Full wwPDB EM Validation Report ⓘ

Nov 7, 2026 – 01:28 pm GMT

PDB ID	:	32PD / pdb_000032pd
EMDB ID	:	EMD-59046
Title	:	Structural characterization of hibernating ribosomes in the Gram-negative pathogen Acinetobacter baumannii with E-site tRNA and no bS21
Authors	:	Vasanthakrishnan, R.K.B.S.; Olivier, D.; Sophie, C.; Yann, L.C.; Sylvie, G.D.; Sassi, M.; Emmanuel, G.; Reynald, G.
Deposited on	:	2026-07-19
Resolution	:	2.70 Å(reported)
Based on initial model	:	8B0X

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:

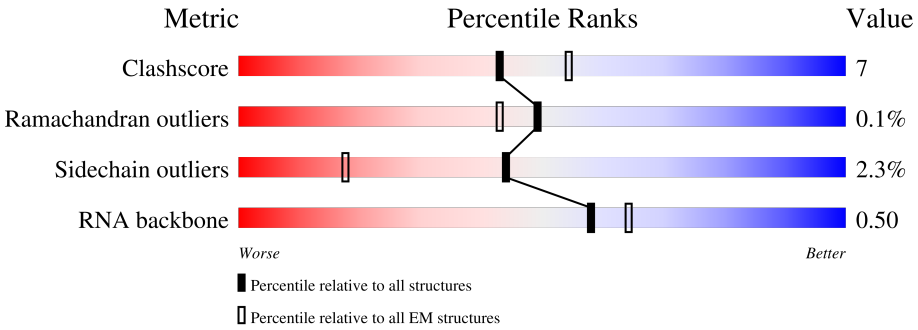
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

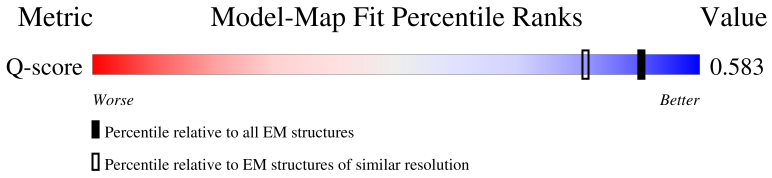
1 Overall quality at a glance

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

The reported resolution of this entry is 2.70 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.





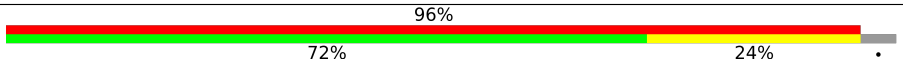
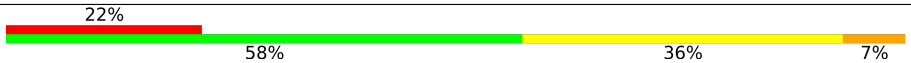
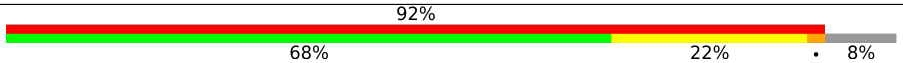
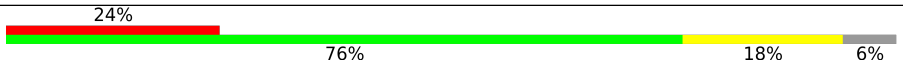
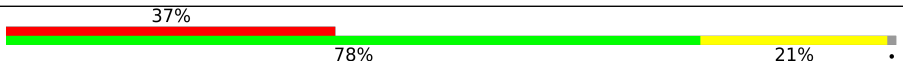
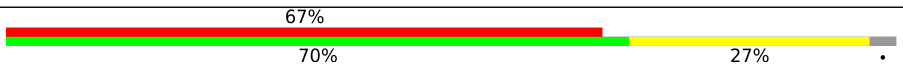
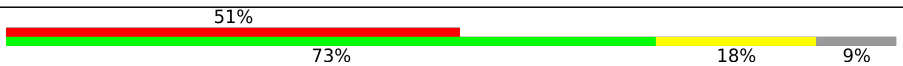
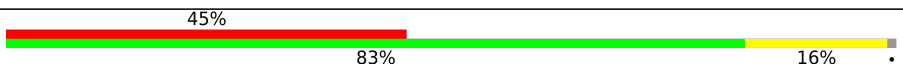
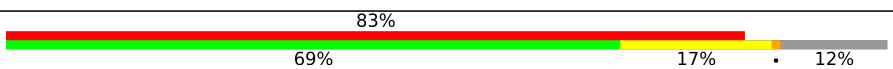
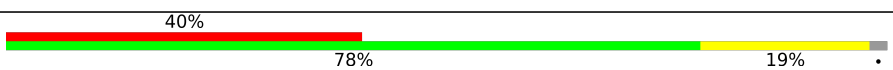
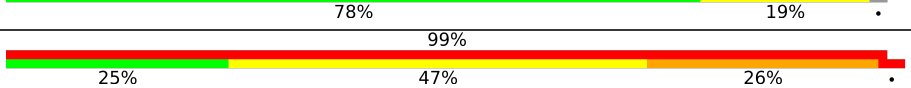
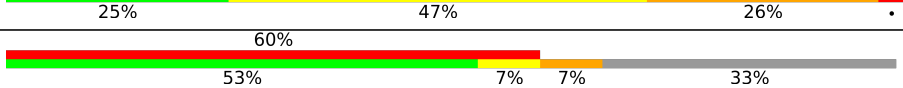
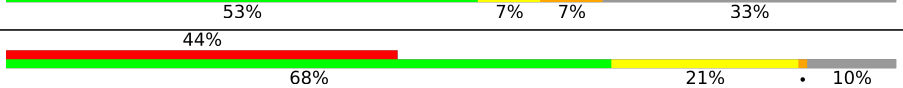
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	10327 (2.20 - 3.20)

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

Mol	Chain	Length	Quality of chain
1	0	51	20% 75% 25%
2	1	44	80% 20%
3	2	64	80% 19%

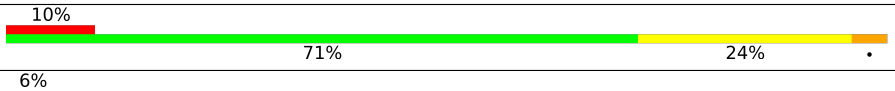
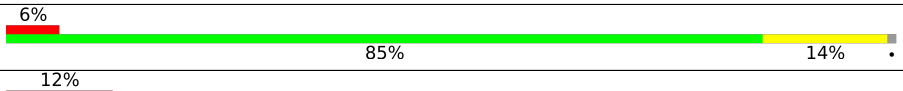
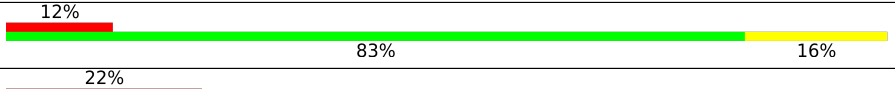
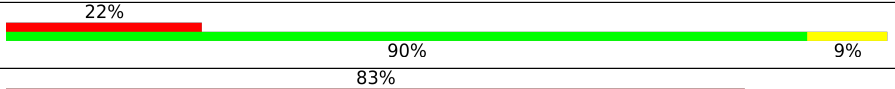
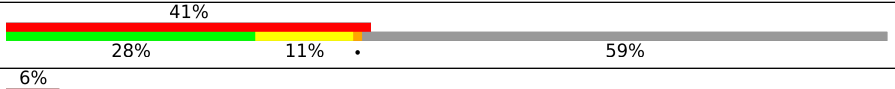
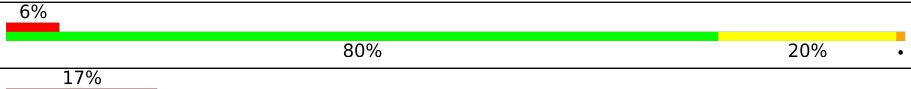
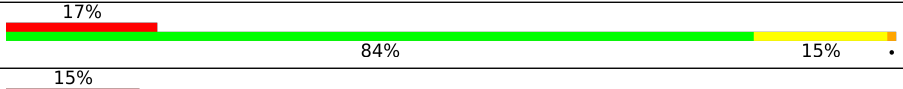
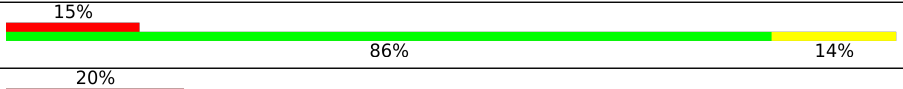
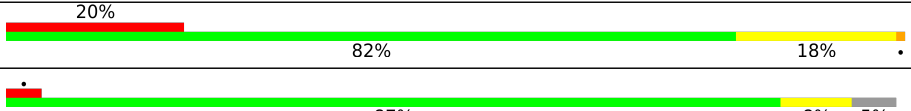
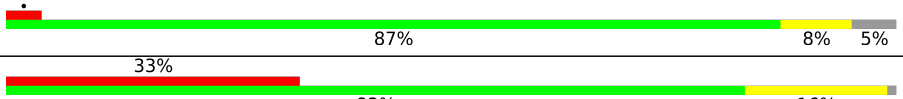
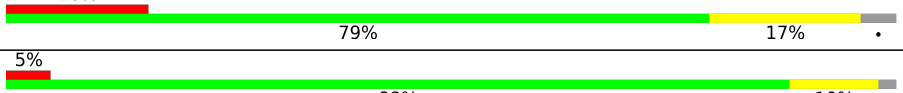
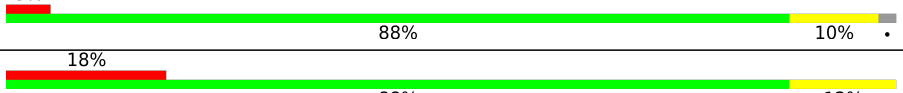
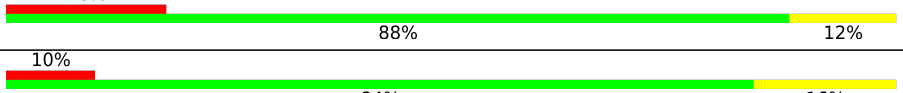
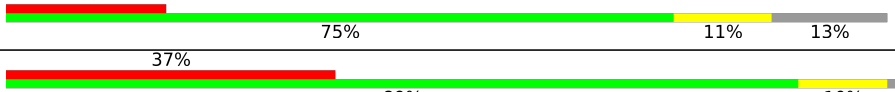
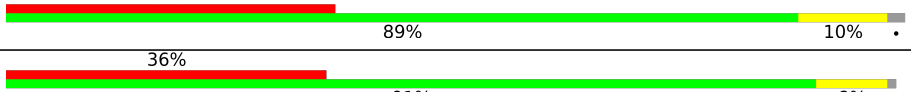
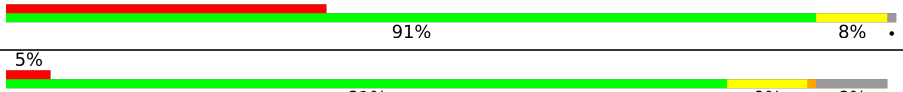
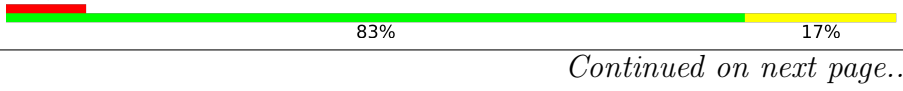
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Mol	Chain	Length	Quality of chain
4	3	38	
5	4	74	
6	A	1537	
7	B	250	
8	C	250	
9	D	208	
10	E	165	
11	F	127	
12	G	156	
13	H	131	
14	I	128	
15	J	103	
16	K	128	
17	L	124	
18	M	118	
19	N	101	
20	O	89	
21	P	83	
22	Q	85	
23	R	75	
24	S	91	
25	T	88	
26	V	77	
27	W	15	
28	X	116	

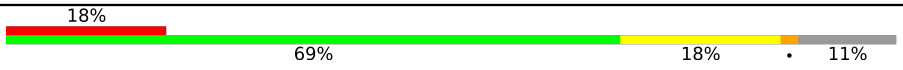
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Mol	Chain	Length	Quality of chain
29	a	2893	
30	b	115	
31	c	274	
32	d	212	
33	e	200	
34	f	178	
35	g	177	
36	h	148	
37	i	142	
38	j	122	
39	k	146	
40	l	137	
41	m	125	
42	n	116	
43	o	122	
44	p	119	
45	q	103	
46	r	109	
47	s	106	
48	t	105	
49	u	98	
50	v	85	
51	w	78	
52	x	65	
53	y	58	

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Mol	Chain	Length	Quality of chain
54	z	61	

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 144018 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	51	427	274	77	73	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	44	363	222	85	54	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	63	509	319	110	76	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	38	295	179	64	48	4	0	0

- Molecule 5 is a protein called Large ribosomal subunit protein bL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	71	552	343	101	102	6	0	0

- Molecule 6 is a RNA chain called 16S rRNA (1536-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	A	1536	32947	14705	6016	10690	1536	0	0

- Molecule 7 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	229	Total	C	N	O	S	0	0
			1801	1130	333	332	6		

- Molecule 8 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	215	Total	C	N	O	S	0	0
			1690	1065	318	299	8		

- Molecule 9 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	207	Total	C	N	O	S	0	0
			1631	1017	313	299	2		

- Molecule 10 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	E	155	Total	C	N	O	S	0	0
			1129	700	217	207	5		

- Molecule 11 is a protein called Small ribosomal subunit protein bS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	106	Total	C	N	O	S	0	0
			878	552	160	162	4		

- Molecule 12 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	153	Total	C	N	O	S	0	0
			1210	758	229	216	7		

- Molecule 13 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	H	130	Total	C	N	O	S	0	0
			985	615	177	187	6		

- Molecule 14 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	127	Total	C	N	O	S	0	0
			995	621	198	175	1		

- Molecule 15 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	100	Total	C	N	O	S	0	0
			801	500	150	148	3		

- Molecule 16 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	117	Total	C	N	O	S	0	0
			862	535	166	160	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	118	IAS	ASN	conflict	UNP D0CD20

- Molecule 17 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	122	Total	C	N	O	S	0	0
			947	581	193	167	6		

- Molecule 18 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	M	116	Total	C	N	O	S	0	0
			912	564	186	159	3		

- Molecule 19 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	N	100	Total	C	N	O	S	0	0
			792	493	158	137	4		

- Molecule 20 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	O	88	Total	C	N	O	S	0	0
			705	434	144	126	1		

- Molecule 21 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	P	82	Total	C	N	O	S	0	0
			644	403	128	112	1		

- Molecule 22 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Q	79	Total	C	N	O	S	0	0
			621	390	116	114	1		

- Molecule 23 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	R	66	Total	C	N	O	S	0	0
			545	349	96	99	1		

- Molecule 24 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	S	84	Total	C	N	O	S	0	0
			657	419	127	109	2		

- Molecule 25 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	T	86	Total	C	N	O	S	0	0
			663	409	139	113	2		

- Molecule 26 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	V	77	Total	C	N	O	P	S	0	0
			1644	734	297	535	77	1		

- Molecule 27 is a RNA chain called Non Stop mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	W	10	Total	C	N	O	P	0	0
			219	97	41	71	10		

- Molecule 28 is a protein called Putative ribosomal subunit interface protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	X	104	Total	C	N	O	S	0	0
			841	519	161	158	3		

- Molecule 29 is a RNA chain called 23S rRNA (2890-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
29	a	2890	Total	C	N	O	P	0	0
			61984	27671	11335	20088	2890		

- Molecule 30 is a RNA chain called 5S rRNA (115-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
30	b	115	Total	C	N	O	P	0	0
			2450	1095	440	800	115		

- Molecule 31 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	c	272	Total	C	N	O	S	0	0
			2111	1302	436	365	8		

- Molecule 32 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	211	Total	C	N	O	S	0	0
			1573	973	297	300	3		

- Molecule 33 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	e	199	Total	C	N	O	S	0	0
			1511	950	280	276	5		

- Molecule 34 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	177	Total	C	N	O	S	0	0
			1395	886	250	251	8		

- Molecule 35 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	g	175	Total	C	N	O	S	0	0
			1327	838	238	250	1		

- Molecule 36 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	h	60	Total	C	N	O	S	0	0
			458	287	84	86	1		

- Molecule 37 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	i	142	Total	C	N	O	S	0	0
			1125	718	200	203	4		

- Molecule 38 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	j	122	Total	C	N	O	S	0	0
			946	592	180	169	5		

- Molecule 39 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	k	146	Total	C	N	O	S	0	0
			1089	673	215	200	1		

- Molecule 40 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	l	137	Total	C	N	O	S	0	0
			1088	687	210	185	6		

- Molecule 41 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	m	119	Total	C	N	O	S	0	0
			942	590	186	163	3		

- Molecule 42 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	n	115	Total	C	N	O	S	0	0
			865	532	175	157	1		

- Molecule 43 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	o	117	Total	C	N	O	0	0
			919	578	177	164		

- Molecule 44 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	p	117	Total	C	N	O	S	0	0
			934	589	197	146	2		

- Molecule 45 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	q	103	Total	C	N	O	S	0	0
			807	506	155	143	3		

- Molecule 46 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	r	109	Total	C	N	O	S	0	0
			826	514	158	150	4		

- Molecule 47 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	s	92	Total	C	N	O	S	0	0
			717	457	129	130	1		

- Molecule 48 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	t	103	Total 766	C 476	N 142	O 148	0	0

- Molecule 49 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	u	97	Total 760	C 477	N 143	O 139	S 1	0	0

- Molecule 50 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	v	78	Total 589	C 365	N 113	O 109	S 2	0	0

- Molecule 51 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	w	77	Total 632	C 395	N 130	O 105	S 2	0	0

- Molecule 52 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	x	62	Total 498	C 308	N 96	O 93	S 1	0	0

- Molecule 53 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	y	58	Total 463	C 286	N 88	O 85	S 4	0	0

- Molecule 54 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	z	54	Total 447	C 265	N 100	O 81	S 1	0	0

- Molecule 55 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
55	1	1	Total K 1 1	0
55	A	45	Total K 45 45	0
55	E	1	Total K 1 1	0
55	L	2	Total K 2 2	0
55	a	111	Total K 111 111	0
55	b	1	Total K 1 1	0
55	c	5	Total K 5 5	0
55	d	1	Total K 1 1	0
55	e	1	Total K 1 1	0
55	t	1	Total K 1 1	0

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
56	3	1	Total Zn 1 1	0
56	4	1	Total Zn 1 1	0

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
57	A	95	Total Mg 95 95	0
57	J	1	Total Mg 1 1	0
57	K	1	Total Mg 1 1	0
57	X	1	Total Mg 1 1	0
57	a	252	Total Mg 252 252	0
57	b	5	Total Mg 5 5	0

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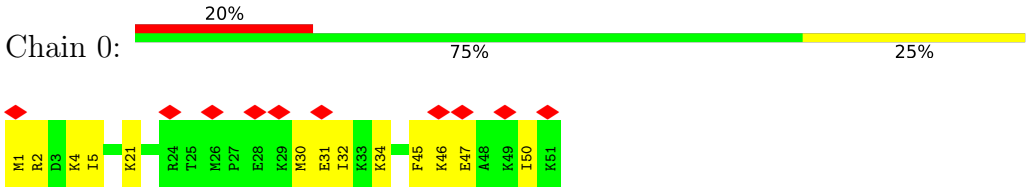
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Mol	Chain	Residues	Atoms	AltConf
57	c	1	Total Mg 1 1	0
57	d	1	Total Mg 1 1	0
57	k	1	Total Mg 1 1	0
57	v	1	Total Mg 1 1	0
57	z	1	Total Mg 1 1	0

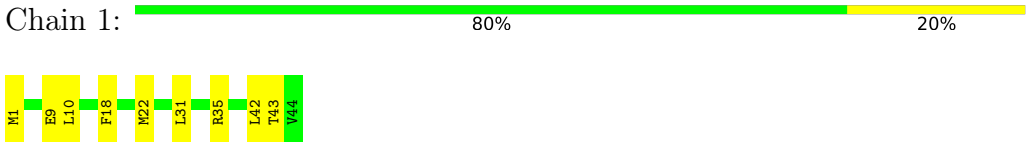
3 Residue-property plots (i)

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

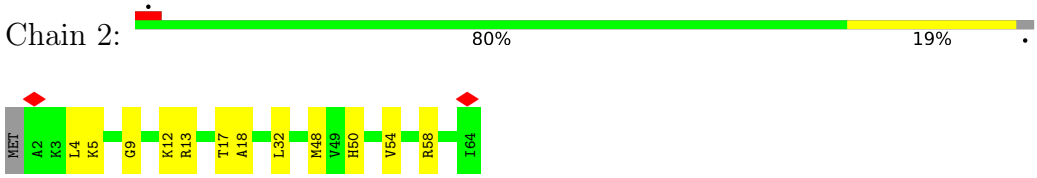
• Molecule 1: Large ribosomal subunit protein bL33



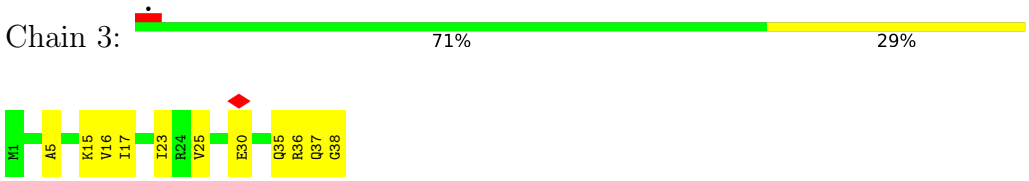
• Molecule 2: Large ribosomal subunit protein bL34



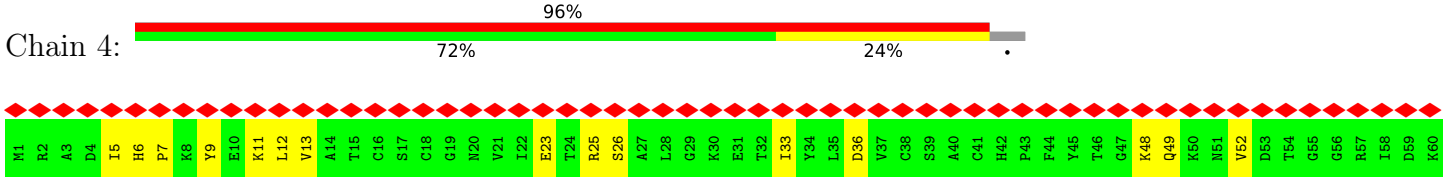
• Molecule 3: Large ribosomal subunit protein bL35

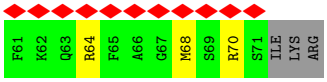


• Molecule 4: Large ribosomal subunit protein bL36



• Molecule 5: Large ribosomal subunit protein bL31

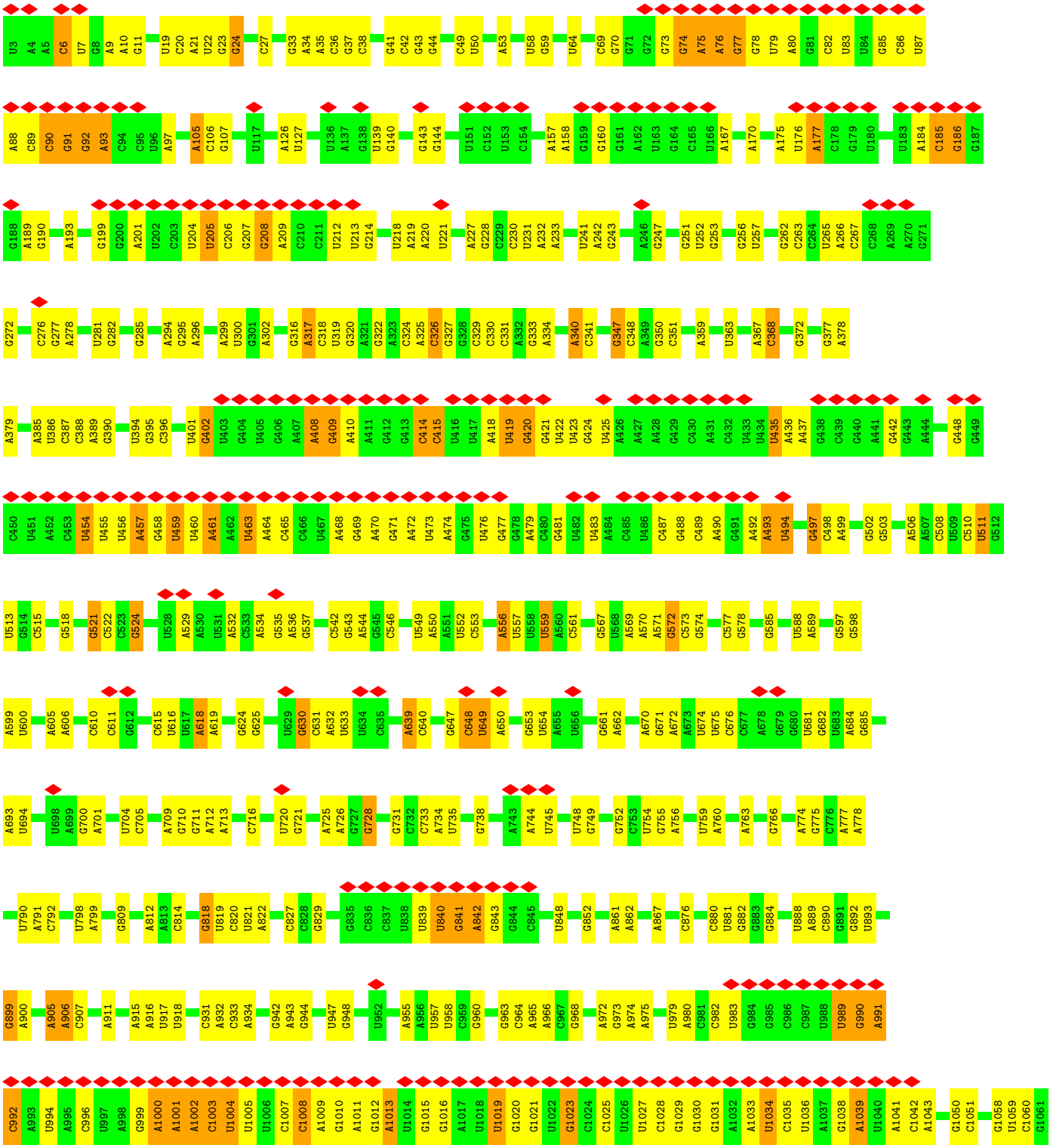


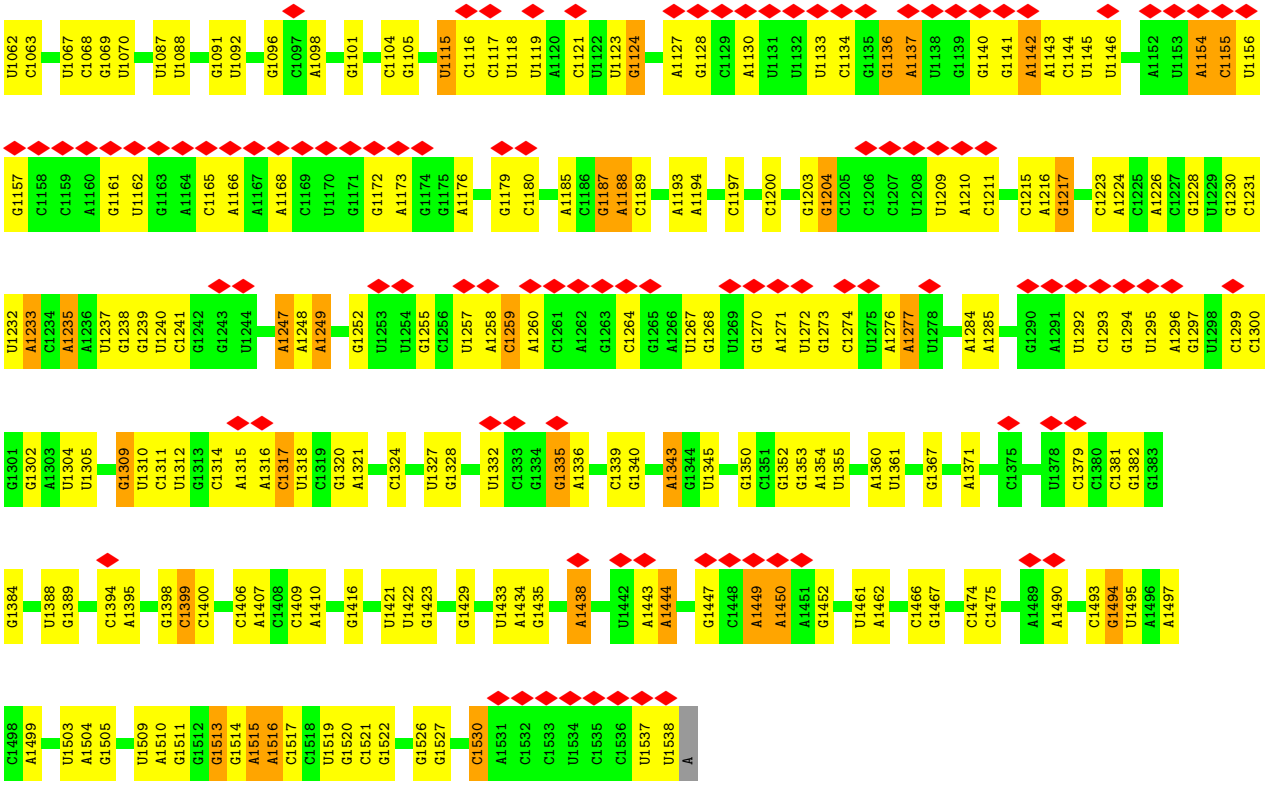


• Molecule 6: 16S rRNA (1536-MER)

Chain A:

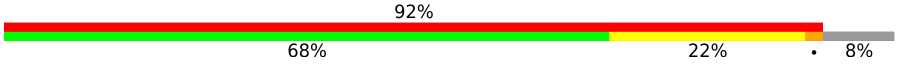


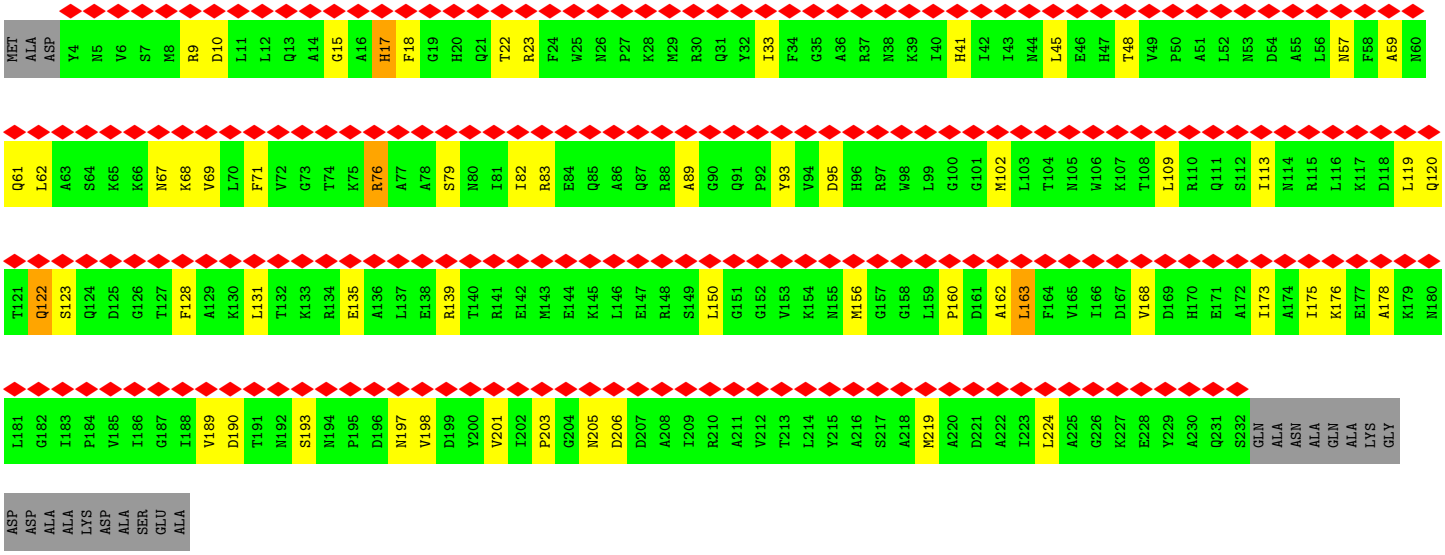




• Molecule 7: Small ribosomal subunit protein uS2

Chain B:

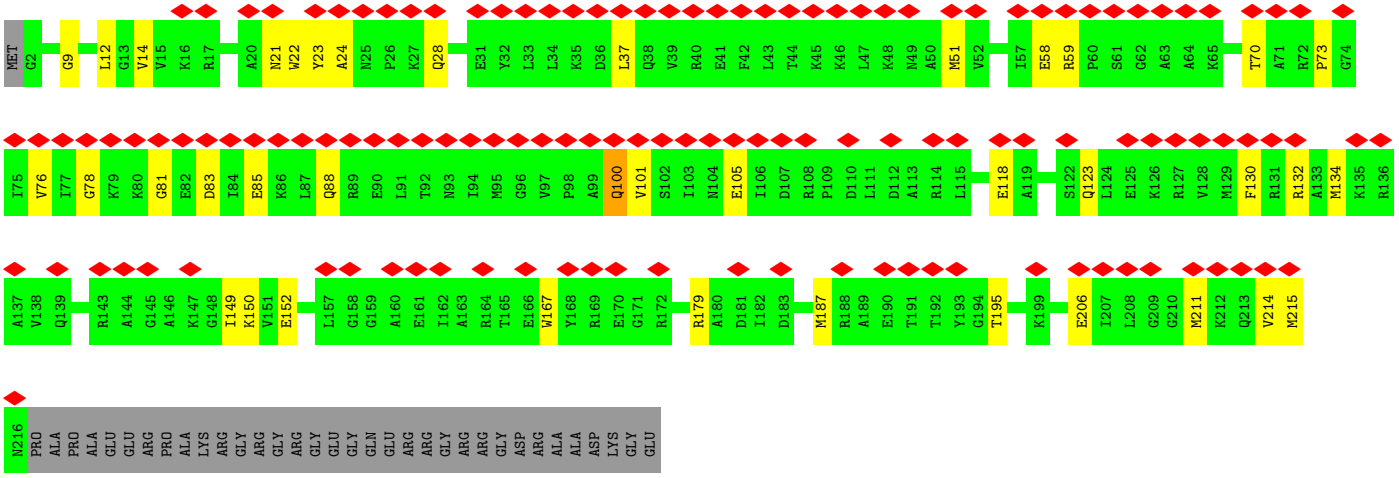




• Molecule 8: Small ribosomal subunit protein uS3

Chain C:

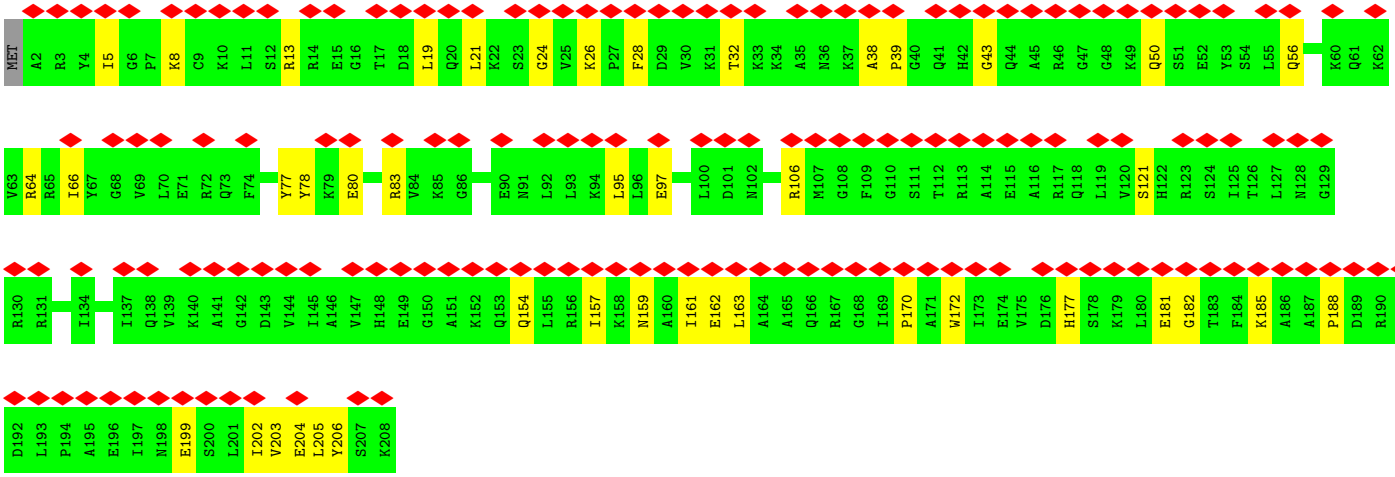




• Molecule 9: Small ribosomal subunit protein uS4

Chain D:

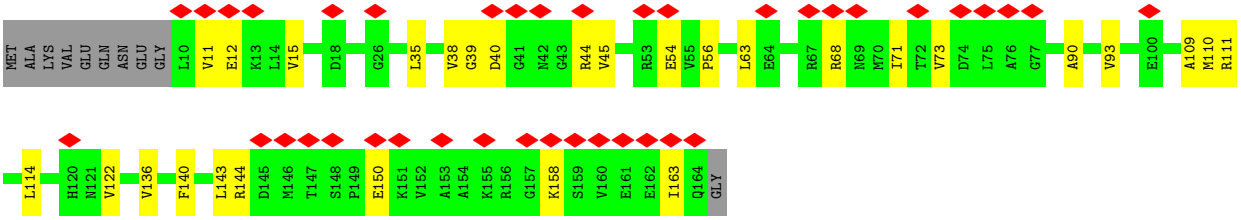




• Molecule 10: Small ribosomal subunit protein uS5

Chain E:

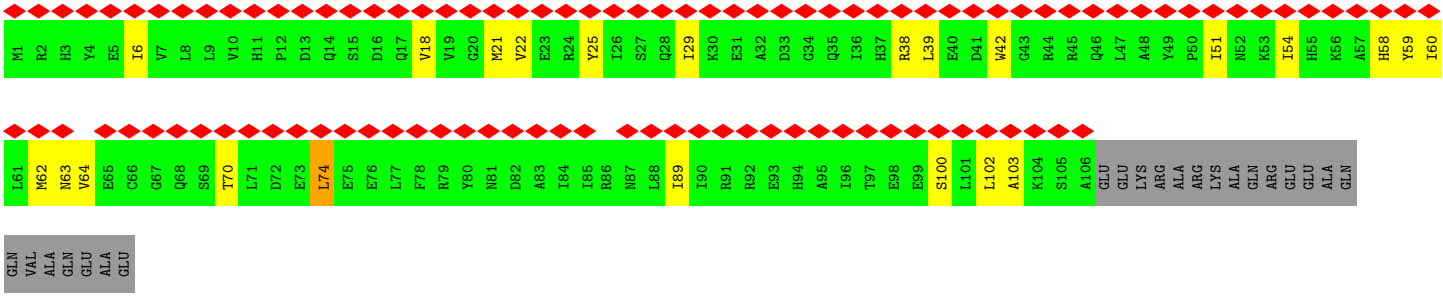




• Molecule 11: Small ribosomal subunit protein bS6

Chain F:

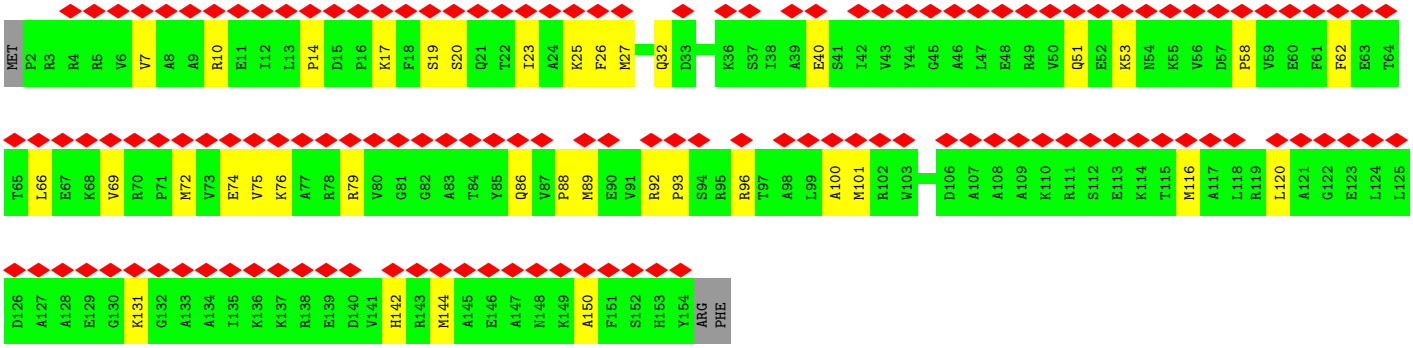




• Molecule 12: Small ribosomal subunit protein uS7

Chain G:

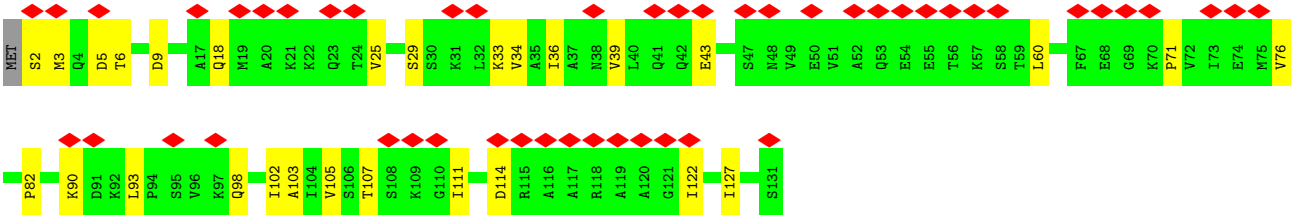




• Molecule 13: Small ribosomal subunit protein uS8

Chain H:

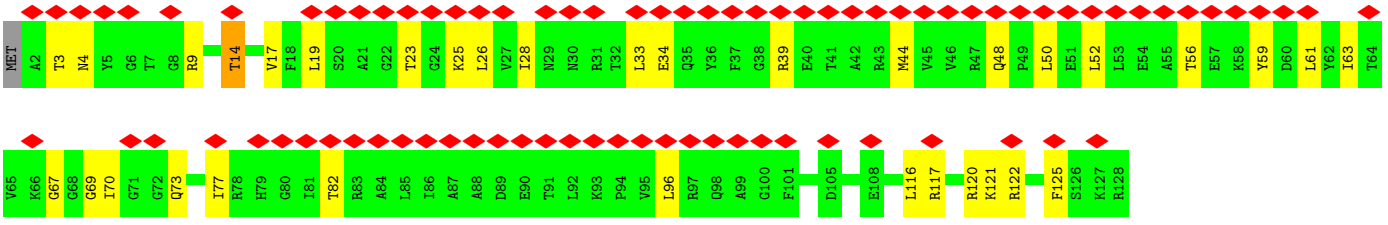




• Molecule 14: Small ribosomal subunit protein uS9

Chain I:

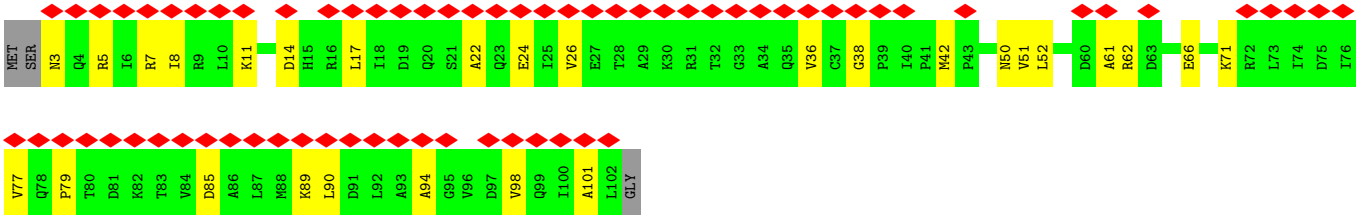




• Molecule 15: Small ribosomal subunit protein uS10

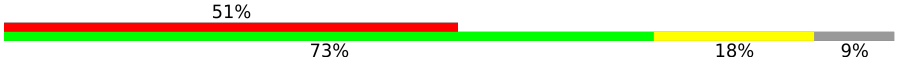
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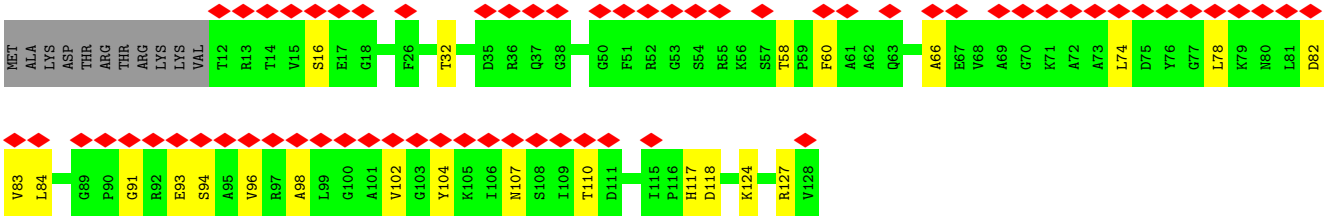




• Molecule 16: Small ribosomal subunit protein uS11

Chain K:

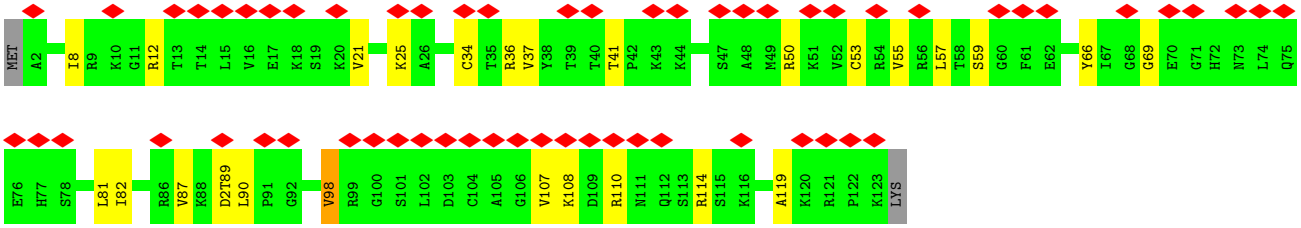




• Molecule 17: Small ribosomal subunit protein uS12

Chain L:

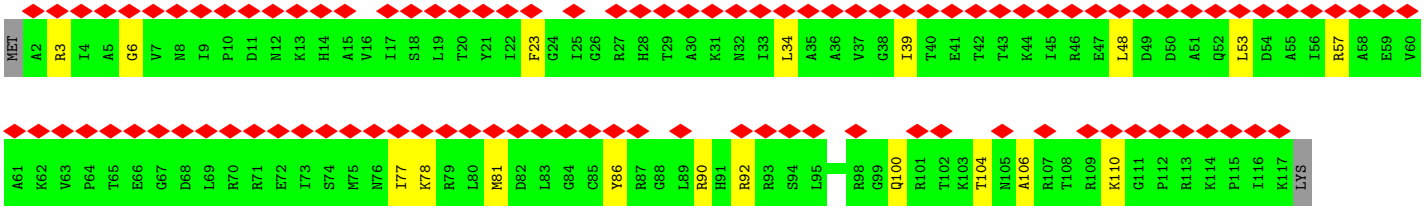




• Molecule 18: Small ribosomal subunit protein uS13

Chain M:

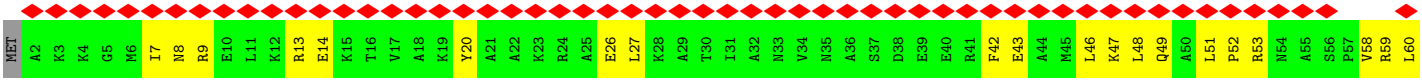


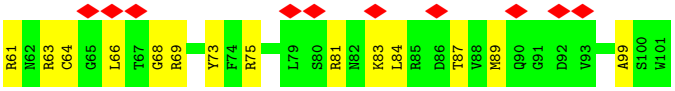


• Molecule 19: Small ribosomal subunit protein uS14

Chain N:



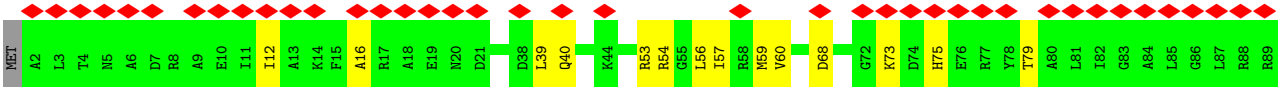




• Molecule 20: Small ribosomal subunit protein uS15

Chain O:

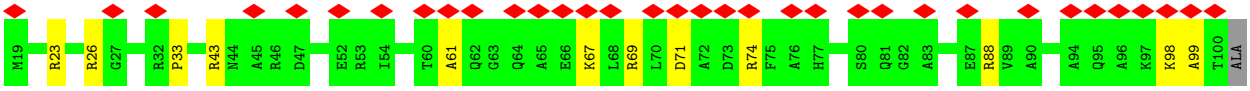




• Molecule 21: Small ribosomal subunit protein bS16

Chain P:

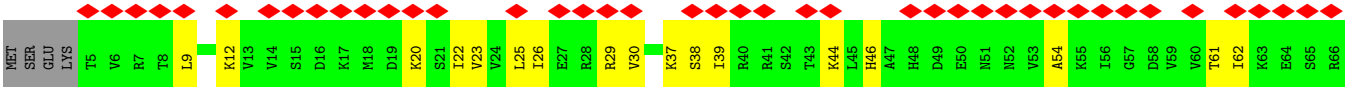


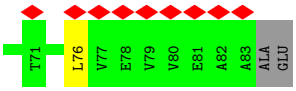


• Molecule 22: Small ribosomal subunit protein uS17

Chain Q:



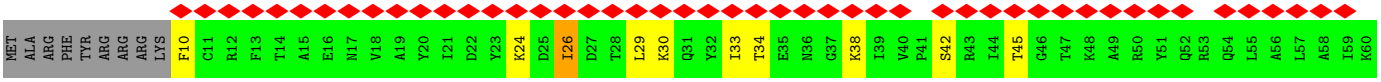


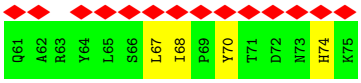


• Molecule 23: Small ribosomal subunit protein bS18

Chain R:



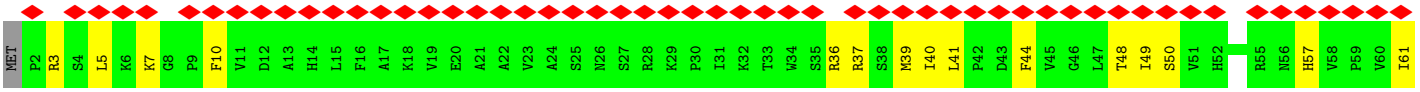


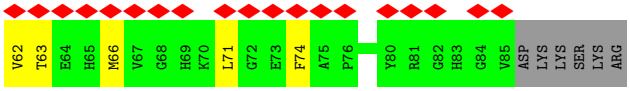


• Molecule 24: Small ribosomal subunit protein uS19

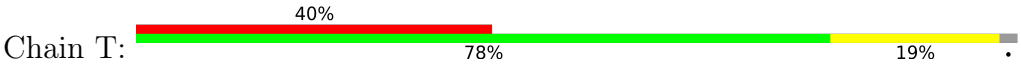
Chain S:

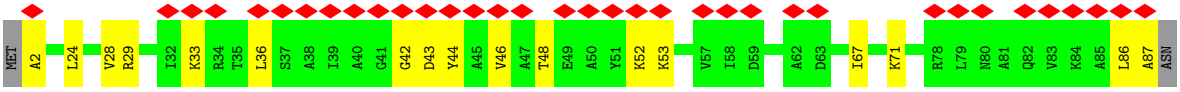






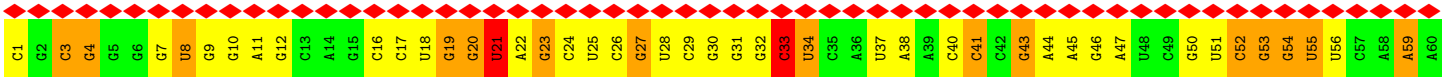
• Molecule 25: Small ribosomal subunit protein bS20





• Molecule 26: tRNA

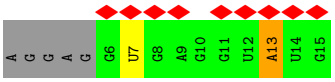




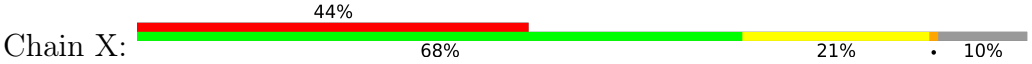


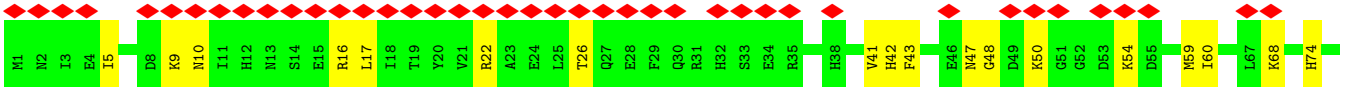
• Molecule 27: Non Stop mRNA

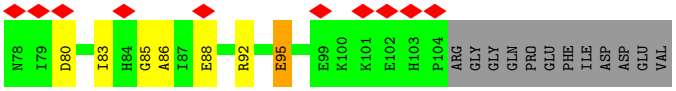




• Molecule 28: Putative ribosomal subunit interface protein

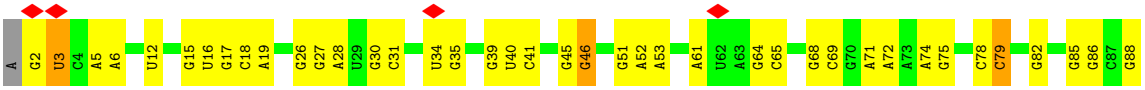


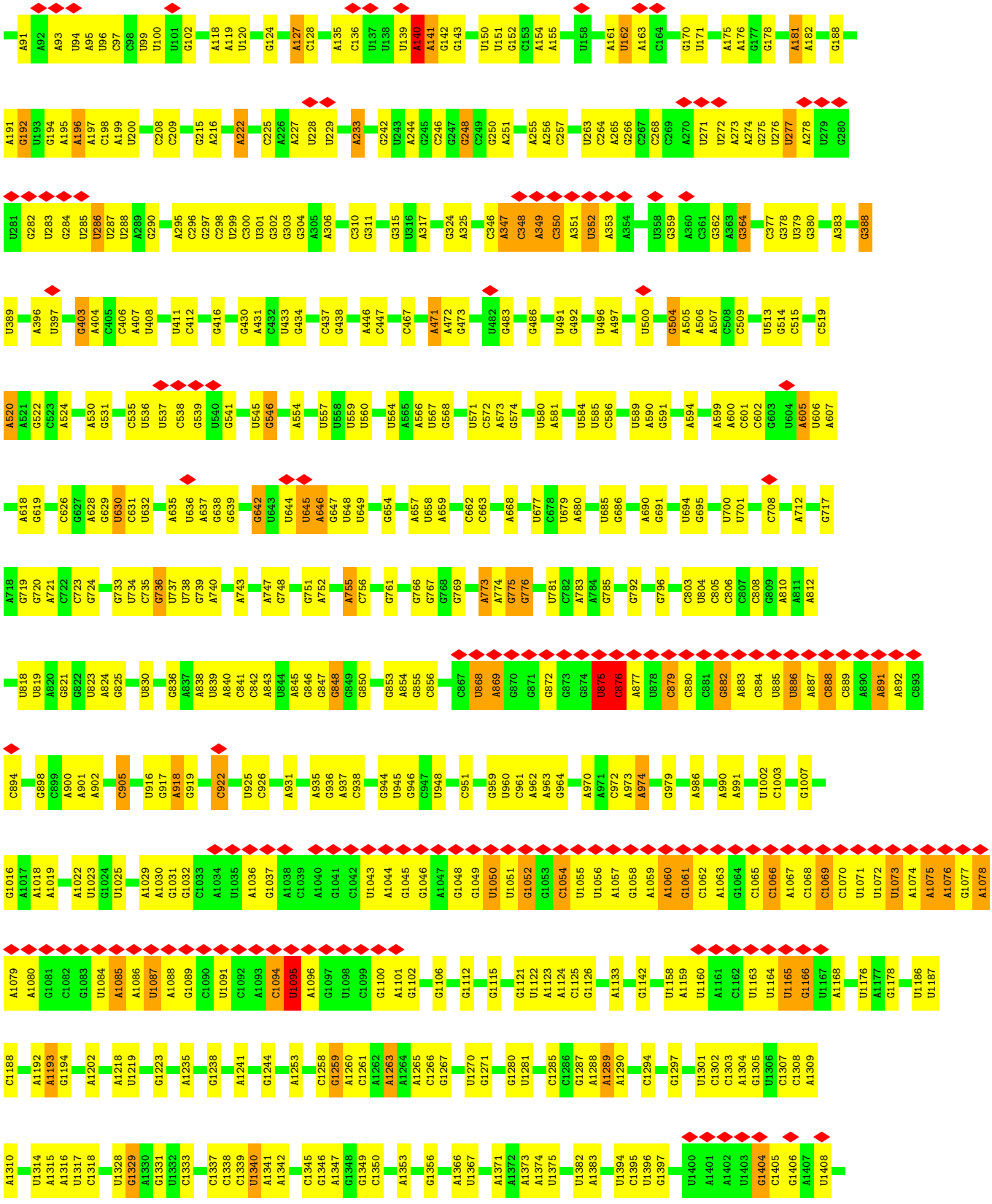


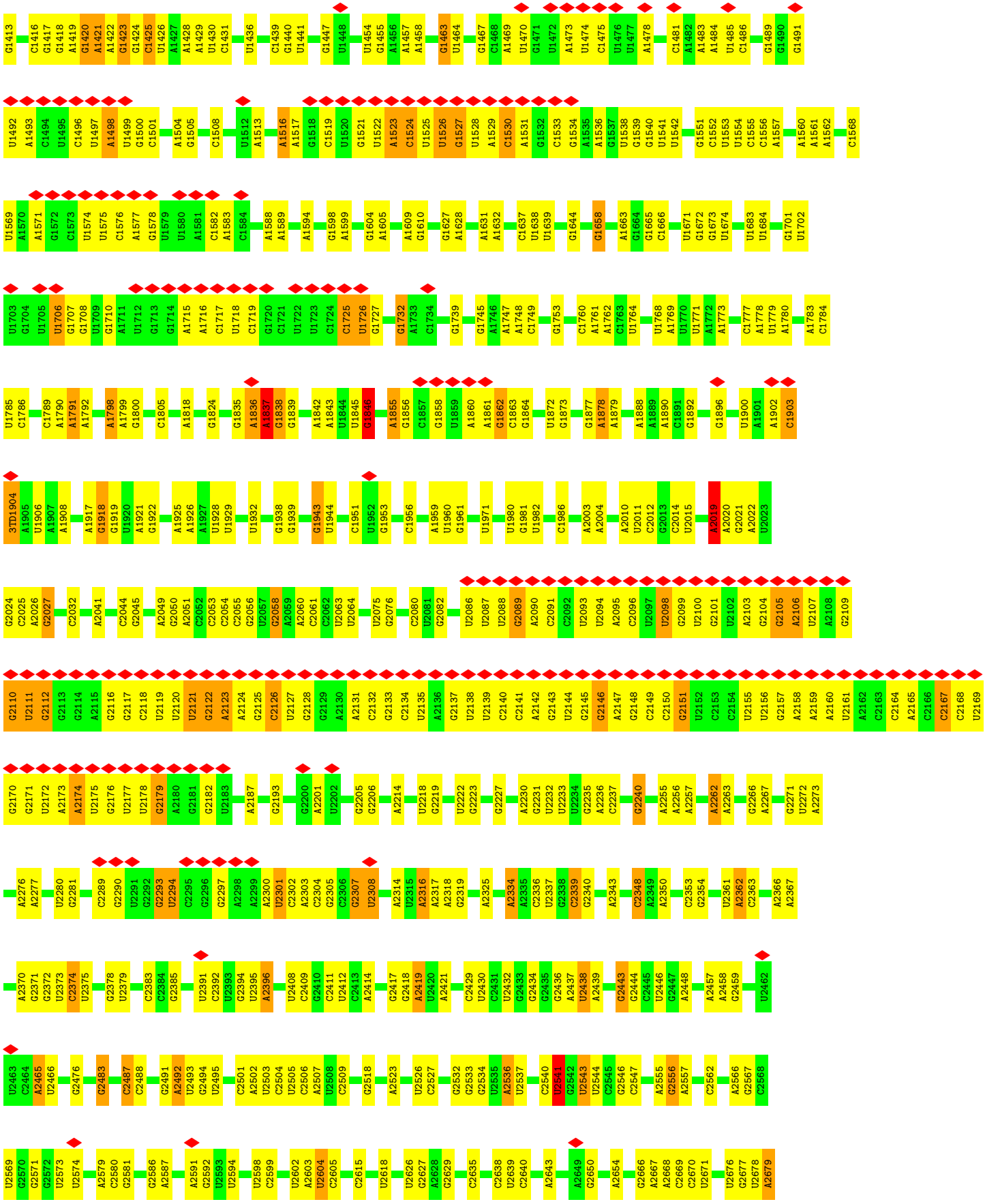


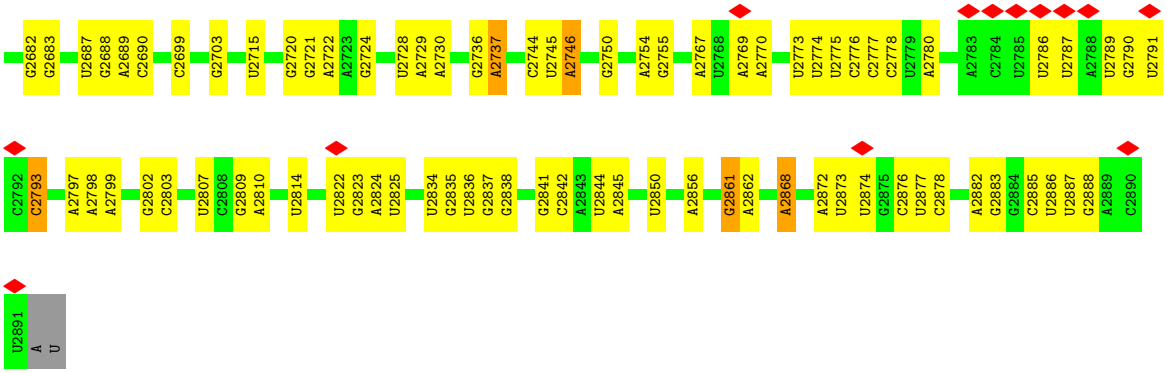
• Molecule 29: 23S rRNA (2890-MER)





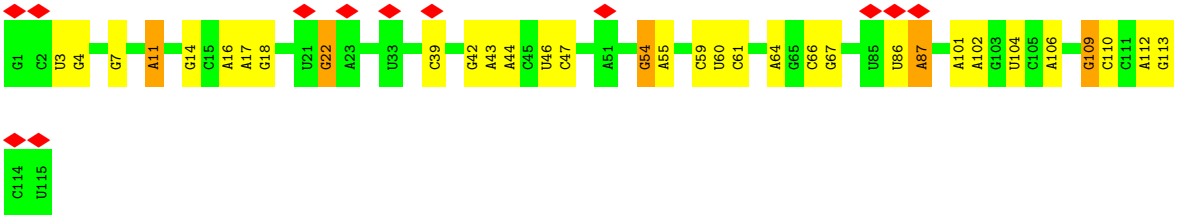



G1413 C1416 G1417 G1418 A1419 G1420 A1421 A1422 G1423 G1424 C1425 U1426 A1427 A1428 A1429 U1430 C1431 U1436 C1439 G1440 U1441 G1447 U1448 U1454 G1455 A1456 A1457 A1458 G1463 U1464 G1467 C1468 A1469 U1470 G1471 U1472 A1473 U1474 C1475 U1476 U1477 A1478 C1481 A1482 A1483 A1484 U1485 C1486 G1489 G1490 G1491
U1492 A1493 C1494 U1495 C1496 U1497 A1498 U1499 G1500 C1501 A1504 G1505 C1508 U1512 A1513 A1516 A1517 G1518 C1519 U1520 G1521 U1522 A1523 C1524 U1525 U1526 G1527 U1528 A1529 C1530 A1531 G1532 C1533 G1534 A1535 A1536 G1537 U1538 G1539 G1540 U1541 U1542 G1551 C1552 U1553 U1554 C1555 C1556 A1557 A1560 A1561 A1562 C1568
U1569 A1570 A1571 G1572 C1573 U1574 U1575 C1576 A1577 G1578 U1579 U1580 A1581 C1582 A1583 C1584 A1588 A1589 A1594 G1598 A1599 G1604 A1605 A1609 G1610 G1627 A1628 A1631 A1632 C1637 U1638 U1639 G1644 G1658 A1663 G1664 G1665 C1666 U1671 G1672 G1673 U1674 U1683 U1684 G1701 U1702
U1703 G1704 U1705 U1706 G1707 G1708 U1709 G1710 A1711 U1712 G1713 G1714 A1715 A1716 C1717 U1718 C1719 G1720 C1721 U1722 U1723 C1724 C1725 U1726 G1727 G1732 A1733 C1734 G1739 G1745 A1746 A1747 A1748 C1749 G1753 C1760 A1761 A1762 C1763 U1764 U1768 A1769 U1770 U1771 A1772 A1773 C1777 A1778 U1779 A1780 A1783 C1784
U1785 C1786 C1789 A1790 A1791 A1792 A1798 A1799 G1800 C1805 A1818 G1824 G1835 A1836 A1837 G1838 G1839 A1842 A1843 U1844 U1845 G1846 A1855 G1856 C1857 G1858 U1859 A1860 A1861 G1862 C1863 G1864 U1872 G1873 G1877 A1878 A1879 A1888 A1889 A1890 C1891 G1892 G1896 U1900 A1901 A1902 C1903
3TD1904 A1905 U1906 A1907 A1908 A1917 G1918 G1919 U1920 A1921 G1922 A1925 A1926 A1927 U1928 U1929 U1932 G1938 G1939 G1943 U1944 C1951 U1952 G1953 C1956 A1959 U1960 G1961 U1971 U1980 G1981 U1982 C1986 A2003 A2004 A2010 U2011 C2012 G2013 C2014 U2015 A2019 A2020 G2021 A2022 U2023
G2024 C2025 A2026 G2027 C2032 A2041 C2044 G2045 A2049 G2050 A2051 C2052 C2053 C2054 C2055 G2056 U2057 G2058 A2059 A2060 C2061 C2062 U2063 U2064 U2075 G2076 C2080 U2081 G2082 U2086 U2087 U2088 G2089 A2090 C2091 C2092 U2093 U2094 A2095 C2096 U2097 U2098 G2099 U2100 G2101 U2102 A2103 G2104 G2105 A2106 U2107 A2108 G2109
G2110 U2111 G2112 G2113 G2114 A2115 G2116 G2117 C2118 U2119 U2120 U2121 G2122 A2123 A2124 G2125 C2126 U2127 G2128 G2129 A2130 A2131 C2132 G2133 C2134 U2135 A2136 G2137 U2138 U2139 C2140 C2141 A2142 G2143 U2144 G2145 G2146 A2147 G2148 C2149 C2150 G2151 U2152 C2153 C2154 U2155 U2156 G2157 A2158 A2159 A2160 U2161 A2162 C2163 C2164 A2165 C2166 C2167 C2168 U2169
G2170 G2171 U2172 A2173 A2174 U2175 G2176 U2177 U2178 G2179 A2180 G2181 G2182 U2183 A2187 G2193 G2200 A2201 U2202 G2205 G2206 A2214 U2218 G2219 U2222 G2223 G2227 A2230 G2231 U2232 U2233 U2234 G2235 A2236 C2237 G2240 A2255 A2256 A2257 A2262 A2263 G2266 A2267 G2271 U2272 A2273
A2276 A2277 U2280 G2281 C2289 G2290 U2291 G2292 G2293 U2294 C2295 G2296 G2297 A2298 A2299 A2300 U2301 C2302 A2303 C2304 G2305 C2306 G2307 U2308 A2314 U2315 A2316 A2317 A2318 G2319 A2325 A2334 A2335 C2336 U2337 G2338 C2339 G2340 A2343 C2348 A2349 A2350 C2353 G2354 U2361 A2362 C2363 A2366 A2367
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U2463 C2464 A2465 U2466 G2476 G2483 C2487 C2488 G2491 A2492 U2493 G2494 U2495 C2501 A2502 U2503 C2504 U2505 C2506 A2507 U2508 C2509 G2518 A2523 U2526 C2527 G2532 G2533 G2534 U2535 A2536 U2537 C2540 U2541 G2542 U2543 U2544 C2545 G2546 C2547 A2555 G2556 A2557 C2562 A2566 G2567 C2568
U2569 G2570 G2571 G2572 U2573 U2574 A2579 C2580 G2581 G2586 A2587 A2591 G2592 U2593 U2594 U2598 C2599 U2602 A2603 U2604 C2605 C2615 U2618 U2626 G2627 A2628 G2629 C2635 C2638 U2639 C2640 A2643 A2649 G2650 A2654 G2666 A2667 A2668 C2669 C2670 U2671 U2676 G2677 U2678 A2679

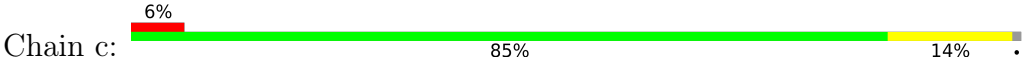


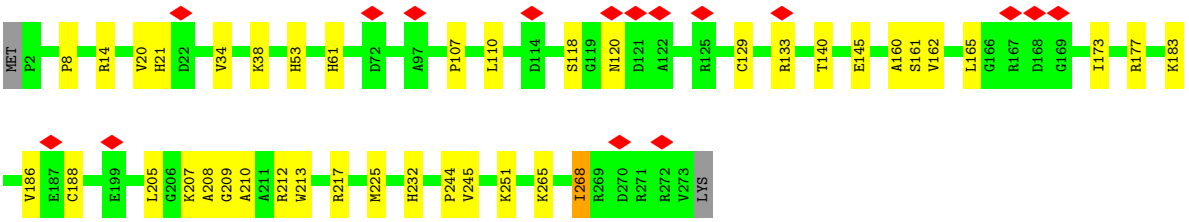
• Molecule 30: 5S rRNA (115-MER)



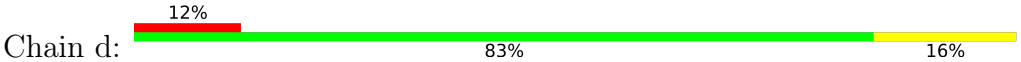


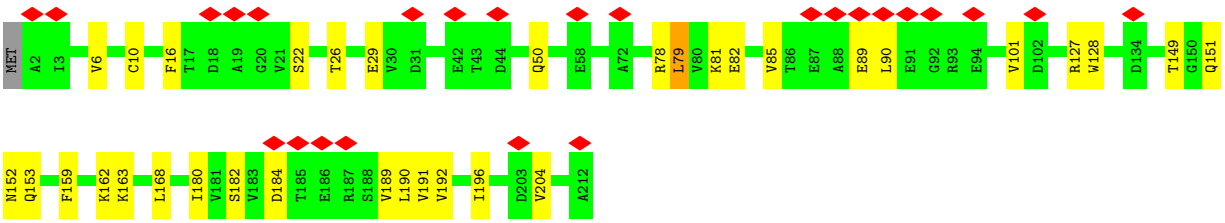
• Molecule 31: Large ribosomal subunit protein uL2



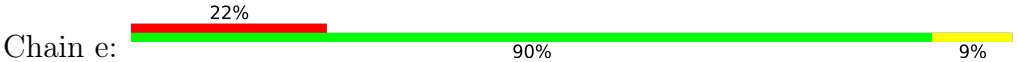


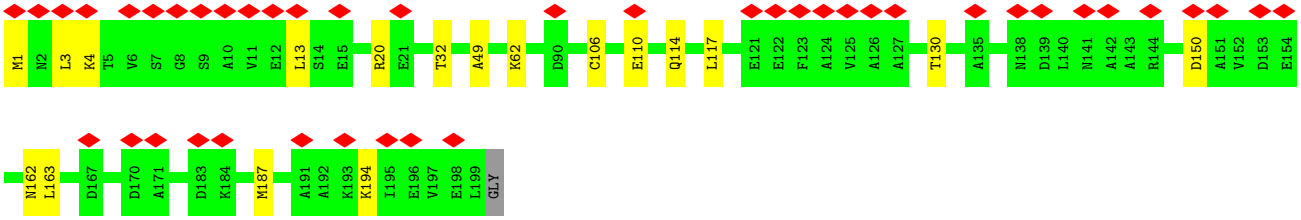
• Molecule 32: Large ribosomal subunit protein uL3





• Molecule 33: Large ribosomal subunit protein uL4

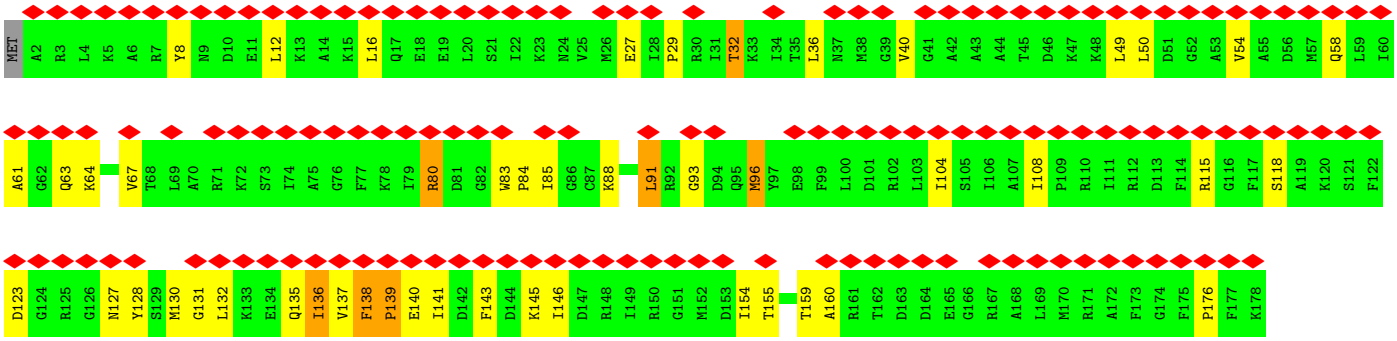




• Molecule 34: Large ribosomal subunit protein uL5

Chain f:

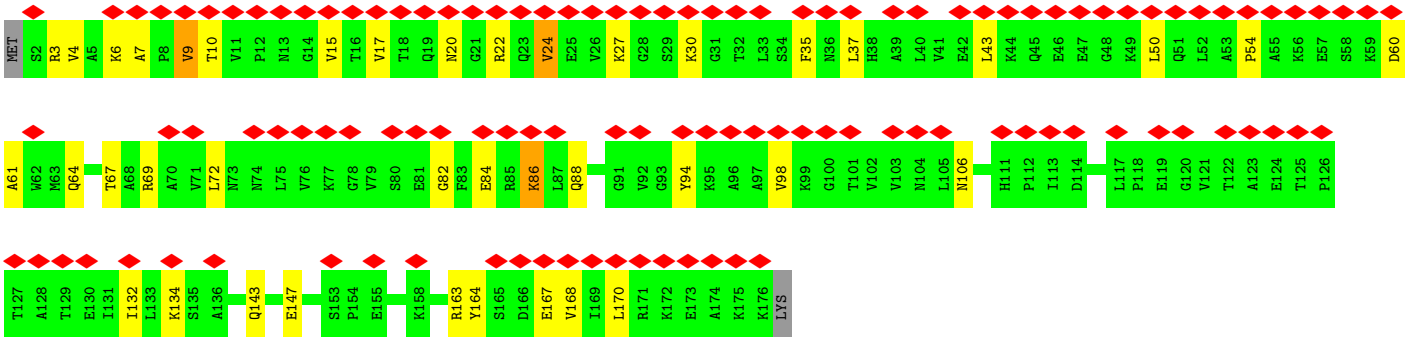




• Molecule 35: Large ribosomal subunit protein uL6

Chain g:

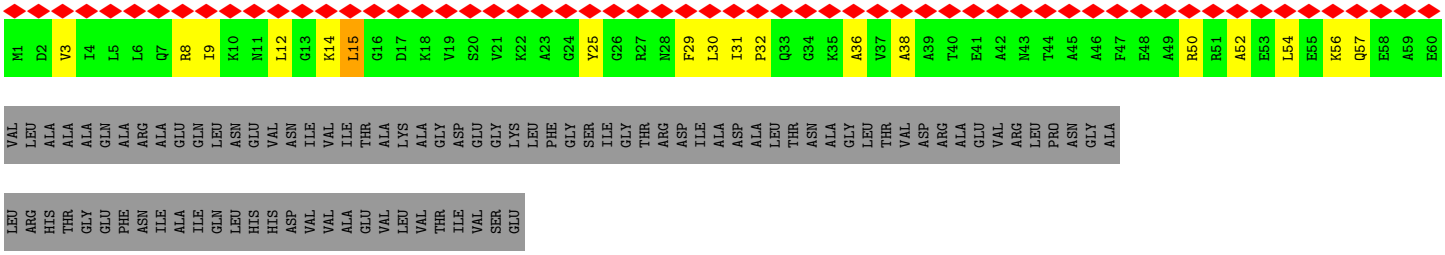




• Molecule 36: Large ribosomal subunit protein bL9

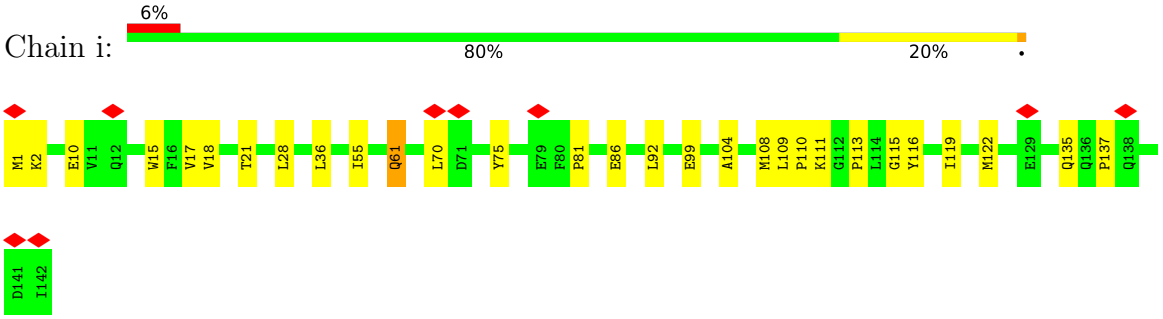
Chain h:





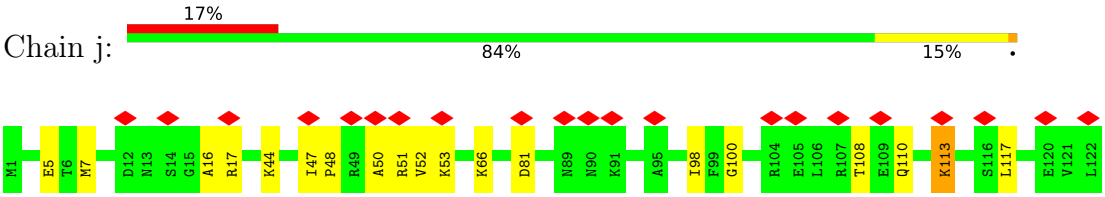
• Molecule 37: Large ribosomal subunit protein uL13

Chain i:



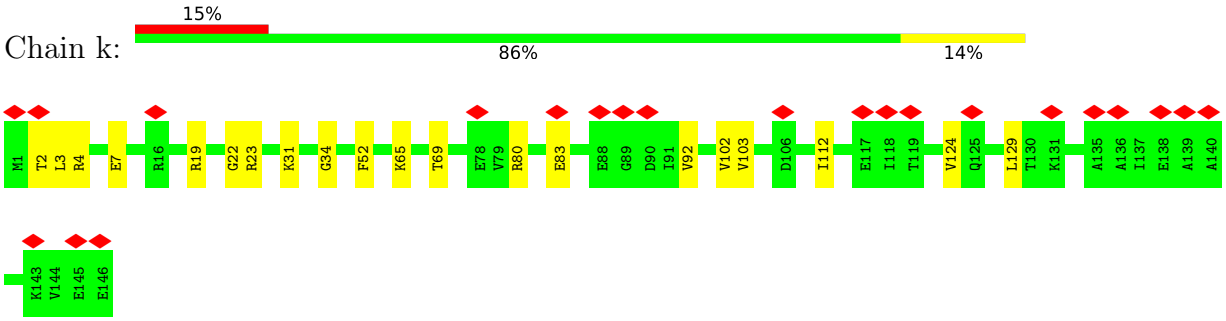
• Molecule 38: Large ribosomal subunit protein uL14

Chain j:



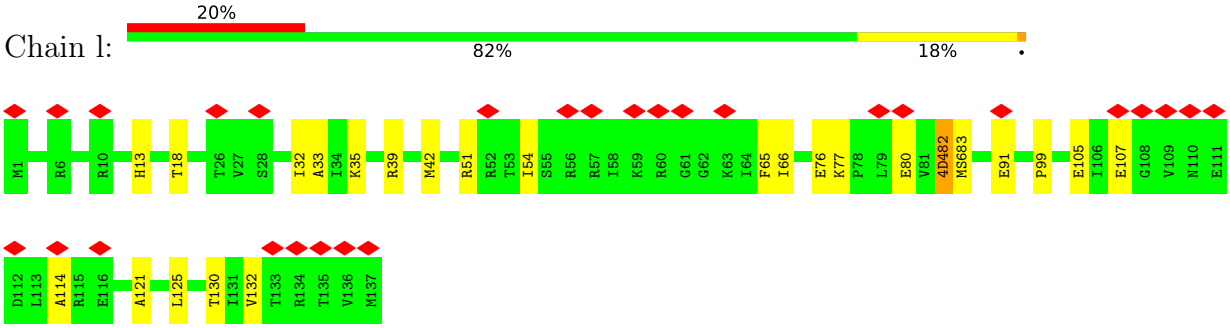
• Molecule 39: Large ribosomal subunit protein uL15

Chain k:



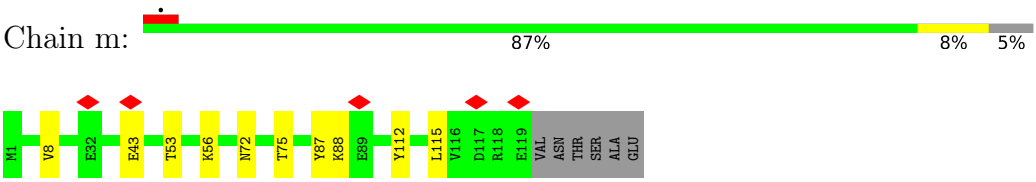
• Molecule 40: Large ribosomal subunit protein uL16

Chain l:



• Molecule 41: Large ribosomal subunit protein bL17

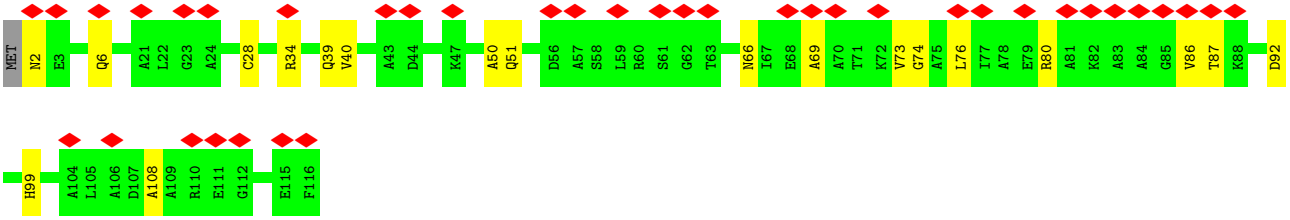
Chain m:



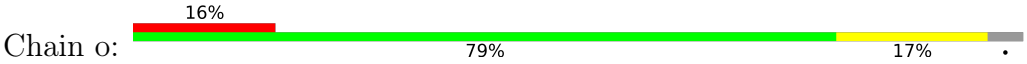
• Molecule 42: Large ribosomal subunit protein uL18

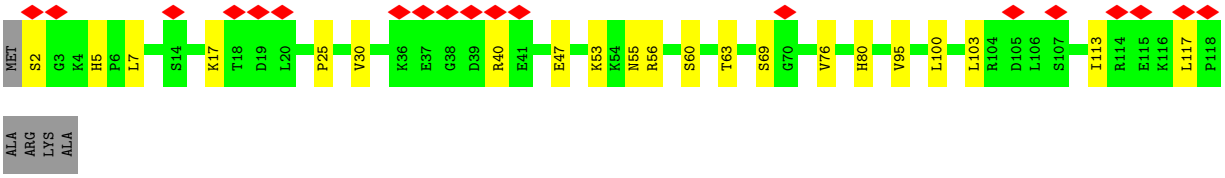
Chain n:



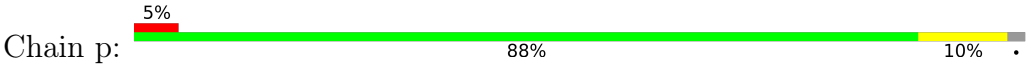


• Molecule 43: Large ribosomal subunit protein bL19



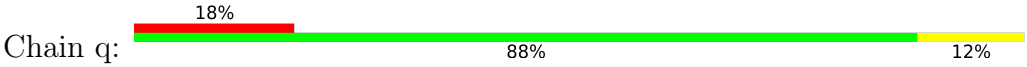


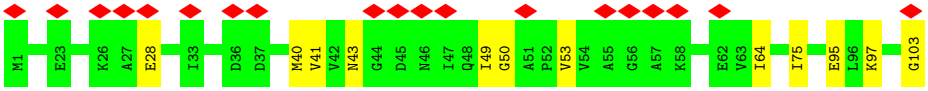
• Molecule 44: Large ribosomal subunit protein bL20



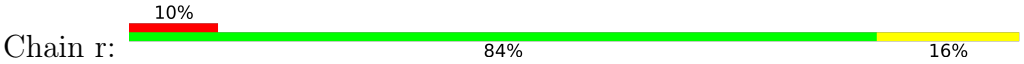


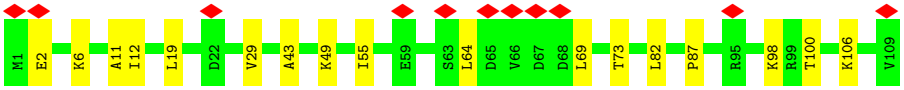
• Molecule 45: Large ribosomal subunit protein bL21



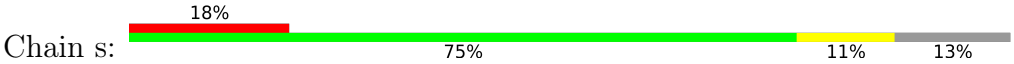


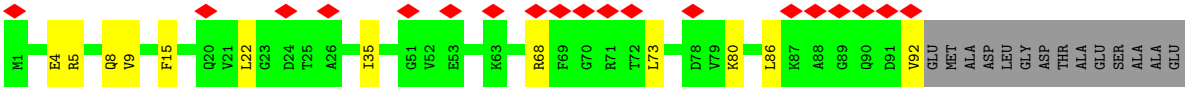
• Molecule 46: Large ribosomal subunit protein uL22





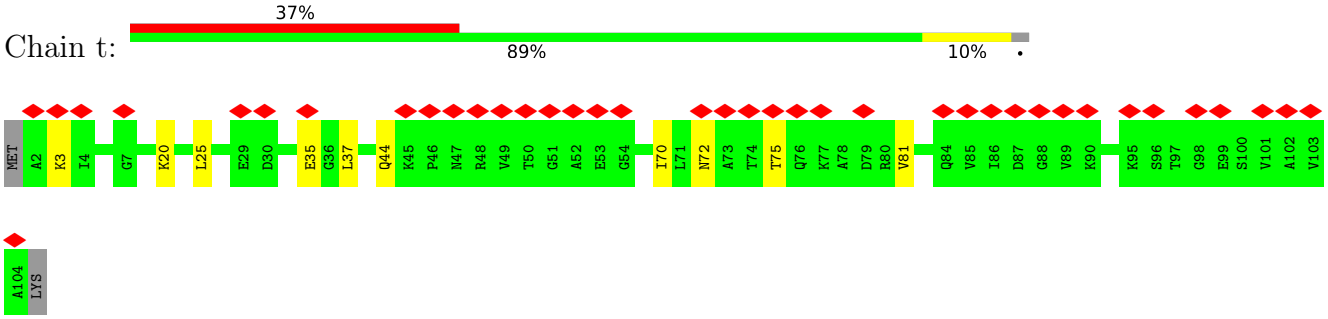
• Molecule 47: Large ribosomal subunit protein uL23





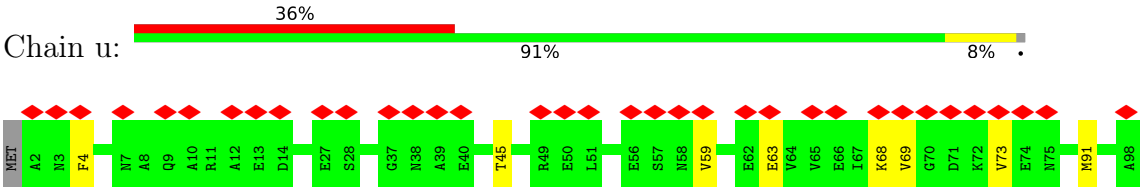
• Molecule 48: Large ribosomal subunit protein uL24

Chain t:



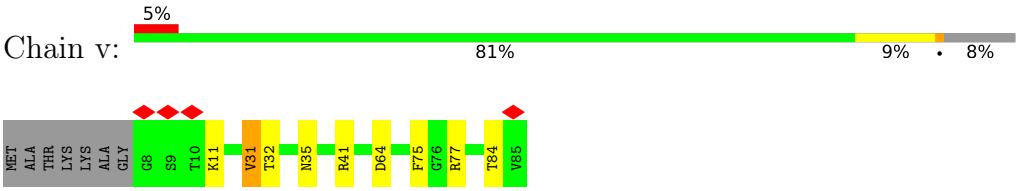
• Molecule 49: Large ribosomal subunit protein bL25

Chain u:



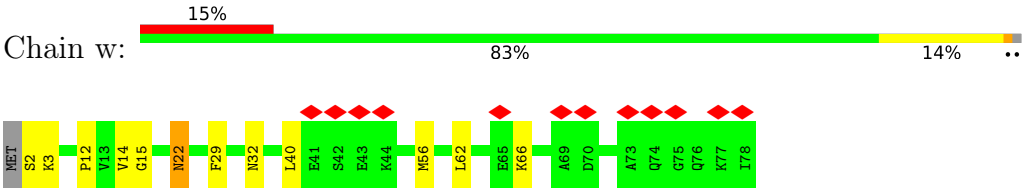
• Molecule 50: Large ribosomal subunit protein bL27

Chain v:



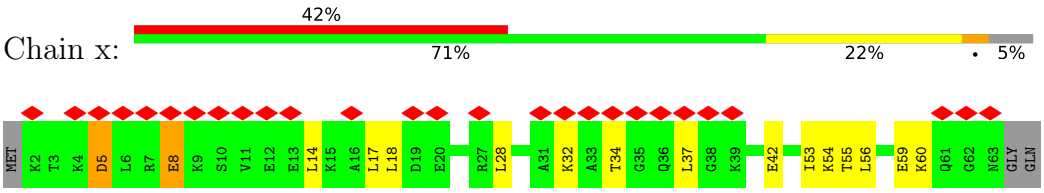
• Molecule 51: Large ribosomal subunit protein bL28

Chain w:



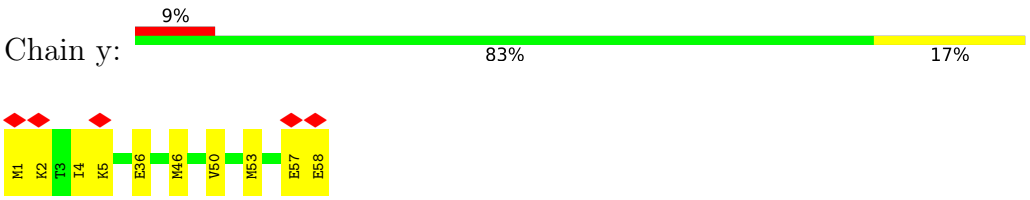
• Molecule 52: Large ribosomal subunit protein uL29

Chain x:



• Molecule 53: Large ribosomal subunit protein uL30

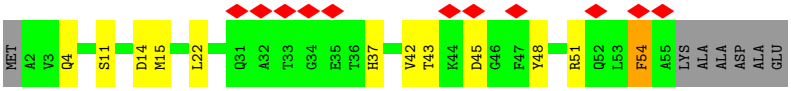
Chain y:



• Molecule 54: Large ribosomal subunit protein bL32

Chain z:




MET
A2
V3
Q4
S11
D14
M15
L22
Q31
A32
T33
G34
E35
T36
H37
V42
T43
K44
D45
G46
F47
Y48
R51
Q52
L53
F54
A55
LYS
ALA
ALA
ASP
ALA
GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	106853	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	35	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.403	Depositor
Minimum map value	-1.048	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.063	Depositor
Recommended contour level	0.45	Depositor
Map size (Å)	542.72, 542.72, 542.72	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OMG, H2U, MEQ, MS6, OMC, 1MG, IAS, 2MA, MG, K, 2MG, 5MC, 4OC, PSU, 6MZ, 4SU, ZN, G7M, 3TD, MA6, D2T, OMU, UR3, 4D4, 5MU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	0	0.21	0/434	0.38	0/573
2	1	0.24	0/367	0.30	0/481
3	2	0.22	0/515	0.34	0/678
4	3	0.22	0/296	0.33	0/389
5	4	0.14	0/561	0.38	0/750
6	A	0.40	0/36630	0.75	5/57129 (0.0%)
7	B	0.14	0/1832	0.34	0/2474
8	C	0.17	0/1714	0.34	0/2304
9	D	0.15	0/1653	0.32	0/2213
10	E	0.20	0/1141	0.37	0/1537
11	F	0.14	0/893	0.34	0/1204
12	G	0.13	0/1229	0.26	0/1647
13	H	0.18	0/993	0.32	0/1331
14	I	0.16	0/1006	0.31	0/1346
15	J	0.17	0/811	0.33	0/1096
16	K	0.17	0/869	0.34	0/1175
17	L	0.17	0/949	0.39	0/1270
18	M	0.15	0/922	0.33	0/1237
19	N	0.15	0/803	0.32	0/1071
20	O	0.16	0/715	0.29	0/958
21	P	0.17	0/655	0.36	0/879
22	Q	0.16	0/628	0.34	0/847
23	R	0.17	0/555	0.32	0/749
24	S	0.14	0/675	0.32	0/912
25	T	0.18	0/669	0.27	0/892
26	V	0.28	0/1724	0.81	1/2687 (0.0%)
27	W	0.29	0/245	0.74	0/381
28	X	0.18	0/858	0.33	0/1150
29	a	0.51	0/68962	0.77	29/107563 (0.0%)
30	b	0.41	0/2739	0.74	0/4266
31	c	0.22	0/2152	0.31	0/2891

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	d	0.22	0/1580	0.33	0/2127
33	e	0.21	0/1532	0.29	0/2068
34	f	0.20	0/1415	0.47	0/1895
35	g	0.15	0/1346	0.27	0/1818
36	h	0.13	0/461	0.36	0/616
37	i	0.21	0/1151	0.32	0/1551
38	j	0.21	0/956	0.31	0/1286
39	k	0.21	0/1097	0.30	0/1461
40	l	0.18	0/1084	0.28	0/1448
41	m	0.22	0/956	0.33	0/1282
42	n	0.18	0/873	0.29	0/1167
43	o	0.20	0/931	0.32	0/1249
44	p	0.23	0/947	0.32	0/1262
45	q	0.22	0/818	0.35	0/1094
46	r	0.21	0/831	0.36	0/1113
47	s	0.19	0/723	0.31	0/967
48	t	0.17	0/770	0.27	0/1034
49	u	0.17	0/770	0.30	0/1036
50	v	0.21	0/597	0.28	0/798
51	w	0.22	0/642	0.30	0/856
52	x	0.17	0/499	0.36	0/662
53	y	0.21	0/468	0.32	0/624
54	z	0.23	0/453	0.32	0/604
All	All	0.41	0/155095	0.68	35/232098 (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
40	l	0	1

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	a	1301	U	C2-N1-C1'	7.28	126.43	117.70
29	a	875	U	N3-C2-O2	-7.24	117.13	122.20
6	A	415	C	N3-C2-O2	-6.94	117.04	121.90
29	a	781	U	C2-N1-C1'	6.20	125.14	117.70
29	a	1837	A	O4'-C1'-N9	6.10	113.08	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	a	876	C	O4'-C1'-N1	5.97	112.98	108.20
29	a	2465	A	O4'-C1'-N9	5.93	112.94	108.20
29	a	504	G	O4'-C1'-N9	5.77	112.54	108.50
29	a	1095	U	C2-N1-C1'	5.63	124.46	117.70
6	A	653	G	O4'-C1'-N9	5.58	112.67	108.20
29	a	2793	C	C2-N1-C1'	5.54	124.90	118.80
6	A	1200	C	C2-N1-C1'	5.54	124.89	118.80
29	a	1301	U	N1-C2-O2	5.54	126.68	122.80
29	a	1301	U	N3-C2-O2	-5.50	118.35	122.20
29	a	2443	G	O4'-C1'-N9	5.45	112.31	108.50
29	a	880	C	N1-C2-O2	5.42	122.15	118.90
29	a	781	U	N1-C2-O2	5.42	126.59	122.80
29	a	739	G	O4'-C1'-N9	5.40	112.28	108.50
29	a	2814	U	C2-N1-C1'	5.39	124.17	117.70
29	a	192	G	C8-N9-C1'	-5.34	120.06	127.00
26	V	41	C	C2-N1-C1'	5.30	124.63	118.80
29	a	880	C	C2-N1-C1'	5.27	124.60	118.80
29	a	471	A	O5'-C5'-C4'	5.22	113.58	109.40
29	a	972	C	C6-N1-C2	-5.20	118.22	120.30
29	a	520	A	C2-N3-C4	-5.19	108.01	110.60
6	A	1155	C	C2-N1-C1'	5.18	124.50	118.80
29	a	1846	G	O4'-C1'-N9	5.18	112.35	108.20
29	a	496	U	N3-C2-O2	-5.16	118.59	122.20
29	a	708	C	C2-N1-C1'	5.15	124.46	118.80
29	a	2443	G	O5'-C5'-C4'	5.13	113.50	109.40
29	a	496	U	N1-C2-O2	5.11	126.38	122.80
6	A	326	C	C2-N1-C1'	5.06	124.37	118.80
29	a	140	A	O5'-C5'-C4'	5.05	113.44	109.40
29	a	1469	A	P-O3'-C3'	5.05	125.76	119.70
29	a	905	C	C2-N1-C1'	5.02	124.32	118.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
40	l	82	4D4	Mainchain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	427	0	462	11	0
2	1	363	0	401	10	0
3	2	509	0	566	11	0
4	3	295	0	326	7	0
5	4	552	0	552	15	0
6	A	32947	0	16583	362	0
7	B	1801	0	1814	33	0
8	C	1690	0	1774	24	0
9	D	1631	0	1691	29	0
10	E	1129	0	1173	17	0
11	F	878	0	878	15	0
12	G	1210	0	1255	29	0
13	H	985	0	1047	15	0
14	I	995	0	1053	22	0
15	J	801	0	832	22	0
16	K	862	0	873	16	0
17	L	947	0	997	18	0
18	M	912	0	975	14	0
19	N	792	0	833	23	0
20	O	705	0	712	5	0
21	P	644	0	655	10	0
22	Q	621	0	665	9	0
23	R	545	0	556	14	0
24	S	657	0	675	17	0
25	T	663	0	714	11	0
26	V	1644	0	842	40	0
27	W	219	0	108	1	0
28	X	841	0	824	17	0
29	a	61984	0	31153	565	0
30	b	2450	0	1241	21	0
31	c	2111	0	2174	22	0
32	d	1573	0	1612	18	0
33	e	1511	0	1566	11	0
34	f	1395	0	1450	34	0
35	g	1327	0	1386	22	0
36	h	458	0	480	8	0
37	i	1125	0	1148	18	0
38	j	946	0	1007	17	0
39	k	1089	0	1158	14	0
40	l	1088	0	1150	15	0
41	m	942	0	987	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	n	865	0	905	10	0
43	o	919	0	973	13	0
44	p	934	0	997	7	0
45	q	807	0	842	7	0
46	r	826	0	894	11	0
47	s	717	0	777	7	0
48	t	766	0	816	6	0
49	u	760	0	783	4	0
50	v	589	0	592	5	0
51	w	632	0	667	10	0
52	x	498	0	537	10	0
53	y	463	0	488	5	0
54	z	447	0	435	8	0
55	1	1	0	0	0	0
55	A	45	0	0	0	0
55	E	1	0	0	0	0
55	L	2	0	0	0	0
55	a	111	0	0	1	0
55	b	1	0	0	0	0
55	c	5	0	0	0	0
55	d	1	0	0	0	0
55	e	1	0	0	0	0
55	t	1	0	0	0	0
56	3	1	0	0	0	0
56	4	1	0	0	0	0
57	A	95	0	0	0	0
57	J	1	0	0	0	0
57	K	1	0	0	0	0
57	X	1	0	0	0	0
57	a	252	0	0	1	0
57	b	5	0	0	0	0
57	c	1	0	0	0	0
57	d	1	0	0	0	0
57	k	1	0	0	0	0
57	v	1	0	0	0	0
57	z	1	0	0	0	0
All	All	144018	0	96054	1569	0

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

All (1569) 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)
26:V:51:U:H3	26:V:65:G:H1	1.02	0.99
29:a:2125:G:H1	29:a:2144:U:H3	1.06	0.96
29:a:140:A:HO2'	29:a:141:A:H8	1.06	0.93
6:A:905:A:HO2'	6:A:906:A:H8	1.07	0.93
13:H:3:MET:HE1	13:H:9:ASP:HB2	1.52	0.90
29:a:536:U:O2	29:a:539:G:O6	1.94	0.85
6:A:201:A:H61	6:A:209:A:H61	1.25	0.85
2:1:1:MET:H2	29:a:1610:G:H21	1.24	0.85
43:o:30:VAL:HG22	43:o:47:GLU:HG3	1.57	0.85
29:a:1925:A:H2	29:a:1932:U:H3	1.24	0.85
29:a:467:C:O2	29:a:471:A:N6	2.11	0.84
24:S:62:VAL:HA	24:S:66:MET:HE2	1.59	0.83
29:a:1059:A:H1'	29:a:1086:A:H4'	1.61	0.83
14:I:19:LEU:HD11	14:I:59:TYR:HB3	1.61	0.82
29:a:1588:A:H5"	29:a:1589:A:H5'	1.62	0.81
39:k:4:ARG:HB2	39:k:7:GLU:HG3	1.63	0.81
6:A:670:A:H2'	6:A:671:G:C8	2.16	0.80
34:f:8:TYR:HA	34:f:12:LEU:HB2	1.63	0.79
7:B:48:THR:HG22	7:B:203:PRO:HG2	1.65	0.78
23:R:26:ILE:HD11	23:R:67:LEU:HB3	1.65	0.78
53:y:1:MET:HE3	53:y:2:LYS:H	1.49	0.76
12:G:86:GLN:HE22	26:V:33:OMC:H4'	1.50	0.75
6:A:74:G:H8	6:A:93:A:H62	1.31	0.75
8:C:118:GLU:HG2	8:C:187:MET:HE2	1.70	0.74
14:I:17:VAL:HG22	14:I:63:ILE:HG12	1.70	0.74
29:a:520:A:H5'	37:i:113:PRO:HG3	1.70	0.74
23:R:30:LYS:HA	23:R:33:ILE:HG12	1.71	0.73
29:a:45:G:H5"	29:a:46:G:H5'	1.71	0.73
29:a:2317:A:H2'	29:a:2318:A:C8	2.24	0.72
26:V:29:C:H2'	26:V:30:G:H8	1.53	0.72
29:a:868:U:O2	29:a:891:A:N7	2.23	0.72
12:G:72:MET:H	12:G:142:HIS:HE1	1.36	0.71
6:A:1068:C:H2'	6:A:1069:G:H8	1.56	0.71
9:D:161:ILE:HG23	9:D:177:HIS:CE1	2.26	0.71
6:A:251:G:H4'	22:Q:20:LYS:HD3	1.72	0.70
45:q:41:VAL:HG11	45:q:103:GLY:HA3	1.73	0.70
29:a:2280:U:H2'	29:a:2281:G:C8	2.26	0.70
15:J:42:MET:HB2	15:J:71:LYS:HB3	1.72	0.70
29:a:2125:G:N2	29:a:2144:U:O2	2.17	0.70
6:A:6:C:H2'	6:A:7:U:H2'	1.73	0.68
6:A:994:U:H3	6:A:1041:A:H62	1.41	0.68
29:a:1837:A:HO2'	29:a:1838:G:H8	1.41	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:z:42:VAL:HG12	54:z:48:TYR:HB2	1.74	0.68
6:A:1353:G:H2'	6:A:1354:A:C8	2.28	0.68
8:C:73:PRO:HG3	8:C:105:GLU:HG3	1.75	0.68
45:q:40:MET:HE3	45:q:49:ILE:HG12	1.74	0.68
6:A:1320:G:H2'	6:A:1321:A:C8	2.28	0.68
9:D:56:GLN:HB3	9:D:205:LEU:HB2	1.76	0.68
19:N:7:ILE:HD11	19:N:68:GLY:HA3	1.76	0.68
29:a:28:A:N6	29:a:504:G:H1'	2.09	0.68
37:i:21:THR:HA	37:i:61:GLN:HB3	1.75	0.68
6:A:1530:C:H42	27:W:13:A:H61	1.41	0.68
36:h:9:ILE:HG13	36:h:12:LEU:HD23	1.76	0.68
46:r:73:THR:HB	46:r:106:LYS:HB2	1.75	0.68
34:f:50:LEU:O	34:f:54:VAL:HG23	1.94	0.67
52:x:56:LEU:O	52:x:60:LYS:HG3	1.94	0.67
5:4:12:LEU:HD11	5:4:33:ILE:HG12	1.78	0.66
44:p:43:GLY:HA3	45:q:75:ILE:HD12	1.78	0.66
29:a:78:C:HO2'	29:a:79:C:H6	1.42	0.66
38:j:17:ARG:HD3	38:j:47:ILE:HD13	1.77	0.66
6:A:536:A:H2'	6:A:537:G:C8	2.31	0.66
29:a:1050:U:H4'	29:a:1052:G:O4'	1.96	0.66
29:a:1627:G:H2'	29:a:1628:A:C8	2.31	0.66
6:A:265:U:H2'	6:A:266:A:C8	2.30	0.66
6:A:661:G:H22	6:A:738:G:H1	1.45	0.65
29:a:902:A:H8	29:a:2266:G:H21	1.43	0.65
26:V:19:G:H21	26:V:59:A:H5'	1.62	0.65
40:l:76:GLU:HB2	40:l:91:GLU:HG3	1.77	0.65
1:0:4:LYS:HB3	1:0:50:ILE:HD13	1.78	0.65
6:A:498:C:H2'	6:A:499:A:H8	1.62	0.65
26:V:29:C:H2'	26:V:30:G:C8	2.30	0.65
23:R:26:ILE:HG23	23:R:30:LYS:HE3	1.79	0.65
29:a:1457:A:H2'	29:a:1458:A:C8	2.31	0.65
6:A:79:U:H2'	6:A:80:A:H8	1.62	0.65
6:A:498:C:H2'	6:A:499:A:C8	2.31	0.65
6:A:73:G:C2	6:A:74:G:H1'	2.32	0.64
29:a:28:A:H61	29:a:504:G:H1'	1.60	0.64
7:B:57:ASN:O	7:B:61:GLN:HG2	1.96	0.64
6:A:733:C:H2'	6:A:734:A:C8	2.32	0.64
35:g:43:LEU:HD11	35:g:50:LEU:HD22	1.79	0.64
15:J:26:VAL:HG13	15:J:36:VAL:HG21	1.79	0.64
29:a:559:U:H1'	29:a:2019:6MZ:H9C1	1.79	0.64
6:A:218:U:H2'	6:A:219:A:H8	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1215:C:H2'	6:A:1216:A:C8	2.32	0.63
6:A:333:G:H2'	6:A:334:A:C8	2.33	0.63
29:a:161:A:H3'	29:a:162:U:H5"	1.79	0.63
6:A:710:G:H2'	6:A:711:G:C8	2.34	0.63
29:a:1178:G:H5'	39:k:34:GLY:HA2	1.81	0.63
32:d:85:VAL:HG21	32:d:90:LEU:HD13	1.80	0.63
6:A:1320:G:H2'	6:A:1321:A:H8	1.63	0.63
39:k:124:VAL:HG11	39:k:129:LEU:HD11	1.80	0.63
9:D:157:ILE:O	9:D:161:ILE:HG12	1.99	0.63
26:V:51:U:O4	26:V:65:G:O6	2.17	0.62
29:a:2075:U:H2'	29:a:2076:G:C8	2.35	0.62
29:a:2088:U:H3	29:a:2179:G:H1	1.44	0.62
29:a:2123:A:H8	29:a:2146:G:H21	1.47	0.62
6:A:943:A:H2'	6:A:944:G:C8	2.34	0.62
33:e:117:LEU:HD11	33:e:187:MET:HE3	1.81	0.62
32:d:159:PHE:HB3	37:i:81:PRO:HG3	1.80	0.62
29:a:2109:G:H2'	29:a:2110:G:H8	1.65	0.62
29:a:875:U:H2'	29:a:876:C:C6	2.35	0.62
6:A:733:C:H2'	6:A:734:A:H8	1.63	0.62
11:F:6:ILE:HG23	11:F:89:ILE:HG12	1.81	0.62
6:A:610:C:H2'	6:A:611:C:C6	2.35	0.62
17:L:34:CYS:HA	17:L:55:VAL:HA	1.80	0.62
29:a:471:A:H4'	29:a:472:A:H5'	1.82	0.62
29:a:1165:U:H4'	29:a:1166:G:C2	2.34	0.62
23:R:42:SER:HA	23:R:45:THR:HG22	1.82	0.62
29:a:1018:A:N6	29:a:1115:G:H2'	2.14	0.62
32:d:184:ASP:HB3	32:d:189:VAL:HG22	1.81	0.62
9:D:77:TYR:HD1	9:D:95:LEU:HD23	1.65	0.61
6:A:333:G:H2'	6:A:334:A:H8	1.65	0.61
7:B:22:THR:HA	7:B:41:HIS:HD2	1.65	0.61
29:a:1018:A:H2'	29:a:1019:A:C8	2.34	0.61
6:A:671:G:H2'	6:A:672:A:H8	1.63	0.61
16:K:78:LEU:HB3	16:K:104:TYR:HE1	1.64	0.61
6:A:1438:A:C4	43:o:117:LEU:HD11	2.35	0.61
15:J:52:LEU:HD23	15:J:62:ARG:HG3	1.82	0.61
36:h:54:LEU:HA	36:h:57:GLN:HG2	1.82	0.61
6:A:19:U:H2'	6:A:20:C:C6	2.35	0.61
6:A:1215:C:H2'	6:A:1216:A:H8	1.65	0.61
31:c:183:LYS:HG3	31:c:268:ILE:HD11	1.83	0.61
6:A:231:U:H2'	6:A:232:A:C8	2.35	0.61
11:F:18:VAL:HA	11:F:21:MET:HE3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:43:G:H2'	6:A:44:G:H8	1.65	0.61
6:A:1068:C:H2'	6:A:1069:G:C8	2.36	0.61
29:a:2318:A:H2'	29:a:2319:G:C8	2.36	0.61
6:A:725:A:H2'	6:A:726:A:C8	2.35	0.61
6:A:766:G:H4'	6:A:1510:A:H4'	1.83	0.61
6:A:1001:A:H5'	6:A:1023:G:H22	1.66	0.60
17:L:87:VAL:HG11	17:L:90:LEU:HD12	1.83	0.60
24:S:10:PHE:HE2	24:S:37:ARG:HG3	1.64	0.60
6:A:550:A:H5"	17:L:21:VAL:HG21	1.83	0.60
8:C:211:MET:O	8:C:215:MET:HE3	2.01	0.60
9:D:38:ALA:HB3	9:D:43:GLY:HA2	1.83	0.60
29:a:1049:G:H3'	29:a:1050:U:C5'	2.31	0.60
6:A:711:G:H2'	6:A:712:A:C8	2.37	0.60
30:b:46:U:H2'	30:b:47:C:C6	2.36	0.60
6:A:458:G:H3'	6:A:459:U:C6	2.37	0.60
26:V:51:U:H2'	26:V:52:C:C6	2.36	0.60
29:a:584:U:H2'	29:a:585:U:C6	2.37	0.60
29:a:2169:U:H2'	29:a:2170:G:C8	2.37	0.60
26:V:27:G:O6	26:V:45:A:N1	2.35	0.60
34:f:67:VAL:HG11	34:f:84:PRO:HB3	1.84	0.60
52:x:28:LEU:HD23	52:x:37:LEU:HD11	1.83	0.60
6:A:252:U:H2'	6:A:253:G:H8	1.66	0.60
6:A:671:G:H21	16:K:117:HIS:HB2	1.66	0.60
6:A:1388:U:H2'	6:A:1389:G:C8	2.37	0.59
29:a:2056:G:H1	29:a:2432:U:H3	1.50	0.59
35:g:9:VAL:HG13	35:g:50:LEU:HB2	1.84	0.59
29:a:2262:A:H2'	29:a:2263:A:C8	2.38	0.59
31:c:107:PRO:HD2	31:c:110:LEU:HD22	1.83	0.59
52:x:18:LEU:HB2	52:x:53:ILE:HG21	1.84	0.59
10:E:40:ASP:OD1	10:E:44:ARG:HB2	2.02	0.59
29:a:2120:U:H5'	29:a:2121:U:H2'	1.83	0.59
52:x:32:LYS:HB2	52:x:37:LEU:HD22	1.84	0.59
6:A:820:C:HO2'	13:H:2:SER:N	2.00	0.59
13:H:39:VAL:HG21	13:H:111:ILE:HG22	1.84	0.59
29:a:733:G:H2'	29:a:734:U:C6	2.37	0.59
37:i:36:LEU:HD11	37:i:122:MET:HB2	1.84	0.59
40:l:39:ARG:HB3	40:l:99:PRO:HD3	1.83	0.59
6:A:77:G:H3'	6:A:78:G:C8	2.37	0.59
6:A:218:U:H2'	6:A:219:A:C8	2.38	0.59
6:A:1315:A:H5"	24:S:3:ARG:NH1	2.18	0.59
28:X:10:ASN:HD22	28:X:48:GLY:HA2	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:127:A:H5”	29:a:128:C:C6	2.37	0.59
29:a:140:A:O2’	29:a:141:A:H8	1.79	0.59
48:t:25:LEU:HD21	48:t:35:GLU:HG2	1.84	0.59
29:a:2483:G:H4’	40:l:80:GLU:HG2	1.85	0.59
1:0:31:GLU:OE2	1:0:46:LYS:HG2	2.03	0.59
6:A:712:A:H2’	6:A:713:A:C8	2.38	0.59
20:O:39:LEU:HD12	20:O:59:MET:HE1	1.84	0.59
29:a:1192:A:H4’	29:a:1193:A:H5”	1.85	0.59
29:a:1474:U:H3	29:a:1491:G:H1	1.51	0.59
29:a:1043:U:H2’	29:a:1044:A:C8	2.38	0.59
29:a:2230:A:H2’	29:a:2231:G:C8	2.38	0.59
11:F:22:VAL:HG13	11:F:62:MET:HE2	1.85	0.58
6:A:420:G:H2’	6:A:421:G:C8	2.38	0.58
29:a:2317:A:H2’	29:a:2318:A:H8	1.66	0.58
36:h:25:TYR:HE1	36:h:29:PHE:HD2	1.51	0.58
29:a:536:U:O2	29:a:539:G:C6	2.56	0.58
29:a:1457:A:H2’	29:a:1458:A:H8	1.68	0.58
6:A:58:U:H2’	6:A:59:G:H8	1.68	0.58
29:a:1304:A:H2’	29:a:1305:G:C8	2.39	0.58
46:r:11:ALA:HA	46:r:100:THR:HG22	1.85	0.58
9:D:19:LEU:HB2	9:D:21:LEU:HG	1.86	0.58
6:A:1247:A:H2’	6:A:1248:A:C8	2.38	0.58
15:J:85:ASP:O	15:J:89:LYS:HG3	2.04	0.58
29:a:273:A:H2’	29:a:274:A:C8	2.36	0.58
29:a:572:C:H2’	29:a:573:A:C8	2.39	0.58
6:A:58:U:H2’	6:A:59:G:C8	2.39	0.58
15:J:24:GLU:OE2	15:J:90:LEU:HD21	2.03	0.58
29:a:2316:A:H2’	29:a:2317:A:C8	2.39	0.58
4:3:36:ARG:HG2	4:3:37:GLN:H	1.68	0.58
12:G:69:VAL:HG13	12:G:100:ALA:HB1	1.85	0.58
29:a:349:A:HO2’	29:a:350:C:H6	1.52	0.58
29:a:990:A:H2’	29:a:991:A:C8	2.39	0.58
6:A:43:G:H2’	6:A:44:G:C8	2.39	0.58
29:a:599:A:H2’	29:a:600:A:C8	2.39	0.58
29:a:2546:G:H2’	29:a:2547:C:C6	2.39	0.58
29:a:2836:U:H2’	29:a:2837:G:O4’	2.03	0.58
1:0:2:ARG:HA	1:0:21:LYS:O	2.03	0.58
4:3:16:VAL:HG22	4:3:25:VAL:HG22	1.86	0.58
11:F:51:ILE:O	11:F:54:ILE:HG13	2.03	0.58
29:a:1785:U:H2’	29:a:1786:C:C6	2.39	0.58
29:a:2294:U:H5”	34:f:131:GLY:HA3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:1071:U:H2'	29:a:1072:U:C6	2.39	0.57
11:F:42:TRP:NE1	11:F:102:LEU:HB2	2.19	0.57
29:a:346:C:H2'	29:a:347:A:H8	1.67	0.57
29:a:2164:C:H2'	29:a:2165:A:C8	2.38	0.57
32:d:6:VAL:HG11	32:d:79:LEU:HD11	1.87	0.57
6:A:1020:G:H2'	6:A:1021:G:C8	2.38	0.57
14:I:63:ILE:HG21	14:I:77:ILE:HG12	1.85	0.57
29:a:1791:A:H2'	29:a:1792:A:C8	2.38	0.57
45:q:64:ILE:HD11	45:q:97:LYS:HB2	1.85	0.57
30:b:11:A:H8	30:b:67:G:H21	1.52	0.57
29:a:839:U:H2'	29:a:840:A:H8	1.69	0.57
29:a:1421:A:H2'	29:a:1422:A:C8	2.38	0.57
29:a:2172:U:H2'	29:a:2173:A:C8	2.39	0.57
29:a:2232:U:H2'	29:a:2233:U:C6	2.39	0.57
6:A:220:A:H2'	6:A:221:U:C6	2.40	0.57
29:a:2116:G:H2'	29:a:2117:G:C8	2.39	0.57
6:A:1353:G:H2'	6:A:1354:A:H8	1.69	0.57
29:a:1043:U:H2'	29:a:1044:A:H8	1.70	0.57
6:A:419:U:H2'	6:A:420:G:O4'	2.04	0.57
6:A:888:U:H2'	6:A:889:A:H8	1.70	0.57
29:a:1527:G:H2'	29:a:1528:U:C6	2.40	0.57
29:a:1836:A:HO2'	29:a:1837:A:H8	1.52	0.57
29:a:2116:G:H2'	29:a:2117:G:H8	1.68	0.57
8:C:78:GLY:HA3	8:C:83:ASP:HB2	1.87	0.56
22:Q:25:LEU:HD12	22:Q:44:LYS:HG3	1.86	0.56
29:a:2175:U:H2'	29:a:2176:G:C8	2.40	0.56
29:a:2526:U:H2'	29:a:2527:C:C6	2.40	0.56
3:2:17:THR:HG21	3:2:48:MET:HE1	1.87	0.56
6:A:1311:C:H2'	6:A:1312:U:C6	2.41	0.56
10:E:54:GLU:HG3	10:E:56:PRO:HD2	1.85	0.56
29:a:630:U:H2'	29:a:631:C:C6	2.39	0.56
29:a:1837:A:O2'	29:a:1838:G:H8	1.88	0.56
1:0:46:LYS:NZ	1:0:46:LYS:HB3	2.19	0.56
29:a:1304:A:H2'	29:a:1305:G:H8	1.68	0.56
6:A:220:A:H2'	6:A:221:U:H6	1.71	0.56
6:A:1519:U:H2'	6:A:1520:G:H8	1.70	0.56
14:I:44:MET:O	14:I:48:GLN:HG2	2.04	0.56
37:i:17:VAL:HG23	37:i:137:PRO:HB2	1.87	0.56
40:l:65:PHE:HE2	40:l:107:GLU:HG2	1.70	0.56
6:A:85:G:H21	6:A:87:U:H3	1.54	0.56
6:A:759:U:H2'	6:A:760:A:C8	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:E:71:ILE:HD12	10:E:144:ARG:HB2	1.86	0.56
14:I:26:LEU:HD22	14:I:33:LEU:HB2	1.87	0.56
29:a:2141:C:H2'	29:a:2142:A:H8	1.71	0.56
29:a:2823:G:H2'	29:a:2868:A:H61	1.71	0.56
35:g:164:TYR:HB2	35:g:167:GLU:HB2	1.88	0.56
8:C:211:MET:HE3	8:C:215:MET:CE	2.35	0.56
29:a:5:A:H2'	29:a:6:A:C8	2.41	0.56
29:a:590:A:H2'	29:a:591:G:H8	1.71	0.56
6:A:1127:A:H2'	6:A:1128:G:H8	1.71	0.56
15:J:14:ASP:HB2	15:J:17:LEU:HB2	1.87	0.56
28:X:22:ARG:O	28:X:26:THR:HG23	2.05	0.56
30:b:46:U:H2'	30:b:47:C:H6	1.70	0.56
37:i:1:MET:N	37:i:1:MET:HE2	2.21	0.56
6:A:1140:G:H2'	6:A:1141:G:H8	1.70	0.56
6:A:1311:C:H2'	6:A:1312:U:H6	1.70	0.56
29:a:885:U:HO2'	29:a:886:U:H6	1.53	0.56
34:f:128:TYR:HE2	34:f:130:MET:HE3	1.71	0.56
44:p:49:ASP:HA	44:p:52:GLN:HB2	1.88	0.56
6:A:414:C:H2'	6:A:415:C:C6	2.41	0.55
6:A:943:A:H2'	6:A:944:G:H8	1.69	0.55
9:D:154:GLN:O	9:D:157:ILE:HG22	2.05	0.55
36:h:30:LEU:HB3	36:h:36:ALA:HB3	1.89	0.55
29:a:2580:C:H2'	29:a:2581:G:C8	2.41	0.55
6:A:1513:2MG:H2'	6:A:1515:MA6:OP2	2.06	0.55
15:J:42:MET:HG3	15:J:71:LYS:HE2	1.88	0.55
29:a:277:U:H3	29:a:353:A:N6	2.04	0.55
29:a:1396:U:H2'	29:a:1397:G:H8	1.70	0.55
34:f:138:PHE:CD2	34:f:139:PRO:HD3	2.42	0.55
6:A:989:U:H4'	6:A:990:G:O5'	2.06	0.55
29:a:1474:U:H2'	29:a:1475:C:C6	2.41	0.55
29:a:1530:C:H2'	29:a:1531:A:C8	2.41	0.55
31:c:165:LEU:HB2	31:c:173:ILE:HG22	1.88	0.55
43:o:5:HIS:HE1	43:o:7:LEU:HD23	1.70	0.55
17:L:37:VAL:HG22	17:L:53:CYS:HB3	1.87	0.55
29:a:181:A:H2'	29:a:182:A:C8	2.42	0.55
29:a:2720:G:H2'	29:a:2721:G:C8	2.41	0.55
6:A:1248:A:H2'	6:A:1249:A:C8	2.41	0.55
9:D:106:ARG:HB3	9:D:170:PRO:HG2	1.88	0.55
16:K:84:LEU:HD23	16:K:110:THR:HB	1.88	0.55
29:a:1783:A:H2'	29:a:1784:C:C6	2.41	0.55
6:A:78:G:H21	6:A:90:C:H41	1.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:F:29:ILE:HD13	11:F:64:VAL:HG21	1.88	0.55
26:V:52:C:H2'	26:V:53:G:O4'	2.07	0.55
26:V:54:G:H3'	26:V:55:5MU:H73	1.89	0.55
29:a:1492:U:H2'	29:a:1493:A:H8	1.71	0.55
29:a:2235:G:H2'	29:a:2236:A:C8	2.42	0.55
6:A:1510:A:H2'	6:A:1511:G:C8	2.42	0.55
29:a:2174:A:H2'	29:a:2175:U:C6	2.41	0.55
29:a:1280:G:H2'	29:a:1281:U:C6	2.42	0.55
29:a:2103:A:H3'	29:a:2104:G:H8	1.71	0.55
34:f:137:VAL:HG13	34:f:140:GLU:H	1.71	0.55
9:D:28:PHE:O	9:D:32:THR:HG22	2.07	0.54
29:a:486:G:H4'	46:r:6:LYS:HB2	1.89	0.54
6:A:1136:G:H4'	6:A:1137:A:H5'	1.88	0.54
11:F:18:VAL:HG21	11:F:58:HIS:CE1	2.42	0.54
29:a:2834:U:H5"	43:o:55:ASN:O	2.07	0.54
40:l:35:LYS:HD2	40:l:132:VAL:HG11	1.89	0.54
29:a:823:U:H2'	29:a:824:A:C8	2.43	0.54
29:a:2111:U:H2'	29:a:2112:G:O4'	2.07	0.54
52:x:28:LEU:HD21	52:x:42:GLU:HB2	1.89	0.54
6:A:27:C:H5'	6:A:521:G:H1'	1.89	0.54
7:B:45:LEU:HA	7:B:48:THR:HG23	1.88	0.54
28:X:5:ILE:HG13	28:X:41:VAL:HB	1.90	0.54
6:A:1504:A:H2'	6:A:1505:G:C8	2.43	0.54
8:C:70:THR:HG21	8:C:76:VAL:HG11	1.90	0.54
12:G:51:GLN:HE22	12:G:58:PRO:HD3	1.71	0.54
26:V:1:C:H42	26:V:73:A:H61	1.55	0.54
29:a:1341:A:H2'	29:a:1342:A:C8	2.42	0.54
29:a:1917:A:H2'	29:a:1918:G:O4'	2.08	0.54
29:a:2222:U:H2'	29:a:2223:G:C8	2.43	0.54
40:l:35:LYS:HG2	40:l:130:THR:HG22	1.90	0.54
42:n:2:ASN:HA	42:n:6:GLN:HG2	1.90	0.54
43:o:56:ARG:H	43:o:60:SER:HB3	1.71	0.54
6:A:266:A:H2'	6:A:267:C:H6	1.72	0.54
7:B:15:GLY:C	7:B:17:HIS:H	2.14	0.54
29:a:824:A:H2'	29:a:825:G:C8	2.43	0.54
29:a:1528:U:H2'	29:a:1529:A:C8	2.43	0.54
6:A:265:U:H2'	6:A:266:A:H8	1.71	0.54
6:A:647:G:H2'	6:A:648:C:H5'	1.89	0.54
6:A:754:U:H2'	6:A:755:G:O4'	2.08	0.54
6:A:1145:U:H2'	6:A:1146:U:O4'	2.08	0.54
19:N:89:MET:HE2	19:N:89:MET:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:17:G:H4'	44:p:25:TYR:HE1	1.73	0.54
29:a:1018:A:H61	29:a:1115:G:H2'	1.73	0.54
29:a:2174:A:H2'	29:a:2175:U:H6	1.71	0.54
31:c:232:HIS:NE2	31:c:244:PRO:HA	2.22	0.54
37:i:92:LEU:HD21	37:i:99:GLU:HG2	1.89	0.54
29:a:700:U:H2'	29:a:701:U:C6	2.43	0.53
43:o:95:VAL:HG11	43:o:100:LEU:HD21	1.90	0.53
3:2:12:LYS:HB3	39:k:65:LYS:HG2	1.91	0.53
17:L:107:VAL:HG23	17:L:110:ARG:HG3	1.90	0.53
29:a:317:A:OP2	33:e:162:ASN:HB2	2.08	0.53
29:a:840:A:H2'	29:a:841:C:C6	2.43	0.53
6:A:670:A:H2'	6:A:671:G:H8	1.67	0.53
22:Q:23:VAL:HG22	22:Q:46:HIS:CD2	2.42	0.53
29:a:2302:C:H5"	34:f:88:LYS:HD3	1.89	0.53
47:s:68:ARG:NH2	47:s:73:LEU:HD22	2.23	0.53
6:A:385:A:H3'	6:A:386:U:H6	1.74	0.53
34:f:40:VAL:HG11	34:f:49:LEU:HB3	1.90	0.53
38:j:98:ILE:HD12	38:j:117:LEU:HB2	1.89	0.53
6:A:1409:C:H2'	6:A:1410:A:C8	2.44	0.53
6:A:1447:G:H21	6:A:1450:A:H2	1.56	0.53
11:F:100:SER:H	11:F:103:ALA:HB3	1.73	0.53
29:a:2798:A:H2'	29:a:2799:A:C8	2.44	0.53
44:p:86:ALA:HB2	44:p:116:ALA:HB2	1.90	0.53
15:J:22:ALA:O	15:J:26:VAL:HG23	2.08	0.53
29:a:513:U:H2'	29:a:514:G:C8	2.44	0.53
29:a:2156:U:H2'	29:a:2157:G:C8	2.43	0.53
29:a:2235:G:H2'	29:a:2236:A:H8	1.74	0.53
29:a:2626:U:H2'	29:a:2627:G:O4'	2.09	0.53
16:K:58:THR:HG22	16:K:60:PHE:H	1.73	0.53
26:V:66:C:H2'	26:V:67:C:C6	2.44	0.53
29:a:773:A:C2	31:c:225:MET:HG2	2.44	0.53
29:a:2362:A:H2'	29:a:2363:C:C6	2.44	0.53
34:f:93:GLY:H	34:f:96:MET:HE3	1.74	0.53
6:A:671:G:H2'	6:A:672:A:C8	2.43	0.53
6:A:1035:C:H2'	6:A:1036:U:H6	1.74	0.53
28:X:10:ASN:ND2	28:X:48:GLY:HA2	2.24	0.53
29:a:52:A:H2'	29:a:53:A:C8	2.44	0.53
29:a:2503:U:H2'	29:a:2504:C:C6	2.43	0.53
6:A:33:G:C5	6:A:302:A:H1'	2.44	0.53
8:C:24:ALA:HB1	8:C:28:GLN:HG3	1.91	0.53
26:V:11:A:H2'	26:V:12:G:C8	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:191:A:H2'	29:a:192:G:N3	2.24	0.53
31:c:20:VAL:HG23	31:c:21:HIS:H	1.74	0.53
6:A:1309:G:H5'	24:S:5:LEU:HD11	1.91	0.53
29:a:1842:A:H2'	29:a:1843:A:C8	2.44	0.53
38:j:47:ILE:HG13	38:j:48:PRO:HD2	1.91	0.53
6:A:388:C:H2'	6:A:389:A:H8	1.75	0.52
6:A:915:A:H2'	6:A:916:A:C8	2.44	0.52
6:A:1267:U:H2'	6:A:1268:G:H8	1.74	0.52
6:A:1352:G:H2'	6:A:1353:G:H8	1.74	0.52
25:T:48:THR:HG22	25:T:52:LYS:HD2	1.90	0.52
29:a:1526:U:H5"	29:a:1527:G:C8	2.45	0.52
29:a:2580:C:H2'	29:a:2581:G:H8	1.71	0.52
29:a:2667:A:H2'	29:a:2668:A:C8	2.44	0.52
6:A:588:U:H2'	6:A:589:A:C8	2.45	0.52
6:A:648:C:HO2'	6:A:649:U:H6	1.55	0.52
26:V:8:4SU:H5"	26:V:50:G:H5'	1.90	0.52
29:a:630:U:H2'	29:a:631:C:H6	1.74	0.52
29:a:2604:U:C2	54:z:4:GLN:HA	2.43	0.52
30:b:87:A:H5'	40:l:18:THR:HG22	1.91	0.52
25:T:43:ASP:HB3	25:T:46:VAL:HG12	1.91	0.52
29:a:154:A:H2'	29:a:155:A:C8	2.44	0.52
29:a:208:C:H2'	29:a:209:C:H6	1.75	0.52
6:A:231:U:H2'	6:A:232:A:H8	1.71	0.52
6:A:552:U:H2'	6:A:553:C:C6	2.44	0.52
6:A:748:U:H2'	6:A:749:G:O4'	2.08	0.52
6:A:818:G:H2'	6:A:819:U:C6	2.44	0.52
8:C:130:PHE:O	8:C:134:MET:HG3	2.10	0.52
10:E:150:GLU:CD	10:E:150:GLU:H	2.17	0.52
13:H:34:VAL:HG22	13:H:60:LEU:HD13	1.90	0.52
16:K:98:ALA:O	16:K:102:VAL:HG23	2.10	0.52
29:a:175:A:H2'	29:a:176:A:C8	2.45	0.52
29:a:2536:A:H2'	29:a:2537:U:C6	2.45	0.52
29:a:2579:A:H2'	29:a:2580:C:C6	2.45	0.52
29:a:2638:C:H2'	29:a:2639:U:H6	1.72	0.52
32:d:10:CYS:SG	32:d:29:GLU:HB3	2.49	0.52
35:g:22:ARG:HH21	35:g:37:LEU:HB3	1.73	0.52
41:m:8:VAL:HG22	41:m:43:GLU:HG2	1.91	0.52
6:A:176:U:H2'	6:A:177:A:H5'	1.92	0.52
6:A:329:C:H2'	6:A:330:C:H6	1.74	0.52
29:a:648:U:H2'	29:a:649:U:C6	2.44	0.52
29:a:2060:A:H2'	29:a:2061:C:C6	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:143:G:H2'	6:A:144:G:C8	2.45	0.52
18:M:77:ILE:HG22	18:M:81:MET:HE2	1.91	0.52
29:a:840:A:H2'	29:a:841:C:H6	1.75	0.52
29:a:1706:U:H3	29:a:1732:G:H1	1.57	0.52
29:a:1903:C:H2'	29:a:1904:3TD:H6	1.92	0.52
6:A:319:U:H2'	6:A:320:G:O4'	2.10	0.52
29:a:348:C:O2'	29:a:349:A:H5'	2.09	0.52
29:a:572:C:H2'	29:a:573:A:H8	1.73	0.52
29:a:1420:G:H2'	29:a:1421:A:C8	2.44	0.52
29:a:1492:U:H2'	29:a:1493:A:C8	2.44	0.52
29:a:1785:U:H2'	29:a:1786:C:H6	1.73	0.52
29:a:2457:A:P	29:a:2465:A:H61	2.33	0.52
29:a:2671:U:H5"	43:o:2:SER:HB2	1.91	0.52
6:A:378:A:H2'	6:A:379:A:C8	2.45	0.52
8:C:22:TRP:HB3	8:C:59:ARG:HB2	1.92	0.52
12:G:75:VAL:HG21	12:G:144:MET:HE3	1.91	0.52
25:T:24:LEU:O	25:T:28:VAL:HG23	2.10	0.52
6:A:37:G:H2'	6:A:38:C:C6	2.45	0.52
7:B:71:PHE:HB3	7:B:82:ILE:HD12	1.92	0.52
26:V:28:U:H2'	26:V:29:C:C6	2.44	0.52
39:k:80:ARG:HB2	39:k:83:GLU:HG3	1.92	0.52
26:V:30:G:H2'	26:V:31:G:H8	1.75	0.51
1:0:30:MET:H	1:0:47:GLU:HB2	1.76	0.51
18:M:78:LYS:HA	18:M:81:MET:HG3	1.91	0.51
29:a:195:A:H61	29:a:198:C:H3'	1.74	0.51
29:a:1673:G:H2'	29:a:1674:U:C6	2.45	0.51
6:A:759:U:H2'	6:A:760:A:H8	1.75	0.51
6:A:1034:U:H2'	6:A:1035:C:H6	1.76	0.51
1:0:1:MET:HG3	29:a:2273:A:OP1	2.09	0.51
6:A:23:G:H2'	6:A:24:G:C8	2.44	0.51
6:A:536:A:H2'	6:A:537:G:H8	1.73	0.51
6:A:1001:A:H5'	6:A:1023:G:N2	2.26	0.51
8:C:58:GLU:HB3	15:J:94:ALA:HB1	1.92	0.51
26:V:10:G:N2	26:V:27:G:H1'	2.25	0.51
29:a:1374:A:H2'	29:a:1375:U:C6	2.45	0.51
32:d:26:THR:HG21	32:d:196:ILE:HG12	1.92	0.51
40:l:65:PHE:CE2	40:l:107:GLU:HG2	2.45	0.51
29:a:513:U:H2'	29:a:514:G:H8	1.75	0.51
29:a:2014:C:H2'	29:a:2015:U:C6	2.45	0.51
29:a:2682:G:H2'	29:a:2683:G:H8	1.75	0.51
6:A:266:A:H2'	6:A:267:C:C6	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:M:106:ALA:HB3	18:M:110:LYS:HD3	1.92	0.51
29:a:2546:G:H2'	29:a:2547:C:H6	1.75	0.51
30:b:109:G:H2'	30:b:110:C:C6	2.46	0.51
6:A:521:G:H2'	6:A:522:C:C6	2.45	0.51
6:A:693:A:H2'	6:A:694:U:H6	1.76	0.51
31:c:53:HIS:HA	31:c:217:ARG:HB2	1.93	0.51
34:f:135:GLN:O	34:f:136:ILE:HG12	2.11	0.51
6:A:1038:G:H2'	6:A:1039:A:C8	2.45	0.51
7:B:168:VAL:HG23	7:B:193:SER:OG	2.11	0.51
14:I:69:GLY:O	14:I:73:GLN:HG3	2.11	0.51
29:a:1484:A:H2'	29:a:1486:C:C5	2.45	0.51
4:3:23:ILE:HD13	29:a:1022:A:H1'	1.92	0.51
8:C:211:MET:O	8:C:214:VAL:HG22	2.11	0.51
29:a:196:A:C2	39:k:52:PHE:HZ	2.29	0.51
29:a:1496:C:H4'	29:a:1498:A:C8	2.46	0.51
29:a:1837:A:C4	29:a:1838:G:C8	2.99	0.51
29:a:2141:C:H2'	29:a:2142:A:C8	2.46	0.51
38:j:47:ILE:HG22	38:j:50:ALA:HB2	1.93	0.51
43:o:17:LYS:HD3	43:o:80:HIS:HA	1.92	0.51
46:r:82:LEU:HB2	46:r:98:LYS:HB2	1.92	0.51
6:A:1381:C:H2'	6:A:1382:G:C8	2.46	0.51
26:V:66:C:H2'	26:V:67:C:H6	1.76	0.51
29:a:2053:C:H2'	29:a:2054:C:C6	2.46	0.51
29:a:2124:A:H4'	29:a:2149:C:H4'	1.93	0.51
29:a:2834:U:H2'	29:a:2835:G:C8	2.46	0.51
5:4:64:ARG:HB3	24:S:5:LEU:HD22	1.93	0.50
6:A:991:A:H3'	6:A:992:C:H5"	1.92	0.50
10:E:73:VAL:HG11	10:E:143:LEU:HB3	1.92	0.50
23:R:30:LYS:HE2	23:R:68:ILE:HG22	1.93	0.50
29:a:64:G:H2'	29:a:65:C:C6	2.46	0.50
29:a:571:U:H2'	29:a:572:C:C6	2.46	0.50
29:a:1725:C:H2'	29:a:1726:U:H6	1.76	0.50
29:a:1760:C:H2'	29:a:1761:A:C8	2.46	0.50
40:l:42:MET:HE3	40:l:125:LEU:HD22	1.93	0.50
46:r:12:ILE:HD13	46:r:43:ALA:HB2	1.93	0.50
6:A:458:G:H3'	6:A:459:U:H6	1.75	0.50
21:P:61:ALA:HB3	21:P:67:LYS:HE2	1.93	0.50
21:P:71:ASP:HB3	21:P:74:ARG:HB2	1.93	0.50
29:a:301:U:H2'	29:a:302:G:O4'	2.12	0.50
29:a:1396:U:H2'	29:a:1397:G:C8	2.47	0.50
29:a:2026:A:H2'	29:a:2027:G:C8	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:2689:A:H2'	29:a:2690:C:H6	1.77	0.50
6:A:821:U:H2'	6:A:822:A:H8	1.77	0.50
6:A:1352:G:H2'	6:A:1353:G:C8	2.47	0.50
29:a:467:C:N3	29:a:471:A:N7	2.59	0.50
29:a:2729:A:H2'	29:a:2730:A:C8	2.46	0.50
31:c:140:THR:HG23	31:c:161:SER:HB2	1.92	0.50
12:G:26:PHE:HE2	12:G:120:LEU:HD21	1.76	0.50
12:G:72:MET:HG3	12:G:142:HIS:NE2	2.26	0.50
18:M:92:ARG:HG2	29:a:879:C:C5	2.45	0.50
37:i:109:LEU:O	37:i:111:LYS:HE3	2.12	0.50
6:A:489:C:H2'	6:A:490:A:C8	2.45	0.50
6:A:674:U:H3	6:A:710:G:H22	1.59	0.50
6:A:1235:A:N7	6:A:1300:C:H1'	2.27	0.50
9:D:8:LYS:HB3	9:D:21:LEU:HB3	1.94	0.50
9:D:199:GLU:HA	9:D:202:ILE:HD12	1.94	0.50
10:E:12:GLU:HG2	10:E:63:LEU:HD22	1.94	0.50
10:E:158:LYS:HB2	10:E:163:ILE:HG23	1.94	0.50
15:J:11:LYS:NZ	15:J:71:LYS:HD2	2.26	0.50
20:O:75:HIS:O	20:O:79:THR:HG23	2.10	0.50
29:a:30:G:H2'	29:a:31:C:C6	2.47	0.50
38:j:108:THR:HG23	38:j:110:GLN:H	1.76	0.50
6:A:408:A:H2'	6:A:409:G:H4'	1.93	0.50
6:A:572:G:O2'	6:A:818:G:H5'	2.11	0.50
25:T:67:ILE:HB	25:T:71:LYS:HD2	1.94	0.50
29:a:78:C:O2'	29:a:79:C:H6	1.95	0.50
29:a:839:U:H2'	29:a:840:A:C8	2.47	0.50
29:a:855:G:H2'	29:a:856:C:C6	2.47	0.50
29:a:1031:G:H2'	29:a:1032:G:H8	1.76	0.50
29:a:2158:A:H2'	29:a:2159:A:C8	2.46	0.50
46:r:2:GLU:HG2	46:r:106:LYS:HD2	1.92	0.50
2:1:10:LEU:HD23	29:a:761:G:H5"	1.94	0.50
6:A:69:C:H2'	6:A:70:G:C8	2.47	0.50
6:A:189:A:H2'	6:A:190:G:C8	2.46	0.50
7:B:83:ARG:HG3	7:B:93:TYR:CE1	2.47	0.50
29:a:2142:A:H2'	29:a:2143:G:H8	1.76	0.50
29:a:2777:C:H2'	29:a:2778:C:C6	2.46	0.50
35:g:24:VAL:HG13	35:g:35:PHE:HB3	1.92	0.50
5:4:11:LYS:HE2	5:4:13:VAL:HG22	1.94	0.50
6:A:1230:G:H2'	6:A:1231:C:C6	2.47	0.50
23:R:70:TYR:HB2	23:R:74:HIS:NE2	2.27	0.50
29:a:1202:A:H61	29:a:1223:G:H1'	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:2532:G:H2'	29:a:2533:G:C8	2.46	0.50
31:c:118:SER:HB3	31:c:129:CYS:HB3	1.92	0.50
3:2:48:MET:HE2	3:2:48:MET:HA	1.93	0.50
6:A:1019:U:H3'	6:A:1020:G:H8	1.77	0.50
29:a:1345:C:H2'	29:a:1346:G:O4'	2.12	0.50
29:a:2041:A:H4'	32:d:151:GLN:O	2.11	0.50
29:a:2132:C:H2'	29:a:2133:G:O4'	2.12	0.50
29:a:2172:U:H2'	29:a:2173:A:H8	1.77	0.50
29:a:2366:A:H2'	29:a:2367:A:C8	2.47	0.50
31:c:173:ILE:HG13	31:c:268:ILE:CD1	2.42	0.50
34:f:141:ILE:HG12	34:f:145:LYS:HG3	1.93	0.50
38:j:113:LYS:O	38:j:117:LEU:HG	2.12	0.50
40:l:32:ILE:HG21	40:l:114:ALA:HB1	1.93	0.50
6:A:35:A:H2'	6:A:36:C:C6	2.47	0.49
7:B:156:MET:HE1	7:B:160:PRO:HD3	1.94	0.49
9:D:181:GLU:HG2	9:D:182:GLY:N	2.27	0.49
10:E:114:LEU:HD13	10:E:122:VAL:HG11	1.93	0.49
29:a:872:G:H1	29:a:886:U:H3	1.58	0.49
29:a:2280:U:H2'	29:a:2281:G:H8	1.73	0.49
42:n:74:GLY:HA3	42:n:108:ALA:HB3	1.94	0.49
6:A:281:U:H2'	6:A:282:G:C8	2.47	0.49
6:A:777:A:H5"	16:K:124:LYS:HD3	1.94	0.49
15:J:66:GLU:HB3	19:N:99:ALA:HB2	1.93	0.49
24:S:3:ARG:NH1	24:S:10:PHE:HB2	2.26	0.49
29:a:925:U:H2'	29:a:926:C:H6	1.77	0.49
29:a:2573:U:H2'	29:a:2574:U:H2'	1.93	0.49
34:f:80:ARG:HD3	34:f:80:ARG:N	2.28	0.49
6:A:201:A:N6	6:A:209:A:H61	2.02	0.49
28:X:60:ILE:HG13	28:X:86:ALA:HB1	1.93	0.49
29:a:545:U:C2'	29:a:546:G:H5'	2.42	0.49
29:a:2689:A:H2'	29:a:2690:C:C6	2.47	0.49
35:g:88:GLN:HB3	35:g:163:ARG:HG2	1.94	0.49
40:l:33:ALA:HB2	40:l:105:GLU:HG2	1.94	0.49
5:4:5:ILE:HB	34:f:64:LYS:HD2	1.93	0.49
6:A:242:A:C2	6:A:278:A:C5	3.00	0.49
6:A:1235:A:H2	6:A:1238:G:N3	2.10	0.49
29:a:847:G:H2'	29:a:848:G:C8	2.48	0.49
29:a:1760:C:H2'	29:a:1761:A:H8	1.77	0.49
46:r:64:LEU:HD23	46:r:69:LEU:HD21	1.95	0.49
12:G:20:SER:HB3	12:G:23:ILE:HB	1.93	0.49
29:a:1561:A:H2'	29:a:1562:A:C8	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:556:A:H4'	6:A:557:U:H3'	1.95	0.49
6:A:1035:C:H2'	6:A:1036:U:C6	2.47	0.49
24:S:49:ILE:HD12	24:S:71:LEU:HD21	1.95	0.49
26:V:24:C:H2'	26:V:25:U:C6	2.47	0.49
29:a:1628:A:H5'	29:a:1749:C:O2'	2.12	0.49
34:f:137:VAL:HG22	34:f:140:GLU:HB3	1.95	0.49
41:m:87:TYR:OH	41:m:115:LEU:HB3	2.13	0.49
29:a:694:U:H2'	29:a:695:G:O4'	2.12	0.49
29:a:1058:G:N1	29:a:1085:A:H1'	2.27	0.49
3:2:32:LEU:HB2	29:a:2408:U:H5"	1.94	0.49
6:A:999:G:H3'	6:A:1000:A:H8	1.78	0.49
6:A:1087:U:H2'	6:A:1088:U:C6	2.48	0.49
14:I:122:ARG:HD3	14:I:125:PHE:HE2	1.77	0.49
29:a:39:G:H2'	29:a:40:U:C6	2.47	0.49
29:a:285:U:H2'	29:a:286:U:C6	2.47	0.49
37:i:104:ALA:O	37:i:108:MET:HG3	2.13	0.49
6:A:1020:G:H2'	6:A:1021:G:H8	1.77	0.49
14:I:50:LEU:HB3	14:I:56:THR:HA	1.95	0.49
15:J:50:ASN:HB3	15:J:62:ARG:HD2	1.95	0.49
17:L:69:GLY:HA3	17:L:107:VAL:HG11	1.94	0.49
24:S:41:LEU:HB2	24:S:44:PHE:CE1	2.48	0.49
29:a:963:A:H5'	29:a:1176:U:H1'	1.94	0.49
34:f:61:ALA:HB1	34:f:91:LEU:HD21	1.95	0.49
34:f:67:VAL:CG1	34:f:84:PRO:HB3	2.43	0.49
39:k:92:VAL:HB	39:k:124:VAL:HG22	1.95	0.49
6:A:675:U:H2'	6:A:676:C:H6	1.77	0.49
6:A:1232:U:H2'	6:A:1233:A:O4'	2.13	0.49
29:a:1783:A:H2'	29:a:1784:C:H6	1.78	0.49
29:a:2383:C:H5"	39:k:65:LYS:HD3	1.93	0.49
29:a:2666:G:H2'	29:a:2667:A:C8	2.48	0.49
38:j:51:ARG:HG2	38:j:51:ARG:HH11	1.77	0.49
3:2:54:VAL:O	3:2:58:ARG:HG3	2.12	0.48
25:T:29:ARG:O	25:T:33:LYS:HG3	2.14	0.48
29:a:2604:U:H2'	29:a:2605:C:H6	1.78	0.48
42:n:69:ALA:O	42:n:73:VAL:HG23	2.13	0.48
26:V:23:G:H2'	26:V:24:C:H6	1.77	0.48
6:A:252:U:H2'	6:A:253:G:C8	2.45	0.48
9:D:172:TRP:CD2	9:D:188:PRO:HB3	2.49	0.48
28:X:92:ARG:HD2	28:X:95:GLU:OE1	2.13	0.48
29:a:483:G:O6	46:r:49:LYS:HE3	2.13	0.48
29:a:1715:A:H2'	29:a:1716:A:H8	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:2336:C:H2'	29:a:2337:U:C6	2.49	0.48
7:B:122:GLN:HG3	7:B:123:SER:N	2.28	0.48
12:G:26:PHE:CD1	12:G:62:PHE:HZ	2.31	0.48
29:a:573:A:H2'	29:a:574:G:C8	2.48	0.48
29:a:1287:G:H5"	29:a:1288:A:H5"	1.94	0.48
29:a:1526:U:H3'	29:a:1527:G:O4'	2.14	0.48
6:A:1140:G:H2'	6:A:1141:G:C8	2.48	0.48
12:G:86:GLN:OE1	12:G:144:MET:HE1	2.13	0.48
29:a:406:C:H2'	29:a:407:A:C8	2.47	0.48
29:a:657:A:H2'	29:a:658:U:C6	2.49	0.48
32:d:127:ARG:HG3	32:d:168:LEU:HD13	1.95	0.48
37:i:15:TRP:CE2	37:i:135:GLN:HG2	2.48	0.48
5:4:36:ASP:HB3	18:M:57:ARG:NH1	2.28	0.48
6:A:942:G:C2	6:A:943:A:C8	3.02	0.48
6:A:947:U:H2'	6:A:948:G:C8	2.49	0.48
6:A:1058:G:H5'	15:J:61:ALA:HB2	1.95	0.48
6:A:1509:U:H2'	6:A:1510:A:C8	2.48	0.48
9:D:5:ILE:O	9:D:5:ILE:HG13	2.13	0.48
14:I:28:ILE:HD13	14:I:77:ILE:HD13	1.96	0.48
26:V:76:C:H5'	26:V:77:A:O5'	2.14	0.48
29:a:151:U:H2'	29:a:152:G:H8	1.79	0.48
29:a:1066:C:H3'	29:a:1067:A:H8	1.78	0.48
6:A:340:A:H5"	6:A:341:C:H5	1.79	0.48
6:A:497:G:H2'	6:A:498:C:C6	2.48	0.48
18:M:3:ARG:CZ	18:M:6:GLY:HA2	2.44	0.48
26:V:23:G:H2'	26:V:24:C:C6	2.48	0.48
29:a:1798:A:H2'	29:a:1799:A:C8	2.49	0.48
29:a:2148:G:H2'	29:a:2149:C:C6	2.48	0.48
36:h:15:LEU:HD23	36:h:56:LYS:HD2	1.95	0.48
47:s:4:GLU:O	47:s:8:GLN:HG2	2.13	0.48
6:A:840:U:H3'	6:A:841:G:C8	2.49	0.48
6:A:1339:C:H2'	6:A:1340:G:C8	2.48	0.48
12:G:72:MET:H	12:G:142:HIS:CE1	2.23	0.48
29:a:590:A:H2'	29:a:591:G:C8	2.47	0.48
29:a:1943:G:N3	29:a:2540:C:H5"	2.29	0.48
29:a:2105:G:H2'	29:a:2106:A:C5	2.49	0.48
6:A:1461:U:H2'	6:A:1462:A:H8	1.78	0.48
7:B:76:ARG:H	7:B:76:ARG:HD3	1.79	0.48
18:M:86:TYR:O	18:M:90:ARG:HG2	2.12	0.48
29:a:1835:G:H5'	29:a:1836:A:OP2	2.14	0.48
29:a:2232:U:H2'	29:a:2233:U:H6	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:g:84:GLU:HB2	35:g:134:LYS:HD3	1.96	0.48
6:A:899:G:H2'	6:A:900:A:H8	1.78	0.48
6:A:1316:A:C8	6:A:1320:G:C6	3.02	0.48
29:a:222:A:C2	29:a:233:A:H5"	2.49	0.48
29:a:2526:U:H2'	29:a:2527:C:H6	1.77	0.48
1:0:32:ILE:HG23	1:0:34:LYS:HG3	1.96	0.47
2:1:1:MET:N	29:a:1610:G:H21	2.05	0.47
6:A:827:C:H4'	7:B:23:ARG:O	2.14	0.47
22:Q:62:ILE:HG22	22:Q:76:LEU:HA	1.95	0.47
29:a:1582:C:H2'	29:a:1583:A:C8	2.49	0.47
29:a:1845:U:H2'	29:a:1846:G:O4'	2.15	0.47
39:k:102:VAL:HG23	39:k:103:VAL:HG23	1.95	0.47
3:2:50:HIS:CG	29:a:2348:C:H5'	2.49	0.47
29:a:856:C:H42	29:a:900:A:H2	1.62	0.47
29:a:1404:G:H2'	29:a:1405:C:H6	1.78	0.47
29:a:1430:U:H2'	29:a:1431:C:C6	2.49	0.47
30:b:109:G:H2'	30:b:110:C:H6	1.78	0.47
6:A:386:U:H2'	6:A:387:C:C6	2.49	0.47
6:A:821:U:H2'	6:A:822:A:C8	2.49	0.47
29:a:1701:G:H2'	29:a:1702:U:C6	2.49	0.47
29:a:1921:A:H2'	29:a:1922:G:O4'	2.14	0.47
29:a:2094:U:H2'	29:a:2095:A:C8	2.50	0.47
29:a:2556:G:H2'	29:a:2557:A:C8	2.49	0.47
6:A:1115:U:H2'	6:A:1116:C:H6	1.79	0.47
17:L:8:ILE:HD11	22:Q:37:LYS:HB3	1.96	0.47
29:a:2019:6MZ:C2	29:a:2488:C:H5"	2.45	0.47
29:a:2139:U:H2'	29:a:2140:C:C6	2.49	0.47
6:A:79:U:H2'	6:A:80:A:C8	2.47	0.47
6:A:559:U:H1'	17:L:12:ARG:HD2	1.95	0.47
6:A:982:C:H2'	6:A:983:U:C6	2.50	0.47
6:A:1188:A:H2'	6:A:1189:C:C6	2.49	0.47
29:a:16:U:H5"	54:z:14:ASP:HB2	1.97	0.47
29:a:875:U:H2'	29:a:876:C:H6	1.78	0.47
29:a:1316:A:H2'	29:a:1318:C:C4	2.49	0.47
29:a:2142:A:H2'	29:a:2143:G:C8	2.49	0.47
29:a:2638:C:H2'	29:a:2639:U:C6	2.48	0.47
30:b:46:U:H4'	42:n:99:HIS:HD2	1.80	0.47
49:u:59:VAL:O	49:u:63:GLU:HB2	2.14	0.47
2:1:1:MET:HE1	29:a:743:A:H3'	1.96	0.47
4:3:15:LYS:HB2	4:3:15:LYS:NZ	2.29	0.47
6:A:1059:U:H2'	6:A:1060:C:C6	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:N:42:PHE:O	19:N:46:LEU:HD23	2.15	0.47
20:O:56:LEU:O	20:O:60:VAL:HG23	2.14	0.47
29:a:589:U:H2'	29:a:590:A:C8	2.50	0.47
38:j:16:ALA:HB2	38:j:52:VAL:HG11	1.96	0.47
2:1:18:PHE:HA	2:1:43:THR:HG21	1.95	0.47
6:A:185:C:H4'	6:A:186:G:O5'	2.14	0.47
6:A:639:A:H2'	6:A:640:C:H6	1.80	0.47
6:A:1115:U:H1'	6:A:1176:A:C5	2.50	0.47
6:A:1399:4OC:H2'	6:A:1400:C:O4'	2.14	0.47
9:D:24:GLY:HA2	9:D:163:LEU:HD22	1.97	0.47
15:J:36:VAL:HG23	15:J:38:GLY:H	1.80	0.47
17:L:25:LYS:HE2	17:L:59:SER:HB2	1.95	0.47
29:a:2:G:H2'	29:a:3:U:C6	2.48	0.47
29:a:12:U:O2	29:a:2615:C:H4'	2.15	0.47
29:a:658:U:H2'	29:a:659:A:O4'	2.15	0.47
29:a:853:G:H2'	29:a:854:A:O4'	2.14	0.47
29:a:2090:A:H2'	29:a:2091:C:H6	1.80	0.47
29:a:2687:U:H2'	29:a:2688:G:C8	2.50	0.47
42:n:34:ARG:HE	42:n:34:ARG:HB3	1.62	0.47
6:A:175:A:H2'	6:A:176:U:C6	2.50	0.47
6:A:1216:A:H2'	6:A:1217:G:C8	2.50	0.47
13:H:18:GLN:HG3	13:H:71:PRO:CB	2.45	0.47
19:N:48:LEU:HD12	19:N:51:LEU:HD12	1.97	0.47
22:Q:22:ILE:HG21	22:Q:54:ALA:HB3	1.96	0.47
29:a:244:A:H5"	39:k:69:THR:HG21	1.96	0.47
29:a:2063:U:H2'	29:a:2064:U:C6	2.50	0.47
6:A:1012:G:H2'	6:A:1013:A:C8	2.50	0.47
6:A:1141:G:N2	6:A:1143:A:H62	2.13	0.47
13:H:5:ASP:HB2	13:H:82:PRO:HG2	1.96	0.47
26:V:50:G:H2'	26:V:51:U:H6	1.80	0.47
29:a:150:U:H2'	29:a:151:U:C6	2.49	0.47
29:a:222:A:N1	29:a:233:A:H5"	2.29	0.47
29:a:585:U:H2'	29:a:586:C:C6	2.49	0.47
29:a:937:A:H2'	29:a:938:C:C6	2.50	0.47
29:a:1473:A:H2'	29:a:1474:U:H6	1.80	0.47
29:a:2802:G:H2'	29:a:2803:C:H6	1.78	0.47
32:d:182:SER:HB2	32:d:191:VAL:HB	1.96	0.47
47:s:5:ARG:O	47:s:9:VAL:HG23	2.15	0.47
6:A:493:A:H2'	6:A:494:U:H5	1.80	0.47
6:A:534:A:H2'	6:A:535:G:H8	1.79	0.47
6:A:1144:C:H2'	6:A:1145:U:C6	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:27:G:H22	29:a:504:G:H2'	1.80	0.47
29:a:805:C:H2'	29:a:806:C:H6	1.80	0.47
54:z:11:SER:O	54:z:15:MET:HG3	2.15	0.47
6:A:327:G:O2'	25:T:2:ALA:HB1	2.15	0.46
6:A:372:G:H4'	21:P:23:ARG:HD2	1.97	0.46
6:A:455:U:H2'	6:A:456:U:C6	2.51	0.46
26:V:30:G:H2'	26:V:31:G:C8	2.49	0.46
29:a:135:A:H2'	29:a:136:C:C6	2.49	0.46
29:a:580:U:H2'	29:a:581:A:C8	2.50	0.46
29:a:1499:U:H2'	29:a:1500:G:C8	2.50	0.46
29:a:2089:G:H2'	29:a:2090:A:C8	2.50	0.46
29:a:2110:G:H2'	29:a:2111:U:C6	2.50	0.46
6:A:1187:G:H4'	6:A:1188:A:OP2	2.14	0.46
19:N:53:ARG:O	19:N:59:ARG:HD2	2.16	0.46
29:a:775:G:H5'	29:a:776:G:OP1	2.14	0.46
29:a:1605:A:C6	46:r:87:PRO:HB3	2.49	0.46
29:a:2579:A:H2'	29:a:2580:C:H6	1.81	0.46
37:i:17:VAL:CG2	37:i:137:PRO:HB2	2.45	0.46
6:A:899:G:H2'	6:A:900:A:C8	2.50	0.46
12:G:76:LYS:HG3	12:G:89:MET:SD	2.55	0.46
14:I:117:ARG:HB2	14:I:121:LYS:HD3	1.97	0.46
21:P:98:LYS:HD2	21:P:99:ALA:N	2.31	0.46
29:a:755:A:H5'	31:c:209:GLY:HA2	1.96	0.46
29:a:946:G:H5"	40:l:77:LYS:HG3	1.96	0.46
29:a:2885:C:H2'	29:a:2886:U:C6	2.50	0.46
52:x:5:ASP:HA	52:x:8:GLU:OE1	2.16	0.46
4:3:25:VAL:HB	4:3:35:GLN:HB2	1.97	0.46
6:A:176:U:C2'	6:A:177:A:H5'	2.46	0.46
11:F:42:TRP:CZ2	23:R:24:LYS:HD3	2.50	0.46
29:a:197:A:H62	29:a:2419:A:H2'	1.79	0.46
29:a:792:G:C8	33:e:49:ALA:HB2	2.51	0.46
29:a:1094:C:H5'	29:a:1095:U:OP2	2.15	0.46
29:a:2164:C:H2'	29:a:2165:A:H8	1.80	0.46
29:a:2307:G:H3'	29:a:2308:U:C6	2.50	0.46
29:a:2541:OMU:OP2	29:a:2541:OMU:H6	2.16	0.46
34:f:83:TRP:N	34:f:83:TRP:CD1	2.84	0.46
34:f:123:ASP:OD2	34:f:127:ASN:HB2	2.15	0.46
35:g:50:LEU:HD13	35:g:72:LEU:HD13	1.98	0.46
53:y:46:MET:O	53:y:50:VAL:HG22	2.16	0.46
1:0:5:ILE:HD13	1:0:47:GLU:HG3	1.97	0.46
5:4:70:ARG:HB3	24:S:41:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:E:93:VAL:HB	10:E:110:MET:HE3	1.98	0.46
12:G:25:LYS:HB3	12:G:101:MET:HE1	1.96	0.46
19:N:20:TYR:HE2	19:N:52:PRO:HG2	1.80	0.46
24:S:39:MET:HE3	24:S:39:MET:HB2	1.83	0.46
29:a:72:A:C8	52:x:54:LYS:HD3	2.50	0.46
29:a:1186:U:H2'	29:a:1187:U:C6	2.51	0.46
29:a:1863:C:H2'	29:a:1864:G:O4'	2.15	0.46
32:d:50:GLN:HG3	32:d:82:GLU:HG3	1.97	0.46
6:A:1217:G:O3'	24:S:36:ARG:HD3	2.16	0.46
6:A:1345:U:H4'	14:I:120:ARG:HG3	1.96	0.46
29:a:1417:G:H2'	29:a:1418:G:H8	1.79	0.46
5:4:6:HIS:CE1	34:f:63:GLN:HG3	2.51	0.46
6:A:201:A:H61	6:A:209:A:N6	2.04	0.46
6:A:615:C:H5'	6:A:616:U:H5"	1.98	0.46
6:A:725:A:H2'	6:A:726:A:H8	1.81	0.46
6:A:1510:A:H2'	6:A:1511:G:H8	1.80	0.46
9:D:19:LEU:HD22	9:D:66:ILE:HG13	1.98	0.46
15:J:51:VAL:HG21	19:N:84:LEU:HD12	1.98	0.46
18:M:53:LEU:HB3	18:M:57:ARG:NH2	2.31	0.46
28:X:80:ASP:O	28:X:83:ILE:HG22	2.16	0.46
29:a:1087:U:C2	29:a:1088:A:C8	3.04	0.46
32:d:78:ARG:HG3	32:d:79:LEU:HD23	1.97	0.46
41:m:72:ASN:HB3	41:m:75:THR:HB	1.97	0.46
6:A:75:A:H1'	6:A:92:G:H22	1.80	0.46
6:A:78:G:H2'	6:A:79:U:C6	2.51	0.46
6:A:295:G:H2'	6:A:296:A:C8	2.50	0.46
6:A:318:C:H2'	6:A:319:U:C6	2.51	0.46
6:A:842:A:H1'	23:R:10:PHE:HD2	1.80	0.46
7:B:71:PHE:HB3	7:B:82:ILE:HG23	1.97	0.46
19:N:43:GLU:O	19:N:47:LYS:HG3	2.16	0.46
29:a:740:A:H4'	29:a:1259:G:N3	2.31	0.46
29:a:1054:C:N3	29:a:1059:A:H8	2.13	0.46
29:a:1516:A:O2'	29:a:1517:A:H8	1.98	0.46
35:g:17:VAL:HG11	35:g:50:LEU:HD11	1.98	0.46
6:A:395:G:H2'	6:A:396:C:C6	2.51	0.46
9:D:161:ILE:HD12	9:D:177:HIS:CE1	2.51	0.46
17:L:34:CYS:HB3	17:L:55:VAL:HG22	1.98	0.46
29:a:1463:G:O2'	29:a:1464:U:H6	1.99	0.46
38:j:51:ARG:HD3	38:j:51:ARG:H	1.80	0.46
38:j:66:LYS:HD2	38:j:81:ASP:HA	1.98	0.46
50:v:75:PHE:HB2	50:v:77:ARG:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:199:G:O2'	6:A:461:A:N1	2.48	0.46
6:A:905:A:O2'	6:A:906:A:H8	1.84	0.46
6:A:1422:U:H2'	6:A:1423:G:H8	1.81	0.46
28:X:68:LYS:HE3	28:X:68:LYS:HB3	1.51	0.46
29:a:263:U:H2'	29:a:264:C:O4'	2.16	0.46
29:a:388:G:H1'	51:w:29:PHE:HB3	1.97	0.46
29:a:589:U:H2'	29:a:590:A:H8	1.80	0.46
29:a:2105:G:H3'	29:a:2106:A:H2'	1.98	0.46
29:a:2120:U:H4'	29:a:2121:U:H5"	1.98	0.46
53:y:5:LYS:HB2	53:y:57:GLU:HB3	1.98	0.46
6:A:256:G:H2'	6:A:257:U:C6	2.51	0.45
6:A:1003:C:N3	6:A:1019:U:O4	2.50	0.45
6:A:1339:C:H2'	6:A:1340:G:H8	1.80	0.45
29:a:389:U:H5"	51:w:32:ASN:HB2	1.98	0.45
29:a:1165:U:H4'	29:a:1166:G:N2	2.31	0.45
29:a:2104:G:H2'	29:a:2106:A:N7	2.30	0.45
29:a:2353:C:H2'	29:a:2354:G:O4'	2.16	0.45
33:e:20:ARG:HD3	33:e:106:CYS:SG	2.56	0.45
35:g:4:VAL:O	35:g:69:ARG:HD3	2.16	0.45
5:4:26:SER:HB2	34:f:139:PRO:HB3	1.98	0.45
6:A:75:A:H4'	6:A:76:A:C8	2.51	0.45
14:I:25:LYS:HB3	14:I:25:LYS:HE2	1.82	0.45
17:L:57:LEU:HD21	17:L:82:ILE:HG12	1.99	0.45
17:L:108:LYS:HB3	17:L:108:LYS:HE2	1.58	0.45
28:X:47:ASN:HB2	28:X:50:LYS:HB2	1.98	0.45
29:a:5:A:H2'	29:a:6:A:H8	1.79	0.45
29:a:227:A:C2	29:a:2396:A:H1'	2.51	0.45
29:a:1404:G:H2'	29:a:1405:C:C6	2.51	0.45
29:a:1582:C:H2'	29:a:1583:A:H8	1.80	0.45
29:a:2303:A:H1'	34:f:155:THR:HG21	1.99	0.45
31:c:34:VAL:HG13	31:c:61:HIS:HB3	1.99	0.45
31:c:208:ALA:O	31:c:212:ARG:HG2	2.16	0.45
34:f:50:LEU:HD23	34:f:50:LEU:HA	1.72	0.45
35:g:143:GLN:O	35:g:147:GLU:HG3	2.16	0.45
36:h:52:ALA:O	36:h:56:LYS:HE2	2.17	0.45
52:x:55:THR:O	52:x:59:GLU:HG3	2.15	0.45
6:A:77:G:H3'	6:A:78:G:H8	1.78	0.45
6:A:459:U:H2'	6:A:460:U:C6	2.51	0.45
6:A:991:A:H8	19:N:8:ASN:HD22	1.64	0.45
6:A:1145:U:O3'	14:I:14:THR:HG21	2.16	0.45
6:A:1259:C:H2'	6:A:1260:A:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:S:48:THR:OG1	24:S:61:ILE:HG22	2.17	0.45
29:a:40:U:H2'	29:a:41:C:C6	2.51	0.45
29:a:350:C:H2'	29:a:351:A:C8	2.51	0.45
6:A:605:A:H2'	6:A:606:A:O4'	2.17	0.45
6:A:1124:G:H1'	6:A:1277:A:C5	2.52	0.45
6:A:1237:U:N3	12:G:32:GLN:HG3	2.32	0.45
6:A:1247:A:O3'	14:I:67:GLY:HA2	2.16	0.45
9:D:159:ASN:O	9:D:162:GLU:HG3	2.15	0.45
14:I:70:ILE:H	14:I:70:ILE:HG13	1.58	0.45
29:a:2138:U:H2'	29:a:2139:U:C6	2.50	0.45
29:a:2150:C:H2'	29:a:2151:G:O4'	2.17	0.45
36:h:31:ILE:HG12	36:h:32:PRO:HD3	1.97	0.45
43:o:63:THR:HG23	43:o:76:VAL:HG22	1.98	0.45
44:p:74:LEU:HD11	44:p:114:LYS:HG3	1.97	0.45
48:t:3:LYS:HD2	48:t:3:LYS:HA	1.68	0.45
6:A:105:A:C6	6:A:322:G:C6	3.05	0.45
6:A:435:U:C2	6:A:436:A:C8	3.04	0.45
13:H:107:THR:HB	13:H:122:ILE:HD12	1.97	0.45
21:P:43:ARG:HE	21:P:43:ARG:HB2	1.52	0.45
21:P:74:ARG:HD2	21:P:74:ARG:HA	1.68	0.45
26:V:11:A:H2'	26:V:12:G:H8	1.81	0.45
26:V:26:C:C4	26:V:27:G:C8	3.05	0.45
29:a:1266:C:H2'	29:a:1267:G:H8	1.81	0.45
29:a:2304:C:H2'	29:a:2305:G:H8	1.80	0.45
47:s:35:ILE:HD12	47:s:80:LYS:HB2	1.98	0.45
6:A:577:C:H2'	6:A:578:G:O4'	2.16	0.45
9:D:161:ILE:HG23	9:D:177:HIS:HE1	1.78	0.45
11:F:21:MET:HG2	11:F:25:TYR:CE2	2.51	0.45
29:a:747:A:H2'	29:a:748:G:O4'	2.16	0.45
30:b:60:U:H2'	30:b:61:C:H6	1.81	0.45
31:c:8:PRO:HB3	31:c:14:ARG:HG3	1.97	0.45
38:j:44:LYS:HA	38:j:44:LYS:HD2	1.74	0.45
6:A:1011:A:H2'	6:A:1012:G:C8	2.52	0.45
6:A:1264:C:O2	6:A:1324:C:H4'	2.16	0.45
14:I:34:GLU:CD	14:I:34:GLU:H	2.24	0.45
15:J:8:ILE:HG23	15:J:98:VAL:HG23	1.99	0.45
17:L:34:CYS:HB3	17:L:55:VAL:CG2	2.47	0.45
24:S:3:ARG:HH21	24:S:7:LYS:HB3	1.80	0.45
29:a:287:U:H2'	29:a:288:U:C6	2.52	0.45
29:a:346:C:H2'	29:a:347:A:C8	2.50	0.45
29:a:351:A:HO2'	29:a:352:U:H6	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:1339:C:H2'	29:a:1340:U:C6	2.51	0.45
29:a:2003:A:H2'	29:a:2004:A:C8	2.52	0.45
30:b:16:A:H2'	30:b:17:A:C8	2.52	0.45
35:g:7:ALA:O	35:g:69:ARG:HD2	2.17	0.45
38:j:100:GLY:HA2	43:o:69:SER:HB2	1.99	0.45
6:A:208:G:H2'	6:A:209:A:H8	1.82	0.45
6:A:1034:U:H2'	6:A:1035:C:C6	2.51	0.45
12:G:74:GLU:O	12:G:88:PRO:HA	2.16	0.45
16:K:16:SER:HA	16:K:78:LEU:HA	1.99	0.45
26:V:50:G:H2'	26:V:51:U:C6	2.51	0.45
29:a:151:U:H2'	29:a:152:G:C8	2.52	0.45
29:a:1473:A:H2'	29:a:1474:U:C6	2.52	0.45
29:a:2374:C:H2'	29:a:2375:U:C6	2.52	0.45
1:0:30:MET:HE2	1:0:30:MET:HB3	1.75	0.45
6:A:454:U:H2'	6:A:455:U:C6	2.52	0.45
6:A:618:A:H2'	6:A:619:A:C8	2.52	0.45
6:A:1115:U:OP1	14:I:9:ARG:HD2	2.17	0.45
17:L:50:ARG:HB3	17:L:66:TYR:HE1	1.81	0.45
29:a:170:G:H2'	29:a:171:U:C6	2.52	0.45
29:a:406:C:H2'	29:a:407:A:H8	1.81	0.45
29:a:804:U:H2'	29:a:805:C:C6	2.52	0.45
29:a:1504:A:H3'	29:a:1505:G:H8	1.82	0.45
29:a:2116:G:N2	29:a:2151:G:H1'	2.32	0.45
32:d:196:ILE:HD12	32:d:204:VAL:HG11	1.98	0.45
34:f:29:PRO:HB3	34:f:160:ALA:HB2	1.99	0.45
6:A:1238:G:H2'	6:A:1239:G:H8	1.82	0.45
8:C:81:GLY:O	8:C:85:GLU:HG3	2.17	0.45
23:R:26:ILE:HG23	23:R:30:LYS:CE	2.47	0.45
26:V:40:C:H2'	26:V:41:C:O4'	2.17	0.45
29:a:139:U:H4'	29:a:140:A:OP1	2.17	0.45
29:a:514:G:H2'	29:a:515:C:C6	2.51	0.45
29:a:733:G:H2'	29:a:734:U:H6	1.78	0.45
29:a:1075:A:H4'	29:a:1076:A:OP1	2.17	0.45
29:a:1528:U:H2'	29:a:1529:A:O4'	2.17	0.45
29:a:2676:U:H2'	29:a:2677:G:O4'	2.16	0.45
29:a:2773:U:H2'	29:a:2774:U:C6	2.52	0.45
29:a:2775:U:H2'	29:a:2776:C:H6	1.82	0.45
34:f:138:PHE:HB2	34:f:139:PRO:HD3	1.99	0.45
6:A:502:G:H2'	6:A:503:G:H8	1.82	0.44
6:A:549:U:H2'	6:A:550:A:H8	1.82	0.44
15:J:3:ASN:HB3	15:J:79:PRO:HD2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:M:92:ARG:HB3	29:a:879:C:OP1	2.17	0.44
20:O:12:ILE:O	20:O:16:ALA:HB2	2.17	0.44
29:a:2604:U:H1'	54:z:4:GLN:HB3	1.99	0.44
36:h:3:VAL:HG12	36:h:38:ALA:HA	1.99	0.44
6:A:631:C:H2'	6:A:632:A:H8	1.82	0.44
6:A:1104:C:C4	6:A:1105:G:C8	3.06	0.44
6:A:1115:U:H2'	6:A:1116:C:C6	2.52	0.44
6:A:1116:C:H2'	6:A:1117:C:H6	1.82	0.44
6:A:1421:U:H2'	6:A:1422:U:C6	2.52	0.44
7:B:189:VAL:O	7:B:203:PRO:HA	2.17	0.44
26:V:33:OMC:H2'	26:V:34:U:C6	2.51	0.44
29:a:567:U:H2'	29:a:568:G:C8	2.52	0.44
29:a:891:A:H3'	29:a:892:A:H8	1.83	0.44
29:a:1309:A:C4	29:a:1310:A:C8	3.05	0.44
29:a:2137:G:H2'	29:a:2138:U:C6	2.51	0.44
43:o:103:LEU:HD11	43:o:113:ILE:HD11	1.99	0.44
6:A:1310:U:H2'	6:A:1311:C:C6	2.51	0.44
6:A:1327:U:H4'	18:M:23:PHE:CE2	2.52	0.44
7:B:190:ASP:HB2	7:B:206:ASP:OD2	2.16	0.44
8:C:9:GLY:HA2	8:C:12:LEU:HG	1.99	0.44
8:C:21:ASN:HB3	8:C:58:GLU:HG2	1.99	0.44
8:C:152:GLU:HG3	8:C:167:TRP:HB3	2.00	0.44
13:H:43:GLU:HG3	13:H:102:ILE:HD13	1.99	0.44
24:S:66:MET:HB3	24:S:74:PHE:CZ	2.52	0.44
29:a:560:U:H5"	29:a:812:A:C2	2.52	0.44
29:a:1054:C:C4	29:a:1059:A:H5"	2.53	0.44
29:a:1187:U:H2'	29:a:1188:C:C6	2.52	0.44
29:a:1394:U:H2'	29:a:1395:C:C6	2.52	0.44
29:a:1516:A:N6	29:a:1534:G:H2'	2.32	0.44
29:a:1554:U:H2'	29:a:1555:C:C6	2.52	0.44
29:a:1715:A:H2'	29:a:1716:A:C8	2.53	0.44
29:a:2090:A:H2'	29:a:2091:C:C6	2.52	0.44
29:a:2118:C:H2'	29:a:2119:U:O4'	2.16	0.44
35:g:86:LYS:HA	35:g:132:ILE:HA	1.99	0.44
42:n:28:CYS:HA	42:n:92:ASP:HB3	2.00	0.44
48:t:20:LYS:HD3	48:t:37:LEU:HD22	2.00	0.44
6:A:917:U:H2'	6:A:918:U:C6	2.52	0.44
6:A:1003:C:H2'	6:A:1004:U:C6	2.52	0.44
7:B:131:LEU:HD23	7:B:135:GLU:HB3	1.99	0.44
19:N:27:LEU:HD21	19:N:47:LYS:HB2	1.98	0.44
22:Q:29:ARG:HD3	22:Q:38:SER:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:315:G:H4'	29:a:317:A:C8	2.52	0.44
29:a:605:A:H5'	29:a:607:A:C6	2.52	0.44
29:a:1048:G:C8	29:a:1050:U:H5	2.36	0.44
29:a:1280:G:H2'	29:a:1281:U:H6	1.82	0.44
29:a:1764:U:O4	29:a:1778:A:H2	2.00	0.44
32:d:128:TRP:CD1	32:d:163:LYS:HB3	2.52	0.44
6:A:329:C:C2	6:A:330:C:C5	3.06	0.44
6:A:502:G:H2'	6:A:503:G:C8	2.53	0.44
6:A:1050:G:H4'	6:A:1051:C:H3'	1.99	0.44
12:G:93:PRO:HA	12:G:96:ARG:HD3	1.99	0.44
28:X:74:HIS:CE1	28:X:85:GLY:HA3	2.52	0.44
29:a:208:C:H2'	29:a:209:C:C6	2.52	0.44
29:a:407:A:H2'	29:a:408:U:C6	2.53	0.44
29:a:1048:G:H2'	29:a:1049:G:H8	1.82	0.44
29:a:1872:U:H2'	29:a:1873:G:O4'	2.17	0.44
29:a:2167:C:H2'	29:a:2168:C:C6	2.52	0.44
29:a:2543:U:H2'	29:a:2544:U:C6	2.53	0.44
37:i:18:VAL:HG11	37:i:28:LEU:HD11	2.00	0.44
38:j:7:MET:HE3	38:j:7:MET:HB3	1.77	0.44
6:A:1002:A:H8	6:A:1020:G:H21	1.63	0.44
6:A:1069:G:H2'	6:A:1070:U:C6	2.53	0.44
8:C:88:GLN:OE1	8:C:100:GLN:HA	2.18	0.44
10:E:11:VAL:HG12	10:E:39:GLY:O	2.17	0.44
14:I:82:THR:HG23	14:I:96:LEU:HD13	2.00	0.44
19:N:43:GLU:OE2	19:N:47:LYS:HE2	2.18	0.44
23:R:34:THR:HG22	23:R:38:LYS:H	1.83	0.44
29:a:18:C:H2'	29:a:19:A:C8	2.53	0.44
29:a:35:G:H1'	29:a:446:A:C4	2.53	0.44
29:a:383:A:H1'	29:a:403:G:O4'	2.18	0.44
29:a:1418:G:H2'	29:a:1419:A:O4'	2.17	0.44
29:a:2080:C:O3'	51:w:56:MET:HE1	2.17	0.44
29:a:2271:G:H4'	29:a:2378:G:O2'	2.17	0.44
41:m:53:THR:HA	41:m:56:LYS:HD2	2.00	0.44
54:z:37:HIS:HB3	54:z:43:THR:HG22	1.99	0.44
6:A:387:C:H5"	21:P:26:ARG:NH1	2.32	0.44
6:A:1237:U:H3	12:G:32:GLN:HG3	1.83	0.44
6:A:1252:G:H3'	6:A:1276:A:H61	1.83	0.44
7:B:69:VAL:HG22	7:B:162:ALA:HB3	2.00	0.44
8:C:132:ARG:HA	8:C:132:ARG:HD3	1.81	0.44
8:C:149:ILE:HG12	8:C:150:LYS:N	2.33	0.44
24:S:40:ILE:HG13	24:S:71:LEU:HG	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:v:41:ARG:HA	50:v:41:ARG:HD3	1.74	0.44
53:y:5:LYS:HE2	53:y:36:GLU:HG3	2.00	0.44
1:0:30:MET:N	1:0:47:GLU:HB2	2.32	0.44
6:A:230:C:H2'	6:A:231:U:H6	1.83	0.44
6:A:1004:U:H2'	6:A:1005:U:C6	2.53	0.44
6:A:1443:A:H1'	6:A:1444:A:H5'	2.00	0.44
15:J:52:LEU:HB2	19:N:81:ARG:HD2	1.99	0.44
17:L:81:LEU:HB3	17:L:98:VAL:CG1	2.48	0.44
26:V:67:C:H2'	26:V:68:C:H6	1.82	0.44
29:a:842:C:H2'	29:a:843:A:C8	2.53	0.44
29:a:1627:G:H2'	29:a:1628:A:H8	1.81	0.44
29:a:1862:G:H2'	29:a:1863:C:C6	2.53	0.44
29:a:2736:G:O6	29:a:2744:C:H5"	2.17	0.44
33:e:1:MET:CB	33:e:13:LEU:O	2.66	0.44
6:A:204:U:H4'	6:A:205:U:C5	2.53	0.44
6:A:251:G:H2'	6:A:252:U:C6	2.53	0.44
6:A:401:U:H3'	6:A:402:G:H5'	2.00	0.44
6:A:889:A:H2'	6:A:890:C:H6	1.83	0.44
6:A:975:A:C2	6:A:1316:A:C4	3.05	0.44
7:B:131:LEU:HD21	7:B:139:ARG:CZ	2.48	0.44
14:I:116:LEU:HD22	14:I:122:ARG:HB2	2.00	0.44
29:a:139:U:H1'	29:a:140:A:H5"	2.00	0.44
30:b:64:A:H61	30:b:104:U:H2'	1.83	0.44
35:g:30:LYS:HD2	35:g:82:GLY:H	1.83	0.44
40:l:51:ARG:HD3	40:l:66:ILE:HD11	1.99	0.44
51:w:62:LEU:HD23	51:w:66:LYS:HG2	1.99	0.44
6:A:476:U:H2'	6:A:477:G:C8	2.52	0.43
6:A:534:A:H2'	6:A:535:G:C8	2.53	0.43
6:A:675:U:H2'	6:A:676:C:C6	2.53	0.43
6:A:798:U:H2'	6:A:799:A:H8	1.83	0.43
6:A:1379:C:H1'	12:G:79:ARG:NH2	2.33	0.43
6:A:1398:G:H2'	6:A:1399:4OC:O4'	2.17	0.43
6:A:1434:A:H2'	6:A:1435:G:H8	1.83	0.43
7:B:113:ILE:HG13	7:B:150:LEU:HD22	1.99	0.43
7:B:205:ASN:OD1	7:B:205:ASN:C	2.61	0.43
9:D:78:TYR:CG	9:D:206:TYR:HD2	2.36	0.43
29:a:1159:A:H2'	29:a:1160:U:C6	2.53	0.43
29:a:1429:A:H2'	29:a:1430:U:C6	2.53	0.43
44:p:58:ARG:HA	44:p:61:TRP:CE3	2.53	0.43
45:q:64:ILE:HD12	45:q:95:GLU:HG2	1.99	0.43
5:4:70:ARG:HD2	5:4:70:ARG:HA	1.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:455:U:H2'	6:A:456:U:H6	1.83	0.43
6:A:1172:G:H2'	6:A:1173:A:H8	1.82	0.43
6:A:1310:U:H2'	6:A:1311:C:H6	1.82	0.43
25:T:36:LEU:HD23	25:T:36:LEU:HA	1.82	0.43
29:a:1060:A:H4'	29:a:1061:G:OP1	2.18	0.43
29:a:1430:U:H2'	29:a:1431:C:H6	1.82	0.43
29:a:1631:A:H2'	29:a:1632:A:C8	2.53	0.43
3:2:9:GLY:O	3:2:13:ARG:HD3	2.18	0.43
6:A:89:C:H5"	6:A:90:C:H6	1.83	0.43
6:A:639:A:H2'	6:A:640:C:C6	2.53	0.43
6:A:1271:A:H2'	6:A:1272:U:C6	2.53	0.43
19:N:73:TYR:CE2	19:N:75:ARG:HA	2.54	0.43
26:V:72:C:H2'	26:V:73:A:C8	2.52	0.43
29:a:64:G:H2'	29:a:65:C:H6	1.83	0.43
29:a:315:G:H4'	29:a:317:A:N7	2.32	0.43
29:a:430:G:H2'	29:a:431:A:C8	2.52	0.43
29:a:1307:C:O2'	29:a:1308:C:H5'	2.17	0.43
29:a:1838:G:H2'	29:a:1839:G:H8	1.81	0.43
29:a:2301:U:O5'	34:f:85:ILE:HD11	2.17	0.43
29:a:2458:A:H2'	29:a:2459:G:O4'	2.18	0.43
32:d:180:ILE:HD12	32:d:190:LEU:HD22	1.99	0.43
40:l:54:ILE:HG13	40:l:121:ALA:HB2	2.01	0.43
6:A:22:U:H2'	6:A:23:G:O4'	2.17	0.43
6:A:157:A:H2'	6:A:158:A:C8	2.53	0.43
6:A:208:G:C4	6:A:209:A:C8	3.07	0.43
6:A:212:U:H2'	6:A:213:U:C6	2.54	0.43
6:A:471:G:C6	6:A:472:A:C6	3.05	0.43
6:A:487:C:H2'	6:A:488:G:H8	1.84	0.43
6:A:716:C:O2'	23:R:38:LYS:HB3	2.18	0.43
6:A:1117:C:H2'	6:A:1118:U:C6	2.54	0.43
6:A:1292:U:H2'	6:A:1293:C:C6	2.53	0.43
11:F:42:TRP:CH2	23:R:24:LYS:HD3	2.53	0.43
13:H:36:ILE:HD11	13:H:127:ILE:HD13	1.99	0.43
29:a:491:U:H2'	29:a:492:G:O4'	2.18	0.43
29:a:845:A:H2'	29:a:846:G:H8	1.82	0.43
29:a:2054:C:H2'	29:a:2055:C:H6	1.84	0.43
30:b:66:C:H2'	30:b:67:G:O4'	2.19	0.43
33:e:3:LEU:HD12	33:e:13:LEU:HD22	2.01	0.43
48:t:25:LEU:HD11	48:t:35:GLU:HG2	2.01	0.43
50:v:31:VAL:HG22	50:v:35:ASN:HB2	2.00	0.43
50:v:64:ASP:O	50:v:84:THR:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:329:C:H2'	6:A:330:C:C6	2.52	0.43
29:a:250:G:H2'	29:a:251:A:C8	2.54	0.43
29:a:285:U:H2'	29:a:286:U:H6	1.82	0.43
29:a:1395:C:H2'	29:a:1396:U:C6	2.53	0.43
35:g:64:GLN:O	35:g:67:THR:HG22	2.17	0.43
45:q:50:GLY:HA3	45:q:53:VAL:C	2.43	0.43
6:A:227:A:H2'	6:A:228:G:H8	1.84	0.43
6:A:632:A:H2'	6:A:633:U:C6	2.53	0.43
6:A:1433:U:H2'	6:A:1434:A:C8	2.53	0.43
6:A:1466:C:H2'	6:A:1467:G:O4'	2.19	0.43
6:A:1521:C:H2'	6:A:1522:G:C8	2.54	0.43
14:I:39:ARG:HE	14:I:39:ARG:HB3	1.65	0.43
28:X:54:LYS:HA	28:X:54:LYS:HD2	1.84	0.43
29:a:1349:G:H2'	29:a:1350:C:C6	2.53	0.43
29:a:2139:U:H2'	29:a:2140:C:H6	1.82	0.43
35:g:54:PRO:HB3	35:g:61:ALA:HB1	2.01	0.43
6:A:91:G:H2'	6:A:92:G:C8	2.53	0.43
6:A:207:G:C2	6:A:208:G:H1'	2.54	0.43
6:A:422:U:H2'	6:A:423:U:C6	2.53	0.43
6:A:684:A:C2	6:A:701:A:C5	3.07	0.43
6:A:933:C:C2	6:A:934:A:C8	3.06	0.43
6:A:1240:U:H2'	6:A:1241:C:C6	2.54	0.43
8:C:23:TYR:CD1	8:C:23:TYR:C	2.97	0.43
8:C:100:GLN:HG2	8:C:101:VAL:N	2.32	0.43
16:K:91:GLY:HA2	16:K:94:SER:HB2	2.00	0.43
22:Q:12:LYS:HB3	22:Q:12:LYS:HE3	1.64	0.43
24:S:50:SER:HB2	24:S:57:HIS:HB3	2.00	0.43
29:a:154:A:H2'	29:a:155:A:H8	1.83	0.43
29:a:1187:U:H2'	29:a:1188:C:H6	1.84	0.43
29:a:2094:U:H2'	29:a:2095:A:H8	1.84	0.43
29:a:2218:U:H2'	29:a:2219:G:H8	1.83	0.43
30:b:22:G:N7	30:b:54:G:H2'	2.33	0.43
30:b:101:A:H2'	30:b:102:A:O4'	2.18	0.43
38:j:51:ARG:HD3	38:j:51:ARG:N	2.34	0.43
4:3:5:ALA:O	4:3:38:GLY:HA2	2.18	0.43
6:A:510:C:H2'	6:A:511:U:C6	2.54	0.43
6:A:681:U:H2'	6:A:682:G:O4'	2.19	0.43
6:A:1141:G:O2'	6:A:1142:A:H5'	2.18	0.43
6:A:1315:A:H1'	24:S:37:ARG:NH2	2.33	0.43
6:A:1343:A:N1	6:A:1371:A:H5"	2.33	0.43
10:E:15:VAL:HB	10:E:35:LEU:HD23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:917:G:H2'	29:a:918:A:H8	1.82	0.43
29:a:1158:U:H2'	29:a:1159:A:C8	2.54	0.43
29:a:2086:U:H2'	29:a:2087:U:H6	1.84	0.43
29:a:2293:G:H5'	29:a:2294:U:OP2	2.19	0.43
29:a:2303:A:H2'	29:a:2304:C:C6	2.53	0.43
29:a:2745:U:H1'	29:a:2746:A:H5"	2.01	0.43
29:a:2790:G:H2'	29:a:2791:U:C6	2.54	0.43
57:a:2960:MG:MG	55:a:3241:K:K	1.55	0.43
31:c:160:ALA:HA	31:c:177:ARG:HD3	2.01	0.43
51:w:15:GLY:HA3	51:w:29:PHE:HE1	1.84	0.43
6:A:377:G:H2'	6:A:378:A:O4'	2.18	0.43
6:A:1237:U:O4	12:G:116:MET:HE2	2.19	0.43
13:H:29:SER:HB2	13:H:60:LEU:HB2	2.01	0.43
25:T:42:GLY:C	25:T:86:LEU:HD21	2.44	0.43
28:X:43:PHE:HZ	28:X:83:ILE:HD13	1.84	0.43
29:a:1261:C:H4'	29:a:1263:A:OP1	2.19	0.43
29:a:1395:C:H2'	29:a:1396:U:H6	1.84	0.43
29:a:1541:U:H2'	29:a:1542:U:C6	2.54	0.43
29:a:1725:C:H2'	29:a:1726:U:C6	2.53	0.43
30:b:60:U:H2'	30:b:61:C:C6	2.54	0.43
31:c:245:VAL:HG12	31:c:251:LYS:HA	2.01	0.43
34:f:36:LEU:HD22	34:f:154:ILE:HG12	2.01	0.43
42:n:40:VAL:HG11	42:n:86:VAL:HG21	2.01	0.43
6:A:299:A:H2'	6:A:300:U:O4'	2.19	0.43
6:A:1497:A:H5"	6:A:1505:G:H5"	2.01	0.43
11:F:59:TYR:O	11:F:60:ILE:HD13	2.19	0.43
12:G:51:GLN:NE2	12:G:58:PRO:HD3	2.34	0.43
18:M:39:ILE:HG21	18:M:48:LEU:HD21	2.00	0.43
26:V:37:U:H2'	26:V:38:A:O4'	2.19	0.43
28:X:88:GLU:OE2	28:X:88:GLU:HA	2.19	0.43
29:a:273:A:H2'	29:a:274:A:H8	1.82	0.43
33:e:150:ASP:OD1	33:e:194:LYS:HD3	2.19	0.43
5:4:52:VAL:HG22	34:f:115:ARG:HH22	1.84	0.42
6:A:21:A:H5"	10:E:90:ALA:HB3	2.01	0.42
6:A:409:G:N2	6:A:424:G:H1'	2.34	0.42
6:A:542:C:P	9:D:64:ARG:HH12	2.42	0.42
6:A:728:G:H5'	6:A:763:A:H4'	2.01	0.42
12:G:92:ARG:O	12:G:96:ARG:HG3	2.19	0.42
29:a:26:G:H1'	29:a:506:A:N6	2.34	0.42
29:a:248:G:H5'	29:a:250:G:N7	2.34	0.42
29:a:580:U:H2'	29:a:581:A:H8	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:599:A:H2'	29:a:600:A:H8	1.82	0.42
29:a:2566:A:H2'	29:a:2603:A:H62	1.83	0.42
30:b:3:U:H2'	30:b:4:G:H8	1.84	0.42
6:A:294:A:H2'	6:A:295:G:C8	2.54	0.42
6:A:597:G:H5"	13:H:90:LYS:HD3	2.01	0.42
6:A:647:G:C2'	6:A:648:C:H5'	2.49	0.42
6:A:1335:G:H2'	6:A:1336:A:C8	2.54	0.42
9:D:97:GLU:HG2	9:D:188:PRO:HG3	2.00	0.42
19:N:64:CYS:HB2	19:N:69:ARG:H	1.84	0.42
19:N:83:LYS:O	19:N:87:THR:HG23	2.19	0.42
26:V:20:G:H4'	26:V:21:H2U:OP2	2.18	0.42
29:a:635:A:H2'	29:a:637:A:C8	2.54	0.42
29:a:888:C:H2'	29:a:889:C:C6	2.54	0.42
32:d:149:THR:HA	32:d:162:LYS:HE3	2.01	0.42
39:k:112:ILE:HD12	39:k:129:LEU:HD11	2.01	0.42
49:u:4:PHE:HE2	49:u:59:VAL:HG23	1.83	0.42
6:A:35:A:H2'	6:A:36:C:H6	1.84	0.42
6:A:367:A:H2'	6:A:368:C:O4'	2.20	0.42
6:A:630:G:H2'	6:A:631:C:H6	1.85	0.42
6:A:704:U:C2	6:A:705:C:C5	3.08	0.42
6:A:881:U:H4'	6:A:882:G:H5"	2.01	0.42
6:A:1267:U:H2'	6:A:1268:G:C8	2.52	0.42
12:G:150:ALA:O	16:K:58:THR:HG21	2.20	0.42
15:J:11:LYS:HZ1	15:J:71:LYS:HD2	1.84	0.42
26:V:33:OMC:HM23	26:V:33:OMC:H1'	1.86	0.42
29:a:188:G:H5'	51:w:14:VAL:HG11	2.00	0.42
29:a:631:C:H2'	29:a:632:U:C6	2.55	0.42
29:a:1051:U:H4'	29:a:1060:A:C4	2.53	0.42
29:a:1073:U:C2	29:a:1075:A:H5'	2.55	0.42
29:a:1121:G:O2'	29:a:2015:U:H5'	2.19	0.42
29:a:2098:U:H2'	29:a:2099:G:O4'	2.20	0.42
29:a:2737:A:H5'	35:g:4:VAL:HG21	2.01	0.42
37:i:1:MET:HE2	37:i:1:MET:H3	1.84	0.42
6:A:316:G:H2'	6:A:317:A:O4'	2.19	0.42
6:A:979:U:H4'	6:A:980:A:O4'	2.20	0.42
6:A:1277:A:H8	15:J:42:MET:HE1	1.84	0.42
16:K:83:VAL:HG21	16:K:96:VAL:HG23	2.01	0.42
17:L:87:VAL:HB	17:L:90:LEU:HB2	2.00	0.42
18:M:106:ALA:O	18:M:110:LYS:HB2	2.20	0.42
26:V:69:C:H2'	26:V:70:C:C6	2.55	0.42
29:a:52:A:H2'	29:a:53:A:H8	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:635:A:H2'	29:a:637:A:N7	2.33	0.42
29:a:1288:A:H4'	29:a:1289:A:H5"	2.00	0.42
29:a:1938:G:H2'	29:a:1939:G:C8	2.54	0.42
29:a:2289:C:H2'	29:a:2290:G:H8	1.85	0.42
29:a:2501:C:H2'	29:a:2502:A:O4'	2.19	0.42
30:b:55:A:H4'	34:f:27:GLU:OE2	2.19	0.42
34:f:138:PHE:CD1	34:f:138:PHE:N	2.87	0.42
6:A:37:G:H2'	6:A:38:C:H6	1.84	0.42
6:A:1127:A:H2'	6:A:1128:G:C8	2.52	0.42
17:L:114:ARG:HG2	17:L:119:ALA:HB3	2.00	0.42
26:V:29:C:C2	26:V:30:G:N7	2.88	0.42
29:a:974:A:N3	29:a:974:A:H2'	2.34	0.42
29:a:1555:C:H2'	29:a:1556:C:C6	2.54	0.42
29:a:1663:A:C2	29:a:2571:G:H5'	2.54	0.42
34:f:108:ILE:HG21	34:f:176:PRO:HG3	2.00	0.42
2:1:35:ARG:HG3	2:1:42:LEU:HD11	2.01	0.42
6:A:189:A:H2'	6:A:190:G:H8	1.85	0.42
21:P:88:ARG:HD2	21:P:88:ARG:HA	1.86	0.42
29:a:364:G:OP2	51:w:62:LEU:HD11	2.19	0.42
29:a:629:G:H2'	29:a:630:U:C6	2.55	0.42
29:a:1843:A:N6	29:a:1877:G:H1'	2.33	0.42
29:a:2086:U:H2'	29:a:2087:U:C6	2.55	0.42
29:a:2378:G:H5"	29:a:2379:U:O4'	2.20	0.42
30:b:3:U:H2'	30:b:4:G:C8	2.54	0.42
30:b:112:A:H2'	30:b:113:G:C8	2.54	0.42
39:k:2:THR:HG22	39:k:3:LEU:H	1.84	0.42
8:C:179:ARG:HD2	8:C:206:GLU:OE1	2.20	0.42
16:K:74:LEU:HD12	16:K:74:LEU:HA	1.84	0.42
16:K:78:LEU:HB3	16:K:104:TYR:CE1	2.50	0.42
22:Q:9:LEU:HD23	22:Q:26:ILE:HG12	2.01	0.42
23:R:29:LEU:O	23:R:33:ILE:HG23	2.20	0.42
29:a:720:G:C8	31:c:207:LYS:HE3	2.54	0.42
29:a:938:C:H1'	29:a:974:A:C8	2.55	0.42
29:a:1779:U:H2'	29:a:1780:A:C5	2.55	0.42
29:a:1878:A:O2'	29:a:2076:G:H5'	2.20	0.42
29:a:2230:A:H2'	29:a:2231:G:H8	1.84	0.42
29:a:2682:G:H2'	29:a:2683:G:C8	2.54	0.42
31:c:145:GLU:HB3	31:c:188:CYS:HB3	2.02	0.42
39:k:22:GLY:O	39:k:23:ARG:HD3	2.20	0.42
43:o:5:HIS:CE1	43:o:7:LEU:HD23	2.52	0.42
6:A:1154:A:H4'	6:A:1155:C:O4'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1273:G:H2'	6:A:1274:C:O4'	2.19	0.42
8:C:211:MET:HE3	8:C:215:MET:HE2	2.02	0.42
13:H:103:ALA:HB3	13:H:114:ASP:HB3	2.02	0.42
16:K:66:ALA:HB3	16:K:98:ALA:HB3	2.02	0.42
17:L:36:ARG:O	17:L:53:CYS:HA	2.20	0.42
29:a:68:G:H2'	29:a:69:C:O4'	2.20	0.42
29:a:297:G:H2'	29:a:298:C:H6	1.84	0.42
29:a:437:C:H2'	29:a:438:G:O4'	2.19	0.42
29:a:645:U:H5'	29:a:646:A:OP2	2.20	0.42
29:a:823:U:H2'	29:a:824:A:H8	1.83	0.42
29:a:842:C:H2'	29:a:843:A:H8	1.84	0.42
29:a:1328:U:H3'	29:a:1329:G:H5'	2.02	0.42
29:a:1568:C:H2'	29:a:1569:U:C6	2.54	0.42
29:a:2533:G:H2'	29:a:2534:G:O4'	2.20	0.42
29:a:2876:C:H2'	29:a:2877:U:C6	2.55	0.42
33:e:194:LYS:HE3	33:e:194:LYS:HB3	1.76	0.42
37:i:75:TYR:CE1	37:i:86:GLU:HG3	2.54	0.42
37:i:110:PRO:O	37:i:115:GLY:HA3	2.20	0.42
51:w:3:LYS:O	51:w:12:PRO:HD3	2.20	0.42
5:4:7:PRO:HG3	34:f:58:GLN:HG2	2.02	0.42
6:A:792:C:H5"	16:K:127:ARG:HH21	1.85	0.42
6:A:905:A:O2'	6:A:906:A:H5"	2.20	0.42
6:A:1355:U:P	19:N:75:ARG:HD2	2.60	0.42
7:B:33:ILE:HG21	7:B:41:HIS:ND1	2.35	0.42
7:B:62:LEU:HD22	7:B:67:ASN:HD22	1.84	0.42
12:G:72:MET:HG3	12:G:142:HIS:CE1	2.55	0.42
14:I:50:LEU:HD11	14:I:61:LEU:HD11	2.00	0.42
18:M:34:LEU:HD13	18:M:39:ILE:HB	2.02	0.42
19:N:61:ARG:O	19:N:63:ARG:HG3	2.19	0.42
29:a:303:G:H2'	29:a:304:G:C8	2.54	0.42
29:a:433:U:H2'	29:a:434:G:C8	2.54	0.42
29:a:925:U:H2'	29:a:926:C:C6	2.54	0.42
29:a:1342:A:H4'	31:c:38:LYS:HD2	2.01	0.42
29:a:1577:A:H2'	29:a:1578:G:O4'	2.20	0.42
29:a:1671:U:H2'	29:a:1672:G:O4'	2.19	0.42
29:a:2334:A:N3	29:a:2370:A:H2'	2.35	0.42
30:b:16:A:H2'	30:b:17:A:H8	1.85	0.42
37:i:116:TYR:O	37:i:119:ILE:HG22	2.20	0.42
1:0:34:LYS:HB2	1:0:45:PHE:CD1	2.54	0.42
6:A:232:A:H2'	6:A:233:A:C8	2.55	0.42
6:A:955:A:H1'	6:A:982:C:O2'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:E:109:ALA:HB1	10:E:136:VAL:HG23	2.02	0.42
29:a:545:U:H2'	29:a:546:G:H5'	2.02	0.42
29:a:808:C:O2'	29:a:830:U:H5"	2.20	0.42
29:a:959:G:H2'	29:a:960:U:C6	2.55	0.42
29:a:1552:C:H2'	29:a:1553:U:C6	2.55	0.42
29:a:2318:A:H2'	29:a:2319:G:H8	1.85	0.42
42:n:40:VAL:HB	42:n:50:ALA:HB3	2.01	0.42
46:r:19:LEU:HB3	54:z:22:LEU:HG	2.01	0.42
48:t:70:ILE:HG21	48:t:81:VAL:HG23	2.02	0.42
50:v:11:LYS:HE3	50:v:11:LYS:HB3	1.68	0.42
53:y:4:ILE:HG22	53:y:58:GLU:HA	2.01	0.42
2:1:42:LEU:HD12	2:1:42:LEU:HA	1.95	0.41
5:4:9:TYR:HD2	5:4:25:ARG:HH21	1.68	0.41
6:A:960:G:H5'	28:X:9:LYS:HD3	2.02	0.41
6:A:1008:C:H4'	6:A:1009:A:H5'	2.01	0.41
7:B:189:VAL:HG13	7:B:193:SER:HB3	2.02	0.41
9:D:80:GLU:CD	9:D:83:ARG:HH12	2.27	0.41
13:H:18:GLN:HG3	13:H:71:PRO:HB2	2.02	0.41
21:P:26:ARG:NE	21:P:33:PRO:HB3	2.34	0.41
29:a:2126:C:H2'	29:a:2127:U:C6	2.55	0.41
29:a:2885:C:H2'	29:a:2886:U:H6	1.85	0.41
30:b:112:A:H4'	42:n:51:GLN:NE2	2.35	0.41
2:1:22:MET:HE2	2:1:31:LEU:HD12	2.02	0.41
6:A:598:G:H2'	6:A:599:A:H8	1.84	0.41
6:A:1270:G:H2'	6:A:1271:A:O4'	2.21	0.41
6:A:1304:U:H2'	6:A:1305:U:C6	2.56	0.41
6:A:1314:C:O2'	19:N:49:GLN:HG2	2.20	0.41
7:B:119:LEU:HA	7:B:122:GLN:HG2	2.01	0.41
10:E:12:GLU:HG2	10:E:38:VAL:HG12	2.01	0.41
13:H:6:THR:HB	13:H:33:LYS:HE2	2.01	0.41
13:H:105:VAL:HG12	13:H:107:THR:HG22	2.01	0.41
26:V:3:C:H2'	26:V:4:G:O4'	2.20	0.41
26:V:70:C:H2'	26:V:71:G:H8	1.84	0.41
28:X:42:HIS:HB2	28:X:59:MET:HE3	2.01	0.41
29:a:1716:A:H2'	29:a:1717:C:O4'	2.20	0.41
30:b:43:A:C4	30:b:44:A:C8	3.08	0.41
44:p:76:TYR:CZ	44:p:80:ILE:HG13	2.55	0.41
52:x:14:LEU:HD23	52:x:14:LEU:HA	1.85	0.41
5:4:48:LYS:HB3	5:4:49:GLN:H	1.79	0.41
6:A:598:G:H2'	6:A:599:A:C8	2.56	0.41
6:A:892:G:H2'	6:A:893:U:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1316:A:C8	6:A:1320:G:C5	3.09	0.41
7:B:102:MET:HA	7:B:109:LEU:HG	2.01	0.41
11:F:29:ILE:HD11	11:F:74:LEU:HD21	2.02	0.41
14:I:3:THR:C	14:I:4:ASN:HD22	2.28	0.41
29:a:601:C:H2'	29:a:602:C:C6	2.55	0.41
29:a:2138:U:H2'	29:a:2139:U:H6	1.85	0.41
3:2:32:LEU:HD13	29:a:2408:U:OP2	2.19	0.41
5:4:68:MET:C	5:4:70:ARG:H	2.27	0.41
6:A:42:C:H2'	6:A:43:G:H8	1.85	0.41
6:A:436:A:C4	6:A:437:A:C8	3.09	0.41
6:A:456:U:H2'	6:A:457:A:C8	2.55	0.41
6:A:610:C:H2'	6:A:611:C:H6	1.82	0.41
6:A:818:G:H2'	6:A:819:U:H6	1.83	0.41
6:A:861:A:H2'	6:A:862:A:C8	2.56	0.41
6:A:1406:C:H2'	6:A:1407:A:H8	1.85	0.41
9:D:172:TRP:O	9:D:185:LYS:HG3	2.20	0.41
23:R:34:THR:HG22	23:R:38:LYS:N	2.35	0.41
29:a:507:A:H1'	29:a:572:C:H1'	2.03	0.41
29:a:882:G:C2	29:a:883:A:C5	3.07	0.41
29:a:1860:A:H2'	29:a:1861:A:C8	2.56	0.41
29:a:2160:A:H1'	29:a:2161:U:C5	2.55	0.41
29:a:2236:A:H2'	29:a:2237:C:H6	1.85	0.41
29:a:2669:C:O2'	29:a:2670:C:H5'	2.21	0.41
29:a:2841:G:H2'	29:a:2842:C:O4'	2.20	0.41
42:n:76:LEU:O	42:n:80:ARG:HG3	2.20	0.41
48:t:72:ASN:HB3	48:t:75:THR:HG22	2.03	0.41
6:A:599:A:H2'	6:A:600:U:C6	2.55	0.41
6:A:1421:U:H2'	6:A:1422:U:H6	1.84	0.41
6:A:1537:U:H2'	6:A:1538:U:O4'	2.21	0.41
10:E:68:ARG:HE	10:E:68:ARG:HB3	1.48	0.41
26:V:43:G:H2'	26:V:44:A:O4'	2.20	0.41
29:a:246:C:O2'	29:a:377:C:H4'	2.20	0.41
29:a:299:U:H2'	29:a:300:C:C6	2.54	0.41
29:a:347:A:H2'	29:a:348:C:H6	1.86	0.41
29:a:411:U:H2'	29:a:412:C:C6	2.56	0.41
29:a:584:U:H2'	29:a:585:U:H6	1.83	0.41
29:a:868:U:H2'	29:a:869:A:H8	1.86	0.41
29:a:922:C:H42	29:a:1158:U:H1'	1.84	0.41
29:a:1069:C:N4	29:a:1078:A:C4	2.89	0.41
29:a:1314:U:H2'	29:a:1315:A:H8	1.86	0.41
29:a:1855:A:H2'	29:a:1856:G:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:2339:C:H2'	29:a:2340:G:O4'	2.19	0.41
29:a:2505:U:H2'	29:a:2506:C:C6	2.55	0.41
32:d:180:ILE:HD13	32:d:192:VAL:HG22	2.02	0.41
51:w:40:LEU:HD12	51:w:40:LEU:HA	1.93	0.41
4:3:36:ARG:HG2	4:3:37:GLN:N	2.34	0.41
6:A:493:A:H2'	6:A:494:U:C5	2.55	0.41
6:A:709:A:H2'	6:A:710:G:C8	2.56	0.41
6:A:1474:C:H2'	6:A:1475:C:C6	2.56	0.41
9:D:13:ARG:NH2	9:D:39:PRO:HA	2.36	0.41
29:a:30:G:H2'	29:a:31:C:H6	1.85	0.41
29:a:557:U:H5"	39:k:31:LYS:HE3	2.03	0.41
29:a:679:U:H2'	29:a:680:A:H8	1.86	0.41
29:a:1337:C:C2	29:a:1338:C:C5	3.09	0.41
29:a:1373:A:H1'	29:a:1374:A:C8	2.56	0.41
29:a:2240:OMG:HM23	29:a:2240:OMG:H1'	1.62	0.41
29:a:2679:A:H5"	29:a:2861:G:N2	2.36	0.41
31:c:205:LEU:HB3	31:c:210:ALA:HB3	2.03	0.41
37:i:15:TRP:HE3	37:i:55:ILE:HD11	1.85	0.41
38:j:53:LYS:HB3	38:j:53:LYS:NZ	2.36	0.41
47:s:15:PHE:HE2	52:x:34:THR:HA	1.84	0.41
2:1:1:MET:H2	29:a:1610:G:N2	2.04	0.41
6:A:497:G:H2'	6:A:498:C:H6	1.86	0.41
6:A:906:A:H2'	6:A:907:C:O4'	2.21	0.41
6:A:1203:G:C4	6:A:1204:2MG:C8	3.09	0.41
10:E:71:ILE:HD13	10:E:140:PHE:CZ	2.56	0.41
12:G:53:LYS:HA	12:G:53:LYS:HD2	1.83	0.41
29:a:1523:A:H4'	29:a:1524:C:C6	2.56	0.41
29:a:2095:A:H2'	29:a:2096:C:C6	2.55	0.41
29:a:2255:A:H4'	29:a:2256:A:N3	2.35	0.41
29:a:2304:C:H2'	29:a:2305:G:C8	2.55	0.41
29:a:2443:G:C5	29:a:2444:G:C8	3.09	0.41
41:m:112:TYR:CZ	54:z:54:PHE:HZ	2.38	0.41
47:s:68:ARG:HE	47:s:68:ARG:HB2	1.68	0.41
49:u:68:LYS:HG2	49:u:73:VAL:HG22	2.02	0.41
3:2:4:LEU:HD23	3:2:4:LEU:HA	1.90	0.41
5:4:11:LYS:HE3	5:4:23:GLU:HB3	2.01	0.41
6:A:389:A:C2	6:A:390:G:C8	3.08	0.41
6:A:989:U:H5	6:A:1041:A:C2	2.39	0.41
6:A:1118:U:H2'	6:A:1119:U:C6	2.55	0.41
7:B:68:LYS:HB3	7:B:68:LYS:HE3	1.77	0.41
9:D:26:LYS:HE3	9:D:26:LYS:HB3	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:131:LYS:HB3	12:G:131:LYS:HE2	1.70	0.41
15:J:7:ARG:HB2	15:J:101:ALA:HB3	2.03	0.41
19:N:64:CYS:HB3	19:N:68:GLY:H	1.86	0.41
29:a:194:G:H2'	29:a:195:A:O4'	2.20	0.41
29:a:530:A:H2'	29:a:531:G:O4'	2.21	0.41
29:a:961:C:H2'	29:a:962:A:O4'	2.20	0.41
29:a:2105:G:H2'	29:a:2106:A:C8	2.55	0.41
31:c:210:ALA:HA	31:c:213:TRP:CE3	2.55	0.41
34:f:32:THR:OG1	34:f:159:THR:HG23	2.20	0.41
35:g:94:TYR:HA	35:g:106:ASN:O	2.21	0.41
43:o:25:PRO:HG3	43:o:53:LYS:HB2	2.03	0.41
6:A:704:U:H2'	6:A:705:C:H6	1.85	0.41
6:A:734:A:H2'	6:A:735:U:H6	1.86	0.41
6:A:1001:A:H8	6:A:1023:G:N2	2.19	0.41
6:A:1011:A:C2	6:A:1216:A:H1'	2.56	0.41
6:A:1449:A:H4'	6:A:1450:A:OP1	2.20	0.41
7:B:79:SER:HB2	7:B:95:ASP:HB2	2.02	0.41
7:B:89:ALA:HA	7:B:224:LEU:HD21	2.03	0.41
7:B:175:ILE:HG22	7:B:197:ASN:HB2	2.03	0.41
12:G:14:PRO:HB2	12:G:19:SER:HA	2.03	0.41
12:G:27:MET:SD	12:G:40:GLU:HG2	2.61	0.41
25:T:44:TYR:CE1	25:T:87:ALA:HB2	2.56	0.41
25:T:53:LYS:HB2	25:T:53:LYS:HE3	1.70	0.41
26:V:28:U:H2'	26:V:29:C:H6	1.85	0.41
29:a:200:U:H4'	51:w:22:ASN:HB3	2.03	0.41
29:a:274:A:H2'	29:a:275:G:O4'	2.21	0.41
29:a:690:A:H2'	29:a:691:G:O4'	2.21	0.41
29:a:1045:G:H2'	29:a:1046:G:O4'	2.20	0.41
29:a:1048:G:H2'	29:a:1049:G:C8	2.56	0.41
29:a:1088:A:H3'	29:a:1089:G:H8	1.86	0.41
29:a:1218:A:H2'	29:a:1219:U:C6	2.56	0.41
29:a:1253:A:OP1	29:a:1253:A:H8	2.03	0.41
29:a:1303:C:H2'	29:a:1304:A:H8	1.86	0.41
29:a:1394:U:H2'	29:a:1395:C:H6	1.86	0.41
29:a:1862:G:H2'	29:a:1863:C:H6	1.85	0.41
29:a:2054:C:H2'	29:a:2055:C:C6	2.56	0.41
29:a:2105:G:O2'	29:a:2106:A:H5'	2.21	0.41
29:a:2586:G:H2'	29:a:2587:A:C8	2.56	0.41
32:d:153:MEQ:HE21	32:d:153:MEQ:HB3	1.69	0.41
33:e:110:GLU:O	33:e:114:GLN:HG3	2.20	0.41
33:e:130:THR:HG23	33:e:163:LEU:HG	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:947:U:H2'	6:A:948:G:H8	1.85	0.41
6:A:1493:C:H2'	6:A:1494:G:O4'	2.21	0.41
7:B:9:ARG:HA	7:B:9:ARG:HD3	1.74	0.41
20:O:53:ARG:O	20:O:57:ILE:HG12	2.21	0.41
29:a:1258:C:H5"	29:a:1259:G:O5'	2.22	0.41
29:a:1382:U:H4'	29:a:1594:A:H4'	2.03	0.41
29:a:1406:G:H21	29:a:1571:A:H62	1.68	0.41
29:a:1424:G:H2'	29:a:1425:C:O4'	2.21	0.41
29:a:2105:G:H2'	29:a:2106:A:C4	2.56	0.41
29:a:2145:G:H3'	29:a:2146:G:C8	2.56	0.41
29:a:2336:C:H2'	29:a:2337:U:H6	1.85	0.41
29:a:2887:U:H2'	29:a:2888:G:H8	1.84	0.41
35:g:3:ARG:HA	35:g:6:LYS:HE2	2.03	0.41
35:g:15:VAL:HA	35:g:27:LYS:O	2.21	0.41
47:s:86:LEU:HD11	47:s:92:VAL:HG23	2.02	0.41
6:A:347:G:OP1	25:T:2:ALA:HB3	2.21	0.40
6:A:460:U:H3	6:A:463:U:P	2.44	0.40
6:A:498:C:H1'	6:A:546:C:H1'	2.03	0.40
6:A:624:G:H2'	6:A:625:G:O4'	2.21	0.40
6:A:1317:C:H2'	6:A:1318:U:C6	2.57	0.40
7:B:176:LYS:HD2	7:B:176:LYS:HA	1.70	0.40
8:C:14:VAL:O	8:C:211:MET:HG2	2.20	0.40
29:a:256:A:H2'	29:a:257:C:H6	1.86	0.40
29:a:662:C:H2'	29:a:663:C:C6	2.55	0.40
29:a:1270:U:H2'	29:a:1271:G:O4'	2.21	0.40
29:a:1285:C:OP1	29:a:2699:C:H4'	2.21	0.40
29:a:1341:A:H2'	29:a:1342:A:H8	1.83	0.40
29:a:1422:A:H2'	29:a:1423:G:O4'	2.21	0.40
29:a:1500:G:H2'	29:a:1501:C:C6	2.57	0.40
29:a:1530:C:H2'	29:a:1531:A:H8	1.86	0.40
29:a:1798:A:H8	29:a:1798:A:OP2	2.04	0.40
29:a:2144:U:C2	29:a:2145:G:C8	3.09	0.40
29:a:2877:U:H2'	29:a:2878:C:C6	2.56	0.40
32:d:16:PHE:CE1	32:d:22:SER:HB2	2.56	0.40
35:g:170:LEU:HD23	35:g:170:LEU:HA	1.96	0.40
37:i:2:LYS:HE2	37:i:2:LYS:HB3	1.56	0.40
45:q:28:GLU:OE2	45:q:28:GLU:HA	2.20	0.40
49:u:91:MET:HE2	49:u:91:MET:HB3	1.93	0.40
7:B:59:ALA:HB2	7:B:219:MET:HE1	2.03	0.40
7:B:163:LEU:HD22	7:B:178:ALA:HB2	2.02	0.40
9:D:204:GLU:CD	10:E:111:ARG:HH12	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:17:LYS:HB2	12:G:17:LYS:HE2	1.89	0.40
16:K:82:ASP:OD1	16:K:107:ASN:HB2	2.21	0.40
18:M:90:ARG:HA	18:M:90:ARG:HD2	1.81	0.40
19:N:60:LEU:HD23	19:N:60:LEU:HA	1.96	0.40
29:a:944:G:H5"	40:l:13:HIS:CG	2.55	0.40
29:a:1658:G:H5"	38:j:5:GLU:O	2.22	0.40
29:a:2121:U:H5'	29:a:2122:G:C4	2.56	0.40
29:a:2176:G:H2'	29:a:2177:U:C6	2.57	0.40
29:a:2205:G:H2'	29:a:2206:G:C8	2.56	0.40
29:a:2639:U:H2'	29:a:2640:C:H6	1.86	0.40
31:c:120:ASN:HD22	31:c:133:ARG:HH12	1.69	0.40
3:2:18:ALA:HB3	29:a:642:G:O5'	2.22	0.40
6:A:330:C:H2'	6:A:331:C:H6	1.86	0.40
6:A:409:G:H22	6:A:424:G:H1'	1.87	0.40
6:A:542:C:H2'	6:A:543:G:O4'	2.20	0.40
6:A:1519:U:H2'	6:A:1520:G:C8	2.53	0.40
8:C:37:LEU:HD13	19:N:66:LEU:HD11	2.02	0.40
11:F:21:MET:HE3	11:F:21:MET:HB3	1.90	0.40
28:X:9:LYS:HG3	28:X:10:ASN:OD1	2.21	0.40
28:X:16:ARG:HG3	28:X:17:LEU:N	2.35	0.40
29:a:347:A:H2'	29:a:348:C:C6	2.57	0.40
29:a:638:G:H2'	29:a:639:G:O4'	2.22	0.40
29:a:2432:U:OP1	33:e:62:LYS:HD3	2.21	0.40
29:a:2887:U:H2'	29:a:2888:G:C8	2.55	0.40
34:f:146:ILE:HD12	34:f:146:ILE:O	2.21	0.40
2:1:9:GLU:HB2	29:a:1297:G:OP1	2.21	0.40
3:2:5:LYS:HG2	29:a:242:G:C8	2.57	0.40
6:A:880:C:O2'	6:A:881:U:H5'	2.22	0.40
11:F:38:ARG:HB3	11:F:63:ASN:HB2	2.04	0.40
15:J:5:ARG:HE	15:J:77:VAL:HG23	1.87	0.40
29:a:277:U:H3	29:a:353:A:H62	1.68	0.40
29:a:735:C:H2'	29:a:736:1MG:O4'	2.21	0.40
29:a:751:G:H2'	29:a:752:A:O4'	2.21	0.40
29:a:1265:A:H2'	29:a:1266:C:C6	2.57	0.40
29:a:1483:A:H2'	29:a:1484:A:C8	2.56	0.40
29:a:2639:U:H2'	29:a:2640:C:C6	2.56	0.40
38:j:51:ARG:HG2	38:j:51:ARG:NH1	2.37	0.40
46:r:29:VAL:HB	46:r:55:ILE:HD11	2.04	0.40
9:D:77:TYR:CD1	9:D:95:LEU:HD23	2.49	0.40
9:D:199:GLU:O	9:D:203:VAL:HG23	2.22	0.40
12:G:66:LEU:HA	12:G:69:VAL:HG12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:K:93:GLU:O	16:K:96:VAL:HG12	2.22	0.40
19:N:9:ARG:O	19:N:13:ARG:HG3	2.22	0.40
21:P:69:ARG:HE	21:P:69:ARG:HB3	1.74	0.40
29:a:297:G:H2'	29:a:298:C:C6	2.56	0.40
29:a:310:C:H2'	29:a:311:G:O4'	2.22	0.40
29:a:723:C:H2'	29:a:724:G:O4'	2.22	0.40
29:a:1420:G:H2'	29:a:1421:A:H8	1.84	0.40
29:a:1747:A:H3'	29:a:1748:A:C8	2.57	0.40
29:a:2121:U:H5'	29:a:2122:G:C5	2.57	0.40
35:g:132:ILE:N	35:g:132:ILE:HD12	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	49/51 (96%)	48 (98%)	1 (2%)	0	100	100
2	1	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
3	2	61/64 (95%)	57 (93%)	4 (7%)	0	100	100
4	3	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
5	4	69/74 (93%)	59 (86%)	10 (14%)	0	100	100
7	B	227/250 (91%)	213 (94%)	13 (6%)	1 (0%)	30	54
8	C	213/250 (85%)	206 (97%)	7 (3%)	0	100	100
9	D	205/208 (99%)	198 (97%)	7 (3%)	0	100	100
10	E	153/165 (93%)	151 (99%)	2 (1%)	0	100	100
11	F	104/127 (82%)	102 (98%)	2 (2%)	0	100	100
12	G	151/156 (97%)	143 (95%)	8 (5%)	0	100	100
13	H	128/131 (98%)	124 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	I	125/128 (98%)	116 (93%)	9 (7%)	0	100	100
15	J	98/103 (95%)	95 (97%)	3 (3%)	0	100	100
16	K	113/128 (88%)	109 (96%)	4 (4%)	0	100	100
17	L	119/124 (96%)	114 (96%)	5 (4%)	0	100	100
18	M	114/118 (97%)	108 (95%)	6 (5%)	0	100	100
19	N	98/101 (97%)	92 (94%)	6 (6%)	0	100	100
20	O	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
21	P	80/83 (96%)	79 (99%)	1 (1%)	0	100	100
22	Q	77/85 (91%)	73 (95%)	4 (5%)	0	100	100
23	R	64/75 (85%)	64 (100%)	0	0	100	100
24	S	82/91 (90%)	80 (98%)	2 (2%)	0	100	100
25	T	84/88 (96%)	84 (100%)	0	0	100	100
28	X	102/116 (88%)	99 (97%)	3 (3%)	0	100	100
31	c	270/274 (98%)	260 (96%)	10 (4%)	0	100	100
32	d	208/212 (98%)	200 (96%)	7 (3%)	1 (0%)	24	48
33	e	197/200 (98%)	196 (100%)	1 (0%)	0	100	100
34	f	175/178 (98%)	161 (92%)	12 (7%)	2 (1%)	11	29
35	g	173/177 (98%)	168 (97%)	4 (2%)	1 (1%)	21	44
36	h	58/148 (39%)	54 (93%)	4 (7%)	0	100	100
37	i	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
38	j	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
39	k	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
40	l	133/137 (97%)	133 (100%)	0	0	100	100
41	m	117/125 (94%)	114 (97%)	3 (3%)	0	100	100
42	n	113/116 (97%)	110 (97%)	3 (3%)	0	100	100
43	o	115/122 (94%)	113 (98%)	2 (2%)	0	100	100
44	p	115/119 (97%)	115 (100%)	0	0	100	100
45	q	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
46	r	107/109 (98%)	105 (98%)	2 (2%)	0	100	100
47	s	90/106 (85%)	87 (97%)	3 (3%)	0	100	100
48	t	101/105 (96%)	97 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	u	95/98 (97%)	91 (96%)	4 (4%)	0	100	100
50	v	76/85 (89%)	75 (99%)	1 (1%)	0	100	100
51	w	75/78 (96%)	75 (100%)	0	0	100	100
52	x	60/65 (92%)	58 (97%)	2 (3%)	0	100	100
53	y	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
54	z	52/61 (85%)	49 (94%)	3 (6%)	0	100	100
All	All	5571/5973 (93%)	5382 (97%)	184 (3%)	5 (0%)	49	73

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
34	f	136	ILE
7	B	128	PHE
32	d	152	ASN
34	f	139	PRO
35	g	86	LYS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	47/47 (100%)	47 (100%)	0	100	100
2	1	36/36 (100%)	36 (100%)	0	100	100
3	2	52/53 (98%)	52 (100%)	0	100	100
4	3	33/33 (100%)	31 (94%)	2 (6%)	17	40
5	4	60/63 (95%)	60 (100%)	0	100	100
7	B	188/200 (94%)	178 (95%)	10 (5%)	20	46
8	C	175/198 (88%)	171 (98%)	4 (2%)	44	73
9	D	170/171 (99%)	168 (99%)	2 (1%)	63	84
10	E	113/120 (94%)	112 (99%)	1 (1%)	70	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
11	F	95/111 (86%)	92 (97%)	3 (3%)	34 64
12	G	125/128 (98%)	123 (98%)	2 (2%)	55 80
13	H	108/109 (99%)	104 (96%)	4 (4%)	30 59
14	I	99/100 (99%)	96 (97%)	3 (3%)	36 66
15	J	89/91 (98%)	89 (100%)	0	100 100
16	K	87/97 (90%)	86 (99%)	1 (1%)	65 85
17	L	103/105 (98%)	101 (98%)	2 (2%)	50 77
18	M	96/98 (98%)	94 (98%)	2 (2%)	47 75
19	N	81/82 (99%)	78 (96%)	3 (4%)	30 59
20	O	71/72 (99%)	67 (94%)	4 (6%)	19 44
21	P	63/63 (100%)	63 (100%)	0	100 100
22	Q	71/76 (93%)	68 (96%)	3 (4%)	26 55
23	R	58/66 (88%)	57 (98%)	1 (2%)	53 79
24	S	71/78 (91%)	70 (99%)	1 (1%)	59 82
25	T	65/67 (97%)	65 (100%)	0	100 100
28	X	92/102 (90%)	91 (99%)	1 (1%)	65 85
31	c	218/220 (99%)	214 (98%)	4 (2%)	51 78
32	d	165/166 (99%)	161 (98%)	4 (2%)	43 72
33	e	155/155 (100%)	153 (99%)	2 (1%)	61 83
34	f	146/147 (99%)	136 (93%)	10 (7%)	14 35
35	g	140/142 (99%)	133 (95%)	7 (5%)	22 48
36	h	45/112 (40%)	41 (91%)	4 (9%)	9 23
37	i	118/118 (100%)	115 (98%)	3 (2%)	42 71
38	j	103/103 (100%)	102 (99%)	1 (1%)	68 86
39	k	108/108 (100%)	107 (99%)	1 (1%)	70 87
40	l	111/111 (100%)	111 (100%)	0	100 100
41	m	96/101 (95%)	95 (99%)	1 (1%)	68 86
42	n	84/85 (99%)	81 (96%)	3 (4%)	31 60
43	o	99/102 (97%)	98 (99%)	1 (1%)	68 86
44	p	85/86 (99%)	85 (100%)	0	100 100
45	q	84/84 (100%)	83 (99%)	1 (1%)	63 84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	r	88/88 (100%)	88 (100%)	0	100	100
47	s	78/87 (90%)	77 (99%)	1 (1%)	61	83
48	t	83/85 (98%)	82 (99%)	1 (1%)	63	84
49	u	79/80 (99%)	77 (98%)	2 (2%)	42	71
50	v	60/64 (94%)	58 (97%)	2 (3%)	33	63
51	w	69/70 (99%)	67 (97%)	2 (3%)	37	67
52	x	54/56 (96%)	51 (94%)	3 (6%)	19	44
53	y	54/54 (100%)	53 (98%)	1 (2%)	50	77
54	z	46/50 (92%)	43 (94%)	3 (6%)	15	37
All	All	4616/4840 (95%)	4510 (98%)	106 (2%)	44	73

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	3	17	ILE
4	3	30	GLU
7	B	10	ASP
7	B	17	HIS
7	B	18	PHE
7	B	76	ARG
7	B	120	GLN
7	B	122	GLN
7	B	163	LEU
7	B	173	ILE
7	B	198	VAL
7	B	201	VAL
8	C	51	MET
8	C	100	GLN
8	C	123	GLN
8	C	195	THR
9	D	50	GLN
9	D	121	SER
10	E	45	VAL
11	F	39	LEU
11	F	70	THR
11	F	74	LEU
12	G	7	VAL
12	G	10	ARG
13	H	25	VAL

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Mol	Chain	Res	Type
13	H	76	VAL
13	H	93	LEU
13	H	98	GLN
14	I	14	THR
14	I	23	THR
14	I	52	LEU
16	K	32	THR
17	L	41	THR
17	L	98	VAL
18	M	100	GLN
18	M	104	THR
19	N	14	GLU
19	N	26	GLU
19	N	58	VAL
20	O	40	GLN
20	O	54	ARG
20	O	68	ASP
20	O	73	LYS
22	Q	30	VAL
22	Q	39	ILE
22	Q	61	THR
23	R	26	ILE
24	S	63	THR
28	X	95	GLU
31	c	162	VAL
31	c	186	VAL
31	c	265	LYS
31	c	268	ILE
32	d	79	LEU
32	d	81	LYS
32	d	89	GLU
32	d	101	VAL
33	e	4	LYS
33	e	32	THR
34	f	16	LEU
34	f	32	THR
34	f	80	ARG
34	f	91	LEU
34	f	96	MET
34	f	104	ILE
34	f	118	SER
34	f	132	LEU

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Mol	Chain	Res	Type
34	f	138	PHE
34	f	143	PHE
35	g	9	VAL
35	g	10	THR
35	g	20	ASN
35	g	24	VAL
35	g	60	ASP
35	g	98	VAL
35	g	168	VAL
36	h	8	ARG
36	h	14	LYS
36	h	15	LEU
36	h	50	ARG
37	i	10	GLU
37	i	61	GLN
37	i	70	LEU
38	j	113	LYS
39	k	19	ARG
41	m	88	LYS
42	n	39	GLN
42	n	66	ASN
42	n	87	THR
43	o	40	ARG
45	q	43	ASN
47	s	22	LEU
48	t	44	GLN
49	u	45	THR
49	u	69	VAL
50	v	31	VAL
50	v	32	THR
51	w	2	SER
51	w	22	ASN
52	x	5	ASP
52	x	8	GLU
52	x	17	LEU
53	y	53	MET
54	z	45	ASP
54	z	51	ARG
54	z	54	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
7	B	38	ASN
7	B	41	HIS
7	B	80	ASN
7	B	120	GLN
7	B	122	GLN
8	C	6	HIS
9	D	154	GLN
9	D	177	HIS
11	F	87	ASN
12	G	51	GLN
12	G	86	GLN
12	G	142	HIS
13	H	4	GLN
14	I	124	GLN
15	J	15	HIS
16	K	21	HIS
16	K	117	HIS
20	O	50	HIS
20	O	62	GLN
21	P	77	HIS
31	c	53	HIS
31	c	134	ASN
31	c	239	ASN
31	c	243	GLN
32	d	129	ASN
33	e	89	GLN
33	e	93	GLN
33	e	141	ASN
35	g	38	HIS
35	g	73	ASN
35	g	106	ASN
35	g	137	ASN
37	i	47	HIS
38	j	82	ASN
40	l	85	ASN
43	o	5	HIS
45	q	6	GLN
45	q	87	GLN
49	u	58	ASN
50	v	57	HIS
51	w	36	HIS
52	x	44	GLN
53	y	8	GLN

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Mol	Chain	Res	Type
54	z	4	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
26	V	76/77 (98%)	30 (39%)	1 (1%)
27	W	9/15 (60%)	2 (22%)	0
29	a	2889/2893 (99%)	550 (19%)	0
30	b	114/115 (99%)	13 (11%)	0
6	A	1534/1537 (99%)	276 (17%)	12 (0%)
All	All	4622/4637 (99%)	871 (18%)	13 (0%)

All (871) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	A	6	C
6	A	9	A
6	A	10	A
6	A	11	G
6	A	24	G
6	A	34	A
6	A	41	G
6	A	49	C
6	A	50	U
6	A	53	A
6	A	64	U
6	A	74	G
6	A	75	A
6	A	76	A
6	A	77	G
6	A	82	C
6	A	83	U
6	A	86	C
6	A	88	A
6	A	90	C
6	A	91	G
6	A	92	G
6	A	93	A
6	A	97	A
6	A	105	A
6	A	106	C

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Mol	Chain	Res	Type
6	A	107	G
6	A	126	A
6	A	127	U
6	A	140	G
6	A	160	G
6	A	167	A
6	A	170	A
6	A	177	A
6	A	184	A
6	A	186	G
6	A	193	A
6	A	205	U
6	A	206	C
6	A	208	G
6	A	214	G
6	A	241	U
6	A	243	G
6	A	247	G
6	A	262	G
6	A	263	C
6	A	272	G
6	A	276	C
6	A	277	G
6	A	285	G
6	A	317	A
6	A	324	C
6	A	325	A
6	A	326	C
6	A	340	A
6	A	347	G
6	A	348	C
6	A	350	G
6	A	351	C
6	A	359	A
6	A	363	U
6	A	368	C
6	A	394	U
6	A	402	G
6	A	408	A
6	A	409	G
6	A	410	A
6	A	414	C

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Mol	Chain	Res	Type
6	A	418	A
6	A	419	U
6	A	420	G
6	A	425	U
6	A	435	U
6	A	442	G
6	A	448	G
6	A	454	U
6	A	457	A
6	A	459	U
6	A	461	A
6	A	463	U
6	A	464	A
6	A	465	C
6	A	468	A
6	A	469	G
6	A	470	A
6	A	473	U
6	A	474	A
6	A	479	A
6	A	481	G
6	A	483	U
6	A	493	A
6	A	494	U
6	A	497	G
6	A	506	A
6	A	508	C
6	A	511	U
6	A	515	C
6	A	518	G
6	A	521	G
6	A	524	G7M
6	A	529	A
6	A	532	A
6	A	544	A
6	A	556	A
6	A	559	U
6	A	561	C
6	A	567	G
6	A	569	A
6	A	570	A
6	A	571	A

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Mol	Chain	Res	Type
6	A	572	G
6	A	573	C
6	A	574	G
6	A	585	G
6	A	630	G
6	A	639	A
6	A	648	C
6	A	649	U
6	A	650	A
6	A	654	U
6	A	662	A
6	A	685	G
6	A	700	G
6	A	720	U
6	A	721	G
6	A	728	G
6	A	731	G
6	A	744	A
6	A	745	U
6	A	752	G
6	A	756	A
6	A	774	A
6	A	778	A
6	A	790	U
6	A	791	A
6	A	809	G
6	A	812	A
6	A	814	C
6	A	818	G
6	A	829	G
6	A	839	U
6	A	840	U
6	A	841	G
6	A	842	A
6	A	843	G
6	A	848	U
6	A	852	G
6	A	867	A
6	A	884	G
6	A	899	G
6	A	906	A
6	A	911	A

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Mol	Chain	Res	Type
6	A	931	C
6	A	932	A
6	A	957	U
6	A	958	U
6	A	965	A
6	A	966	A
6	A	968	G
6	A	972	A
6	A	973	G
6	A	974	A
6	A	990	G
6	A	991	A
6	A	992	C
6	A	996	C
6	A	1000	A
6	A	1001	A
6	A	1002	A
6	A	1003	C
6	A	1004	U
6	A	1007	C
6	A	1008	C
6	A	1010	G
6	A	1013	A
6	A	1015	G
6	A	1016	G
6	A	1019	U
6	A	1023	G
6	A	1025	C
6	A	1027	U
6	A	1028	C
6	A	1029	G
6	A	1030	G
6	A	1031	G
6	A	1033	A
6	A	1034	U
6	A	1039	A
6	A	1042	C
6	A	1043	A
6	A	1062	U
6	A	1063	C
6	A	1067	U
6	A	1091	G

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Mol	Chain	Res	Type
6	A	1092	U
6	A	1096	G
6	A	1098	A
6	A	1101	G
6	A	1115	U
6	A	1121	C
6	A	1123	U
6	A	1124	G
6	A	1130	A
6	A	1133	U
6	A	1134	C
6	A	1136	G
6	A	1137	A
6	A	1142	A
6	A	1154	A
6	A	1156	U
6	A	1157	G
6	A	1161	G
6	A	1162	U
6	A	1165	C
6	A	1166	A
6	A	1168	A
6	A	1180	C
6	A	1185	A
6	A	1188	A
6	A	1193	A
6	A	1194	A
6	A	1197	C
6	A	1209	U
6	A	1210	A
6	A	1211	C
6	A	1217	G
6	A	1223	C
6	A	1224	A
6	A	1226	A
6	A	1228	G
6	A	1233	A
6	A	1235	A
6	A	1247	A
6	A	1249	A
6	A	1255	G
6	A	1257	U

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Mol	Chain	Res	Type
6	A	1258	A
6	A	1259	C
6	A	1277	A
6	A	1284	A
6	A	1285	A
6	A	1294	G
6	A	1295	U
6	A	1296	A
6	A	1297	G
6	A	1299	C
6	A	1302	G
6	A	1309	G
6	A	1317	C
6	A	1328	G
6	A	1332	U
6	A	1335	G
6	A	1343	A
6	A	1350	G
6	A	1360	A
6	A	1361	U
6	A	1367	G
6	A	1384	G
6	A	1394	C
6	A	1395	A
6	A	1416	G
6	A	1429	G
6	A	1438	A
6	A	1444	A
6	A	1450	A
6	A	1452	G
6	A	1490	A
6	A	1494	G
6	A	1499	A
6	A	1503	U
6	A	1514	G
6	A	1516	MA6
6	A	1517	C
6	A	1526	G
6	A	1527	G
6	A	1530	C
26	V	3	C
26	V	4	G

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Mol	Chain	Res	Type
26	V	7	G
26	V	9	G
26	V	16	C
26	V	17	C
26	V	18	U
26	V	19	G
26	V	20	G
26	V	21	H2U
26	V	22	A
26	V	23	G
26	V	27	G
26	V	32	G
26	V	33	OMC
26	V	34	U
26	V	43	G
26	V	46	G
26	V	47	A
26	V	52	C
26	V	53	G
26	V	54	G
26	V	59	A
26	V	64	G
26	V	65	G
26	V	66	C
26	V	73	A
26	V	75	C
26	V	76	C
26	V	77	A
27	W	7	U
27	W	13	A
29	a	3	U
29	a	15	G
29	a	34	U
29	a	46	G
29	a	51	G
29	a	61	A
29	a	71	A
29	a	74	A
29	a	75	G
29	a	79	C
29	a	82	G
29	a	85	G

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Mol	Chain	Res	Type
29	a	86	G
29	a	88	G
29	a	91	A
29	a	93	A
29	a	94	U
29	a	95	A
29	a	96	U
29	a	97	C
29	a	99	U
29	a	100	U
29	a	102	G
29	a	118	A
29	a	119	A
29	a	120	U
29	a	124	G
29	a	127	A
29	a	140	A
29	a	141	A
29	a	142	G
29	a	143	G
29	a	162	U
29	a	163	A
29	a	178	G
29	a	181	A
29	a	196	A
29	a	199	A
29	a	215	G
29	a	216	A
29	a	222	A
29	a	225	C
29	a	228	U
29	a	229	U
29	a	233	A
29	a	248	G
29	a	255	A
29	a	265	A
29	a	266	G
29	a	268	C
29	a	271	U
29	a	272	U
29	a	276	U
29	a	277	U

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Mol	Chain	Res	Type
29	a	278	A
29	a	282	G
29	a	283	U
29	a	284	G
29	a	286	U
29	a	290	G
29	a	295	A
29	a	296	C
29	a	306	A
29	a	324	G
29	a	325	A
29	a	347	A
29	a	348	C
29	a	349	A
29	a	350	C
29	a	352	U
29	a	359	G
29	a	362	G
29	a	364	G
29	a	378	G
29	a	379	U
29	a	380	G
29	a	388	G
29	a	396	A
29	a	397	U
29	a	403	G
29	a	404	A
29	a	416	G
29	a	447	C
29	a	473	G
29	a	497	A
29	a	500	U
29	a	505	A
29	a	509	C
29	a	519	C
29	a	522	G
29	a	524	A
29	a	535	C
29	a	537	U
29	a	538	C
29	a	541	G
29	a	546	G

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Mol	Chain	Res	Type
29	a	554	A
29	a	564	U
29	a	566	A
29	a	594	A
29	a	605	A
29	a	606	U
29	a	618	A
29	a	619	G
29	a	626	C
29	a	628	A
29	a	630	U
29	a	636	U
29	a	642	G
29	a	644	U
29	a	645	U
29	a	646	A
29	a	647	G
29	a	654	G
29	a	668	A
29	a	677	U
29	a	685	U
29	a	686	G
29	a	712	A
29	a	717	G
29	a	719	G
29	a	721	A
29	a	738	U
29	a	755	A
29	a	756	C
29	a	766	G
29	a	767	G
29	a	769	G
29	a	773	A
29	a	774	A
29	a	775	G
29	a	776	G
29	a	783	A
29	a	785	G
29	a	796	G
29	a	803	C
29	a	810	A
29	a	818	U

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Mol	Chain	Res	Type
29	a	819	U
29	a	821	G
29	a	836	G
29	a	838	A
29	a	848	G
29	a	850	G
29	a	868	U
29	a	869	A
29	a	875	U
29	a	876	C
29	a	877	A
29	a	879	C
29	a	882	G
29	a	884	C
29	a	886	U
29	a	887	A
29	a	888	C
29	a	891	A
29	a	894	C
29	a	898	G
29	a	901	A
29	a	905	C
29	a	916	U
29	a	918	A
29	a	919	G
29	a	922	C
29	a	931	A
29	a	935	A
29	a	936	G
29	a	948	U
29	a	951	C
29	a	964	G
29	a	970	A
29	a	973	A
29	a	974	A
29	a	979	G
29	a	986	A
29	a	1002	U
29	a	1003	C
29	a	1007	G
29	a	1016	G
29	a	1023	U

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Mol	Chain	Res	Type
29	a	1025	U
29	a	1029	A
29	a	1030	A
29	a	1036	A
29	a	1037	G
29	a	1050	U
29	a	1052	G
29	a	1054	C
29	a	1055	U
29	a	1056	U
29	a	1057	A
29	a	1060	A
29	a	1061	G
29	a	1062	C
29	a	1063	A
29	a	1065	C
29	a	1066	C
29	a	1068	C
29	a	1069	C
29	a	1070	C
29	a	1073	U
29	a	1074	A
29	a	1075	A
29	a	1076	A
29	a	1077	G
29	a	1078	A
29	a	1079	A
29	a	1080	A
29	a	1084	U
29	a	1085	A
29	a	1087	U
29	a	1091	U
29	a	1094	C
29	a	1095	U
29	a	1096	A
29	a	1100	G
29	a	1101	A
29	a	1102	G
29	a	1106	G
29	a	1112	G
29	a	1122	U
29	a	1123	A

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Mol	Chain	Res	Type
29	a	1124	A
29	a	1125	C
29	a	1126	G
29	a	1133	A
29	a	1142	G
29	a	1163	U
29	a	1164	U
29	a	1165	U
29	a	1166	G
29	a	1168	A
29	a	1193	A
29	a	1194	G
29	a	1235	A
29	a	1238	G
29	a	1241	A
29	a	1244	G
29	a	1259	G
29	a	1260	A
29	a	1263	A
29	a	1289	A
29	a	1290	A
29	a	1294	C
29	a	1302	C
29	a	1317	U
29	a	1329	G
29	a	1331	G
29	a	1333	C
29	a	1340	U
29	a	1347	A
29	a	1353	A
29	a	1356	G
29	a	1366	A
29	a	1367	U
29	a	1371	A
29	a	1383	A
29	a	1404	G
29	a	1408	U
29	a	1413	G
29	a	1416	C
29	a	1420	G
29	a	1421	A
29	a	1423	G

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Mol	Chain	Res	Type
29	a	1425	C
29	a	1426	U
29	a	1428	A
29	a	1436	U
29	a	1439	C
29	a	1440	G
29	a	1441	U
29	a	1447	G
29	a	1454	U
29	a	1455	G
29	a	1463	G
29	a	1467	G
29	a	1470	U
29	a	1478	A
29	a	1481	C
29	a	1485	U
29	a	1489	G
29	a	1497	U
29	a	1498	A
29	a	1508	C
29	a	1513	A
29	a	1516	A
29	a	1519	C
29	a	1521	G
29	a	1522	U
29	a	1523	A
29	a	1524	C
29	a	1525	U
29	a	1526	U
29	a	1527	G
29	a	1530	C
29	a	1533	C
29	a	1536	A
29	a	1538	U
29	a	1539	G
29	a	1540	G
29	a	1551	G
29	a	1557	A
29	a	1560	A
29	a	1574	U
29	a	1575	U
29	a	1576	C

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Mol	Chain	Res	Type
29	a	1598	G
29	a	1599	A
29	a	1604	G
29	a	1609	A
29	a	1637	C
29	a	1638	U
29	a	1639	U
29	a	1644	G
29	a	1658	G
29	a	1665	G
29	a	1666	C
29	a	1683	U
29	a	1684	U
29	a	1706	U
29	a	1707	G
29	a	1708	G
29	a	1710	G
29	a	1718	U
29	a	1719	C
29	a	1725	C
29	a	1726	U
29	a	1727	G
29	a	1732	G
29	a	1739	G
29	a	1745	G
29	a	1753	G
29	a	1762	A
29	a	1768	U
29	a	1769	A
29	a	1771	U
29	a	1773	A
29	a	1777	C
29	a	1789	C
29	a	1790	A
29	a	1791	A
29	a	1798	A
29	a	1800	G
29	a	1805	C
29	a	1818	A
29	a	1824	G
29	a	1836	A
29	a	1837	A

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Mol	Chain	Res	Type
29	a	1838	G
29	a	1846	G
29	a	1855	A
29	a	1858	G
29	a	1862	G
29	a	1878	A
29	a	1879	A
29	a	1888	A
29	a	1890	A
29	a	1892	G
29	a	1896	G
29	a	1902	A
29	a	1903	C
29	a	1908	A
29	a	1918	G
29	a	1919	G
29	a	1926	A
29	a	1929	U
29	a	1943	G
29	a	1944	U
29	a	1951	C
29	a	1953	G
29	a	1956	C
29	a	1959	A
29	a	1960	U
29	a	1961	G
29	a	1971	U
29	a	1980	U
29	a	1981	G
29	a	1982	U
29	a	1986	C
29	a	2010	A
29	a	2011	U
29	a	2012	C
29	a	2019	6MZ
29	a	2020	A
29	a	2021	G
29	a	2022	A
29	a	2024	G
29	a	2025	C
29	a	2027	G
29	a	2032	C

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Mol	Chain	Res	Type
29	a	2044	C
29	a	2045	G
29	a	2049	A
29	a	2050	G
29	a	2051	A
29	a	2058	G7M
29	a	2082	G
29	a	2089	G
29	a	2093	U
29	a	2098	U
29	a	2100	U
29	a	2101	G
29	a	2105	G
29	a	2106	A
29	a	2107	U
29	a	2110	G
29	a	2111	U
29	a	2112	G
29	a	2121	U
29	a	2122	G
29	a	2123	A
29	a	2126	C
29	a	2128	G
29	a	2131	A
29	a	2134	C
29	a	2135	U
29	a	2146	G
29	a	2147	A
29	a	2151	G
29	a	2155	U
29	a	2167	C
29	a	2171	G
29	a	2174	A
29	a	2178	U
29	a	2179	G
29	a	2182	G
29	a	2187	A
29	a	2193	G
29	a	2201	A
29	a	2214	A
29	a	2227	G
29	a	2257	A

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Mol	Chain	Res	Type
29	a	2262	A
29	a	2267	A
29	a	2272	U
29	a	2276	A
29	a	2277	A
29	a	2293	G
29	a	2294	U
29	a	2297	G
29	a	2300	A
29	a	2301	U
29	a	2307	G
29	a	2308	U
29	a	2314	A
29	a	2316	A
29	a	2325	A
29	a	2334	A
29	a	2339	C
29	a	2343	A
29	a	2348	C
29	a	2350	A
29	a	2361	U
29	a	2362	A
29	a	2371	G
29	a	2372	G
29	a	2373	U
29	a	2374	C
29	a	2385	G
29	a	2391	U
29	a	2392	C
29	a	2394	G
29	a	2395	U
29	a	2396	A
29	a	2409	C
29	a	2411	C
29	a	2412	U
29	a	2414	A
29	a	2417	G
29	a	2418	G
29	a	2419	A
29	a	2421	A
29	a	2429	C
29	a	2430	U

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Mol	Chain	Res	Type
29	a	2436	G
29	a	2437	A
29	a	2438	H2U
29	a	2439	A
29	a	2448	A
29	a	2466	U
29	a	2476	G
29	a	2483	G
29	a	2487	OMC
29	a	2491	G
29	a	2492	2MA
29	a	2494	G
29	a	2495	U
29	a	2507	A
29	a	2509	C
29	a	2518	G
29	a	2523	A
29	a	2536	A
29	a	2541	OMU
29	a	2543	U
29	a	2555	A
29	a	2556	G
29	a	2562	C
29	a	2567	G
29	a	2591	A
29	a	2592	G
29	a	2598	U
29	a	2599	C
29	a	2602	U
29	a	2604	U
29	a	2618	U
29	a	2629	G
29	a	2635	C
29	a	2643	A
29	a	2650	G
29	a	2654	A
29	a	2678	U
29	a	2679	A
29	a	2703	G
29	a	2715	U
29	a	2722	A
29	a	2724	G

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Mol	Chain	Res	Type
29	a	2728	U
29	a	2737	A
29	a	2746	A
29	a	2750	G
29	a	2754	A
29	a	2755	G
29	a	2767	A
29	a	2769	A
29	a	2770	A
29	a	2780	A
29	a	2786	U
29	a	2787	U
29	a	2789	U
29	a	2793	C
29	a	2797	A
29	a	2807	U
29	a	2809	G
29	a	2810	A
29	a	2822	U
29	a	2824	A
29	a	2825	U
29	a	2838	G
29	a	2844	U
29	a	2845	A
29	a	2850	U
29	a	2856	A
29	a	2861	G
29	a	2862	A
29	a	2868	A
29	a	2872	A
29	a	2873	U
29	a	2874	U
29	a	2882	A
29	a	2883	G
30	b	7	G
30	b	11	A
30	b	14	G
30	b	18	G
30	b	22	G
30	b	39	C
30	b	42	G
30	b	54	G

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Mol	Chain	Res	Type
30	b	59	C
30	b	86	U
30	b	87	A
30	b	106	A
30	b	109	G

All (13) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	A	139	U
6	A	185	C
6	A	492	A
6	A	618	A
6	A	775	G
6	A	876	C
6	A	905	A
6	A	989	U
6	A	1123	U
6	A	1179	G
6	A	1187	G
6	A	1449	A
26	V	20	G

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

39 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	$\#\|Z\| > 2$
17	D2T	L	89	17	7,9,10	1.28	1 (14%)	6,11,13	1.58	1 (16%)
6	4OC	A	1399	6	20,23,24	2.23	3 (15%)	26,32,35	1.03	2 (7%)
32	MEQ	d	153	32	8,9,10	0.87	0	5,10,12	0.55	0
6	5MC	A	964	6	18,22,23	1.88	6 (33%)	26,32,35	1.33	2 (7%)
6	MA6	A	1516	6	23,26,27	1.19	3 (13%)	34,38,41	2.25	9 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	4SU	V	8	26	18,21,22	3.75	8 (44%)	26,30,33	2.13	5 (19%)
26	OMC	V	33	26	19,22,23	1.76	3 (15%)	26,31,34	0.89	1 (3%)
29	PSU	a	1900	29	18,21,22	1.99	7 (38%)	22,30,33	1.84	3 (13%)
40	4D4	l	82	40	9,11,12	0.81	0	8,13,15	1.69	2 (25%)
16	IAS	K	118	16	6,7,8	1.79	1 (16%)	6,8,10	2.51	1 (16%)
29	H2U	a	2438	29	18,21,22	4.15	5 (27%)	21,30,33	5.13	7 (33%)
29	PSU	a	1906	29	18,21,22	2.02	7 (38%)	22,30,33	1.85	4 (18%)
26	5MU	V	55	26	19,22,23	2.35	7 (36%)	28,32,35	3.75	10 (35%)
6	2MG	A	1204	6,55	23,26,27	2.56	4 (17%)	32,38,41	2.13	10 (31%)
29	1MG	a	736	29	22,26,27	2.50	5 (22%)	33,39,42	2.02	7 (21%)
29	2MG	a	2434	29	23,26,27	2.59	6 (26%)	32,38,41	2.06	11 (34%)
6	UR3	A	1495	6	19,22,23	2.55	6 (31%)	26,32,35	1.30	2 (7%)
6	G7M	A	524	6,55	23,26,27	2.17	5 (21%)	35,39,42	1.84	7 (20%)
6	2MG	A	1513	6	23,26,27	2.57	6 (26%)	32,38,41	2.13	12 (37%)
29	PSU	a	945	29	18,21,22	2.06	7 (38%)	22,30,33	1.84	4 (18%)
29	PSU	a	737	57,29	18,21,22	2.07	7 (38%)	22,30,33	1.84	3 (13%)
29	G7M	a	2058	29	23,26,27	2.17	5 (21%)	35,39,42	1.89	7 (20%)
29	PSU	a	2446	29	18,21,22	2.14	7 (38%)	22,30,33	1.84	5 (22%)
29	3TD	a	1904	29	18,22,23	2.72	7 (38%)	22,32,35	1.71	2 (9%)
6	MA6	A	1515	6	23,26,27	1.19	3 (13%)	34,38,41	2.23	9 (26%)
26	H2U	V	21	26	18,21,22	4.37	5 (27%)	21,30,33	4.73	7 (33%)
29	PSU	a	2569	29	18,21,22	2.13	8 (44%)	22,30,33	1.96	5 (22%)
40	MS6	l	83	40	5,7,8	0.57	0	2,7,9	1.83	1 (50%)
26	PSU	V	56	26	18,21,22	1.94	7 (38%)	22,30,33	1.80	3 (13%)
29	OMC	a	2487	57,29	19,22,23	1.77	3 (15%)	26,31,34	1.02	2 (7%)
29	PSU	a	2493	55,29	18,21,22	2.07	7 (38%)	22,30,33	1.79	4 (18%)
29	OMU	a	2541	29	19,22,23	2.62	7 (36%)	26,31,34	1.75	5 (19%)
29	6MZ	a	2019	29	22,25,26	2.33	3 (13%)	30,36,39	2.43	10 (33%)
29	OMG	a	2240	55,29	23,26,27	2.35	6 (26%)	33,38,41	1.88	10 (30%)
6	2MG	A	963	6	23,26,27	2.56	4 (17%)	32,38,41	2.09	10 (31%)
6	PSU	A	513	6	18,21,22	2.02	8 (44%)	22,30,33	1.85	4 (18%)
29	2MA	a	2492	55,29	22,25,26	1.35	3 (13%)	33,37,40	2.04	7 (21%)
29	PSU	a	2594	29	18,21,22	2.08	7 (38%)	22,30,33	1.91	3 (13%)
29	5MU	a	1928	55,29	19,22,23	2.51	7 (36%)	28,32,35	3.77	10 (35%)

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
17	D2T	L	89	17	-	4/7/12/14	-
6	4OC	A	1399	6	-	0/9/29/30	0/2/2/2
32	MEQ	d	153	32	-	3/8/9/11	-
6	5MC	A	964	6	-	0/7/25/26	0/2/2/2
6	MA6	A	1516	6	-	2/11/29/30	0/3/3/3
26	4SU	V	8	26	-	0/7/25/26	0/2/2/2
26	OMC	V	33	26	-	0/9/27/28	0/2/2/2
29	PSU	a	1900	29	-	0/7/25/26	0/2/2/2
40	4D4	l	82	40	-	0/11/12/14	-
16	IAS	K	118	16	-	2/7/7/8	-
29	H2U	a	2438	29	-	4/7/38/39	0/2/2/2
29	PSU	a	1906	29	-	0/7/25/26	0/2/2/2
26	5MU	V	55	26	-	0/7/25/26	0/2/2/2
6	2MG	A	1204	6,55	-	2/9/27/28	0/3/3/3
29	1MG	a	736	29	-	0/7/25/26	0/3/3/3
29	2MG	a	2434	29	-	1/9/27/28	0/3/3/3
6	UR3	A	1495	6	-	0/7/25/26	0/2/2/2
6	G7M	A	524	6,55	-	3/7/25/26	0/3/3/3
6	2MG	A	1513	6	-	0/9/27/28	0/3/3/3
29	PSU	a	945	29	-	0/7/25/26	0/2/2/2
29	PSU	a	737	57,29	-	1/7/25/26	0/2/2/2
29	G7M	a	2058	29	-	2/7/25/26	0/3/3/3
29	PSU	a	2446	29	-	0/7/25/26	0/2/2/2
29	3TD	a	1904	29	-	0/7/25/26	0/2/2/2
6	MA6	A	1515	6	-	0/11/29/30	0/3/3/3
26	H2U	V	21	26	-	4/7/38/39	0/2/2/2
29	PSU	a	2569	29	-	0/7/25/26	0/2/2/2
40	MS6	l	83	40	-	2/4/6/8	-
26	PSU	V	56	26	-	0/7/25/26	0/2/2/2
29	OMC	a	2487	57,29	-	0/9/27/28	0/2/2/2
29	PSU	a	2493	55,29	-	2/7/25/26	0/2/2/2
29	OMU	a	2541	29	-	2/9/27/28	0/2/2/2
29	6MZ	a	2019	29	-	2/9/27/28	0/3/3/3
29	OMG	a	2240	55,29	-	1/9/27/28	0/3/3/3
6	2MG	A	963	6	-	0/9/27/28	0/3/3/3
6	PSU	A	513	6	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	2MA	a	2492	55,29	-	3/7/25/26	0/3/3/3
29	PSU	a	2594	29	-	0/7/25/26	0/2/2/2
29	5MU	a	1928	55,29	-	0/7/25/26	0/2/2/2

All (194) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	V	21	H2U	O4-C4	10.25	1.44	1.23
29	a	2438	H2U	O4-C4	9.92	1.43	1.23
29	a	2019	6MZ	C6-N6	9.58	1.44	1.34
6	A	1204	2MG	O6-C6	9.15	1.41	1.23
6	A	1513	2MG	O6-C6	9.07	1.40	1.23
6	A	963	2MG	O6-C6	9.03	1.40	1.23
29	a	2434	2MG	O6-C6	8.99	1.40	1.23
26	V	21	H2U	C2-N1	8.88	1.48	1.35
6	A	1495	UR3	O4-C4	8.72	1.42	1.23
26	V	21	H2U	O2-C2	8.54	1.38	1.23
29	a	2240	OMG	O6-C6	8.41	1.39	1.23
29	a	2438	H2U	C2-N1	8.33	1.47	1.35
29	a	2438	H2U	O2-C2	8.22	1.38	1.23
29	a	1904	3TD	O4-C4	8.22	1.40	1.23
29	a	2541	OMU	O4-C4	8.01	1.40	1.24
29	a	2058	G7M	O6-C6	8.00	1.38	1.23
29	a	736	1MG	O6-C6	7.99	1.40	1.23
6	A	524	G7M	O6-C6	7.96	1.38	1.23
26	V	8	4SU	C4-N3	7.75	1.45	1.37
26	V	21	H2U	C2-N3	7.42	1.51	1.38
26	V	8	4SU	C2-N3	7.20	1.50	1.38
29	a	2438	H2U	C2-N3	6.90	1.50	1.38
26	V	8	4SU	C4-S4	-6.74	1.55	1.68
6	A	1399	4OC	O2-C2	6.53	1.35	1.23
29	a	1928	5MU	C2-N1	-6.10	1.28	1.38
29	a	736	1MG	C2-N2	6.04	1.45	1.34
6	A	963	2MG	C2-N2	6.01	1.46	1.33
6	A	1204	2MG	C2-N2	5.95	1.46	1.33
6	A	1513	2MG	C2-N2	5.92	1.46	1.33
29	a	2434	2MG	C2-N2	5.84	1.46	1.33
6	A	1399	4OC	C4-N4	5.50	1.47	1.35
26	V	55	5MU	C2-N1	-5.45	1.29	1.38
26	V	21	H2U	C4-N3	5.41	1.46	1.37
26	V	8	4SU	C6-C5	5.06	1.46	1.35
29	a	2438	H2U	C4-N3	4.99	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	V	33	OMC	C4-N4	4.98	1.45	1.33
26	V	8	4SU	C2-N1	4.95	1.46	1.38
29	a	1928	5MU	C2-N3	-4.78	1.29	1.38
29	a	2487	OMC	C4-N4	4.74	1.45	1.33
26	V	55	5MU	C2-N3	-4.50	1.29	1.38
29	a	2492	2MA	C6-N6	4.46	1.45	1.34
29	a	1928	5MU	C6-N1	-4.29	1.30	1.38
6	A	964	5MC	C4-N4	4.16	1.44	1.34
29	a	2240	OMG	C2-N2	4.14	1.44	1.34
26	V	55	5MU	C6-N1	-4.13	1.31	1.38
26	V	33	OMC	C2-N1	-4.06	1.31	1.40
29	a	2541	OMU	C2-N1	-4.05	1.32	1.38
29	a	2446	PSU	C4-N3	-4.03	1.31	1.38
29	a	2487	OMC	C2-N1	-4.03	1.31	1.40
26	V	8	4SU	C5-C4	4.02	1.47	1.42
26	V	8	4SU	C6-N1	4.00	1.47	1.38
29	a	2569	PSU	C2-N1	-3.96	1.31	1.36
29	a	1904	3TD	C2-N1	-3.93	1.32	1.37
29	a	736	1MG	C6-N1	-3.89	1.32	1.40
29	a	2240	OMG	C6-N1	-3.87	1.31	1.38
29	a	2594	PSU	C4-N3	-3.85	1.31	1.38
29	a	945	PSU	C4-N3	-3.78	1.31	1.38
29	a	2446	PSU	C2-N1	-3.76	1.31	1.36
6	A	513	PSU	C2-N1	-3.76	1.31	1.36
29	a	1904	3TD	C4-N3	-3.75	1.32	1.40
29	a	737	PSU	C4-N3	-3.74	1.31	1.38
29	a	2493	PSU	C4-N3	-3.74	1.31	1.38
6	A	964	5MC	C2-N1	-3.73	1.31	1.40
29	a	2541	OMU	C4-N3	-3.70	1.31	1.38
29	a	2569	PSU	C4-N3	-3.69	1.32	1.38
29	a	2493	PSU	C2-N1	-3.68	1.31	1.36
29	a	737	PSU	C2-N1	-3.66	1.31	1.36
29	a	2594	PSU	C2-N1	-3.65	1.31	1.36
26	V	55	5MU	C6-C5	3.64	1.40	1.34
29	a	1906	PSU	C4-N3	-3.64	1.32	1.38
6	A	1495	UR3	C4-N3	-3.64	1.32	1.40
16	K	118	IAS	OD1-CG	3.63	1.40	1.19
29	a	2446	PSU	C2-N3	-3.61	1.31	1.37
29	a	945	PSU	C2-N1	-3.61	1.31	1.36
29	a	1928	5MU	C6-C5	3.60	1.40	1.34
29	a	1900	PSU	C4-N3	-3.60	1.32	1.38
29	a	2541	OMU	C2-N3	-3.58	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1399	4OC	C2-N1	-3.57	1.32	1.40
26	V	8	4SU	O2-C2	-3.54	1.16	1.23
29	a	2594	PSU	C2-N3	-3.53	1.31	1.37
29	a	1906	PSU	C2-N1	-3.52	1.32	1.36
29	a	1900	PSU	C2-N1	-3.51	1.32	1.36
26	V	56	PSU	C4-N3	-3.50	1.32	1.38
6	A	513	PSU	C4-N3	-3.48	1.32	1.38
29	a	2493	PSU	C2-N3	-3.46	1.31	1.37
29	a	737	PSU	C2-N3	-3.45	1.31	1.37
6	A	524	G7M	C5-N7	-3.45	1.35	1.39
29	a	945	PSU	C2-N3	-3.44	1.31	1.37
29	a	2569	PSU	C2-N3	-3.40	1.31	1.37
29	a	2058	G7M	C5-N7	-3.38	1.35	1.39
26	V	56	PSU	C6-C5	3.37	1.39	1.35
6	A	1516	MA6	C6-N6	3.37	1.46	1.36
29	a	1906	PSU	C2-N3	-3.35	1.31	1.37
29	a	1928	5MU	C4-N3	-3.35	1.32	1.38
6	A	1515	MA6	C6-N6	3.33	1.46	1.36
29	a	1900	PSU	C2-N3	-3.31	1.31	1.37
6	A	524	G7M	C6-N1	-3.30	1.32	1.38
26	V	56	PSU	C2-N1	-3.28	1.32	1.36
6	A	513	PSU	C2-N3	-3.24	1.31	1.37
29	a	1904	3TD	C6-C5	3.24	1.39	1.35
6	A	524	G7M	C2-N2	3.22	1.41	1.34
29	a	2058	G7M	C6-N1	-3.22	1.32	1.38
6	A	1515	MA6	C8-N9	-3.14	1.31	1.37
26	V	55	5MU	C4-N3	-3.14	1.33	1.38
26	V	56	PSU	C2-N3	-3.14	1.32	1.37
29	a	2493	PSU	C6-C5	3.12	1.39	1.35
6	A	1516	MA6	C8-N9	-3.12	1.31	1.37
29	a	2019	6MZ	C8-N9	-3.10	1.32	1.37
29	a	1900	PSU	C6-C5	3.10	1.38	1.35
29	a	1906	PSU	C6-C5	3.10	1.38	1.35
29	a	2058	G7M	C2-N2	3.08	1.41	1.34
6	A	1495	UR3	C2-N3	-3.08	1.33	1.39
6	A	964	5MC	C6-N1	-3.03	1.32	1.38
29	a	2446	PSU	C6-C5	3.02	1.38	1.35
29	a	2594	PSU	C6-C5	3.02	1.38	1.35
29	a	945	PSU	C6-C5	3.00	1.38	1.35
6	A	1495	UR3	C2-N1	-2.97	1.34	1.38
29	a	2434	2MG	C6-N1	-2.96	1.33	1.38
29	a	737	PSU	C6-C5	2.96	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	1904	3TD	C2-N3	-2.94	1.32	1.38
6	A	963	2MG	C6-N1	-2.93	1.33	1.38
6	A	513	PSU	C6-C5	2.91	1.38	1.35
6	A	1513	2MG	C6-N1	-2.86	1.33	1.38
6	A	1204	2MG	C6-N1	-2.85	1.33	1.38
29	a	2434	2MG	C5-N7	-2.83	1.33	1.39
29	a	2240	OMG	C8-N9	-2.81	1.31	1.37
6	A	964	5MC	O2-C2	-2.80	1.18	1.23
29	a	1928	5MU	O4-C4	-2.79	1.18	1.23
29	a	2569	PSU	C6-C5	2.78	1.38	1.35
6	A	1204	2MG	C5-N7	-2.78	1.33	1.39
29	a	2594	PSU	O4-C4	-2.76	1.18	1.23
6	A	963	2MG	C5-N7	-2.75	1.33	1.39
29	a	2446	PSU	O4-C4	-2.75	1.18	1.23
29	a	945	PSU	O4-C4	-2.73	1.18	1.23
29	a	1906	PSU	O4-C4	-2.70	1.18	1.23
29	a	2493	PSU	O4-C4	-2.69	1.18	1.23
29	a	2569	PSU	C6-N1	-2.66	1.31	1.36
6	A	964	5MC	C6-C5	2.66	1.39	1.34
29	a	2569	PSU	O4-C4	-2.65	1.18	1.23
29	a	737	PSU	C6-N1	-2.62	1.31	1.36
29	a	2019	6MZ	C5-N7	-2.60	1.34	1.39
6	A	513	PSU	O4-C4	-2.60	1.18	1.23
29	a	2541	OMU	O2-C2	-2.59	1.18	1.23
6	A	1513	2MG	C5-N7	-2.59	1.34	1.39
29	a	737	PSU	O4-C4	-2.57	1.18	1.23
29	a	1900	PSU	O4-C4	-2.57	1.18	1.23
29	a	2594	PSU	C6-N1	-2.56	1.32	1.36
26	V	55	5MU	O4-C4	-2.55	1.18	1.23
26	V	56	PSU	O4-C4	-2.55	1.18	1.23
29	a	945	PSU	C6-N1	-2.54	1.32	1.36
29	a	2569	PSU	O4'-C1'	-2.53	1.40	1.43
29	a	2240	OMG	C5-N7	-2.51	1.34	1.39
29	a	2541	OMU	C6-N1	-2.50	1.31	1.38
29	a	736	1MG	C8-N9	-2.50	1.32	1.37
29	a	1928	5MU	O2-C2	-2.48	1.18	1.23
29	a	2446	PSU	C6-N1	-2.47	1.32	1.36
29	a	2446	PSU	O2-C2	-2.44	1.18	1.23
6	A	513	PSU	C6-N1	-2.44	1.32	1.36
29	a	2493	PSU	C6-N1	-2.42	1.32	1.36
29	a	736	1MG	C5-N7	-2.40	1.34	1.39
29	a	2569	PSU	O2-C2	-2.39	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	2058	G7M	C2-N1	-2.39	1.31	1.37
6	A	524	G7M	C2-N1	-2.39	1.31	1.37
29	a	1904	3TD	C6-N1	-2.38	1.32	1.36
29	a	945	PSU	O2-C2	-2.37	1.18	1.23
29	a	2594	PSU	O2-C2	-2.36	1.18	1.23
29	a	1906	PSU	C6-N1	-2.35	1.32	1.36
29	a	2493	PSU	O2-C2	-2.34	1.18	1.23
29	a	2541	OMU	C5-C4	-2.33	1.38	1.43
29	a	1900	PSU	C6-N1	-2.33	1.32	1.36
29	a	1904	3TD	O2-C2	-2.32	1.18	1.23
6	A	1495	UR3	O2-C2	2.32	1.26	1.22
6	A	513	PSU	O2-C2	-2.27	1.18	1.23
26	V	56	PSU	C6-N1	-2.27	1.32	1.36
29	a	1906	PSU	O2-C2	-2.27	1.18	1.23
29	a	1900	PSU	O2-C2	-2.27	1.18	1.23
29	a	737	PSU	O2-C2	-2.26	1.18	1.23
29	a	2434	2MG	C4-N9	-2.25	1.32	1.38
26	V	55	5MU	O2-C2	-2.23	1.19	1.23
6	A	1513	2MG	C4-N9	-2.23	1.32	1.38
29	a	2487	OMC	C5-C4	-2.20	1.37	1.42
6	A	1495	UR3	C6-N1	-2.18	1.32	1.38
29	a	2240	OMG	C2-N1	-2.18	1.32	1.37
26	V	56	PSU	O2-C2	-2.13	1.18	1.23
6	A	513	PSU	O4'-C1'	-2.11	1.40	1.43
6	A	1515	MA6	C5-N7	-2.08	1.35	1.39
6	A	1516	MA6	C5-N7	-2.08	1.35	1.39
29	a	2434	2MG	CM2-N2	-2.05	1.41	1.45
26	V	33	OMC	C6-C5	2.04	1.39	1.35
6	A	1513	2MG	CM2-N2	-2.04	1.42	1.45
17	L	89	D2T	CB-CG	2.03	1.55	1.52
6	A	964	5MC	C2-N3	-2.02	1.32	1.36
29	a	2492	2MA	C5-N7	-2.02	1.35	1.39
29	a	2492	2MA	C8-N9	-2.01	1.33	1.37

All (207) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	a	2438	H2U	C4-N3-C2	-15.73	112.74	125.79
26	V	21	H2U	C4-N3-C2	-12.97	115.03	125.79
26	V	21	H2U	O2-C2-N1	-11.52	108.64	123.11
29	a	2438	H2U	O2-C2-N1	-10.64	109.75	123.11
29	a	1928	5MU	C4-N3-C2	-8.75	116.02	127.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	V	55	5MU	C5M-C5-C4	8.60	128.23	118.77
29	a	1928	5MU	N3-C2-N1	8.43	126.08	114.89
26	V	55	5MU	C4-N3-C2	-8.26	116.65	127.35
26	V	55	5MU	N3-C2-N1	8.08	125.61	114.89
29	a	1928	5MU	C5-C6-N1	-7.77	115.35	123.34
29	a	1928	5MU	C5M-C5-C4	7.71	127.25	118.77
29	a	2438	H2U	O4-C4-N3	-7.65	108.15	120.28
26	V	8	4SU	C4-N3-C2	-7.33	120.22	127.34
6	A	1204	2MG	C2-N3-C4	7.33	121.13	112.04
26	V	21	H2U	O2-C2-N3	-7.31	107.89	121.50
6	A	1513	2MG	C2-N3-C4	7.22	120.99	112.04
29	a	2492	2MA	C5-C4-N3	-7.17	119.12	127.19
6	A	963	2MG	C2-N3-C4	7.17	120.92	112.04
26	V	55	5MU	C5-C6-N1	-7.11	116.02	123.34
29	a	2434	2MG	C2-N3-C4	7.10	120.84	112.04
26	V	21	H2U	O4-C4-N3	-7.09	109.04	120.28
29	a	736	1MG	C5-C4-N3	-6.95	117.19	128.46
26	V	55	5MU	C5M-C5-C6	-6.76	113.83	122.85
29	a	1904	3TD	N1-C2-N3	6.59	121.34	116.14
29	a	1928	5MU	C5-C4-N3	6.55	120.90	115.31
29	a	2438	H2U	O2-C2-N3	-6.45	109.48	121.50
26	V	21	H2U	O4-C4-C5	-6.44	108.41	122.17
29	a	2438	H2U	O4-C4-C5	-6.38	108.54	122.17
29	a	2438	H2U	N3-C2-N1	-6.20	110.10	116.65
26	V	55	5MU	C5-C4-N3	6.13	120.54	115.31
29	a	1928	5MU	C5M-C5-C6	-6.12	114.67	122.85
29	a	2019	6MZ	C9-N6-C6	-6.07	117.64	122.87
6	A	1516	MA6	C5-C4-N3	-5.84	119.13	126.75
29	a	2569	PSU	N1-C2-N3	5.77	121.67	115.13
29	a	2594	PSU	N1-C2-N3	5.77	121.67	115.13
29	a	737	PSU	N1-C2-N3	5.77	121.66	115.13
29	a	2446	PSU	N1-C2-N3	5.67	121.55	115.13
6	A	1515	MA6	C5-C4-N3	-5.63	119.41	126.75
29	a	945	PSU	N1-C2-N3	5.61	121.49	115.13
29	a	1900	PSU	N1-C2-N3	5.54	121.41	115.13
29	a	1906	PSU	N1-C2-N3	5.52	121.39	115.13
26	V	56	PSU	N1-C2-N3	5.50	121.36	115.13
16	K	118	IAS	OD1-CG-CB	-5.49	109.44	125.43
29	a	2541	OMU	N3-C2-N1	5.45	122.12	114.89
29	a	2240	OMG	C5-C4-N3	-5.43	119.65	128.46
6	A	1204	2MG	C5-C4-N3	-5.41	119.68	128.46
29	a	2493	PSU	N1-C2-N3	5.39	121.24	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	513	PSU	N1-C2-N3	5.34	121.18	115.13
29	a	2058	G7M	C2-N3-C4	5.28	121.70	112.30
6	A	524	G7M	C2-N3-C4	5.25	121.65	112.30
6	A	964	5MC	C5-C6-N1	-5.24	117.94	123.34
6	A	963	2MG	C5-C4-N3	-5.20	120.03	128.46
29	a	2492	2MA	N3-C4-N9	5.16	134.15	126.99
29	a	736	1MG	C2-N3-C4	5.14	123.53	111.98
26	V	8	4SU	C5-C4-N3	5.09	119.41	114.69
29	a	2019	6MZ	N1-C2-N3	-4.96	120.84	128.60
6	A	1516	MA6	N1-C2-N3	-4.96	120.85	128.60
6	A	1515	MA6	N1-C2-N3	-4.92	120.91	128.60
29	a	2019	6MZ	C5-C4-N3	-4.86	120.41	126.75
29	a	736	1MG	N9-C4-N3	4.83	135.65	125.94
6	A	524	G7M	C5-C4-N3	-4.79	118.97	128.15
29	a	2434	2MG	C5-C4-N3	-4.76	120.74	128.46
6	A	1513	2MG	C5-C4-N3	-4.75	120.75	128.46
6	A	1495	UR3	C4-N3-C2	-4.62	120.21	124.56
29	a	2240	OMG	C2-N3-C4	4.60	120.50	112.30
6	A	1516	MA6	N3-C4-N9	4.49	134.48	127.08
6	A	1515	MA6	N3-C4-N9	4.43	134.39	127.08
29	a	2058	G7M	C5-C4-N3	-4.31	119.89	128.15
6	A	1516	MA6	C2-N3-C4	4.26	121.80	111.75
6	A	524	G7M	C5-C6-N1	4.22	120.61	111.79
29	a	2058	G7M	C5-C6-N1	4.21	120.58	111.79
6	A	1515	MA6	C2-N1-C6	4.20	121.68	111.75
29	a	2541	OMU	C4-N3-C2	-4.19	121.06	126.58
29	a	1928	5MU	O2-C2-N1	-4.16	117.26	122.79
6	A	1515	MA6	C2-N3-C4	4.14	121.52	111.75
6	A	1516	MA6	C2-N1-C6	4.11	121.46	111.75
29	a	2058	G7M	C6-C5-N7	4.11	137.21	132.25
29	a	2019	6MZ	C6-C5-N7	3.99	136.71	132.39
29	a	2594	PSU	C4-N3-C2	-3.98	120.60	126.34
29	a	2240	OMG	N9-C4-N3	3.96	133.88	125.94
26	V	55	5MU	O4-C4-N3	-3.93	112.58	120.12
6	A	524	G7M	N9-C4-N3	3.87	133.71	125.94
29	a	2019	6MZ	C2-N3-C4	3.85	120.83	111.75
26	V	8	4SU	N3-C2-N1	3.82	119.96	114.89
29	a	1928	5MU	O4-C4-N3	-3.81	112.81	120.12
29	a	737	PSU	C4-N3-C2	-3.75	120.94	126.34
29	a	1900	PSU	C4-N3-C2	-3.70	121.01	126.34
29	a	1906	PSU	C4-N3-C2	-3.69	121.02	126.34
6	A	1515	MA6	N9-C8-N7	-3.68	108.88	113.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	963	2MG	N9-C4-N3	3.61	133.19	125.94
26	V	56	PSU	C4-N3-C2	-3.60	121.15	126.34
29	a	945	PSU	C4-N3-C2	-3.60	121.15	126.34
6	A	1516	MA6	N9-C8-N7	-3.59	109.00	113.91
29	a	2569	PSU	C4-N3-C2	-3.59	121.17	126.34
26	V	21	H2U	N3-C2-N1	-3.58	112.86	116.65
6	A	1204	2MG	N9-C4-N3	3.56	133.08	125.94
6	A	513	PSU	C4-N3-C2	-3.51	121.28	126.34
29	a	2019	6MZ	C5-N7-C8	3.49	108.46	103.51
6	A	1515	MA6	C4-N9-C8	3.47	109.49	105.73
29	a	2569	PSU	O2-C2-N1	-3.47	118.97	122.79
6	A	1515	MA6	C5-N7-C8	3.46	108.43	103.51
6	A	1516	MA6	C5-N7-C8	3.46	108.42	103.51
29	a	2493	PSU	C4-N3-C2	-3.44	121.38	126.34
29	a	2446	PSU	C4-N3-C2	-3.44	121.39	126.34
6	A	1513	2MG	C6-C5-N7	3.43	136.63	130.25
29	a	2058	G7M	O6-C6-C5	-3.42	120.34	128.06
29	a	2019	6MZ	C4-C5-N7	-3.42	106.46	110.62
6	A	524	G7M	O6-C6-C5	-3.38	120.43	128.06
6	A	513	PSU	O2-C2-N1	-3.34	119.11	122.79
29	a	737	PSU	O2-C2-N1	-3.32	119.13	122.79
40	l	82	4D4	NE-CZ-NH2	3.30	126.50	120.70
29	a	2019	6MZ	N9-C8-N7	-3.24	109.48	113.91
29	a	2434	2MG	N9-C4-N3	3.24	132.44	125.94
6	A	1516	MA6	C4-N9-C8	3.23	109.23	105.73
29	a	2058	G7M	N9-C4-N3	3.19	132.35	125.94
29	a	2594	PSU	O2-C2-N1	-3.16	119.31	122.79
29	a	2438	H2U	C5-C4-N3	-3.15	113.11	116.65
26	V	8	4SU	C5-C4-S4	-3.15	120.41	124.47
29	a	1900	PSU	O2-C2-N1	-3.14	119.34	122.79
26	V	55	5MU	O2-C2-N3	-3.12	115.68	121.50
29	a	1906	PSU	O2-C2-N1	-3.11	119.37	122.79
29	a	945	PSU	O2-C2-N1	-3.09	119.39	122.79
26	V	55	5MU	O2-C2-N1	-3.07	118.70	122.79
29	a	2492	2MA	N9-C8-N7	-3.02	109.78	113.91
6	A	524	G7M	C6-C5-N7	3.01	135.89	132.25
6	A	1516	MA6	C4-C5-N7	-3.01	106.95	110.62
29	a	2019	6MZ	N3-C4-N9	3.00	132.03	127.08
29	a	2492	2MA	C5-N7-C8	2.98	107.74	103.51
29	a	2434	2MG	C6-C5-N7	2.98	135.79	130.25
6	A	1515	MA6	C4-C5-N7	-2.98	106.99	110.62
26	V	56	PSU	O2-C2-N1	-2.97	119.52	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1513	2MG	N9-C4-N3	2.86	131.68	125.94
29	a	2487	OMC	O2-C2-N3	-2.83	117.73	122.33
29	a	2493	PSU	O2-C2-N1	-2.82	119.69	122.79
29	a	2446	PSU	O2-C2-N1	-2.79	119.72	122.79
6	A	963	2MG	C6-C5-N7	2.78	135.42	130.25
17	L	89	D2T	OD1-CG-CB	-2.75	116.67	122.44
6	A	1513	2MG	C4-C5-N7	-2.73	106.40	110.72
6	A	1204	2MG	C6-C5-N7	2.70	135.27	130.25
29	a	2492	2MA	C4-C5-N7	-2.68	107.36	110.62
6	A	524	G7M	C2-N1-C6	-2.67	120.24	125.10
29	a	2240	OMG	C6-C5-N7	2.62	135.13	130.25
6	A	1399	4OC	O2-C2-N3	-2.60	118.10	122.33
29	a	1928	5MU	O2-C2-N3	-2.60	116.66	121.50
29	a	2569	PSU	O4'-C1'-C2'	2.58	108.78	105.14
29	a	2058	G7M	C2-N1-C6	-2.58	120.40	125.10
29	a	736	1MG	C5-C6-N1	2.56	119.86	114.91
29	a	1904	3TD	C4-N3-C2	-2.54	121.85	124.61
40	l	83	MS6	CE-SD-CG	2.51	109.01	100.40
26	V	55	5MU	C1'-N1-C6	-2.50	116.97	121.12
29	a	2434	2MG	O6-C6-C5	-2.49	119.98	126.60
40	l	82	4D4	NH1-CZ-NE	-2.49	113.45	119.19
29	a	2240	OMG	C8-N7-C5	2.47	108.72	104.24
29	a	2240	OMG	O6-C6-C5	-2.46	120.06	126.60
29	a	2492	2MA	C4-N9-C8	2.46	108.39	105.73
6	A	1204	2MG	C4-C5-N7	-2.45	106.84	110.72
29	a	2541	OMU	O4-C4-C5	-2.45	120.85	125.16
29	a	2240	OMG	C5-C6-N1	2.43	119.37	113.19
29	a	736	1MG	C4-C5-N7	-2.42	106.88	110.72
29	a	2541	OMU	C5-C4-N3	2.41	118.44	114.84
6	A	1204	2MG	C2-N1-C6	-2.40	121.72	124.48
29	a	2434	2MG	N1-C2-N3	-2.37	120.28	123.95
29	a	2240	OMG	C4-C5-N7	-2.36	106.98	110.72
29	a	2240	OMG	N9-C8-N7	-2.33	109.01	113.39
6	A	963	2MG	C4-C5-N7	-2.32	107.04	110.72
29	a	2541	OMU	O2-C2-N1	-2.32	119.70	122.79
29	a	2492	2MA	N3-C2-N1	-2.31	121.47	125.72
6	A	513	PSU	O4'-C1'-C2'	2.31	108.40	105.14
6	A	1513	2MG	N1-C2-N3	-2.31	120.39	123.95
29	a	2434	2MG	C4-C5-N7	-2.30	107.08	110.72
6	A	1204	2MG	CM2-N2-C2	-2.29	118.81	123.86
29	a	736	1MG	C6-C5-N7	2.29	134.53	129.35
26	V	8	4SU	C1'-N1-C2	2.28	121.70	117.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	V	21	H2U	C5-C4-N3	-2.28	114.09	116.65
6	A	1204	2MG	O6-C6-C5	-2.27	120.58	126.60
6	A	964	5MC	C5-C4-N3	-2.25	119.24	121.67
29	a	1928	5MU	C6-N1-C2	2.25	123.58	121.30
6	A	1513	2MG	C8-N7-C5	2.25	108.31	104.24
6	A	963	2MG	O6-C6-C5	-2.23	120.67	126.60
6	A	1495	UR3	C5-C6-N1	-2.23	118.07	121.81
26	V	33	OMC	O2-C2-N3	-2.22	118.72	122.33
6	A	963	2MG	C5-C6-N1	2.22	118.83	113.19
29	a	2569	PSU	C6-N1-C2	-2.21	120.42	122.68
6	A	1513	2MG	O6-C6-C5	-2.21	120.75	126.60
6	A	1513	2MG	C5-C6-N1	2.20	118.78	113.19
29	a	2487	OMC	N1-C2-N3	2.19	122.80	118.81
29	a	2446	PSU	O4'-C1'-C2'	2.19	108.23	105.14
29	a	2240	OMG	C2-N1-C6	-2.17	121.13	125.10
6	A	963	2MG	C2-N1-C6	-2.17	121.98	124.48
29	a	2446	PSU	C6-N1-C2	-2.17	120.47	122.68
6	A	1204	2MG	C5-C6-N1	2.16	118.68	113.19
29	a	2434	2MG	C5-C6-N1	2.16	118.67	113.19
6	A	1399	4OC	C5-C4-N3	-2.14	119.15	122.59
29	a	2019	6MZ	C4-N9-C8	2.13	108.04	105.73
29	a	736	1MG	C8-N7-C5	2.11	108.06	104.24
6	A	963	2MG	C8-N7-C5	2.11	108.05	104.24
6	A	963	2MG	N1-C2-N3	-2.10	120.70	123.95
6	A	1513	2MG	N9-C8-N7	-2.10	109.44	113.39
6	A	1204	2MG	C8-N7-C5	2.09	108.03	104.24
29	a	2434	2MG	C8-N7-C5	2.09	108.03	104.24
29	a	2434	2MG	N9-C8-N7	-2.08	109.47	113.39
6	A	1513	2MG	C2-N1-C6	-2.05	122.12	124.48
29	a	945	PSU	C6-N1-C2	-2.05	120.59	122.68
29	a	1906	PSU	O4'-C1'-C2'	2.03	108.00	105.14
6	A	1513	2MG	CM2-N2-C2	-2.02	119.41	123.86
29	a	2434	2MG	CM2-N2-C2	-2.01	119.42	123.86
29	a	2493	PSU	C6-N1-C2	-2.01	120.63	122.68

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	524	G7M	C3'-C4'-C5'-O5'
6	A	1204	2MG	N1-C2-N2-CM2
6	A	1204	2MG	N3-C2-N2-CM2

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Mol	Chain	Res	Type	Atoms
17	L	89	D2T	CA-CB-CG-OD2
26	V	21	H2U	O4'-C4'-C5'-O5'
26	V	21	H2U	C3'-C4'-C5'-O5'
26	V	21	H2U	O4'-C1'-N1-C2
26	V	21	H2U	O4'-C1'-N1-C6
32	d	153	MEQ	O-C-CA-CB
29	a	2240	OMG	C1'-C2'-O2'-CM2
29	a	2019	6MZ	O4'-C4'-C5'-O5'
29	a	2019	6MZ	C3'-C4'-C5'-O5'
29	a	2541	OMU	C3'-C4'-C5'-O5'
29	a	2541	OMU	O4'-C4'-C5'-O5'
32	d	153	MEQ	NE2-CD-CG-CB
32	d	153	MEQ	OE1-CD-CG-CB
40	l	83	MS6	CB-CG-SD-CE
6	A	524	G7M	O4'-C4'-C5'-O5'
29	a	2492	2MA	O4'-C4'-C5'-O5'
40	l	83	MS6	CA-CB-CG-SD
29	a	2493	PSU	O4'-C4'-C5'-O5'
29	a	2492	2MA	C3'-C4'-C5'-O5'
17	L	89	D2T	CG-CB-SB-CB1
17	L	89	D2T	CA-CB-CG-OD1
6	A	1516	MA6	C4'-C5'-O5'-P
6	A	524	G7M	C4'-C5'-O5'-P
16	K	118	IAS	N-CA-CB-CG
29	a	2438	H2U	O4'-C4'-C5'-O5'
17	L	89	D2T	SB-CB-CG-OD2
29	a	2493	PSU	C3'-C4'-C5'-O5'
6	A	1516	MA6	C5-C6-N6-C10
29	a	2434	2MG	C3'-C4'-C5'-O5'
29	a	737	PSU	O4'-C1'-C5-C6
29	a	2438	H2U	C2'-C1'-N1-C2
29	a	2438	H2U	O4'-C1'-N1-C2
29	a	2492	2MA	C4'-C5'-O5'-P
29	a	2438	H2U	C3'-C4'-C5'-O5'
16	K	118	IAS	CA-CB-CG-OD1
29	a	2058	G7M	O4'-C4'-C5'-O5'
29	a	2058	G7M	C4'-C5'-O5'-P

There are no ring outliers.

14 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1399	4OC	2	0
32	d	153	MEQ	1	0
26	V	8	4SU	1	0
26	V	33	OMC	3	0
26	V	55	5MU	1	0
6	A	1204	2MG	1	0
29	a	736	1MG	1	0
6	A	1513	2MG	1	0
29	a	1904	3TD	1	0
6	A	1515	MA6	1	0
26	V	21	H2U	1	0
29	a	2541	OMU	1	0
29	a	2019	6MZ	2	0
29	a	2240	OMG	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 531 ligands modelled in this entry, 531 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
6	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1530:C	O3’	1531:A	P	4.72

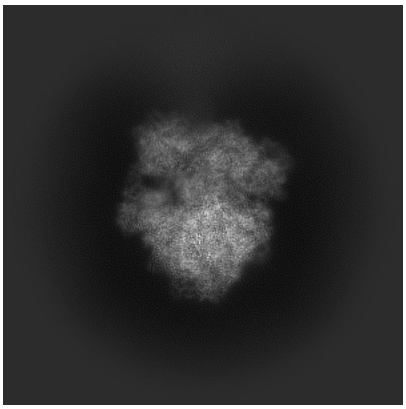
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-59046. These allow visual inspection of the internal detail of the map and identification of artifacts.

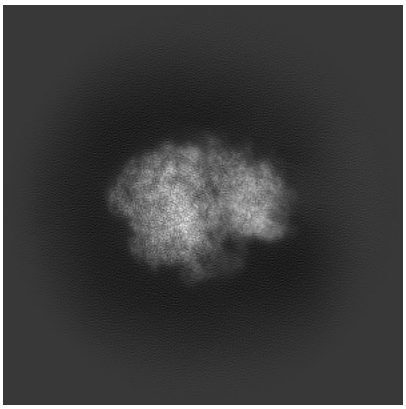
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

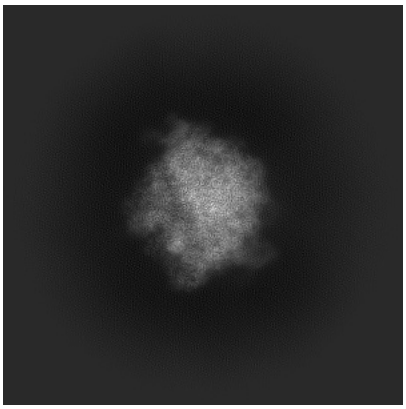
6.1.1 Primary map



X

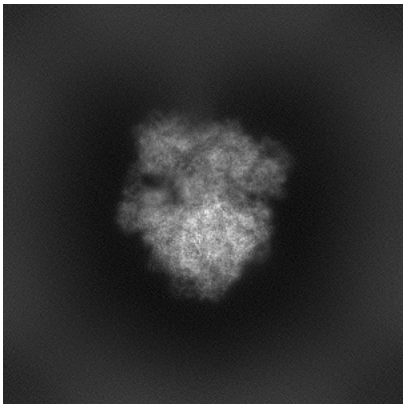


Y

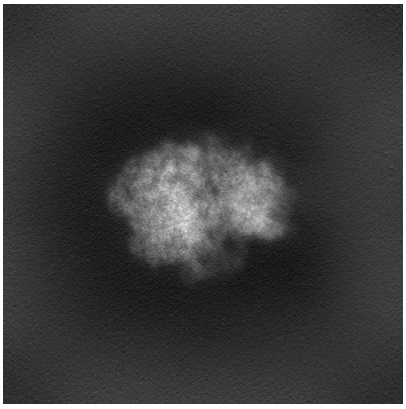


Z

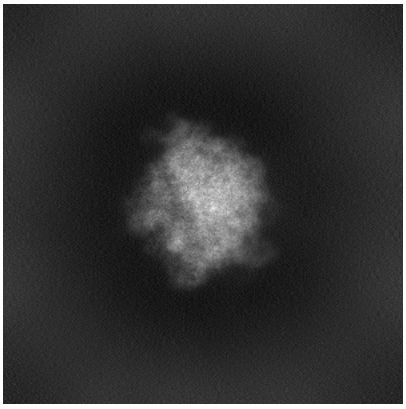
6.1.2 Raw map



X



Y

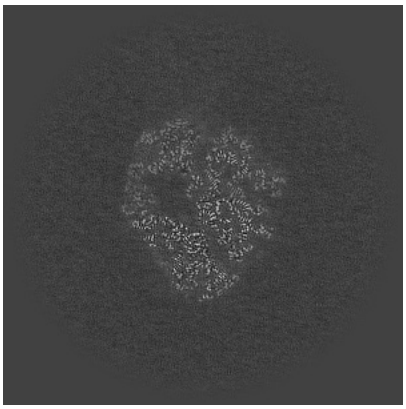


Z

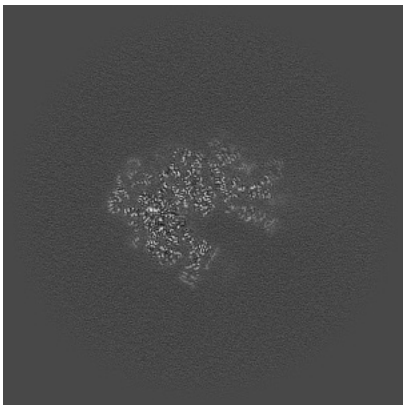
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

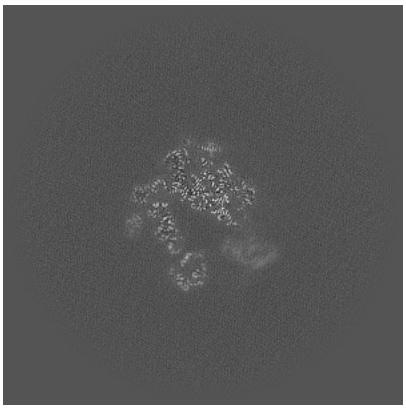
6.2.1 Primary map



X Index: 256

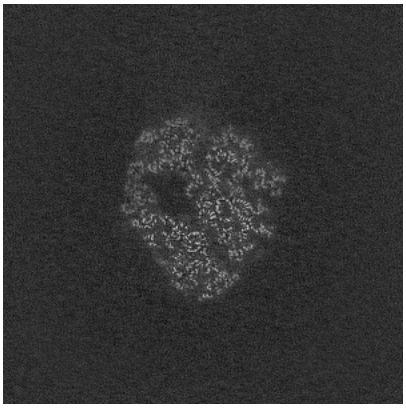


Y Index: 256

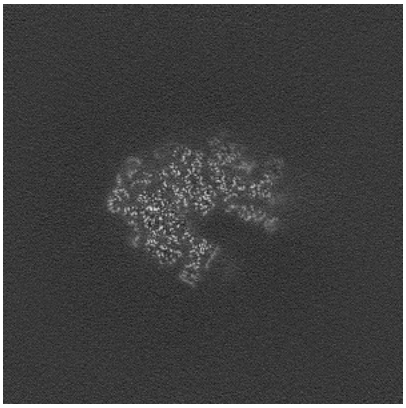


Z Index: 256

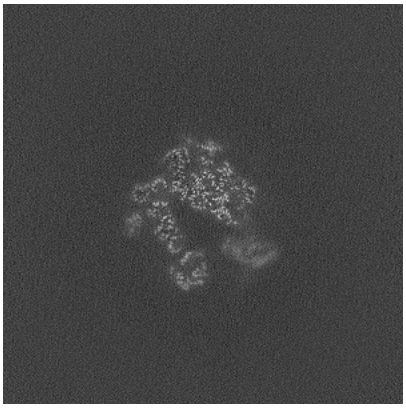
6.2.2 Raw map



X Index: 256



Y Index: 256

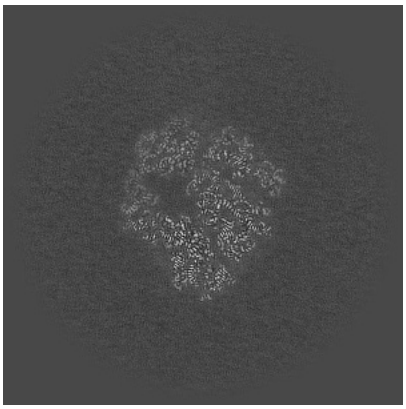


Z Index: 256

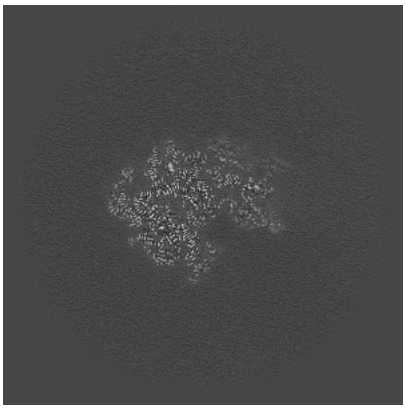
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

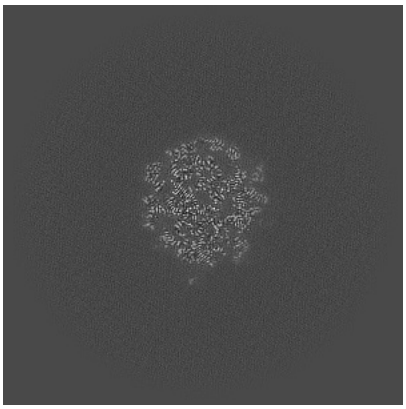
6.3.1 Primary map



X Index: 253

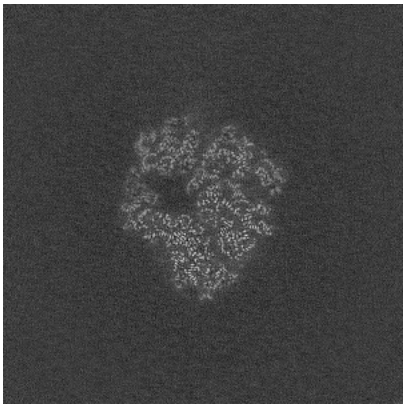


Y Index: 263

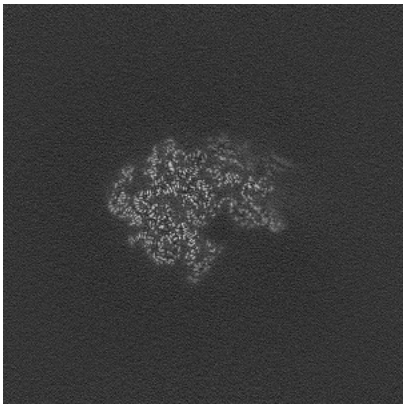


Z Index: 216

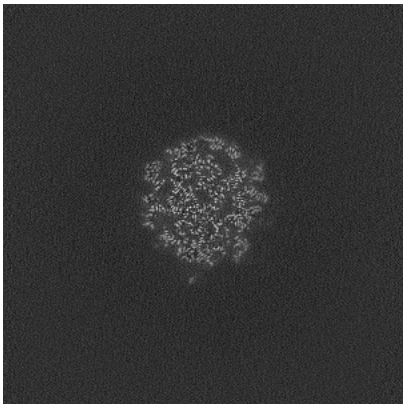
6.3.2 Raw map



X Index: 252



Y Index: 263

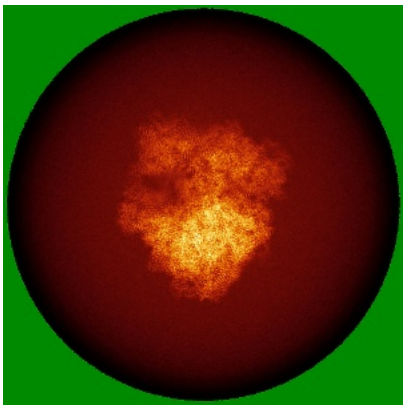


Z Index: 216

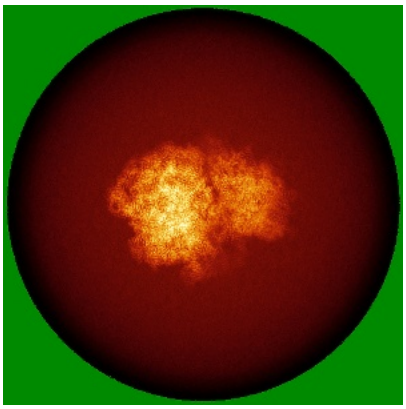
The images above show the largest variance slices of the map in three orthogonal directions.

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

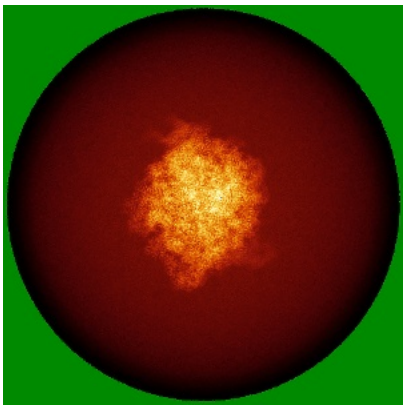
6.4.1 Primary map



X

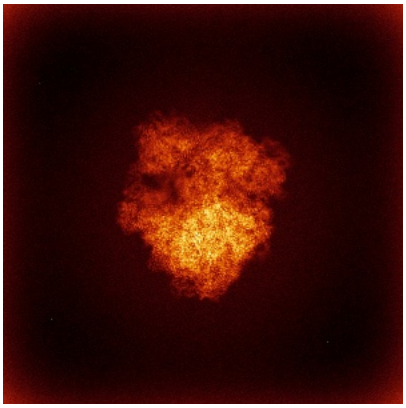


Y

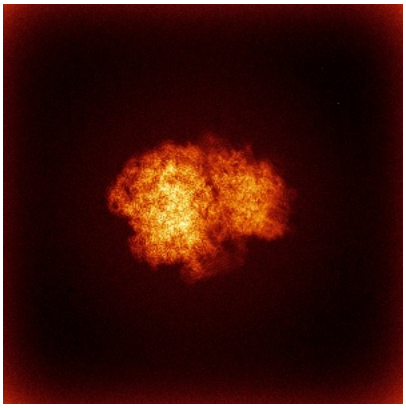


Z

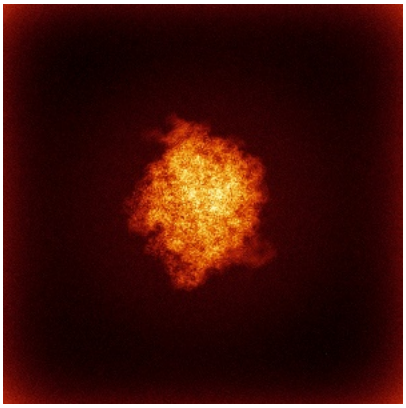
6.4.2 Raw map



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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.45. 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



X Y Z

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.

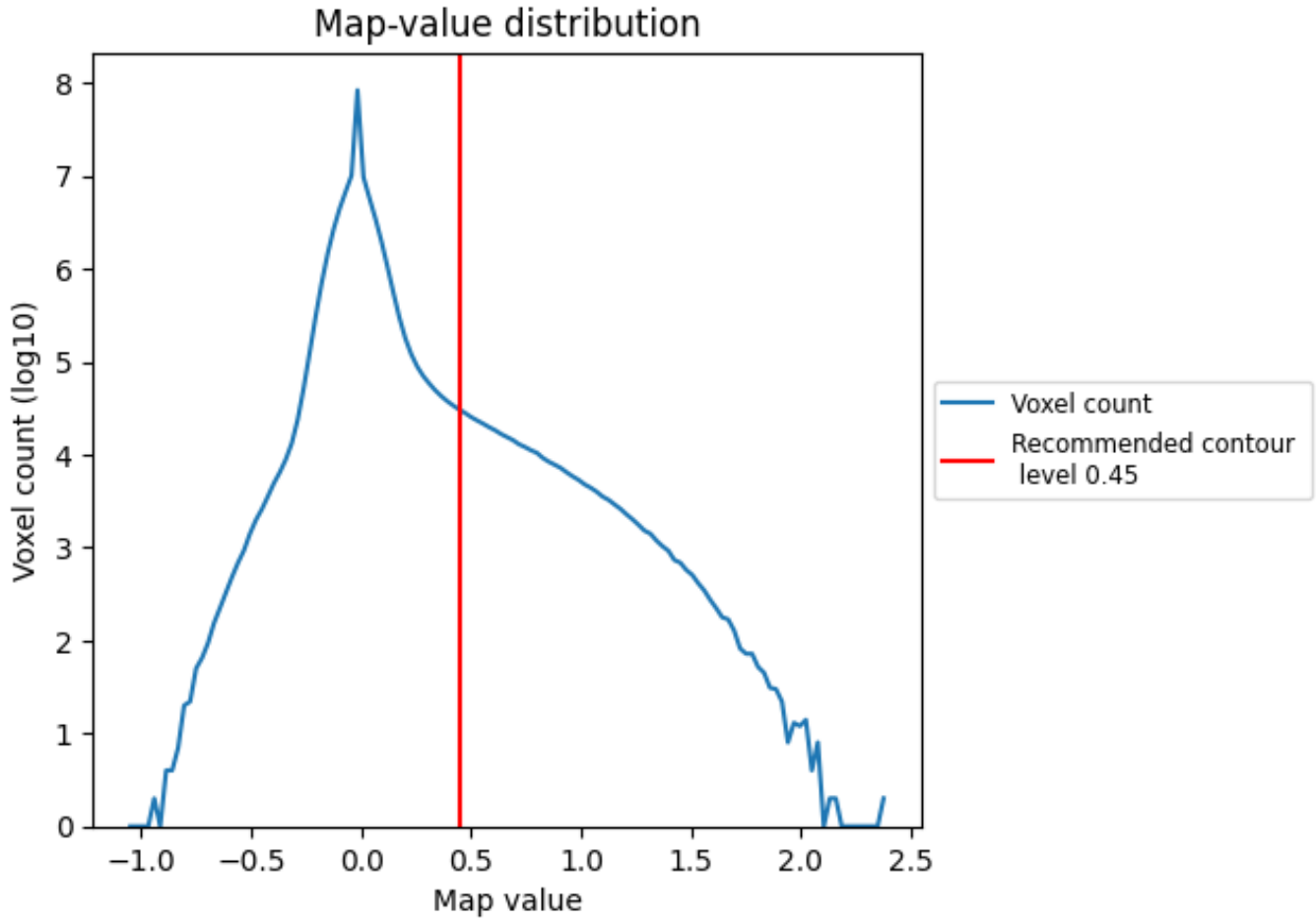
6.6 Mask visualisation (i)

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

7 Map analysis

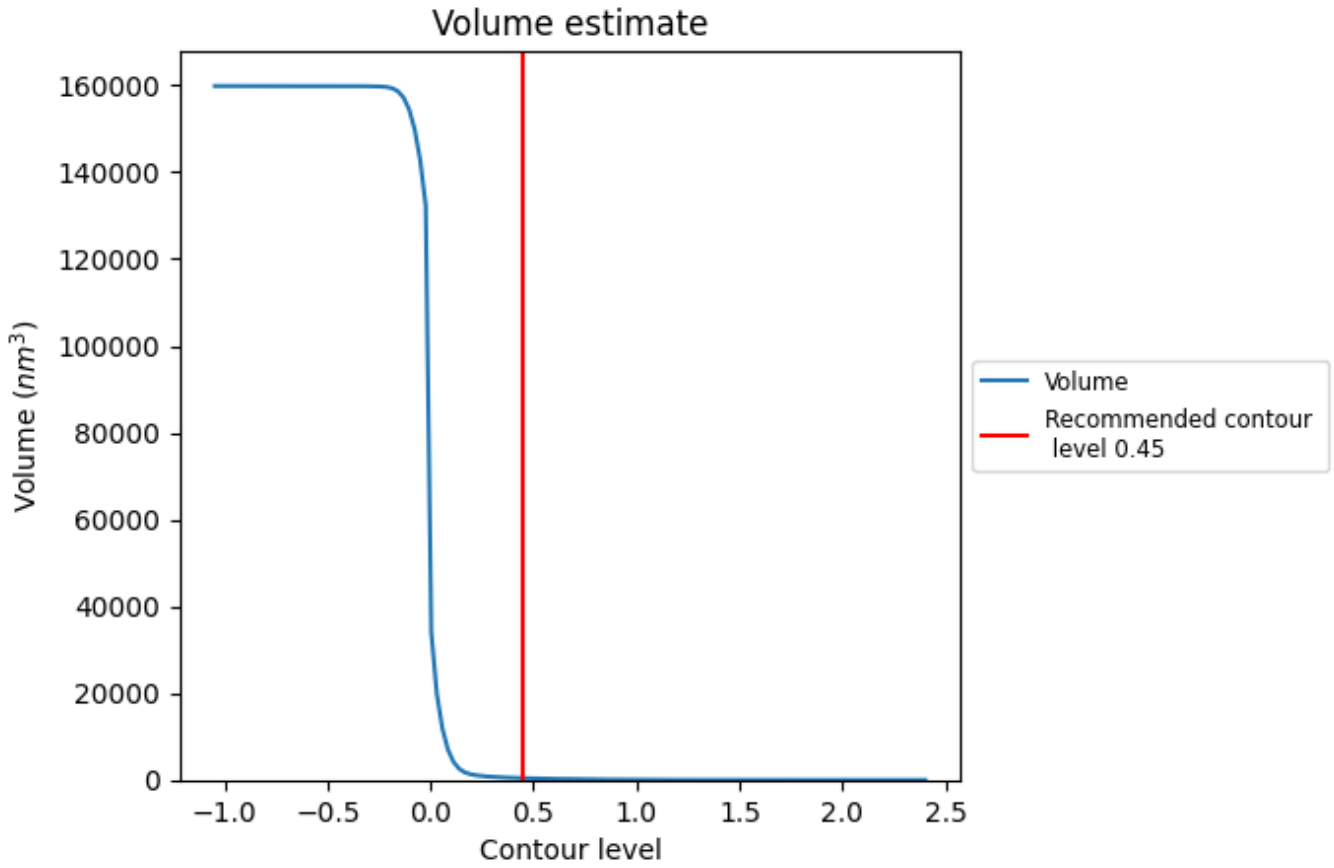
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

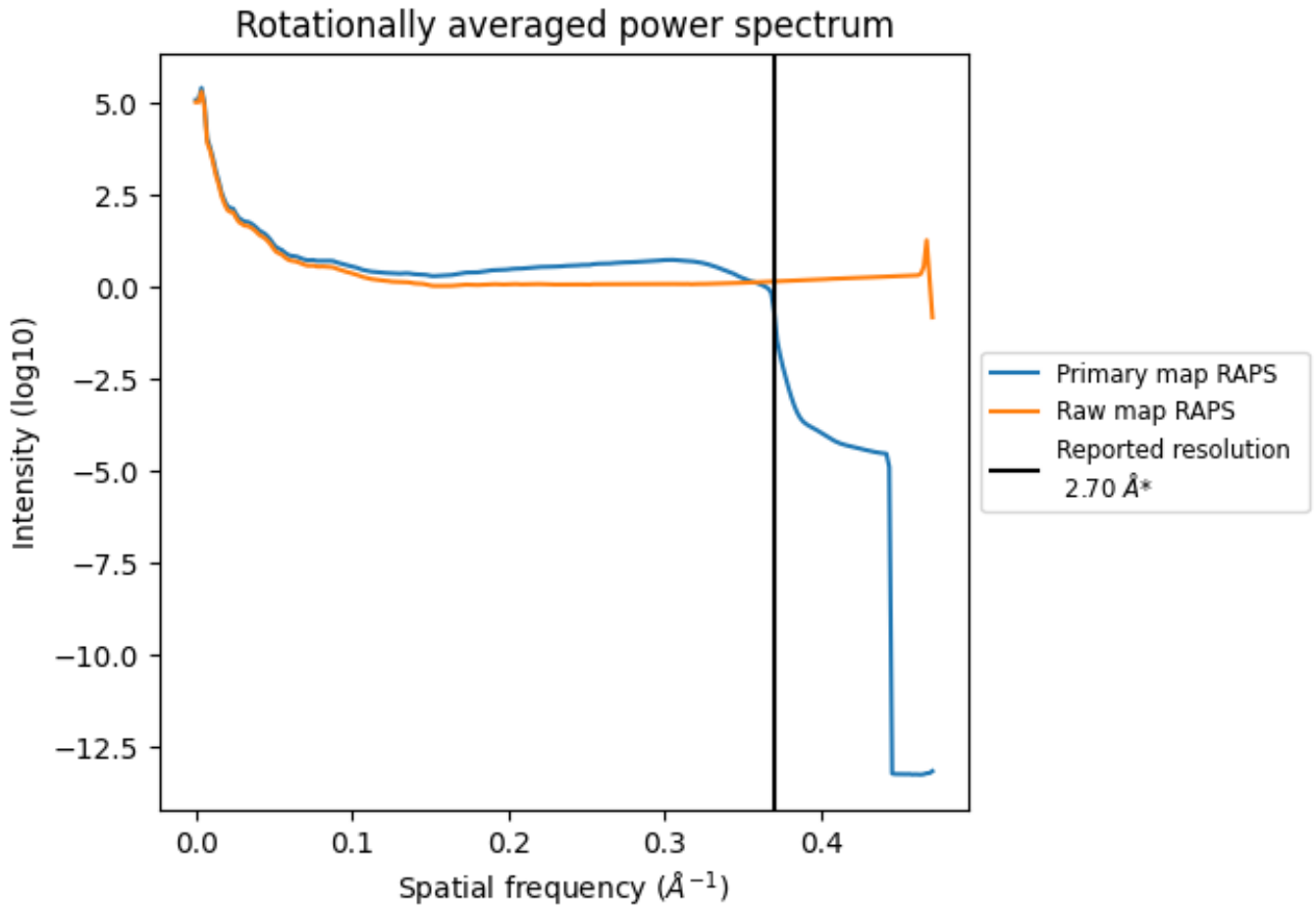
7.2 Volume estimate



The volume at the recommended contour level is 416 nm^3; this corresponds to an approximate mass of 376 kDa.

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

7.3 Rotationally averaged power spectrum (i)

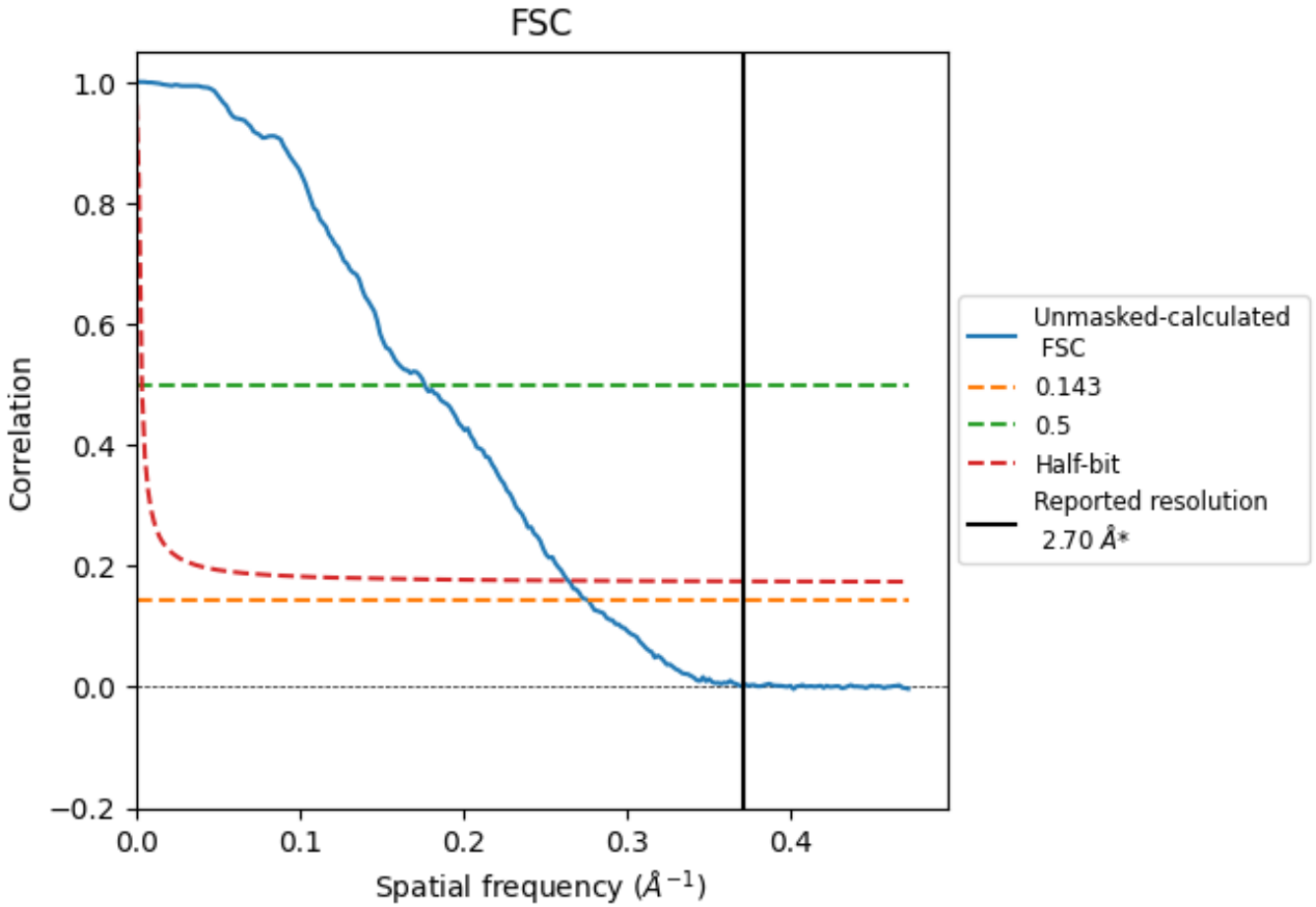


*Reported resolution corresponds to spatial frequency of 0.370 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

8.2 Resolution estimates (i)

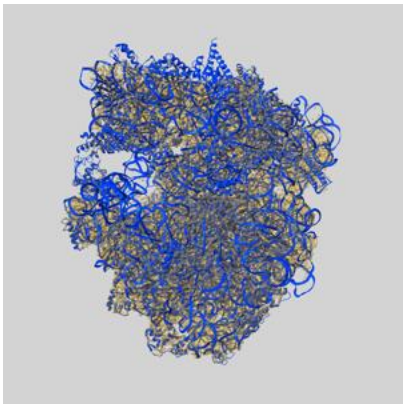
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.62	5.68	3.79

*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 3.62 differs from the reported value 2.7 by more than 10 %

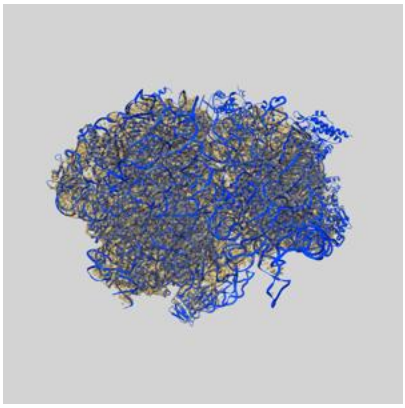
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-59046 and PDB model 32PD. Per-residue inclusion information can be found in section 3 on page 16.

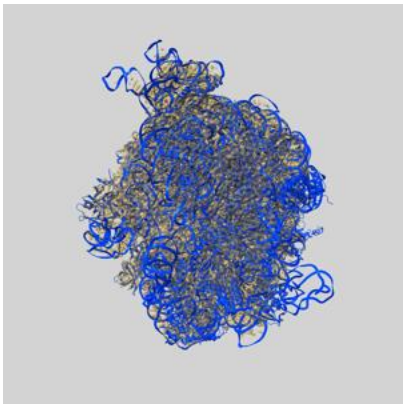
9.1 Map-model overlay



X



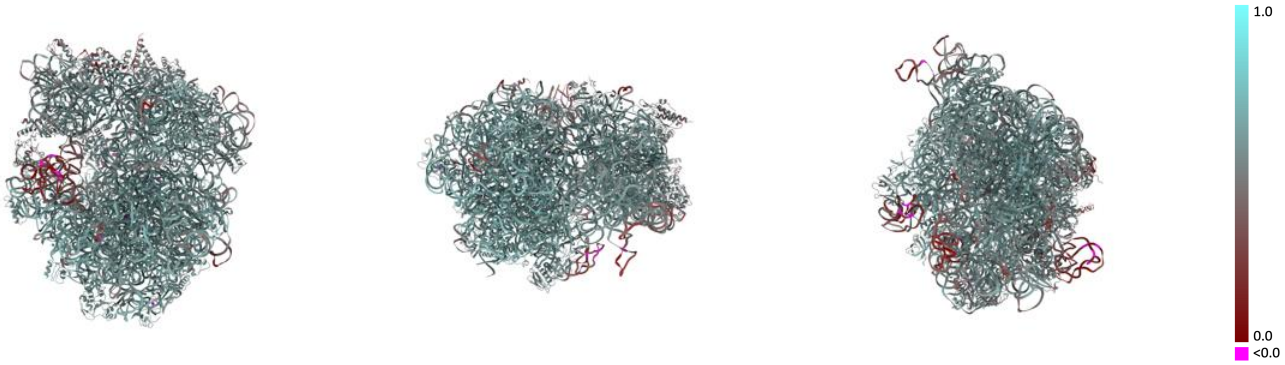
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

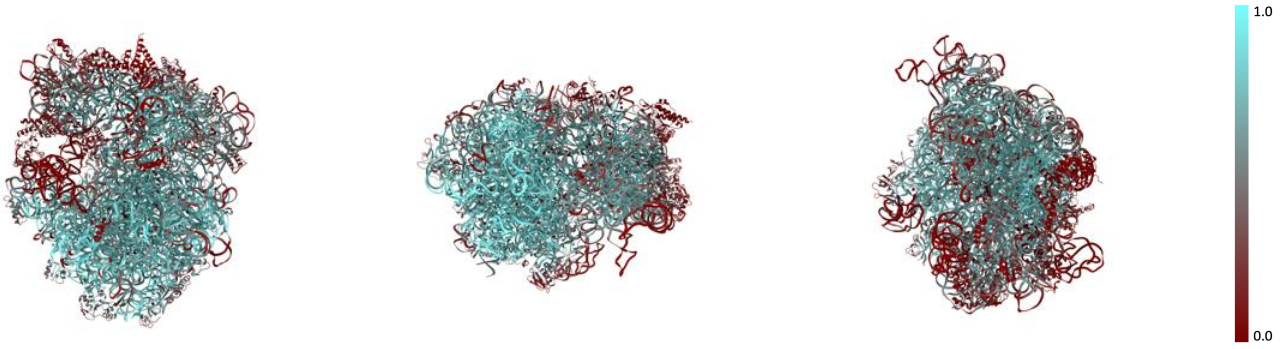
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

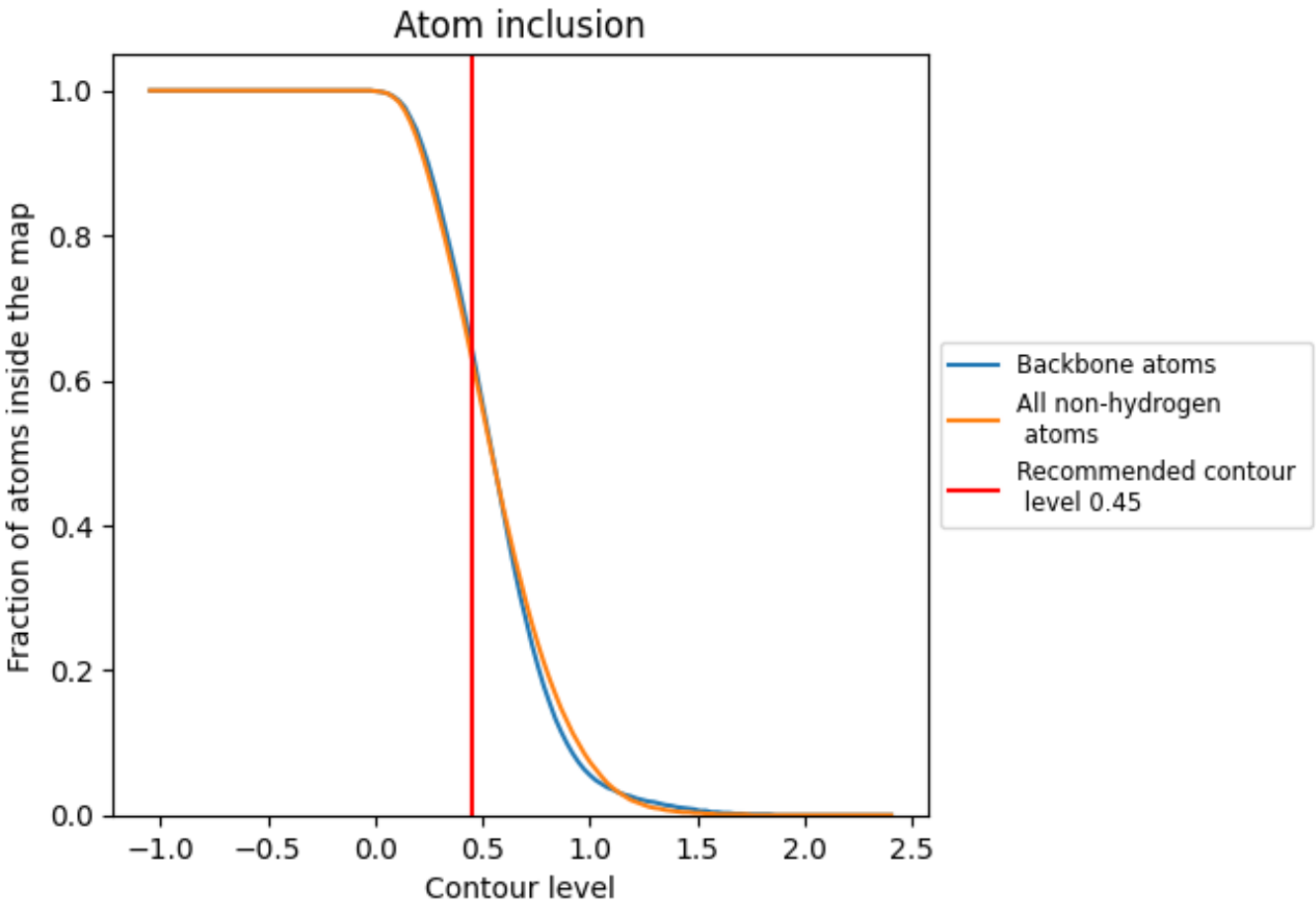
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.45).

9.4 Atom inclusion (i)



At the recommended contour level, 64% of all backbone atoms, 63% 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 (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6310	0.5830
0	0.6190	0.6230
1	0.8230	0.6430
2	0.8440	0.6520
3	0.6960	0.6310
4	0.0060	0.4100
A	0.6030	0.5680
B	0.0020	0.4540
C	0.3430	0.5590
D	0.2380	0.5330
E	0.5500	0.6100
F	0.0410	0.5100
G	0.1900	0.5290
H	0.4830	0.6010
I	0.3100	0.5510
J	0.2720	0.5200
K	0.3360	0.5590
L	0.4460	0.5940
M	0.1910	0.5260
N	0.3100	0.5490
O	0.4630	0.5870
P	0.4440	0.5740
Q	0.3410	0.5760
R	0.1120	0.5160
S	0.1470	0.5330
T	0.4410	0.5830
V	0.0320	0.3600
W	0.1870	0.5090
X	0.4150	0.5900
a	0.7750	0.5980
b	0.6740	0.5970
c	0.7460	0.6430
d	0.7350	0.6370
e	0.6320	0.6220
f	0.1680	0.5120



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Chain	Atom inclusion	Q-score
g	0.3150	0.5620
h	0.0070	0.3720
i	0.7250	0.6370
j	0.6460	0.6320
k	0.6840	0.6280
l	0.6420	0.6270
m	0.7780	0.6480
n	0.5400	0.6000
o	0.6400	0.6240
p	0.7960	0.6500
q	0.6860	0.6300
r	0.7310	0.6340
s	0.5790	0.6160
t	0.4470	0.5730
u	0.5130	0.6000
v	0.7690	0.6490
w	0.6720	0.6280
x	0.4450	0.5880
y	0.7020	0.6320
z	0.7000	0.6350