	6:f:43:ALA:HB2	1.83	0.60
1:a:849:A:H2'	1:a:850:U:C6	2.36	0.60
3:c:150:LYS:HD2	3:c:153:GLN:NE2	2.16	0.60
1:a:848:C:H2'	1:a:849:A:C8	2.37	0.60
1:a:1889:A:H2'	1:a:1890:A:C8	2.36	0.60
1:a:357:C:H2'	1:a:358:U:C6	2.36	0.60
1:a:1168:G:H2'	1:a:1169:A:H8	1.66	0.60
1:a:288:U:H2'	1:a:289:G:C8	2.37	0.60
1:a:807:U:OP2	9:k:41:ARG:NH1	2.34	0.60
2:b:48:U:P	11:n:30:ARG:HH12	2.25	0.60
6:f:16:LEU:HD12	6:f:28:VAL:HG13	1.83	0.60
19:v:33:ALA:N	19:v:64:ASP:OD1	2.33	0.60
1:a:1808:A:O2'	20:w:3:ARG:NH1	2.34	0.60
2:b:2:G:H2'	2:b:3:C:H6	1.66	0.60
4:d:116:LYS:HB2	4:d:165:MET:HB3	1.83	0.60
10:m:4:ARG:NH1	29:m:203:HOH:O	2.32	0.60
1:a:988:A:P	22:y:12:SER:HB3	2.41	0.59
1:a:2058:A:H2'	1:a:2059:A:C8	2.36	0.59
17:t:86:ARG:NH1	17:t:102:THR:OG1	2.35	0.59
6:f:115:ARG:O	6:f:178:ARG:NE	2.28	0.59
8:j:25:LEU:HD12	8:j:38:ILE:HG22	1.84	0.59
15:r:48:LYS:O	15:r:52:GLU:HG3	2.02	0.59
1:a:639:U:H2'	1:a:640:C:H6	1.66	0.59
1:a:832:U:H2'	1:a:833:A:H8	1.66	0.59
1:a:1032:A:H2	1:a:1122:G:H22	1.51	0.59
1:a:1197:G:H2'	1:a:1198:U:H6	1.67	0.59
1:a:948:C:H2'	1:a:949:G:H8	1.67	0.59
1:a:2680:U:O2'	1:a:2681:C:H5'	2.03	0.59
3:c:6:CYS:SG	3:c:13:ARG:NH2	2.76	0.59
1:a:2329:U:H2'	1:a:2330:G:C8	2.38	0.59
1:a:1000:A:H2'	1:a:1001:A:C8	2.38	0.59
1:a:2419:U:H4'	24:o:22:THR:HG21	1.85	0.59
3:c:163:GLN:HG2	3:c:175:ARG:HH21	1.67	0.59
1:a:64:A:H2'	1:a:65:U:C6	2.38	0.59
1:a:221:A:N1	1:a:265:A:O2'	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1837:C:O2'	1:a:1927:A:N3	2.32	0.59
7:i:110:PRO:O	7:i:115:GLY:HA3	2.03	0.59
13:p:50:ARG:O	13:p:54:LYS:NZ	2.32	0.59
15:r:29:VAL:HB	15:r:55:ILE:HD11	1.84	0.59
21:x:27:ASN:O	21:x:31:GLN:HG3	2.03	0.59
10:m:49:GLU:OE1	10:m:95:THR:OG1	2.20	0.58
20:w:10:LYS:HE3	20:w:54:LYS:HD3	1.83	0.58
26:2:15:LYS:HB2	26:2:23:LYS:HE3	1.85	0.58
2:b:60:C:H2'	2:b:61:G:H8	1.68	0.58
9:k:123:ARG:HA	9:k:143:GLU:HB2	1.85	0.58
18:u:77:VAL:HG22	18:u:89:ILE:HD12	1.85	0.58
2:b:2:G:H2'	2:b:3:C:C6	2.38	0.58
1:a:592:A:HO2'	26:2:64:TYR:HH	1.49	0.58
1:a:1432:G:H2'	1:a:1433:A:C8	2.38	0.58
8:j:13:ASN:HD22	8:j:98:ARG:HE	1.50	0.58
1:a:719:C:H6	1:a:719:C:O5'	1.87	0.58
1:a:917:A:H5''	1:a:2268:A:H61	1.69	0.58
1:a:2333:A:OP1	19:v:77:ARG:NH1	2.29	0.58
1:a:2821:A:OP1	4:d:115:GLY:N	2.21	0.58
2:b:109:A:N1	29:b:335:HOH:O	2.32	0.58
6:f:26:MET:O	6:f:30:ARG:NH1	2.35	0.58
1:a:1386:C:H2'	1:a:1387:A:C8	2.38	0.58
1:a:1808:A:H3'	1:a:1809:A:C8	2.39	0.58
1:a:1834:U:H5''	1:a:1835:2MG:H5'	1.86	0.58
1:a:2191:A:H2'	1:a:2192:U:C6	2.39	0.58
2:b:115:A:N3	29:b:333:HOH:O	2.32	0.58
10:m:8:ARG:NH1	10:m:43:GLU:OE1	2.37	0.58
27:h:51:ARG:HA	27:h:55:GLU:OE1	2.04	0.58
1:a:1494:A:H2'	1:a:1495:A:C8	2.38	0.58
1:a:278:A:N6	1:a:362:A:N7	2.52	0.57
1:a:642:U:O2'	1:a:644:A:N7	2.31	0.57
1:a:1255:U:C4	5:e:69:ARG:HD2	2.38	0.57
1:a:1484:U:H2'	1:a:1485:U:C6	2.38	0.57
1:a:1918:A:O2'	1:a:1920:C:N4	2.36	0.57
6:f:148:ARG:HB3	6:f:150:ARG:NH1	2.19	0.57
24:0:33:LYS:HG3	24:0:51:GLU:HB3	1.86	0.57
1:a:2285:C:OP2	24:0:6:ARG:NH1	2.36	0.57
1:a:2291:U:H2'	1:a:2292:U:C6	2.39	0.57
2:b:18:G:H1	2:b:65:U:H3	1.52	0.57
1:a:1417:C:HO2'	1:a:1587:G:HO2'	1.51	0.57
1:a:643:A:N1	1:a:2369:A:O2'	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:u:2:PHE:HE2	18:u:53:LYS:HE2	1.69	0.57
1:a:2345:G:H5'	1:a:2347:C:O4'	2.05	0.57
2:b:66:A:H61	2:b:107:G:H2'	1.68	0.57
6:f:66:LEU:HB3	6:f:88:LYS:HB2	1.85	0.57
1:a:568:U:H1'	1:a:2030:6MZ:H9C1	1.87	0.57
26:2:32:ILE:HG22	26:2:32:ILE:O	2.05	0.57
1:a:644:A:H2'	1:a:645:C:O4'	2.05	0.57
1:a:871:U:H2'	1:a:872:U:C6	2.39	0.57
1:a:964:C:O2'	1:a:2273:A:N3	2.34	0.57
1:a:1924:C:H2'	1:a:1925:C:O4'	2.05	0.57
7:i:125:TYR:OH	7:i:132:HIS:NE2	2.25	0.57
1:a:926:G:H2'	1:a:927:A:C8	2.40	0.57
1:a:1570:A:H2'	1:a:1571:A:C8	2.39	0.57
1:a:1614:A:C6	15:r:87:PRO:HB3	2.39	0.57
1:a:2649:C:H2'	1:a:2650:U:H6	1.70	0.57
2:b:48:U:H2'	2:b:49:C:C6	2.40	0.57
1:a:2315:G:OP1	6:f:33:LYS:NZ	2.30	0.57
1:a:2654:A:N1	1:a:2665:A:H5''	2.20	0.57
3:c:155:ALA:HB2	3:c:162:VAL:HG23	1.85	0.57
6:f:56:ASP:O	6:f:60:ILE:HD12	2.05	0.57
8:j:87:LEU:HD21	8:j:112:PHE:HE1	1.70	0.57
11:n:26:LEU:HD23	11:n:92:PHE:HD1	1.69	0.57
1:a:1340:U:OP2	16:s:82:LYS:NZ	2.37	0.56
1:a:613:A:H2'	1:a:614:A:O4'	2.05	0.56
1:a:782:A:N1	3:c:225:MET:HE2	2.20	0.56
2:b:28:C:H2'	2:b:29:A:C8	2.40	0.56
2:b:28:C:OP1	11:n:36:TYR:OH	2.23	0.56
2:b:51:G:H5''	11:n:64:TYR:CD2	2.40	0.56
1:a:1266:G:O2'	1:a:2012:G:O6	2.20	0.56
1:a:1794:A:H2'	1:a:1795:C:H6	1.69	0.56
1:a:2190:G:H2'	1:a:2191:A:H8	1.69	0.56
1:a:2649:C:H2'	1:a:2650:U:C6	2.40	0.56
1:a:244:A:OP2	26:2:8:ARG:NH2	2.30	0.56
1:a:1484:U:H2'	1:a:1485:U:H6	1.71	0.56
1:a:1920:C:H2'	1:a:1921:G:H8	1.71	0.56
2:b:16:G:N2	2:b:69:G:H1'	2.21	0.56
6:f:56:ASP:OD2	6:f:150:ARG:NE	2.36	0.56
1:a:155:A:H2'	1:a:156:A:C8	2.41	0.56
1:a:742:A:H2'	1:a:743:A:C8	2.41	0.56
6:f:62:GLY:O	6:f:95:ARG:NH2	2.38	0.56
6:f:62:GLY:C	6:f:95:ARG:HH22	2.13	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:414:C:H2'	1:a:415:A:H8	1.71	0.56
1:a:1417:C:O2'	1:a:1587:G:O2'	2.22	0.56
12:o:75:GLN:NE2	29:o:201:HOH:O	2.21	0.56
1:a:189:G:OP2	20:w:26:LYS:NZ	2.38	0.56
1:a:310:A:H5''	17:t:15:THR:OG1	2.05	0.56
1:a:909:A:H2'	1:a:912:C:H5	1.71	0.56
3:c:165:VAL:HG11	3:c:175:ARG:HG3	1.88	0.56
6:f:38:MET:HE1	6:f:57:LEU:CD1	2.36	0.56
1:a:861:A:H2'	1:a:862:G:O4'	2.06	0.56
1:a:1911:PSU:O4	1:a:1919:A:N6	2.39	0.56
3:c:133:ARG:NH1	3:c:187:ASP:OD1	2.32	0.56
1:a:1532:A:H2'	1:a:1533:C:H6	1.71	0.55
1:a:1548:A:H2'	1:a:1549:A:H8	1.70	0.55
2:b:57:A:O4'	6:f:24:SER:OG	2.23	0.55
1:a:414:C:H2'	1:a:415:A:C8	2.41	0.55
1:a:753:A:H5'	25:l:1:MET:SD	2.46	0.55
1:a:2803:G:H2'	1:a:2804:U:H6	1.70	0.55
8:j:38:ILE:HD11	8:j:112:PHE:HZ	1.71	0.55
27:h:78:VAL:HB	27:h:144:VAL:HG13	1.87	0.55
1:a:511:U:H4'	1:a:1235:G:H4'	1.88	0.55
1:a:2788:C:H2'	1:a:2789:C:C6	2.42	0.55
5:e:102:ARG:O	5:e:106:LYS:HG3	2.07	0.55
1:a:1908:C:O2	1:a:1922:G:N2	2.25	0.55
4:d:48:ILE:HG23	4:d:84:LEU:HD11	1.87	0.55
6:f:90:THR:HG21	6:f:92:ARG:NH1	2.21	0.55
27:h:130:VAL:HB	27:h:142:VAL:HG13	1.86	0.55
1:a:197:A:N6	1:a:2430:A:O2'	2.39	0.55
1:a:832:U:H2'	1:a:833:A:C8	2.42	0.55
1:a:871:U:H2'	1:a:872:U:H6	1.72	0.55
1:a:995:C:O2	7:i:3:THR:OG1	2.21	0.55
1:a:1149:G:H2'	1:a:1150:C:C6	2.40	0.55
1:a:2780:G:OP2	7:i:120:ARG:HD3	2.07	0.55
1:a:29:U:H2'	1:a:30:G:C8	2.42	0.55
1:a:57:C:H2'	1:a:58:G:O4'	2.07	0.55
1:a:788:A:OP1	1:a:791:C:N4	2.30	0.55
21:x:42:LEU:O	21:x:46:VAL:HG23	2.07	0.55
1:a:542:C:H2'	1:a:543:G:C8	2.42	0.55
1:a:2728:U:HO2'	1:a:2729:G:H8	1.55	0.55
3:c:66:ASP:OD2	3:c:102:ARG:NH1	2.39	0.55
1:a:586:A:N1	1:a:809:G:O2'	2.35	0.54
1:a:918:A:H5''	2:b:97:C:O2'	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:2065:C:H2'	1:a:2066:C:C6	2.42	0.54
1:a:657:U:H2'	1:a:658:U:C6	2.43	0.54
1:a:1198:U:H2'	1:a:1199:U:C6	2.42	0.54
1:a:1846:G:H2'	1:a:1847:A:C8	2.42	0.54
1:a:2303:G:H4'	6:f:121:SER:HA	1.89	0.54
2:b:39:A:N1	29:b:337:HOH:O	2.34	0.54
2:b:41:G:P	2:b:43:C:H41	2.30	0.54
4:d:35:THR:HG22	4:d:73:VAL:HG21	1.88	0.54
1:a:1506:U:H2'	1:a:1507:C:C6	2.43	0.54
1:a:356:G:H2'	1:a:357:C:C6	2.42	0.54
1:a:1792:G:H5'	3:c:204:VAL:HG13	1.89	0.54
7:i:21:THR:HG22	7:i:61:LYS:HE2	1.90	0.54
9:k:63:LYS:HA	26:2:12:LYS:O	2.08	0.54
9:k:78:ARG:HG2	9:k:113:ALA:HB3	1.88	0.54
12:o:5:ILE:O	12:o:9:GLU:HG3	2.07	0.54
27:h:47:PHE:HA	27:h:51:ARG:HB2	1.89	0.54
1:a:589:U:H2'	1:a:590:A:C8	2.42	0.54
1:a:1028:A:H2'	1:a:1028:A:N3	2.22	0.54
1:a:2619:C:OP1	4:d:157:LYS:NZ	2.33	0.54
27:h:6:LEU:H	27:h:36:ALA:HA	1.72	0.54
1:a:2186:G:H2'	1:a:2187:U:C6	2.42	0.54
3:c:29:PRO:HG2	3:c:34:LEU:HD11	1.90	0.54
1:a:1801:A:H5'	1:a:2203:U:O2'	2.07	0.54
1:a:139:U:H5''	1:a:140:C:H5	1.72	0.54
1:a:52:A:H2'	1:a:53:A:C8	2.43	0.53
1:a:813:U:H2'	1:a:814:C:H6	1.73	0.53
1:a:1394:U:H4'	1:a:1603:A:H4'	1.91	0.53
1:a:2020:A:H5'	23:z:9:THR:CG2	2.38	0.53
11:n:51:ALA:HB3	11:n:78:VAL:HB	1.90	0.53
22:y:31:ARG:HG2	22:y:34:HIS:HB2	1.88	0.53
1:a:358:U:H2'	1:a:359:G:H8	1.74	0.53
1:a:2740:A:H2'	1:a:2741:A:C8	2.44	0.53
9:k:36:LYS:NZ	29:k:206:HOH:O	2.36	0.53
12:o:96:LYS:NZ	29:o:203:HOH:O	2.41	0.53
13:p:76:TYR:CZ	13:p:80:ILE:HG13	2.43	0.53
1:a:278:A:N1	1:a:361:G:O2'	2.40	0.53
1:a:590:A:H2'	1:a:591:U:C6	2.44	0.53
1:a:1338:G:O2'	1:a:1393:A:N1	2.32	0.53
1:a:2334:U:H1'	11:n:13:ARG:HD2	1.90	0.53
1:a:272:A:H2'	1:a:273:G:H8	1.73	0.53
1:a:947:A:H2'	1:a:948:C:C6	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:2898:U:H2'	1:a:2899:A:C8	2.43	0.53
18:u:53:LYS:HZ2	18:u:55:GLU:HG3	1.73	0.53
20:w:3:ARG:HD2	20:w:30:LEU:HD22	1.90	0.53
1:a:548:G:H2'	1:a:549:G:C1'	2.39	0.53
1:a:926:G:H2'	1:a:927:A:H8	1.72	0.53
1:a:927:A:H2'	1:a:928:A:C8	2.44	0.53
1:a:2204:G:OP2	3:c:147:LYS:NZ	2.33	0.53
3:c:100:GLU:OE2	3:c:102:ARG:NE	2.42	0.53
6:f:66:LEU:O	6:f:88:LYS:N	2.41	0.53
11:n:28:VAL:HG21	11:n:103:VAL:HG13	1.90	0.53
1:a:1199:U:H2'	1:a:1200:C:H6	1.74	0.53
1:a:1747:U:H2'	1:a:1748:C:C6	2.44	0.53
1:a:2070:A:H2'	1:a:2071:A:C8	2.44	0.53
1:a:2291:U:H2'	1:a:2292:U:H6	1.74	0.53
1:a:2373:G:H2'	1:a:2374:C:C6	2.43	0.53
2:b:1:U:H2'	2:b:2:G:C8	2.44	0.53
9:k:77:ILE:CD1	9:k:108:ALA:HB1	2.36	0.53
2:b:48:U:H4'	11:n:100:HIS:ND1	2.23	0.53
8:j:14:SER:OG	8:j:86:LEU:HD12	2.09	0.53
22:y:44:ILE:HA	22:y:47:MET:HE3	1.90	0.53
1:a:645:C:O2'	1:a:646:U:H5''	2.09	0.53
1:a:2648:G:H2'	1:a:2649:C:H6	1.74	0.53
4:d:25:THR:HG21	4:d:193:VAL:HG22	1.91	0.53
7:i:24:THR:HG21	7:i:27:ARG:HD2	1.91	0.53
10:m:37:THR:OG1	10:m:40:LYS:HG3	2.09	0.53
27:h:76:GLU:HA	27:h:142:VAL:HG23	1.90	0.53
1:a:1123:C:H2'	1:a:1124:G:H8	1.74	0.53
2:b:14:U:OP2	2:b:70:C:O2'	2.27	0.53
1:a:284:U:H3	1:a:356:G:H1	1.57	0.52
1:a:1433:A:H2'	1:a:1434:A:C8	2.44	0.52
1:a:1667:G:O2'	1:a:1991:U:O4	2.21	0.52
27:h:122:LEU:HD13	27:h:146:VAL:HG21	1.91	0.52
1:a:491:G:O6	15:r:49:LYS:HE2	2.09	0.52
1:a:532:A:H4'	1:a:533:G:C8	2.44	0.52
1:a:1289:C:H2'	1:a:1290:C:C6	2.44	0.52
12:o:4:ILE:O	12:o:8:LEU:HD23	2.09	0.52
1:a:99:U:O2	17:t:7:ARG:NH1	2.42	0.52
1:a:2698:U:H2'	1:a:2699:C:C6	2.44	0.52
6:f:103:LEU:HD12	6:f:107:ALA:HB3	1.91	0.52
16:s:11:LEU:HD22	16:s:32:LEU:HD13	1.91	0.52
1:a:219:A:N3	1:a:234:U:O2'	2.32	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:r:24:ILE:HD13	15:r:36:LEU:HD11	1.92	0.52
1:a:1419:A:O2'	1:a:1421:G:N7	2.37	0.52
1:a:2627:G:O2'	1:a:2781:A:N1	2.32	0.52
1:a:2883:A:OP2	23:z:50:ARG:NH1	2.43	0.52
1:a:2012:G:P	15:r:11:ARG:HH22	2.33	0.52
1:a:2346:A:H3'	1:a:2347:C:H5''	1.92	0.52
1:a:26:G:H1'	1:a:514:A:N6	2.25	0.52
1:a:1689:A:H2'	1:a:1690:A:C8	2.45	0.52
1:a:1847:A:OP2	1:a:1847:A:H8	1.92	0.52
1:a:1869:G:N2	1:a:1873:G:C5	2.77	0.52
1:a:306:U:H2'	1:a:307:G:O4'	2.09	0.52
1:a:1156:A:C8	13:p:51:ARG:HG2	2.45	0.52
5:e:23:PHE:CD1	5:e:111:GLU:HG3	2.44	0.52
6:f:148:ARG:HB3	6:f:150:ARG:HH11	1.75	0.52
15:r:23:LEU:HD21	23:z:22:LEU:HB2	1.90	0.52
1:a:12:U:O2	1:a:12:U:H2'	2.10	0.52
1:a:2303:G:O6	1:a:2314:A:N6	2.43	0.52
4:d:12:THR:HG22	4:d:13:ARG:N	2.23	0.52
15:r:11:ARG:HH21	15:r:98:LYS:CE	2.22	0.52
1:a:277:G:H4'	1:a:278:A:O5'	2.10	0.52
3:c:72:ASP:OD1	3:c:189:ARG:NH1	2.43	0.52
12:o:9:GLU:OE2	12:o:56:HIS:NE2	2.43	0.52
1:a:580:U:H2'	1:a:581:C:C6	2.45	0.51
1:a:2062:A:N1	1:a:2448:A:H2	2.07	0.51
1:a:2079:U:H2'	1:a:2080:A:O4'	2.10	0.51
1:a:2204:G:O6	1:a:2221:G:C5	2.63	0.51
1:a:2898:U:H2'	1:a:2899:A:H8	1.75	0.51
2:b:106:G:H2'	2:b:107:G:O4'	2.10	0.51
11:n:49:VAL:HG21	11:n:81:ARG:HB3	1.91	0.51
1:a:479:A:N3	1:a:481:G:H5''	2.25	0.51
1:a:588:U:H2'	1:a:589:U:C6	2.45	0.51
2:b:10:G:N2	29:b:335:HOH:O	2.42	0.51
2:b:45:A:C4	2:b:46:A:C8	2.98	0.51
18:u:32:GLY:O	18:u:93:ARG:NH1	2.41	0.51
24:0:11:LEU:HD21	24:0:34:LEU:HD23	1.91	0.51
1:a:828:U:H4'	1:a:831:G:N1	2.26	0.51
1:a:848:C:H2'	1:a:849:A:H8	1.72	0.51
1:a:1328:A:H2'	1:a:1330:C:C4	2.45	0.51
1:a:1485:U:H2'	1:a:1486:U:H6	1.76	0.51
3:c:163:GLN:HG2	3:c:175:ARG:NH2	2.25	0.51
3:c:245:VAL:HG12	3:c:251:GLN:HA	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:u:9:ARG:NH2	18:u:40:ILE:O	2.44	0.51
1:a:337:C:OP2	17:t:4:LYS:NZ	2.34	0.51
1:a:632:A:H2'	1:a:633:A:C8	2.46	0.51
1:a:856:G:H2'	1:a:857:G:C8	2.46	0.51
1:a:863:A:N3	29:a:6321:HOH:O	2.34	0.51
2:b:50:A:OP2	11:n:67:ASN:HA	2.10	0.51
21:x:10:SER:OG	21:x:13:GLU:OE1	2.29	0.51
1:a:613:A:H8	1:a:613:A:OP1	1.94	0.51
1:a:2309:A:H2'	1:a:2310:C:O4'	2.10	0.51
1:a:2885:G:N7	23:z:40:ARG:NH2	2.47	0.51
3:c:150:LYS:CD	3:c:153:GLN:NE2	2.73	0.51
6:f:40:VAL:HG12	6:f:40:VAL:O	2.09	0.51
1:a:194:G:H2'	1:a:195:A:O4'	2.11	0.51
1:a:1589:U:H2'	1:a:1590:A:C8	2.45	0.51
1:a:1910:G:N2	1:a:1920:C:N3	2.49	0.51
1:a:2193:G:H2'	1:a:2194:U:C6	2.46	0.51
2:b:28:C:H2'	2:b:29:A:H8	1.76	0.51
1:a:39:G:H2'	1:a:40:U:C6	2.46	0.51
1:a:273:G:H2'	1:a:274:C:C6	2.46	0.51
1:a:670:A:H3'	9:k:43:GLY:HA2	1.93	0.51
1:a:2070:A:H2'	1:a:2071:A:H8	1.76	0.51
1:a:2291:U:O2'	1:a:2374:C:O2	2.28	0.51
6:f:111:ILE:HG23	6:f:114:PHE:HB2	1.93	0.51
13:p:94:ILE:O	13:p:98:ILE:HG13	2.10	0.51
1:a:2:G:H2'	1:a:3:U:H6	1.74	0.51
1:a:279:A:H61	1:a:361:G:H1'	1.76	0.51
1:a:594:U:H2'	1:a:595:C:H6	1.75	0.51
1:a:1824:G:O3'	3:c:247:PRO:HD3	2.11	0.51
1:a:1880:U:H2'	1:a:1881:C:C6	2.46	0.51
2:b:64:G:N7	29:b:340:HOH:O	2.34	0.51
3:c:121:ASP:HB3	27:h:91:PHE:HE1	1.76	0.51
3:c:150:LYS:O	3:c:150:LYS:HG2	2.11	0.51
5:e:75:SER:HB3	5:e:78:TRP:CD1	2.46	0.51
7:i:95:ARG:HE	7:i:96:ARG:HH22	1.59	0.51
8:j:2:ILE:HD12	8:j:6:THR:HG21	1.92	0.51
22:y:11:ARG:HB2	22:y:54:MET:HB2	1.92	0.51
1:a:248:G:O5'	1:a:249:C:H5''	2.11	0.51
1:a:903:C:H2'	1:a:904:G:C8	2.46	0.51
1:a:1429:G:H2'	1:a:1430:G:H8	1.76	0.51
1:a:1677:A:H2'	1:a:1678:A:C8	2.46	0.51
1:a:2333:A:H4'	1:a:2334:U:H5''	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:48:U:OP1	11:n:30:ARG:NH1	2.38	0.51
2:b:66:A:N6	2:b:107:G:H2'	2.26	0.51
11:n:102:ARG:NH1	29:n:201:HOH:O	2.34	0.51
12:o:25:THR:HB	12:o:88:ARG:HB3	1.93	0.51
1:a:833:A:H2'	1:a:834:G:C8	2.46	0.50
1:a:973:A:H5''	14:q:81:LYS:HD2	1.93	0.50
1:a:1035:U:H2'	1:a:1036:G:C8	2.46	0.50
1:a:1141:U:H4'	1:a:1142:A:O4'	2.10	0.50
1:a:1734:G:H2'	1:a:1735:A:H8	1.76	0.50
1:a:2017:U:H4'	23:z:5:GLN:O	2.11	0.50
2:b:97:C:H2'	2:b:98:G:O4'	2.11	0.50
6:f:37:ASN:OD1	6:f:38:MET:N	2.43	0.50
7:i:24:THR:CG2	7:i:27:ARG:HB2	2.41	0.50
11:n:10:ARG:NH1	11:n:96:GLY:O	2.40	0.50
27:h:82:SER:HB3	27:h:94:ILE:HD11	1.92	0.50
27:h:114:GLU:O	27:h:114:GLU:HG2	2.12	0.50
1:a:917:A:H5''	1:a:2268:A:N6	2.25	0.50
10:m:65:LEU:HB3	10:m:69:ARG:NH2	2.25	0.50
1:a:593:U:H2'	1:a:594:U:C6	2.46	0.50
1:a:845:A:N3	1:a:845:A:C3'	2.73	0.50
1:a:1589:U:H2'	1:a:1590:A:H8	1.74	0.50
1:a:1853:A:H2'	1:a:1854:A:C8	2.46	0.50
1:a:1932:A:H2'	1:a:1933:G:O4'	2.12	0.50
1:a:2038:G:H2'	1:a:2039:U:O4'	2.10	0.50
2:b:13:G:N2	2:b:69:G:O2'	2.44	0.50
18:u:66:ASP:HB2	18:u:68:LYS:HE2	1.94	0.50
5:e:170:ARG:HG2	5:e:174:GLY:O	2.12	0.50
6:f:130:MET:HB2	6:f:154:ILE:HB	1.94	0.50
11:n:48:LEU:O	11:n:85:LYS:HE2	2.11	0.50
1:a:855:G:C6	1:a:923:G:C6	2.99	0.50
1:a:967:U:H2'	1:a:968:C:C6	2.47	0.50
1:a:1009:A:N3	1:a:1153:C:O2'	2.40	0.50
5:e:147:LEU:HD11	5:e:170:ARG:HD3	1.92	0.50
3:c:5:LYS:NZ	29:c:415:HOH:O	2.45	0.50
3:c:234:GLY:O	29:c:401:HOH:O	2.20	0.50
18:u:61:LEU:O	18:u:72:VAL:N	2.34	0.50
1:a:272:A:H2'	1:a:273:G:C8	2.46	0.50
1:a:365:U:H2'	1:a:366:C:C6	2.46	0.50
1:a:549:G:H2'	1:a:550:C:H6	1.75	0.50
1:a:634:C:H2'	1:a:635:C:C6	2.47	0.50
1:a:1132:U:OP2	1:a:1133:A:H2'	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1199:U:H2'	1:a:1200:C:C6	2.47	0.50
2:b:118:C:H2'	2:b:119:A:H8	1.77	0.50
9:k:81:ASP:HA	9:k:84:LYS:NZ	2.21	0.50
9:k:82:LEU:HD22	9:k:90:VAL:HG21	1.93	0.50
1:a:353:C:H6	1:a:353:C:C5'	2.19	0.50
1:a:1183:U:H2'	1:a:1184:U:C6	2.46	0.50
1:a:2025:C:H2'	1:a:2026:U:C6	2.46	0.50
1:a:2636:C:H2'	1:a:2637:U:C6	2.47	0.50
3:c:133:ARG:HA	3:c:167:ARG:NH2	2.26	0.50
4:d:4:LEU:HD11	4:d:100:LEU:HD13	1.93	0.50
8:j:15:GLY:N	29:j:201:HOH:O	2.26	0.50
1:a:2328:A:H2'	1:a:2329:U:H6	1.73	0.50
1:a:2359:C:O2'	26:2:54:ASP:OD2	2.27	0.50
6:f:12:VAL:HG22	6:f:172:ALA:HB1	1.94	0.50
18:u:75:GLN:HB2	18:u:92:VAL:HG23	1.94	0.50
1:a:5:A:H2'	1:a:6:A:C8	2.47	0.49
1:a:163:C:H2'	1:a:164:C:C6	2.47	0.49
1:a:546:U:H5'	1:a:547:A:C8	2.47	0.49
1:a:1278:C:H2'	1:a:1279:G:H8	1.77	0.49
1:a:1447:C:H2'	1:a:1448:G:C8	2.47	0.49
2:b:70:C:H2'	2:b:71:C:H6	1.77	0.49
14:q:86:GLN:HB3	29:q:201:HOH:O	2.12	0.49
25:1:35:ARG:NH1	29:1:102:HOH:O	2.30	0.49
1:a:171:U:H2'	1:a:172:A:H8	1.77	0.49
1:a:716:A:O5'	1:a:716:A:H8	1.95	0.49
1:a:1912:A:N6	1:a:1917:PSU:HN3	2.09	0.49
4:d:184:ARG:HG3	4:d:186:LEU:HG	1.94	0.49
1:a:839:U:H2'	1:a:840:C:C6	2.48	0.49
1:a:928:A:H2'	1:a:929:U:O4'	2.12	0.49
1:a:2091:C:H4'	20:w:56:MET:CE	2.41	0.49
11:n:7:ARG:HD2	11:n:97:PHE:CE1	2.47	0.49
20:w:41:GLU:OE2	20:w:44:LYS:NZ	2.32	0.49
1:a:78:U:H2'	1:a:79:C:C6	2.47	0.49
1:a:1637:A:H5'	1:a:1760:C:O2'	2.13	0.49
1:a:2210:U:H4'	1:a:2211:A:H5'	1.94	0.49
1:a:2639:A:H2'	1:a:2640:G:O4'	2.13	0.49
1:a:713:G:H2'	1:a:714:U:C6	2.48	0.49
1:a:784:G:H4'	1:a:785:G:O5'	2.12	0.49
1:a:2014:A:H2'	1:a:2015:A:C8	2.48	0.49
1:a:2312:U:O2'	6:f:37:ASN:ND2	2.44	0.49
2:b:52:A:N7	11:n:64:TYR:OH	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:232:HIS:NE2	3:c:244:PRO:HA	2.28	0.49
8:j:10:VAL:HG12	8:j:12:ASP:H	1.77	0.49
1:a:1590:A:H2'	1:a:1591:A:C8	2.48	0.49
1:a:1920:C:H2'	1:a:1921:G:C8	2.47	0.49
1:a:2780:G:O6	7:i:99:ARG:NH1	2.46	0.49
1:a:28:A:H1'	1:a:513:A:C2	2.48	0.49
1:a:471:A:H2'	1:a:472:A:O4'	2.12	0.49
1:a:851:C:H2'	1:a:852:U:C6	2.48	0.49
1:a:1019:U:O2'	1:a:1021:A:N7	2.37	0.49
1:a:2065:C:H2'	1:a:2066:C:H6	1.76	0.49
1:a:2317:A:C4	1:a:2318:G:C8	3.01	0.49
15:r:20:VAL:HG11	15:r:44:ALA:HA	1.95	0.49
1:a:499:U:H2'	1:a:500:G:O4'	2.12	0.49
1:a:1563:U:H2'	1:a:1564:C:C6	2.48	0.49
1:a:2307:G:O6	6:f:41:GLY:N	2.45	0.49
1:a:2773:C:OP1	4:d:169:ARG:NE	2.44	0.49
1:a:739:A:H1'	1:a:740:C:H5	1.78	0.49
1:a:1123:C:H2'	1:a:1124:G:C8	2.48	0.49
1:a:1269:A:H2'	1:a:1270:C:C6	2.48	0.49
1:a:1688:U:O2'	1:a:1700:A:N7	2.42	0.49
6:f:56:ASP:OD2	6:f:150:ARG:NH2	2.45	0.49
8:j:13:ASN:ND2	8:j:98:ARG:HB2	2.28	0.49
1:a:2204:G:H4'	3:c:150:LYS:HG3	1.95	0.49
3:c:162:VAL:HG11	3:c:174:LEU:HD13	1.95	0.49
3:c:175:ARG:HG2	3:c:181:MET:SD	2.52	0.49
27:h:65:ALA:HA	27:h:68:ARG:HD2	1.95	0.49
1:a:608:A:H2'	1:a:609:A:C8	2.48	0.48
1:a:1182:G:H2'	1:a:1183:U:O4'	2.13	0.48
1:a:1529:G:H2'	1:a:1530:G:C8	2.48	0.48
1:a:2901:C:H2'	1:a:2902:C:C6	2.47	0.48
7:i:114:LEU:HG	7:i:118:MET:HE3	1.95	0.48
10:m:29:VAL:O	10:m:78:LYS:NZ	2.41	0.48
11:n:27:VAL:HG13	11:n:95:SER:OG	2.13	0.48
17:t:86:ARG:HG3	17:t:95:PHE:CE1	2.47	0.48
1:a:279:A:N6	1:a:361:G:H1'	2.28	0.48
1:a:493:G:H2'	1:a:494:G:O4'	2.12	0.48
1:a:1035:U:H2'	1:a:1036:G:H8	1.77	0.48
1:a:2303:G:N2	29:a:6312:HOH:O	2.26	0.48
2:b:42:C:O2'	6:f:63:GLN:HG2	2.13	0.48
1:a:263:G:H2'	1:a:264:C:O4'	2.13	0.48
1:a:1394:U:H2'	1:a:1395:A:O4'	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1561:C:H2'	1:a:1562:U:C6	2.48	0.48
4:d:181:ASP:CG	4:d:184:ARG:HG2	2.38	0.48
11:n:79:ALA:HB2	11:n:110:ALA:HA	1.95	0.48
11:n:87:ILE:HG13	11:n:88:LYS:N	2.27	0.48
1:a:1231:U:H2'	1:a:1232:G:H8	1.77	0.48
12:o:103:ARG:HD2	12:o:107:ALA:HB1	1.95	0.48
1:a:839:U:H1'	1:a:1191:G:H1'	1.94	0.48
1:a:2243:U:H2'	1:a:2244:U:C6	2.48	0.48
1:a:2636:C:H2'	1:a:2637:U:H6	1.78	0.48
1:a:2743:U:OP2	1:a:2755:C:N4	2.45	0.48
2:b:48:U:P	11:n:30:ARG:HH22	2.34	0.48
6:f:17:MET:SD	6:f:22:TYR:HB2	2.53	0.48
8:j:71:ARG:HH22	8:j:123:LEU:C	2.22	0.48
20:w:54:LYS:O	20:w:58:VAL:HG23	2.14	0.48
1:a:3:U:H2'	1:a:4:U:C6	2.49	0.48
1:a:948:C:H2'	1:a:949:G:C8	2.47	0.48
1:a:2047:C:H2'	1:a:2048:G:H8	1.79	0.48
1:a:2329:U:H2'	1:a:2330:G:H8	1.77	0.48
5:e:48:THR:HG22	5:e:86:ALA:HB3	1.94	0.48
7:i:31:GLU:HA	7:i:31:GLU:OE1	2.14	0.48
12:o:34:GLU:CD	12:o:39:ARG:HH22	2.21	0.48
14:q:1:MET:SD	14:q:43:ASN:ND2	2.87	0.48
14:q:28:ALA:HB3	14:q:31:GLU:HG2	1.94	0.48
20:w:43:GLU:OE2	20:w:45:ARG:NH2	2.39	0.48
1:a:714:U:O5'	1:a:714:U:H6	1.97	0.48
1:a:2071:A:H2'	1:a:2072:C:C6	2.48	0.48
1:a:2087:G:H2'	1:a:2088:A:H8	1.79	0.48
1:a:2295:C:OP2	11:n:9:ARG:NH2	2.47	0.48
6:f:4:LEU:HD13	6:f:100:PHE:HD2	1.78	0.48
23:z:43:ILE:HG22	23:z:49:TYR:HB2	1.95	0.48
1:a:282:A:H2'	1:a:283:G:H8	1.78	0.48
1:a:1527:G:N1	1:a:1544:A:OP2	2.42	0.48
1:a:1604:C:O2'	1:a:1610:A:N1	2.39	0.48
1:a:1859:U:H2'	1:a:1860:G:C8	2.49	0.48
1:a:2291:U:OP1	1:a:2380:C:O2'	2.25	0.48
1:a:2813:A:H2'	1:a:2814:A:C8	2.49	0.48
9:k:49:GLY:HA3	9:k:58:TYR:HE2	1.78	0.48
18:u:51:GLN:HA	18:u:56:PHE:CG	2.48	0.48
1:a:581:C:H2'	1:a:582:A:C8	2.48	0.48
1:a:677:A:O2'	1:a:2071:A:H5'	2.13	0.48
1:a:1340:U:OP1	16:s:84:TYR:OH	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1734:G:H2'	1:a:1735:A:C8	2.49	0.48
1:a:2648:G:H2'	1:a:2649:C:C6	2.48	0.48
2:b:76:G:H2'	2:b:77:U:H6	1.79	0.48
4:d:8:LYS:NZ	4:d:195:GLY:O	2.33	0.48
5:e:91:ASP:OD2	5:e:93:SER:OG	2.25	0.48
15:r:46:LEU:O	15:r:50:VAL:HG23	2.14	0.48
16:s:6:ARG:HH22	16:s:37:ASP:CG	2.21	0.48
1:a:367:G:H2'	1:a:368:A:C8	2.49	0.48
1:a:560:C:H2'	1:a:561:G:O4'	2.14	0.48
1:a:1441:G:H2'	1:a:1442:U:C6	2.49	0.48
1:a:1599:U:H2'	1:a:1600:C:C6	2.49	0.48
1:a:1720:U:H2'	1:a:1721:G:O4'	2.13	0.48
1:a:2192:U:H2'	1:a:2193:G:H8	1.79	0.48
1:a:2753:A:H2'	1:a:2754:U:O4'	2.14	0.48
4:d:1:MET:HA	4:d:88:GLU:OE2	2.14	0.48
18:u:78:GLN:HB3	18:u:87:GLN:HB2	1.96	0.48
1:a:810:U:C4	9:k:29:LYS:O	2.67	0.47
1:a:973:A:H5'	1:a:1188:U:H1'	1.95	0.47
1:a:1980:G:O2'	1:a:1982:U:OP2	2.29	0.47
1:a:2784:U:H4'	4:d:43:ASP:OD1	2.14	0.47
1:a:151:C:H2'	1:a:152:A:H8	1.78	0.47
1:a:749:A:H4'	1:a:1271:G:N3	2.29	0.47
1:a:1199:U:H1'	13:p:4:VAL:HG22	1.96	0.47
1:a:1447:C:O2'	1:a:1544:A:N3	2.40	0.47
1:a:2720:U:OP1	12:o:53:ARG:NH2	2.29	0.47
6:f:68:THR:CG2	6:f:88:LYS:HG2	2.43	0.47
17:t:35:ILE:HD13	17:t:64:ALA:HA	1.96	0.47
27:h:41:LYS:O	27:h:44:ILE:N	2.47	0.47
1:a:17:G:H2'	1:a:18:U:C6	2.49	0.47
1:a:960:A:H5''	1:a:961:C:OP1	2.14	0.47
1:a:1131:G:N2	1:a:1132:U:O4	2.35	0.47
1:a:1447:C:H2'	1:a:1448:G:H8	1.80	0.47
1:a:1689:A:H61	1:a:1697:G:H2'	1.79	0.47
2:b:7:G:O2'	11:n:38:GLN:OE1	2.22	0.47
2:b:28:C:H2'	2:b:29:A:O4'	2.15	0.47
3:c:161:TYR:HB3	3:c:194:GLU:HG3	1.96	0.47
5:e:7:ASP:OD2	5:e:122:GLU:HG3	2.14	0.47
5:e:106:LYS:NZ	5:e:200:LEU:HB3	2.29	0.47
1:a:322:A:OP2	5:e:163:ASN:HB2	2.14	0.47
1:a:548:G:H2'	1:a:549:G:H1'	1.97	0.47
1:a:635:C:O2'	1:a:639:U:OP1	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1590:A:H2'	1:a:1591:A:H8	1.79	0.47
1:a:2702:G:H2'	1:a:2703:C:H6	1.80	0.47
2:b:41:G:OP2	29:b:301:HOH:O	2.20	0.47
6:f:158:THR:HG22	6:f:160:ALA:H	1.79	0.47
1:a:65:U:H2'	1:a:66:C:H6	1.77	0.47
1:a:363:G:H2'	1:a:364:C:C6	2.49	0.47
1:a:729:G:C6	3:c:207:LYS:HB2	2.50	0.47
1:a:924:G:H2'	1:a:925:A:C8	2.47	0.47
1:a:1710:G:H4'	1:a:2858:C:O2	2.14	0.47
1:a:2311:A:C2	6:f:77:PHE:HB3	2.49	0.47
17:t:8:ASP:HB3	17:t:24:LYS:HZ1	1.79	0.47
26:2:26:HIS:NE2	26:2:48:ALA:HB2	2.29	0.47
1:a:26:G:H2'	1:a:27:G:O4'	2.13	0.47
1:a:68:G:H2'	1:a:69:C:O4'	2.15	0.47
1:a:171:U:H2'	1:a:172:A:C8	2.49	0.47
1:a:352:A:H2'	1:a:353:C:C6	2.48	0.47
1:a:1282:U:H2'	1:a:1283:G:O4'	2.15	0.47
1:a:1361:G:H2'	1:a:1362:C:C6	2.49	0.47
1:a:1928:A:H2'	1:a:1929:G:O4'	2.14	0.47
3:c:150:LYS:CD	3:c:153:GLN:HE22	2.27	0.47
20:w:3:ARG:O	20:w:12:PRO:HD3	2.14	0.47
23:z:8:PRO:O	29:z:201:HOH:O	2.20	0.47
1:a:538:A:H5''	7:i:7:LYS:HE3	1.96	0.47
1:a:600:G:H2'	1:a:601:C:C6	2.49	0.47
1:a:813:U:OP1	29:a:6301:HOH:O	2.20	0.47
1:a:923:G:H2'	1:a:924:G:H8	1.79	0.47
1:a:1353:A:H2'	1:a:1354:A:C8	2.50	0.47
1:a:1482:G:H1'	1:a:1509:A:H61	1.79	0.47
1:a:1857:G:O2'	1:a:1884:G:N2	2.44	0.47
1:a:1889:A:H2'	1:a:1890:A:H8	1.77	0.47
1:a:2373:G:H2'	1:a:2374:C:H6	1.78	0.47
1:a:2700:A:H2'	1:a:2701:U:C6	2.50	0.47
2:b:60:C:H2'	2:b:61:G:C8	2.48	0.47
3:c:107:PRO:HD2	3:c:110:LEU:HD22	1.95	0.47
16:s:1:MET:HE3	16:s:1:MET:HB3	1.83	0.47
19:v:59:LEU:HD12	19:v:80:ILE:HD12	1.97	0.47
27:h:14:SER:N	27:h:17:ASP:OD2	2.43	0.47
1:a:151:C:H2'	1:a:152:A:C8	2.50	0.47
1:a:465:G:H2'	1:a:466:A:C8	2.50	0.47
1:a:1532:A:C6	1:a:1540:G:C6	3.03	0.47
1:a:1873:G:H2'	1:a:1874:C:C6	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:2057:G:H2'	1:a:2058:A:C8	2.50	0.47
1:a:2386:A:H4'	19:v:56:ASP:HA	1.95	0.47
3:c:37:ASN:HB2	3:c:62:TYR:HB2	1.96	0.47
1:a:589:U:H2'	1:a:590:A:H8	1.79	0.47
1:a:1427:A:H4'	1:a:1428:C:O4'	2.14	0.47
1:a:1534:U:H5''	1:a:1535:A:OP1	2.15	0.47
1:a:2244:U:H2'	1:a:2245:U:O4'	2.15	0.47
2:b:59:A:H2'	2:b:60:C:C6	2.50	0.47
6:f:63:GLN:OE1	6:f:95:ARG:NH1	2.48	0.47
12:o:106:LYS:O	12:o:109:ARG:NE	2.36	0.47
26:2:33:LEU:HB3	26:2:41:LYS:HD3	1.97	0.47
26:2:52:LYS:HA	26:2:55:LEU:HD12	1.95	0.47
27:h:70:GLU:HG2	27:h:134:VAL:HG21	1.97	0.47
1:a:143:C:H2'	1:a:144:A:C8	2.50	0.47
1:a:1792:G:O2'	1:a:1830:C:OP1	2.32	0.47
1:a:2065:C:H4'	1:a:2251:OMG:HM22	1.97	0.47
1:a:2674:G:H5'	8:j:30:ARG:NH1	2.30	0.47
1:a:2688:G:H1'	1:a:2721:A:N6	2.30	0.47
3:c:43:ARG:HA	3:c:48:ARG:O	2.15	0.47
9:k:37:GLY:O	9:k:41:ARG:HG2	2.15	0.47
18:u:51:GLN:HA	18:u:56:PHE:CD2	2.49	0.47
18:u:78:GLN:O	18:u:87:GLN:N	2.45	0.47
1:a:323:C:H6	1:a:1205:A:C2	2.33	0.46
1:a:1860:G:H2'	1:a:1861:G:C8	2.49	0.46
1:a:2342:C:O2'	1:a:2374:C:H5''	2.14	0.46
1:a:2656:U:O2	1:a:2665:A:C5	2.68	0.46
3:c:59:LYS:NZ	29:c:418:HOH:O	2.48	0.46
5:e:7:ASP:OD1	5:e:7:ASP:N	2.48	0.46
1:a:286:U:C2	1:a:287:G:C8	3.02	0.46
1:a:563:A:OP2	14:q:79:ARG:NH2	2.41	0.46
1:a:819:A:H5''	1:a:973:A:N1	2.31	0.46
1:a:675:A:N3	1:a:2443:C:O2'	2.42	0.46
1:a:805:G:OP2	1:a:806:C:N4	2.40	0.46
1:a:2293:G:H2'	1:a:2294:G:O4'	2.15	0.46
1:a:2447:G:H3'	1:a:2448:A:C8	2.50	0.46
1:a:2786:U:OP1	4:d:70:LYS:HE3	2.16	0.46
10:m:107:ASN:OD1	15:r:40:ASN:HB3	2.15	0.46
18:u:65:VAL:O	18:u:68:LYS:N	2.36	0.46
21:x:18:LEU:HB2	21:x:53:VAL:HG11	1.97	0.46
1:a:565:C:H2'	1:a:566:U:O4'	2.15	0.46
1:a:1012:U:O4	7:i:30:THR:OG1	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1856:U:H2'	1:a:1857:G:O4'	2.15	0.46
2:b:117:G:OP1	11:n:56:LYS:NZ	2.32	0.46
1:a:81:G:H2'	1:a:82:U:O4'	2.16	0.46
1:a:207:A:H2'	1:a:208:C:O4'	2.15	0.46
1:a:717:C:H3'	1:a:718:A:C8	2.45	0.46
1:a:729:G:OP1	3:c:10:SER:OG	2.34	0.46
1:a:1860:G:H2'	1:a:1861:G:H8	1.80	0.46
1:a:2242:G:H2'	1:a:2243:U:O4'	2.16	0.46
5:e:1:MET:HE2	5:e:113:VAL:HG11	1.97	0.46
7:i:9:GLU:HG2	7:i:10:THR:HG23	1.97	0.46
20:w:38:PHE:HZ	20:w:56:MET:HG2	1.80	0.46
27:h:4:ILE:CD1	27:h:18:GLN:HG2	2.45	0.46
27:h:67:ALA:O	27:h:70:GLU:HG3	2.15	0.46
1:a:128:C:H2'	1:a:129:C:H6	1.81	0.46
1:a:299:A:N3	1:a:319:G:O2'	2.43	0.46
1:a:811:U:H2'	9:k:21:ARG:HA	1.96	0.46
1:a:1680:U:H2'	1:a:1681:G:O4'	2.16	0.46
1:a:1682:G:H2'	1:a:1683:U:C6	2.51	0.46
1:a:1779:U:OP2	1:a:1784:A:N6	2.34	0.46
1:a:2098:U:H2'	1:a:2099:U:O4'	2.15	0.46
1:a:2204:G:C6	1:a:2221:G:C4	3.04	0.46
3:c:150:LYS:HD2	3:c:153:GLN:HE22	1.78	0.46
1:a:340:A:H2'	1:a:341:C:O4'	2.15	0.46
1:a:673:C:N4	29:a:6327:HOH:O	2.40	0.46
1:a:760:G:H2'	1:a:761:A:O4'	2.15	0.46
1:a:1872:A:OP2	1:a:1872:A:H8	1.98	0.46
1:a:2902:C:H2'	1:a:2903:U:O4'	2.14	0.46
10:m:35:LYS:NZ	10:m:100:CYS:SG	2.89	0.46
1:a:323:C:C4	1:a:333:G:C8	3.04	0.46
1:a:1187:G:H5''	14:q:83:TYR:CE1	2.51	0.46
1:a:1278:C:H2'	1:a:1279:G:C8	2.50	0.46
1:a:1485:U:H2'	1:a:1486:U:C6	2.51	0.46
1:a:1842:G:H1'	3:c:243:HIS:CD2	2.50	0.46
1:a:2277:G:P	19:v:12:ASN:HD22	2.38	0.46
13:p:58:ARG:HA	13:p:61:TRP:CE3	2.51	0.46
1:a:709:U:H2'	1:a:710:U:C6	2.51	0.46
1:a:1428:C:C5	1:a:1569:A:H5''	2.51	0.46
1:a:1475:G:O2'	1:a:1514:G:O6	2.34	0.46
2:b:42:C:O2	6:f:90:THR:N	2.34	0.46
2:b:104:A:H2'	2:b:105:G:O4'	2.15	0.46
3:c:76:ALA:HB2	3:c:96:TYR:CD1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:u:29:ILE:HD12	18:u:38:LEU:O	2.16	0.46
1:a:1469:A:H2'	1:a:1470:A:H8	1.77	0.46
1:a:1529:G:H2'	1:a:1530:G:H8	1.81	0.46
1:a:1773:A:N7	1:a:1829:A:H1'	2.31	0.46
1:a:1790:C:H2'	1:a:1791:A:C5	2.50	0.46
2:b:98:G:N1	29:b:302:HOH:O	2.21	0.46
10:m:67:PHE:O	10:m:71:ARG:HD2	2.16	0.46
1:a:512:G:OP1	1:a:1234:U:O2'	2.21	0.45
1:a:2895:G:H2'	1:a:2896:C:C6	2.51	0.45
4:d:123:LYS:NZ	29:d:304:HOH:O	2.36	0.45
5:e:56:GLY:C	5:e:57:LYS:HD2	2.41	0.45
6:f:160:ALA:HB1	6:f:165:GLU:HB2	1.97	0.45
15:r:83:LYS:HD3	15:r:95:ARG:HD3	1.97	0.45
1:a:930:G:H1'	22:y:25:LEU:HD21	1.97	0.45
1:a:2074:U:H2'	1:a:2075:U:C6	2.51	0.45
1:a:2233:U:H2'	1:a:2234:G:C8	2.50	0.45
2:b:29:A:OP2	29:b:304:HOH:O	2.21	0.45
16:s:30:ILE:HG13	16:s:85:VAL:HB	1.97	0.45
18:u:9:ARG:HH22	18:u:27:PRO:HA	1.81	0.45
27:h:94:ILE:HG23	27:h:98:ASP:HB3	1.97	0.45
1:a:710:U:N3	1:a:722:A:C2	2.84	0.45
1:a:1725:U:H2'	1:a:1726:C:C6	2.51	0.45
5:e:154:ASP:OD1	5:e:155:GLU:N	2.49	0.45
9:k:91:ASP:HB2	9:k:94:THR:HG23	1.97	0.45
20:w:6:GLN:O	20:w:74:ARG:NH1	2.44	0.45
27:h:6:LEU:HD23	27:h:6:LEU:O	2.17	0.45
1:a:225:C:H2'	1:a:226:A:O4'	2.17	0.45
1:a:868:U:C4	1:a:869:G:N7	2.84	0.45
1:a:1197:G:H2'	1:a:1198:U:C6	2.47	0.45
1:a:2301:C:H2'	1:a:2302:U:C6	2.52	0.45
1:a:2394:C:H5''	9:k:63:LYS:HD2	1.99	0.45
13:p:49:ASP:HA	13:p:52:GLN:HB2	1.98	0.45
14:q:34:GLU:OE2	14:q:60:LYS:HG2	2.17	0.45
1:a:419:U:H2'	1:a:420:C:C6	2.51	0.45
1:a:606:U:OP2	5:e:99:LYS:HE2	2.17	0.45
1:a:609:A:H2'	1:a:610:C:O4'	2.17	0.45
1:a:843:G:H2'	1:a:844:A:C8	2.51	0.45
1:a:910:A:H2'	1:a:911:A:C8	2.51	0.45
1:a:1223:G:OP1	14:q:68:ARG:NH2	2.47	0.45
1:a:1486:U:H2'	1:a:1487:U:C6	2.51	0.45
1:a:2245:U:H5''	1:a:2246:G:H5'	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:2799:A:O2'	1:a:2800:A:H5''	2.17	0.45
11:n:94:ARG:NH2	11:n:97:PHE:O	2.42	0.45
1:a:191:A:H2'	1:a:192:C:C6	2.51	0.45
1:a:240:C:OP2	1:a:241:A:O2'	2.20	0.45
1:a:372:G:O2'	1:a:400:G:O6	2.22	0.45
1:a:532:A:N1	1:a:2020:A:H1'	2.31	0.45
1:a:1015:U:H2'	1:a:1016:G:C8	2.52	0.45
1:a:1316:U:H2'	1:a:1317:G:C8	2.52	0.45
1:a:1730:C:O2'	1:a:1731:G:C4	2.70	0.45
1:a:2318:G:H3'	1:a:2319:G:C8	2.52	0.45
2:b:35:C:H2'	2:b:36:C:O4'	2.15	0.45
4:d:3:GLY:O	4:d:4:LEU:HD12	2.16	0.45
6:f:22:TYR:HB3	6:f:27:GLN:HB3	1.98	0.45
6:f:105:THR:OG1	6:f:106:ILE:HD12	2.17	0.45
14:q:71:LYS:HA	14:q:90:ARG:HG2	1.98	0.45
17:t:85:PHE:CE1	17:t:94:ARG:HG2	2.52	0.45
18:u:9:ARG:HH22	18:u:27:PRO:HB3	1.81	0.45
1:a:155:A:H2'	1:a:156:A:H8	1.80	0.45
1:a:172:A:H2'	1:a:173:A:C8	2.51	0.45
1:a:458:G:C8	25:1:37:LYS:HG2	2.51	0.45
1:a:651:G:OP1	26:2:19:LYS:HB2	2.17	0.45
1:a:2072:C:H2'	1:a:2073:C:H6	1.82	0.45
1:a:2705:A:H2'	1:a:2706:A:O4'	2.16	0.45
3:c:226:ASN:HA	3:c:234:GLY:N	2.32	0.45
6:f:58:ALA:O	6:f:62:GLY:HA2	2.17	0.45
6:f:101:GLU:HA	6:f:104:ILE:HG12	1.98	0.45
1:a:353:C:C6	1:a:353:C:C5'	2.93	0.45
1:a:383:C:N4	1:a:386:G:OP2	2.48	0.45
1:a:1715:G:O2'	1:a:1743:G:O6	2.30	0.45
1:a:2087:G:H2'	1:a:2088:A:C8	2.52	0.45
2:b:8:C:O3'	11:n:25:ARG:NH1	2.26	0.45
3:c:133:ARG:NH2	3:c:167:ARG:HH12	2.15	0.45
6:f:106:ILE:C	6:f:109:PRO:HD2	2.41	0.45
10:m:55:ALA:HA	10:m:80:PHE:CE2	2.52	0.45
1:a:287:G:H2'	1:a:288:U:C6	2.52	0.45
1:a:445:C:H2'	1:a:446:G:O4'	2.17	0.45
1:a:782:A:C6	3:c:225:MET:HE2	2.51	0.45
1:a:1363:C:O2'	1:a:1809:A:N3	2.46	0.45
9:k:3:LEU:HD23	9:k:3:LEU:HA	1.84	0.45
27:h:114:GLU:OE1	27:h:132:PHE:HB3	2.17	0.45
1:a:743:A:O2'	1:a:1659:G:OP1	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1545:A:H2'	1:a:1546:G:O4'	2.16	0.45
3:c:219:THR:OG1	29:c:403:HOH:O	2.21	0.45
8:j:107:LEU:O	8:j:109:SER:N	2.50	0.45
12:o:106:LYS:HA	12:o:109:ARG:NE	2.32	0.45
16:s:33:LYS:HE2	16:s:80:TRP:CZ3	2.52	0.45
27:h:30:LEU:HB3	27:h:36:ALA:HB3	1.98	0.45
1:a:729:G:C5	3:c:207:LYS:HB2	2.53	0.44
1:a:862:G:O2'	2:b:78:A:N3	2.50	0.44
1:a:872:U:H2'	1:a:873:C:H6	1.83	0.44
1:a:1239:G:H2'	1:a:1240:U:O4'	2.17	0.44
1:a:2377:A:O2'	11:n:117:PHE:O	2.21	0.44
18:u:9:ARG:NH2	18:u:27:PRO:HA	2.32	0.44
23:z:54:VAL:HG23	23:z:55:ILE:HG23	1.99	0.44
1:a:145:C:H2'	1:a:146:A:C8	2.52	0.44
1:a:363:G:H2'	1:a:364:C:H6	1.82	0.44
1:a:855:G:C6	1:a:856:G:C5	3.05	0.44
1:a:1366:A:H2'	1:a:1367:A:O4'	2.18	0.44
1:a:1372:U:O2'	1:a:2212:A:N3	2.47	0.44
1:a:2064:C:H2'	1:a:2065:C:H6	1.82	0.44
1:a:2655:G:H1'	1:a:2656:U:H5	1.81	0.44
2:b:74:U:H2'	2:b:75:G:O4'	2.17	0.44
9:k:109:LYS:HE2	9:k:128:THR:HG22	1.99	0.44
10:m:38:LEU:HD11	10:m:42:LYS:HE2	1.99	0.44
15:r:55:ILE:O	15:r:59:GLU:HG3	2.17	0.44
18:u:3:THR:HA	18:u:62:THR:HG23	1.99	0.44
1:a:30:G:H2'	1:a:31:C:C6	2.52	0.44
1:a:250:G:H2'	1:a:251:A:C8	2.53	0.44
1:a:1850:G:H2'	1:a:1851:U:C6	2.52	0.44
3:c:225:MET:SD	3:c:230:HIS:HB2	2.57	0.44
3:c:251:GLN:HE22	3:c:253:LYS:HB2	1.83	0.44
8:j:24:VAL:HG13	8:j:33:ALA:HB2	1.99	0.44
8:j:116:ILE:HG23	8:j:122:VAL:HG21	1.98	0.44
11:n:7:ARG:HG2	11:n:7:ARG:HH11	1.82	0.44
11:n:79:ALA:HB3	11:n:113:ALA:HB3	1.99	0.44
1:a:381:G:OP1	20:w:18:ARG:NH1	2.44	0.44
1:a:454:A:H4'	1:a:455:C:OP2	2.17	0.44
1:a:1558:C:O4'	1:a:1560:G:C8	2.70	0.44
1:a:1731:G:C6	1:a:1733:G:C5	3.05	0.44
1:a:2020:A:H5'	23:z:9:THR:HG21	1.99	0.44
1:a:2756:U:H1'	1:a:2757:A:H5''	1.99	0.44
1:a:2804:U:H2'	1:a:2805:C:C6	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:2836:U:H2'	1:a:2837:A:C8	2.53	0.44
16:s:11:LEU:O	21:x:29:ARG:NH2	2.50	0.44
25:1:25:LYS:O	25:1:29:GLN:HG3	2.17	0.44
27:h:135:HIS:ND1	27:h:137:GLU:HG2	2.32	0.44
1:a:614:A:H3'	1:a:615:U:C5'	2.47	0.44
1:a:1026:G:H2'	1:a:1027:A:H8	1.83	0.44
1:a:1799:G:OP1	3:c:258:ARG:NH1	2.38	0.44
1:a:2250:G:OP1	1:a:2275:C:O2'	2.35	0.44
1:a:2842:G:H2'	1:a:2843:G:O4'	2.17	0.44
6:f:8:TYR:HB2	6:f:173:PHE:HZ	1.83	0.44
1:a:152:A:H2'	1:a:153:U:C6	2.53	0.44
1:a:1739:A:H2'	1:a:1740:G:O4'	2.18	0.44
1:a:1805:A:N3	3:c:50:THR:HB	2.32	0.44
1:a:1869:G:C2	1:a:1873:G:C6	3.05	0.44
1:a:2054:A:C2'	23:z:5:GLN:HE22	2.23	0.44
1:a:2314:A:C4	1:a:2315:G:C8	3.05	0.44
1:a:2315:G:O2'	6:f:123:ASP:OD2	2.35	0.44
1:a:2333:A:H3'	19:v:75:LYS:NZ	2.33	0.44
6:f:5:HIS:HB2	6:f:97:TRP:CD1	2.52	0.44
12:o:9:GLU:HB3	12:o:55:LEU:HB2	1.98	0.44
1:a:56:A:H2'	1:a:57:C:O4'	2.18	0.44
1:a:596:U:H2'	1:a:597:G:H8	1.82	0.44
1:a:903:C:N4	1:a:904:G:O6	2.51	0.44
1:a:1001:A:H2'	1:a:1002:G:O4'	2.17	0.44
1:a:1328:A:H2'	1:a:1330:C:C5	2.52	0.44
1:a:1385:A:O2'	1:a:1396:U:O2	2.36	0.44
1:a:1495:A:H2'	1:a:1496:A:C8	2.53	0.44
1:a:1544:A:H2'	1:a:1545:A:C8	2.52	0.44
1:a:2252:G:C4	1:a:2253:G:C8	3.06	0.44
20:w:40:VAL:HG12	20:w:43:GLU:H	1.83	0.44
27:h:3:VAL:CG1	27:h:36:ALA:HB1	2.47	0.44
1:a:120:U:H5''	1:a:122:G:OP2	2.18	0.44
1:a:678:C:H2'	1:a:679:C:C6	2.53	0.44
1:a:796:C:H2'	1:a:797:G:C8	2.52	0.44
1:a:817:C:O2'	1:a:839:U:H5''	2.17	0.44
1:a:952:G:C6	1:a:966:G:C6	3.06	0.44
1:a:1406:U:H2'	1:a:1407:G:C8	2.52	0.44
1:a:1656:C:H2'	1:a:1657:U:H6	1.82	0.44
1:a:2241:A:H2'	1:a:2242:G:C8	2.53	0.44
1:a:2694:G:H2'	1:a:2695:U:O4'	2.18	0.44
15:r:70:LYS:HE2	15:r:70:LYS:HB2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:u:4:ILE:HD11	18:u:61:LEU:HD23	1.99	0.44
27:h:125:THR:OG1	27:h:148:ALA:HB2	2.18	0.44
1:a:40:U:H2'	1:a:41:C:C6	2.52	0.44
1:a:139:U:H5''	1:a:140:C:C5	2.52	0.44
1:a:144:A:H2'	1:a:145:C:C6	2.53	0.44
1:a:700:G:O2'	1:a:1632:A:N3	2.50	0.44
1:a:739:A:N3	1:a:740:C:N4	2.54	0.44
1:a:747:5MU:O2	1:a:2014:A:H1'	2.17	0.44
1:a:866:A:C8	1:a:914:G:C5	3.06	0.44
1:a:935:C:H2'	1:a:936:A:C8	2.53	0.44
1:a:1588:G:H2'	1:a:1589:U:C6	2.53	0.44
1:a:1841:U:C2	1:a:1842:G:C8	3.06	0.44
1:a:1880:U:H2'	1:a:1881:C:H6	1.81	0.44
1:a:2377:A:OP2	1:a:2377:A:H8	2.00	0.44
2:b:116:G:H2'	2:b:117:G:C8	2.53	0.44
27:h:40:THR:O	27:h:44:ILE:HD12	2.18	0.44
1:a:128:C:H2'	1:a:129:C:C6	2.53	0.43
1:a:646:U:C4	1:a:2368:C:H1'	2.52	0.43
1:a:1505:A:H2'	1:a:1506:U:O4'	2.18	0.43
1:a:2657:A:H2'	1:a:2658:C:O4'	2.18	0.43
6:f:79:ILE:HD12	6:f:79:ILE:HA	1.87	0.43
10:m:53:THR:O	10:m:56:LYS:HB2	2.18	0.43
25:l:12:ARG:NH2	25:l:12:ARG:HG3	2.33	0.43
27:h:2:GLN:OE1	27:h:20:ASN:HB2	2.17	0.43
1:a:457:A:N1	1:a:470:A:H5''	2.33	0.43
1:a:1409:U:O2'	1:a:1410:G:H5'	2.18	0.43
1:a:1480:C:H2'	1:a:1481:U:O4'	2.18	0.43
1:a:1636:U:H2'	1:a:1637:A:C8	2.53	0.43
1:a:1831:G:H2'	1:a:1832:C:C6	2.53	0.43
1:a:2302:U:H2'	1:a:2303:G:C8	2.53	0.43
1:a:2609:U:H2'	1:a:2610:C:O4'	2.18	0.43
1:a:2795:C:H2'	1:a:2796:U:C6	2.53	0.43
3:c:218:PRO:O	29:c:402:HOH:O	2.21	0.43
4:d:124:ARG:HA	4:d:165:MET:SD	2.57	0.43
7:i:92:MET:SD	7:i:96:ARG:HD2	2.57	0.43
16:s:56:GLU:OE1	16:s:88:LYS:HG2	2.18	0.43
18:u:80:HIS:HB3	18:u:83:LYS:O	2.18	0.43
20:w:12:PRO:HB3	20:w:30:LEU:HD23	2.00	0.43
21:x:12:GLU:HG2	21:x:13:GLU:N	2.32	0.43
22:y:12:SER:HB2	22:y:32:ILE:HD11	2.00	0.43
1:a:244:A:H2'	1:a:245:G:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:276:U:H2'	1:a:277:G:H8	1.84	0.43
1:a:647:G:N2	1:a:2350:C:O2'	2.50	0.43
1:a:753:A:H2'	1:a:754:U:C6	2.53	0.43
1:a:2047:C:H2'	1:a:2048:G:C8	2.53	0.43
1:a:2391:G:O6	1:a:2425:A:H8	2.02	0.43
17:t:86:ARG:HG3	17:t:95:PHE:CD1	2.54	0.43
1:a:208:C:H2'	1:a:209:C:C6	2.53	0.43
1:a:417:C:H2'	1:a:418:C:C6	2.53	0.43
1:a:685:A:O2'	1:a:773:U:O4	2.34	0.43
1:a:1357:C:H2'	1:a:1358:G:O4'	2.18	0.43
1:a:1757:A:O2'	1:a:1758:U:OP1	2.29	0.43
1:a:2047:C:O2'	1:a:2823:A:N1	2.47	0.43
1:a:2192:U:H2'	1:a:2193:G:C8	2.53	0.43
1:a:2193:G:H2'	1:a:2194:U:H6	1.82	0.43
6:f:53:ALA:O	6:f:56:ASP:HB2	2.18	0.43
6:f:79:ILE:HD11	6:f:83:TYR:HB3	2.00	0.43
10:m:86:ARG:NH2	10:m:117:ASP:OD1	2.28	0.43
11:n:17:LYS:O	11:n:21:LEU:HG	2.18	0.43
18:u:27:PRO:O	18:u:88:HIS:HA	2.17	0.43
18:u:53:LYS:NZ	18:u:55:GLU:HG3	2.32	0.43
19:v:37:ILE:HG21	19:v:80:ILE:HG21	1.99	0.43
26:2:26:HIS:CE1	26:2:48:ALA:HB2	2.53	0.43
1:a:58:G:O2'	1:a:73:A:N1	2.43	0.43
1:a:173:A:H2'	1:a:174:U:C6	2.54	0.43
1:a:347:A:H2'	1:a:348:A:C8	2.54	0.43
1:a:1289:C:H2'	1:a:1290:C:H6	1.83	0.43
1:a:1442:U:H2'	1:a:1443:U:C6	2.53	0.43
1:a:1681:G:N3	1:a:1762:A:H2'	2.33	0.43
1:a:1839:G:C2	1:a:1840:G:C8	3.06	0.43
1:a:2840:C:H5''	10:m:53:THR:OG1	2.18	0.43
2:b:8:C:H2'	2:b:9:G:O4'	2.18	0.43
2:b:42:C:N3	6:f:90:THR:OG1	2.47	0.43
7:i:24:THR:HG23	7:i:27:ARG:HB2	1.99	0.43
1:a:273:G:C6	1:a:274:C:N4	2.87	0.43
1:a:476:G:N1	1:a:479:A:OP2	2.50	0.43
1:a:764:A:H2	3:c:218:PRO:HG3	1.83	0.43
1:a:874:G:H2'	1:a:875:G:H8	1.84	0.43
1:a:1429:G:H2'	1:a:1430:G:C8	2.53	0.43
1:a:1607:C:H4'	1:a:1608:A:O5'	2.19	0.43
1:a:2055:C:O4'	23:z:5:GLN:NE2	2.52	0.43
1:a:2099:U:H2'	1:a:2100:G:H8	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:i:43:GLU:N	7:i:43:GLU:OE1	2.51	0.43
17:t:11:VAL:HG12	17:t:72:ILE:HD13	2.01	0.43
23:z:33:THR:HB	23:z:51:GLY:HA2	2.00	0.43
1:a:1443:U:H2'	1:a:1444:G:C8	2.54	0.43
1:a:2271:G:OP1	19:v:18:ALA:HB1	2.17	0.43
1:a:721:A:C3'	1:a:722:A:H8	2.28	0.43
1:a:963:U:H1'	1:a:2250:G:O6	2.18	0.43
1:a:1853:A:N1	1:a:2087:G:H1'	2.34	0.43
1:a:2228:G:H2'	1:a:2229:U:C6	2.54	0.43
1:a:2317:A:H3'	1:a:2318:G:H8	1.84	0.43
1:a:2702:G:H2'	1:a:2703:C:C6	2.54	0.43
3:c:144:VAL:HG12	3:c:145:GLU:O	2.18	0.43
3:c:271:ARG:O	3:c:272:SER:OG	2.30	0.43
5:e:41:GLN:HG2	5:e:43:THR:HG23	2.00	0.43
11:n:90:VAL:O	11:n:117:PHE:HB3	2.18	0.43
1:a:285:G:C6	1:a:356:G:C6	3.06	0.43
1:a:391:A:O2'	1:a:410:G:OP1	2.30	0.43
1:a:566:U:H2'	1:a:567:U:O4'	2.19	0.43
1:a:680:C:H2'	1:a:681:G:C8	2.54	0.43
1:a:1122:G:N3	1:a:1122:G:H2'	2.33	0.43
1:a:1212:G:O2'	1:a:1236:G:N2	2.44	0.43
1:a:1349:C:C2	1:a:1350:C:C5	3.07	0.43
1:a:2438:U:O3'	1:a:2439:A:H3'	2.18	0.43
2:b:118:C:H2'	2:b:119:A:C8	2.54	0.43
3:c:205:LEU:HB3	3:c:210:ALA:HB3	2.00	0.43
8:j:77:ILE:HD11	12:o:72:ARG:NH1	2.34	0.43
20:w:16:ASN:ND2	20:w:24:ALA:HB1	2.33	0.43
1:a:231:A:H2'	1:a:232:G:O4'	2.19	0.43
1:a:284:U:O2	1:a:356:G:N2	2.44	0.43
1:a:624:C:O2'	1:a:657:U:OP1	2.28	0.43
1:a:676:A:C2	1:a:2069:G7M:H2'	2.53	0.43
1:a:1131:G:O2'	1:a:2025:C:O2'	2.20	0.43
1:a:1248:G:OP1	5:e:44:ARG:NH2	2.52	0.43
1:a:1536:C:H4'	1:a:1537:G:C4	2.53	0.43
1:a:1541:C:H2'	1:a:1542:U:C6	2.54	0.43
1:a:2037:A:H2'	1:a:2038:G:C8	2.54	0.43
1:a:2290:G:H2'	1:a:2291:U:C6	2.54	0.43
1:a:2372:U:H2'	1:a:2373:G:H8	1.84	0.43
1:a:2700:A:H2'	1:a:2701:U:H6	1.84	0.43
1:a:2849:U:H4'	1:a:2868:A:C2	2.53	0.43
5:e:177:PRO:O	5:e:181:ILE:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:u:77:VAL:HG22	18:u:89:ILE:CD1	2.49	0.43
1:a:542:C:H2'	1:a:543:G:H8	1.83	0.42
1:a:721:A:C3'	1:a:722:A:C8	3.01	0.42
1:a:1171:G:H2'	1:a:1172:C:C6	2.54	0.42
1:a:1319:C:O2'	1:a:1320:C:H5'	2.18	0.42
1:a:2005:A:C8	1:a:2006:C:C5	3.07	0.42
1:a:2345:G:N3	1:a:2381:A:H2'	2.33	0.42
2:b:9:G:OP1	11:n:15:ARG:HD3	2.19	0.42
2:b:18:G:H2'	2:b:19:C:C6	2.53	0.42
2:b:30:C:OP2	29:b:305:HOH:O	2.22	0.42
3:c:153:GLN:NE2	29:c:404:HOH:O	2.21	0.42
8:j:105:ARG:HH21	8:j:108:ARG:HD3	1.84	0.42
18:u:53:LYS:HZ2	18:u:55:GLU:C	2.26	0.42
27:h:69:ALA:HA	27:h:72:ILE:HD12	2.01	0.42
27:h:84:ALA:HA	27:h:91:PHE:N	2.22	0.42
1:a:52:A:H2'	1:a:53:A:H8	1.84	0.42
1:a:546:U:H5'	1:a:547:A:H8	1.85	0.42
1:a:667:U:H2'	1:a:668:A:O4'	2.18	0.42
1:a:992:C:OP1	13:p:47:TYR:OH	2.25	0.42
1:a:1022:G:N2	1:a:1023:U:O4	2.39	0.42
1:a:1292:G:H2'	1:a:1293:C:C6	2.53	0.42
1:a:1538:G:C2	1:a:1539:U:C2	3.07	0.42
1:a:2661:G:H8	1:a:2661:G:OP2	2.02	0.42
7:i:31:GLU:OE1	7:i:34:ARG:HD3	2.19	0.42
27:h:110:VAL:HG21	27:h:114:GLU:OE2	2.19	0.42
1:a:439:A:H2'	1:a:440:C:O4'	2.18	0.42
1:a:780:G:H2'	1:a:782:A:N7	2.34	0.42
1:a:1443:U:H2'	1:a:1444:G:H8	1.85	0.42
1:a:1614:A:C2	15:r:93:ALA:HB2	2.55	0.42
1:a:1683:U:H2'	1:a:1684:G:C8	2.54	0.42
1:a:2747:G:H2'	1:a:2748:A:C8	2.54	0.42
1:a:2896:C:H2'	1:a:2897:U:C6	2.55	0.42
1:a:5:A:H2'	1:a:6:A:H8	1.84	0.42
1:a:95:A:H2'	1:a:96:C:O4'	2.19	0.42
1:a:244:A:C2	1:a:255:A:C4	3.08	0.42
1:a:391:A:H1'	1:a:411:G:O4'	2.19	0.42
1:a:476:G:H4'	1:a:502:A:N1	2.35	0.42
1:a:846:U:H3'	1:a:846:U:O2	2.19	0.42
1:a:1181:U:H2'	1:a:1182:G:C8	2.54	0.42
1:a:1361:G:H2'	1:a:1362:C:H6	1.84	0.42
1:a:1421:G:O2'	1:a:1494:A:N6	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1882:U:H2'	1:a:1883:U:C6	2.55	0.42
1:a:2032:G:H4'	1:a:2033:A:OP1	2.19	0.42
1:a:2277:G:O5'	19:v:12:ASN:ND2	2.52	0.42
1:a:2307:G:H4'	1:a:2308:G:O4'	2.19	0.42
1:a:2333:A:H5'	1:a:2335:A:H1'	2.02	0.42
1:a:2358:A:H2'	1:a:2359:C:O4'	2.20	0.42
1:a:2659:G:O2'	1:a:2661:G:N7	2.49	0.42
11:n:115:LEU:HA	11:n:115:LEU:HD23	1.85	0.42
15:r:109:ASP:OD1	15:r:109:ASP:N	2.43	0.42
1:a:679:C:H2'	1:a:680:C:H6	1.84	0.42
1:a:1130:U:N3	1:a:2025:C:OP1	2.39	0.42
1:a:1754:A:O2'	12:o:103:ARG:NH2	2.51	0.42
1:a:1792:G:C5'	3:c:204:VAL:HG13	2.49	0.42
1:a:2199:A:N1	1:a:2226:C:N4	2.65	0.42
5:e:149:ILE:HG22	5:e:192:ALA:HB1	2.02	0.42
7:i:40:HIS:NE2	7:i:52:ASP:OD2	2.50	0.42
9:k:91:ASP:OD1	9:k:123:ARG:HB3	2.19	0.42
1:a:24:G:O2'	15:r:78:GLU:O	2.33	0.42
1:a:666:A:H2'	1:a:667:U:C6	2.55	0.42
1:a:671:C:H2'	1:a:672:C:C6	2.54	0.42
1:a:719:C:H2'	1:a:720:U:C6	2.55	0.42
1:a:984:A:N3	1:a:984:A:H2'	2.35	0.42
1:a:1223:G:C6	1:a:1227:G:C6	3.08	0.42
1:a:1403:A:H2'	1:a:1404:C:O4'	2.19	0.42
1:a:1511:G:H2'	1:a:1512:C:C6	2.55	0.42
5:e:23:PHE:HB2	5:e:111:GLU:OE2	2.19	0.42
5:e:122:GLU:OE2	5:e:123:LYS:HG2	2.20	0.42
8:j:13:ASN:ND2	8:j:98:ARG:HE	2.17	0.42
23:z:29:SER:OG	23:z:40:ARG:NH1	2.40	0.42
1:a:678:C:H2'	1:a:679:C:H6	1.83	0.42
1:a:740:C:O5'	1:a:740:C:H6	2.02	0.42
1:a:846:U:O2	1:a:846:U:H5''	2.20	0.42
1:a:957:C:O2'	1:a:959:A:H8	2.02	0.42
1:a:960:A:H8	1:a:960:A:O5'	2.03	0.42
1:a:1405:U:H2'	1:a:1406:U:H6	1.80	0.42
1:a:1436:G:H2'	1:a:1437:C:O4'	2.20	0.42
1:a:1791:A:N6	1:a:1828:G:O2'	2.44	0.42
1:a:2039:U:H2'	1:a:2040:G:C8	2.55	0.42
1:a:2282:G:H4'	1:a:2389:G:O2'	2.20	0.42
1:a:2820:A:N3	1:a:2820:A:H2'	2.35	0.42
3:c:133:ARG:HA	3:c:167:ARG:HH22	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:j:1:MET:HE3	8:j:32:TYR:CE2	2.55	0.42
19:v:20:ARG:O	19:v:24:LYS:NZ	2.51	0.42
22:y:41:THR:O	22:y:45:ARG:HG2	2.20	0.42
27:h:25:TYR:CE2	27:h:30:LEU:HD11	2.55	0.42
1:a:108:G:H2'	1:a:109:C:O4'	2.20	0.42
1:a:224:U:OP2	1:a:408:G:N2	2.36	0.42
1:a:290:U:H2'	1:a:291:G:O4'	2.20	0.42
1:a:1019:U:OP1	1:a:1035:U:O2'	2.34	0.42
1:a:1359:A:OP2	1:a:1371:G:N1	2.37	0.42
1:a:1585:C:H2'	1:a:1586:A:O4'	2.19	0.42
4:d:110:THR:CG2	4:d:202:ILE:HB	2.50	0.42
1:a:38:A:H2'	1:a:39:G:O4'	2.18	0.42
1:a:961:C:P	1:a:961:C:H3'	2.60	0.42
1:a:1827:U:OP2	3:c:221:ARG:HD2	2.20	0.42
1:a:2081:U:H2'	1:a:2082:A:C8	2.55	0.42
1:a:2311:A:O2'	1:a:2312:U:O4'	2.36	0.42
1:a:2830:C:H5''	4:d:56:LYS:HE3	2.01	0.42
2:b:29:A:H2'	2:b:30:C:C6	2.54	0.42
4:d:3:GLY:C	4:d:4:LEU:HD12	2.44	0.42
6:f:9:LYS:HB2	6:f:9:LYS:HE3	1.91	0.42
7:i:36:LEU:O	7:i:51:GLY:HA3	2.19	0.42
21:x:20:ASN:OD1	21:x:23:ARG:NH1	2.52	0.42
27:h:31:VAL:N	27:h:32:PRO:HD2	2.35	0.42
1:a:619:G:OP2	1:a:620:G:N2	2.44	0.42
1:a:906:U:H2'	1:a:907:G:O4'	2.20	0.42
1:a:1242:U:H2'	1:a:1243:C:C6	2.54	0.42
1:a:1989:G:H2'	1:a:1990:C:O4'	2.19	0.42
1:a:2312:U:C2'	6:f:37:ASN:HD21	2.32	0.42
1:a:2420:C:H4'	24:0:54:ILE:HG21	2.02	0.42
2:b:70:C:H2'	2:b:71:C:C6	2.55	0.42
11:n:80:GLU:O	11:n:83:LEU:HB2	2.19	0.42
13:p:106:PHE:O	13:p:110:VAL:HG23	2.20	0.42
25:1:42:LEU:HD23	25:1:42:LEU:HA	1.88	0.42
27:h:24:GLY:O	27:h:28:ASN:HB2	2.19	0.42
1:a:276:U:H2'	1:a:277:G:C8	2.55	0.41
1:a:547:A:H4'	1:a:548:G:O4'	2.20	0.41
1:a:598:U:H2'	1:a:599:A:H8	1.85	0.41
1:a:669:G:H2'	1:a:670:A:N7	2.35	0.41
1:a:686:U:H6	1:a:788:A:N1	2.18	0.41
1:a:838:C:H2'	1:a:839:U:H6	1.85	0.41
1:a:2443:C:H2'	1:a:2444:G:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:2651:C:C2	1:a:2670:A:C2	3.08	0.41
1:a:2687:U:H2'	1:a:2688:G:O4'	2.19	0.41
3:c:182:ARG:HG2	3:c:183:LYS:N	2.35	0.41
17:t:74:ASN:ND2	17:t:81:ASP:OD2	2.53	0.41
18:u:2:PHE:CE2	18:u:53:LYS:HE2	2.53	0.41
26:2:12:LYS:HE2	29:2:102:HOH:O	2.19	0.41
1:a:26:G:H1'	1:a:514:A:H61	1.85	0.41
1:a:1900:A:H5'	1:a:1970:A:H5'	2.02	0.41
1:a:2389:G:H5''	1:a:2390:U:O4'	2.20	0.41
5:e:46:GLN:O	5:e:88:ARG:NH1	2.53	0.41
21:x:7:ARG:NH1	21:x:59:GLU:OE1	2.53	0.41
21:x:19:LEU:HD23	21:x:19:LEU:HA	1.87	0.41
25:1:12:ARG:HG3	25:1:12:ARG:HH21	1.84	0.41
25:1:43:THR:OG1	25:1:45:SER:HB2	2.20	0.41
1:a:197:A:H2	1:a:2434:A:H62	1.69	0.41
1:a:265:A:N1	1:a:427:U:O2'	2.47	0.41
1:a:484:C:OP1	17:t:48:PRO:HG3	2.21	0.41
1:a:640:C:H2'	1:a:641:U:C6	2.56	0.41
1:a:874:G:H2'	1:a:875:G:C8	2.55	0.41
1:a:1641:A:H2'	1:a:1642:G:O4'	2.20	0.41
1:a:1725:U:H2'	1:a:1726:C:H6	1.85	0.41
1:a:2676:C:P	8:j:31:ARG:HH22	2.42	0.41
1:a:2743:U:H2'	1:a:2744:G:O4'	2.19	0.41
2:b:74:U:O4	2:b:102:G:N2	2.51	0.41
8:j:101:GLY:HA2	12:o:66:ASN:HB2	2.02	0.41
8:j:107:LEU:HB2	8:j:116:ILE:HD11	2.01	0.41
10:m:30:ARG:HH12	10:m:74:GLU:HG2	1.86	0.41
14:q:83:TYR:OH	14:q:85:LYS:HE3	2.20	0.41
25:1:29:GLN:HG2	29:1:124:HOH:O	2.19	0.41
1:a:208:C:H2'	1:a:209:C:H6	1.85	0.41
1:a:278:A:C6	1:a:362:A:C8	3.08	0.41
1:a:534:U:H2'	1:a:535:G:H8	1.85	0.41
1:a:569:U:OP1	1:a:945:A:O2'	2.28	0.41
1:a:592:A:C2	26:2:4:ILE:HD11	2.55	0.41
1:a:987:C:H2'	1:a:988:A:O4'	2.21	0.41
1:a:1348:C:C5	1:a:1349:C:C5	3.09	0.41
1:a:1809:A:H2'	1:a:1810:A:C8	2.55	0.41
1:a:2315:G:H2'	1:a:2316:G:H8	1.85	0.41
1:a:2395:C:OP1	9:k:63:LYS:NZ	2.53	0.41
6:f:6:ASP:HA	6:f:9:LYS:HE3	2.02	0.41
1:a:308:G:H2'	1:a:309:A:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1026:G:H2'	1:a:1027:A:C8	2.56	0.41
1:a:1655:A:H1'	4:d:118:PHE:CD1	2.56	0.41
1:a:2291:U:H5''	1:a:2380:C:O2'	2.21	0.41
1:a:2303:G:O2'	6:f:129:SER:HB2	2.20	0.41
5:e:122:GLU:OE2	5:e:123:LYS:NZ	2.53	0.41
8:j:98:ARG:HE	8:j:98:ARG:HB2	1.67	0.41
9:k:48:ARG:HE	9:k:48:ARG:HB2	1.56	0.41
27:h:76:GLU:C	27:h:142:VAL:HG23	2.45	0.41
1:a:300:A:H2'	1:a:334:C:H1'	2.02	0.41
1:a:569:U:H5''	1:a:821:A:C2	2.54	0.41
1:a:742:A:H2'	1:a:743:A:H8	1.83	0.41
1:a:1013:C:H2'	1:a:1014:A:H8	1.84	0.41
1:a:1430:G:H2'	1:a:1431:A:O4'	2.20	0.41
1:a:1676:A:H2'	1:a:1677:A:O4'	2.20	0.41
1:a:2077:A:H2'	1:a:2078:C:C6	2.56	0.41
1:a:2348:U:OP1	26:2:38:THR:HG21	2.20	0.41
3:c:83:TYR:CD1	3:c:83:TYR:C	2.99	0.41
4:d:73:VAL:CG1	4:d:93:GLY:HA2	2.50	0.41
24:0:5:ILE:HD13	24:0:28:ARG:NH2	2.35	0.41
27:h:12:LEU:H	27:h:12:LEU:HD23	1.84	0.41
1:a:593:U:H2'	1:a:594:U:H6	1.86	0.41
1:a:637:A:H4'	1:a:638:G:O5'	2.20	0.41
1:a:671:C:OP1	9:k:43:GLY:N	2.43	0.41
1:a:1591:A:H2'	1:a:1592:C:O4'	2.20	0.41
1:a:1775:U:O4	1:a:1789:A:H2	2.04	0.41
1:a:1838:C:C2	1:a:1898:U:C4	3.09	0.41
1:a:2046:G:H1'	23:z:19:HIS:CD2	2.55	0.41
1:a:2305:U:H2'	1:a:2306:C:O4'	2.21	0.41
1:a:2350:C:H2'	1:a:2351:G:O4'	2.21	0.41
1:a:2900:A:H2'	1:a:2901:C:C6	2.55	0.41
2:b:33:G:C6	2:b:50:A:C6	3.08	0.41
2:b:60:C:C2	2:b:61:G:C8	3.09	0.41
4:d:39:ASP:OD1	4:d:39:ASP:N	2.50	0.41
8:j:19:VAL:HB	8:j:41:ILE:HD12	2.02	0.41
16:s:53:VAL:HG11	16:s:93:LEU:HG	2.02	0.41
18:u:21:ARG:HA	18:u:25:LYS:O	2.20	0.41
20:w:37:ARG:HG2	20:w:48:THR:OG1	2.21	0.41
27:h:41:LYS:HA	27:h:44:ILE:HD13	2.02	0.41
1:a:184:C:H2'	1:a:185:G:C8	2.56	0.41
1:a:363:G:C6	1:a:364:C:C4	3.09	0.41
1:a:460:A:H2'	1:a:461:C:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:513:A:H5''	1:a:1216:G:O2'	2.21	0.41
1:a:923:G:C2	1:a:924:G:C8	3.08	0.41
1:a:1542:U:H2'	1:a:1543:G:O4'	2.21	0.41
1:a:1918:A:O5'	1:a:1918:A:H8	2.04	0.41
1:a:2315:G:H2'	1:a:2316:G:C8	2.56	0.41
1:a:2765:A:H2	1:a:2766:A:O4'	2.03	0.41
1:a:2812:G:H2'	1:a:2813:A:O4'	2.21	0.41
3:c:66:ASP:OD1	3:c:66:ASP:C	2.64	0.41
6:f:79:ILE:HG12	6:f:85:ILE:HD13	2.02	0.41
8:j:102:PRO:HB3	8:j:121:GLU:HB2	2.02	0.41
21:x:19:LEU:O	21:x:23:ARG:HG3	2.21	0.41
24:0:25:LYS:NZ	24:0:32:GLU:O	2.45	0.41
1:a:150:U:H2'	1:a:151:C:C6	2.55	0.41
1:a:483:A:HO2'	17:t:57:GLY:H	1.61	0.41
1:a:610:C:H2'	1:a:611:C:H6	1.84	0.41
1:a:814:C:H1'	1:a:1225:G:N2	2.36	0.41
1:a:1029:A:N6	1:a:1125:G:O2'	2.54	0.41
1:a:1351:C:H2'	1:a:1352:U:O4'	2.21	0.41
1:a:1370:C:H2'	1:a:1371:G:O4'	2.20	0.41
1:a:1386:C:H2'	1:a:1387:A:H8	1.83	0.41
1:a:1446:C:H2'	1:a:1447:C:C6	2.56	0.41
1:a:1519:G:H2'	1:a:1520:U:O4'	2.21	0.41
1:a:1594:U:H2'	1:a:1595:C:C6	2.56	0.41
1:a:2364:C:H2'	1:a:2365:G:O4'	2.20	0.41
1:a:2642:G:H5'	7:i:80:HIS:CE1	2.56	0.41
1:a:2784:U:H2'	1:a:2785:C:C6	2.56	0.41
1:a:2834:G:H1'	1:a:2883:A:N6	2.36	0.41
1:a:2895:G:H2'	1:a:2896:C:H6	1.85	0.41
3:c:105:LEU:O	3:c:107:PRO:HD3	2.21	0.41
5:e:12:LEU:HD12	5:e:12:LEU:HA	1.95	0.41
9:k:29:LYS:O	9:k:29:LYS:HG2	2.20	0.41
13:p:85:LYS:HB2	13:p:116:ALA:HB1	2.03	0.41
16:s:88:LYS:C	16:s:89:GLU:OE1	2.64	0.41
26:2:31:HIS:HD1	26:2:31:HIS:H	1.68	0.41
1:a:143:C:H2'	1:a:144:A:H8	1.85	0.41
1:a:224:U:O4	1:a:419:U:O2'	2.36	0.41
1:a:652:U:OP2	26:2:19:LYS:HE3	2.21	0.41
1:a:2075:U:OP1	29:a:6302:HOH:O	2.22	0.41
1:a:2082:A:H2'	1:a:2083:G:O4'	2.20	0.41
1:a:2204:G:C5	1:a:2221:G:N2	2.89	0.41
1:a:2259:U:H2'	1:a:2260:C:H6	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:2840:C:H2'	1:a:2841:C:H6	1.86	0.41
2:b:29:A:H2'	2:b:30:C:O4'	2.21	0.41
2:b:77:U:H3'	29:b:345:HOH:O	2.20	0.41
3:c:73:GLY:HA2	3:c:117:GLN:HE21	1.86	0.41
4:d:46:ARG:NH1	4:d:86:GLU:HA	2.36	0.41
6:f:68:THR:O	6:f:84:PRO:HA	2.21	0.41
9:k:2:ARG:HD3	9:k:2:ARG:HA	1.80	0.41
9:k:89:VAL:HG11	9:k:123:ARG:NH2	2.36	0.41
1:a:20:C:H2'	1:a:21:A:C8	2.56	0.40
1:a:65:U:H2'	1:a:66:C:C6	2.55	0.40
1:a:766:U:H2'	1:a:767:U:C6	2.56	0.40
1:a:934:U:H2'	1:a:935:C:C6	2.56	0.40
1:a:1684:G:H2'	1:a:1685:C:C6	2.57	0.40
1:a:2392:A:H2'	1:a:2393:U:O4'	2.22	0.40
2:b:26:C:H2'	2:b:27:C:O4'	2.21	0.40
2:b:61:G:O2'	29:b:306:HOH:O	2.22	0.40
3:c:107:PRO:HB3	3:c:142:HIS:CE1	2.56	0.40
8:j:51:LYS:HE2	8:j:51:LYS:HB3	1.88	0.40
11:n:7:ARG:HG3	11:n:10:ARG:NH1	2.36	0.40
12:o:60:THR:OG1	12:o:73:VAL:HG22	2.21	0.40
22:y:16:ARG:NH1	29:y:103:HOH:O	2.32	0.40
1:a:413:C:H2'	1:a:414:C:H6	1.86	0.40
1:a:591:U:H1'	26:2:2:PRO:N	2.36	0.40
1:a:610:C:H2'	1:a:611:C:C6	2.56	0.40
1:a:612:G:O2'	1:a:614:A:N7	2.47	0.40
1:a:654:A:H3'	1:a:654:A:N3	2.35	0.40
1:a:687:C:H2'	1:a:688:U:O4'	2.21	0.40
1:a:756:A:H2'	1:a:757:G:O4'	2.21	0.40
1:a:817:C:H2'	1:a:818:G:O4'	2.21	0.40
1:a:972:A:OP2	1:a:973:A:O2'	2.35	0.40
1:a:1295:C:H2'	1:a:1296:G:C8	2.56	0.40
1:a:1829:A:C8	1:a:1830:C:C5	3.10	0.40
1:a:2773:C:H2'	1:a:2774:C:C6	2.56	0.40
2:b:6:G:H2'	2:b:7:G:C8	2.56	0.40
2:b:75:G:H2'	2:b:76:G:O4'	2.21	0.40
4:d:38:LYS:HG2	4:d:43:ASP:OD2	2.20	0.40
6:f:116:GLY:HA3	6:f:178:ARG:HB2	2.03	0.40
8:j:75:SER:HB2	12:o:73:VAL:O	2.21	0.40
9:k:122:VAL:HG21	9:k:135:ILE:HD13	2.03	0.40
1:a:360:U:H2'	1:a:361:G:O4'	2.22	0.40
1:a:956:G:N2	1:a:959:A:H3'	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:963:U:H2'	1:a:964:C:C6	2.55	0.40
1:a:1257:C:H4'	5:e:78:TRP:CD2	2.57	0.40
1:a:1572:A:H2'	1:a:1573:G:H8	1.87	0.40
1:a:1689:A:H2'	1:a:1690:A:H8	1.87	0.40
1:a:1813:G:H1'	3:c:50:THR:OG1	2.21	0.40
1:a:2290:G:H4'	1:a:2381:A:O2'	2.22	0.40
1:a:2345:G:C5	1:a:2381:A:C2	3.10	0.40
1:a:2787:C:O3'	4:d:62:LYS:HE3	2.21	0.40
1:a:2813:A:H2'	1:a:2814:A:H8	1.86	0.40
2:b:93:C:H2'	2:b:94:A:C8	2.57	0.40
6:f:108:VAL:O	6:f:111:ILE:HG22	2.21	0.40
6:f:115:ARG:HH21	6:f:178:ARG:HG2	1.85	0.40
8:j:69:VAL:HG21	8:j:106:GLU:HG2	2.03	0.40
17:t:48:PRO:HA	17:t:55:PRO:O	2.22	0.40
1:a:493:G:O2'	15:r:7:HIS:HA	2.21	0.40
1:a:581:C:H2'	1:a:582:A:H8	1.86	0.40
1:a:841:G:H2'	1:a:842:U:C6	2.57	0.40
1:a:1795:C:H2'	1:a:1796:U:O4'	2.21	0.40
1:a:1881:C:H2'	1:a:1882:U:O4'	2.21	0.40
1:a:2196:C:O2'	1:a:2197:U:H5'	2.21	0.40
1:a:2292:U:H2'	1:a:2293:G:H8	1.87	0.40
1:a:2318:G:C6	1:a:2319:G:C6	3.10	0.40
1:a:2334:U:N3	11:n:16:ARG:HG3	2.37	0.40
13:p:14:HIS:O	13:p:18:LEU:HD23	2.21	0.40
19:v:70:GLU:O	19:v:79:PHE:N	2.44	0.40
1:a:1:G:H2'	1:a:2:G:C8	2.56	0.40
1:a:479:A:H4'	1:a:480:A:OP1	2.22	0.40
1:a:592:A:N3	26:2:4:ILE:HD11	2.36	0.40
1:a:834:G:H1'	1:a:2358:A:N3	2.37	0.40
1:a:854:C:H2'	1:a:855:G:H8	1.85	0.40
1:a:1418:G:N1	1:a:1579:A:OP2	2.35	0.40
1:a:1575:C:H2'	1:a:1576:U:O4'	2.21	0.40
1:a:1586:A:H3'	1:a:1587:G:H8	1.86	0.40
1:a:1908:C:H2'	1:a:1909:C:C6	2.56	0.40
2:b:23:G:N2	29:b:332:HOH:O	2.54	0.40
2:b:101:A:H2'	2:b:102:G:O4'	2.22	0.40
3:c:162:VAL:CG1	3:c:174:LEU:HB3	2.52	0.40
8:j:106:GLU:OE1	8:j:106:GLU:N	2.54	0.40
11:n:80:GLU:O	11:n:84:GLU:OE1	2.39	0.40
14:q:43:ASN:N	14:q:46:GLU:O	2.38	0.40
16:s:67:VAL:CG1	16:s:74:ILE:HD11	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:v:47:ALA:HB1	19:v:51:VAL:O	2.22	0.40
27:h:100:ALA:HB2	27:h:115:VAL:HG21	2.03	0.40
27:h:132:PHE:CE2	27:h:142:VAL:HG11	2.56	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	
3	c	261/273 (96%)	256 (98%)	5 (2%)	0	100	100
4	d	182/209 (87%)	181 (100%)	1 (0%)	0	100	100
5	e	189/201 (94%)	184 (97%)	5 (3%)	0	100	100
6	f	175/179 (98%)	163 (93%)	12 (7%)	0	100	100
7	i	140/142 (99%)	140 (100%)	0	0	100	100
8	j	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
9	k	142/144 (99%)	136 (96%)	6 (4%)	0	100	100
10	m	116/127 (91%)	109 (94%)	7 (6%)	0	100	100
11	n	114/117 (97%)	113 (99%)	1 (1%)	0	100	100
12	o	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
13	p	115/118 (98%)	115 (100%)	0	0	100	100
14	q	101/103 (98%)	96 (95%)	5 (5%)	0	100	100
15	r	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
16	s	91/100 (91%)	87 (96%)	4 (4%)	0	100	100
17	t	100/104 (96%)	93 (93%)	7 (7%)	0	100	100
18	u	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
19	v	73/85 (86%)	70 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	w	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
21	x	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
22	y	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
23	z	54/57 (95%)	54 (100%)	0	0	100	100
24	0	49/55 (89%)	49 (100%)	0	0	100	100
25	1	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
26	2	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
27	h	147/149 (99%)	126 (86%)	21 (14%)	0	100	100
All	All	2779/2916 (95%)	2676 (96%)	103 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	
3	c	212/218 (97%)	210 (99%)	2 (1%)	70	87
4	d	145/164 (88%)	145 (100%)	0	100	100
5	e	159/165 (96%)	159 (100%)	0	100	100
6	f	148/150 (99%)	146 (99%)	2 (1%)	59	81
7	i	116/116 (100%)	116 (100%)	0	100	100
8	j	104/104 (100%)	104 (100%)	0	100	100
9	k	103/103 (100%)	102 (99%)	1 (1%)	68	86
10	m	98/103 (95%)	98 (100%)	0	100	100
11	n	86/87 (99%)	86 (100%)	0	100	100
12	o	99/100 (99%)	98 (99%)	1 (1%)	68	86
13	p	89/90 (99%)	89 (100%)	0	100	100
14	q	84/84 (100%)	84 (100%)	0	100	100
15	r	93/93 (100%)	93 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	s	80/84 (95%)	80 (100%)	0	100	100
17	t	83/85 (98%)	83 (100%)	0	100	100
18	u	78/78 (100%)	78 (100%)	0	100	100
19	v	56/63 (89%)	56 (100%)	0	100	100
20	w	67/68 (98%)	67 (100%)	0	100	100
21	x	54/55 (98%)	53 (98%)	1 (2%)	50	75
22	y	48/49 (98%)	48 (100%)	0	100	100
23	z	47/48 (98%)	47 (100%)	0	100	100
24	0	46/49 (94%)	46 (100%)	0	100	100
25	1	38/38 (100%)	37 (97%)	1 (3%)	40	68
26	2	51/52 (98%)	49 (96%)	2 (4%)	28	55
27	h	114/114 (100%)	114 (100%)	0	100	100
All	All	2298/2360 (97%)	2288 (100%)	10 (0%)	81	93

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	c	125	LYS
3	c	270	ARG
6	f	69	LYS
6	f	162	SER
9	k	42	SER
12	o	11	GLU
21	x	47	ARG
25	1	45	SER
26	2	32	ILE
26	2	33	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
3	c	53	HIS
3	c	134	ASN
3	c	153	GLN
4	d	42	ASN
4	d	94	GLN
4	d	126	ASN

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Mol	Chain	Res	Type
5	e	92	HIS
5	e	94	GLN
6	f	5	HIS
6	f	21	ASN
8	j	13	ASN
8	j	88	ASN
9	k	35	HIS
10	m	73	ASN
12	o	3	ASN
12	o	75	GLN
13	p	72	ASN
14	q	86	GLN
15	r	9	HIS
16	s	28	ASN
17	t	74	ASN
18	u	49	ASN
19	v	12	ASN
23	z	6	ASN
27	h	73	ASN
27	h	133	GLN
27	h	145	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	2504/2904 (86%)	328 (13%)	0
2	b	118/120 (98%)	13 (11%)	0
All	All	2622/3024 (86%)	341 (13%)	0

All (341) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	10	A
1	a	15	G
1	a	34	U
1	a	42	A
1	a	45	G
1	a	51	G
1	a	58	G
1	a	63	A
1	a	71	A

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Mol	Chain	Res	Type
1	a	74	A
1	a	75	G
1	a	80	G
1	a	101	A
1	a	102	U
1	a	103	A
1	a	110	G
1	a	118	A
1	a	119	A
1	a	120	U
1	a	125	A
1	a	139	U
1	a	142	A
1	a	164	C
1	a	181	A
1	a	196	A
1	a	199	A
1	a	215	G
1	a	216	A
1	a	221	A
1	a	222	A
1	a	248	G
1	a	265	A
1	a	272	A
1	a	274	C
1	a	278	A
1	a	281	C
1	a	285	G
1	a	288	U
1	a	294	A
1	a	311	A
1	a	329	G
1	a	330	A
1	a	345	A
1	a	352	A
1	a	357	C
1	a	361	G
1	a	362	A
1	a	386	G
1	a	396	G
1	a	405	U
1	a	411	G

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Mol	Chain	Res	Type
1	a	412	A
1	a	455	C
1	a	481	G
1	a	491	G
1	a	501	A
1	a	504	A
1	a	505	A
1	a	508	A
1	a	509	C
1	a	512	G
1	a	513	A
1	a	532	A
1	a	545	U
1	a	546	U
1	a	547	A
1	a	549	G
1	a	563	A
1	a	569	U
1	a	573	U
1	a	575	A
1	a	588	U
1	a	603	A
1	a	614	A
1	a	615	U
1	a	627	A
1	a	637	A
1	a	645	C
1	a	647	G
1	a	654	A
1	a	655	A
1	a	664	G
1	a	667	U
1	a	685	A
1	a	686	U
1	a	712	G
1	a	716	A
1	a	717	C
1	a	721	A
1	a	723	C
1	a	730	A
1	a	738	G
1	a	747	5MU

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Mol	Chain	Res	Type
1	a	764	A
1	a	775	G
1	a	776	G
1	a	782	A
1	a	784	G
1	a	785	G
1	a	792	A
1	a	805	G
1	a	812	C
1	a	827	U
1	a	828	U
1	a	845	A
1	a	846	U
1	a	847	U
1	a	857	G
1	a	859	G
1	a	903	C
1	a	905	A
1	a	907	G
1	a	910	A
1	a	914	G
1	a	915	C
1	a	946	C
1	a	958	U
1	a	961	C
1	a	974	G
1	a	983	A
1	a	989	G
1	a	996	A
1	a	1005	C
1	a	1012	U
1	a	1013	C
1	a	1016	G
1	a	1026	G
1	a	1028	A
1	a	1033	U
1	a	1122	G
1	a	1130	U
1	a	1132	U
1	a	1133	A
1	a	1134	A
1	a	1135	C

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Mol	Chain	Res	Type
1	a	1142	A
1	a	1169	A
1	a	1171	G
1	a	1250	G
1	a	1253	A
1	a	1256	G
1	a	1271	G
1	a	1272	A
1	a	1288	G
1	a	1300	G
1	a	1301	A
1	a	1306	C
1	a	1321	A
1	a	1329	U
1	a	1352	U
1	a	1365	A
1	a	1378	A
1	a	1379	U
1	a	1383	A
1	a	1386	C
1	a	1395	A
1	a	1410	G
1	a	1411	U
1	a	1416	G
1	a	1417	C
1	a	1419	A
1	a	1421	G
1	a	1427	A
1	a	1428	C
1	a	1437	C
1	a	1452	G
1	a	1453	A
1	a	1460	U
1	a	1482	G
1	a	1493	C
1	a	1508	A
1	a	1509	A
1	a	1510	G
1	a	1515	A
1	a	1533	C
1	a	1534	U
1	a	1535	A

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Mol	Chain	Res	Type
1	a	1536	C
1	a	1537	G
1	a	1544	A
1	a	1554	U
1	a	1566	A
1	a	1569	A
1	a	1578	U
1	a	1584	U
1	a	1585	C
1	a	1608	A
1	a	1613	G
1	a	1634	A
1	a	1647	U
1	a	1648	U
1	a	1649	G
1	a	1664	A
1	a	1667	G
1	a	1674	G
1	a	1715	G
1	a	1729	U
1	a	1730	C
1	a	1732	C
1	a	1738	G
1	a	1744	A
1	a	1764	C
1	a	1773	A
1	a	1786	A
1	a	1800	C
1	a	1801	A
1	a	1808	A
1	a	1816	C
1	a	1829	A
1	a	1847	A
1	a	1858	A
1	a	1868	C
1	a	1870	C
1	a	1871	A
1	a	1872	A
1	a	1873	G
1	a	1906	G
1	a	1907	G
1	a	1912	A

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Mol	Chain	Res	Type
1	a	1917	PSU
1	a	1929	G
1	a	1930	G
1	a	1931	U
1	a	1967	C
1	a	1970	A
1	a	1971	U
1	a	1972	G
1	a	1991	U
1	a	1993	U
1	a	2023	C
1	a	2030	6MZ
1	a	2031	A
1	a	2032	G
1	a	2033	A
1	a	2043	C
1	a	2049	G
1	a	2069	G7M
1	a	2070	A
1	a	2080	A
1	a	2093	G
1	a	2095	A
1	a	2096	C
1	a	2098	U
1	a	2100	G
1	a	2101	A
1	a	2189	U
1	a	2198	A
1	a	2203	U
1	a	2204	G
1	a	2211	A
1	a	2225	A
1	a	2238	G
1	a	2239	G
1	a	2268	A
1	a	2279	G
1	a	2283	C
1	a	2287	A
1	a	2288	A
1	a	2305	U
1	a	2307	G
1	a	2308	G

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Mol	Chain	Res	Type
1	a	2309	A
1	a	2312	U
1	a	2314	A
1	a	2322	A
1	a	2325	G
1	a	2333	A
1	a	2334	U
1	a	2335	A
1	a	2344	U
1	a	2345	G
1	a	2347	C
1	a	2350	C
1	a	2357	G
1	a	2358	A
1	a	2361	G
1	a	2377	A
1	a	2383	G
1	a	2385	C
1	a	2392	A
1	a	2402	U
1	a	2403	C
1	a	2406	A
1	a	2422	C
1	a	2425	A
1	a	2429	G
1	a	2435	A
1	a	2441	U
1	a	2446	G
1	a	2612	C
1	a	2613	U
1	a	2615	U
1	a	2629	U
1	a	2630	G
1	a	2639	A
1	a	2646	C
1	a	2656	U
1	a	2661	G
1	a	2671	G
1	a	2681	C
1	a	2689	U
1	a	2690	U
1	a	2714	G

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Mol	Chain	Res	Type
1	a	2716	C
1	a	2726	A
1	a	2733	A
1	a	2744	G
1	a	2748	A
1	a	2752	C
1	a	2757	A
1	a	2765	A
1	a	2778	A
1	a	2790	U
1	a	2798	U
1	a	2818	U
1	a	2820	A
1	a	2821	A
1	a	2833	U
1	a	2835	A
1	a	2849	U
1	a	2861	U
1	a	2872	A
1	a	2873	A
1	a	2879	A
1	a	2884	U
1	a	2891	U
1	a	2899	A
1	a	2902	C
2	b	9	G
2	b	13	G
2	b	24	G
2	b	27	C
2	b	35	C
2	b	36	C
2	b	56	G
2	b	58	A
2	b	67	G
2	b	89	U
2	b	90	C
2	b	99	A
2	b	109	A

There are no RNA pucker outliers to report.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	a	955	1	18,21,22	1.03	1 (5%)	22,30,33	2.03	5 (22%)
1	PSU	a	1917	1	18,21,22	1.11	1 (5%)	22,30,33	1.71	5 (22%)
1	PSU	a	746	1	18,21,22	1.00	2 (11%)	22,30,33	2.13	5 (22%)
1	6MZ	a	2030	1	22,25,26	1.36	4 (18%)	30,36,39	2.32	11 (36%)
1	5MU	a	747	1	19,22,23	1.42	4 (21%)	28,32,35	2.16	6 (21%)
1	2MG	a	1835	1	23,26,27	1.32	3 (13%)	32,38,41	2.27	9 (28%)
1	G7M	a	2069	1	23,26,27	1.57	4 (17%)	35,39,42	1.68	5 (14%)
1	OMG	a	2251	1	23,26,27	1.22	3 (13%)	33,38,41	1.98	7 (21%)
1	PSU	a	1911	1	18,21,22	1.09	1 (5%)	22,30,33	1.91	5 (22%)
1	6MZ	a	1618	1	22,25,26	1.43	4 (18%)	30,36,39	2.28	10 (33%)
1	1MG	a	745	1	22,26,27	1.12	3 (13%)	33,39,42	1.75	6 (18%)
1	2MG	a	2445	1	23,26,27	1.35	3 (13%)	32,38,41	2.21	7 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	a	955	1	-	0/7/25/26	0/2/2/2
1	PSU	a	1917	1	-	2/7/25/26	0/2/2/2
1	PSU	a	746	1	-	0/7/25/26	0/2/2/2
1	6MZ	a	2030	1	-	2/9/27/28	0/3/3/3
1	5MU	a	747	1	-	2/7/25/26	0/2/2/2
1	G7M	a	2069	1	3/3/5/5	1/7/25/26	0/3/3/3
1	2MG	a	1835	1	-	2/9/27/28	0/3/3/3
1	OMG	a	2251	1	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	a	1911	1	-	2/7/25/26	0/2/2/2
1	6MZ	a	1618	1	-	0/9/27/28	0/3/3/3
1	1MG	a	745	1	-	0/7/25/26	0/3/3/3
1	2MG	a	2445	1	-	0/9/27/28	0/3/3/3

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	2069	G7M	C5-N7	-5.32	1.33	1.39
1	a	1911	PSU	C6-C5	3.53	1.39	1.35
1	a	1917	PSU	C6-C5	3.53	1.39	1.35
1	a	1618	6MZ	C5-C4	3.44	1.45	1.39
1	a	2030	6MZ	C5-C4	3.38	1.45	1.39
1	a	747	5MU	C4-N3	-3.38	1.32	1.38
1	a	2445	2MG	C6-N1	-3.13	1.33	1.38
1	a	1618	6MZ	C5-N7	-3.05	1.33	1.39
1	a	2251	OMG	C5-C4	2.98	1.47	1.38
1	a	1835	2MG	C6-N1	-2.96	1.33	1.38
1	a	747	5MU	C6-N1	-2.95	1.33	1.38
1	a	745	1MG	C5-N7	-2.85	1.33	1.39
1	a	1618	6MZ	C4-N9	-2.81	1.31	1.37
1	a	2030	6MZ	C4-N9	-2.79	1.31	1.37
1	a	955	PSU	C6-C5	2.78	1.38	1.35
1	a	2069	G7M	C6-N1	-2.78	1.33	1.38
1	a	747	5MU	C2-N3	-2.71	1.33	1.38
1	a	2445	2MG	C5-C4	2.67	1.46	1.38
1	a	1835	2MG	C5-C4	2.66	1.46	1.38
1	a	2251	OMG	C6-N1	-2.65	1.33	1.38
1	a	2445	2MG	C5-N7	-2.64	1.34	1.39
1	a	1835	2MG	C5-N7	-2.63	1.34	1.39
1	a	2030	6MZ	C5-N7	-2.60	1.34	1.39
1	a	2069	G7M	C5-C4	2.55	1.44	1.38
1	a	745	1MG	C5-C4	2.51	1.45	1.38
1	a	1618	6MZ	C8-N9	-2.45	1.33	1.37
1	a	746	PSU	C6-C5	2.31	1.38	1.35
1	a	2251	OMG	C5-N7	-2.31	1.34	1.39
1	a	746	PSU	C4-C5	-2.23	1.37	1.44
1	a	2069	G7M	C4-N9	-2.20	1.32	1.38
1	a	2030	6MZ	C8-N9	-2.16	1.33	1.37
1	a	745	1MG	C4-N9	-2.13	1.32	1.38
1	a	747	5MU	C6-C5	2.01	1.37	1.34

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1835	2MG	C2-N3-C4	7.25	121.02	112.04
1	a	2445	2MG	C2-N3-C4	6.99	120.71	112.04
1	a	2251	OMG	C5-C4-N3	-6.38	118.11	128.46
1	a	2445	2MG	C5-C4-N3	-6.34	118.17	128.46
1	a	1835	2MG	C5-C4-N3	-6.28	118.27	128.46
1	a	1618	6MZ	C5-C4-N3	-5.57	119.49	126.75
1	a	1618	6MZ	C9-N6-C6	-5.42	118.20	122.87
1	a	955	PSU	N1-C2-N3	5.36	121.20	115.13
1	a	747	5MU	C4-N3-C2	-5.32	120.46	127.35
1	a	746	PSU	C4-N3-C2	-5.31	118.69	126.34
1	a	746	PSU	N1-C2-N3	5.22	121.04	115.13
1	a	745	1MG	C5-C4-N3	-5.13	120.14	128.46
1	a	2251	OMG	C2-N3-C4	5.06	121.32	112.30
1	a	2030	6MZ	C5-C4-N3	-5.01	120.22	126.75
1	a	747	5MU	N3-C2-N1	4.98	121.51	114.89
1	a	2030	6MZ	C9-N6-C6	-4.98	118.58	122.87
1	a	1911	PSU	C4-N3-C2	-4.97	119.17	126.34
1	a	955	PSU	C4-N3-C2	-4.96	119.19	126.34
1	a	2069	G7M	N9-C4-N3	4.87	135.71	125.94
1	a	2069	G7M	C5-C4-N3	-4.78	118.98	128.15
1	a	2445	2MG	N9-C4-N3	4.78	135.53	125.94
1	a	2251	OMG	N9-C4-N3	4.77	135.52	125.94
1	a	1911	PSU	N1-C2-N3	4.74	120.50	115.13
1	a	747	5MU	C5-C4-N3	4.64	119.27	115.31
1	a	1835	2MG	N9-C4-N3	4.59	135.15	125.94
1	a	745	1MG	C2-N3-C4	4.40	121.87	111.98
1	a	2069	G7M	C2-N3-C4	4.37	120.09	112.30
1	a	1618	6MZ	N3-C4-N9	4.37	134.28	127.08
1	a	1917	PSU	N1-C2-N3	4.31	120.02	115.13
1	a	747	5MU	O4-C4-C5	-4.18	120.06	124.90
1	a	2030	6MZ	N3-C4-N9	4.14	133.91	127.08
1	a	2030	6MZ	C6-C5-N7	4.10	136.83	132.39
1	a	1917	PSU	C4-N3-C2	-4.09	120.44	126.34
1	a	745	1MG	N9-C4-N3	4.06	134.09	125.94
1	a	747	5MU	C5-C6-N1	-4.01	119.21	123.34
1	a	2030	6MZ	C4-N9-C8	3.80	109.84	105.73
1	a	1618	6MZ	C2-N3-C4	3.76	120.63	111.75
1	a	1618	6MZ	C6-C5-N7	3.73	136.43	132.39
1	a	2030	6MZ	C2-N3-C4	3.62	120.29	111.75
1	a	2030	6MZ	N1-C2-N3	-3.55	123.04	128.60
1	a	746	PSU	O2-C2-N1	-3.33	119.13	122.79
1	a	1618	6MZ	N1-C2-N3	-3.23	123.56	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1835	2MG	C6-C5-N7	3.20	136.19	130.25
1	a	746	PSU	C6-C5-C4	3.09	120.36	118.20
1	a	1618	6MZ	C4-C5-N7	-3.07	106.87	110.62
1	a	2030	6MZ	C4-C5-N7	-3.06	106.89	110.62
1	a	2251	OMG	C6-C5-N7	3.03	135.89	130.25
1	a	1618	6MZ	C4-N9-C8	2.98	108.96	105.73
1	a	955	PSU	O2-C2-N1	-2.92	119.58	122.79
1	a	2030	6MZ	N9-C8-N7	-2.85	110.02	113.91
1	a	2445	2MG	C6-C5-N7	2.84	135.53	130.25
1	a	1917	PSU	O2-C2-N1	-2.83	119.68	122.79
1	a	1835	2MG	C4-C5-N7	-2.76	106.35	110.72
1	a	1917	PSU	C6-N1-C2	-2.75	119.87	122.68
1	a	955	PSU	C6-N1-C2	-2.75	119.87	122.68
1	a	2030	6MZ	C5-N7-C8	2.72	107.38	103.51
1	a	745	1MG	C6-C5-N7	2.67	135.39	129.35
1	a	1835	2MG	CM2-N2-C2	-2.65	118.00	123.86
1	a	2069	G7M	O6-C6-C5	-2.64	122.10	128.06
1	a	1835	2MG	C2-N1-C6	-2.64	121.44	124.48
1	a	747	5MU	O2-C2-N1	-2.64	119.28	122.79
1	a	1911	PSU	O2-C2-N1	-2.60	119.93	122.79
1	a	2445	2MG	C4-C5-N7	-2.59	106.63	110.72
1	a	955	PSU	C6-C5-C4	2.52	119.96	118.20
1	a	2251	OMG	C4-C5-N7	-2.51	106.74	110.72
1	a	1618	6MZ	C5-N7-C8	2.48	107.04	103.51
1	a	1911	PSU	O4'-C1'-C2'	2.37	108.49	105.14
1	a	2445	2MG	C2-N1-C6	-2.32	121.81	124.48
1	a	745	1MG	C4-C5-N7	-2.30	107.07	110.72
1	a	746	PSU	C6-N1-C2	-2.24	120.39	122.68
1	a	1618	6MZ	N9-C8-N7	-2.21	110.89	113.91
1	a	745	1MG	C6-C5-C4	-2.20	117.54	119.97
1	a	2069	G7M	C5-C6-N1	2.17	116.32	111.79
1	a	1911	PSU	C6-C5-C4	2.12	119.68	118.20
1	a	2251	OMG	O6-C6-C5	-2.12	120.98	126.60
1	a	1917	PSU	O4'-C1'-C2'	2.09	108.09	105.14
1	a	2445	2MG	O6-C6-C5	-2.09	121.06	126.60
1	a	1835	2MG	O6-C6-C5	-2.06	121.13	126.60
1	a	1835	2MG	C5-C6-N1	2.05	118.41	113.19
1	a	2030	6MZ	C2-N1-C6	2.04	122.11	115.25
1	a	2251	OMG	C5-C6-N1	2.03	118.33	113.19

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	a	2069	G7M	C2'
1	a	2069	G7M	C4'
1	a	2069	G7M	C3'

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	a	1917	PSU	C3'-C4'-C5'-O5'
1	a	1917	PSU	O4'-C4'-C5'-O5'
1	a	747	5MU	C3'-C4'-C5'-O5'
1	a	747	5MU	O4'-C4'-C5'-O5'
1	a	2030	6MZ	O4'-C4'-C5'-O5'
1	a	2030	6MZ	C3'-C4'-C5'-O5'
1	a	1911	PSU	C3'-C4'-C5'-O5'
1	a	1835	2MG	O4'-C4'-C5'-O5'
1	a	1835	2MG	C3'-C4'-C5'-O5'
1	a	1911	PSU	O4'-C4'-C5'-O5'
1	a	2069	G7M	O4'-C4'-C5'-O5'

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	a	1917	PSU	1	0
1	a	2030	6MZ	1	0
1	a	747	5MU	1	0
1	a	1835	2MG	1	0
1	a	2069	G7M	1	0
1	a	2251	OMG	1	0
1	a	1911	PSU	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 210 ligands modelled in this entry, 210 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

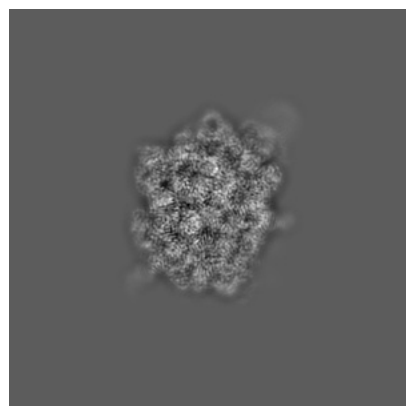
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35939. These allow visual inspection of the internal detail of the map and identification of artifacts.

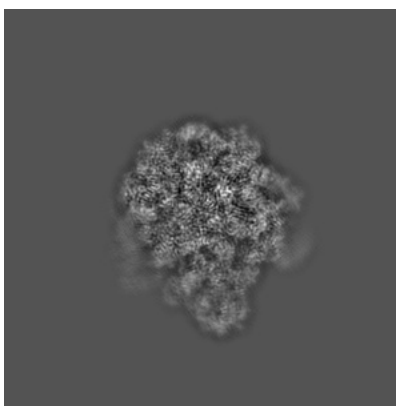
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

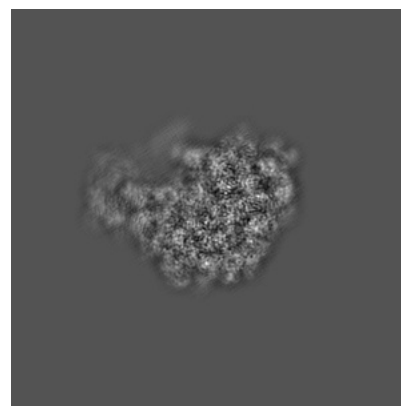
6.1.1 Primary map



X

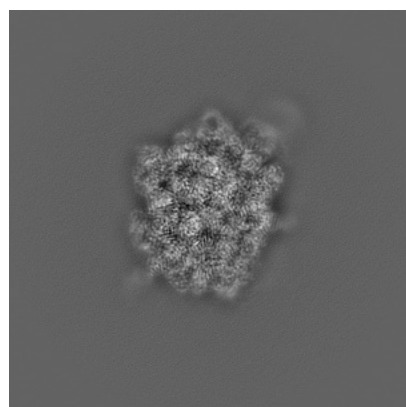


Y

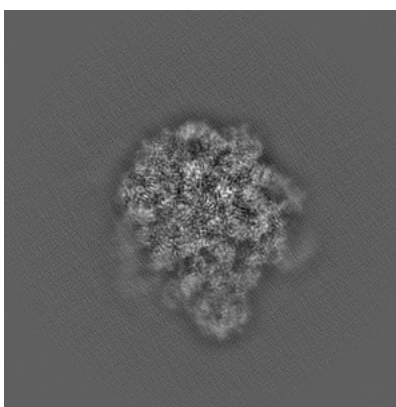


Z

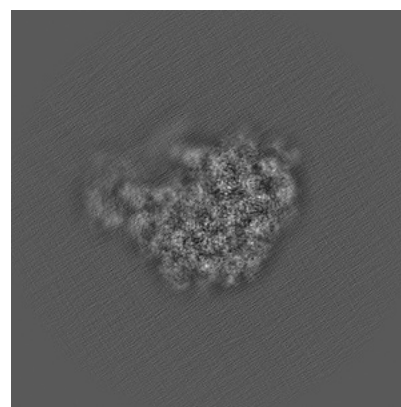
6.1.2 Raw map



X



Y

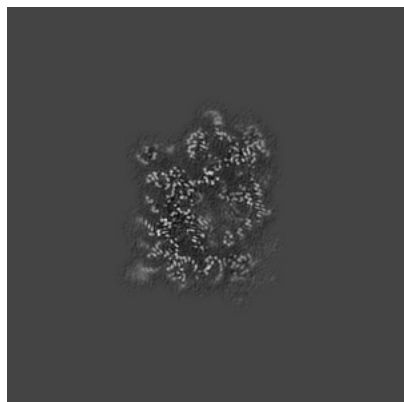


Z

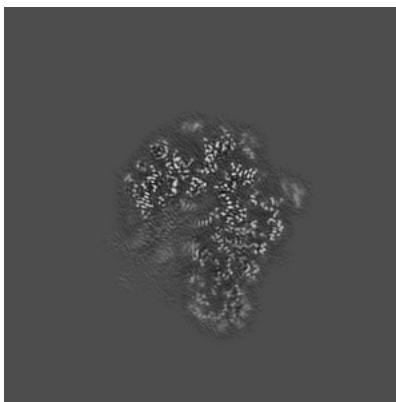
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

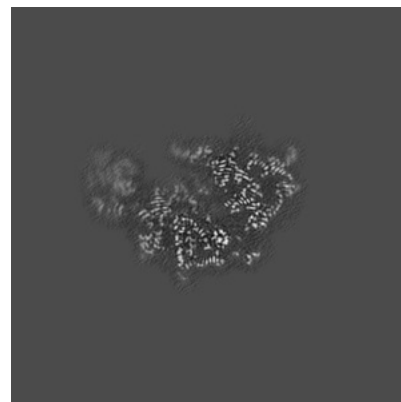
6.2.1 Primary map



X Index: 192

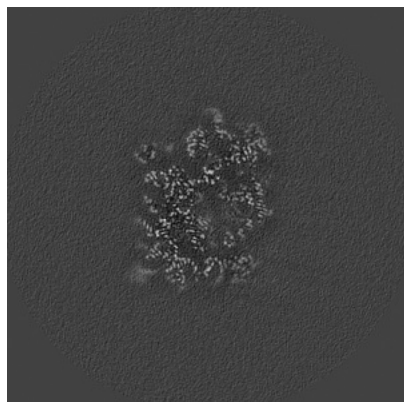


Y Index: 192

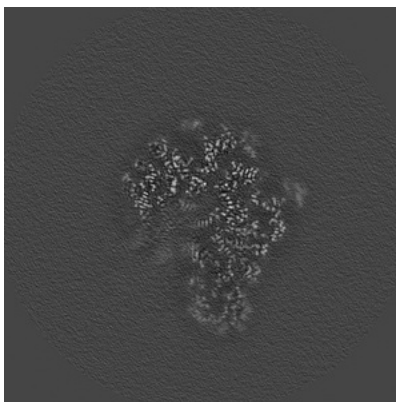


Z Index: 192

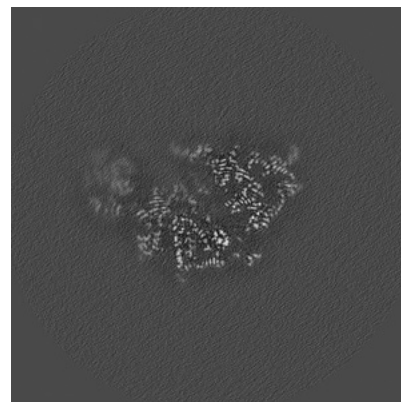
6.2.2 Raw map



X Index: 192



Y Index: 192

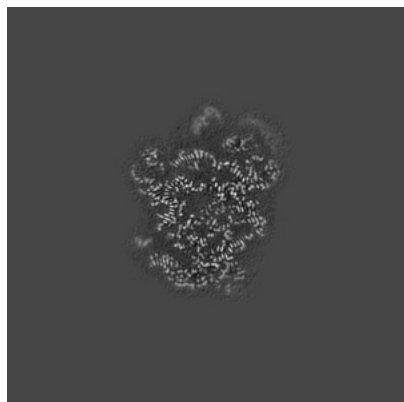


Z Index: 192

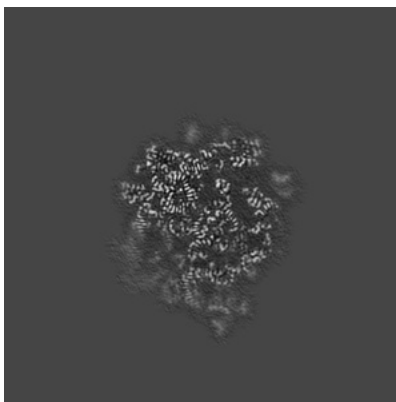
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

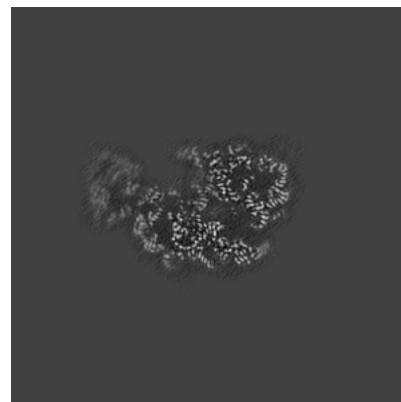
6.3.1 Primary map



X Index: 205

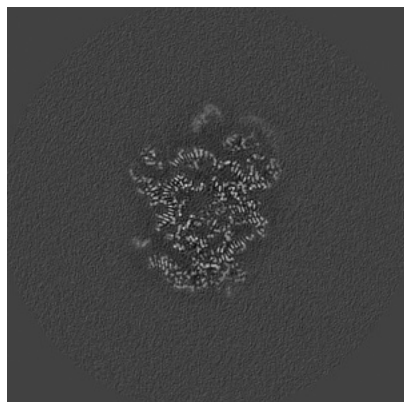


Y Index: 179

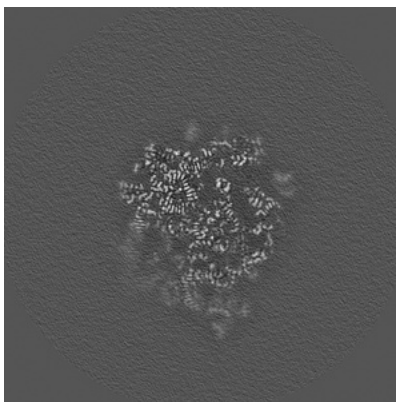


Z Index: 199

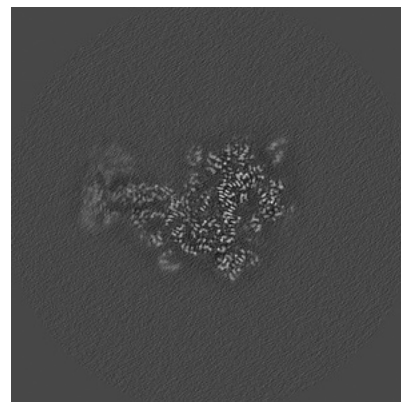
6.3.2 Raw map



X Index: 205



Y Index: 179

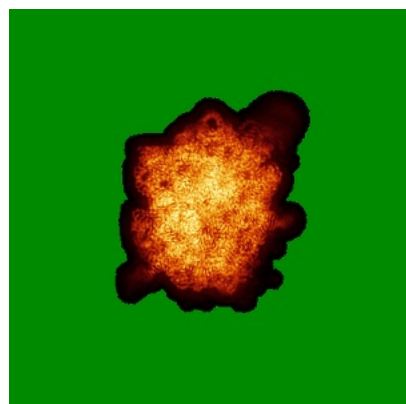


Z Index: 209

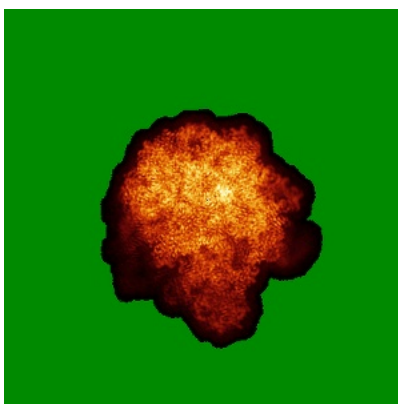
The images above show the largest variance slices of the map in three orthogonal directions.

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

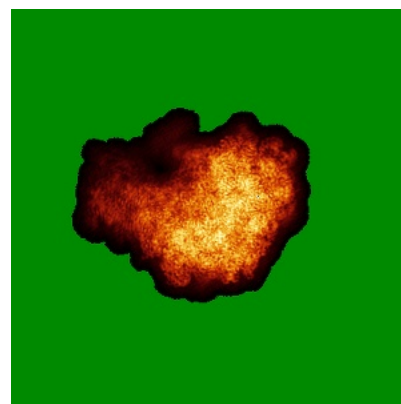
6.4.1 Primary map



X

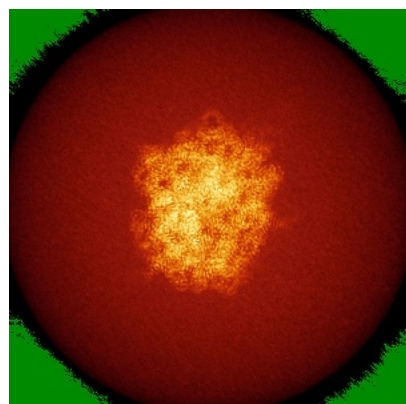


Y

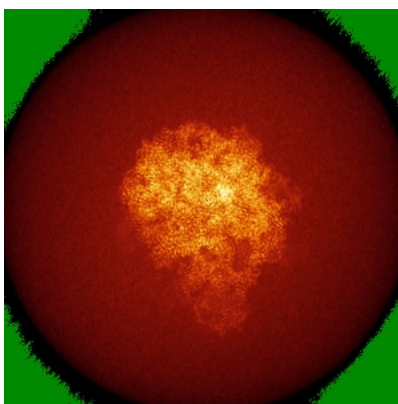


Z

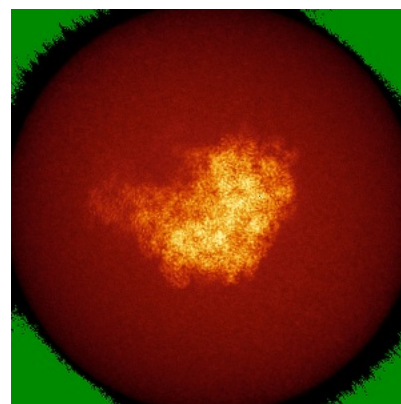
6.4.2 Raw map



X



Y

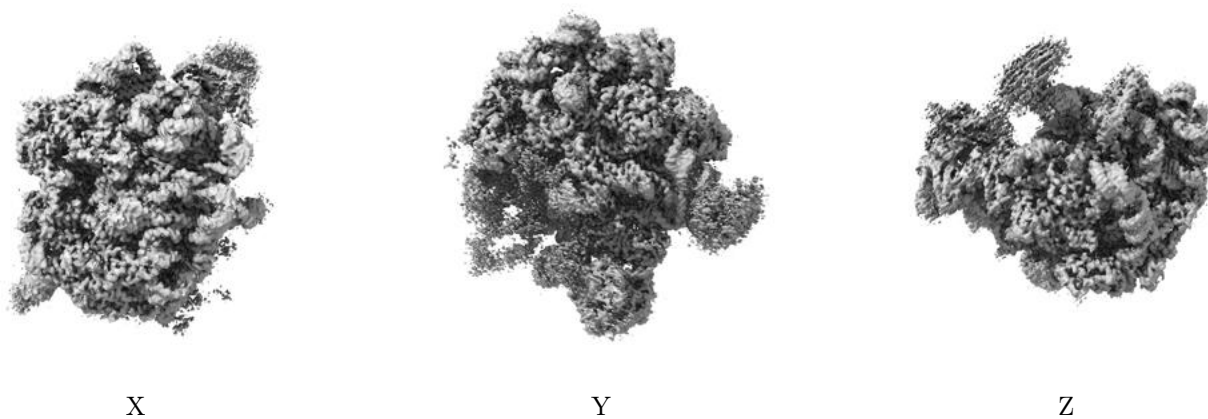


Z

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.

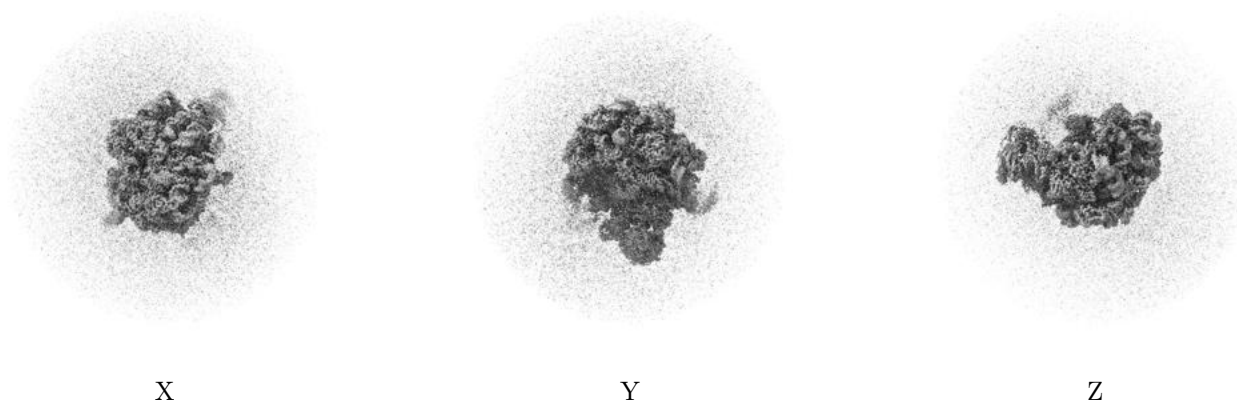
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. 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.

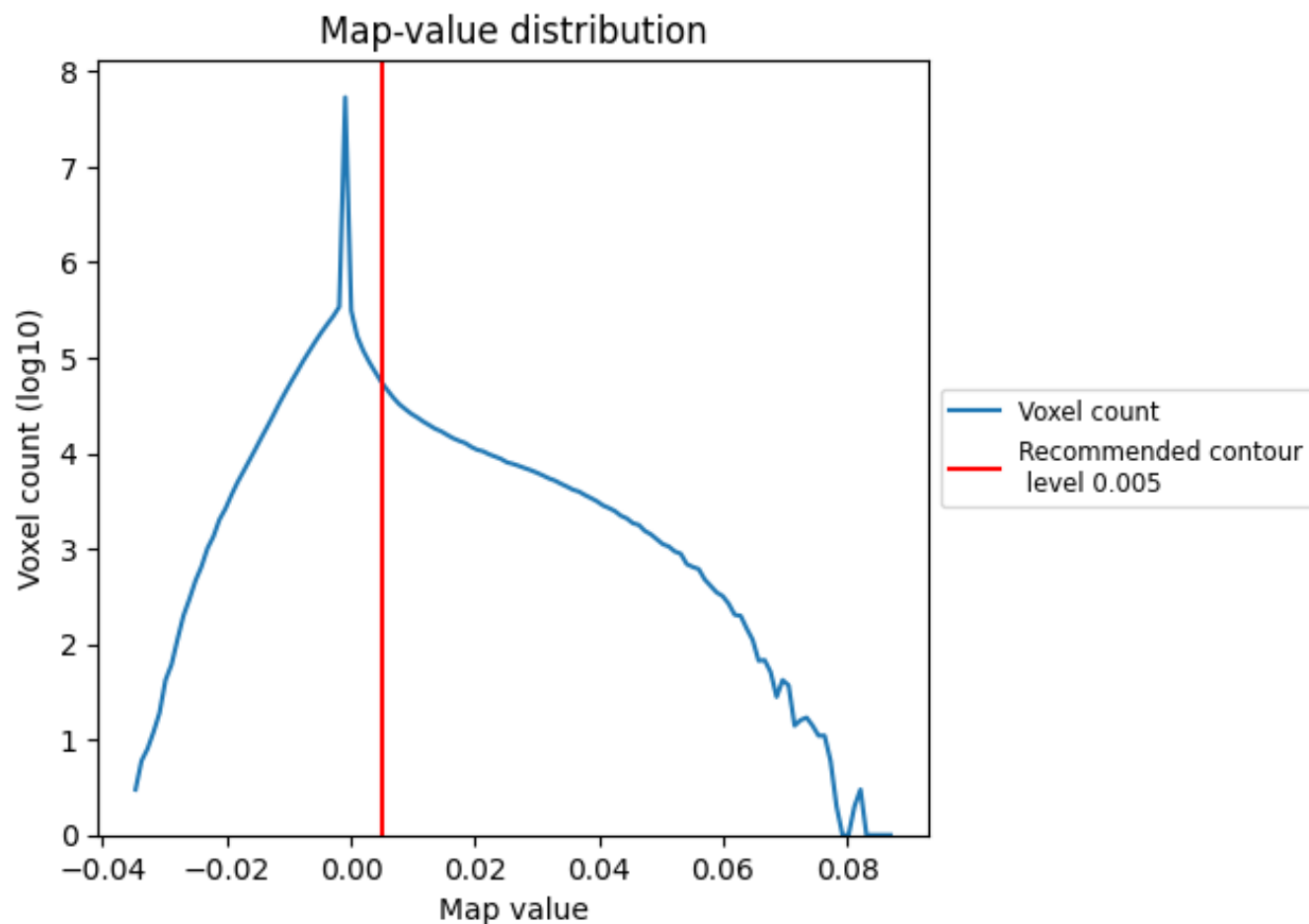
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

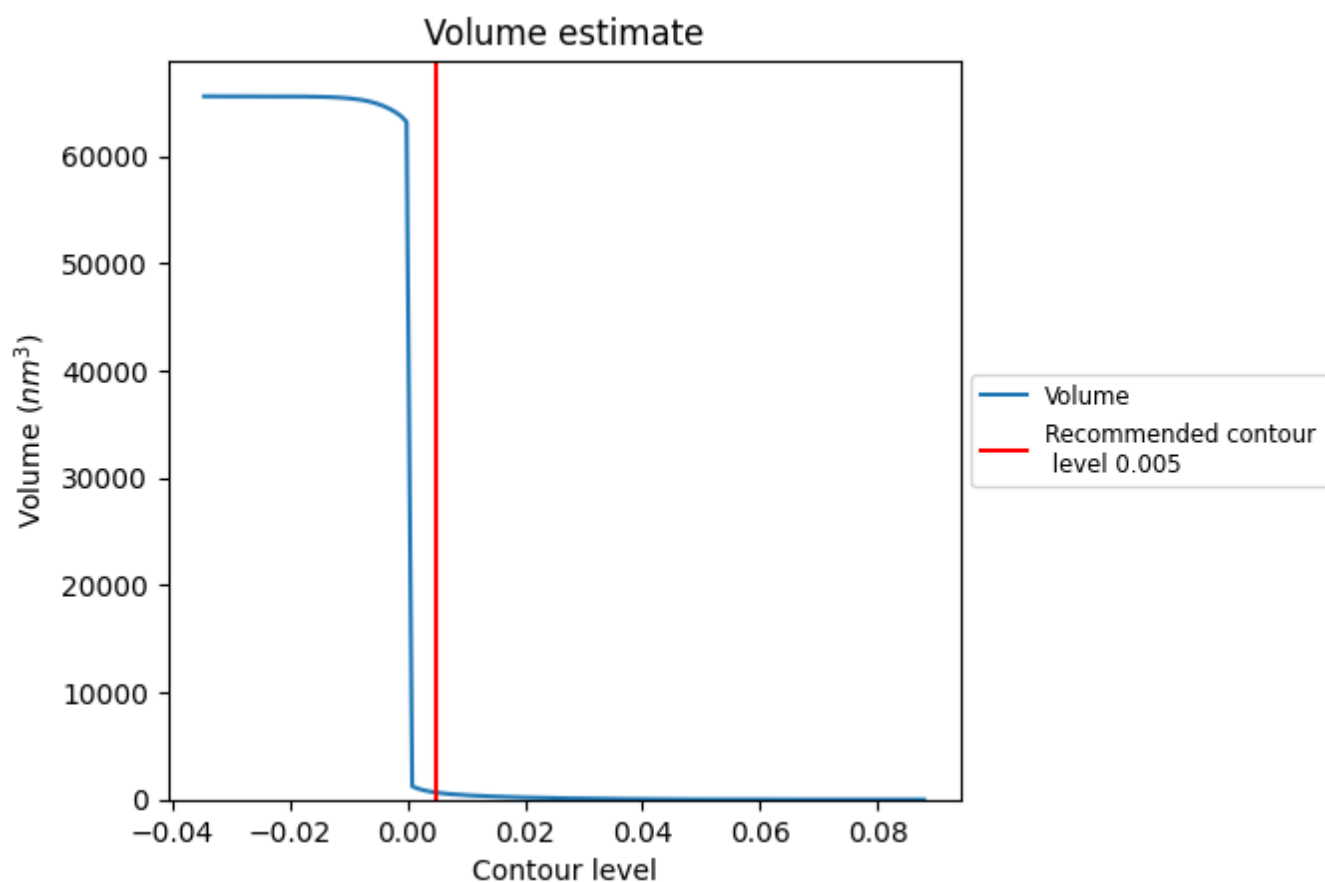
This section contains the results of statistical analysis of the map.

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.

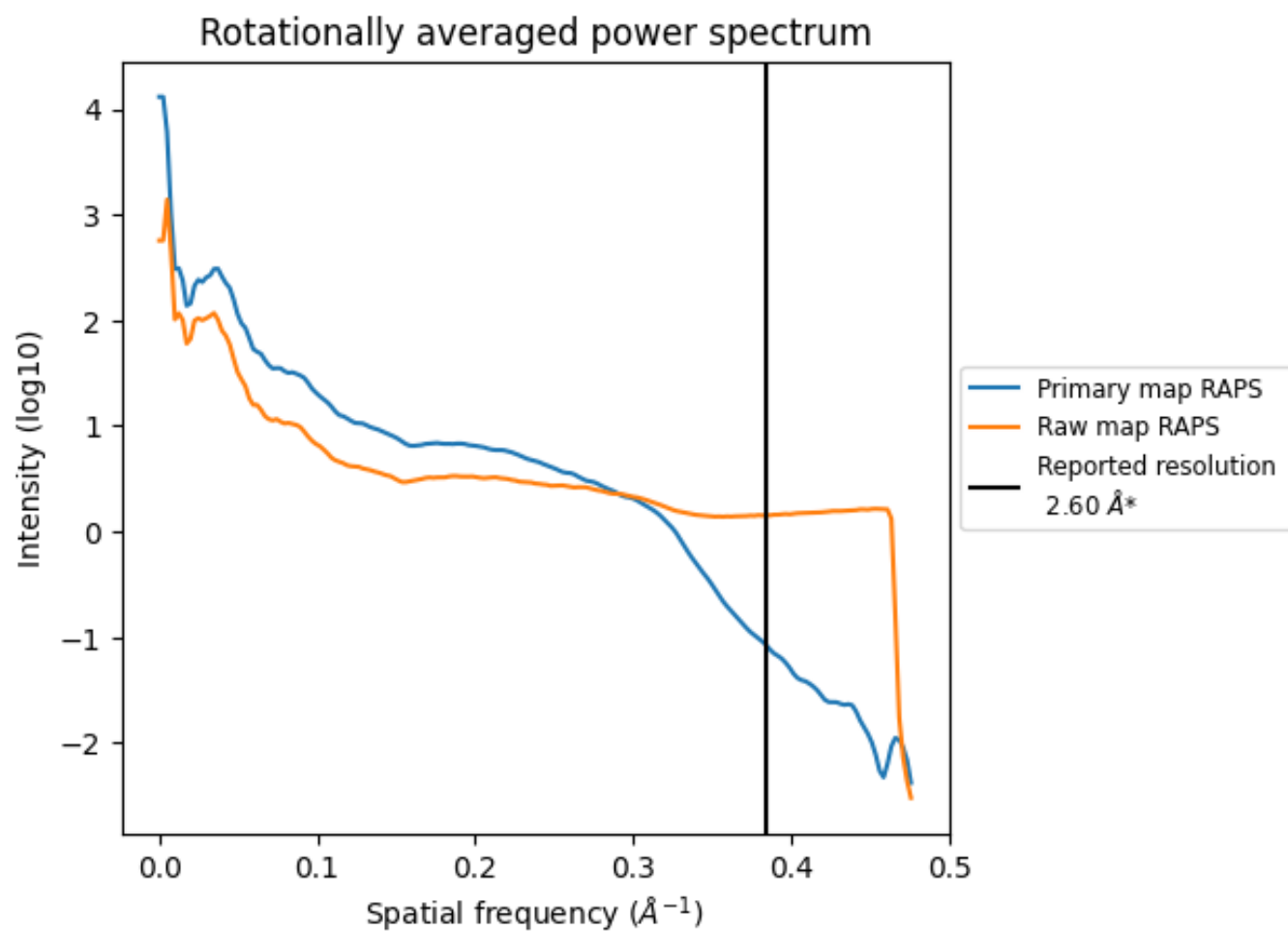
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 647 nm^3 ; this corresponds to an approximate mass of 584 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 ⓘ

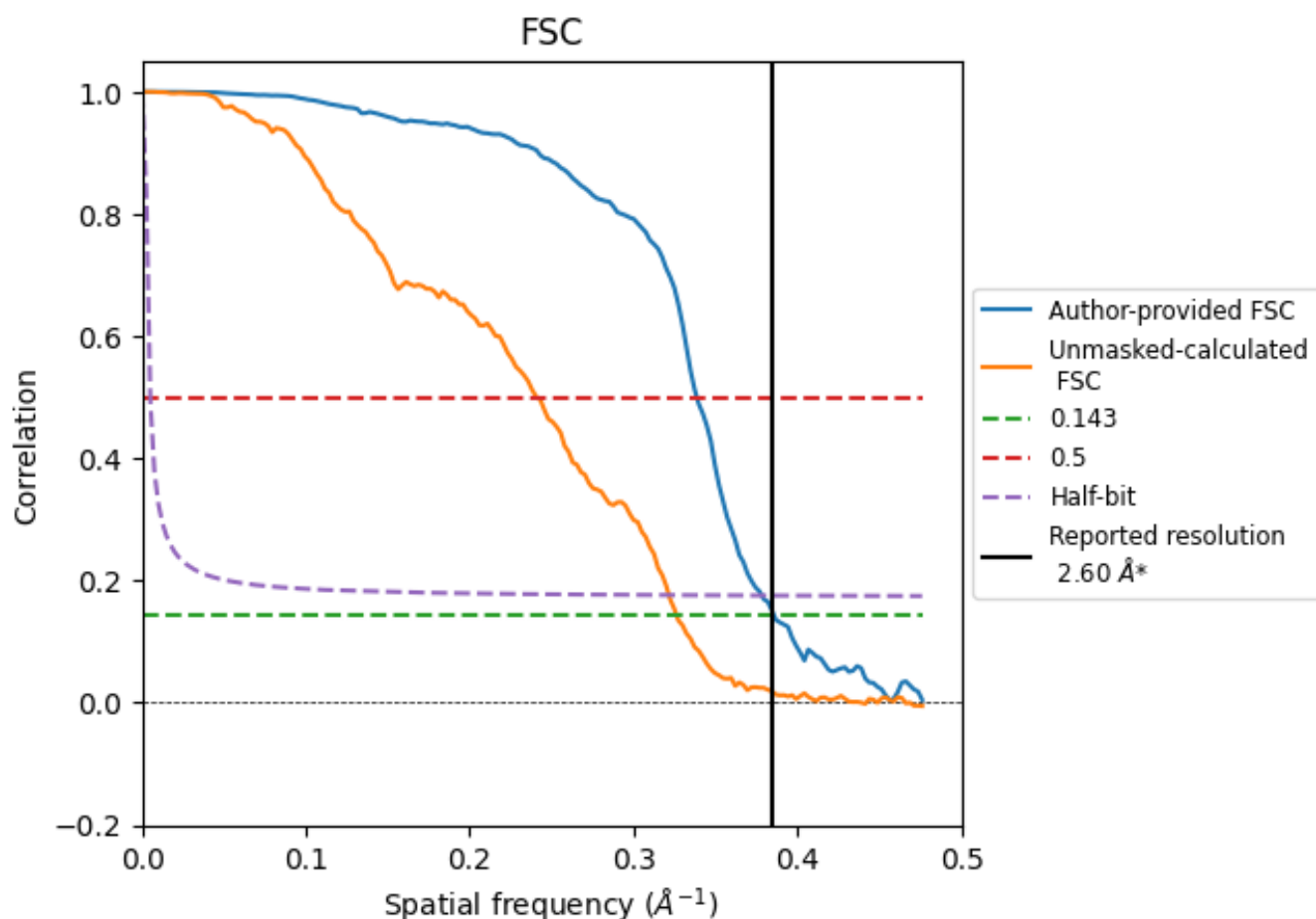


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

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 0.385 $\text{\AA}^{-1}$

8.2 Resolution estimates

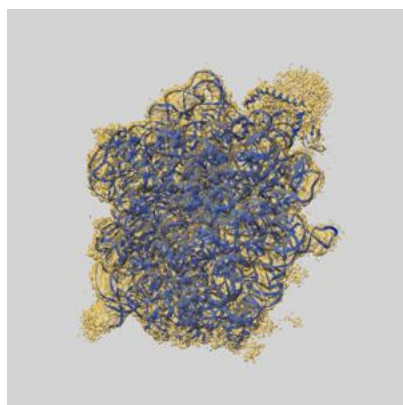
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.59	2.95	2.64
Unmasked-calculated*	3.06	4.15	3.11

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.06 differs from the reported value 2.6 by more than 10 %

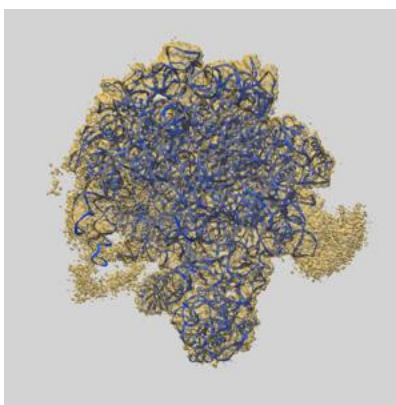
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-35939 and PDB model 8J1Z. Per-residue inclusion information can be found in section 3 on page 11.

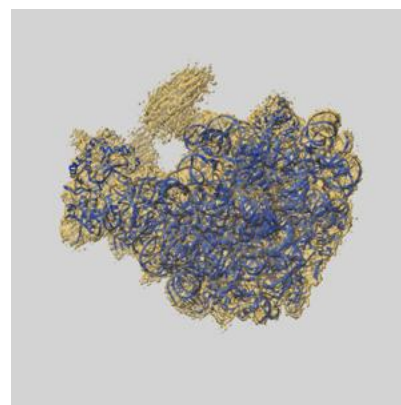
9.1 Map-model overlay [i](#)



X



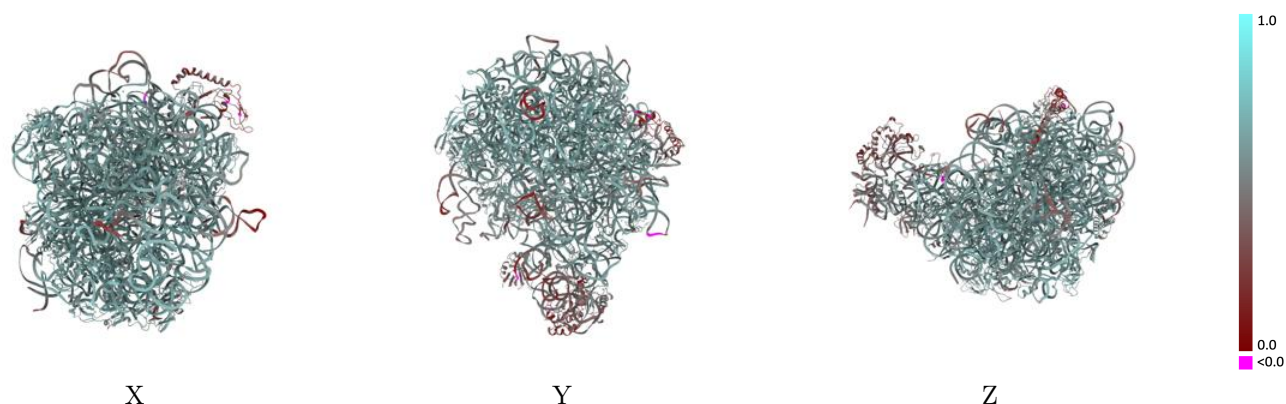
Y



Z

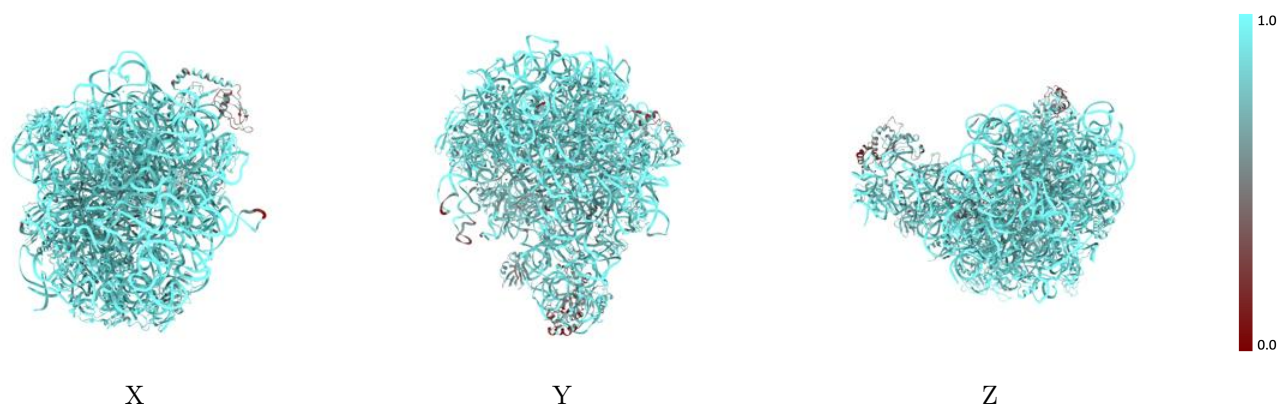
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



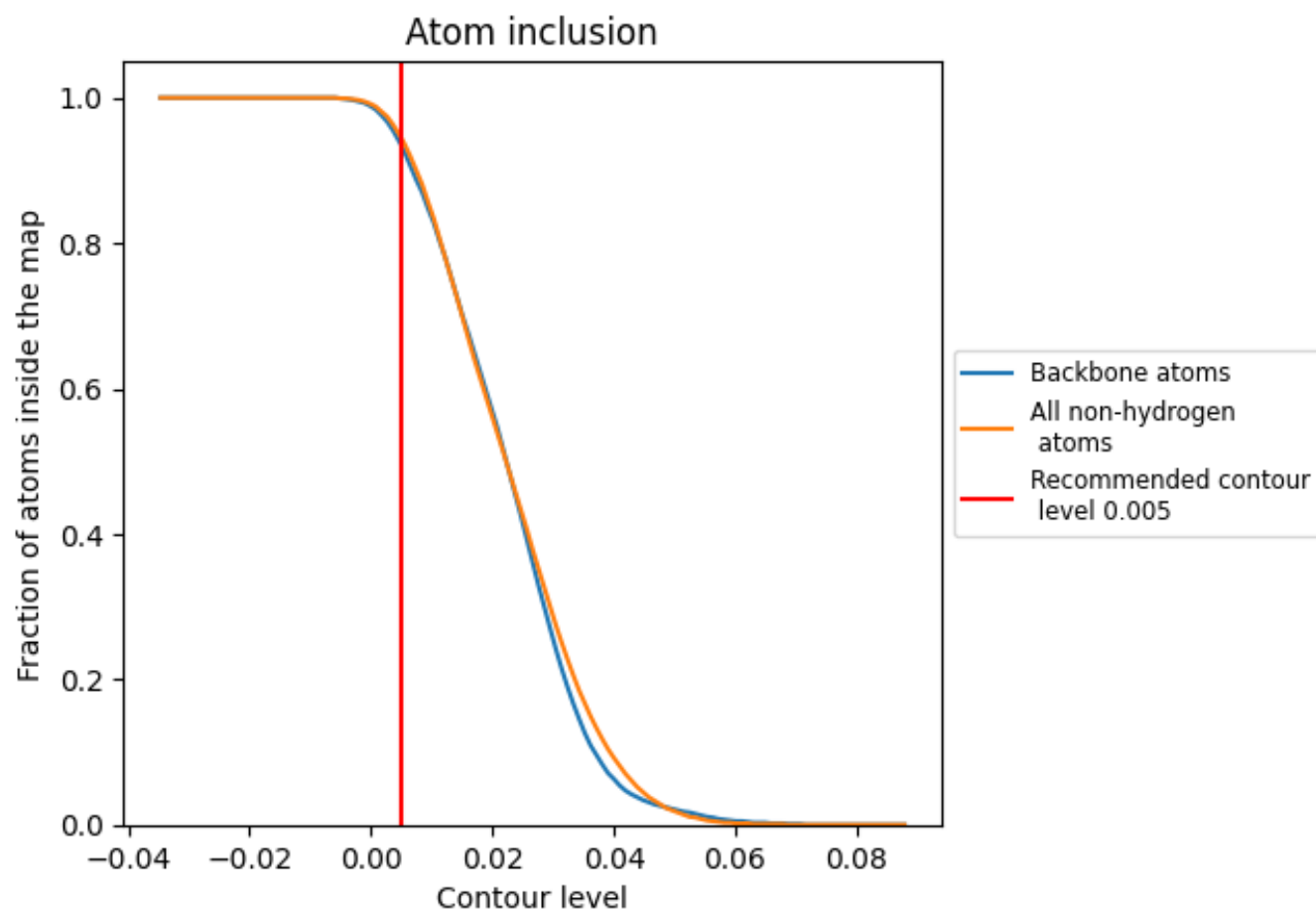
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.005).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 94% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9450	 0.5820
0	 0.7510	 0.5440
1	 0.9490	 0.6370
2	 0.7350	 0.6080
a	 0.9750	 0.5950
b	 0.9390	 0.4940
c	 0.9420	 0.6210
d	 0.9480	 0.6120
e	 0.9370	 0.5910
f	 0.5340	 0.3220
h	 0.6290	 0.3420
i	 0.9370	 0.6090
j	 0.9020	 0.5730
k	 0.9160	 0.5950
m	 0.9700	 0.6350
n	 0.8510	 0.4790
o	 0.9230	 0.5860
p	 0.9640	 0.6350
q	 0.9560	 0.6090
r	 0.9410	 0.6230
s	 0.9240	 0.5990
t	 0.9560	 0.5880
u	 0.7210	 0.3970
v	 0.8830	 0.5820
w	 0.9300	 0.6100
x	 0.9300	 0.5640
y	 0.9200	 0.5810
z	 0.9370	 0.6130

