Full wwPDB EM Validation Report ⓘ

Nov 7, 2026 – 01:29 pm GMT

PDB ID	:	9T8U / pdb_00009t8u
EMDB ID	:	EMD-55712
Title	:	Structural characterization of hibernating ribosomes in the Gram-negative pathogen Pseudomonas aeruginosa with 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	:	2025-11-13
Resolution	:	2.79 Å(reported)
Based on initial model	:	7UNW

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:

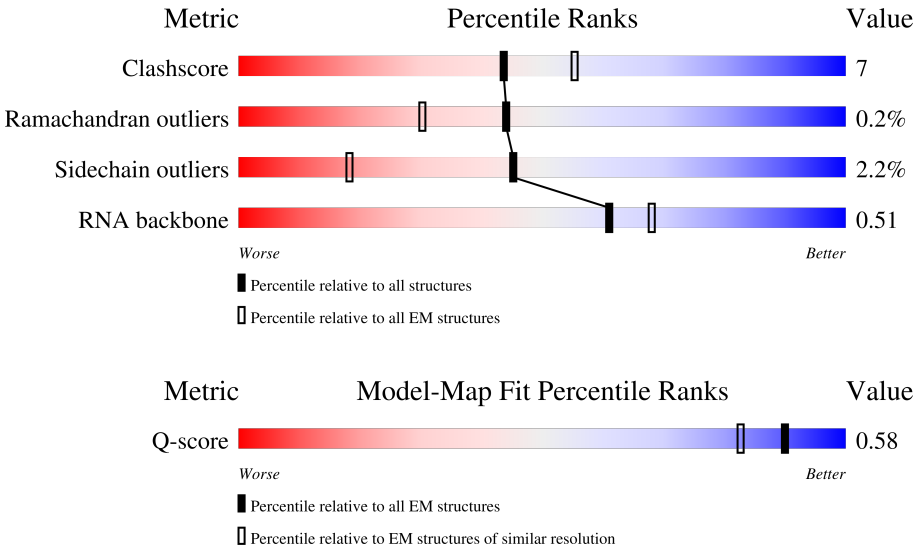
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal 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

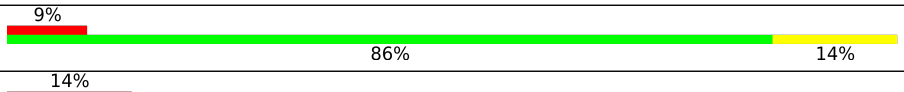
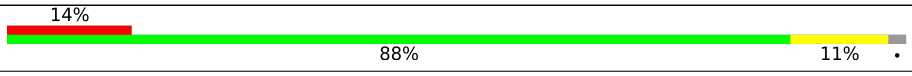
The reported resolution of this entry is 2.79 Å.

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.



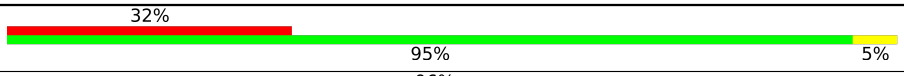
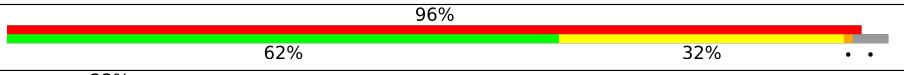
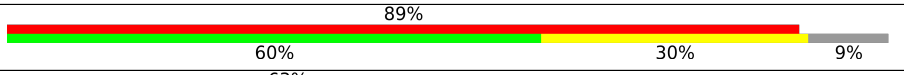
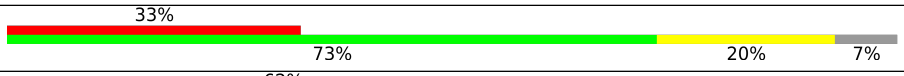
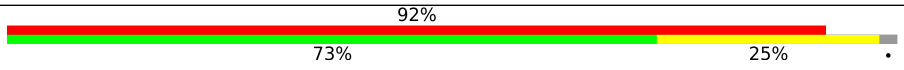
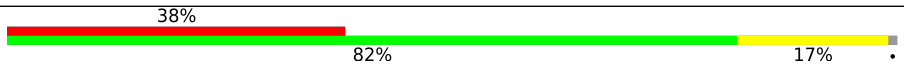
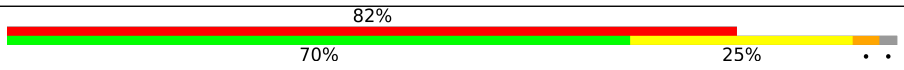
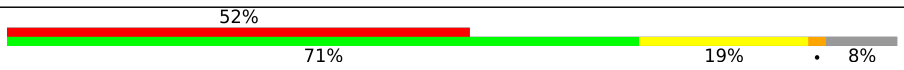
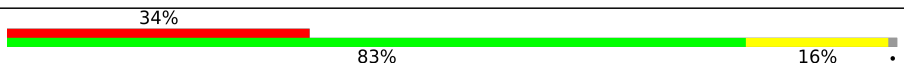
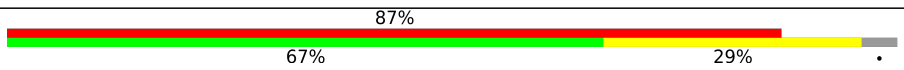
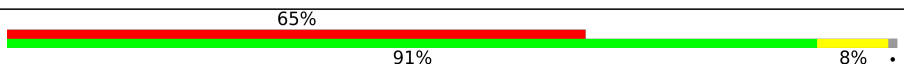
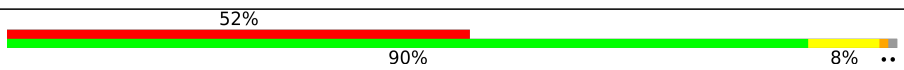
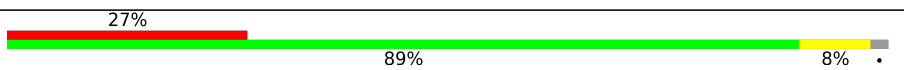
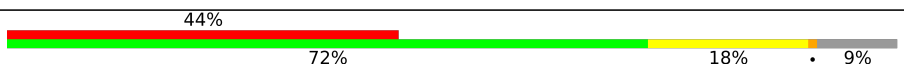
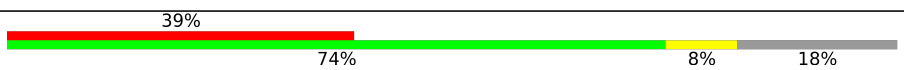
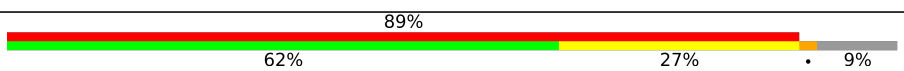
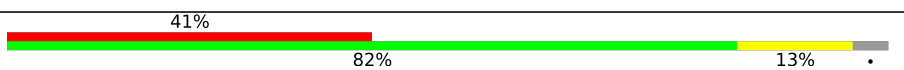
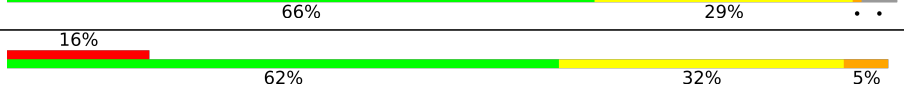
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	10811 (2.29 - 3.29)

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	
2	1	44	
3	2	64	

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Mol	Chain	Length	Quality of chain
4	3	38	
5	4	71	
6	A	1536	
7	B	246	
8	C	228	
9	D	206	
10	E	166	
11	F	139	
12	G	156	
13	H	130	
14	I	130	
15	J	103	
16	K	129	
17	L	123	
18	M	118	
19	N	101	
20	O	89	
21	P	83	
22	Q	88	
23	R	76	
24	S	91	
25	T	91	
26	U	71	
27	X	102	
28	a	2891	

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Mol	Chain	Length	Quality of chain
29	b	120	40% 58% 33% 7%
30	c	273	14% 86% 14%
31	d	211	17% 81% 18%
32	e	200	34% 82% 18%
33	f	179	97% 68% 29%
34	g	177	90% 84% 14%
35	h	148	49% 41% 7% 51%
36	i	142	15% 87% 12%
37	j	122	30% 82% 17%
38	k	144	26% 87% 13%
39	l	137	30% 82% 18%
40	m	129	11% 78% 15% 7%
41	n	116	66% 79% 20%
42	o	116	28% 86% 12%
43	p	118	17% 86% 13%
44	q	103	36% 89% 10%
45	r	110	20% 95% 5%
46	s	99	36% 80% 15% 5%
47	t	104	58% 85% 14%
48	u	204	70% 74% 19% 7%
49	v	85	16% 85% 5% 11%
50	w	78	36% 78% 19%
51	x	63	49% 86% 10%
52	y	58	17% 90% 7%
53	z	60	32% 78% 13% 8%

2 Entry composition (i)

There are 56 unique types of molecules in this entry. The entry contains 143222 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
1	0	51	Total	C	N	O	S	0	0
			426	272	78	75	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	44	Total	C	N	O	S	0	0
			365	222	87	54	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	63	Total	C	N	O	S	0	0
			506	314	108	81	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	38	Total	C	N	O	S	0	0
			307	186	69	48	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	68	Total	C	N	O	S	0	0
			531	334	95	96	6		

- Molecule 6 is a RNA chain called 16S rRNA (1527-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	1527	Total	C	N	O	P	0	0
			32783	14628	6016	10612	1527		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	224	Total	C	N	O	S	0	0
			1763	1112	322	319	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	208	Total	C	N	O	S	0	0
			1664	1052	315	292	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	205	Total	C	N	O	S	0	0
			1627	1003	316	303	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	E	154	Total	C	N	O	S	0	0
			1134	711	210	207	6		

- 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
			868	539	159	164	6		

- 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
			1199	752	232	210	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	H	129	Total	C	N	O	S	0	0
			982	618	173	185	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
			1010	625	203	181	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	99	Total	C	N	O	S	0	0
			793	496	150	146	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	119	Total	C	N	O	S	0	0
			882	546	171	163	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	IAS	ASN	conflict	UNP E2RXU4

- 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
			961	589	198	169	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	M	113	Total	C	N	O	S	0	0
			883	541	178	160	4		

- 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
			804	496	167	138	3		

- 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
			703	434	139	129	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	P	81	Total	C	N	O	S	0	0
			637	398	125	113	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Q	80	Total	C	N	O	S	0	0
			645	404	124	115	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
23	R	62	Total	C	N	O	0	0
			494	316	86	92		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	S	83	Total	C	N	O	S	0	0
			663	422	129	109	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	T	87	Total	C	N	O	S	0	0
			671	414	138	117	2		

- Molecule 26 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	U	62	Total	C	N	O	S	0	0
			506	316	103	86	1		

- Molecule 27 is a protein called Ribosome hibernation promoting factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	X	98	Total	C	N	O	S	0	0
			796	498	143	152	3		

- Molecule 28 is a RNA chain called 23S rRNA (2890-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
28	a	2890	Total	C	N	O	P	0	0
			62019	27677	11363	20089	2890		

- Molecule 29 is a RNA chain called 5S rRNA (117-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	117	Total	C	N	O	P	0	0
			2495	1114	448	816	117		

- Molecule 30 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	c	272	Total	C	N	O	S	0	0
			2072	1276	426	364	6		

- Molecule 31 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	d	211	Total	C	N	O	S	0	0
			1589	982	304	297	6		

- Molecule 32 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	e	200	Total	C	N	O	S	0	0
			1524	956	283	282	3		

- Molecule 33 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	f	177	Total	C	N	O	S	0	0
			1418	905	253	256	4		

- Molecule 34 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	g	175	Total	C	N	O	S	0	0
			1326	835	244	245	2		

- Molecule 35 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	h	72	Total	C	N	O	S	0	0
			533	334	98	100	1		

- Molecule 36 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	i	142	Total	C	N	O	S	0	0
			1130	718	206	202	4		

- Molecule 37 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	j	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 38 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	k	144	Total	C	N	O	S	0	0
			1066	654	215	194	3		

- Molecule 39 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	l	137	Total	C	N	O	S	0	0
			1086	689	211	181	5		

- Molecule 40 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	m	120	Total	C	N	O	S	0	0
			959	600	192	162	5		

- Molecule 41 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	n	115	Total	C	N	O	S	0	0
			881	544	174	161	2		

- Molecule 42 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	o	114	Total	C	N	O	S	0	0
			902	568	171	162	1		

- Molecule 43 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	p	117	Total	C	N	O	0	0
			936	592	196	148		

- Molecule 44 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	q	103	Total	C	N	O	S	0	0
			822	521	156	143	2		

- Molecule 45 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	r	110	Total	C	N	O	S	0	0
			833	515	161	153	4		

- Molecule 46 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	s	94	Total	C	N	O	S	0	0
			739	472	134	132	1		

- Molecule 47 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	t	103	Total	C	N	O	S	0	0
			800	503	152	143	2		

- Molecule 48 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	u	190	Total	C	N	O	S	0	0
			1446	915	262	266	3		

- Molecule 49 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	v	76	Total	C	N	O	0	0
			575	364	111	100		

- Molecule 50 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	w	77	Total	C	N	O	S	0	0
			630	391	134	103	2		

- Molecule 51 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	x	61	Total	C	N	O	S	0	0
			490	301	96	91	2		

- Molecule 52 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	y	57	Total	C	N	O	S	0	0
			445	277	87	79	2		

- Molecule 53 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	z	55	Total	C	N	O	S	0	0
			440	264	93	82	1		

- Molecule 54 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
54	3	1	Total	Zn	0
			1	1	
54	4	1	Total	Zn	0
			1	1	

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
55	A	93	Total Mg 93 93	0
55	M	1	Total Mg 1 1	0
55	X	1	Total Mg 1 1	0
55	a	251	Total Mg 251 251	0
55	b	5	Total Mg 5 5	0
55	c	1	Total Mg 1 1	0
55	p	1	Total Mg 1 1	0
55	z	1	Total Mg 1 1	0

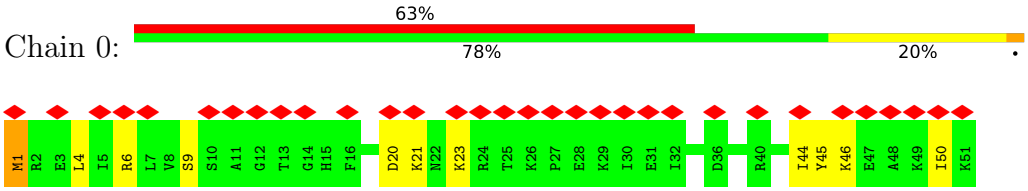
- Molecule 56 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
56	A	49	Total K 49 49	0
56	a	114	Total K 114 114	0
56	b	1	Total K 1 1	0
56	c	3	Total K 3 3	0
56	e	1	Total K 1 1	0
56	f	1	Total K 1 1	0

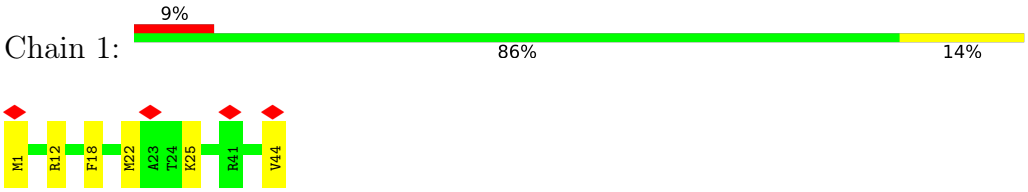
3 Residue-property plots (i)

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.

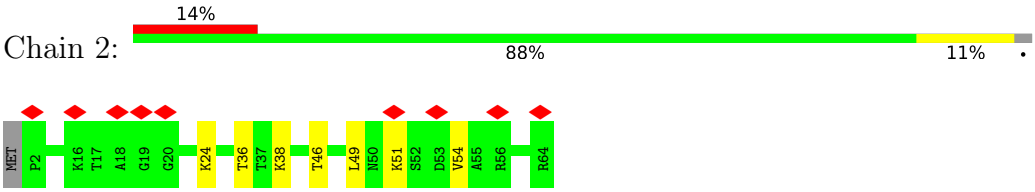
• Molecule 1: Large ribosomal subunit protein bL33



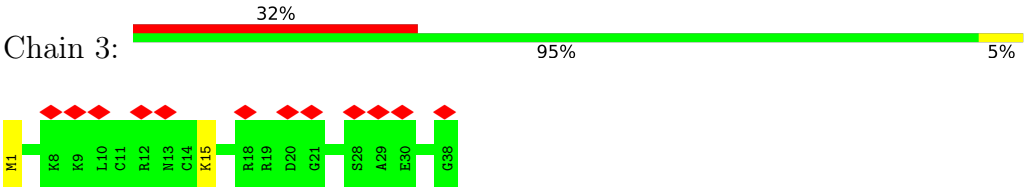
• Molecule 2: Large ribosomal subunit protein bL34



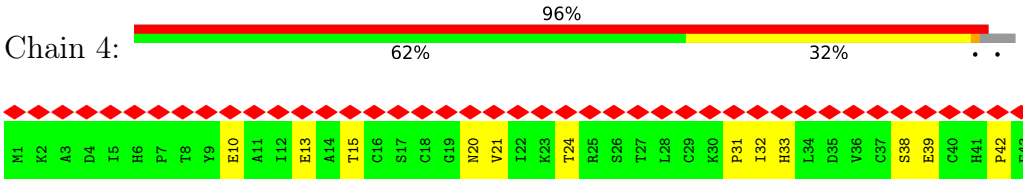
• Molecule 3: Large ribosomal subunit protein bL35

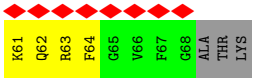


• Molecule 4: Large ribosomal subunit protein bL36



• Molecule 5: Large ribosomal subunit protein bL31

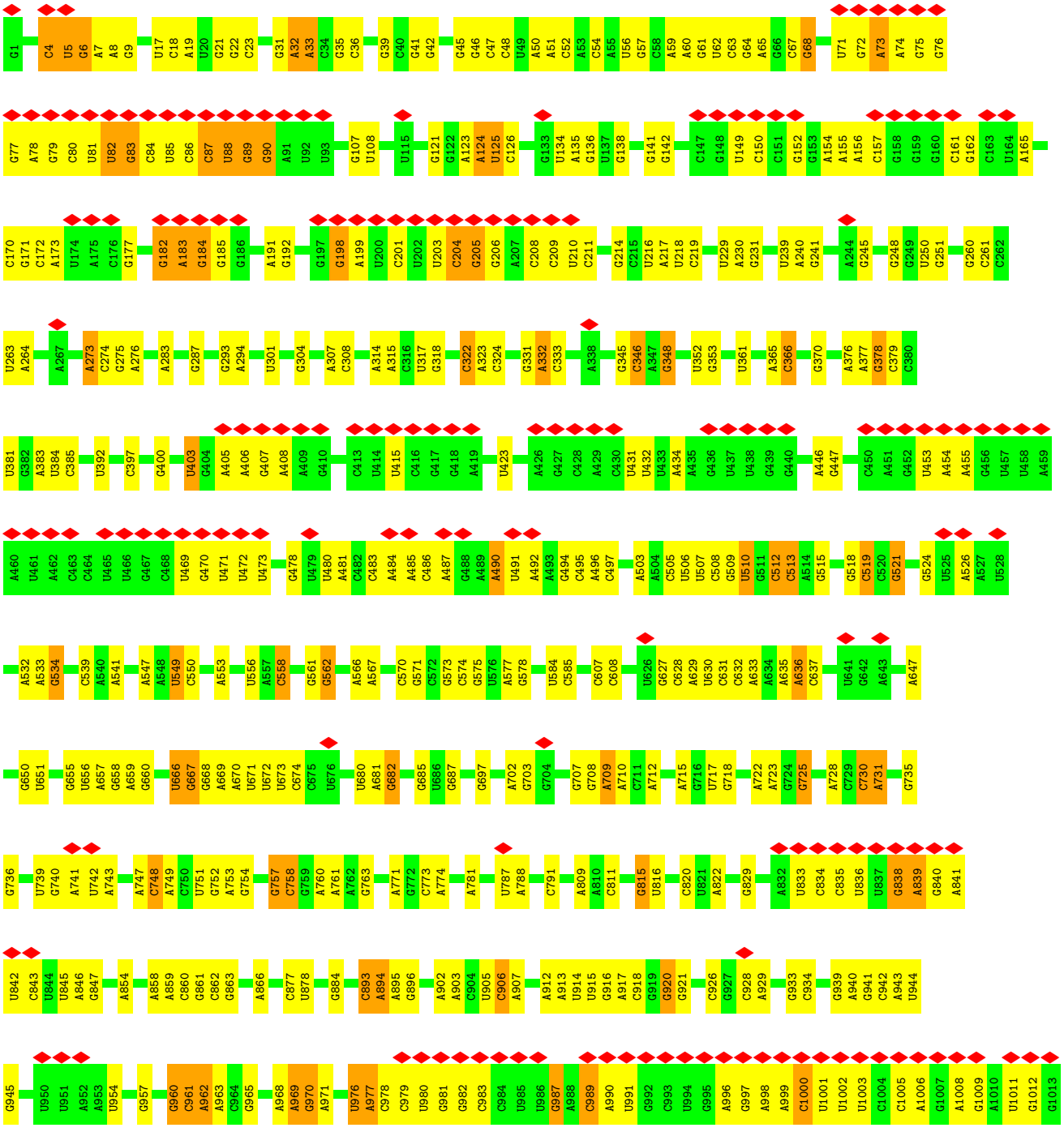


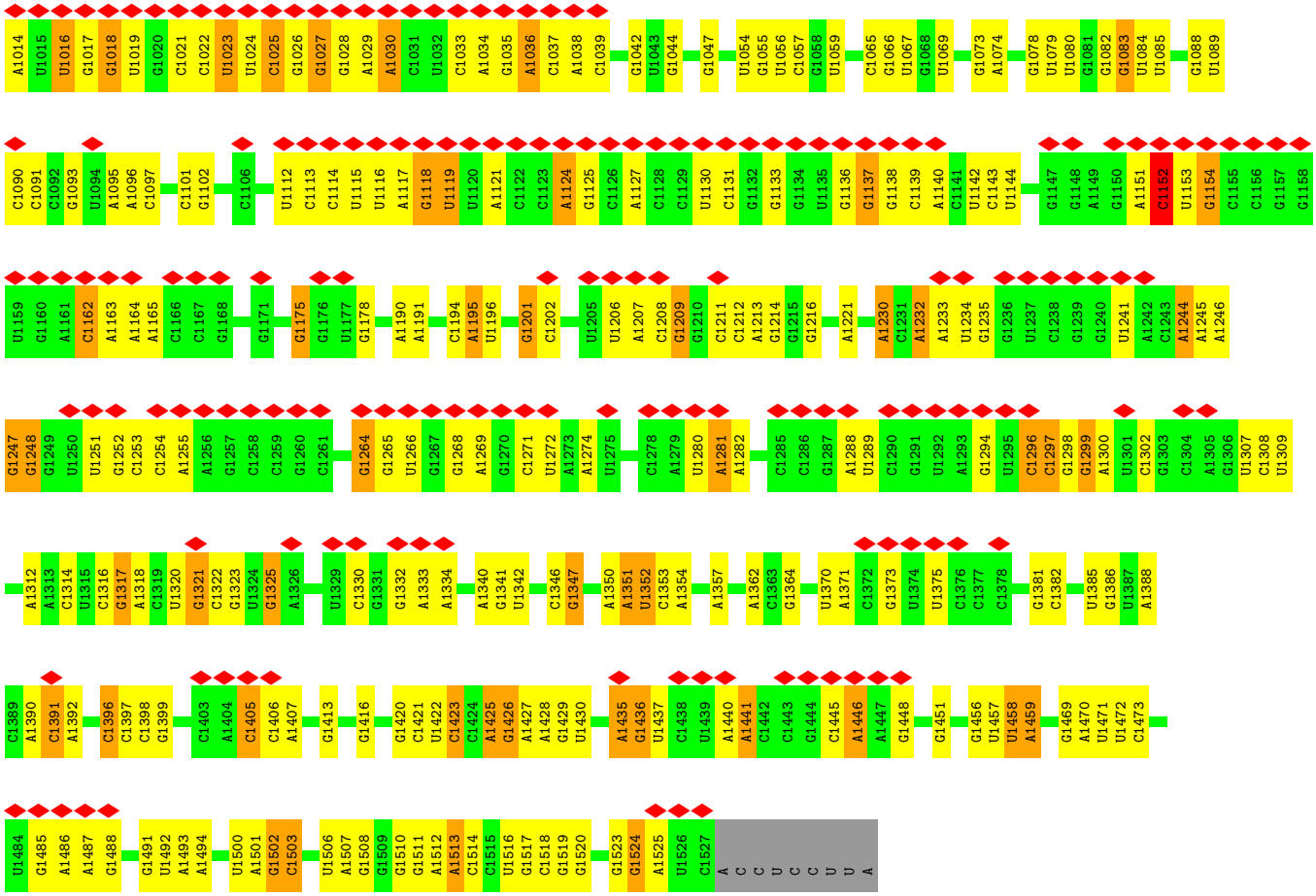


• Molecule 6: 16S rRNA (1527-MER)

Chain A:

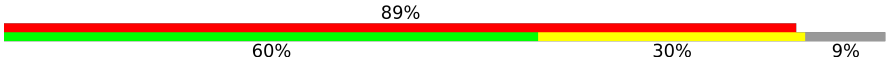






• Molecule 7: Small ribosomal subunit protein uS2

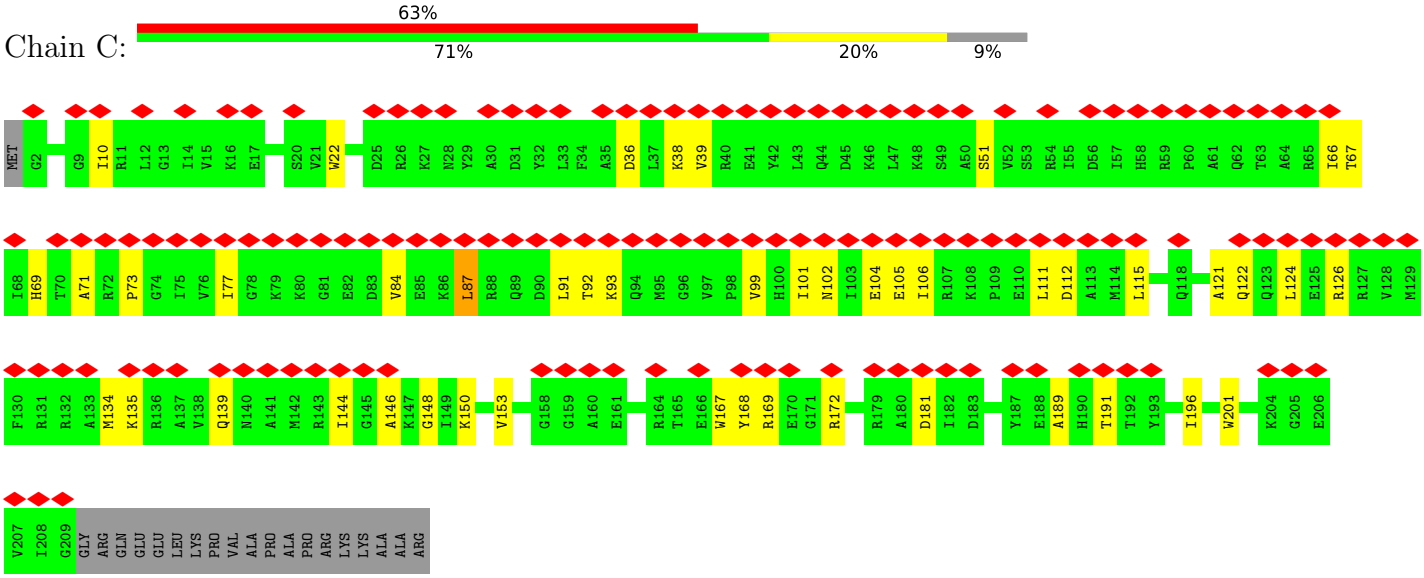
Chain B:





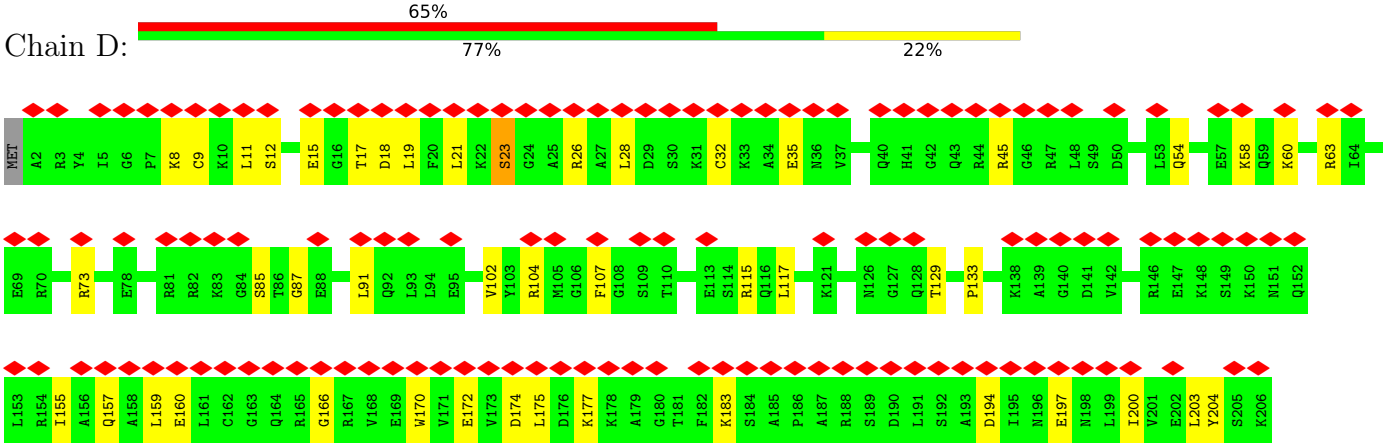
• Molecule 8: Small ribosomal subunit protein uS3

Chain C:



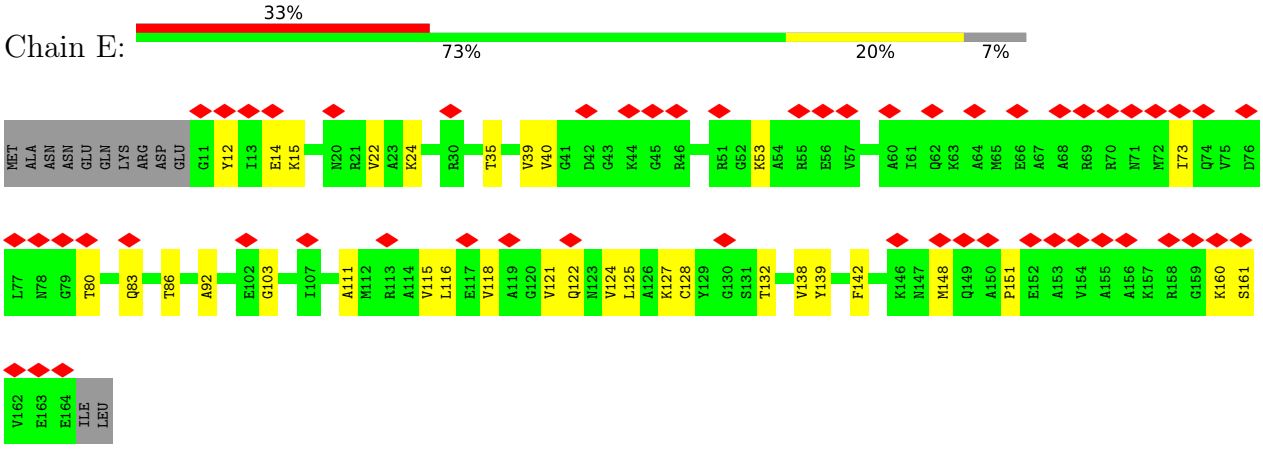
• Molecule 9: Small ribosomal subunit protein uS4

Chain D:



• Molecule 10: Small ribosomal subunit protein uS5

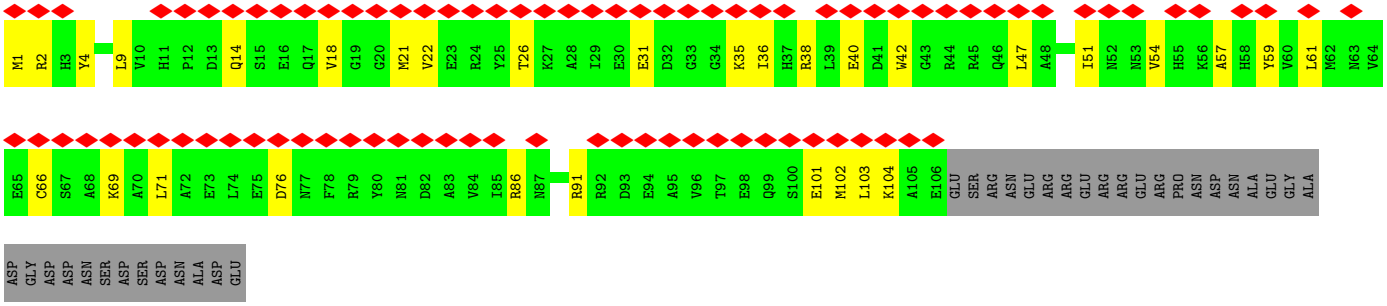
Chain E:



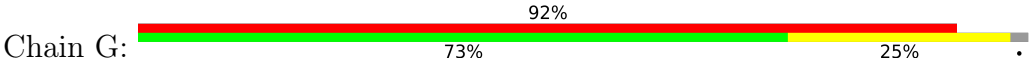
• Molecule 11: Small ribosomal subunit protein bS6

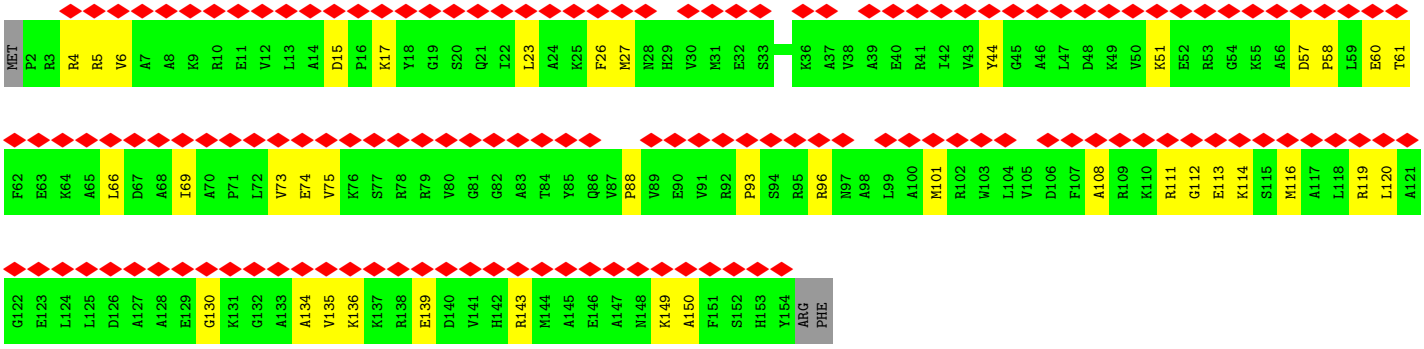
Chain F:



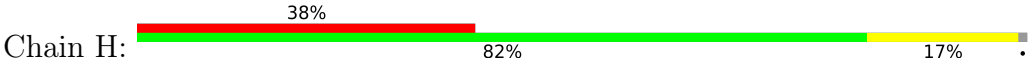


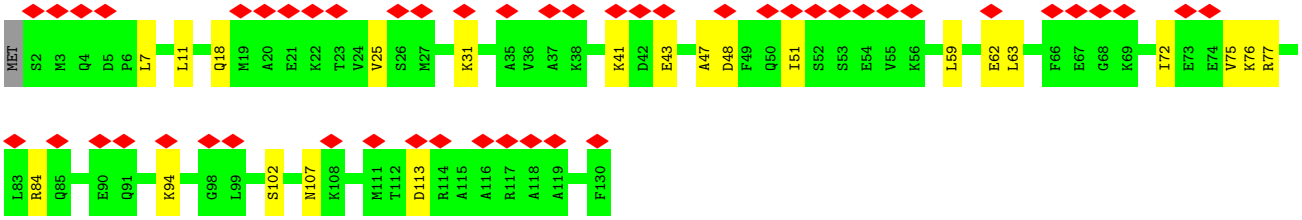
• Molecule 12: Small ribosomal subunit protein uS7



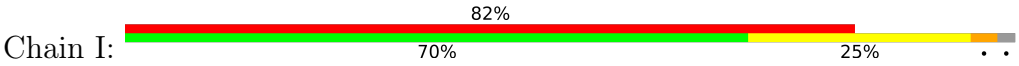


• Molecule 13: Small ribosomal subunit protein uS8





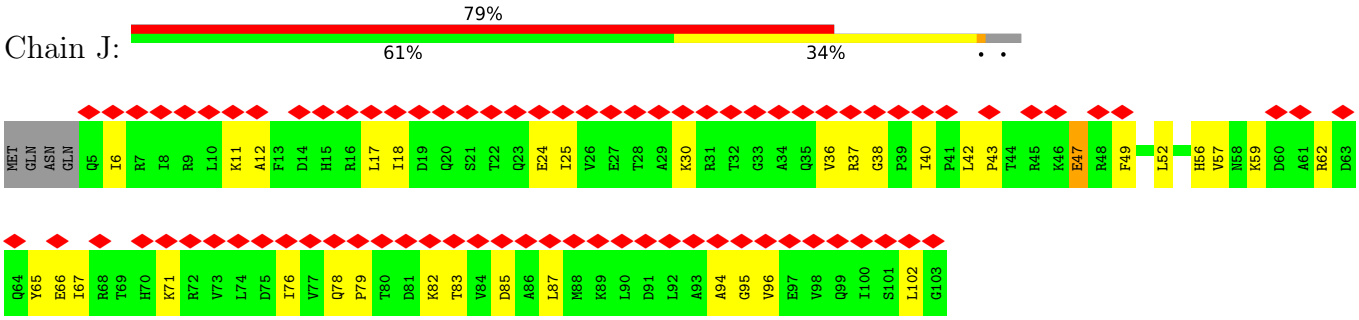
• Molecule 14: Small ribosomal subunit protein uS9





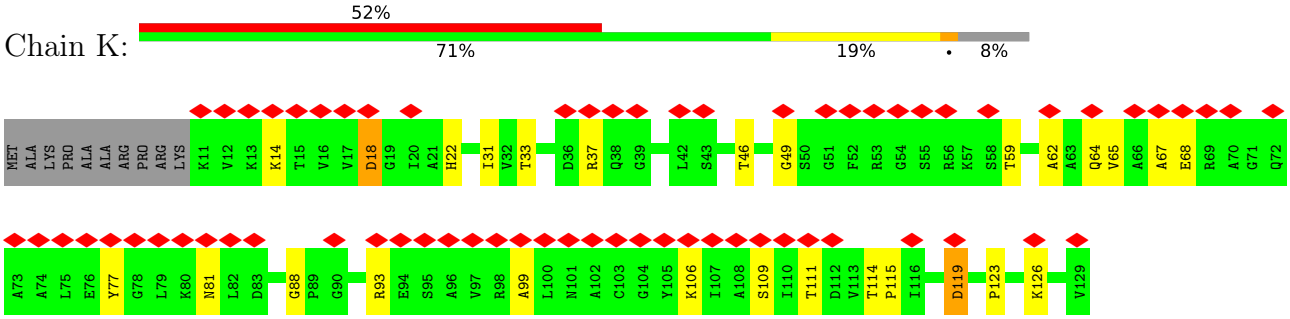
• Molecule 15: Small ribosomal subunit protein uS10

Chain J:



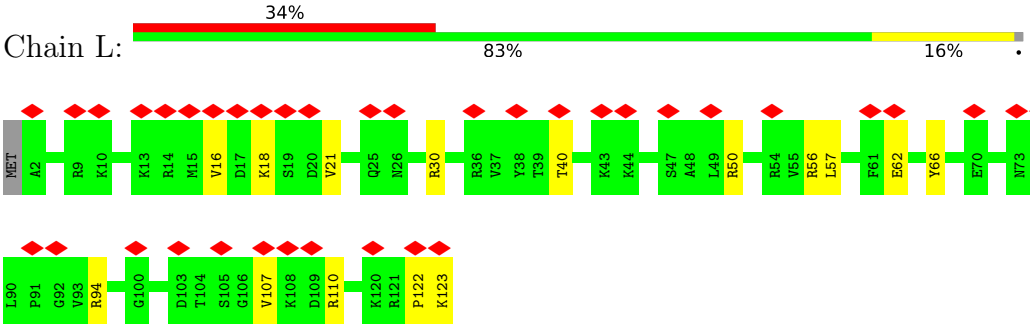
• Molecule 16: Small ribosomal subunit protein uS11

Chain K:



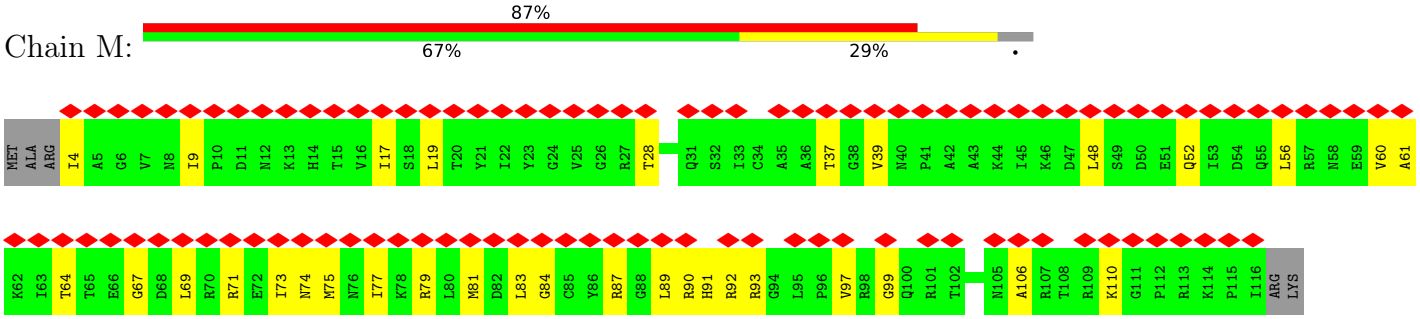
• Molecule 17: Small ribosomal subunit protein uS12

Chain L:



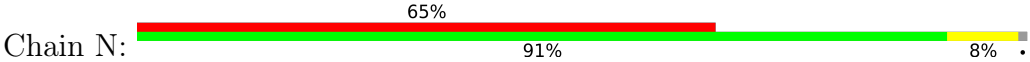
• Molecule 18: Small ribosomal subunit protein uS13

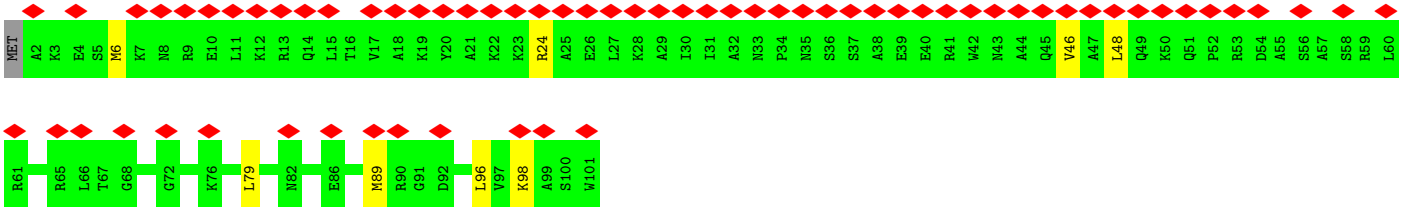
Chain M:



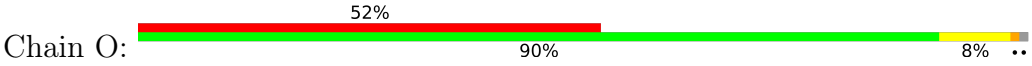
• Molecule 19: Small ribosomal subunit protein uS14

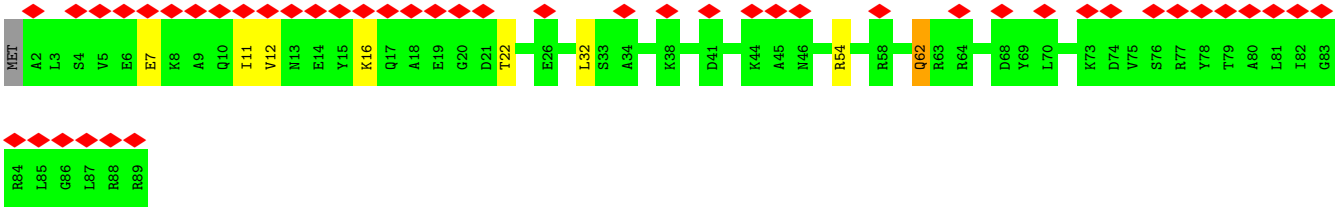
Chain N:



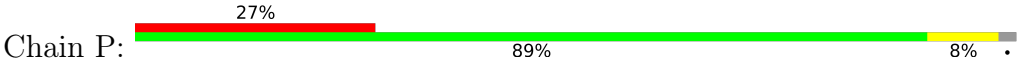


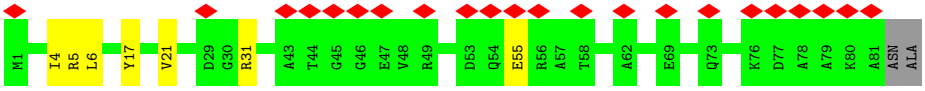
• Molecule 20: Small ribosomal subunit protein uS15





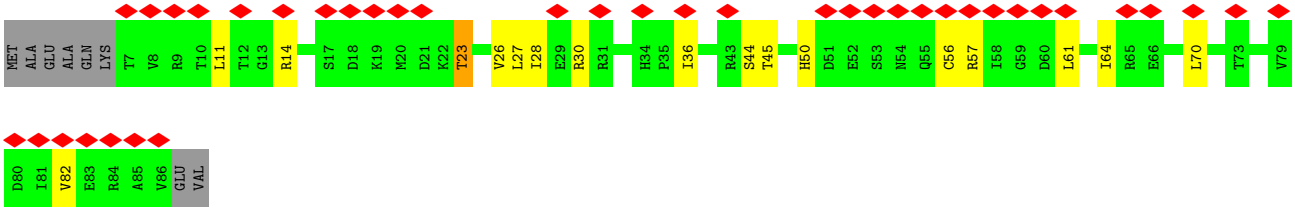
• Molecule 21: Small ribosomal subunit protein bS16





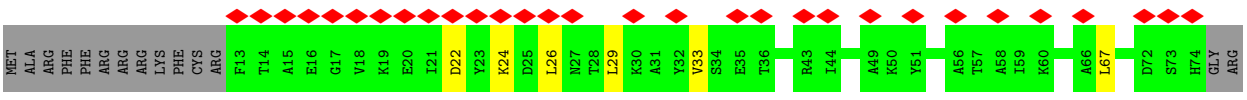
• Molecule 22: Small ribosomal subunit protein uS17



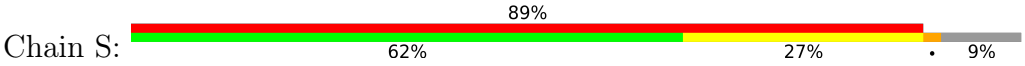


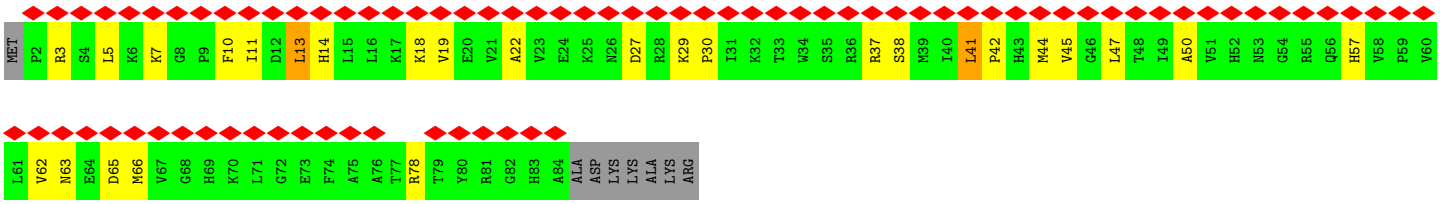
• Molecule 23: Small ribosomal subunit protein bS18





• Molecule 24: Small ribosomal subunit protein uS19

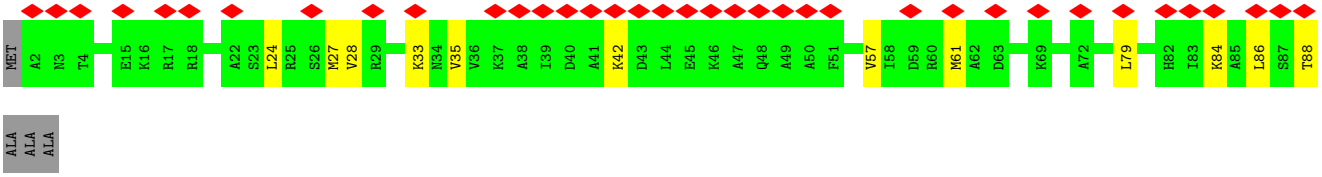




• Molecule 25: Small ribosomal subunit protein bS20

Chain T:

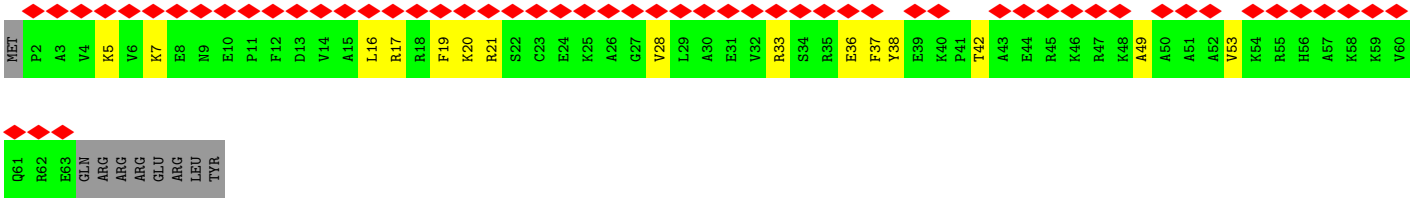




• Molecule 26: Small ribosomal subunit protein bS21

Chain U:

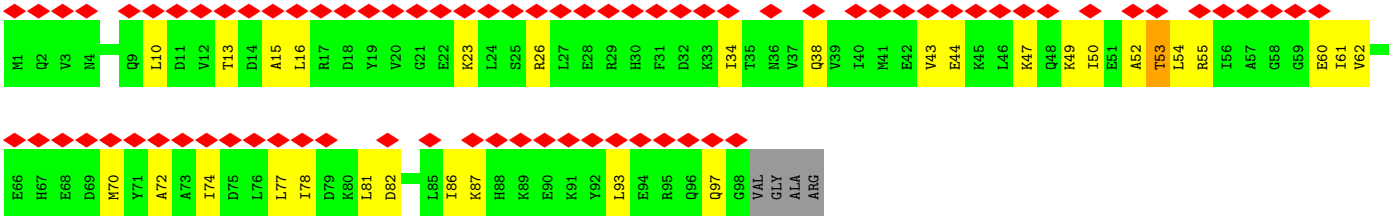




• Molecule 27: Ribosome hibernation promoting factor

Chain X:

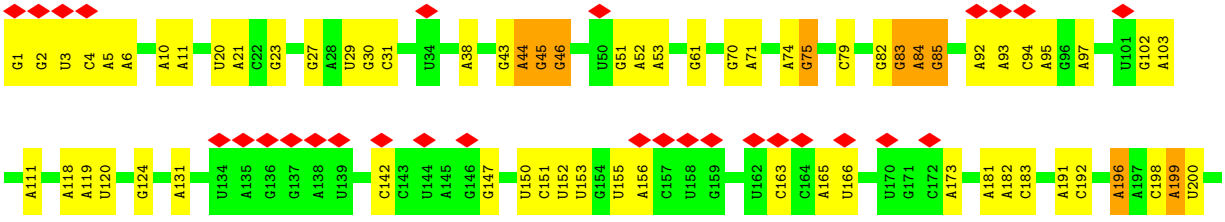


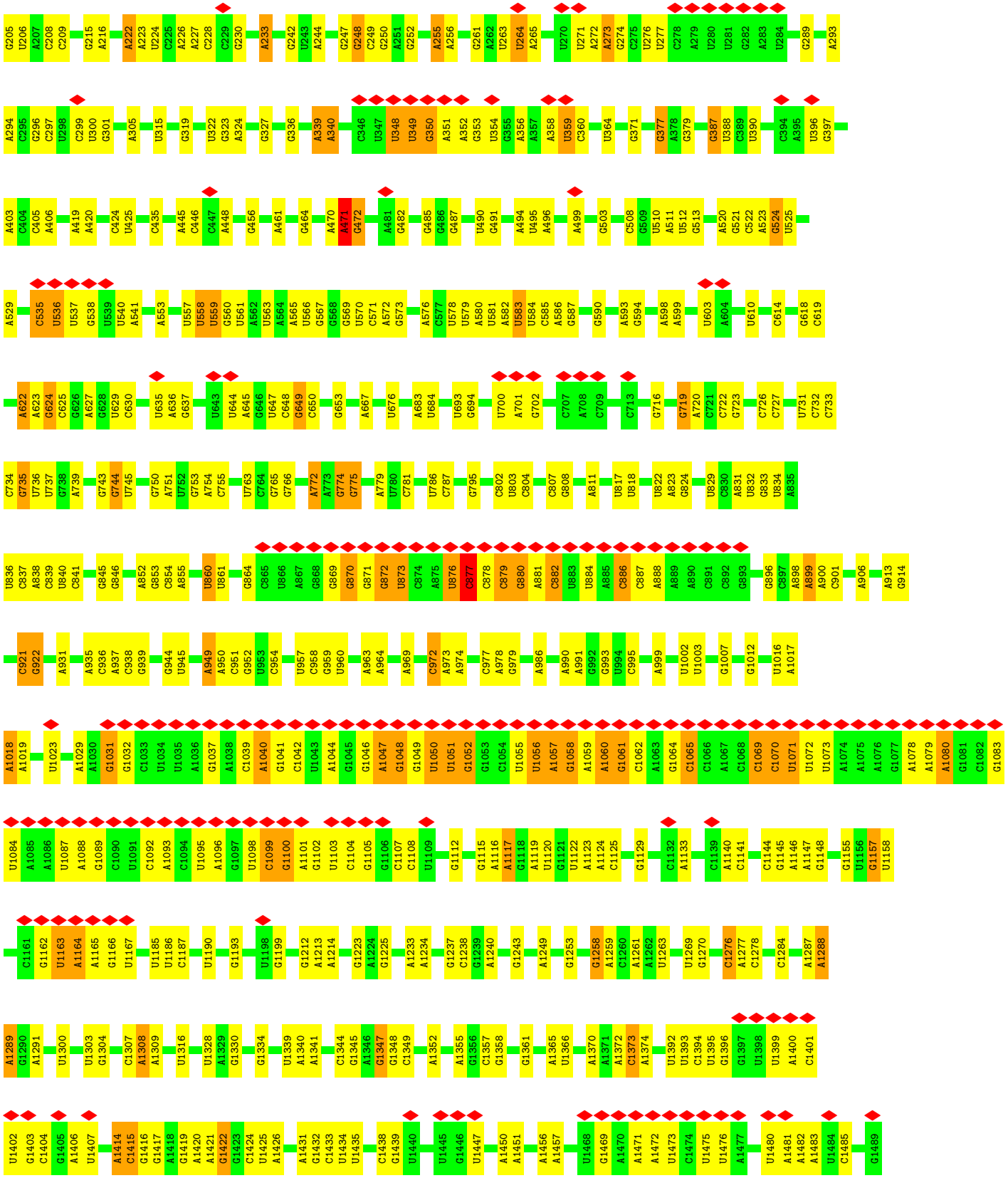


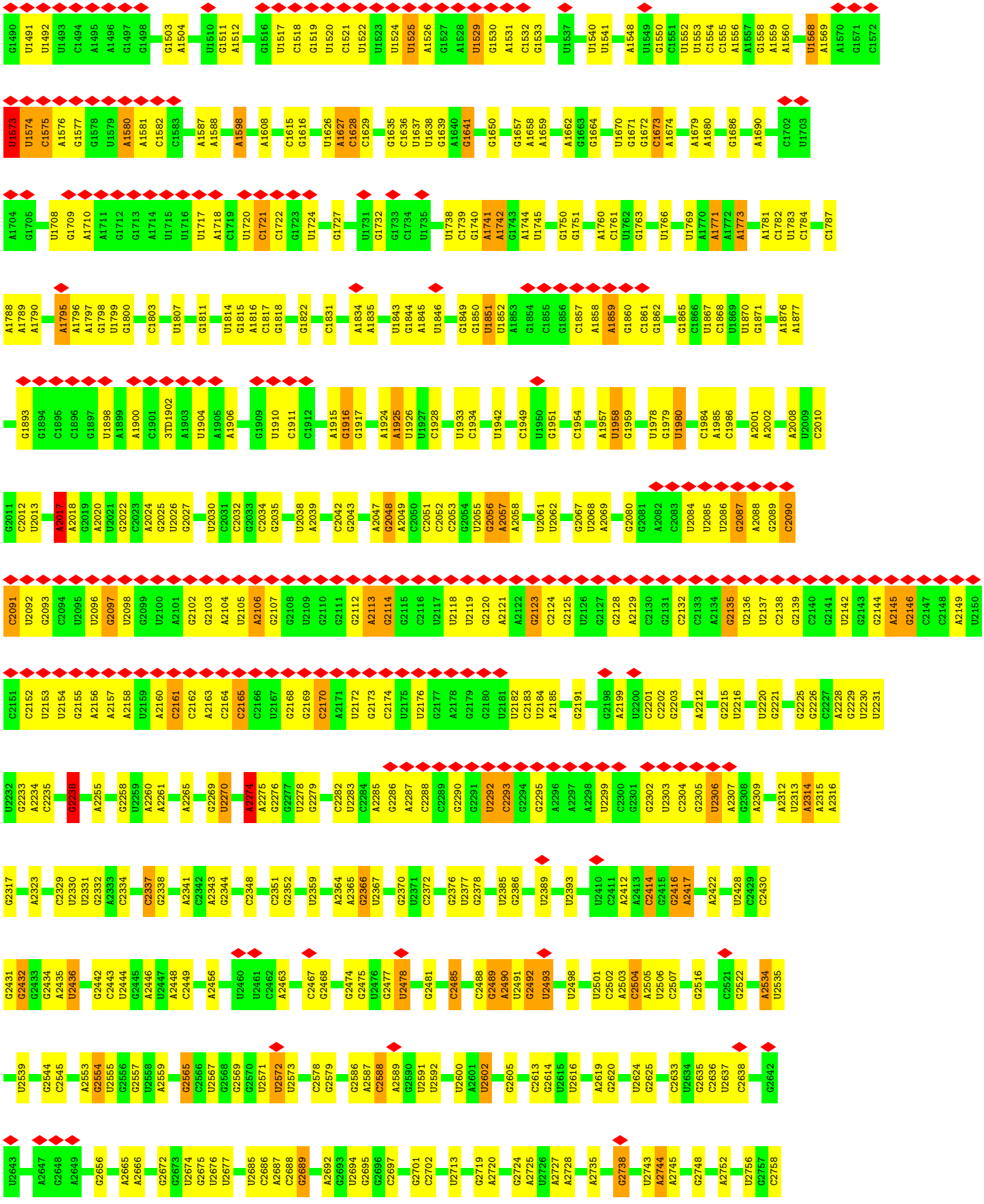
• Molecule 28: 23S rRNA (2890-MER)

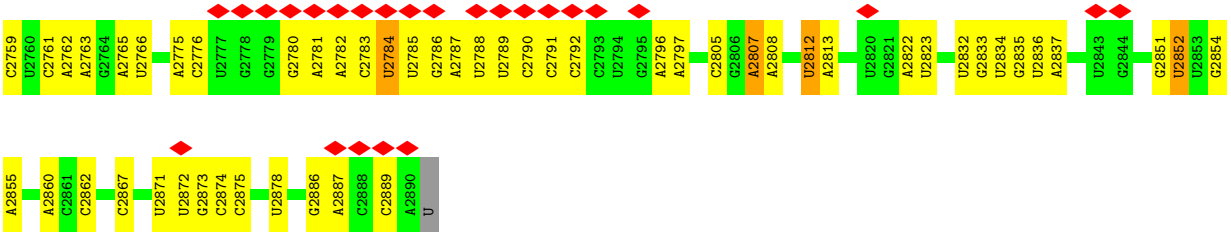
Chain a:







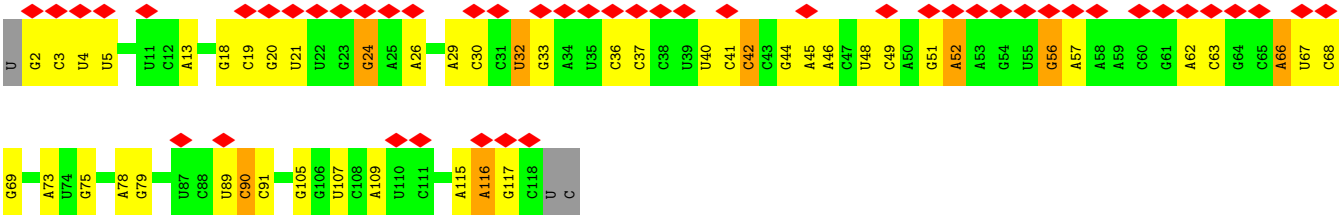

G1490 U1491 U1492 U1493 C1494 A1495 A1496 G1497 G1498 G1503 A1504 U1510 G1511 A1512 G1516 U1517 C1518 G1519 U1520 C1521 U1522 U1523 U1524 U1525 A1526 G1527 A1528 U1529 G1530 A1531 C1532 G1533 U1537 U1540 U1541 A1548 U1549 G1550 C1551 U1552 U1553 C1554 C1555 A1556 A1557 G1558 A1559 A1560 U1568 A1569 A1570 G1571 C1572
U1573 U1574 C1575 A1576 G1577 G1578 U1579 A1580 A1581 C1582 C1583 A1587 A1588 A1598 A1608 C1615 G1616 U1626 A1627 C1628 C1629 G1635 C1636 U1637 U1638 G1639 A1640 G1641 G1650 G1657 A1658 A1659 A1662 G1663 G1664 U1670 G1671 G1672 C1673 A1674 A1679 A1680 G1686 A1690 C1702 U1703
A1704 G1705 U1708 G1709 A1710 A1711 G1712 G1713 A1714 U1715 U1716 U1717 A1718 C1719 U1720 C1721 C1722 G1723 U1724 G1727 U1731 G1732 G1733 C1734 U1735 U1738 C1739 G1740 A1741 A1742 G1743 A1744 U1745 G1750 G1751 A1760 C1761 U1762 G1763 U1766 U1769 A1770 A1771 A1772 A1773 A1781 C1782 U1783 C1784 C1787
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G2011 C2012 U2013 A2017 A2018 G2019 A2020 U2021 G2022 C2023 A2024 G2025 U2026 G2027 U2030 C2031 C2032 G2033 C2034 G2035 U2038 A2039 C2042 G2043 A2047 G2048 A2049 C2050 C2051 C2052 C2053 G2054 U2055 G2056 A2057 A2058 U2061 U2062 G2067 U2068 A2069 G2080 G2081 A2082 C2083 U2084 U2085 U2086 G2087 A2088 G2089 C2090
C2091 U2092 G2093 C2094 U2095 U2096 G2097 U2098 G2099 U2100 A2101 G2102 G2103 A2104 U2105 A2106 G2107 G2108 U2109 G2110 G2111 G2112 A2113 G2114 G2115 C2116 U2117 U2118 U2119 G2120 A2121 A2122 G2123 C2124 G2125 U2126 G2127 G2128 A2129 C2130 G2131 C2132 C2133 A2134 G2135 U2136 U2137 C2138 G2139 C2140 G2141 U2142 G2143 G2144 A2145 G2146 C2147 C2148 A2149 U2150
C2151 C2152 U2153 U2154 G2155 A2156 A2157 A2158 U2159 A2160 C2161 C2162 A2163 C2164 C2165 C2166 U2167 G2168 G2169 C2170 A2171 U2172 G2173 C2174 U2175 U2176 G2177 A2178 G2179 G2180 U2181 U2182 C2183 U2184 A2185 G2191 G2198 A2199 U2200 C2201 C2202 G2203 A2212 G2215 U2216 U2220 G2221 G2225 G2226 C2227 A2228 G2229 U2230 U2231
U2232 G2233 A2234 C2235 G2238 A2255 G2258 U2259 A2260 A2261 A2265 G2269 U2270 A2274 A2275 G2276 G2277 U2278 G2279 C2282 U2283 C2284 A2285 G2286 A2287 C2288 C2289 G2290 G2291 U2292 C2293 G2294 G2295 A2296 A2297 A2298 U2299 C2300 G2301 G2302 U2303 C2304 G2305 U2306 A2307 G2308 A2309 A2312 U2313 A2314 A2315 A2316
G2317 A2323 C2329 U2330 U2331 G2332 A2333 C2334 C2337 G2338 A2341 C2342 A2343 G2344 C2348 C2351 G2352 U2359 A2364 A2365 G2366 U2367 G2370 U2371 C2372 G2376 U2377 G2378 U2385 G2386 U2389 U2393 U2410 C2411 A2412 A2413 C2414 G2415 G2416 A2417 A2422 U2428 C2429 C2430
G2431 G2432 G2433 G2434 A2435 U2436 G2442 C2443 U2444 G2445 A2446 U2447 A2448 C2449 A2456 U2460 U2461 C2462 A2463 C2467 G2468 G2474 G2475 U2476 G2477 U2478 G2481 C2485 C2488 G2489 A2490 U2491 G2492 U2493 U2498 U2501 C2502 A2503 C2504 A2505 U2506 C2507 G2516 C2521 G2522 A2534 U2535
U2539 G2544 C2545 A2553 G2554 U2555 G2556 G2557 U2558 A2559 G2565 C2566 U2567 G2568 G2569 G2570 U2571 U2572 U2573 C2578 G2579 G2586 A2587 C2588 A2589 G2590 U2591 U2592 U2600 A2601 U2602 G2605 C2613 G2614 U2615 U2616 A2619 G2620 U2624 G2625 C2633 U2634 G2635 C2636 U2637 C2638 G2642
U2643 A2647 G2648 A2649 G2656 A2665 A2666 G2672 G2673 U2674 G2675 U2676 U2677 U2685 C2686 A2687 C2688 G2689 A2692 G2693 U2694 G2695 G2696 C2697 G2701 C2702 U2713 G2719 A2720 G2724 A2725 U2726 A2727 A2728 A2735 G2738 U2743 A2744 A2745 G2748 A2752 U2756 G2757 C2758



• Molecule 29: 5S rRNA (117-MER)

Chain b:

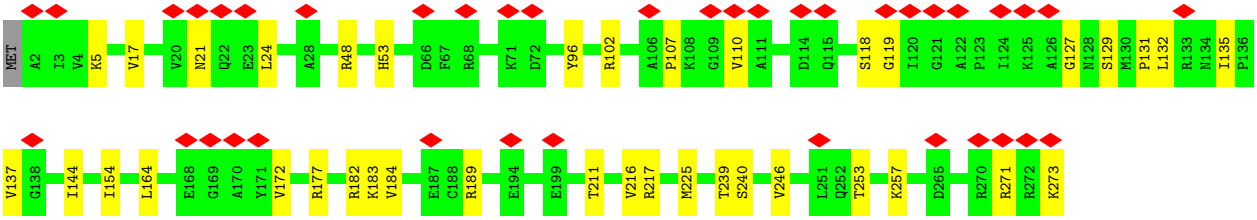




• Molecule 30: Large ribosomal subunit protein uL2

Chain c:

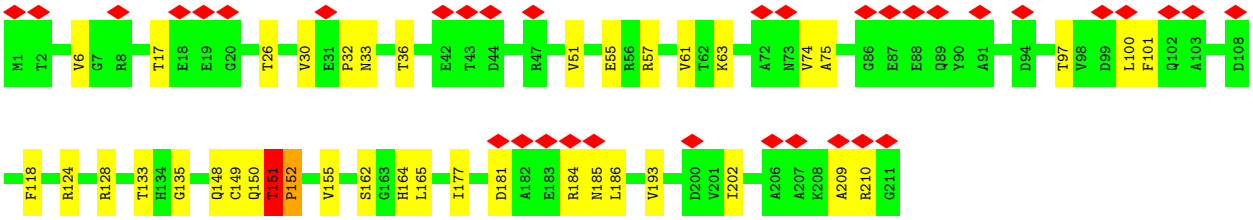




• Molecule 31: Large ribosomal subunit protein uL3

Chain d:

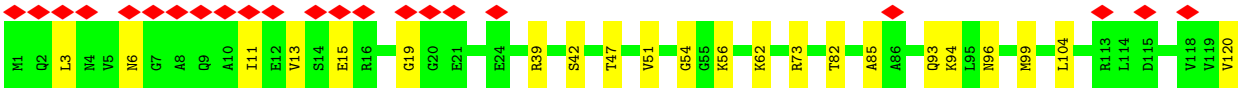




• Molecule 32: Large ribosomal subunit protein uL4

Chain e:

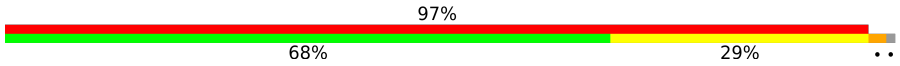


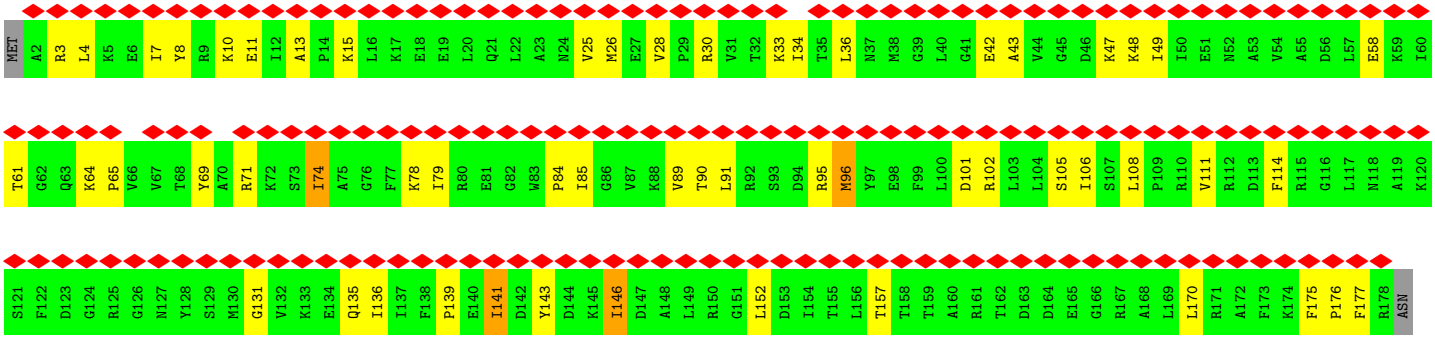




• Molecule 33: Large ribosomal subunit protein uL5

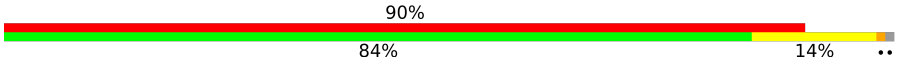
Chain f:

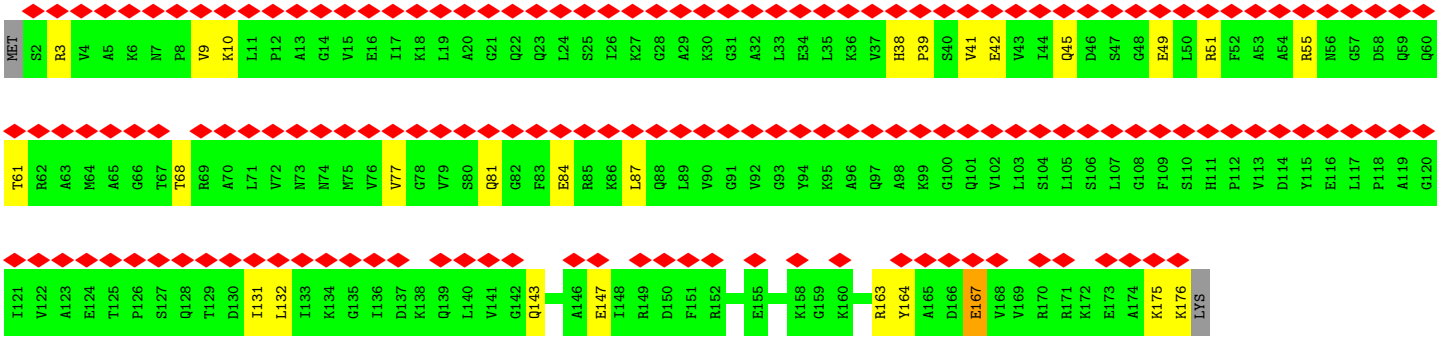




• Molecule 34: Large ribosomal subunit protein uL6

Chain g:

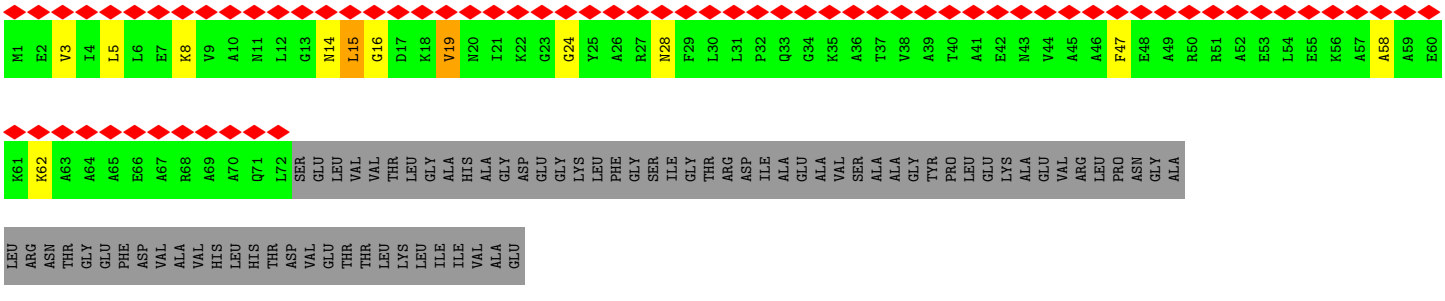




• Molecule 35: Large ribosomal subunit protein bL9

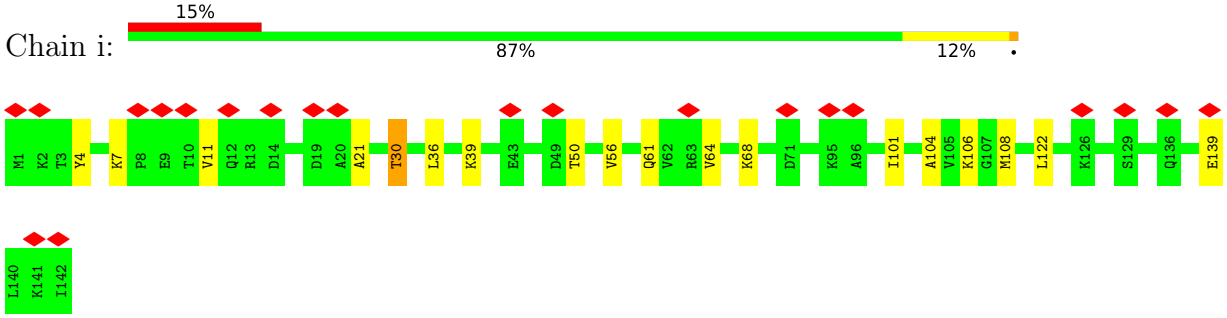
Chain h:





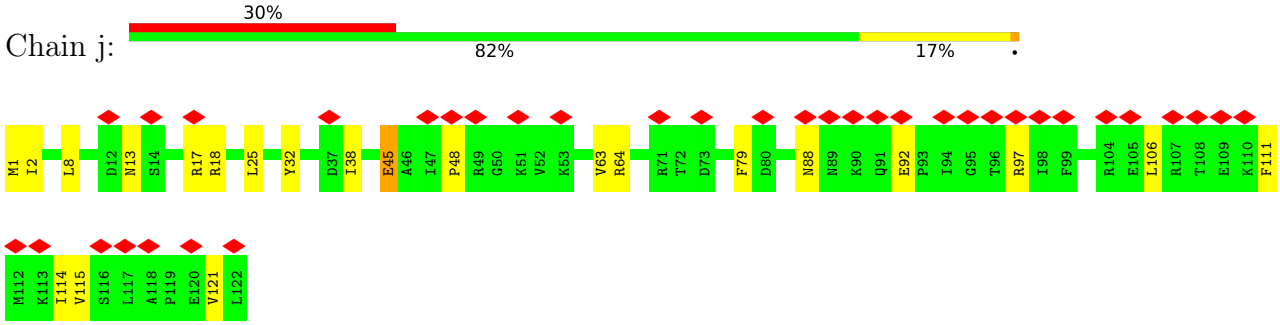
• Molecule 36: Large ribosomal subunit protein uL13

Chain i:



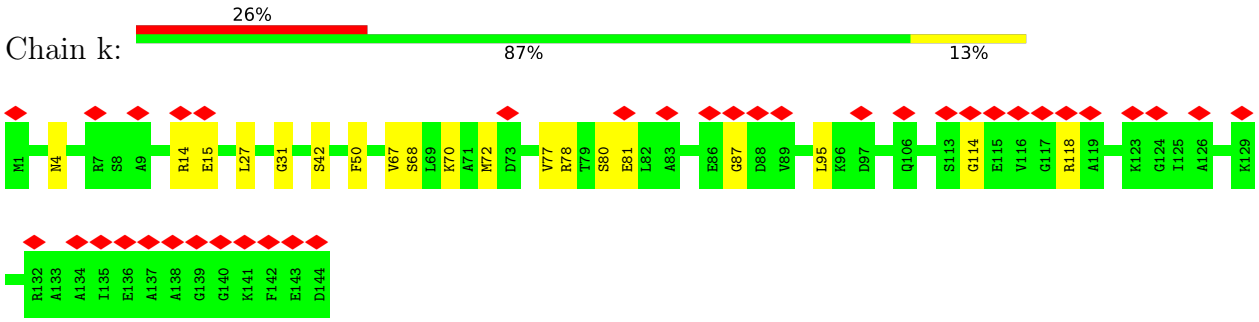
• Molecule 37: Large ribosomal subunit protein uL14

Chain j:



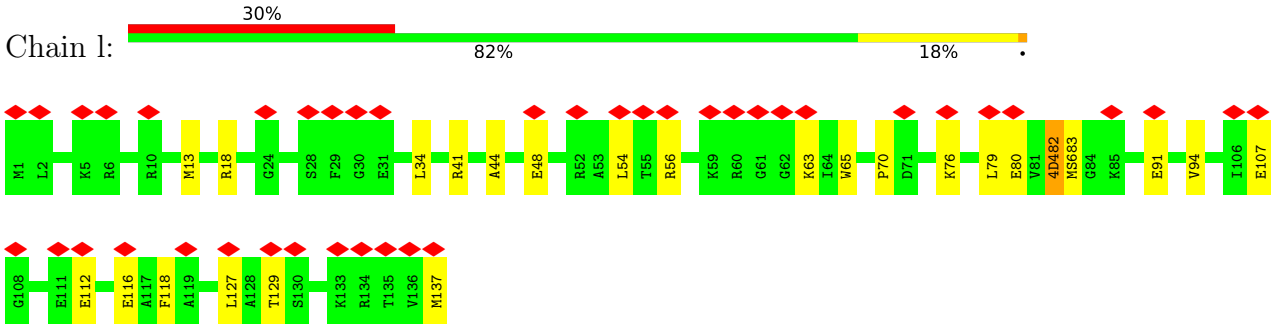
• Molecule 38: Large ribosomal subunit protein uL15

Chain k:



• Molecule 39: Large ribosomal subunit protein uL16

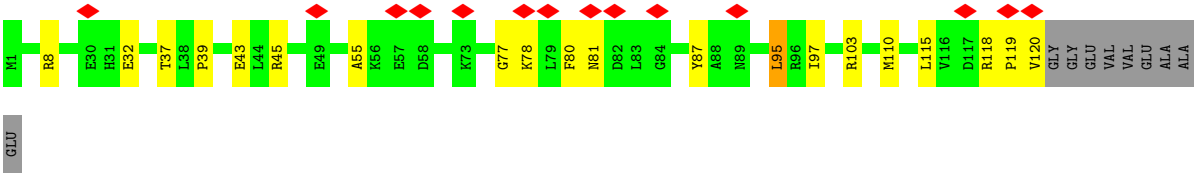
Chain l:



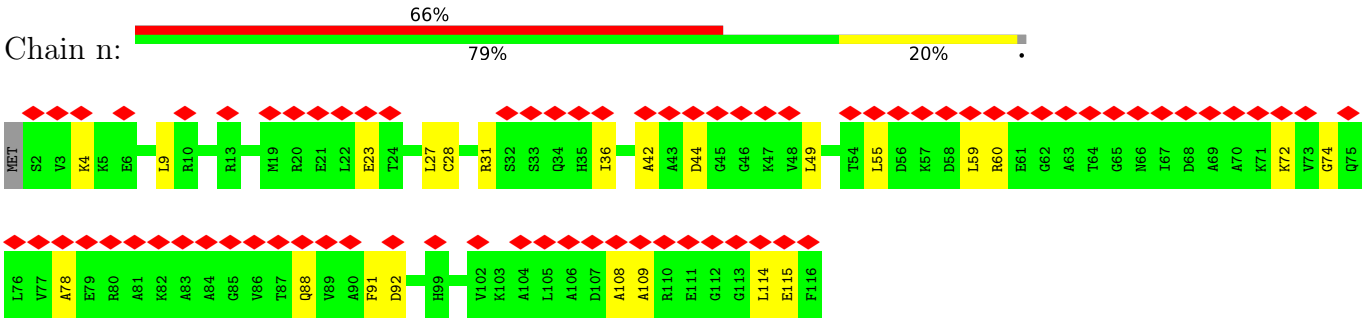
• Molecule 40: Large ribosomal subunit protein bL17

Chain m:

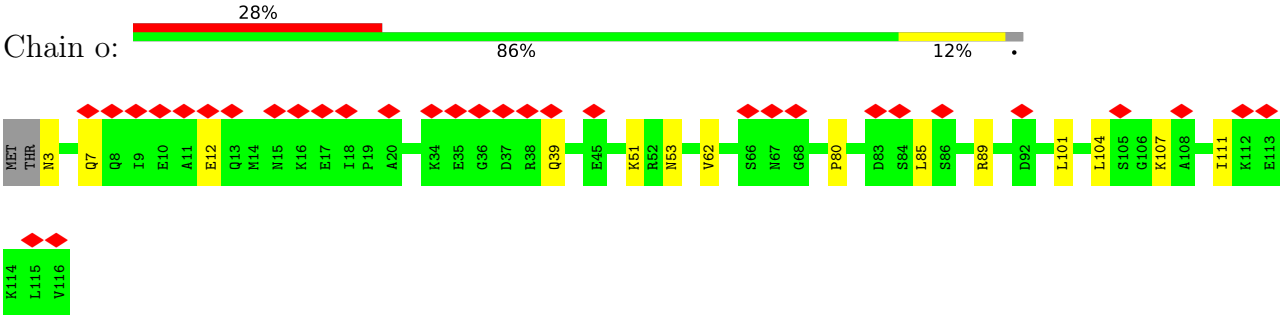




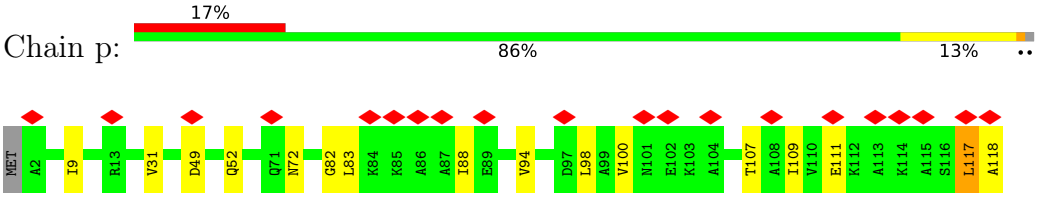
• Molecule 41: Large ribosomal subunit protein uL18



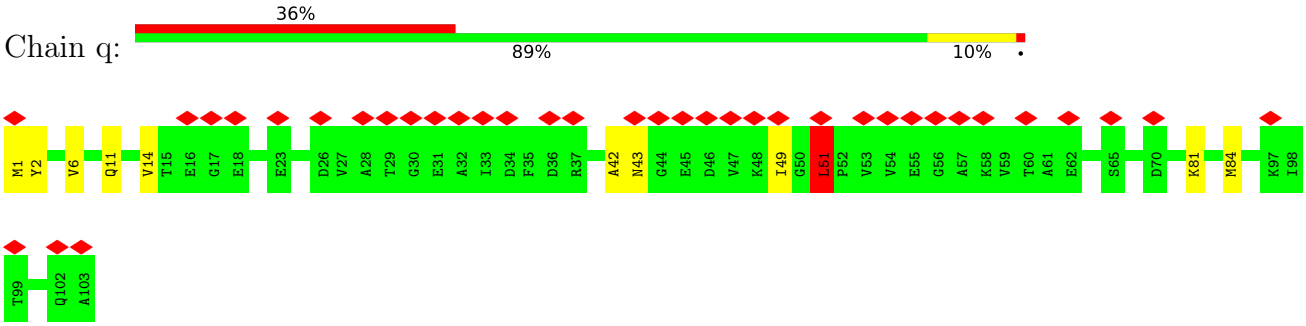
• Molecule 42: Large ribosomal subunit protein bL19



• Molecule 43: Large ribosomal subunit protein bL20

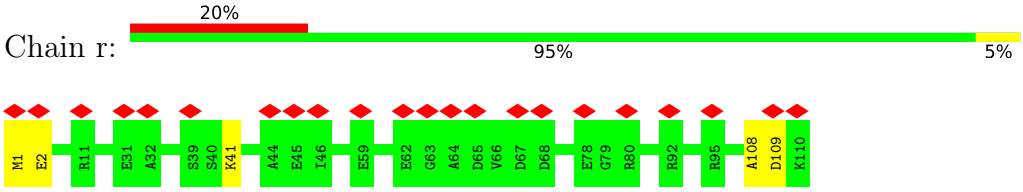


• Molecule 44: Large ribosomal subunit protein bL21



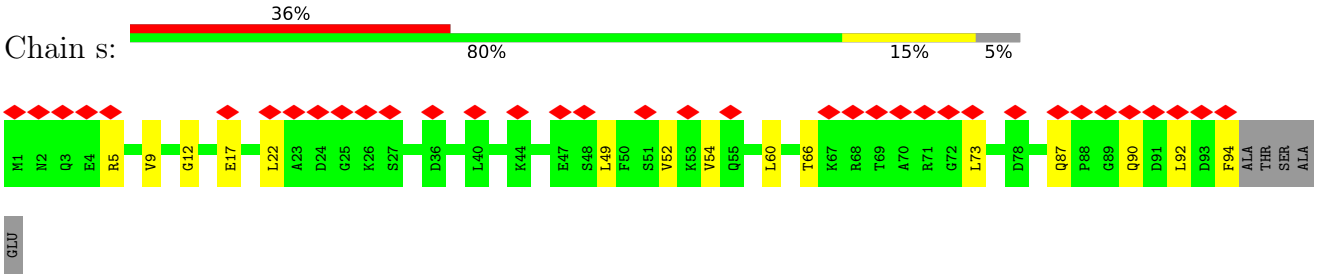
• Molecule 45: Large ribosomal subunit protein uL22

Chain r:



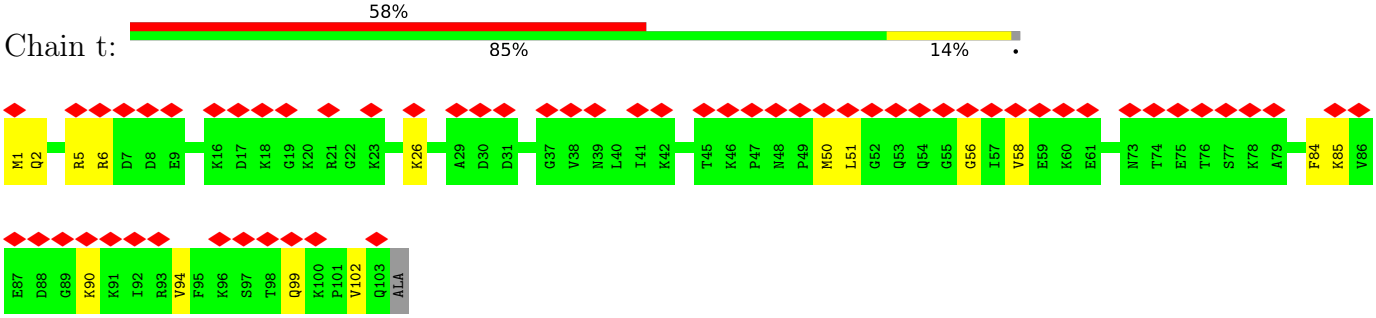
• Molecule 46: Large ribosomal subunit protein uL23

Chain s:



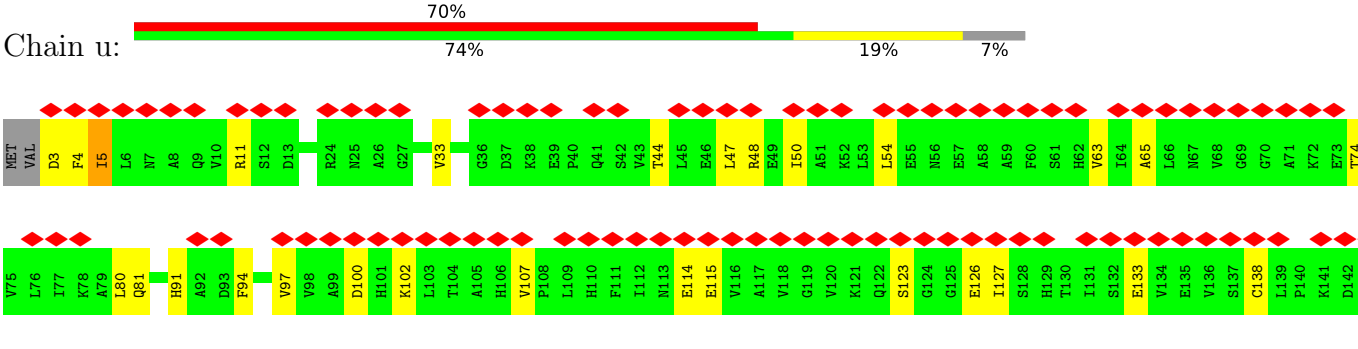
• Molecule 47: Large ribosomal subunit protein uL24

Chain t:



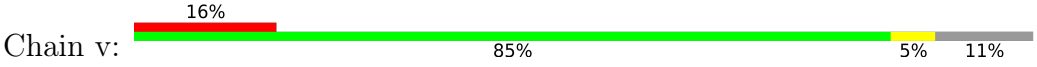
• Molecule 48: Large ribosomal subunit protein bL25

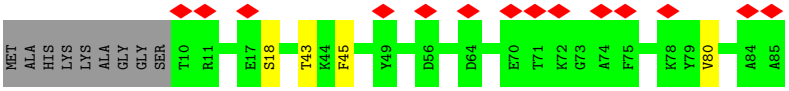
Chain u:



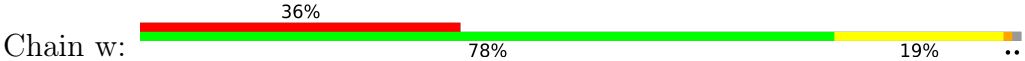
• Molecule 49: Large ribosomal subunit protein bL27

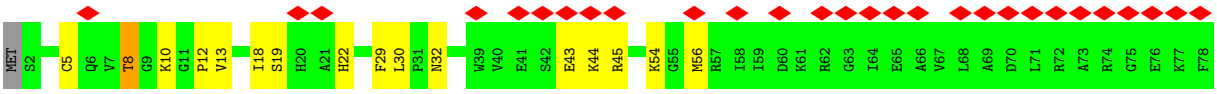
Chain v:



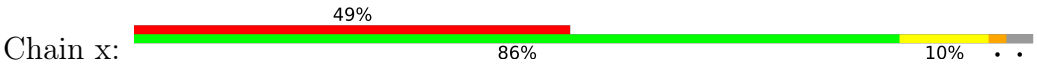


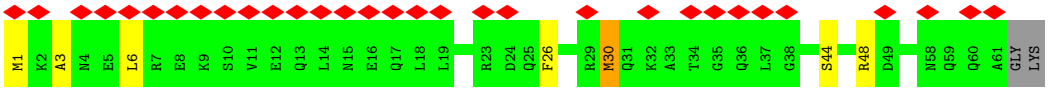
• Molecule 50: Large ribosomal subunit protein bL28



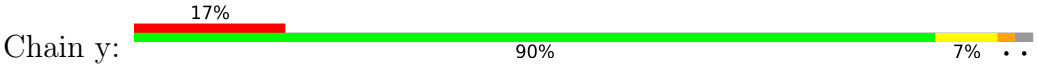


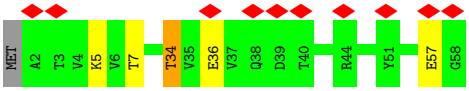
• Molecule 51: Large ribosomal subunit protein uL29



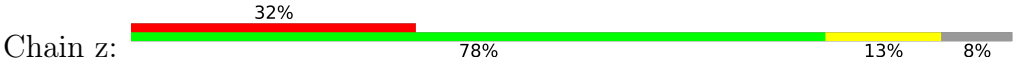


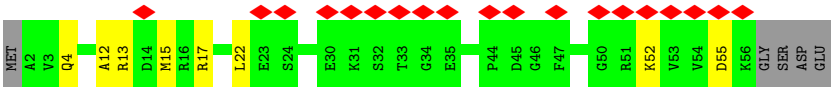
• Molecule 52: Large ribosomal subunit protein uL30





• Molecule 53: Large ribosomal subunit protein bL32





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	50773	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	2.311	Depositor
Minimum map value	-0.980	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.073	Depositor
Recommended contour level	0.55	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: IAS, 4OC, MG, MS6, 5MU, 2MG, 7MG, G7M, ZN, OMC, 2MA, H2U, K, OMG, PSU, 5MC, 1MG, UR3, 3TD, 4D4, MEQ, 6MZ, OMU, MA6, D2T

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	0.18	0/433	0.34	0/576
2	1	0.22	0/368	0.32	0/482
3	2	0.19	0/511	0.29	0/668
4	3	0.19	0/308	0.30	0/404
5	4	0.16	0/542	0.48	0/728
6	A	0.43	0/36453	0.74	10/56863 (0.0%)
7	B	0.16	0/1791	0.38	0/2405
8	C	0.17	0/1693	0.33	0/2279
9	D	0.16	0/1646	0.35	1/2201 (0.0%)
10	E	0.19	0/1148	0.38	0/1544
11	F	0.16	0/882	0.38	0/1186
12	G	0.15	0/1217	0.31	0/1627
13	H	0.18	0/993	0.32	0/1332
14	I	0.16	0/1022	0.35	0/1365
15	J	0.20	0/803	0.42	0/1083
16	K	0.18	0/889	0.36	0/1199
17	L	0.18	0/964	0.33	0/1289
18	M	0.16	0/892	0.35	0/1199
19	N	0.17	0/816	0.34	0/1087
20	O	0.17	0/710	0.27	0/947
21	P	0.18	0/648	0.30	0/872
22	Q	0.16	0/653	0.31	0/881
23	R	0.17	0/502	0.31	0/677
24	S	0.14	0/678	0.30	0/912
25	T	0.21	0/678	0.30	0/904
26	U	0.16	0/513	0.41	0/680
27	X	0.19	0/803	0.39	0/1075
28	a	0.49	0/68901	0.74	16/107478 (0.0%)
29	b	0.38	0/2789	0.71	1/4345 (0.0%)
30	c	0.21	0/2108	0.31	0/2831
31	d	0.22	0/1601	0.41	1/2152 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	e	0.21	0/1544	0.36	0/2079
33	f	0.16	0/1439	0.39	0/1932
34	g	0.15	0/1344	0.36	0/1809
35	h	0.10	0/536	0.28	0/719
36	i	0.20	0/1156	0.31	0/1559
37	j	0.20	0/947	0.30	0/1268
38	k	0.18	0/1078	0.29	0/1436
39	l	0.20	0/1085	0.34	0/1449
40	m	0.21	0/975	0.33	0/1304
41	n	0.18	0/888	0.35	0/1183
42	o	0.20	0/911	0.29	0/1218
43	p	0.22	0/946	0.30	0/1257
44	q	0.20	0/835	0.36	0/1117
45	r	0.19	0/837	0.33	0/1114
46	s	0.18	0/749	0.36	0/1002
47	t	0.17	0/808	0.39	0/1079
48	u	0.18	0/1469	0.34	0/1988
49	v	0.22	0/583	0.34	0/774
50	w	0.21	0/641	0.32	0/854
51	x	0.17	0/491	0.33	0/654
52	y	0.19	0/449	0.34	0/602
53	z	0.21	0/446	0.35	0/594
All	All	0.40	0/154112	0.66	29/230262 (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
31	d	0	1
39	l	0	1
44	q	0	1
All	All	0	3

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	a	2087	G	OP1-P-O3'	-11.03	74.91	108.00
28	a	2087	G	OP2-P-O3'	-10.27	77.19	108.00
6	A	1000	C	N3-C2-O2	-7.73	116.49	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	a	359	U	C2-N1-C1'	7.54	126.75	117.70
28	a	1300	U	C2-N1-C1'	7.15	126.28	117.70
31	d	151	THR	C-N-CD	-7.00	96.29	125.00
6	A	1000	C	N1-C2-O2	6.88	123.03	118.90
28	a	359	U	N1-C2-O2	6.56	127.39	122.80
28	a	503	G	O4'-C1'-N9	6.03	113.03	108.20
28	a	359	U	N3-C2-O2	-6.02	117.99	122.20
28	a	879	C	O4'-C1'-N1	5.97	112.68	108.50
28	a	1573	U	O5'-C5'-C4'	5.92	114.13	109.40
28	a	877	C	O4'-C1'-N1	5.74	112.52	108.50
6	A	6	G	P-O3'-C3'	5.63	126.46	119.70
6	A	1405	C	C2-N1-C1'	5.59	124.95	118.80
6	A	748	C	C2-N1-C1'	5.51	124.86	118.80
28	a	860	U	O5'-C5'-C4'	5.34	113.67	109.40
28	a	348	U	C2-N1-C1'	5.28	124.03	117.70
28	a	1300	U	N1-C2-O2	5.23	126.46	122.80
6	A	631	C	C2-N1-C1'	5.22	124.54	118.80
9	D	166	GLY	N-CA-C	5.17	117.33	111.85
6	A	1152	C	C2-N1-C1'	5.17	124.49	118.80
28	a	471	A	O5'-C5'-C4'	5.15	113.52	109.40
6	A	322	C	P-O3'-C3'	5.15	125.88	119.70
6	A	1503	C	C2-N1-C1'	5.05	124.36	118.80
29	b	42	C	C2-N1-C1'	5.05	124.35	118.80
28	a	1300	U	N3-C2-O2	-5.03	118.68	122.20
28	a	2274	A	P-O3'-C3'	5.01	125.71	119.70
6	A	490	A	O4'-C1'-N9	5.00	112.00	108.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
31	d	151	THR	Peptide
39	l	82	4D4	Mainchain
44	q	51	LEU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	426	0	457	8	0
2	1	365	0	409	4	0
3	2	506	0	569	4	0
4	3	307	0	342	2	0
5	4	531	0	529	20	0
6	A	32783	0	16501	372	0
7	B	1763	0	1811	44	0
8	C	1664	0	1723	27	0
9	D	1627	0	1665	27	0
10	E	1134	0	1181	24	0
11	F	868	0	846	21	0
12	G	1199	0	1253	24	0
13	H	982	0	1036	14	0
14	I	1010	0	1052	25	0
15	J	793	0	833	28	0
16	K	882	0	897	19	0
17	L	961	0	1010	9	0
18	M	883	0	929	25	0
19	N	804	0	841	5	0
20	O	703	0	727	4	0
21	P	637	0	648	4	0
22	Q	645	0	689	12	0
23	R	494	0	514	4	0
24	S	663	0	697	25	0
25	T	671	0	722	7	0
26	U	506	0	535	13	0
27	X	796	0	818	26	0
28	a	62019	0	31187	556	0
29	b	2495	0	1263	28	0
30	c	2072	0	2152	25	0
31	d	1589	0	1605	21	0
32	e	1524	0	1582	27	0
33	f	1418	0	1486	41	0
34	g	1326	0	1388	15	0
35	h	533	0	560	7	0
36	i	1130	0	1160	11	0
37	j	938	0	1012	12	0
38	k	1066	0	1112	10	0
39	l	1086	0	1145	15	0
40	m	959	0	1005	12	0
41	n	881	0	920	12	0
42	o	902	0	960	10	0
43	p	936	0	1025	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	q	822	0	858	7	0
45	r	833	0	897	4	0
46	s	739	0	788	9	0
47	t	800	0	863	7	0
48	u	1446	0	1486	22	0
49	v	575	0	598	2	0
50	w	630	0	653	12	0
51	x	490	0	520	5	0
52	y	445	0	472	3	0
53	z	440	0	437	6	0
54	3	1	0	0	0	0
54	4	1	0	0	0	0
55	A	93	0	0	0	0
55	M	1	0	0	0	0
55	X	1	0	0	0	0
55	a	251	0	0	0	0
55	b	5	0	0	0	0
55	c	1	0	0	0	0
55	p	1	0	0	0	0
55	z	1	0	0	0	0
56	A	49	0	0	0	0
56	a	114	0	0	0	0
56	b	1	0	0	0	0
56	c	3	0	0	0	0
56	e	1	0	0	0	0
56	f	1	0	0	0	0
All	All	143222	0	96368	1564	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 (1564) 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)
6:A:74:A:H62	6:A:89:G:N2	1.53	1.06
6:A:74:A:N6	6:A:89:G:H21	1.60	0.98
6:A:75:G:H1	6:A:88:U:H3	1.14	0.94
28:a:1834:A:HO2'	28:a:1835:A:H8	1.06	0.92
6:A:74:A:H62	6:A:89:G:H21	0.92	0.92
5:4:51:LEU:HD23	5:4:52:ASP:H	1.33	0.90
28:a:1095:U:H2'	28:a:1096:A:H8	1.34	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:2128:G:H1	28:a:2137:U:H3	1.17	0.89
6:A:1080:U:H3	6:A:1093:G:H22	1.24	0.85
7:B:57:VAL:HG21	7:B:217:MET:HE1	1.58	0.84
28:a:2414:C:H5"	28:a:2416:G:H5'	1.60	0.83
12:G:113:GLU:HB2	12:G:119:ARG:HG2	1.62	0.82
6:A:969:A:H4'	6:A:970:G:H5"	1.62	0.81
12:G:150:ALA:HB1	16:K:59:THR:HG21	1.63	0.80
9:D:159:LEU:HD13	9:D:175:LEU:HG	1.64	0.80
53:z:52:LYS:HE3	53:z:55:ASP:HA	1.64	0.78
6:A:667:G:H2'	6:A:668:G:C8	2.18	0.78
33:f:58:GLU:HG3	33:f:65:PRO:HD3	1.66	0.77
28:a:2456:A:H4'	39:l:56:ARG:HD2	1.66	0.77
28:a:2571:U:H2'	28:a:2572:U:H2'	1.66	0.77
15:J:36:VAL:HG12	15:J:76:ILE:HG22	1.65	0.77
28:a:845:G:H2'	28:a:846:G:C8	2.20	0.76
40:m:37:THR:HG22	40:m:39:PRO:HD2	1.67	0.76
16:K:106:LYS:HE3	16:K:106:LYS:HA	1.68	0.76
28:a:2315:A:H2'	28:a:2316:A:C8	2.21	0.76
52:y:5:LYS:HB2	52:y:57:GLU:HB2	1.67	0.76
12:G:57:ASP:HB3	12:G:60:GLU:HG2	1.68	0.75
28:a:2605:G:H21	31:d:155:VAL:HG21	1.51	0.74
33:f:111:VAL:HG21	33:f:114:PHE:HB3	1.68	0.74
9:D:197:GLU:HA	9:D:200:ILE:HD12	1.66	0.74
6:A:1299:G:H22	6:A:1325:G:H2'	1.52	0.73
1:0:4:LEU:HB3	1:0:50:ILE:HD13	1.70	0.73
22:Q:14:ARG:HH21	22:Q:61:LEU:HB2	1.53	0.72
34:g:164:TYR:HB2	34:g:167:GLU:HB3	1.71	0.72
7:B:112:LYS:HD2	7:B:115:ARG:HH21	1.55	0.72
6:A:1350:A:H2'	6:A:1351:A:H8	1.54	0.71
7:B:76:ALA:HA	7:B:79:ILE:HD12	1.72	0.71
28:a:1048:G:N1	28:a:1071:U:N3	2.39	0.71
14:I:65:VAL:HG21	14:I:79:ILE:HG12	1.72	0.70
15:J:12:ALA:HB3	15:J:18:ILE:HG12	1.73	0.70
28:a:1672:G:H2'	28:a:1673:C:C6	2.27	0.70
35:h:8:LYS:HG2	35:h:14:ASN:HA	1.72	0.70
6:A:1124:A:H2'	6:A:1125:G:H8	1.54	0.70
11:F:9:LEU:HD13	11:F:86:ARG:HB3	1.73	0.70
37:j:63:VAL:HG23	37:j:106:LEU:HD11	1.73	0.70
18:M:90:ARG:HB2	18:M:97:VAL:HG12	1.74	0.70
14:I:21:LEU:HD22	14:I:86:ALA:HB1	1.73	0.70
24:S:11:ILE:HD12	24:S:38:SER:HB3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:O:12:VAL:HG21	20:O:22:THR:HG22	1.75	0.69
28:a:1018:A:H2'	28:a:1019:A:C8	2.27	0.69
52:y:7:THR:HG23	52:y:34:THR:HG22	1.75	0.69
18:M:83:LEU:HD11	24:S:65:ASP:HB3	1.74	0.68
10:E:80:THR:HB	10:E:122:GLN:HG3	1.75	0.68
31:d:124:ARG:HG3	31:d:165:LEU:HB2	1.76	0.68
28:a:371:G:H5'	50:w:18:ILE:HD12	1.76	0.68
27:X:82:ASP:O	27:X:86:ILE:HG12	1.94	0.67
28:a:558:U:H1'	28:a:2017:6MZ:H9C1	1.76	0.67
14:I:57:THR:HG21	14:I:87:LEU:HD21	1.76	0.67
44:q:6:VAL:HG22	44:q:11:GLN:HG2	1.76	0.67
6:A:666:U:H2'	6:A:667:G:H8	1.59	0.67
6:A:1118:G:H4'	15:J:40:ILE:HD11	1.77	0.67
43:p:9:ILE:HD12	43:p:9:ILE:H	1.61	0.67
7:B:32:PHE:HB2	7:B:42:ASN:HB3	1.77	0.66
28:a:1116:A:H4'	28:a:1117:A:H5"	1.76	0.66
6:A:1342:U:H4'	14:I:122:ARG:HG3	1.77	0.66
6:A:1244:A:H2'	6:A:1245:A:C8	2.30	0.66
7:B:28:GLY:HA2	7:B:31:ILE:HD12	1.78	0.66
6:A:248:G:H4'	22:Q:23:THR:HG21	1.77	0.66
10:E:83:GLN:H	10:E:148:MET:HE1	1.61	0.66
8:C:135:LYS:O	8:C:139:GLN:HG2	1.96	0.66
28:a:2278:U:H2'	28:a:2279:G:C8	2.31	0.66
52:y:5:LYS:HD3	52:y:36:GLU:OE1	1.96	0.66
9:D:12:SER:HA	9:D:19:LEU:HD13	1.78	0.65
6:A:1350:A:H2'	6:A:1351:A:C8	2.32	0.65
6:A:940:A:H2'	6:A:941:G:C8	2.32	0.65
9:D:28:LEU:O	9:D:32:CYS:HB3	1.96	0.65
6:A:668:G:H2'	6:A:669:A:H8	1.61	0.65
9:D:58:LYS:HG3	9:D:200:ILE:HG23	1.79	0.65
6:A:263:U:H2'	6:A:264:A:C8	2.32	0.64
28:a:837:C:H2'	28:a:838:A:H8	1.61	0.64
34:g:45:GLN:HE22	34:g:51:ARG:HE	1.45	0.64
51:x:1:MET:HE2	51:x:6:LEU:HG	1.79	0.64
7:B:100:MET:HA	7:B:107:ILE:HG13	1.79	0.64
7:B:111:ILE:HG13	7:B:148:LEU:HD13	1.79	0.64
6:A:730:C:H2'	6:A:731:A:H8	1.63	0.64
27:X:23:LYS:HB3	27:X:78:ILE:HG13	1.80	0.64
27:X:55:ARG:HG2	27:X:60:GLU:HG2	1.79	0.64
7:B:70:VAL:HG12	7:B:92:VAL:HB	1.79	0.64
8:C:92:THR:HG23	8:C:99:VAL:HG22	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:740:G:H2'	6:A:741:A:C8	2.32	0.64
18:M:4:ILE:HD12	18:M:9:ILE:HG22	1.80	0.64
28:a:2481:G:H4'	39:l:80:GLU:HG2	1.80	0.64
50:w:10:LYS:HE3	50:w:54:LYS:HD2	1.80	0.64
28:a:2154:U:O2	28:a:2158:A:N7	2.31	0.64
6:A:486:C:H2'	6:A:487:A:C8	2.33	0.63
6:A:1194:C:H5"	6:A:1195:A:H3'	1.80	0.63
28:a:2092:U:H2'	28:a:2093:G:H8	1.63	0.63
12:G:66:LEU:HD21	12:G:101:MET:HE3	1.80	0.63
6:A:658:G:H22	6:A:735:G:H1	1.45	0.63
6:A:707:G:H2'	6:A:708:G:C8	2.34	0.63
6:A:1320:U:H2'	6:A:1321:G:H8	1.64	0.63
10:E:151:PRO:HB2	10:E:160:LYS:HE2	1.80	0.63
28:a:5:A:H2'	28:a:6:A:C8	2.34	0.63
28:a:529:A:H4'	36:i:7:LYS:HG2	1.78	0.63
39:l:44:ALA:HB2	39:l:70:PRO:HG2	1.81	0.63
28:a:1420:A:H2'	28:a:1421:A:C8	2.34	0.63
5:4:61:LYS:HE3	24:S:42:PRO:HG3	1.81	0.63
6:A:961:5MC:H2'	6:A:962:A:C2	2.33	0.63
6:A:331:G:H2'	6:A:332:A:C8	2.34	0.62
28:a:1529:U:H2'	28:a:1530:G:H8	1.62	0.62
6:A:453:U:H2'	6:A:454:A:H8	1.64	0.62
7:B:173:ILE:O	7:B:177:ASN:ND2	2.31	0.62
6:A:141:G:H2'	6:A:142:G:C8	2.34	0.62
28:a:1518:C:H2'	28:a:1519:G:C8	2.34	0.62
28:a:1233:A:H4'	32:e:39:ARG:HH12	1.64	0.62
3:2:36:THR:HG22	3:2:38:LYS:H	1.65	0.62
28:a:2299:U:H5'	33:f:85:ILE:HD11	1.81	0.62
31:d:118:PHE:HA	31:d:164:HIS:H	1.64	0.62
6:A:86:C:H2'	6:A:87:C:H6	1.65	0.62
23:R:22:ASP:OD2	23:R:24:LYS:HG2	2.00	0.62
28:a:2092:U:H2'	28:a:2093:G:C8	2.35	0.62
7:B:142:GLU:O	7:B:146:ARG:HG2	2.00	0.61
28:a:2135:G:H2'	28:a:2136:U:C6	2.35	0.61
47:t:50:MET:HE3	47:t:51:LEU:O	2.00	0.61
14:I:129:LYS:HG3	27:X:60:GLU:OE1	1.99	0.61
28:a:823:A:H2'	28:a:824:G:C8	2.35	0.61
28:a:1789:A:H2'	28:a:1790:A:C8	2.34	0.61
28:a:2128:G:N2	28:a:2137:U:O2	2.21	0.61
6:A:107:G:H1'	6:A:348:G:H5'	1.83	0.61
12:G:108:ALA:HA	12:G:111:ARG:HG3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:S:3:ARG:HH11	24:S:10:PHE:HB2	1.66	0.61
28:a:1673:C:H2'	28:a:1674:A:H8	1.66	0.61
28:a:963:A:H5"	44:q:81:LYS:HD2	1.82	0.61
6:A:1117:A:H4'	15:J:38:GLY:HA3	1.83	0.61
6:A:17:U:H2'	6:A:18:C:C6	2.36	0.60
6:A:454:A:H2'	6:A:455:A:H8	1.66	0.60
11:F:102:MET:HA	11:F:102:MET:HE3	1.81	0.60
28:a:1587:A:H5"	28:a:1588:A:H5'	1.83	0.60
6:A:1201:2MG:H2'	6:A:1202:C:H6	1.66	0.60
6:A:1212:C:H2'	6:A:1213:A:C8	2.36	0.60
7:B:43:LEU:HA	7:B:46:THR:HG22	1.82	0.60
7:B:83:GLU:HG2	7:B:214:LEU:HB3	1.83	0.60
11:F:101:GLU:HA	11:F:104:LYS:HB2	1.83	0.60
33:f:4:LEU:HG	33:f:101:ASP:HB3	1.82	0.60
6:A:708:G:H2'	6:A:709:A:C8	2.36	0.60
27:X:50:ILE:HG23	27:X:77:LEU:HD13	1.83	0.60
6:A:1281:A:H2'	6:A:1282:A:C8	2.37	0.60
9:D:54:GLN:HB3	9:D:203:LEU:HB2	1.82	0.60
28:a:786:U:H2'	28:a:787:C:C6	2.35	0.60
6:A:549:U:H2'	6:A:550:C:C6	2.36	0.60
13:H:18:GLN:HE21	13:H:63:LEU:HB3	1.66	0.60
28:a:822:U:H2'	28:a:823:A:H8	1.66	0.60
6:A:453:U:H2'	6:A:454:A:C8	2.37	0.60
6:A:687:G:C6	27:X:97:GLN:HG2	2.37	0.60
15:J:24:GLU:OE1	15:J:25:ILE:HD12	2.00	0.60
6:A:21:G:H2'	6:A:22:G:C8	2.36	0.59
6:A:86:C:H2'	6:A:87:C:C6	2.37	0.59
12:G:93:PRO:HA	12:G:96:ARG:HD3	1.82	0.59
23:R:29:LEU:O	23:R:33:VAL:HG23	2.01	0.59
28:a:200:U:H4'	50:w:22:HIS:HB3	1.84	0.59
6:A:1069:U:H5"	7:B:178:LYS:HE2	1.84	0.59
6:A:1494:A:H5"	6:A:1502:G:H5'	1.84	0.59
28:a:571:C:H2'	28:a:572:A:H8	1.67	0.59
28:a:1672:G:H2'	28:a:1673:C:H6	1.68	0.59
14:I:28:ILE:HA	14:I:63:ILE:HB	1.84	0.59
28:a:491:G:H22	28:a:494:A:H5'	1.66	0.59
28:a:822:U:H2'	28:a:823:A:C8	2.37	0.59
28:a:2051:C:H2'	28:a:2052:C:C6	2.37	0.59
28:a:2260:A:H2'	28:a:2261:A:C8	2.38	0.59
48:u:175:GLN:HG3	48:u:182:LEU:HD11	1.84	0.59
7:B:100:MET:HE3	7:B:151:ILE:HD12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:2086:U:H2'	28:a:2087:G:C8	2.38	0.59
28:a:2172:U:H2'	28:a:2173:G:C8	2.37	0.59
28:a:2315:A:H2'	28:a:2316:A:H8	1.68	0.59
39:l:137:MET:HE3	48:u:80:LEU:HB2	1.83	0.59
6:A:84:C:H2'	6:A:85:U:C6	2.37	0.59
28:a:1673:C:H2'	28:a:1674:A:C8	2.37	0.59
32:e:11:ILE:HG23	32:e:13:VAL:HG13	1.84	0.59
38:k:78:ARG:HB2	38:k:81:GLU:HG2	1.83	0.59
48:u:74:THR:HG23	48:u:97:VAL:HB	1.85	0.59
6:A:741:A:H2'	6:A:742:U:C6	2.37	0.59
28:a:1766:U:H5	28:a:1771:A:N7	2.01	0.59
6:A:763:G:H4'	6:A:1507:A:H4'	1.85	0.59
28:a:5:A:H2'	28:a:6:A:H8	1.65	0.59
44:q:51:LEU:H	44:q:51:LEU:HD22	1.68	0.59
6:A:77:G:H2'	6:A:78:A:C8	2.37	0.58
2:1:12:ARG:HH21	2:1:44:VAL:HG21	1.69	0.58
6:A:1471:U:H2'	6:A:1472:U:C6	2.38	0.58
10:E:14:GLU:HG2	10:E:40:VAL:HG22	1.85	0.58
28:a:1288:A:H2	28:a:1616:G:H21	1.50	0.58
28:a:1518:C:H2'	28:a:1519:G:H8	1.67	0.58
6:A:533:A:H2'	6:A:534:G:C8	2.38	0.58
27:X:13:THR:HB	27:X:16:LEU:HD12	1.83	0.58
28:a:873:U:O2	28:a:880:G:O6	2.21	0.58
28:a:2057:A:H2'	28:a:2058:A:H8	1.68	0.58
28:a:2173:G:H2'	28:a:2174:C:C6	2.38	0.58
5:4:15:THR:HG23	5:4:21:VAL:HG22	1.86	0.58
22:Q:11:LEU:HD13	22:Q:28:ILE:HD13	1.86	0.58
28:a:512:U:H2'	28:a:513:G:H8	1.67	0.58
28:a:700:U:H2'	28:a:701:A:C8	2.39	0.58
28:a:852:A:H2'	28:a:853:G:C8	2.37	0.58
28:a:2057:A:H2'	28:a:2058:A:C8	2.39	0.58
28:a:629:U:H2'	28:a:630:C:C6	2.39	0.58
28:a:1095:U:H2'	28:a:1096:A:C8	2.27	0.58
28:a:1340:A:H2'	28:a:1341:A:C8	2.39	0.58
28:a:1635:G:H5"	28:a:1636:C:H5'	1.84	0.58
30:c:118:SER:HA	30:c:129:SER:O	2.03	0.58
34:g:41:VAL:HB	34:g:61:THR:HG23	1.85	0.58
5:4:42:PRO:HG3	5:4:49:LYS:HG3	1.84	0.58
28:a:2230:U:H2'	28:a:2231:U:C6	2.39	0.58
6:A:893:C:H2'	6:A:894:A:C8	2.39	0.58
6:A:1255:A:N6	6:A:1268:G:H1'	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1317:G:H2'	6:A:1318:A:C8	2.38	0.58
11:F:38:ARG:HG2	11:F:40:GLU:HG2	1.85	0.58
28:a:571:C:H2'	28:a:572:A:C8	2.38	0.57
32:e:160:ALA:HA	32:e:163:LEU:HB2	1.86	0.57
9:D:85:SER:HA	10:E:103:GLY:HA3	1.86	0.57
33:f:36:LEU:HB2	33:f:89:VAL:HG12	1.86	0.57
37:j:17:ARG:HB2	37:j:45:GLU:HB2	1.86	0.57
6:A:83:G:H2'	6:A:84:C:C6	2.39	0.57
6:A:1487:A:H5"	28:a:1900:A:H62	1.69	0.57
8:C:73:PRO:HG3	8:C:105:GLU:HB3	1.85	0.57
18:M:87:ARG:HG3	18:M:97:VAL:HB	1.85	0.57
28:a:864:G:H5"	48:u:159:ILE:HG13	1.86	0.57
6:A:216:U:H2'	6:A:217:A:C8	2.39	0.57
28:a:1050:U:H5"	28:a:1051:U:H5'	1.86	0.57
28:a:1783:U:H2'	28:a:1784:C:C6	2.39	0.57
28:a:2775:A:H2'	28:a:2776:C:C6	2.39	0.57
6:A:1352:U:H5'	6:A:1353:C:OP2	2.05	0.57
16:K:109:SER:HB3	26:U:5:LYS:HD2	1.85	0.57
28:a:1402:U:H3	28:a:1577:G:H1	1.51	0.57
28:a:1581:A:H2'	28:a:1582:C:C6	2.40	0.57
6:A:730:C:H2'	6:A:731:A:C8	2.39	0.57
28:a:512:U:H2'	28:a:513:G:C8	2.40	0.57
28:a:2061:U:H2'	28:a:2062:U:C6	2.40	0.57
28:a:2172:U:H2'	28:a:2173:G:H8	1.70	0.57
6:A:1436:G:H2'	6:A:1437:U:C6	2.40	0.57
6:A:668:G:H2'	6:A:669:A:C8	2.39	0.57
11:F:91:ARG:HH11	11:F:91:ARG:HG2	1.70	0.57
28:a:470:A:N3	28:a:472:G:H5"	2.19	0.57
28:a:2489:G:H5"	28:a:2490:2MA:H5"	1.86	0.57
28:a:1373:C:H2'	28:a:1374:A:C8	2.40	0.56
6:A:666:U:H2'	6:A:667:G:C8	2.40	0.56
28:a:899:A:H2'	28:a:900:A:C8	2.40	0.56
28:a:1061:G:H1'	28:a:1079:A:H2'	1.86	0.56
28:a:2292:U:H5"	33:f:131:GLY:HA3	1.86	0.56
28:a:2862:C:H4'	42:o:3:ASN:HB3	1.87	0.56
39:l:54:LEU:HD11	39:l:118:PHE:HE1	1.70	0.56
15:J:6:ILE:HG22	15:J:102:LEU:HA	1.87	0.56
28:a:1529:U:H2'	28:a:1530:G:C8	2.41	0.56
28:a:2685:U:H2'	28:a:2686:C:C6	2.40	0.56
6:A:1320:U:H2'	6:A:1321:G:C8	2.41	0.56
10:E:160:LYS:NZ	10:E:161:SER:H	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:1303:U:H2'	28:a:1304:G:H8	1.70	0.56
28:a:579:U:H2'	28:a:580:A:H8	1.71	0.56
1:0:21:LYS:HD3	1:0:23:LYS:HD3	1.86	0.56
29:b:42:C:H5	33:f:90:THR:HB	1.70	0.56
3:2:24:LYS:HG2	3:2:46:THR:HG22	1.87	0.56
15:J:11:LYS:HG2	15:J:71:LYS:HG2	1.88	0.56
28:a:2873:G:H2'	28:a:2874:C:C6	2.41	0.56
6:A:19:A:H5"	10:E:92:ALA:HB3	1.87	0.56
28:a:969:A:H2'	28:a:972:C:H42	1.69	0.56
28:a:2128:G:H2'	28:a:2129:A:C8	2.40	0.56
47:t:2:GLN:HE21	47:t:5:ARG:HA	1.71	0.56
6:A:712:A:H5'	16:K:119:IAS:HA	1.87	0.56
6:A:1245:A:H2'	6:A:1246:A:C8	2.39	0.55
8:C:112:ASP:OD2	8:C:115:LEU:HB2	2.06	0.55
31:d:36:THR:HG22	31:d:74:VAL:HG11	1.88	0.55
43:p:49:ASP:HA	43:p:52:GLN:HB2	1.88	0.55
48:u:33:VAL:HG22	48:u:94:PHE:HB2	1.88	0.55
6:A:454:A:H2'	6:A:455:A:C8	2.40	0.55
6:A:845:U:H2'	6:A:846:A:C8	2.41	0.55
6:A:1124:A:H2'	6:A:1125:G:C8	2.38	0.55
28:a:300:U:H2'	28:a:301:G:O4'	2.07	0.55
28:a:1071:U:H2'	28:a:1072:U:C6	2.42	0.55
32:e:146:LEU:HD11	32:e:169:ARG:HG3	1.87	0.55
35:h:24:GLY:O	35:h:28:ASN:HB2	2.06	0.55
5:4:56:ARG:HD3	5:4:59:ARG:HB3	1.87	0.55
16:K:65:VAL:O	16:K:68:GLU:HG3	2.07	0.55
28:a:2124:C:H2'	28:a:2125:G:C8	2.41	0.55
28:a:2788:U:H2'	28:a:2789:U:H6	1.72	0.55
31:d:30:VAL:O	31:d:185:ASN:HB3	2.07	0.55
35:h:16:GLY:HA2	35:h:47:PHE:CZ	2.42	0.55
6:A:1065:C:H2'	6:A:1066:G:H8	1.71	0.55
6:A:1119:U:C6	15:J:40:ILE:HD13	2.42	0.55
28:a:272:A:H2'	28:a:273:A:C8	2.40	0.55
6:A:384:U:H2'	6:A:385:C:C6	2.42	0.55
13:H:18:GLN:HG3	13:H:63:LEU:HD13	1.88	0.55
28:a:700:U:H2'	28:a:701:A:H8	1.71	0.55
28:a:2781:A:H2'	28:a:2782:A:H8	1.72	0.55
6:A:210:U:H2'	6:A:211:C:C6	2.41	0.55
18:M:106:ALA:HB3	18:M:110:LYS:HD2	1.88	0.55
28:a:1048:G:N1	28:a:1071:U:C2	2.74	0.55
28:a:1424:C:H2'	28:a:1425:U:C6	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:e:3:LEU:HB2	32:e:11:ILE:HG22	1.89	0.55
8:C:51:SER:HB2	8:C:71:ALA:HB3	1.89	0.55
9:D:87:GLY:HA3	9:D:197:GLU:HG3	1.88	0.55
47:t:1:MET:HG3	47:t:84:PHE:CE1	2.42	0.55
6:A:198:G:H2'	6:A:199:A:H8	1.72	0.54
28:a:2086:U:H2'	28:a:2087:G:H8	1.70	0.54
7:B:120:GLN:HA	7:B:124:GLY:HA3	1.89	0.54
14:I:19:VAL:HG22	14:I:65:VAL:HB	1.89	0.54
6:A:725:G:H5'	6:A:760:A:H4'	1.90	0.54
28:a:1419:G:H2'	28:a:1420:A:C8	2.42	0.54
28:a:2026:U:H2'	28:a:2027:G:C8	2.43	0.54
41:n:78:ALA:HB2	41:n:109:ALA:HA	1.88	0.54
43:p:82:GLY:HA2	43:p:118:ALA:HB3	1.89	0.54
48:u:54:LEU:HD13	48:u:80:LEU:HD21	1.90	0.54
6:A:1385:U:H2'	6:A:1386:G:C8	2.43	0.54
6:A:1524:G:H2'	6:A:1525:A:C8	2.42	0.54
28:a:949:A:H2'	28:a:950:A:C8	2.42	0.54
28:a:1721:C:H2'	28:a:1722:C:C6	2.42	0.54
53:z:12:ALA:HA	53:z:15:MET:HG3	1.90	0.54
12:G:116:MET:HE2	12:G:116:MET:HA	1.88	0.54
28:a:244:A:H5"	38:k:67:VAL:HG11	1.90	0.54
28:a:1520:U:H2'	28:a:1521:C:C6	2.42	0.54
28:a:2578:C:H2'	28:a:2579:G:C8	2.42	0.54
28:a:2687:A:H2'	28:a:2688:C:C6	2.43	0.54
28:a:1099:C:H3'	28:a:1100:G:C8	2.42	0.54
28:a:1519:G:H2'	28:a:1520:U:C6	2.42	0.54
29:b:48:U:H2'	29:b:49:C:C6	2.43	0.54
37:j:1:MET:HB2	37:j:32:TYR:HB3	1.88	0.54
6:A:331:G:H2'	6:A:332:A:H8	1.72	0.54
7:B:16:PHE:HB2	7:B:203:ASN:HD22	1.73	0.54
6:A:940:A:H2'	6:A:941:G:H8	1.71	0.54
9:D:11:LEU:HB3	9:D:63:ARG:HD3	1.89	0.54
12:G:15:ASP:HB2	12:G:27:MET:HE1	1.90	0.54
28:a:1018:A:N6	28:a:1115:G:H2'	2.23	0.54
28:a:1795:A:H3'	28:a:1796:A:C8	2.43	0.54
28:a:470:A:H1'	28:a:471:A:H5"	1.89	0.54
28:a:2788:U:H2'	28:a:2789:U:C6	2.43	0.54
33:f:43:ALA:HB2	33:f:49:ILE:HG13	1.90	0.54
6:A:208:C:H2'	6:A:209:C:H6	1.73	0.53
6:A:912:A:H2'	6:A:913:A:C8	2.44	0.53
28:a:540:U:H2'	28:a:541:A:H8	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:853:G:H2'	28:a:854:C:C6	2.43	0.53
28:a:2578:C:H2'	28:a:2579:G:H8	1.73	0.53
30:c:132:LEU:HA	30:c:135:ILE:HG13	1.90	0.53
6:A:656:U:H2'	6:A:657:A:C8	2.43	0.53
18:M:75:MET:O	18:M:79:ARG:HG2	2.09	0.53
20:O:7:GLU:O	20:O:11:ILE:HG13	2.08	0.53
28:a:2024:A:H2'	28:a:2025:G:C8	2.44	0.53
28:a:2162:C:H2'	28:a:2163:A:C8	2.43	0.53
6:A:470:G:H2'	6:A:471:U:C6	2.43	0.53
6:A:840:G:H2'	6:A:841:A:H8	1.73	0.53
28:a:990:A:H2'	28:a:991:A:C8	2.43	0.53
28:a:1373:C:H2'	28:a:1374:A:H8	1.73	0.53
28:a:2781:A:H2'	28:a:2782:A:C8	2.42	0.53
6:A:56:U:H2'	6:A:57:G:H8	1.72	0.53
24:S:14:HIS:O	24:S:18:LYS:HG3	2.08	0.53
50:w:13:VAL:HG23	50:w:29:PHE:HB2	1.89	0.53
15:J:17:LEU:HD13	15:J:95:GLY:HA3	1.91	0.53
28:a:1069:C:H2'	28:a:1070:C:O4'	2.08	0.53
28:a:1080:A:N1	28:a:1092:C:H1'	2.24	0.53
32:e:6:ASN:HB3	32:e:120:VAL:HG12	1.89	0.53
32:e:147:ILE:HG23	32:e:186:LEU:HD22	1.91	0.53
9:D:17:THR:HG22	9:D:18:ASP:H	1.74	0.53
12:G:112:GLY:H	12:G:119:ARG:HD3	1.73	0.53
28:a:535:C:H2'	28:a:536:U:H5"	1.90	0.53
28:a:1519:G:H1	28:a:1529:U:H3	1.55	0.53
28:a:1641:G:H5'	40:m:39:PRO:HG2	1.89	0.53
6:A:484:A:H2'	6:A:485:A:H8	1.74	0.53
28:a:1:G:H2'	28:a:2:G:H8	1.72	0.53
28:a:388:U:H5"	50:w:32:ASN:HB2	1.91	0.53
14:I:124:ARG:HH11	14:I:124:ARG:HB2	1.74	0.53
28:a:2124:C:H2'	28:a:2125:G:H8	1.73	0.53
28:a:2796:A:H2'	28:a:2797:A:C8	2.43	0.53
6:A:670:A:H5"	16:K:115:PRO:HB3	1.91	0.53
8:C:150:LYS:HG2	8:C:201:TRP:CE3	2.44	0.53
28:a:1029:A:H5"	48:u:48:ARG:NH1	2.23	0.53
28:a:2162:C:H2'	28:a:2163:A:H8	1.73	0.53
5:4:51:LEU:CD2	5:4:52:ASP:H	2.12	0.53
5:4:60:PHE:O	5:4:63:ARG:HB3	2.09	0.53
6:A:204:C:H4'	6:A:205:G:H21	1.74	0.53
6:A:1518:C:H2'	6:A:1519:G:C8	2.44	0.53
7:B:4:VAL:N	7:B:47:LEU:HD11	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:44:GLU:HB2	27:X:49:LYS:HD2	1.91	0.53
28:a:1416:G:H2'	28:a:1417:G:H8	1.74	0.53
33:f:36:LEU:HD23	33:f:152:LEU:HD23	1.91	0.53
48:u:156:LEU:HD23	48:u:187:ILE:HG22	1.91	0.53
6:A:1268:G:HO2'	6:A:1269:A:H8	1.56	0.52
6:A:1507:A:H2'	6:A:1508:G:C8	2.44	0.52
8:C:148:GLY:HA3	8:C:172:ARG:O	2.09	0.52
28:a:629:U:H2'	28:a:630:C:H6	1.72	0.52
28:a:1708:U:H2'	28:a:1709:G:O4'	2.08	0.52
28:a:1811:G:O2'	30:c:253:THR:HG21	2.09	0.52
28:a:2738:G:C4	34:g:3:ARG:HD3	2.44	0.52
28:a:2790:C:H2'	28:a:2791:C:C6	2.45	0.52
32:e:11:ILE:HD11	32:e:189:VAL:HG13	1.91	0.52
6:A:88:U:H2'	6:A:89:G:C8	2.45	0.52
12:G:5:ARG:HD3	12:G:5:ARG:O	2.09	0.52
14:I:71:GLY:O	14:I:75:GLN:HG3	2.08	0.52
28:a:1185:U:H2'	28:a:1186:U:C6	2.43	0.52
28:a:1456:A:H2'	28:a:1457:A:C8	2.44	0.52
28:a:2145:A:H1'	28:a:2146:G:C8	2.45	0.52
34:g:41:VAL:HA	34:g:55:ARG:HB2	1.91	0.52
7:B:85:ALA:C	7:B:87:CYS:H	2.17	0.52
8:C:111:LEU:HD22	8:C:146:ALA:HB2	1.91	0.52
27:X:93:LEU:O	27:X:97:GLN:HB3	2.09	0.52
28:a:1395:U:H2'	28:a:1396:G:H8	1.73	0.52
28:a:2128:G:H2'	28:a:2129:A:H8	1.74	0.52
28:a:2302:G:H2'	28:a:2303:U:C6	2.45	0.52
28:a:2724:G:H2'	28:a:2725:A:C8	2.44	0.52
32:e:54:GLY:HA3	32:e:73:ARG:HG2	1.91	0.52
18:M:77:ILE:O	18:M:81:MET:HG2	2.09	0.52
6:A:914:U:H2'	6:A:915:U:C6	2.44	0.52
6:A:1028:G:H2'	6:A:1029:A:H8	1.75	0.52
7:B:31:ILE:HD13	7:B:39:HIS:HD2	1.75	0.52
10:E:116:LEU:HD22	10:E:124:VAL:HG21	1.92	0.52
16:K:123:PRO:HD2	26:U:38:TYR:HD1	1.74	0.52
28:a:572:A:H2'	28:a:573:G:C8	2.45	0.52
28:a:579:U:H2'	28:a:580:A:C8	2.44	0.52
28:a:1103:U:H2'	28:a:1104:C:C6	2.44	0.52
28:a:1157:G:H2'	28:a:1158:U:C6	2.45	0.52
28:a:1481:A:H2'	28:a:1482:A:C8	2.45	0.52
33:f:78:LYS:HD3	33:f:78:LYS:N	2.24	0.52
6:A:352:U:H2'	6:A:353:G:H8	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:533:A:H2'	6:A:534:G:H8	1.75	0.52
24:S:19:VAL:HG21	24:S:44:MET:HG2	1.91	0.52
27:X:26:ARG:HD2	27:X:26:ARG:C	2.34	0.52
35:h:5:LEU:HB3	35:h:15:LEU:HA	1.91	0.52
6:A:957:G:N2	15:J:57:VAL:HG11	2.25	0.52
13:H:41:LYS:HD2	13:H:48:ASP:HA	1.92	0.52
28:a:693:U:H2'	28:a:694:G:O4'	2.09	0.52
6:A:1247:G:H2'	6:A:1248:G:H8	1.75	0.52
15:J:65:TYR:HB3	19:N:96:LEU:HD11	1.90	0.52
28:a:823:A:H2'	28:a:824:G:H8	1.73	0.52
28:a:2812:U:H3'	28:a:2813:A:H8	1.75	0.52
1:0:1:MET:HE1	28:a:2270:U:H5'	1.92	0.52
12:G:51:LYS:HB3	12:G:58:PRO:HG3	1.92	0.52
28:a:1915:A:H2'	28:a:1916:G:O4'	2.10	0.52
28:a:2096:U:H2'	28:a:2097:G:O4'	2.09	0.52
36:i:56:VAL:HG11	36:i:101:ILE:HD13	1.92	0.52
9:D:172:GLU:HG3	9:D:183:LYS:HD3	1.92	0.52
18:M:81:MET:HE3	28:a:876:U:C2	2.45	0.52
27:X:70:MET:O	27:X:74:ILE:HG13	2.10	0.52
28:a:82:G:O2'	28:a:83:G:H5'	2.09	0.52
28:a:1773:A:H1'	28:a:1925:A:N6	2.24	0.52
6:A:1308:C:H2'	6:A:1309:U:C6	2.45	0.51
18:M:48:LEU:HD13	18:M:52:GLN:HB3	1.92	0.51
28:a:1781:A:H2'	28:a:1782:C:C6	2.44	0.51
28:a:2796:A:H2'	28:a:2797:A:H8	1.76	0.51
6:A:607:C:H2'	6:A:608:C:C6	2.45	0.51
6:A:352:U:H2'	6:A:353:G:C8	2.46	0.51
6:A:999:A:C5	6:A:1000:C:H1'	2.45	0.51
6:A:1021:C:H2'	6:A:1022:C:C6	2.45	0.51
7:B:114:LEU:HB2	7:B:144:LEU:HD23	1.93	0.51
14:I:80:ARG:HD2	14:I:103:TYR:CD2	2.46	0.51
28:a:572:A:H2'	28:a:573:G:H8	1.75	0.51
28:a:586:A:H2'	28:a:587:G:H8	1.76	0.51
28:a:622:A:H5'	38:k:68:SER:HB2	1.92	0.51
28:a:647:U:H2'	28:a:648:C:C6	2.45	0.51
28:a:1303:U:H2'	28:a:1304:G:C8	2.45	0.51
28:a:2292:U:H2'	28:a:2293:C:C6	2.46	0.51
33:f:170:LEU:HD23	33:f:177:PHE:HZ	1.75	0.51
9:D:28:LEU:O	9:D:32:CYS:CB	2.59	0.51
18:M:89:LEU:HD13	18:M:93:ARG:HH21	1.76	0.51
28:a:2085:U:H2'	28:a:2086:U:O4'	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:U:19:PHE:HD2	26:U:20:LYS:HE3	1.74	0.51
28:a:1055:U:H2'	28:a:1056:U:O4'	2.11	0.51
6:A:229:U:H2'	6:A:230:A:C8	2.44	0.51
6:A:636:A:N7	13:H:107:ASN:HA	2.25	0.51
6:A:651:U:H5	6:A:743:A:N1	2.09	0.51
14:I:47:VAL:HG13	14:I:80:ARG:HE	1.74	0.51
18:M:92:ARG:HG2	28:a:876:U:O4'	2.09	0.51
28:a:584:U:H2'	28:a:585:C:C6	2.45	0.51
28:a:772:A:C2	30:c:225:MET:HG2	2.45	0.51
28:a:2012:C:H2'	28:a:2013:U:C6	2.45	0.51
29:b:90:C:H5'	39:l:18:ARG:HG2	1.93	0.51
41:n:55:LEU:HA	41:n:60:ARG:HD2	1.92	0.51
42:o:101:LEU:HD11	42:o:111:ILE:HD11	1.92	0.51
6:A:134:U:H2'	6:A:135:A:C8	2.46	0.51
6:A:742:U:H2'	6:A:743:A:C8	2.45	0.51
6:A:1255:A:H61	6:A:1268:G:H1'	1.72	0.51
15:J:59:LYS:O	15:J:62:ARG:HD3	2.11	0.51
28:a:598:A:H2'	28:a:599:A:C8	2.46	0.51
34:g:45:GLN:NE2	34:g:51:ARG:HE	2.07	0.51
6:A:208:C:H2'	6:A:209:C:C6	2.46	0.51
6:A:1005:C:H2'	6:A:1006:A:C8	2.45	0.51
24:S:62:VAL:HA	24:S:66:MET:SD	2.50	0.51
28:a:803:U:H2'	28:a:804:C:C6	2.46	0.51
28:a:2228:A:H2'	28:a:2229:G:C8	2.46	0.51
41:n:59:LEU:HD11	41:n:72:LYS:HB3	1.93	0.51
28:a:191:A:H2'	28:a:192:C:C6	2.46	0.51
28:a:831:A:H2'	28:a:832:U:C6	2.45	0.51
28:a:1933:U:H2'	28:a:1934:C:C6	2.46	0.51
28:a:2051:C:H2'	28:a:2052:C:H6	1.76	0.51
28:a:2233:G:H2'	28:a:2234:A:C8	2.46	0.51
37:j:18:ARG:HB2	37:j:45:GLU:HG3	1.93	0.51
6:A:250:U:H2'	6:A:251:G:H8	1.77	0.50
6:A:263:U:H2'	6:A:264:A:H8	1.73	0.50
22:Q:56:CYS:O	22:Q:57:ARG:HD2	2.11	0.50
6:A:378:G:H2'	6:A:379:C:C6	2.47	0.50
6:A:670:A:H2'	6:A:671:U:H6	1.77	0.50
6:A:1440:A:HO2'	6:A:1441:A:H8	1.58	0.50
17:L:74:LEU:HD11	17:L:80:VAL:HG11	1.93	0.50
19:N:46:VAL:HG22	24:S:13:LEU:HD21	1.93	0.50
19:N:89:MET:HE1	19:N:98:LYS:HD2	1.93	0.50
6:A:149:U:H2'	6:A:150:C:C6	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1406:C:H2'	6:A:1407:A:C8	2.46	0.50
14:I:84:THR:HG23	14:I:98:LEU:HD13	1.92	0.50
16:K:64:GLN:HG2	16:K:99:ALA:HB2	1.91	0.50
25:T:24:LEU:O	25:T:28:VAL:HG23	2.12	0.50
28:a:1276:C:H2'	28:a:1277:A:H8	1.75	0.50
28:a:2220:U:H2'	28:a:2221:G:C8	2.46	0.50
28:a:2278:U:H2'	28:a:2279:G:H8	1.75	0.50
28:a:2417:A:H2'	28:a:2417:A:N3	2.26	0.50
28:a:2534:A:H2'	28:a:2535:U:C6	2.46	0.50
34:g:143:GLN:O	34:g:147:GLU:HG3	2.11	0.50
45:r:2:GLU:HG2	45:r:108:ALA:HB2	1.93	0.50
14:I:47:VAL:HA	14:I:50:GLN:HG3	1.92	0.50
28:a:559:U:H5"	28:a:811:A:C2	2.47	0.50
28:a:774:G:H5'	28:a:775:G:OP1	2.12	0.50
28:a:869:G:C5	28:a:870:G:H1'	2.46	0.50
28:a:1581:A:H2'	28:a:1582:C:H6	1.76	0.50
28:a:2067:G:H5'	50:w:19:SER:HB2	1.92	0.50
29:b:29:A:H2'	29:b:30:C:C6	2.46	0.50
7:B:151:ILE:HG13	7:B:154:MET:HE2	1.93	0.50
15:J:83:THR:O	15:J:87:LEU:HB2	2.12	0.50
28:a:75:G:H22	28:a:111:A:H2	1.60	0.50
28:a:1627:A:H2'	28:a:1628:C:C6	2.46	0.50
28:a:1814:U:H2'	28:a:1815:G:O4'	2.12	0.50
23:R:26:LEU:HD11	23:R:67:LEU:HB3	1.93	0.50
25:T:42:LYS:HA	25:T:86:LEU:HD11	1.94	0.50
27:X:52:ALA:HB2	27:X:77:LEU:HD21	1.92	0.50
28:a:840:U:H2'	28:a:841:C:C6	2.47	0.50
28:a:1047:A:H2'	28:a:1048:G:C8	2.47	0.50
33:f:25:VAL:O	33:f:28:VAL:HG23	2.11	0.50
34:g:84:GLU:HB2	34:g:132:LEU:HD11	1.93	0.50
40:m:45:ARG:HD3	40:m:97:ILE:HD11	1.94	0.50
9:D:9:CYS:HB3	9:D:32:CYS:SG	2.51	0.50
17:L:56:ARG:HB2	17:L:62:GLU:HG3	1.94	0.50
28:a:1876:A:H2'	28:a:1877:A:C8	2.47	0.50
29:b:2:G:H2'	29:b:3:C:C6	2.47	0.50
30:c:119:GLY:HA2	30:c:189:ARG:HH21	1.77	0.50
40:m:87:TYR:OH	40:m:115:LEU:HB3	2.11	0.50
6:A:916:G:H2'	6:A:917:A:C8	2.47	0.50
28:a:45:G:H5'	28:a:46:G:H5'	1.94	0.50
28:a:1058:G:H2'	28:a:1059:A:O4'	2.12	0.50
28:a:2554:G:H2'	28:a:2555:U:C6	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:2636:C:H2'	28:a:2637:U:H6	1.75	0.50
28:a:2790:C:H2'	28:a:2791:C:H6	1.76	0.50
6:A:834:C:H2'	6:A:835:C:C6	2.46	0.50
6:A:1308:C:H2'	6:A:1309:U:H6	1.75	0.50
6:A:1334:A:N3	14:I:130:ARG:HD3	2.27	0.50
28:a:570:U:H2'	28:a:571:C:C6	2.47	0.50
41:n:28:CYS:HA	41:n:92:ASP:HB3	1.94	0.50
6:A:64:G:H4'	6:A:65:A:H3'	1.93	0.49
6:A:125:U:H2'	6:A:126:C:C6	2.47	0.49
10:E:160:LYS:HZ3	10:E:161:SER:H	1.59	0.49
28:a:1958:U:C2	30:c:240:SER:HB3	2.47	0.49
28:a:2665:A:H2'	28:a:2666:A:C8	2.47	0.49
40:m:8:ARG:HD2	40:m:43:GLU:HG2	1.94	0.49
28:a:2182:U:H2'	28:a:2183:C:H6	1.77	0.49
35:h:16:GLY:HA2	35:h:47:PHE:HZ	1.76	0.49
5:4:56:ARG:NH1	5:4:60:PHE:HA	2.27	0.49
6:A:495:C:H2'	6:A:496:A:C8	2.47	0.49
6:A:990:A:H2'	6:A:991:U:C6	2.47	0.49
6:A:1037:C:H2'	6:A:1038:A:C8	2.47	0.49
6:A:1436:G:H2'	6:A:1437:U:H6	1.75	0.49
15:J:52:LEU:HD21	15:J:59:LYS:HD2	1.94	0.49
22:Q:26:VAL:HG21	22:Q:64:ILE:HD13	1.94	0.49
28:a:649:G:H4'	32:e:94:LYS:HG2	1.93	0.49
28:a:1980:U:H4'	31:d:133:THR:OG1	2.12	0.49
31:d:184:ARG:HB2	31:d:186:LEU:HD13	1.94	0.49
45:r:1:MET:HG2	45:r:109:ASP:CG	2.37	0.49
6:A:83:G:H2'	6:A:84:C:H6	1.77	0.49
6:A:722:A:H2'	6:A:723:A:C8	2.48	0.49
6:A:1037:C:H2'	6:A:1038:A:H8	1.78	0.49
16:K:31:ILE:HG12	16:K:46:THR:HG22	1.94	0.49
29:b:66:A:H61	29:b:107:U:H2'	1.76	0.49
40:m:8:ARG:HH11	40:m:43:GLU:HG2	1.77	0.49
6:A:56:U:H2'	6:A:57:G:C8	2.48	0.49
6:A:518:G:H2'	6:A:519:C:C6	2.47	0.49
28:a:623:A:H5"	38:k:70:LYS:HD3	1.95	0.49
33:f:33:LYS:HG2	33:f:157:THR:HB	1.93	0.49
48:u:123:SER:OG	48:u:156:LEU:HG	2.13	0.49
28:a:1186:U:H2'	28:a:1187:C:H6	1.77	0.49
28:a:2102:G:O2'	28:a:2154:U:H1'	2.13	0.49
28:a:2287:A:H2'	28:a:2288:C:H6	1.78	0.49
29:b:2:G:H2'	29:b:3:C:H6	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:m:77:GLY:O	40:m:81:ASN:HB2	2.13	0.49
6:A:73:A:H8	6:A:90:G:H21	1.58	0.49
6:A:383:A:H3'	6:A:384:U:H6	1.77	0.49
17:L:50:ARG:HB3	17:L:66:TYR:HE1	1.77	0.49
28:a:1843:U:H2'	28:a:1844:G:O4'	2.13	0.49
6:A:41:G:H2'	6:A:42:G:H8	1.78	0.49
6:A:574:C:H2'	6:A:575:G:O4'	2.12	0.49
6:A:757:G:H2'	6:A:758:C:C6	2.48	0.49
11:F:40:GLU:HB3	11:F:103:LEU:HD12	1.95	0.49
24:S:3:ARG:HH21	24:S:7:LYS:HD2	1.78	0.49
28:a:2161:C:H2'	28:a:2162:C:C6	2.47	0.49
28:a:2834:U:H2'	28:a:2835:G:O4'	2.12	0.49
32:e:96:ASN:HB2	32:e:99:MET:HG3	1.94	0.49
6:A:484:A:H2'	6:A:485:A:C8	2.48	0.49
28:a:52:A:H2'	28:a:53:A:C8	2.48	0.49
28:a:339:A:H1'	28:a:340:A:C2	2.48	0.49
5:4:56:ARG:HH11	5:4:60:PHE:HA	1.77	0.49
6:A:75:G:O6	6:A:88:U:O4	2.31	0.49
6:A:512:C:H4'	6:A:513:C:O5'	2.12	0.49
23:R:26:LEU:HD23	23:R:29:LEU:HD12	1.94	0.49
28:a:29:U:H2'	28:a:30:G:C8	2.48	0.49
28:a:1088:A:C2	28:a:1089:G:H1'	2.48	0.49
28:a:2832:U:H5"	42:o:53:ASN:O	2.12	0.49
30:c:239:THR:HG22	30:c:240:SER:H	1.78	0.49
6:A:1390:A:H4'	6:A:1391:C:H5"	1.94	0.48
28:a:837:C:H2'	28:a:838:A:C8	2.45	0.48
28:a:1348:G:H2'	28:a:1349:C:C6	2.47	0.48
30:c:21:ASN:HB3	30:c:24:LEU:HG	1.94	0.48
6:A:170:C:H2'	6:A:171:G:N3	2.27	0.48
6:A:317:U:H2'	6:A:318:G:O4'	2.12	0.48
6:A:532:A:H2'	6:A:533:A:H8	1.78	0.48
6:A:1016:U:H2'	6:A:1017:G:O4'	2.14	0.48
6:A:1114:C:H2'	6:A:1115:U:C6	2.48	0.48
14:I:67:VAL:HG11	14:I:79:ILE:HD11	1.95	0.48
28:a:2164:C:H2'	28:a:2165:C:O4'	2.13	0.48
28:a:2559:A:N7	31:d:150:MEQ:HB3	2.28	0.48
5:4:13:GLU:HG2	5:4:31:PRO:HA	1.95	0.48
6:A:198:G:H2'	6:A:199:A:C8	2.48	0.48
6:A:216:U:H2'	6:A:217:A:H8	1.75	0.48
6:A:920:G:C6	27:X:87:LYS:HG3	2.49	0.48
6:A:1435:A:O2'	6:A:1436:G:C8	2.67	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:101:LEU:HB3	7:B:179:LEU:HD12	1.96	0.48
28:a:650:C:H5"	32:e:93:GLN:HB3	1.95	0.48
28:a:1424:C:H2'	28:a:1425:U:H6	1.77	0.48
28:a:2832:U:H2'	28:a:2833:G:C8	2.48	0.48
40:m:32:GLU:HB3	40:m:118:ARG:HD3	1.95	0.48
28:a:155:U:H2'	28:a:156:A:C8	2.47	0.48
28:a:263:U:H2'	28:a:264:U:O4'	2.13	0.48
28:a:1425:U:H2'	28:a:1426:A:H8	1.78	0.48
48:u:5:ILE:HD12	48:u:65:ALA:HB3	1.95	0.48
11:F:4:TYR:CZ	11:F:71:LEU:HD22	2.48	0.48
28:a:45:G:H5'	28:a:46:G:OP1	2.13	0.48
28:a:299:C:H2'	28:a:300:U:C6	2.49	0.48
28:a:2114:G:N2	28:a:2149:A:H1'	2.29	0.48
28:a:2286:G:H2'	28:a:2287:A:H8	1.79	0.48
5:4:64:PHE:CG	24:S:5:LEU:HD13	2.49	0.48
6:A:370:G:H4'	21:P:5:ARG:HD3	1.95	0.48
9:D:15:GLU:HB2	9:D:19:LEU:HD11	1.96	0.48
12:G:58:PRO:HA	12:G:61:THR:HG22	1.96	0.48
28:a:1276:C:H2'	28:a:1277:A:C8	2.48	0.48
31:d:209:ALA:HB1	31:d:210:ARG:HH21	1.78	0.48
48:u:102:LYS:HZ2	48:u:138:CYS:HA	1.78	0.48
6:A:999:A:H62	6:A:1018:G:N2	2.11	0.48
6:A:1470:A:H2'	6:A:1471:U:C6	2.48	0.48
14:I:42:GLU:O	14:I:46:MET:HG3	2.14	0.48
17:L:57:LEU:HD21	17:L:82:ILE:HG12	1.94	0.48
28:a:1781:A:H2'	28:a:1782:C:H6	1.78	0.48
28:a:2173:G:H2'	28:a:2174:C:H6	1.78	0.48
28:a:2220:U:H2'	28:a:2221:G:H8	1.79	0.48
41:n:27:LEU:HD23	41:n:91:PHE:HD1	1.78	0.48
6:A:293:G:H2'	6:A:294:A:C8	2.48	0.48
6:A:495:C:H2'	6:A:496:A:H8	1.79	0.48
6:A:636:A:H2'	6:A:637:C:H6	1.79	0.48
6:A:1516:U:H2'	6:A:1517:G:H8	1.77	0.48
8:C:134:MET:HE2	8:C:168:TYR:HD2	1.77	0.48
10:E:15:LYS:HE3	10:E:15:LYS:HB3	1.56	0.48
14:I:6:ASN:ND2	14:I:90:TYR:HA	2.27	0.48
16:K:18:ASP:HB2	16:K:81:ASN:HB2	1.96	0.48
30:c:144:ILE:HB	30:c:154:ILE:HB	1.95	0.48
36:i:11:VAL:HG11	36:i:50:THR:HA	1.96	0.48
1:0:6:ARG:HG3	1:0:50:ILE:HA	1.95	0.48
1:0:44:ILE:HG22	1:0:46:LYS:HD3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:51:LYS:HE2	3:2:51:LYS:HB2	1.69	0.48
7:B:70:VAL:HG23	7:B:163:VAL:HA	1.96	0.48
9:D:174:ASP:OD2	9:D:177:LYS:HG3	2.13	0.48
19:N:24:ARG:HG3	19:N:48:LEU:HD11	1.96	0.48
28:a:1431:A:H2'	28:a:1432:G:C8	2.49	0.48
28:a:1580:A:H2'	28:a:1581:A:H8	1.78	0.48
28:a:2026:U:H2'	28:a:2027:G:H8	1.79	0.48
29:b:3:C:H2'	29:b:4:U:H6	1.78	0.48
43:p:83:LEU:HD22	43:p:88:ILE:HD12	1.96	0.48
6:A:840:G:H2'	6:A:841:A:C8	2.49	0.48
6:A:1034:A:H2'	6:A:1035:G:H8	1.78	0.48
6:A:1216:G:H5"	24:S:78:ARG:HE	1.79	0.48
8:C:22:TRP:HA	15:J:94:ALA:O	2.14	0.48
12:G:111:ARG:HD3	12:G:119:ARG:O	2.14	0.48
12:G:130:GLY:HA2	12:G:135:VAL:HG21	1.96	0.48
16:K:88:GLY:O	16:K:93:ARG:HD2	2.14	0.48
21:P:4:ILE:HG12	21:P:21:VAL:HG22	1.96	0.48
28:a:840:U:H2'	28:a:841:C:H6	1.79	0.48
28:a:1064:G:H2'	28:a:1065:C:C6	2.49	0.48
44:q:2:TYR:CE1	44:q:42:ALA:HB3	2.47	0.48
2:1:18:PHE:CZ	2:1:22:MET:HE3	2.49	0.47
6:A:981:G:H2'	6:A:982:G:H8	1.79	0.47
13:H:7:LEU:HD23	13:H:77:ARG:NH1	2.29	0.47
28:a:198:C:H2'	28:a:199:A:H5"	1.96	0.47
28:a:731:U:H2'	28:a:732:C:C6	2.48	0.47
28:a:1083:G:H2'	28:a:1084:U:C6	2.49	0.47
28:a:2624:U:H2'	28:a:2625:G:O4'	2.13	0.47
29:b:115:A:H2'	29:b:116:A:C8	2.48	0.47
37:j:111:PHE:HB3	37:j:114:ILE:HD12	1.96	0.47
6:A:858:A:H2'	6:A:859:A:C8	2.50	0.47
6:A:1201:2MG:H2'	6:A:1202:C:C6	2.47	0.47
6:A:1247:G:H2'	6:A:1248:G:C8	2.49	0.47
6:A:1299:G:N2	6:A:1325:G:H2'	2.25	0.47
7:B:117:LEU:HG	7:B:141:LEU:HG	1.96	0.47
28:a:1580:A:H2'	28:a:1581:A:C8	2.49	0.47
28:a:2285:A:OP1	33:f:71:ARG:HD2	2.14	0.47
6:A:507:U:H2'	6:A:508:C:C6	2.49	0.47
6:A:976:U:H3'	19:N:6:MET:HE1	1.96	0.47
6:A:978:C:H2'	6:A:979:C:H6	1.79	0.47
28:a:1044:A:H62	28:a:1095:U:H3	1.62	0.47
29:b:48:U:H2'	29:b:49:C:H6	1.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:u:144:PRO:HD3	48:u:171:VAL:HG21	1.96	0.47
6:A:1008:A:C2	6:A:1213:A:H1'	2.49	0.47
6:A:1232:A:H2	6:A:1235:G:N3	2.12	0.47
7:B:82:GLU:O	7:B:86:ARG:HB2	2.14	0.47
13:H:11:LEU:HD13	13:H:75:VAL:HG22	1.96	0.47
28:a:1395:U:H2'	28:a:1396:G:C8	2.48	0.47
28:a:1679:A:H2'	28:a:1680:A:C8	2.50	0.47
28:a:2282:C:H2'	28:a:2283:U:C6	2.49	0.47
43:p:109:ILE:HG12	44:q:49:ILE:HG12	1.96	0.47
6:A:751:U:H2'	6:A:752:G:O4'	2.15	0.47
6:A:944:U:H2'	6:A:945:G:C8	2.49	0.47
28:a:586:A:H2'	28:a:587:G:C8	2.49	0.47
28:a:1807:U:H5	30:c:177:ARG:HH12	1.60	0.47
28:a:2182:U:H2'	28:a:2183:C:C6	2.49	0.47
29:b:3:C:H2'	29:b:4:U:C6	2.49	0.47
35:h:58:ALA:O	35:h:62:LYS:HG3	2.15	0.47
6:A:862:C:H2'	6:A:863:G:O4'	2.14	0.47
9:D:159:LEU:HD23	9:D:159:LEU:HA	1.81	0.47
28:a:1471:A:H2'	28:a:1472:A:H8	1.77	0.47
28:a:1870:U:H2'	28:a:1871:G:O4'	2.15	0.47
28:a:2001:A:H2'	28:a:2002:A:C8	2.49	0.47
30:c:211:THR:HG23	30:c:216:VAL:HB	1.96	0.47
33:f:106:ILE:HG21	33:f:139:PRO:HG3	1.96	0.47
39:l:48:GLU:OE2	39:l:48:GLU:HA	2.15	0.47
41:n:31:ARG:HG3	41:n:36:ILE:HD12	1.97	0.47
48:u:11:ARG:HD3	48:u:44:THR:HG22	1.95	0.47
6:A:365:A:H2'	6:A:366:C:O4'	2.15	0.47
6:A:815:G:H2'	6:A:816:U:C6	2.49	0.47
6:A:842:U:H2'	6:A:843:C:H6	1.80	0.47
6:A:1458:U:H2'	6:A:1459:A:H8	1.80	0.47
7:B:66:LYS:HA	7:B:89:MET:HE1	1.96	0.47
16:K:14:LYS:HB2	16:K:77:TYR:HE1	1.79	0.47
28:a:349:U:O2'	28:a:350:G:H8	1.97	0.47
28:a:1185:U:H2'	28:a:1186:U:H6	1.79	0.47
28:a:1626:U:H2'	28:a:1627:A:C8	2.49	0.47
28:a:2430:C:H2'	28:a:2431:G:H8	1.78	0.47
31:d:6:VAL:HG22	31:d:202:ILE:HG12	1.96	0.47
32:e:171:VAL:HG21	32:e:194:LYS:HB3	1.97	0.47
44:q:84:MET:HB2	44:q:84:MET:HE2	1.82	0.47
6:A:845:U:H2'	6:A:846:A:H8	1.80	0.47
10:E:15:LYS:HB2	10:E:39:VAL:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:O:32:LEU:HD11	20:O:62:GLN:HG2	1.97	0.47
28:a:1540:U:H2'	28:a:1541:U:C6	2.50	0.47
28:a:2084:U:H2'	28:a:2085:U:C6	2.50	0.47
45:r:41:LYS:HE2	53:z:22:LEU:HD11	1.97	0.47
6:A:82:U:H4'	6:A:83:G:C8	2.50	0.47
11:F:2:ARG:HE	11:F:91:ARG:HH21	1.62	0.47
28:a:852:A:H2'	28:a:853:G:H8	1.77	0.47
28:a:1394:C:H2'	28:a:1395:U:C6	2.49	0.47
28:a:1845:A:H2'	28:a:1846:U:O4'	2.14	0.47
28:a:2351:C:H2'	28:a:2352:G:O4'	2.15	0.47
29:b:46:A:H5"	41:n:4:LYS:HD2	1.96	0.47
42:o:101:LEU:HD23	42:o:104:LEU:HD12	1.96	0.47
6:A:346:C:H4'	6:A:348:G:OP1	2.14	0.47
6:A:469:U:H2'	6:A:470:G:H8	1.80	0.47
6:A:1152:C:C5	6:A:1154:G:H1'	2.50	0.47
6:A:1472:U:H2'	6:A:1473:C:C6	2.50	0.47
7:B:19:GLN:HA	7:B:38:ILE:HA	1.97	0.47
17:L:30:ARG:HD2	17:L:30:ARG:HA	1.61	0.47
28:a:43:G:C2'	28:a:44:A:H5'	2.45	0.47
28:a:273:A:H2'	28:a:274:G:O4'	2.15	0.47
28:a:733:C:OP1	31:d:135:GLY:HA2	2.14	0.47
28:a:2234:A:H2'	28:a:2235:C:H6	1.79	0.47
28:a:2258:G:OP1	49:v:18:SER:HB3	2.15	0.47
29:b:78:A:H2'	29:b:79:G:O4'	2.15	0.47
31:d:32:PRO:HB3	31:d:97:THR:HG22	1.97	0.47
48:u:114:GLU:OE1	48:u:127:ILE:HG21	2.15	0.47
6:A:471:U:H2'	6:A:472:U:C6	2.50	0.46
15:J:12:ALA:HB2	15:J:96:VAL:HA	1.97	0.46
17:L:86:ARG:HA	17:L:94:ARG:HA	1.97	0.46
28:a:719:G:O2'	28:a:753:G:H4'	2.16	0.46
28:a:2789:U:H2'	28:a:2790:C:H6	1.81	0.46
30:c:132:LEU:HD23	30:c:135:ILE:HD12	1.97	0.46
6:A:1112:U:H2'	6:A:1113:C:H6	1.80	0.46
28:a:150:U:H2'	28:a:151:C:C6	2.50	0.46
28:a:566:U:H2'	28:a:567:G:C8	2.50	0.46
28:a:937:A:H2'	28:a:938:C:C6	2.49	0.46
28:a:1721:C:H2'	28:a:1722:C:H6	1.80	0.46
28:a:1783:U:H2'	28:a:1784:C:H6	1.78	0.46
28:a:2316:A:H2'	28:a:2317:G:C8	2.51	0.46
28:a:2743:U:H1'	28:a:2744:A:H5"	1.96	0.46
38:k:80:SER:HB3	38:k:114:GLY:HA3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:218:U:H2'	6:A:219:C:H6	1.79	0.46
6:A:960:2MG:C2	27:X:62:VAL:HG21	2.51	0.46
6:A:1396:4OC:H2'	6:A:1397:C:O4'	2.15	0.46
22:Q:30:ARG:HE	22:Q:45:THR:HG23	1.79	0.46
28:a:155:U:H2'	28:a:156:A:H8	1.80	0.46
28:a:1434:U:H2'	28:a:1435:U:C6	2.51	0.46
28:a:1933:U:H2'	28:a:1934:C:H6	1.80	0.46
34:g:87:LEU:HB2	34:g:131:ILE:HB	1.97	0.46
6:A:532:A:H2'	6:A:533:A:C8	2.49	0.46
6:A:1507:A:H2'	6:A:1508:G:H8	1.79	0.46
13:H:76:LYS:HB2	13:H:76:LYS:HE2	1.71	0.46
28:a:1104:C:H2'	28:a:1105:G:C8	2.51	0.46
28:a:1867:U:H2'	28:a:1868:C:C6	2.51	0.46
38:k:87:GLY:HA2	38:k:118:ARG:HH22	1.80	0.46
6:A:230:A:H2'	6:A:231:G:C8	2.50	0.46
6:A:667:G:H5"	11:F:86:ARG:NH2	2.31	0.46
6:A:1002:U:H4'	6:A:1003:U:C5	2.50	0.46
11:F:47:LEU:HD21	11:F:57:ALA:HB3	1.97	0.46
24:S:3:ARG:HE	24:S:7:LYS:HD2	1.79	0.46
26:U:49:ALA:O	26:U:53:VAL:HG13	2.15	0.46
28:a:838:A:H2'	28:a:839:C:C6	2.51	0.46
28:a:2233:G:H2'	28:a:2234:A:H8	1.81	0.46
6:A:41:G:H2'	6:A:42:G:C8	2.51	0.46
6:A:939:G:C2	6:A:940:A:C8	3.03	0.46
10:E:39:VAL:HB	10:E:118:VAL:HG21	1.96	0.46
14:I:130:ARG:C	27:X:55:ARG:HD2	2.40	0.46
28:a:4:C:H2'	28:a:5:A:H8	1.81	0.46
28:a:150:U:H2'	28:a:151:C:H6	1.80	0.46
28:a:1615:C:H2'	28:a:1616:G:O4'	2.16	0.46
28:a:2087:G:H22	28:a:2176:U:H3	1.63	0.46
32:e:125:VAL:HG21	32:e:133:LEU:HD13	1.97	0.46
32:e:163:LEU:HD13	32:e:166:VAL:HG21	1.98	0.46
40:m:45:ARG:HB3	40:m:95:LEU:HD11	1.98	0.46
6:A:4:C:O2'	6:A:5:U:H3'	2.16	0.46
7:B:97:LEU:HB2	7:B:100:MET:HG3	1.97	0.46
11:F:51:ILE:O	11:F:54:VAL:HG22	2.16	0.46
12:G:69:ILE:HD12	12:G:134:ALA:HB3	1.98	0.46
28:a:731:U:H2'	28:a:732:C:H6	1.81	0.46
28:a:2238:OMG:HM23	28:a:2238:OMG:H1'	1.62	0.46
6:A:75:G:H2'	6:A:76:G:H8	1.81	0.46
6:A:833:U:H2'	6:A:834:C:C6	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1518:C:H2'	6:A:1519:G:H8	1.81	0.46
25:T:27:MET:SD	25:T:61:MET:HE3	2.56	0.46
28:a:152:U:H2'	28:a:153:U:C6	2.51	0.46
28:a:1670:U:H2'	28:a:1671:G:O4'	2.16	0.46
28:a:2215:G:H2'	28:a:2216:U:C6	2.51	0.46
28:a:2286:G:H2'	28:a:2287:A:C8	2.51	0.46
29:b:68:C:H2'	29:b:69:G:O4'	2.16	0.46
30:c:271:ARG:HE	30:c:273:LYS:NZ	2.14	0.46
37:j:13:ASN:ND2	37:j:97:ARG:HB2	2.31	0.46
42:o:3:ASN:O	42:o:7:GLN:HG3	2.15	0.46
6:A:229:U:H2'	6:A:230:A:H8	1.81	0.46
6:A:636:A:C8	13:H:107:ASN:HA	2.49	0.46
6:A:905:U:H2'	6:A:906:C:C6	2.51	0.46
6:A:1426:G:H5"	42:o:107:LYS:HG3	1.97	0.46
13:H:51:ILE:HG13	13:H:59:LEU:HD13	1.98	0.46
28:a:938:C:H2'	28:a:939:G:H8	1.80	0.46
29:b:20:G:H2'	29:b:21:U:C6	2.50	0.46
29:b:51:G:H2'	29:b:52:A:C8	2.50	0.46
31:d:101:PHE:HB3	31:d:177:ILE:HD13	1.98	0.46
33:f:34:ILE:HG13	33:f:96:MET:HG3	1.98	0.46
33:f:135:GLN:HG3	33:f:141:ILE:HD12	1.98	0.46
5:4:38:SER:OG	33:f:105:SER:HA	2.16	0.46
6:A:1113:C:H2'	6:A:1114:C:H6	1.81	0.46
6:A:1213:A:H2'	6:A:1214:G:C8	2.52	0.46
12:G:23:LEU:O	12:G:27:MET:HG3	2.16	0.46
18:M:64:THR:HG22	18:M:69:LEU:HB2	1.97	0.46
28:a:1018:A:H2'	28:a:1019:A:H8	1.79	0.46
37:j:115:VAL:HG13	37:j:121:VAL:HG21	1.98	0.46
39:l:54:LEU:HD11	39:l:118:PHE:CE1	2.51	0.46
6:A:154:A:H2'	6:A:155:A:O4'	2.16	0.45
6:A:240:A:C2	6:A:276:A:C5	3.03	0.45
6:A:1005:C:H2'	6:A:1006:A:H8	1.80	0.45
6:A:1416:G:H5'	37:j:48:PRO:HB3	1.98	0.45
15:J:52:LEU:HD23	15:J:62:ARG:HD2	1.98	0.45
27:X:47:LYS:HB2	27:X:47:LYS:HE3	1.66	0.45
28:a:85:G:OP2	47:t:6:ARG:HB2	2.16	0.45
28:a:351:A:H2'	28:a:352:A:C8	2.52	0.45
28:a:511:A:H2'	28:a:512:U:C6	2.51	0.45
28:a:1186:U:H2'	28:a:1187:C:C6	2.51	0.45
6:A:672:U:H2'	6:A:673:U:H6	1.81	0.45
7:B:47:LEU:HB3	7:B:48:PRO:HD3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:167:TRP:HZ3	8:C:169:ARG:HG2	1.80	0.45
12:G:136:LYS:HB3	12:G:136:LYS:HE3	1.64	0.45
28:a:2314:A:H2'	28:a:2315:A:C8	2.51	0.45
28:a:2761:C:H2'	28:a:2762:A:O4'	2.16	0.45
29:b:30:C:H1'	29:b:57:A:H61	1.81	0.45
30:c:5:LYS:HE3	30:c:5:LYS:HB3	1.68	0.45
47:t:90:LYS:HE3	47:t:90:LYS:HB2	1.75	0.45
6:A:509:G:H2'	6:A:510:PSU:H6	1.81	0.45
6:A:859:A:H2'	6:A:860:C:C6	2.51	0.45
6:A:1029:A:H2'	6:A:1030:A:C8	2.51	0.45
6:A:1346:C:H2'	6:A:1347:G:C8	2.51	0.45
28:a:1394:C:H2'	28:a:1395:U:H6	1.81	0.45
28:a:2138:C:H2'	28:a:2139:G:H8	1.81	0.45
28:a:2687:A:H2'	28:a:2688:C:H6	1.81	0.45
33:f:69:TYR:HE1	33:f:84:PRO:HG3	1.81	0.45
50:w:12:PRO:HB3	50:w:30:LEU:HD23	1.98	0.45
6:A:62:U:H2'	6:A:63:C:C6	2.52	0.45
6:A:773:C:H2'	6:A:774:A:O4'	2.16	0.45
28:a:2:G:H2'	28:a:3:U:C6	2.51	0.45
28:a:52:A:H2'	28:a:53:A:H8	1.81	0.45
28:a:913:A:H2'	28:a:914:G:C8	2.51	0.45
28:a:2636:C:H2'	28:a:2637:U:C6	2.50	0.45
28:a:2873:G:H2'	28:a:2874:C:H6	1.80	0.45
43:p:117:LEU:HD13	43:p:117:LEU:HA	1.80	0.45
5:4:20:ASN:ND2	5:4:39:GLU:HG3	2.32	0.45
6:A:59:A:H5"	6:A:381:U:H5"	1.99	0.45
7:B:67:ILE:HG13	7:B:160:ALA:HB3	1.98	0.45
27:X:13:THR:HG22	27:X:15:ALA:H	1.81	0.45
28:a:1431:A:H2'	28:a:1432:G:H8	1.81	0.45
28:a:1483:A:H2'	28:a:1485:C:C5	2.51	0.45
28:a:2544:G:H2'	28:a:2545:C:C6	2.52	0.45
33:f:170:LEU:HD23	33:f:177:PHE:CZ	2.52	0.45
34:g:42:GLU:HG2	34:g:68:THR:HG21	1.99	0.45
1:0:21:LYS:HE3	1:0:21:LYS:HB2	1.56	0.45
6:A:32:A:H2'	6:A:33:A:C8	2.52	0.45
6:A:483:C:H2'	6:A:484:A:H8	1.80	0.45
6:A:1138:G:N2	6:A:1140:A:H62	2.15	0.45
6:A:1212:C:H2'	6:A:1213:A:H8	1.78	0.45
6:A:1398:C:H2'	6:A:1399:G:C8	2.51	0.45
8:C:93:LYS:HA	8:C:93:LYS:HD3	1.66	0.45
11:F:42:TRP:HB2	11:F:59:TYR:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Q:14:ARG:HE	22:Q:61:LEU:HB2	1.81	0.45
26:U:16:LEU:O	26:U:20:LYS:HG2	2.16	0.45
28:a:339:A:H1'	28:a:340:A:H2	1.80	0.45
28:a:2602:U:C2	53:z:4:GLN:HA	2.50	0.45
36:i:36:LEU:HD11	36:i:122:LEU:HB2	1.99	0.45
2:1:12:ARG:HE	2:1:44:VAL:HG22	1.80	0.45
5:4:61:LYS:NZ	24:S:42:PRO:HD3	2.32	0.45
6:A:506:U:H2'	6:A:507:U:C6	2.51	0.45
6:A:1028:G:H2'	6:A:1029:A:C8	2.51	0.45
6:A:1034:A:H2'	6:A:1035:G:C8	2.52	0.45
6:A:1114:C:H2'	6:A:1115:U:H6	1.81	0.45
6:A:1370:U:H2'	6:A:1371:A:C8	2.52	0.45
7:B:71:GLY:HA2	7:B:164:ILE:HG12	1.98	0.45
7:B:84:ALA:CB	7:B:91:TYR:HB3	2.46	0.45
14:I:79:ILE:O	14:I:83:ILE:HD12	2.17	0.45
15:J:56:HIS:CD2	15:J:57:VAL:HG22	2.52	0.45
22:Q:50:HIS:HB2	22:Q:70:LEU:HD13	1.98	0.45
28:a:786:U:OP1	32:e:56:LYS:HE2	2.16	0.45
28:a:2202:C:H2'	28:a:2203:G:H8	1.82	0.45
28:a:2635:G:H2'	28:a:2636:C:C6	2.52	0.45
28:a:2783:C:H4'	28:a:2784:U:OP1	2.17	0.45
33:f:61:THR:HG21	33:f:89:VAL:HG11	1.97	0.45
33:f:136:ILE:H	33:f:136:ILE:HG12	1.59	0.45
50:w:44:LYS:HD2	50:w:44:LYS:HA	1.75	0.45
6:A:84:C:H2'	6:A:85:U:H6	1.82	0.45
6:A:628:C:H2'	6:A:629:A:H8	1.82	0.45
6:A:987:G:H2'	6:A:989:C:H41	1.82	0.45
6:A:1396:4OC:H6	6:A:1396:4OC:O5'	2.16	0.45
9:D:157:GLN:O	9:D:160:GLU:HG2	2.15	0.45
16:K:22:HIS:HB2	16:K:33:THR:HG22	1.99	0.45
22:Q:27:LEU:HD11	22:Q:44:SER:HB2	1.98	0.45
28:a:387:G:H1'	50:w:29:PHE:HB3	1.99	0.45
28:a:2183:C:H2'	28:a:2184:U:C6	2.51	0.45
1:0:4:LEU:HD23	1:0:20:ASP:HB3	1.99	0.45
3:2:49:LEU:HD23	3:2:54:VAL:HA	1.97	0.45
6:A:981:G:H2'	6:A:982:G:C8	2.52	0.45
6:A:1142:U:H2'	6:A:1143:C:O4'	2.16	0.45
9:D:102:VAL:HG13	9:D:107:PHE:HB2	1.98	0.45
10:E:111:ALA:HB1	10:E:138:VAL:HG23	1.98	0.45
13:H:47:ALA:HB3	13:H:62:GLU:HG2	1.99	0.45
14:I:18:ARG:O	14:I:65:VAL:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:J:42:LEU:HD12	15:J:43:PRO:HD2	1.98	0.45
17:L:107:VAL:HG23	17:L:110:ARG:HB2	1.98	0.45
18:M:9:ILE:HD11	18:M:19:LEU:HA	1.98	0.45
22:Q:14:ARG:NH2	22:Q:61:LEU:HB2	2.28	0.45
28:a:1450:A:H2'	28:a:1451:A:C8	2.52	0.45
28:a:1574:U:H4'	28:a:1575:C:O5'	2.17	0.45
28:a:2068:U:H2'	28:a:2069:A:H8	1.82	0.45
28:a:2376:G:H5"	28:a:2377:U:O4'	2.17	0.45
33:f:48:LYS:HD2	33:f:48:LYS:HA	1.75	0.45
48:u:115:GLU:H	48:u:115:GLU:CD	2.25	0.45
6:A:672:U:H2'	6:A:673:U:C6	2.52	0.45
6:A:1316:C:H5"	18:M:99:GLY:HA3	1.98	0.45
8:C:77:ILE:HA	8:C:84:VAL:HG23	1.98	0.45
8:C:122:GLN:O	8:C:126:ARG:HG3	2.17	0.45
12:G:17:LYS:HB2	12:G:44:TYR:CZ	2.52	0.45
24:S:13:LEU:HD13	24:S:13:LEU:HA	1.85	0.45
27:X:34:ILE:HD13	27:X:54:LEU:HD11	1.98	0.45
27:X:50:ILE:HD13	27:X:77:LEU:HD22	1.99	0.45
28:a:1525:U:H2'	28:a:1526:A:O4'	2.17	0.45
28:a:1739:C:H2'	28:a:1740:G:C8	2.52	0.45
31:d:17:THR:O	42:o:80:PRO:HG2	2.17	0.45
32:e:104:LEU:HD23	32:e:104:LEU:HA	1.82	0.45
37:j:2:ILE:HG13	37:j:8:LEU:HD21	1.98	0.45
6:A:35:G:H2'	6:A:36:C:C6	2.52	0.44
6:A:307:A:H2'	6:A:308:C:C6	2.52	0.44
7:B:5:ASN:OD1	7:B:7:ARG:HB2	2.17	0.44
9:D:91:LEU:HD23	9:D:91:LEU:HA	1.85	0.44
24:S:29:LYS:HD2	24:S:30:PRO:HD2	1.99	0.44
28:a:1328:U:H5'	46:s:60:LEU:HB3	1.98	0.44
28:a:1433:C:H2'	28:a:1434:U:C6	2.51	0.44
37:j:25:LEU:HD12	37:j:38:ILE:HG22	1.99	0.44
46:s:17:GLU:CD	46:s:17:GLU:H	2.25	0.44
53:z:13:ARG:HD3	53:z:17:ARG:CZ	2.47	0.44
6:A:45:G:H5"	6:A:301:U:O2'	2.17	0.44
6:A:273:A:H5"	6:A:275:G:O4'	2.17	0.44
6:A:1082:G:H2'	6:A:1083:G:O4'	2.17	0.44
10:E:116:LEU:HB3	10:E:121:VAL:CG2	2.46	0.44
28:a:803:U:H2'	28:a:804:C:H6	1.80	0.44
28:a:2305:G:H5"	28:a:2306:U:OP2	2.18	0.44
33:f:108:LEU:HD23	33:f:108:LEU:HA	1.68	0.44
39:l:76:LYS:HE2	39:l:76:LYS:HB2	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1151:A:C2	6:A:1175:G:C5	3.05	0.44
6:A:1264:G:H2'	6:A:1265:G:H8	1.82	0.44
7:B:218:ALA:HA	7:B:221:VAL:HG12	1.99	0.44
28:a:151:C:H2'	28:a:152:U:H6	1.81	0.44
28:a:222:A:N1	28:a:233:A:H5"	2.32	0.44
28:a:833:G:H2'	28:a:834:U:C6	2.52	0.44
28:a:1284:C:OP1	28:a:2697:C:H4'	2.18	0.44
28:a:1858:A:H2'	28:a:1859:A:C8	2.53	0.44
28:a:2287:A:H2'	28:a:2288:C:C6	2.52	0.44
29:b:24:G:N7	29:b:56:G:H2'	2.33	0.44
30:c:96:TYR:HE2	30:c:102:ARG:HG3	1.83	0.44
31:d:151:THR:HG22	31:d:152:PRO:CD	2.47	0.44
6:A:107:G:H2'	6:A:108:U:C6	2.52	0.44
6:A:183:A:H4'	6:A:184:G:O5'	2.17	0.44
6:A:739:U:H5'	6:A:829:G:N2	2.31	0.44
6:A:838:G:H2'	6:A:839:A:O4'	2.18	0.44
6:A:968:A:H5'	6:A:970:G:OP1	2.17	0.44
7:B:141:LEU:HD23	7:B:141:LEU:HA	1.74	0.44
10:E:73:ILE:HD13	10:E:142:PHE:CE2	2.53	0.44
14:I:39:PHE:HE2	14:I:48:VAL:HG21	1.82	0.44
18:M:81:MET:SD	18:M:91:HIS:HB3	2.58	0.44
28:a:272:A:H2'	28:a:273:A:H8	1.80	0.44
28:a:578:U:H2'	28:a:579:U:C6	2.52	0.44
28:a:580:A:H2'	28:a:581:U:C6	2.52	0.44
28:a:614:C:O2'	28:a:647:U:H5"	2.18	0.44
28:a:921:C:H4'	28:a:922:G:H5'	1.99	0.44
28:a:1425:U:H2'	28:a:1426:A:C8	2.52	0.44
28:a:1831:C:H5"	30:c:257:LYS:HG3	1.98	0.44
28:a:2169:G:H2'	28:a:2170:C:H6	1.82	0.44
30:c:107:PRO:HG2	30:c:127:GLY:HA2	2.00	0.44
30:c:137:VAL:HA	30:c:164:LEU:HD22	1.99	0.44
33:f:13:ALA:HA	33:f:28:VAL:HG11	1.99	0.44
1:0:9:SER:HB3	1:0:45:TYR:CZ	2.52	0.44
6:A:1074:A:H5"	10:E:22:VAL:HG21	1.99	0.44
6:A:1307:U:H2'	6:A:1308:C:C6	2.52	0.44
6:A:1312:A:H1'	24:S:37:ARG:HH11	1.82	0.44
8:C:191:THR:HG21	8:C:196:ILE:HD12	2.00	0.44
10:E:116:LEU:HD13	10:E:124:VAL:HG21	1.99	0.44
18:M:56:LEU:O	18:M:60:VAL:HG23	2.18	0.44
26:U:5:LYS:HE3	26:U:5:LYS:HB3	1.83	0.44
27:X:38:GLN:HB3	27:X:53:THR:HG23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:1056:U:H2'	28:a:1058:G:N7	2.33	0.44
28:a:2366:G:H2'	28:a:2367:U:C6	2.53	0.44
33:f:47:LYS:HZ2	33:f:84:PRO:HD2	1.81	0.44
38:k:77:VAL:HG21	38:k:95:LEU:HD13	2.00	0.44
45:r:1:MET:HG2	45:r:109:ASP:OD2	2.18	0.44
46:s:87:GLN:HB2	46:s:90:GLN:OE1	2.17	0.44
47:t:56:GLY:O	47:t:58:VAL:HG23	2.17	0.44
48:u:126:GLU:CD	48:u:190:SER:HA	2.43	0.44
5:4:49:LYS:HD3	18:M:61:ALA:HB1	2.00	0.44
6:A:1506:U:H2'	6:A:1507:A:C8	2.53	0.44
18:M:67:GLY:O	18:M:71:ARG:HG3	2.17	0.44
28:a:763:U:O2'	30:c:48:ARG:HD3	2.18	0.44
28:a:898:A:H2'	28:a:901:C:C5	2.51	0.44
28:a:1532:C:H2'	28:a:1533:G:O4'	2.17	0.44
28:a:1554:C:H2'	28:a:1555:C:C6	2.53	0.44
28:a:2052:C:H2'	28:a:2053:C:H6	1.82	0.44
28:a:2442:G:H2'	28:a:2443:C:C6	2.53	0.44
28:a:2791:C:H2'	28:a:2792:C:H6	1.82	0.44
32:e:15:GLU:HG3	32:e:19:GLY:HA3	1.99	0.44
33:f:3:ARG:O	33:f:7:ILE:HG13	2.18	0.44
33:f:91:LEU:HD12	33:f:95:ARG:HB3	2.00	0.44
46:s:66:THR:HB	46:s:73:LEU:HD22	2.00	0.44
6:A:942:C:H5'	6:A:1300:A:O2'	2.18	0.44
6:A:1445:C:H2'	6:A:1446:A:O4'	2.18	0.44
28:a:744:G:H2'	28:a:745:U:C6	2.52	0.44
28:a:1031:G:H2'	28:a:1032:G:H8	1.81	0.44
28:a:1340:A:H2'	28:a:1341:A:H8	1.81	0.44
28:a:1357:C:H2'	28:a:1358:G:O4'	2.18	0.44
28:a:2113:A:H4'	28:a:2114:G:H5'	1.98	0.44
28:a:2152:C:H2'	28:a:2153:U:H6	1.83	0.44
28:a:2330:U:H2'	28:a:2331:U:C6	2.53	0.44
31:d:63:LYS:HB3	31:d:63:LYS:HE3	1.75	0.44
32:e:167:ASP:HB2	32:e:182:TYR:OH	2.17	0.44
39:l:76:LYS:HB3	39:l:91:GLU:HG3	1.98	0.44
6:A:78:A:H2'	6:A:79:G:C8	2.53	0.44
6:A:894:A:H2'	6:A:895:A:C8	2.53	0.44
6:A:1487:A:O2'	27:X:72:ALA:HA	2.18	0.44
7:B:8:ASP:HB2	7:B:212:LEU:HD11	1.99	0.44
17:L:122:PRO:O	17:L:123:LYS:HG2	2.17	0.44
28:a:38:A:N3	32:e:42:SER:HB3	2.33	0.44
28:a:248:G:H5'	28:a:250:G:N7	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:1517:U:H2'	28:a:1518:C:O4'	2.17	0.44
28:a:1568:U:H2'	28:a:1569:A:H8	1.83	0.44
28:a:2097:G:H5'	28:a:2105:U:H3	1.83	0.44
28:a:2498:U:OP1	31:d:128:ARG:HD2	2.18	0.44
30:c:172:VAL:HG12	30:c:184:VAL:O	2.18	0.44
5:4:56:ARG:HD3	5:4:59:ARG:HE	1.83	0.44
6:A:1501:A:H2'	6:A:1502:G:C8	2.53	0.44
8:C:10:ILE:HD12	8:C:10:ILE:HA	1.87	0.44
28:a:1399:U:H2'	28:a:1400:A:H8	1.83	0.44
28:a:1910:U:H2'	28:a:1911:C:C6	2.53	0.44
28:a:2039:A:H4'	31:d:148:GLN:O	2.18	0.44
28:a:2467:C:H2'	28:a:2468:G:O4'	2.17	0.44
28:a:2727:A:H2'	28:a:2728:A:C8	2.52	0.44
29:b:32:U:H2'	29:b:33:G:H8	1.83	0.44
35:h:3:VAL:HG23	35:h:19:VAL:HG23	2.00	0.44
6:A:218:U:H2'	6:A:219:C:C6	2.52	0.43
6:A:702:A:H2'	6:A:703:G:H8	1.82	0.43
8:C:69:HIS:HB3	8:C:106:ILE:HD11	2.00	0.43
9:D:8:LYS:HB3	9:D:21:LEU:HB3	1.99	0.43
24:S:22:ALA:HB1	24:S:47:LEU:HD21	1.99	0.43
25:T:84:LYS:O	25:T:88:THR:HG23	2.17	0.43
28:a:84:A:C2	28:a:103:A:C5	3.06	0.43
28:a:2688:C:H3'	28:a:2689:G:H5"	2.00	0.43
32:e:47:THR:HG22	32:e:85:ALA:HB3	2.00	0.43
36:i:21:ALA:HA	36:i:61:GLN:HB2	1.99	0.43
42:o:51:LYS:HB3	42:o:51:LYS:HE2	1.70	0.43
6:A:8:A:H5"	10:E:127:LYS:HD2	2.00	0.43
6:A:22:G:H2'	6:A:23:C:C6	2.52	0.43
6:A:496:A:H2'	6:A:497:C:O4'	2.19	0.43
6:A:547:A:H5"	17:L:21:VAL:HG21	2.00	0.43
6:A:979:C:H2'	6:A:980:U:C6	2.53	0.43
28:a:2138:C:H2'	28:a:2139:G:C8	2.53	0.43
34:g:175:LYS:HG3	34:g:176:LYS:N	2.32	0.43
50:w:43:GLU:HB3	50:w:45:ARG:HG2	1.99	0.43
51:x:44:SER:O	51:x:48:ARG:HG2	2.18	0.43
6:A:149:U:H2'	6:A:150:C:H6	1.82	0.43
6:A:933:G:H2'	6:A:934:C:C6	2.52	0.43
6:A:1115:U:H2'	6:A:1116:U:C6	2.54	0.43
6:A:1230:A:H4'	6:A:1298:G:H4'	2.00	0.43
9:D:15:GLU:HB3	9:D:60:LYS:HG3	2.00	0.43
26:U:16:LEU:HD23	26:U:16:LEU:HA	1.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:151:C:H2'	28:a:152:U:C6	2.53	0.43
28:a:1521:C:H2'	28:a:1522:U:O4'	2.19	0.43
28:a:2478:U:H5"	28:a:2557:G:H5'	1.99	0.43
28:a:2619:A:H2'	28:a:2620:G:C8	2.53	0.43
31:d:57:ARG:O	31:d:61:VAL:HG23	2.18	0.43
40:m:55:ALA:HA	40:m:80:PHE:CE1	2.53	0.43
6:A:75:G:H2'	6:A:76:G:C8	2.53	0.43
6:A:172:C:C2	6:A:173:A:C8	3.05	0.43
6:A:304:G:H5"	21:P:31:ARG:HB2	2.00	0.43
6:A:1008:A:H2'	6:A:1009:G:C8	2.53	0.43
6:A:1112:U:H2'	6:A:1113:C:C6	2.53	0.43
24:S:62:VAL:HG13	24:S:66:MET:HG3	2.00	0.43
28:a:84:A:H8	28:a:84:A:OP2	2.02	0.43
28:a:490:U:H2'	28:a:491:G:O4'	2.18	0.43
28:a:2112:G:H2'	28:a:2113:A:C5	2.53	0.43
28:a:2448:A:H2'	28:a:2449:C:C6	2.54	0.43
31:d:33:ASN:HB3	31:d:51:VAL:HG13	2.00	0.43
6:A:480:U:H2'	6:A:481:A:H8	1.83	0.43
6:A:1036:A:H2'	6:A:1037:C:C6	2.52	0.43
13:H:102:SER:HB3	13:H:113:ASP:HB3	2.00	0.43
16:K:59:THR:HG23	16:K:62:ALA:H	1.83	0.43
24:S:45:VAL:HG13	24:S:63:ASN:HA	2.00	0.43
28:a:255:A:H2'	28:a:256:A:O4'	2.18	0.43
28:a:405:C:H2'	28:a:406:A:C8	2.54	0.43
28:a:1212:G:H2'	28:a:1213:A:C8	2.54	0.43
28:a:1471:A:H2'	28:a:1472:A:C8	2.52	0.43
28:a:2034:C:H2'	28:a:2035:G:H8	1.82	0.43
29:b:18:G:H2'	29:b:19:C:C6	2.54	0.43
33:f:10:LYS:HB3	33:f:11:GLU:OE1	2.19	0.43
6:A:739:U:H2'	6:A:740:G:C8	2.54	0.43
6:A:1143:C:H2'	6:A:1144:U:C6	2.54	0.43
6:A:1321:G:H2'	6:A:1322:C:H6	1.84	0.43
6:A:1420:G:H2'	6:A:1421:C:H6	1.84	0.43
28:a:569:G:H2'	28:a:570:U:C6	2.54	0.43
28:a:1374:A:H5'	28:a:1456:A:H1'	1.99	0.43
28:a:1519:G:H2'	28:a:1520:U:H6	1.81	0.43
28:a:2152:C:H2'	28:a:2153:U:C6	2.54	0.43
28:a:2343:A:H2'	28:a:2344:G:O4'	2.18	0.43
40:m:103:ARG:HG3	40:m:110:MET:SD	2.58	0.43
43:p:94:VAL:O	43:p:98:LEU:HG	2.18	0.43
6:A:507:U:H2'	6:A:508:C:H6	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1302:C:OP1	18:M:97:VAL:HG22	2.18	0.43
6:A:1352:U:H5"	6:A:1353:C:C5	2.54	0.43
15:J:37:ARG:HA	15:J:37:ARG:HD2	1.88	0.43
28:a:405:C:H2'	28:a:406:A:H8	1.83	0.43
28:a:1344:C:H2'	28:a:1345:G:O4'	2.18	0.43
28:a:2156:A:H2'	28:a:2157:A:C8	2.53	0.43
6:A:494:G:H2'	6:A:495:C:C6	2.53	0.43
6:A:960:2MG:C5	27:X:62:VAL:HG11	2.54	0.43
8:C:124:LEU:HD11	8:C:153:VAL:HG21	2.01	0.43
10:E:39:VAL:HG11	10:E:115:VAL:HG22	2.01	0.43
11:F:21:MET:HB2	11:F:21:MET:HE2	1.70	0.43
18:M:74:ASN:HA	18:M:77:ILE:HD12	2.00	0.43
28:a:1472:A:H2'	28:a:1473:U:C6	2.53	0.43
28:a:1475:U:H2'	28:a:1476:U:C6	2.54	0.43
28:a:1761:C:O2	28:a:1761:C:H2'	2.18	0.43
30:c:183:LYS:HB3	30:c:183:LYS:HE2	1.65	0.43
36:i:4:TYR:CD1	43:p:100:VAL:HG11	2.53	0.43
6:A:735:G:H2'	6:A:736:G:O4'	2.18	0.43
6:A:815:G:H2'	6:A:816:U:H6	1.84	0.43
6:A:877:C:O2'	6:A:878:U:H5'	2.19	0.43
6:A:1056:U:H2'	6:A:1057:C:C6	2.54	0.43
6:A:1066:G:H2'	6:A:1067:U:C6	2.54	0.43
9:D:115:ARG:HG3	9:D:133:PRO:HB3	2.01	0.43
12:G:139:GLU:O	12:G:143:ARG:HG2	2.17	0.43
28:a:30:G:H2'	28:a:31:C:C6	2.54	0.43
28:a:296:G:H2'	28:a:297:C:H6	1.83	0.43
28:a:1048:G:C2	28:a:1071:U:O2	2.72	0.43
28:a:1084:U:H1'	28:a:1087:U:H5	1.84	0.43
28:a:2503:A:O2'	28:a:2504:C:H5'	2.19	0.43
30:c:131:PRO:HA	30:c:189:ARG:HA	2.00	0.43
33:f:136:ILE:HD12	33:f:143:TYR:HD1	1.84	0.43
6:A:926:C:H5"	12:G:4:ARG:HE	1.83	0.43
20:O:12:VAL:O	20:O:16:LYS:HB3	2.19	0.43
24:S:11:ILE:HD13	24:S:41:LEU:HD21	2.01	0.43
26:U:33:ARG:HG3	26:U:36:GLU:OE2	2.18	0.43
28:a:524:G:H2'	28:a:525:U:C6	2.53	0.43
28:a:957:U:H2'	28:a:958:C:C6	2.54	0.43
28:a:977:C:H2'	28:a:978:A:O4'	2.19	0.43
28:a:1392:U:H2'	28:a:1393:U:C6	2.54	0.43
28:a:2123:G:H1	28:a:2142:U:H3	1.66	0.43
28:a:2168:G:H2'	28:a:2169:G:H8	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:2492:G:O2'	28:a:2493:U:H5"	2.19	0.43
29:b:36:C:N4	29:b:37:C:H41	2.17	0.43
34:g:163:ARG:HG3	34:g:164:TYR:O	2.19	0.43
36:i:39:LYS:HE2	36:i:39:LYS:HB3	1.75	0.43
6:A:230:A:H2'	6:A:231:G:H8	1.84	0.42
6:A:250:U:H2'	6:A:251:G:C8	2.54	0.42
6:A:944:U:H2'	6:A:945:G:H8	1.82	0.42
6:A:1042:G:H1'	6:A:1209:G:H5"	2.01	0.42
6:A:1119:U:C2	6:A:1121:A:C8	3.07	0.42
6:A:1136:G:H2'	6:A:1137:G:O4'	2.19	0.42
11:F:69:LYS:HE2	11:F:69:LYS:HB2	1.72	0.42
14:I:6:ASN:HD22	14:I:90:TYR:HA	1.84	0.42
18:M:73:ILE:O	18:M:77:ILE:HD12	2.18	0.42
28:a:2202:C:H2'	28:a:2203:G:C8	2.54	0.42
28:a:2874:C:H2'	28:a:2875:C:C6	2.54	0.42
33:f:8:TYR:OH	33:f:30:ARG:HB3	2.19	0.42
51:x:3:ALA:HA	51:x:6:LEU:HB2	2.00	0.42
2:1:25:LYS:HB3	2:1:25:LYS:HE3	1.80	0.42
6:A:709:A:H2'	6:A:710:A:C8	2.54	0.42
6:A:1299:G:HO2'	6:A:1300:A:H8	1.66	0.42
6:A:1352:U:H5"	6:A:1353:C:H5	1.85	0.42
9:D:45:ARG:HE	9:D:45:ARG:HA	1.84	0.42
10:E:148:MET:HB3	10:E:148:MET:HE3	1.67	0.42
21:P:6:LEU:HB3	21:P:17:TYR:HB3	2.01	0.42
28:a:871:G:H2'	28:a:872:G:C8	2.54	0.42
28:a:2048:G:H2'	28:a:2488:C:O2'	2.19	0.42
28:a:2502:C:H2'	28:a:2503:A:H8	1.84	0.42
28:a:2886:G:H2'	28:a:2887:A:C8	2.54	0.42
46:s:12:GLY:HA2	51:x:30:MET:SD	2.60	0.42
6:A:558:C:C5	22:Q:36:ILE:HD11	2.54	0.42
6:A:685:G:O2'	6:A:791:C:H4'	2.19	0.42
6:A:902:A:H2'	6:A:903:A:C8	2.54	0.42
6:A:942:C:H2'	6:A:943:A:H8	1.84	0.42
6:A:1034:A:C2	6:A:1035:G:C5	3.08	0.42
6:A:1101:C:C4	6:A:1102:G:C8	3.07	0.42
9:D:104:ARG:HD2	9:D:170:TRP:HZ2	1.85	0.42
27:X:26:ARG:HD2	27:X:26:ARG:O	2.18	0.42
28:a:510:U:C2	28:a:511:A:C8	3.07	0.42
28:a:887:C:H2'	28:a:888:A:O4'	2.20	0.42
28:a:2364:A:H2'	28:a:2365:A:C8	2.54	0.42
29:b:4:U:H2'	29:b:5:U:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:e:82:THR:HB	32:e:85:ALA:HB2	2.01	0.42
32:e:143:LYS:HA	32:e:143:LYS:HD3	1.82	0.42
6:A:483:C:H2'	6:A:484:A:C8	2.54	0.42
6:A:1381:G:H2'	6:A:1382:C:C6	2.54	0.42
8:C:91:LEU:HB2	8:C:99:VAL:HG21	2.02	0.42
11:F:1:MET:HG2	11:F:66:CYS:C	2.44	0.42
28:a:726:C:H2'	28:a:727:C:C6	2.54	0.42
28:a:750:G:H2'	28:a:751:A:O4'	2.19	0.42
28:a:1144:C:H2'	28:a:1145:G:O4'	2.19	0.42
46:s:5:ARG:O	46:s:9:VAL:HG23	2.20	0.42
6:A:31:G:H3'	6:A:32:A:H5"	2.00	0.42
6:A:376:A:H2'	6:A:377:A:C8	2.54	0.42
10:E:35:THR:HG22	10:E:53:LYS:HG3	2.01	0.42
10:E:116:LEU:HD13	10:E:124:VAL:HG11	2.02	0.42
24:S:66:MET:HE2	24:S:66:MET:HB3	1.94	0.42
28:a:348:U:H2'	28:a:349:U:H5'	2.02	0.42
28:a:557:U:H2'	28:a:558:U:O4'	2.19	0.42
28:a:1039:C:H2'	28:a:1040:A:O4'	2.19	0.42
28:a:2430:C:H2'	28:a:2431:G:C8	2.53	0.42
29:b:45:A:C4	29:b:46:A:C8	3.07	0.42
32:e:163:LEU:HD23	32:e:163:LEU:HA	1.79	0.42
37:j:64:ARG:HB2	37:j:79:PHE:CD1	2.55	0.42
6:A:22:G:H2'	6:A:23:C:H6	1.85	0.42
6:A:1084:U:H2'	6:A:1085:U:C6	2.55	0.42
6:A:1420:G:H2'	6:A:1421:C:C6	2.55	0.42
7:B:56:PHE:HA	7:B:59:ARG:HE	1.84	0.42
7:B:203:ASN:OD1	7:B:203:ASN:C	2.62	0.42
24:S:50:ALA:HB1	24:S:57:HIS:HB3	2.01	0.42
26:U:17:ARG:HG2	26:U:21:ARG:NH1	2.35	0.42
28:a:540:U:H2'	28:a:541:A:C8	2.51	0.42
28:a:734:C:H2'	28:a:735:1MG:O4'	2.19	0.42
28:a:1048:G:C2	28:a:1071:U:C2	3.08	0.42
28:a:1185:U:H4'	43:p:9:ILE:HD11	2.01	0.42
28:a:1520:U:H2'	28:a:1521:C:H6	1.85	0.42
28:a:2135:G:H2'	28:a:2136:U:C5	2.54	0.42
33:f:42:GLU:H	33:f:42:GLU:CD	2.27	0.42
34:g:38:HIS:ND1	34:g:39:PRO:HD2	2.34	0.42
46:s:5:ARG:HG3	46:s:9:VAL:HG23	2.01	0.42
46:s:49:LEU:HD13	51:x:26:PHE:CE2	2.54	0.42
6:A:508:C:H2'	6:A:509:G:H8	1.83	0.42
6:A:636:A:H2'	6:A:637:C:C6	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:976:U:H4'	6:A:977:A:O5'	2.19	0.42
6:A:1027:G:O5'	6:A:1027:G:H8	2.03	0.42
6:A:1138:G:H21	6:A:1140:A:H62	1.67	0.42
6:A:1425:A:H3'	6:A:1426:G:C8	2.54	0.42
11:F:35:LYS:HE2	11:F:35:LYS:HB3	1.91	0.42
12:G:26:PHE:CE2	12:G:120:LEU:HD21	2.54	0.42
28:a:182:A:H2'	28:a:183:C:H6	1.84	0.42
28:a:226:A:H3'	28:a:227:A:H8	1.85	0.42
28:a:1018:A:H61	28:a:1115:G:H2'	1.85	0.42
28:a:1985:A:H2'	28:a:1986:C:C6	2.54	0.42
6:A:1271:C:H2'	6:A:1272:U:H5"	2.01	0.42
8:C:66:ILE:O	8:C:101:ILE:HA	2.20	0.42
11:F:18:VAL:O	11:F:22:VAL:HG13	2.20	0.42
16:K:18:ASP:OD2	16:K:37:ARG:HD3	2.19	0.42
28:a:424:C:O2'	28:a:425:U:H5'	2.19	0.42
28:a:1269:U:H2'	28:a:1270:G:O4'	2.20	0.42
28:a:1540:U:H5'	28:a:1727:G:N2	2.34	0.42
28:a:1796:A:H2'	28:a:1797:A:C8	2.54	0.42
28:a:1817:C:H2'	28:a:1818:G:H8	1.84	0.42
28:a:2038:U:H5'	28:a:2565:G:O4'	2.20	0.42
28:a:2168:G:H2'	28:a:2169:G:C8	2.54	0.42
28:a:2169:G:H2'	28:a:2170:C:C6	2.54	0.42
30:c:53:HIS:HA	30:c:217:ARG:HB2	2.00	0.42
44:q:1:MET:SD	44:q:43:ASN:HB3	2.59	0.42
6:A:577:A:H2'	6:A:578:G:O4'	2.20	0.42
6:A:1090:C:H2'	6:A:1091:C:H6	1.85	0.42
6:A:1096:A:H2'	6:A:1097:C:C6	2.54	0.42
6:A:1322:C:OP1	18:M:28:THR:HG21	2.20	0.42
8:C:38:LYS:HD2	8:C:38:LYS:HA	1.61	0.42
15:J:82:LYS:HE2	15:J:85:ASP:HB3	2.02	0.42
28:a:247:G:H4'	28:a:377:G:C5	2.55	0.42
28:a:590:G:H1'	32:e:99:MET:HG2	2.01	0.42
28:a:1098:U:H2'	28:a:1099:C:C6	2.55	0.42
28:a:1400:A:H2'	28:a:1401:C:C6	2.55	0.42
28:a:1662:A:C2	28:a:2569:G:H5'	2.54	0.42
28:a:2329:C:H2'	28:a:2330:U:O4'	2.20	0.42
28:a:2613:C:H2'	28:a:2614:G:C8	2.54	0.42
42:o:89:ARG:HE	42:o:89:ARG:HB3	1.70	0.42
7:B:85:ALA:C	7:B:87:CYS:N	2.77	0.42
16:K:126:LYS:HD2	26:U:37:PHE:CE1	2.55	0.42
28:a:511:A:H2'	28:a:512:U:H6	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:860:U:H2'	28:a:861:U:C6	2.55	0.42
28:a:880:G:H1'	28:a:882:C:H5	1.85	0.42
28:a:2282:C:H2'	28:a:2283:U:H6	1.84	0.42
28:a:2501:U:H2'	28:a:2502:C:C6	2.55	0.42
28:a:2851:G:H2'	28:a:2852:U:C6	2.55	0.42
29:b:75:G:N2	48:u:81:GLN:HE22	2.18	0.42
39:l:34:LEU:HD11	39:l:129:THR:HB	2.01	0.42
40:m:32:GLU:OE1	40:m:119:PRO:HD2	2.20	0.42
43:p:72:ASN:OD1	43:p:107:THR:HG23	2.20	0.42
6:A:673:U:H2'	6:A:674:C:H6	1.84	0.41
6:A:1011:U:H2'	6:A:1012:G:C8	2.55	0.41
6:A:1253:C:H2'	6:A:1254:C:O4'	2.20	0.41
6:A:1296:C:C5	18:M:17:ILE:HG13	2.55	0.41
7:B:80:VAL:HG23	7:B:214:LEU:HD21	2.01	0.41
9:D:117:LEU:HD11	9:D:155:ILE:HD11	2.01	0.41
24:S:3:ARG:NH1	24:S:10:PHE:HB2	2.35	0.41
28:a:944:G:O3'	39:l:13:MET:HG2	2.20	0.41
28:a:2832:U:H2'	28:a:2833:G:H8	1.85	0.41
31:d:26:THR:HG21	31:d:193:VAL:HB	2.02	0.41
32:e:62:LYS:HE3	32:e:62:LYS:HB3	1.83	0.41
33:f:175:PHE:HA	33:f:176:PRO:HD3	1.89	0.41
39:l:63:LYS:HE3	39:l:65:TRP:CZ2	2.54	0.41
48:u:162:LEU:HD23	48:u:162:LEU:HA	1.87	0.41
49:v:45:PHE:HB3	49:v:80:VAL:HG23	2.02	0.41
5:4:24:THR:HA	33:f:3:ARG:HH21	1.85	0.41
6:A:470:G:H2'	6:A:471:U:H6	1.85	0.41
7:B:6:MET:HE2	7:B:6:MET:HB2	1.79	0.41
28:a:1107:C:H2'	28:a:1108:C:C6	2.55	0.41
28:a:1277:A:H2'	28:a:1278:C:C6	2.56	0.41
28:a:1399:U:H2'	28:a:1400:A:C8	2.55	0.41
28:a:1491:U:H2'	28:a:1492:U:C6	2.55	0.41
28:a:2269:G:H4'	28:a:2376:G:O2'	2.20	0.41
6:A:45:G:H2'	6:A:46:G:C8	2.55	0.41
6:A:1033:C:H2'	6:A:1034:A:H8	1.85	0.41
10:E:24:LYS:HB2	10:E:24:LYS:HE2	1.65	0.41
18:M:37:THR:O	18:M:39:VAL:HG13	2.21	0.41
25:T:57:VAL:O	25:T:61:MET:HG2	2.20	0.41
27:X:61:ILE:HG22	27:X:81:LEU:HD23	2.03	0.41
28:a:353:G:H2'	28:a:354:U:O4'	2.20	0.41
28:a:876:U:C5	28:a:877:C:H1'	2.56	0.41
6:A:906:C:H2'	6:A:907:A:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:F:40:GLU:HG3	11:F:61:LEU:HD23	2.02	0.41
13:H:18:GLN:OE1	13:H:72:ILE:HB	2.20	0.41
15:J:71:LYS:HB2	15:J:71:LYS:HE2	1.78	0.41
28:a:624:G:H2'	28:a:625:C:C6	2.56	0.41
28:a:744:G:H2'	28:a:745:U:H6	1.85	0.41
28:a:838:A:H2'	28:a:839:C:H6	1.85	0.41
28:a:1060:A:C6	28:a:1087:U:H4'	2.54	0.41
28:a:1857:C:H3'	28:a:1858:A:H8	1.85	0.41
28:a:2089:G:H2'	28:a:2090:C:O4'	2.21	0.41
28:a:2587:A:O2'	28:a:2588:C:H5'	2.20	0.41
6:A:1354:A:H8	6:A:1354:A:OP1	2.03	0.41
6:A:1429:G:H2'	6:A:1430:U:C6	2.55	0.41
12:G:88:PRO:HG3	12:G:149:LYS:HA	2.03	0.41
13:H:43:GLU:OE1	13:H:43:GLU:HA	2.19	0.41
15:J:11:LYS:HB3	15:J:11:LYS:HE3	1.85	0.41
28:a:869:G:H22	28:a:886:C:H2'	1.85	0.41
28:a:1041:G:C6	28:a:1042:C:C4	3.08	0.41
28:a:1163:U:H4'	28:a:1164:A:OP1	2.19	0.41
28:a:1867:U:H2'	28:a:1868:C:H6	1.85	0.41
28:a:2234:A:H2'	28:a:2235:C:C6	2.55	0.41
28:a:2414:C:OP2	28:a:2414:C:H6	2.03	0.41
29:b:32:U:H2'	29:b:33:G:C8	2.55	0.41
33:f:101:ASP:OD2	33:f:102:ARG:N	2.53	0.41
37:j:88:ASN:HD21	37:j:92:GLU:HB3	1.86	0.41
41:n:42:ALA:HB2	41:n:49:LEU:HD21	2.01	0.41
41:n:114:LEU:HD23	41:n:114:LEU:HA	1.82	0.41
47:t:85:LYS:HD3	47:t:94:VAL:HG11	2.03	0.41
50:w:5:CYS:HB3	50:w:8:THR:HG22	2.02	0.41
6:A:549:U:H2'	6:A:550:C:H6	1.82	0.41
6:A:980:U:H2'	6:A:981:G:O4'	2.21	0.41
28:a:807:C:H2'	28:a:808:G:O4'	2.21	0.41
28:a:995:C:O2'	36:i:30:THR:HG21	2.21	0.41
28:a:1190:U:H1'	38:k:4:ASN:HB3	2.03	0.41
28:a:1573:U:H5'	28:a:1574:U:OP1	2.20	0.41
28:a:1658:A:H4'	28:a:1659:A:O5'	2.20	0.41
28:a:1741:A:H2'	28:a:1742:A:C8	2.56	0.41
28:a:2032:C:H5"	53:z:15:MET:HE3	2.01	0.41
28:a:2168:G:C4	28:a:2169:G:C8	3.08	0.41
28:a:2836:U:H4'	28:a:2855:A:C2	2.56	0.41
29:b:29:A:H2'	29:b:30:C:H6	1.86	0.41
33:f:64:LYS:HA	33:f:65:PRO:HD3	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:i:104:ALA:O	36:i:108:MET:HG3	2.21	0.41
39:l:79:LEU:HD23	39:l:80:GLU:N	2.35	0.41
41:n:9:LEU:HD23	41:n:9:LEU:HA	1.85	0.41
6:A:83:G:O5'	6:A:83:G:H8	2.04	0.41
15:J:49:PHE:HE2	15:J:67:ILE:HG13	1.86	0.41
25:T:33:LYS:HE2	25:T:33:LYS:HB2	1.89	0.41
25:T:35:VAL:HG11	25:T:79:LEU:HD13	2.03	0.41
26:U:17:ARG:HG2	26:U:21:ARG:HH12	1.85	0.41
28:a:196:A:C2	38:k:50:PHE:HZ	2.39	0.41
28:a:807:C:O2'	28:a:829:U:H5"	2.21	0.41
28:a:974:A:N3	28:a:974:A:H2'	2.35	0.41
28:a:1421:A:H2'	28:a:1422:G:O4'	2.21	0.41
28:a:1482:A:H2'	28:a:1483:A:C8	2.56	0.41
39:l:112:GLU:O	39:l:116:GLU:HG3	2.20	0.41
42:o:39:GLN:HE21	42:o:39:GLN:HB3	1.67	0.41
6:A:67:C:H2'	6:A:68:G:C8	2.56	0.41
6:A:79:G:H2'	6:A:80:C:C6	2.56	0.41
6:A:561:G:H2'	6:A:562:G:O4'	2.21	0.41
8:C:102:ASN:O	8:C:104:GLU:HG2	2.20	0.41
13:H:94:LYS:HE2	13:H:94:LYS:HB3	1.80	0.41
14:I:35:LEU:HD21	14:I:45:ARG:HB3	2.03	0.41
28:a:921:C:H4'	28:a:922:G:C5'	2.51	0.41
28:a:959:G:H2'	28:a:960:U:C6	2.55	0.41
29:b:115:A:H2'	29:b:116:A:H8	1.85	0.41
41:n:74:GLY:HA3	41:n:108:ALA:HB3	2.03	0.41
4:3:1:MET:HE2	4:3:1:MET:HB2	1.89	0.41
5:4:32:ILE:HG13	5:4:33:HIS:N	2.36	0.41
5:4:44:TYR:OH	33:f:176:PRO:HG3	2.20	0.41
5:4:61:LYS:HE3	24:S:42:PRO:CG	2.50	0.41
6:A:584:U:H2'	6:A:585:C:C6	2.56	0.41
6:A:629:A:H2'	6:A:630:U:C6	2.55	0.41
6:A:682:G:H5'	16:K:49:GLY:HA2	2.01	0.41
6:A:841:A:H2'	6:A:842:U:H6	1.84	0.41
6:A:1021:C:H2'	6:A:1022:C:H6	1.83	0.41
6:A:1232:A:N7	6:A:1297:C:H1'	2.36	0.41
8:C:121:ALA:HB1	8:C:189:ALA:HB2	2.02	0.41
11:F:26:THR:HG23	11:F:36:ILE:HD13	2.02	0.41
11:F:42:TRP:HZ2	11:F:61:LEU:HD22	1.86	0.41
15:J:47:GLU:O	15:J:66:GLU:HA	2.21	0.41
27:X:10:LEU:HD22	27:X:43:VAL:HG23	2.03	0.41
27:X:93:LEU:O	27:X:97:GLN:CB	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:10:A:H2'	28:a:11:A:C8	2.55	0.41
28:a:419:A:H2'	28:a:420:A:C8	2.56	0.41
28:a:570:U:H2'	28:a:571:C:H6	1.86	0.41
28:a:683:A:H2'	28:a:684:U:C6	2.56	0.41
28:a:722:C:H2'	28:a:723:G:O4'	2.21	0.41
28:a:1140:A:H2'	28:a:1141:C:C6	2.56	0.41
28:a:1289:A:H5'	28:a:1598:A:P	2.61	0.41
28:a:1414:A:H4'	28:a:1415:C:O5'	2.21	0.41
28:a:1420:A:H2'	28:a:1421:A:H8	1.83	0.41
28:a:1799:U:H2'	28:a:1800:G:H8	1.85	0.41
28:a:1850:G:H2'	28:a:1851:U:C6	2.56	0.41
28:a:1861:C:H2'	28:a:1862:G:O4'	2.21	0.41
28:a:2337:C:H2'	28:a:2338:G:O4'	2.20	0.41
28:a:2385:U:H2'	28:a:2386:G:H8	1.86	0.41
28:a:2637:U:H2'	28:a:2638:C:H6	1.85	0.41
28:a:2791:C:H2'	28:a:2792:C:C6	2.56	0.41
29:b:62:A:H2'	29:b:63:C:C6	2.55	0.41
33:f:15:LYS:HE2	33:f:15:LYS:HB3	1.92	0.41
33:f:26:MET:HE3	33:f:26:MET:HB3	1.88	0.41
36:i:64:VAL:HB	36:i:68:LYS:HE3	2.03	0.41
50:w:56:MET:HE3	50:w:56:MET:HB2	1.86	0.41
6:A:123:A:H1'	6:A:124:A:C8	2.56	0.41
6:A:403:U:OP1	9:D:23:SER:HB3	2.21	0.41
6:A:512:C:H5"	6:A:513:C:C6	2.56	0.41
6:A:760:A:H2'	6:A:761:A:O4'	2.21	0.41
6:A:1312:A:O2'	24:S:37:ARG:HD2	2.21	0.41
6:A:1317:G:H2'	6:A:1318:A:H8	1.83	0.41
7:B:73:LYS:HB3	7:B:73:LYS:HE2	1.88	0.41
7:B:171:ILE:O	7:B:175:GLU:HG3	2.21	0.41
8:C:36:ASP:O	8:C:39:VAL:HG12	2.21	0.41
8:C:87:LEU:O	8:C:91:LEU:HG	2.22	0.41
9:D:73:ARG:HE	9:D:204:TYR:HE1	1.68	0.41
10:E:128:CYS:SG	10:E:132:THR:HG22	2.61	0.41
15:J:78:GLN:N	15:J:79:PRO:HD3	2.36	0.41
18:M:84:GLY:HA2	18:M:92:ARG:HH21	1.86	0.41
28:a:583:U:H2'	28:a:584:U:C6	2.56	0.41
28:a:1050:U:H4'	28:a:1052:G:O5'	2.21	0.41
28:a:1416:G:H2'	28:a:1417:G:C8	2.54	0.41
28:a:1503:G:C2	28:a:1504:A:C8	3.09	0.41
28:a:2274:A:C5	28:a:2276:G:C8	3.08	0.41
30:c:5:LYS:HG3	30:c:17:VAL:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:e:47:THR:O	32:e:51:VAL:HG23	2.21	0.41
38:k:27:LEU:O	38:k:31:GLY:HA2	2.21	0.41
41:n:88:GLN:HA	41:n:115:GLU:HB2	2.03	0.41
6:A:1023:U:H2'	6:A:1025:C:C4	2.56	0.40
6:A:1268:G:O2'	6:A:1269:A:H8	2.04	0.40
6:A:1320:U:O2'	6:A:1321:G:H5'	2.21	0.40
12:G:26:PHE:HZ	12:G:120:LEU:HD11	1.86	0.40
15:J:30:LYS:HB2	15:J:30:LYS:HE2	1.88	0.40
16:K:114:THR:HA	16:K:115:PRO:HD3	1.92	0.40
28:a:618:G:H2'	28:a:619:C:C6	2.56	0.40
28:a:1017:A:C2	28:a:2475:G:H5'	2.57	0.40
28:a:1393:U:H2'	28:a:1394:C:C6	2.56	0.40
28:a:1393:U:H2'	28:a:1394:C:H6	1.86	0.40
28:a:1530:G:C6	28:a:1531:A:C5	3.09	0.40
28:a:1738:U:H2'	28:a:1739:C:C6	2.56	0.40
28:a:1876:A:H2'	28:a:1877:A:H8	1.86	0.40
30:c:182:ARG:HG3	30:c:183:LYS:N	2.36	0.40
36:i:106:LYS:HB2	36:i:106:LYS:HE3	1.73	0.40
48:u:3:ASP:HB3	48:u:4:PHE:H	1.78	0.40
48:u:107:VAL:HG11	48:u:147:ILE:HG13	2.03	0.40
6:A:472:U:H2'	6:A:473:U:C6	2.56	0.40
6:A:667:G:H2'	6:A:668:G:H8	1.79	0.40
6:A:1113:C:H2'	6:A:1114:C:C6	2.56	0.40
6:A:1162:C:H6	6:A:1162:C:H2'	1.70	0.40
6:A:1288:A:H2'	6:A:1289:U:C6	2.56	0.40
28:a:93:A:H2'	28:a:94:C:C6	2.56	0.40
28:a:870:G:H2'	28:a:871:G:C8	2.56	0.40
28:a:938:C:H1'	28:a:974:A:C8	2.56	0.40
28:a:1056:U:H3'	28:a:1057:A:C5'	2.51	0.40
28:a:2304:C:H2'	28:a:2305:G:O4'	2.21	0.40
28:a:2807:A:N3	28:a:2807:A:H2'	2.37	0.40
33:f:74:ILE:HB	33:f:79:ILE:HG13	2.03	0.40
34:g:9:VAL:O	34:g:10:LYS:HG2	2.22	0.40
46:s:52:VAL:HG21	46:s:92:LEU:HD12	2.03	0.40
48:u:47:LEU:HA	48:u:50:ILE:HG22	2.03	0.40
4:3:15:LYS:HE2	4:3:15:LYS:HB3	1.70	0.40
6:A:155:A:H2'	6:A:156:A:C8	2.56	0.40
6:A:1054:U:H2'	6:A:1055:G:H8	1.85	0.40
6:A:1307:U:H2'	6:A:1308:C:H6	1.86	0.40
8:C:181:ASP:O	8:C:181:ASP:OD2	2.39	0.40
11:F:76:ASP:OD1	11:F:76:ASP:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:26:PHE:HE2	12:G:120:LEU:HD21	1.85	0.40
15:J:42:LEU:CD1	15:J:43:PRO:HD2	2.51	0.40
28:a:44:A:O2'	28:a:45:G:H5"	2.21	0.40
28:a:208:C:H2'	28:a:209:C:C6	2.56	0.40
28:a:296:G:H2'	28:a:297:C:C6	2.57	0.40
28:a:348:U:C2'	28:a:349:U:H5'	2.52	0.40
28:a:349:U:H2'	28:a:349:U:OP2	2.21	0.40
28:a:584:U:H2'	28:a:585:C:H6	1.85	0.40
28:a:906:A:H5"	28:a:2255:A:H61	1.85	0.40
28:a:2674:U:H2'	28:a:2675:G:O4'	2.21	0.40
28:a:2758:C:H2'	28:a:2759:C:H6	1.86	0.40
6:A:182:G:H5'	6:A:183:A:N7	2.36	0.40
6:A:210:U:H2'	6:A:211:C:H6	1.83	0.40
6:A:917:A:H2'	6:A:918:C:C6	2.56	0.40
6:A:1332:G:H2'	6:A:1333:A:C8	2.56	0.40
6:A:1422:U:H2'	6:A:1423:C:O4'	2.22	0.40
7:B:42:ASN:ND2	7:B:45:LYS:HG3	2.37	0.40
14:I:52:LEU:HB3	14:I:58:VAL:HB	2.04	0.40
14:I:129:LYS:HD2	14:I:129:LYS:HA	1.62	0.40
22:Q:11:LEU:HD23	22:Q:11:LEU:HA	1.93	0.40
26:U:20:LYS:HA	26:U:20:LYS:HD3	1.91	0.40
28:a:165:A:H2'	28:a:166:U:C6	2.56	0.40
28:a:1552:U:H2'	28:a:1553:U:O4'	2.22	0.40
28:a:2091:C:H2'	28:a:2092:U:O4'	2.21	0.40
28:a:2106:A:C2	28:a:2158:A:H5'	2.57	0.40
33:f:146:ILE:HA	33:f:146:ILE:HD13	1.66	0.40
34:g:77:VAL:HG13	34:g:81:GLN:HE21	1.86	0.40
6:A:902:A:H2'	6:A:903:A:H8	1.86	0.40
6:A:996:A:C6	6:A:997:G:C5	3.10	0.40
6:A:1520:G:OP2	26:U:42:THR:HG23	2.21	0.40
8:C:112:ASP:OD2	8:C:112:ASP:O	2.39	0.40
16:K:67:ALA:HB3	16:K:99:ALA:HB3	2.04	0.40
28:a:20:U:H2'	28:a:21:A:C8	2.56	0.40
28:a:510:U:H2'	28:a:511:A:H8	1.86	0.40
28:a:739:A:H4'	28:a:1258:G:N3	2.37	0.40
28:a:1308:A:C4	28:a:1309:A:C8	3.10	0.40
28:a:1347:G:N7	28:a:1348:G:C8	2.90	0.40
28:a:2135:G:C2	28:a:2136:U:C4	3.09	0.40
28:a:2694:U:H2'	28:a:2695:G:C8	2.57	0.40
48:u:81:GLN:HB2	48:u:91:HIS:HB3	2.04	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%)	49 (100%)	0	0	100	100
2	1	42/44 (96%)	39 (93%)	3 (7%)	0	100	100
3	2	61/64 (95%)	60 (98%)	1 (2%)	0	100	100
4	3	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
5	4	66/71 (93%)	56 (85%)	9 (14%)	1 (2%)	8	28
7	B	222/246 (90%)	201 (90%)	20 (9%)	1 (0%)	24	55
8	C	206/228 (90%)	192 (93%)	14 (7%)	0	100	100
9	D	203/206 (98%)	191 (94%)	12 (6%)	0	100	100
10	E	152/166 (92%)	144 (95%)	8 (5%)	0	100	100
11	F	104/139 (75%)	102 (98%)	2 (2%)	0	100	100
12	G	151/156 (97%)	144 (95%)	7 (5%)	0	100	100
13	H	127/130 (98%)	117 (92%)	9 (7%)	1 (1%)	16	44
14	I	125/130 (96%)	117 (94%)	7 (6%)	1 (1%)	16	44
15	J	97/103 (94%)	92 (95%)	5 (5%)	0	100	100
16	K	115/129 (89%)	107 (93%)	7 (6%)	1 (1%)	14	41
17	L	119/123 (97%)	111 (93%)	8 (7%)	0	100	100
18	M	111/118 (94%)	102 (92%)	9 (8%)	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	79/83 (95%)	79 (100%)	0	0	100	100
22	Q	78/88 (89%)	77 (99%)	1 (1%)	0	100	100
23	R	60/76 (79%)	54 (90%)	6 (10%)	0	100	100
24	S	81/91 (89%)	78 (96%)	3 (4%)	0	100	100
25	T	85/91 (93%)	85 (100%)	0	0	100	100
26	U	60/71 (84%)	56 (93%)	3 (5%)	1 (2%)	7	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	X	96/102 (94%)	91 (95%)	5 (5%)	0	100	100
30	c	270/273 (99%)	262 (97%)	8 (3%)	0	100	100
31	d	208/211 (99%)	194 (93%)	11 (5%)	3 (1%)	9	30
32	e	198/200 (99%)	188 (95%)	10 (5%)	0	100	100
33	f	175/179 (98%)	160 (91%)	14 (8%)	1 (1%)	21	51
34	g	173/177 (98%)	160 (92%)	13 (8%)	0	100	100
35	h	70/148 (47%)	63 (90%)	7 (10%)	0	100	100
36	i	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
37	j	120/122 (98%)	119 (99%)	1 (1%)	0	100	100
38	k	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
39	l	133/137 (97%)	128 (96%)	5 (4%)	0	100	100
40	m	118/129 (92%)	115 (98%)	3 (2%)	0	100	100
41	n	113/116 (97%)	103 (91%)	10 (9%)	0	100	100
42	o	112/116 (97%)	105 (94%)	7 (6%)	0	100	100
43	p	115/118 (98%)	112 (97%)	3 (3%)	0	100	100
44	q	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
45	r	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
46	s	92/99 (93%)	86 (94%)	6 (6%)	0	100	100
47	t	101/104 (97%)	90 (89%)	11 (11%)	0	100	100
48	u	188/204 (92%)	182 (97%)	6 (3%)	0	100	100
49	v	74/85 (87%)	72 (97%)	2 (3%)	0	100	100
50	w	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
51	x	59/63 (94%)	59 (100%)	0	0	100	100
52	y	55/58 (95%)	54 (98%)	1 (2%)	0	100	100
53	z	53/60 (88%)	52 (98%)	1 (2%)	0	100	100
All	All	5702/6110 (93%)	5407 (95%)	285 (5%)	10 (0%)	44	72

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
31	d	149	CYS
31	d	152	PRO
7	B	126	PHE

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Mol	Chain	Res	Type
26	U	28	VAL
13	H	84	ARG
16	K	18	ASP
31	d	75	ALA
33	f	74	ILE
5	4	57	ILE
14	I	28	ILE

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%)	46 (98%)	1 (2%)	47 79
2	1	37/37 (100%)	36 (97%)	1 (3%)	39 74
3	2	54/55 (98%)	54 (100%)	0	100 100
4	3	34/34 (100%)	34 (100%)	0	100 100
5	4	59/61 (97%)	56 (95%)	3 (5%)	21 54
7	B	187/202 (93%)	182 (97%)	5 (3%)	39 74
8	C	172/187 (92%)	169 (98%)	3 (2%)	53 83
9	D	173/174 (99%)	168 (97%)	5 (3%)	37 73
10	E	113/124 (91%)	109 (96%)	4 (4%)	32 67
11	F	91/119 (76%)	89 (98%)	2 (2%)	45 78
12	G	119/122 (98%)	114 (96%)	5 (4%)	26 61
13	H	108/109 (99%)	106 (98%)	2 (2%)	50 81
14	I	104/106 (98%)	99 (95%)	5 (5%)	23 56
15	J	88/92 (96%)	87 (99%)	1 (1%)	65 87
16	K	90/97 (93%)	89 (99%)	1 (1%)	65 87
17	L	105/106 (99%)	102 (97%)	3 (3%)	37 73
18	M	95/99 (96%)	95 (100%)	0	100 100
19	N	81/82 (99%)	80 (99%)	1 (1%)	63 87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	O	74/75 (99%)	72 (97%)	2 (3%)	39	74
21	P	64/65 (98%)	63 (98%)	1 (2%)	55	83
22	Q	73/79 (92%)	71 (97%)	2 (3%)	39	74
23	R	52/64 (81%)	52 (100%)	0	100	100
24	S	72/78 (92%)	69 (96%)	3 (4%)	26	61
25	T	69/70 (99%)	69 (100%)	0	100	100
26	U	51/60 (85%)	50 (98%)	1 (2%)	48	80
27	X	86/88 (98%)	85 (99%)	1 (1%)	63	87
30	c	212/213 (100%)	210 (99%)	2 (1%)	70	89
31	d	161/161 (100%)	157 (98%)	4 (2%)	42	76
32	e	158/158 (100%)	158 (100%)	0	100	100
33	f	151/153 (99%)	148 (98%)	3 (2%)	48	80
34	g	139/141 (99%)	137 (99%)	2 (1%)	59	85
35	h	49/107 (46%)	47 (96%)	2 (4%)	27	62
36	i	119/119 (100%)	117 (98%)	2 (2%)	53	83
37	j	102/102 (100%)	101 (99%)	1 (1%)	68	88
38	k	106/106 (100%)	102 (96%)	4 (4%)	29	64
39	l	108/108 (100%)	104 (96%)	4 (4%)	30	65
40	m	99/104 (95%)	96 (97%)	3 (3%)	36	72
41	n	86/87 (99%)	84 (98%)	2 (2%)	44	78
42	o	96/98 (98%)	93 (97%)	3 (3%)	35	70
43	p	87/88 (99%)	84 (97%)	3 (3%)	32	68
44	q	86/86 (100%)	84 (98%)	2 (2%)	44	78
45	r	87/87 (100%)	87 (100%)	0	100	100
46	s	79/82 (96%)	76 (96%)	3 (4%)	29	64
47	t	88/88 (100%)	85 (97%)	3 (3%)	32	68
48	u	155/165 (94%)	150 (97%)	5 (3%)	34	70
49	v	56/61 (92%)	55 (98%)	1 (2%)	51	82
50	w	66/67 (98%)	65 (98%)	1 (2%)	57	84
51	x	54/55 (98%)	53 (98%)	1 (2%)	50	81
52	y	48/49 (98%)	47 (98%)	1 (2%)	47	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
53	z	48/52 (92%)	48 (100%)	0	100 100
All	All	4738/4969 (95%)	4634 (98%)	104 (2%)	45 78

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	1	MET
2	1	1	MET
5	4	10	GLU
5	4	52	ASP
5	4	62	GLN
7	B	26	LYS
7	B	122	GLN
7	B	143	LYS
7	B	164	ILE
7	B	199	VAL
8	C	67	THR
8	C	87	LEU
8	C	144	ILE
9	D	23	SER
9	D	26	ARG
9	D	35	GLU
9	D	129	THR
9	D	194	ASP
10	E	12	TYR
10	E	86	THR
10	E	125	LEU
10	E	139	TYR
11	F	14	GLN
11	F	31	GLU
12	G	6	VAL
12	G	73	VAL
12	G	74	GLU
12	G	75	VAL
12	G	114	LYS
13	H	25	VAL
13	H	31	LYS
14	I	16	THR
14	I	30	ILE
14	I	58	VAL
14	I	65	VAL
14	I	83	ILE

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Mol	Chain	Res	Type
15	J	47	GLU
16	K	111	THR
17	L	16	VAL
17	L	18	LYS
17	L	40	THR
19	N	79	LEU
20	O	54	ARG
20	O	62	GLN
21	P	55	GLU
22	Q	23	THR
22	Q	82	VAL
24	S	13	LEU
24	S	27	ASP
24	S	41	LEU
26	U	7	LYS
27	X	53	THR
30	c	110	VAL
30	c	246	VAL
31	d	55	GLU
31	d	100	LEU
31	d	162	SER
31	d	181	ASP
33	f	96	MET
33	f	141	ILE
33	f	146	ILE
34	g	49	GLU
34	g	167	GLU
35	h	15	LEU
35	h	19	VAL
36	i	30	THR
36	i	139	GLU
37	j	45	GLU
38	k	14	ARG
38	k	15	GLU
38	k	42	SER
38	k	72	MET
39	l	41	ARG
39	l	94	VAL
39	l	107	GLU
39	l	127	LEU
40	m	78	LYS
40	m	95	LEU

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Mol	Chain	Res	Type
40	m	120	VAL
41	n	23	GLU
41	n	44	ASP
42	o	12	GLU
42	o	62	VAL
42	o	85	LEU
43	p	31	VAL
43	p	111	GLU
43	p	117	LEU
44	q	14	VAL
44	q	51	LEU
46	s	22	LEU
46	s	54	VAL
46	s	94	PHE
47	t	26	LYS
47	t	99	GLN
47	t	102	VAL
48	u	5	ILE
48	u	63	VAL
48	u	100	ASP
48	u	133	GLU
48	u	192	VAL
49	v	43	THR
50	w	8	THR
51	x	30	MET
52	y	34	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
8	C	3	GLN
8	C	6	HIS
8	C	123	GLN
9	D	77	GLN
9	D	128	GLN
10	E	62	GLN
10	E	133	ASN
10	E	136	ASN
11	F	52	ASN
15	J	78	GLN
16	K	38	GLN
17	L	26	ASN

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Mol	Chain	Res	Type
17	L	77	HIS
18	M	8	ASN
18	M	55	GLN
18	M	105	ASN
19	N	45	GLN
19	N	49	GLN
21	P	26	ASN
22	Q	48	HIS
22	Q	55	GLN
24	S	14	HIS
25	T	3	ASN
27	X	2	GLN
27	X	9	GLN
30	c	53	HIS
30	c	153	GLN
30	c	226	ASN
30	c	261	ASN
31	d	65	GLN
31	d	126	ASN
31	d	136	ASN
33	f	37	ASN
34	g	38	HIS
34	g	45	GLN
34	g	59	GLN
34	g	81	GLN
34	g	111	HIS
35	h	20	ASN
36	i	130	HIS
37	j	56	GLN
39	l	96	GLN
41	n	88	GLN
42	o	39	GLN
42	o	67	ASN
45	r	23	GLN
47	t	2	GLN
48	u	41	GLN
48	u	56	ASN
48	u	67	ASN
48	u	81	GLN
48	u	129	HIS
48	u	158	GLN
48	u	175	GLN

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Mol	Chain	Res	Type
48	u	180	ASN
49	v	57	HIS
50	w	36	HIS
51	x	15	ASN
51	x	39	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
28	a	2889/2891 (99%)	521 (18%)	0
29	b	116/120 (96%)	19 (16%)	0
6	A	1526/1536 (99%)	291 (19%)	22 (1%)
All	All	4531/4547 (99%)	831 (18%)	22 (0%)

All (831) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	A	4	C
6	A	5	U
6	A	6	G
6	A	7	A
6	A	9	G
6	A	32	A
6	A	33	A
6	A	39	G
6	A	47	C
6	A	48	C
6	A	50	A
6	A	51	A
6	A	52	C
6	A	54	C
6	A	60	A
6	A	61	G
6	A	68	G
6	A	71	U
6	A	72	G
6	A	73	A
6	A	81	U
6	A	82	U
6	A	83	G
6	A	87	C

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Mol	Chain	Res	Type
6	A	88	U
6	A	89	G
6	A	90	G
6	A	121	G
6	A	124	A
6	A	125	U
6	A	136	G
6	A	138	G
6	A	152	G
6	A	157	C
6	A	161	C
6	A	162	G
6	A	165	A
6	A	177	G
6	A	182	G
6	A	184	G
6	A	185	G
6	A	191	A
6	A	192	G
6	A	198	G
6	A	201	C
6	A	203	U
6	A	204	C
6	A	205	G
6	A	206	G
6	A	214	G
6	A	239	U
6	A	241	G
6	A	245	G
6	A	260	G
6	A	261	C
6	A	273	A
6	A	274	C
6	A	283	A
6	A	287	G
6	A	315	A
6	A	322	C
6	A	323	A
6	A	324	C
6	A	333	C
6	A	345	G
6	A	346	C

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Mol	Chain	Res	Type
6	A	348	G
6	A	361	U
6	A	366	C
6	A	378	G
6	A	392	U
6	A	397	C
6	A	400	G
6	A	403	U
6	A	405	A
6	A	406	A
6	A	407	G
6	A	408	A
6	A	415	U
6	A	423	U
6	A	431	U
6	A	432	U
6	A	446	A
6	A	447	G
6	A	478	G
6	A	490	A
6	A	491	U
6	A	492	A
6	A	503	A
6	A	505	C
6	A	512	C
6	A	513	C
6	A	515	G
6	A	519	C
6	A	521	G7M
6	A	524	G
6	A	526	A
6	A	534	G
6	A	539	C
6	A	541	A
6	A	549	U
6	A	553	A
6	A	556	U
6	A	558	C
6	A	562	G
6	A	566	A
6	A	567	A
6	A	570	C

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Mol	Chain	Res	Type
6	A	571	G
6	A	573	G
6	A	627	G
6	A	632	C
6	A	633	A
6	A	635	A
6	A	636	A
6	A	647	A
6	A	650	G
6	A	655	G
6	A	659	A
6	A	660	G
6	A	667	G
6	A	680	U
6	A	681	A
6	A	682	G
6	A	697	G
6	A	709	A
6	A	715	A
6	A	717	U
6	A	718	G
6	A	725	G
6	A	728	A
6	A	730	C
6	A	731	A
6	A	747	A
6	A	748	C
6	A	749	A
6	A	753	A
6	A	754	G
6	A	758	C
6	A	771	A
6	A	781	A
6	A	787	U
6	A	788	A
6	A	809	A
6	A	811	C
6	A	815	G
6	A	820	C
6	A	822	A
6	A	836	U
6	A	838	G

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Mol	Chain	Res	Type
6	A	839	A
6	A	847	G
6	A	854	A
6	A	861	G
6	A	866	A
6	A	884	G
6	A	894	A
6	A	896	G
6	A	906	C
6	A	920	G
6	A	921	G
6	A	928	C
6	A	929	A
6	A	954	U
6	A	962	A
6	A	963	A
6	A	965	G
6	A	969	A
6	A	970	G
6	A	971	A
6	A	977	A
6	A	983	C
6	A	987	G
6	A	989	C
6	A	998	A
6	A	1001	U
6	A	1014	A
6	A	1016	U
6	A	1018	G
6	A	1019	U
6	A	1023	U
6	A	1024	U
6	A	1025	C
6	A	1026	G
6	A	1027	G
6	A	1030	A
6	A	1036	A
6	A	1039	C
6	A	1044	G
6	A	1047	G
6	A	1059	U
6	A	1073	G

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Mol	Chain	Res	Type
6	A	1078	G
6	A	1079	U
6	A	1083	G
6	A	1088	G
6	A	1089	U
6	A	1095	A
6	A	1118	G
6	A	1119	U
6	A	1124	A
6	A	1127	A
6	A	1130	U
6	A	1131	C
6	A	1133	G
6	A	1137	G
6	A	1139	C
6	A	1152	C
6	A	1153	U
6	A	1154	G
6	A	1162	C
6	A	1163	A
6	A	1165	A
6	A	1175	G
6	A	1178	G
6	A	1190	A
6	A	1191	A
6	A	1196	U
6	A	1206	U
6	A	1207	A
6	A	1208	C
6	A	1209	G
6	A	1211	C
6	A	1221	A
6	A	1230	A
6	A	1232	A
6	A	1234	U
6	A	1241	U
6	A	1244	A
6	A	1248	G
6	A	1251	U
6	A	1252	G
6	A	1264	G
6	A	1266	U

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Mol	Chain	Res	Type
6	A	1274	A
6	A	1280	U
6	A	1281	A
6	A	1294	G
6	A	1296	C
6	A	1297	C
6	A	1299	G
6	A	1314	C
6	A	1317	G
6	A	1321	G
6	A	1323	G
6	A	1325	G
6	A	1330	C
6	A	1340	A
6	A	1341	G
6	A	1347	G
6	A	1351	A
6	A	1352	U
6	A	1357	A
6	A	1362	A
6	A	1364	G
6	A	1373	G
6	A	1375	U
6	A	1388	A
6	A	1391	C
6	A	1392	A
6	A	1405	C
6	A	1413	G
6	A	1423	C
6	A	1425	A
6	A	1426	G
6	A	1427	A
6	A	1428	A
6	A	1435	A
6	A	1436	G
6	A	1441	A
6	A	1446	A
6	A	1448	G
6	A	1451	G
6	A	1456	G
6	A	1457	U
6	A	1458	U

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Mol	Chain	Res	Type
6	A	1459	A
6	A	1469	G
6	A	1485	G
6	A	1486	A
6	A	1488	G
6	A	1491	G
6	A	1493	A
6	A	1500	U
6	A	1502	G
6	A	1503	C
6	A	1511	G
6	A	1513	MA6
6	A	1514	C
6	A	1523	G
6	A	1524	G
28	a	23	G
28	a	27	G
28	a	44	A
28	a	45	G
28	a	46	G
28	a	51	G
28	a	61	G
28	a	70	G
28	a	71	A
28	a	74	A
28	a	75	G
28	a	79	C
28	a	83	G
28	a	84	A
28	a	85	G
28	a	92	A
28	a	95	A
28	a	97	A
28	a	102	G
28	a	118	A
28	a	119	A
28	a	120	U
28	a	124	G
28	a	131	A
28	a	142	C
28	a	147	G
28	a	163	C

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Mol	Chain	Res	Type
28	a	173	A
28	a	181	A
28	a	196	A
28	a	199	A
28	a	205	G
28	a	206	U
28	a	215	G
28	a	216	A
28	a	222	A
28	a	223	A
28	a	224	U
28	a	228	C
28	a	230	G
28	a	233	A
28	a	242	G
28	a	248	G
28	a	249	C
28	a	252	G
28	a	255	A
28	a	261	G
28	a	264	U
28	a	265	A
28	a	271	U
28	a	273	A
28	a	276	U
28	a	277	U
28	a	289	G
28	a	293	A
28	a	294	A
28	a	305	A
28	a	315	U
28	a	319	G
28	a	322	U
28	a	323	G
28	a	324	A
28	a	327	G
28	a	336	G
28	a	339	A
28	a	340	A
28	a	349	U
28	a	350	G
28	a	356	A

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Mol	Chain	Res	Type
28	a	358	A
28	a	359	U
28	a	360	C
28	a	364	U
28	a	377	G
28	a	379	G
28	a	387	G
28	a	390	U
28	a	396	U
28	a	397	G
28	a	403	A
28	a	435	C
28	a	445	A
28	a	446	C
28	a	448	A
28	a	456	G
28	a	461	A
28	a	464	G
28	a	471	A
28	a	472	G
28	a	482	G
28	a	485	G
28	a	487	G
28	a	495	U
28	a	496	A
28	a	499	A
28	a	508	C
28	a	520	A
28	a	521	G
28	a	522	C
28	a	523	A
28	a	524	G
28	a	535	C
28	a	536	U
28	a	537	U
28	a	538	G
28	a	553	A
28	a	558	U
28	a	559	U
28	a	560	G
28	a	561	U
28	a	563	U

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Mol	Chain	Res	Type
28	a	565	A
28	a	576	A
28	a	582	A
28	a	583	U
28	a	593	A
28	a	594	G
28	a	603	U
28	a	610	U
28	a	622	A
28	a	624	G
28	a	627	A
28	a	635	U
28	a	636	A
28	a	637	G
28	a	644	U
28	a	645	A
28	a	649	G
28	a	653	G
28	a	667	A
28	a	676	U
28	a	702	G
28	a	716	G
28	a	719	G
28	a	720	A
28	a	737	U
28	a	743	G
28	a	744	G
28	a	754	A
28	a	755	C
28	a	765	G
28	a	766	G
28	a	772	A
28	a	774	G
28	a	775	G
28	a	779	A
28	a	781	C
28	a	795	G
28	a	802	C
28	a	817	U
28	a	818	U
28	a	836	U
28	a	855	A

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Mol	Chain	Res	Type
28	a	870	G
28	a	872	G
28	a	873	U
28	a	876	U
28	a	877	C
28	a	878	C
28	a	879	C
28	a	880	G
28	a	881	A
28	a	882	C
28	a	884	U
28	a	886	C
28	a	896	G
28	a	899	A
28	a	921	C
28	a	922	G
28	a	931	A
28	a	935	A
28	a	936	C
28	a	949	A
28	a	951	C
28	a	952	G
28	a	954	C
28	a	964	A
28	a	972	C
28	a	973	A
28	a	979	G
28	a	986	A
28	a	993	G
28	a	999	A
28	a	1002	U
28	a	1003	U
28	a	1007	G
28	a	1012	G
28	a	1016	U
28	a	1018	A
28	a	1023	U
28	a	1031	G
28	a	1037	G
28	a	1040	A
28	a	1046	G
28	a	1047	A

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Mol	Chain	Res	Type
28	a	1048	G
28	a	1049	G
28	a	1050	U
28	a	1051	U
28	a	1052	G
28	a	1056	U
28	a	1057	A
28	a	1058	G
28	a	1060	A
28	a	1061	G
28	a	1062	C
28	a	1065	C
28	a	1069	C
28	a	1070	C
28	a	1071	U
28	a	1073	U
28	a	1078	A
28	a	1080	A
28	a	1093	A
28	a	1099	C
28	a	1100	G
28	a	1101	A
28	a	1102	G
28	a	1112	G
28	a	1117	A
28	a	1119	A
28	a	1120	U
28	a	1122	U
28	a	1123	A
28	a	1124	A
28	a	1125	C
28	a	1129	G
28	a	1133	A
28	a	1146	A
28	a	1147	A
28	a	1148	G
28	a	1155	G
28	a	1157	G
28	a	1162	G
28	a	1163	U
28	a	1164	A
28	a	1165	A

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Mol	Chain	Res	Type
28	a	1166	G
28	a	1167	U
28	a	1193	G
28	a	1199	G
28	a	1214	A
28	a	1223	G
28	a	1225	G
28	a	1234	A
28	a	1237	G
28	a	1238	C
28	a	1240	A
28	a	1243	G
28	a	1249	A
28	a	1253	G
28	a	1258	G
28	a	1259	A
28	a	1261	A
28	a	1263	U
28	a	1276	C
28	a	1287	A
28	a	1288	A
28	a	1289	A
28	a	1291	A
28	a	1307	C
28	a	1308	A
28	a	1316	U
28	a	1330	G
28	a	1334	G
28	a	1339	U
28	a	1347	G
28	a	1352	A
28	a	1355	A
28	a	1361	G
28	a	1365	A
28	a	1366	U
28	a	1370	A
28	a	1372	A
28	a	1373	C
28	a	1403	G
28	a	1404	C
28	a	1406	A
28	a	1407	U

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Mol	Chain	Res	Type
28	a	1414	A
28	a	1415	C
28	a	1422	G
28	a	1438	C
28	a	1439	G
28	a	1447	U
28	a	1469	G
28	a	1480	U
28	a	1511	G
28	a	1512	A
28	a	1524	U
28	a	1525	U
28	a	1529	U
28	a	1548	A
28	a	1550	G
28	a	1556	A
28	a	1558	G
28	a	1559	A
28	a	1560	A
28	a	1568	U
28	a	1573	U
28	a	1574	U
28	a	1575	C
28	a	1576	A
28	a	1580	A
28	a	1598	A
28	a	1627	A
28	a	1628	C
28	a	1629	C
28	a	1637	U
28	a	1638	U
28	a	1639	G
28	a	1641	G
28	a	1650	G
28	a	1657	G
28	a	1664	G
28	a	1673	C
28	a	1686	G
28	a	1690	A
28	a	1710	A
28	a	1717	U
28	a	1718	A

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Mol	Chain	Res	Type
28	a	1720	U
28	a	1721	C
28	a	1724	U
28	a	1732	G
28	a	1741	A
28	a	1742	A
28	a	1744	A
28	a	1745	U
28	a	1750	G
28	a	1751	G
28	a	1760	A
28	a	1763	G
28	a	1769	U
28	a	1771	A
28	a	1773	A
28	a	1787	C
28	a	1788	A
28	a	1795	A
28	a	1798	G
28	a	1803	C
28	a	1816	A
28	a	1849	G
28	a	1851	U
28	a	1852	U
28	a	1859	A
28	a	1860	G
28	a	1865	G
28	a	1893	G
28	a	1906	A
28	a	1916	G
28	a	1917	G
28	a	1924	A
28	a	1925	A
28	a	1928	C
28	a	1942	U
28	a	1951	G
28	a	1954	C
28	a	1957	A
28	a	1958	U
28	a	1959	G
28	a	1978	U
28	a	1979	G

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Mol	Chain	Res	Type
28	a	1980	U
28	a	1984	C
28	a	2008	A
28	a	2010	C
28	a	2017	6MZ
28	a	2018	A
28	a	2020	A
28	a	2022	G
28	a	2030	U
28	a	2042	C
28	a	2043	G
28	a	2047	A
28	a	2048	G
28	a	2049	A
28	a	2055	U
28	a	2056	7MG
28	a	2057	A
28	a	2080	G
28	a	2088	A
28	a	2090	C
28	a	2091	C
28	a	2097	G
28	a	2098	U
28	a	2103	G
28	a	2104	A
28	a	2106	A
28	a	2107	G
28	a	2113	A
28	a	2114	G
28	a	2118	U
28	a	2119	U
28	a	2120	G
28	a	2121	A
28	a	2123	G
28	a	2132	C
28	a	2135	G
28	a	2144	G
28	a	2145	A
28	a	2146	G
28	a	2155	G
28	a	2160	A
28	a	2161	C

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Mol	Chain	Res	Type
28	a	2165	C
28	a	2170	C
28	a	2185	A
28	a	2191	G
28	a	2199	A
28	a	2201	C
28	a	2212	A
28	a	2225	G
28	a	2226	G
28	a	2238	OMG
28	a	2265	A
28	a	2270	U
28	a	2274	A
28	a	2275	A
28	a	2290	G
28	a	2292	U
28	a	2293	C
28	a	2295	G
28	a	2306	U
28	a	2307	A
28	a	2309	A
28	a	2312	A
28	a	2313	U
28	a	2314	A
28	a	2323	A
28	a	2332	G
28	a	2334	C
28	a	2337	C
28	a	2341	A
28	a	2348	C
28	a	2359	U
28	a	2366	G
28	a	2370	G
28	a	2372	C
28	a	2378	G
28	a	2389	U
28	a	2393	U
28	a	2412	A
28	a	2414	C
28	a	2416	G
28	a	2417	A
28	a	2422	A

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Mol	Chain	Res	Type
28	a	2428	U
28	a	2432	2MG
28	a	2434	G
28	a	2435	A
28	a	2436	H2U
28	a	2446	A
28	a	2463	A
28	a	2474	G
28	a	2477	G
28	a	2478	U
28	a	2485	OMC
28	a	2489	G
28	a	2492	G
28	a	2493	U
28	a	2504	C
28	a	2505	A
28	a	2506	U
28	a	2507	C
28	a	2516	G
28	a	2522	G
28	a	2534	A
28	a	2553	A
28	a	2554	G
28	a	2565	G
28	a	2572	U
28	a	2573	U
28	a	2586	G
28	a	2588	C
28	a	2589	A
28	a	2600	U
28	a	2602	U
28	a	2616	U
28	a	2633	C
28	a	2656	G
28	a	2672	G
28	a	2676	U
28	a	2677	U
28	a	2689	G
28	a	2692	A
28	a	2701	G
28	a	2702	C
28	a	2713	U

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Mol	Chain	Res	Type
28	a	2719	G
28	a	2720	A
28	a	2735	A
28	a	2738	G
28	a	2744	A
28	a	2745	A
28	a	2748	G
28	a	2752	A
28	a	2756	U
28	a	2763	A
28	a	2765	A
28	a	2766	U
28	a	2780	G
28	a	2784	U
28	a	2785	U
28	a	2786	G
28	a	2787	A
28	a	2805	C
28	a	2807	A
28	a	2808	A
28	a	2812	U
28	a	2822	A
28	a	2823	U
28	a	2837	A
28	a	2852	U
28	a	2854	G
28	a	2860	A
28	a	2867	C
28	a	2871	U
28	a	2872	U
28	a	2878	U
28	a	2889	C
29	b	13	A
29	b	24	G
29	b	26	A
29	b	32	U
29	b	40	U
29	b	41	C
29	b	44	G
29	b	52	A
29	b	56	G
29	b	66	A

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Mol	Chain	Res	Type
29	b	67	U
29	b	73	A
29	b	89	U
29	b	90	C
29	b	91	C
29	b	105	G
29	b	109	A
29	b	116	A
29	b	117	G

All (22) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	A	5	U
6	A	6	G
6	A	83	G
6	A	87	C
6	A	183	A
6	A	273	A
6	A	314	A
6	A	322	C
6	A	332	A
6	A	434	A
6	A	491	U
6	A	512	C
6	A	666	U
6	A	757	G
6	A	893	C
6	A	976	U
6	A	1039	C
6	A	1162	C
6	A	1164	A
6	A	1195	A
6	A	1233	A
6	A	1247	G

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

38 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	$\#\|Z\| > 2$
28	PSU	a	945	28	18,21,22	2.08	7 (38%)	22,30,33	1.87	4 (18%)
28	6MZ	a	2017	28	22,25,26	2.38	3 (13%)	30,36,39	2.39	9 (30%)
6	2MG	A	960	6	23,26,27	2.58	4 (17%)	32,38,41	2.08	9 (28%)
28	PSU	a	1898	28	18,21,22	1.97	7 (38%)	22,30,33	1.86	3 (13%)
28	2MG	a	2432	28	23,26,27	2.57	6 (26%)	32,38,41	2.08	11 (34%)
31	MEQ	d	150	31	8,9,10	0.84	0	5,10,12	0.42	0
28	PSU	a	2444	28	18,21,22	2.09	7 (38%)	22,30,33	1.83	5 (22%)
28	7MG	a	2056	28	22,26,27	1.20	1 (4%)	29,39,42	0.93	1 (3%)
28	OMC	a	2485	55,28	19,22,23	1.76	4 (21%)	26,31,34	0.97	2 (7%)
28	6MZ	a	1608	28	22,25,26	2.40	3 (13%)	30,36,39	2.21	10 (33%)
28	1MG	a	735	28	22,26,27	2.51	5 (22%)	33,39,42	2.01	6 (18%)
28	PSU	a	1904	28	18,21,22	1.98	7 (38%)	22,30,33	1.79	4 (18%)
17	D2T	L	89	17	7,9,10	1.24	1 (14%)	6,11,13	1.54	1 (16%)
28	2MG	a	1822	28	23,26,27	2.57	5 (21%)	32,38,41	2.06	10 (31%)
6	PSU	A	510	55,6,56	18,21,22	2.02	7 (38%)	22,30,33	1.82	5 (22%)
6	MA6	A	1513	6	23,26,27	1.21	3 (13%)	34,38,41	2.24	9 (26%)
6	4OC	A	1396	6	20,23,24	2.22	3 (15%)	26,32,35	0.95	2 (7%)
28	OMU	a	2539	56,28	19,22,23	2.61	7 (36%)	26,31,34	1.76	5 (19%)
28	PSU	a	2491	56,28	18,21,22	2.07	7 (38%)	22,30,33	1.84	4 (18%)
6	MA6	A	1512	6	23,26,27	1.20	3 (13%)	34,38,41	2.26	9 (26%)
28	3TD	a	1902	28	18,22,23	2.68	7 (38%)	22,32,35	1.70	2 (9%)
28	5MU	a	1926	56,28	19,22,23	2.50	7 (36%)	28,32,35	3.87	10 (35%)
28	5MC	a	1949	56,28	18,22,23	1.89	5 (27%)	26,32,35	1.29	2 (7%)
28	2MA	a	2490	55,56,28	22,25,26	1.33	2 (9%)	33,37,40	2.00	8 (24%)
28	PSU	a	2591	28	18,21,22	2.05	7 (38%)	22,30,33	1.80	3 (13%)
28	PSU	a	2592	28	18,21,22	2.05	7 (38%)	22,30,33	1.84	3 (13%)
39	MS6	l	83	39	5,7,8	0.56	0	2,7,9	1.66	1 (50%)
6	5MC	A	961	6	18,22,23	1.90	6 (33%)	26,32,35	1.30	2 (7%)
28	PSU	a	2567	28	18,21,22	2.11	8 (44%)	22,30,33	1.90	5 (22%)
28	H2U	a	2436	28	18,21,22	4.20	5 (27%)	21,30,33	4.70	6 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
39	4D4	l	82	39	9,11,12	0.78	0	8,13,15	1.64	2 (25%)
6	2MG	A	1201	6,56	23,26,27	2.57	4 (17%)	32,38,41	2.12	12 (37%)
28	OMG	a	2238	56,28	23,26,27	2.34	6 (26%)	33,38,41	1.81	10 (30%)
6	UR3	A	1492	6	19,22,23	2.56	6 (31%)	26,32,35	1.29	2 (7%)
6	2MG	A	1510	6,56	23,26,27	2.58	5 (21%)	32,38,41	2.11	10 (31%)
16	IAS	K	119	16,26	6,7,8	1.73	1 (16%)	6,8,10	2.58	1 (16%)
6	G7M	A	521	6,56	23,26,27	2.16	5 (21%)	35,39,42	1.88	7 (20%)
28	PSU	a	736	55,28	18,21,22	2.03	7 (38%)	22,30,33	1.79	3 (13%)

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
28	PSU	a	945	28	-	0/7/25/26	0/2/2/2
28	6MZ	a	2017	28	-	2/9/27/28	0/3/3/3
6	2MG	A	960	6	-	0/9/27/28	0/3/3/3
28	PSU	a	1898	28	-	0/7/25/26	0/2/2/2
28	2MG	a	2432	28	-	2/9/27/28	0/3/3/3
31	MEQ	d	150	31	-	3/8/9/11	-
28	PSU	a	2444	28	-	0/7/25/26	0/2/2/2
28	7MG	a	2056	28	-	2/7/37/38	0/3/3/3
28	OMC	a	2485	55,28	-	1/9/27/28	0/2/2/2
28	6MZ	a	1608	28	-	0/9/27/28	0/3/3/3
28	1MG	a	735	28	-	0/7/25/26	0/3/3/3
28	PSU	a	1904	28	-	0/7/25/26	0/2/2/2
17	D2T	L	89	17	-	4/7/12/14	-
28	2MG	a	1822	28	-	0/9/27/28	0/3/3/3
6	PSU	A	510	55,6,56	-	0/7/25/26	0/2/2/2
6	MA6	A	1513	6	-	2/11/29/30	0/3/3/3
6	4OC	A	1396	6	-	1/9/29/30	0/2/2/2
28	OMU	a	2539	56,28	-	0/9/27/28	0/2/2/2
28	PSU	a	2491	56,28	-	0/7/25/26	0/2/2/2
6	MA6	A	1512	6	-	0/11/29/30	0/3/3/3
28	3TD	a	1902	28	-	3/7/25/26	0/2/2/2
28	5MU	a	1926	56,28	-	0/7/25/26	0/2/2/2
28	5MC	a	1949	56,28	-	0/7/25/26	0/2/2/2
28	2MA	a	2490	55,56,28	-	2/7/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	PSU	a	2591	28	-	0/7/25/26	0/2/2/2
28	PSU	a	2592	28	-	0/7/25/26	0/2/2/2
39	MS6	l	83	39	-	2/4/6/8	-
6	5MC	A	961	6	-	0/7/25/26	0/2/2/2
28	PSU	a	2567	28	-	1/7/25/26	0/2/2/2
28	H2U	a	2436	28	-	1/7/38/39	0/2/2/2
39	4D4	l	82	39	-	4/11/12/14	-
6	2MG	A	1201	6,56	-	0/9/27/28	0/3/3/3
28	OMG	a	2238	56,28	-	3/9/27/28	0/3/3/3
6	UR3	A	1492	6	-	0/7/25/26	0/2/2/2
6	2MG	A	1510	6,56	-	0/9/27/28	0/3/3/3
16	IAS	K	119	16,26	-	4/7/7/8	-
6	G7M	A	521	6,56	-	3/7/25/26	0/3/3/3
28	PSU	a	736	55,28	-	1/7/25/26	0/2/2/2

All (178) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	1608	6MZ	C6-N6	10.12	1.45	1.34
28	a	2436	H2U	O4-C4	10.01	1.43	1.23
28	a	2017	6MZ	C6-N6	9.91	1.44	1.34
6	A	1201	2MG	O6-C6	9.15	1.41	1.23
6	A	960	2MG	O6-C6	9.10	1.40	1.23
6	A	1510	2MG	O6-C6	9.08	1.40	1.23
28	a	1822	2MG	O6-C6	8.99	1.40	1.23
28	a	2432	2MG	O6-C6	8.95	1.40	1.23
6	A	1492	UR3	O4-C4	8.78	1.42	1.23
28	a	2238	OMG	O6-C6	8.45	1.39	1.23
28	a	2436	H2U	O2-C2	8.32	1.38	1.23
28	a	2436	H2U	C2-N1	8.26	1.47	1.35
28	a	1902	3TD	O4-C4	8.13	1.40	1.23
28	a	735	1MG	O6-C6	8.09	1.40	1.23
28	a	2539	OMU	O4-C4	8.03	1.40	1.24
6	A	521	G7M	O6-C6	7.94	1.38	1.23
28	a	2436	H2U	C2-N3	7.09	1.50	1.38
6	A	1396	4OC	O2-C2	6.38	1.35	1.23
28	a	1926	5MU	C2-N1	-6.08	1.28	1.38
28	a	735	1MG	C2-N2	6.05	1.45	1.34
6	A	1201	2MG	C2-N2	5.94	1.46	1.33
6	A	960	2MG	C2-N2	5.94	1.46	1.33
6	A	1510	2MG	C2-N2	5.91	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	1822	2MG	C2-N2	5.90	1.46	1.33
28	a	2432	2MG	C2-N2	5.78	1.46	1.33
6	A	1396	4OC	C4-N4	5.55	1.47	1.35
28	a	2436	H2U	C4-N3	5.18	1.46	1.37
28	a	2056	7MG	C5-N7	4.83	1.41	1.35
28	a	1926	5MU	C2-N3	-4.78	1.29	1.38
28	a	2485	OMC	C4-N4	4.74	1.45	1.33
28	a	2490	2MA	C6-N6	4.54	1.45	1.34
28	a	1926	5MU	C6-N1	-4.49	1.30	1.38
6	A	961	5MC	C4-N4	4.19	1.45	1.34
28	a	2539	OMU	C2-N1	-4.17	1.31	1.38
28	a	1949	5MC	C4-N4	4.13	1.44	1.34
28	a	2238	OMG	C2-N2	4.09	1.43	1.34
28	a	2485	OMC	C2-N1	-4.02	1.31	1.40
28	a	1902	3TD	C2-N1	-3.87	1.32	1.37
28	a	2238	OMG	C6-N1	-3.86	1.31	1.38
28	a	735	1MG	C6-N1	-3.86	1.32	1.40
28	a	2444	PSU	C4-N3	-3.84	1.31	1.38
28	a	2567	PSU	C2-N1	-3.81	1.31	1.36
28	a	2591	PSU	C4-N3	-3.80	1.31	1.38
28	a	2592	PSU	C4-N3	-3.80	1.31	1.38
28	a	945	PSU	C2-N1	-3.78	1.31	1.36
28	a	945	PSU	C4-N3	-3.75	1.31	1.38
28	a	2567	PSU	C4-N3	-3.75	1.31	1.38
6	A	510	PSU	C2-N1	-3.75	1.31	1.36
28	a	2491	PSU	C2-N1	-3.74	1.31	1.36
28	a	2491	PSU	C4-N3	-3.73	1.31	1.38
6	A	1396	4OC	C2-N1	-3.73	1.31	1.40
6	A	961	5MC	C2-N1	-3.72	1.31	1.40
28	a	736	PSU	C2-N1	-3.70	1.31	1.36
28	a	2444	PSU	C2-N1	-3.69	1.31	1.36
28	a	1949	5MC	C2-N1	-3.69	1.32	1.40
28	a	2539	OMU	C4-N3	-3.65	1.32	1.38
28	a	2592	PSU	C2-N3	-3.63	1.31	1.37
28	a	1902	3TD	C4-N3	-3.63	1.32	1.40
16	K	119	IAS	OD1-CG	3.62	1.40	1.19
28	a	2591	PSU	C2-N3	-3.61	1.31	1.37
6	A	510	PSU	C4-N3	-3.60	1.32	1.38
28	a	1904	PSU	C4-N3	-3.60	1.32	1.38
6	A	1492	UR3	C4-N3	-3.60	1.32	1.40
28	a	2444	PSU	C2-N3	-3.60	1.31	1.37
28	a	736	PSU	C4-N3	-3.59	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	2592	PSU	C2-N1	-3.58	1.31	1.36
28	a	2591	PSU	C2-N1	-3.58	1.31	1.36
28	a	1898	PSU	C4-N3	-3.58	1.32	1.38
28	a	2539	OMU	C2-N3	-3.55	1.31	1.38
6	A	521	G7M	C5-N7	-3.51	1.35	1.39
28	a	1904	PSU	C2-N1	-3.48	1.32	1.36
28	a	2491	PSU	C2-N3	-3.47	1.31	1.37
28	a	1926	5MU	C6-C5	3.44	1.40	1.34
6	A	1512	MA6	C6-N6	3.42	1.46	1.36
28	a	2567	PSU	C2-N3	-3.41	1.31	1.37
6	A	1513	MA6	C6-N6	3.40	1.46	1.36
28	a	945	PSU	C2-N3	-3.39	1.31	1.37
28	a	1898	PSU	C2-N1	-3.36	1.32	1.36
6	A	510	PSU	C2-N3	-3.33	1.31	1.37
28	a	1926	5MU	C4-N3	-3.33	1.32	1.38
28	a	1902	3TD	C6-C5	3.32	1.39	1.35
6	A	1492	UR3	C2-N3	-3.32	1.32	1.39
6	A	521	G7M	C6-N1	-3.27	1.32	1.38
28	a	1904	PSU	C2-N3	-3.26	1.31	1.37
28	a	736	PSU	C2-N3	-3.24	1.32	1.37
28	a	1898	PSU	C2-N3	-3.24	1.32	1.37
28	a	2432	2MG	C6-N1	-3.23	1.32	1.38
6	A	1512	MA6	C8-N9	-3.21	1.31	1.37
6	A	521	G7M	C2-N2	3.18	1.41	1.34
28	a	1822	2MG	C6-N1	-3.16	1.33	1.38
6	A	961	5MC	C6-N1	-3.14	1.32	1.38
6	A	1513	MA6	C8-N9	-3.12	1.31	1.37
28	a	2017	6MZ	C8-N9	-3.11	1.31	1.37
28	a	1949	5MC	C6-N1	-3.11	1.32	1.38
28	a	1898	PSU	C6-C5	3.09	1.38	1.35
28	a	1904	PSU	C6-C5	3.09	1.38	1.35
28	a	1608	6MZ	C8-N9	-3.02	1.32	1.37
28	a	2591	PSU	C6-C5	2.98	1.38	1.35
6	A	960	2MG	C6-N1	-2.98	1.33	1.38
28	a	945	PSU	C6-C5	2.95	1.38	1.35
28	a	1902	3TD	C2-N3	-2.95	1.32	1.38
6	A	1510	2MG	C6-N1	-2.94	1.33	1.38
28	a	736	PSU	C6-C5	2.92	1.38	1.35
28	a	1949	5MC	O2-C2	-2.90	1.18	1.23
6	A	1201	2MG	C6-N1	-2.90	1.33	1.38
28	a	2491	PSU	C6-C5	2.88	1.38	1.35
6	A	510	PSU	C6-C5	2.87	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	1822	2MG	C5-N7	-2.87	1.33	1.39
28	a	2444	PSU	C6-C5	2.86	1.38	1.35
6	A	1492	UR3	C2-N1	-2.81	1.34	1.38
6	A	960	2MG	C5-N7	-2.80	1.33	1.39
28	a	2592	PSU	C6-C5	2.78	1.38	1.35
28	a	2567	PSU	C6-C5	2.77	1.38	1.35
28	a	2432	2MG	C5-N7	-2.76	1.33	1.39
6	A	961	5MC	O2-C2	-2.75	1.18	1.23
28	a	2567	PSU	C6-N1	-2.71	1.31	1.36
28	a	945	PSU	O4-C4	-2.70	1.18	1.23
28	a	2592	PSU	O4-C4	-2.69	1.18	1.23
28	a	2491	PSU	O4-C4	-2.68	1.18	1.23
28	a	2591	PSU	O4-C4	-2.68	1.18	1.23
28	a	2567	PSU	O4-C4	-2.68	1.18	1.23
28	a	2444	PSU	O4-C4	-2.67	1.18	1.23
28	a	1926	5MU	O4-C4	-2.66	1.18	1.23
6	A	961	5MC	C6-C5	2.66	1.39	1.34
28	a	2238	OMG	C8-N9	-2.65	1.31	1.37
28	a	1898	PSU	O4-C4	-2.64	1.18	1.23
6	A	1201	2MG	C5-N7	-2.63	1.34	1.39
6	A	1510	2MG	C5-N7	-2.63	1.34	1.39
28	a	736	PSU	O4-C4	-2.62	1.18	1.23
28	a	2017	6MZ	C5-N7	-2.61	1.34	1.39
28	a	1949	5MC	C6-C5	2.61	1.38	1.34
28	a	2491	PSU	C6-N1	-2.59	1.31	1.36
28	a	2539	OMU	O2-C2	-2.59	1.18	1.23
28	a	945	PSU	C6-N1	-2.58	1.31	1.36
28	a	1904	PSU	O4-C4	-2.58	1.18	1.23
6	A	510	PSU	O4-C4	-2.57	1.18	1.23
28	a	736	PSU	C6-N1	-2.55	1.32	1.36
28	a	2238	OMG	C5-N7	-2.52	1.34	1.39
28	a	2444	PSU	C6-N1	-2.51	1.32	1.36
28	a	2567	PSU	O4'-C1'	-2.51	1.40	1.43
28	a	1608	6MZ	C5-N7	-2.49	1.34	1.39
6	A	510	PSU	C6-N1	-2.48	1.32	1.36
28	a	1926	5MU	O2-C2	-2.45	1.18	1.23
28	a	735	1MG	C5-N7	-2.44	1.34	1.39
28	a	2444	PSU	O2-C2	-2.43	1.18	1.23
28	a	2592	PSU	C6-N1	-2.41	1.32	1.36
28	a	735	1MG	C8-N9	-2.40	1.32	1.37
6	A	521	G7M	C2-N1	-2.36	1.31	1.37
28	a	2591	PSU	C6-N1	-2.36	1.32	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	2539	OMU	C6-N1	-2.35	1.32	1.38
28	a	2491	PSU	O2-C2	-2.34	1.18	1.23
28	a	1902	3TD	O2-C2	-2.34	1.18	1.23
28	a	945	PSU	O2-C2	-2.34	1.18	1.23
28	a	2592	PSU	O2-C2	-2.34	1.18	1.23
28	a	2591	PSU	O2-C2	-2.31	1.18	1.23
28	a	1904	PSU	C6-N1	-2.30	1.32	1.36
28	a	2567	PSU	O2-C2	-2.30	1.18	1.23
28	a	1898	PSU	C6-N1	-2.28	1.32	1.36
28	a	1902	3TD	C6-N1	-2.27	1.32	1.36
28	a	2238	OMG	C2-N1	-2.27	1.32	1.37
6	A	1510	2MG	C4-N9	-2.24	1.32	1.38
28	a	2539	OMU	C5-C4	-2.23	1.38	1.43
6	A	1492	UR3	O2-C2	2.23	1.26	1.22
28	a	1898	PSU	O2-C2	-2.23	1.18	1.23
6	A	510	PSU	O2-C2	-2.22	1.18	1.23
28	a	736	PSU	O2-C2	-2.20	1.18	1.23
6	A	1492	UR3	C6-N1	-2.20	1.32	1.38
28	a	1904	PSU	O2-C2	-2.18	1.18	1.23
28	a	2485	OMC	C5-C4	-2.17	1.38	1.42
6	A	1513	MA6	C5-N7	-2.17	1.34	1.39
6	A	1512	MA6	C5-N7	-2.12	1.35	1.39
28	a	2432	2MG	C4-N9	-2.07	1.32	1.38
28	a	2432	2MG	CM2-N2	-2.06	1.41	1.45
17	L	89	D2T	CB-CG	2.05	1.55	1.52
28	a	1822	2MG	CM2-N2	-2.05	1.41	1.45
28	a	2490	2MA	C5-N7	-2.03	1.35	1.39
6	A	961	5MC	C2-N3	-2.02	1.32	1.36
28	a	2485	OMC	C6-C5	2.02	1.39	1.35

All (198) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	a	2436	H2U	C4-N3-C2	-12.79	115.18	125.79
28	a	2436	H2U	O2-C2-N1	-11.13	109.14	123.11
28	a	1926	5MU	C4-N3-C2	-8.75	116.03	127.35
28	a	1926	5MU	C5M-C5-C4	8.47	128.09	118.77
28	a	1926	5MU	N3-C2-N1	8.38	126.01	114.89
28	a	1926	5MU	C5-C6-N1	-7.77	115.35	123.34
28	a	2436	H2U	O4-C4-N3	-7.41	108.54	120.28
6	A	1510	2MG	C2-N3-C4	7.21	120.98	112.04
6	A	1201	2MG	C2-N3-C4	7.20	120.97	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	960	2MG	C2-N3-C4	7.20	120.97	112.04
28	a	2432	2MG	C2-N3-C4	7.14	120.89	112.04
28	a	1822	2MG	C2-N3-C4	7.07	120.81	112.04
28	a	2490	2MA	C5-C4-N3	-7.07	119.24	127.19
28	a	735	1MG	C5-C4-N3	-6.89	117.29	128.46
28	a	2436	H2U	O4-C4-C5	-6.80	107.66	122.17
28	a	1926	5MU	C5M-C5-C6	-6.79	113.78	122.85
28	a	2436	H2U	O2-C2-N3	-6.60	109.22	121.50
28	a	1902	3TD	N1-C2-N3	6.46	121.24	116.14
28	a	1926	5MU	C5-C4-N3	6.33	120.72	115.31
6	A	1512	MA6	C5-C4-N3	-5.95	118.99	126.75
6	A	1513	MA6	C5-C4-N3	-5.82	119.16	126.75
16	K	119	IAS	OD1-CG-CB	-5.71	108.78	125.43
28	a	945	PSU	N1-C2-N3	5.65	121.53	115.13
28	a	2491	PSU	N1-C2-N3	5.61	121.48	115.13
28	a	2444	PSU	N1-C2-N3	5.59	121.46	115.13
28	a	1898	PSU	N1-C2-N3	5.53	121.39	115.13
28	a	2567	PSU	N1-C2-N3	5.51	121.37	115.13
28	a	2017	6MZ	C9-N6-C6	-5.50	118.13	122.87
28	a	736	PSU	N1-C2-N3	5.48	121.34	115.13
28	a	2539	OMU	N3-C2-N1	5.47	122.14	114.89
28	a	2592	PSU	N1-C2-N3	5.46	121.32	115.13
28	a	2591	PSU	N1-C2-N3	5.46	121.31	115.13
6	A	510	PSU	N1-C2-N3	5.39	121.23	115.13
28	a	1608	6MZ	C5-C4-N3	-5.34	119.78	126.75
28	a	1904	PSU	N1-C2-N3	5.32	121.16	115.13
6	A	521	G7M	C2-N3-C4	5.29	121.73	112.30
28	a	2238	OMG	C5-C4-N3	-5.28	119.90	128.46
28	a	2017	6MZ	C5-C4-N3	-5.21	119.95	126.75
28	a	1822	2MG	C5-C4-N3	-5.17	120.07	128.46
6	A	960	2MG	C5-C4-N3	-5.16	120.08	128.46
6	A	961	5MC	C5-C6-N1	-5.13	118.06	123.34
28	a	2432	2MG	C5-C4-N3	-5.08	120.22	128.46
6	A	1201	2MG	C5-C4-N3	-5.07	120.23	128.46
28	a	735	1MG	C2-N3-C4	5.07	123.38	111.98
28	a	2017	6MZ	N1-C2-N3	-5.07	120.67	128.60
28	a	2490	2MA	N3-C4-N9	4.98	133.90	126.99
28	a	735	1MG	N9-C4-N3	4.91	135.80	125.94
28	a	1608	6MZ	N1-C2-N3	-4.89	120.96	128.60
6	A	1513	MA6	N1-C2-N3	-4.88	120.97	128.60
28	a	2436	H2U	N3-C2-N1	-4.87	111.50	116.65
6	A	1512	MA6	N1-C2-N3	-4.84	121.03	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1510	2MG	C5-C4-N3	-4.81	120.65	128.46
6	A	521	G7M	C5-C4-N3	-4.70	119.13	128.15
28	a	1949	5MC	C5-C6-N1	-4.63	118.57	123.34
6	A	1512	MA6	N3-C4-N9	4.62	134.69	127.08
6	A	1492	UR3	C4-N3-C2	-4.53	120.30	124.56
28	a	2238	OMG	C2-N3-C4	4.51	120.33	112.30
6	A	521	G7M	C5-C6-N1	4.31	120.79	111.79
28	a	2539	OMU	C4-N3-C2	-4.31	120.89	126.58
6	A	1513	MA6	N3-C4-N9	4.25	134.09	127.08
28	a	1926	5MU	O2-C2-N1	-4.23	117.17	122.79
6	A	1512	MA6	C2-N3-C4	4.21	121.69	111.75
6	A	1513	MA6	C2-N3-C4	4.18	121.62	111.75
6	A	1513	MA6	C2-N1-C6	4.12	121.48	111.75
6	A	1512	MA6	C2-N1-C6	4.08	121.39	111.75
28	a	2017	6MZ	C2-N3-C4	4.00	121.20	111.75
28	a	1926	5MU	O4-C4-N3	-3.97	112.51	120.12
28	a	1898	PSU	C4-N3-C2	-3.92	120.69	126.34
28	a	1608	6MZ	C2-N3-C4	3.88	120.91	111.75
28	a	2592	PSU	C4-N3-C2	-3.84	120.80	126.34
28	a	2017	6MZ	C6-C5-N7	3.79	136.49	132.39
28	a	2238	OMG	N9-C4-N3	3.73	133.44	125.94
28	a	736	PSU	C4-N3-C2	-3.73	120.96	126.34
6	A	1512	MA6	N9-C8-N7	-3.72	108.83	113.91
6	A	521	G7M	N9-C4-N3	3.69	133.36	125.94
28	a	2491	PSU	C4-N3-C2	-3.66	121.07	126.34
28	a	1608	6MZ	N3-C4-N9	3.64	133.09	127.08
28	a	2591	PSU	C4-N3-C2	-3.62	121.12	126.34
6	A	1512	MA6	C5-N7-C8	3.62	108.66	103.51
6	A	1513	MA6	C5-N7-C8	3.61	108.64	103.51
6	A	1513	MA6	N9-C8-N7	-3.60	108.98	113.91
28	a	1822	2MG	N9-C4-N3	3.60	133.16	125.94
28	a	945	PSU	C4-N3-C2	-3.57	121.19	126.34
28	a	2444	PSU	C4-N3-C2	-3.57	121.19	126.34
28	a	2567	PSU	C4-N3-C2	-3.54	121.24	126.34
6	A	521	G7M	O6-C6-C5	-3.49	120.18	128.06
28	a	1904	PSU	C4-N3-C2	-3.44	121.38	126.34
28	a	2017	6MZ	C4-C5-N7	-3.42	106.46	110.62
28	a	736	PSU	O2-C2-N1	-3.41	119.04	122.79
28	a	2017	6MZ	C5-N7-C8	3.40	108.34	103.51
28	a	2567	PSU	O2-C2-N1	-3.39	119.06	122.79
6	A	960	2MG	N9-C4-N3	3.38	132.74	125.94
28	a	2432	2MG	N9-C4-N3	3.38	132.73	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	510	PSU	C4-N3-C2	-3.37	121.48	126.34
6	A	1512	MA6	C4-N9-C8	3.37	109.38	105.73
28	a	1608	6MZ	C9-N6-C6	-3.34	119.99	122.87
6	A	1510	2MG	C6-C5-N7	3.32	136.43	130.25
39	l	82	4D4	NE-CZ-NH2	3.29	126.48	120.70
6	A	521	G7M	C6-C5-N7	3.29	136.22	132.25
28	a	1608	6MZ	C5-N7-C8	3.29	108.18	103.51
28	a	2017	6MZ	N3-C4-N9	3.27	132.47	127.08
6	A	1201	2MG	N9-C4-N3	3.26	132.48	125.94
6	A	1513	MA6	C4-C5-N7	-3.25	106.66	110.62
6	A	510	PSU	O2-C2-N1	-3.22	119.25	122.79
28	a	945	PSU	O2-C2-N1	-3.17	119.30	122.79
28	a	2491	PSU	O2-C2-N1	-3.15	119.32	122.79
28	a	1898	PSU	O2-C2-N1	-3.13	119.34	122.79
6	A	1512	MA6	C4-C5-N7	-3.12	106.82	110.62
28	a	1608	6MZ	C4-C5-N7	-3.10	106.84	110.62
6	A	1201	2MG	C6-C5-N7	3.10	136.01	130.25
28	a	1608	6MZ	C6-C5-N7	3.09	135.74	132.39
28	a	1608	6MZ	N9-C8-N7	-2.99	109.82	113.91
6	A	1513	MA6	C4-N9-C8	2.99	108.97	105.73
28	a	2017	6MZ	N9-C8-N7	-2.96	109.87	113.91
28	a	1904	PSU	O2-C2-N1	-2.96	119.53	122.79
6	A	1510	2MG	N9-C4-N3	2.96	131.88	125.94
28	a	2490	2MA	N9-C8-N7	-2.94	109.90	113.91
28	a	2432	2MG	C6-C5-N7	2.92	135.68	130.25
28	a	2490	2MA	C5-N7-C8	2.92	107.65	103.51
28	a	2444	PSU	O2-C2-N1	-2.89	119.61	122.79
28	a	2485	OMC	O2-C2-N3	-2.84	117.71	122.33
28	a	2592	PSU	O2-C2-N1	-2.82	119.69	122.79
6	A	960	2MG	C6-C5-N7	2.79	135.43	130.25
6	A	521	G7M	C2-N1-C6	-2.77	120.04	125.10
28	a	2238	OMG	C6-C5-N7	2.77	135.40	130.25
28	a	2539	OMU	O2-C2-N1	-2.75	119.13	122.79
28	a	2591	PSU	O2-C2-N1	-2.75	119.76	122.79
17	L	89	D2T	OD1-CG-CB	-2.72	116.75	122.44
28	a	1822	2MG	C6-C5-N7	2.70	135.27	130.25
28	a	2490	2MA	C4-C5-N7	-2.67	107.37	110.62
6	A	1510	2MG	C4-C5-N7	-2.64	106.55	110.72
6	A	1201	2MG	C4-C5-N7	-2.62	106.58	110.72
28	a	2539	OMU	C5-C4-N3	2.55	118.66	114.84
28	a	735	1MG	C5-C6-N1	2.54	119.81	114.91
28	a	2539	OMU	O4-C4-C5	-2.52	120.72	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	a	1926	5MU	O2-C2-N3	-2.51	116.82	121.50
28	a	2567	PSU	O4'-C1'-C2'	2.51	108.68	105.14
28	a	1902	3TD	C4-N3-C2	-2.46	121.94	124.61
28	a	1926	5MU	C6-N1-C2	2.45	123.77	121.30
39	l	82	4D4	NH1-CZ-NE	-2.43	113.59	119.19
28	a	2056	7MG	C5-C4-N9	2.42	109.49	106.35
28	a	2238	OMG	C5-C6-N1	2.41	119.30	113.19
28	a	945	PSU	C6-N1-C2	-2.39	120.24	122.68
28	a	2432	2MG	CM2-N2-C2	-2.39	118.58	123.86
28	a	2432	2MG	C4-C5-N7	-2.35	107.01	110.72
28	a	1949	5MC	C5-C4-N3	-2.33	119.16	121.67
28	a	2238	OMG	C8-N7-C5	2.31	108.43	104.24
6	A	961	5MC	C5-C4-N3	-2.31	119.18	121.67
28	a	2238	OMG	C4-C5-N7	-2.31	107.06	110.72
28	a	2490	2MA	C4-N9-C8	2.30	108.22	105.73
6	A	960	2MG	O6-C6-C5	-2.30	120.50	126.60
6	A	960	2MG	C4-C5-N7	-2.30	107.08	110.72
39	l	83	MS6	CE-SD-CG	2.29	108.28	100.40
6	A	1201	2MG	C8-N7-C5	2.27	108.35	104.24
6	A	1510	2MG	N1-C2-N3	-2.26	120.45	123.95
28	a	2490	2MA	N3-C2-N1	-2.26	121.56	125.72
6	A	510	PSU	O4'-C1'-C2'	2.25	108.32	105.14
28	a	1822	2MG	C4-C5-N7	-2.25	107.16	110.72
6	A	1201	2MG	CM2-N2-C2	-2.25	118.89	123.86
28	a	2238	OMG	O6-C6-C5	-2.22	120.70	126.60
6	A	1396	4OC	O2-C2-N3	-2.22	118.72	122.33
6	A	960	2MG	C5-C6-N1	2.21	118.80	113.19
28	a	2432	2MG	O6-C6-C5	-2.21	120.75	126.60
28	a	2432	2MG	C5-C6-N1	2.20	118.79	113.19
6	A	1396	4OC	C5-C4-N3	-2.20	119.06	122.59
28	a	1822	2MG	C5-C6-N1	2.19	118.76	113.19
6	A	1510	2MG	O6-C6-C5	-2.19	120.80	126.60
28	a	1904	PSU	O4'-C1'-C2'	2.18	108.22	105.14
28	a	735	1MG	C4-C5-N7	-2.18	107.27	110.72
6	A	1510	2MG	C8-N7-C5	2.18	108.18	104.24
6	A	1201	2MG	C2-N1-C6	-2.18	121.98	124.48
28	a	735	1MG	C6-C5-N7	2.18	134.27	129.35
6	A	1201	2MG	C5-C6-N1	2.17	118.71	113.19
6	A	1510	2MG	C5-C6-N1	2.17	118.69	113.19
6	A	960	2MG	N1-C2-N3	-2.16	120.61	123.95
6	A	1201	2MG	O6-C6-C5	-2.15	120.89	126.60
6	A	510	PSU	C6-N1-C2	-2.15	120.48	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1492	UR3	C5-C6-N1	-2.14	118.22	121.81
28	a	2432	2MG	N1-C2-N3	-2.14	120.64	123.95
28	a	1822	2MG	O6-C6-C5	-2.14	120.92	126.60
28	a	1608	6MZ	C4-N9-C8	2.12	108.03	105.73
28	a	1822	2MG	N1-C2-N3	-2.11	120.69	123.95
6	A	960	2MG	C2-N1-C6	-2.11	122.05	124.48
6	A	1201	2MG	N1-C2-N3	-2.11	120.69	123.95
28	a	2444	PSU	O4'-C1'-C2'	2.08	108.08	105.14
28	a	2238	OMG	N9-C8-N7	-2.08	109.48	113.39
28	a	1822	2MG	C2-N1-C6	-2.07	122.10	124.48
28	a	2485	OMC	N1-C2-N3	2.05	122.55	118.81
28	a	2490	2MA	N6-C6-N1	2.04	119.92	117.03
28	a	1822	2MG	C8-N7-C5	2.04	107.94	104.24
6	A	1510	2MG	N9-C8-N7	-2.04	109.56	113.39
28	a	2432	2MG	C8-N7-C5	2.03	107.92	104.24
28	a	2432	2MG	C2-N1-C6	-2.03	122.15	124.48
28	a	2238	OMG	C2-N1-C6	-2.02	121.41	125.10
28	a	2567	PSU	C6-N1-C2	-2.02	120.62	122.68
28	a	2491	PSU	C6-N1-C2	-2.01	120.63	122.68
28	a	2444	PSU	C6-N1-C2	-2.01	120.63	122.68
6	A	1201	2MG	N9-C8-N7	-2.00	109.62	113.39

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	L	89	D2T	CA-CB-CG-OD1
17	L	89	D2T	CA-CB-CG-OD2
39	l	82	4D4	O-C-CA-CB
39	l	82	4D4	CA-CB-CG-CD
16	K	119	IAS	N-CA-CB-CG
16	K	119	IAS	C-CA-CB-CG
28	a	1902	3TD	O4'-C1'-C5-C4
28	a	1902	3TD	O4'-C1'-C5-C6
28	a	2017	6MZ	O4'-C4'-C5'-O5'
28	a	2238	OMG	O4'-C4'-C5'-O5'
28	a	2238	OMG	C1'-C2'-O2'-CM2
28	a	2432	2MG	C3'-C4'-C5'-O5'
6	A	1513	MA6	O4'-C4'-C5'-O5'
28	a	2056	7MG	O4'-C4'-C5'-O5'
28	a	2056	7MG	C3'-C4'-C5'-O5'
28	a	2238	OMG	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
6	A	521	G7M	C3'-C4'-C5'-O5'
6	A	1513	MA6	C3'-C4'-C5'-O5'
28	a	2017	6MZ	C3'-C4'-C5'-O5'
28	a	2432	2MG	O4'-C4'-C5'-O5'
39	l	82	4D4	OB-CB-CG-CD
6	A	521	G7M	O4'-C4'-C5'-O5'
39	l	83	MS6	CB-CG-SD-CE
17	L	89	D2T	CG-CB-SB-CB1
31	d	150	MEQ	N-CA-CB-CG
6	A	521	G7M	C4'-C5'-O5'-P
31	d	150	MEQ	OE1-CD-CG-CB
39	l	82	4D4	NE-CD-CG-CB
16	K	119	IAS	O-C-CA-N
28	a	2490	2MA	O4'-C4'-C5'-O5'
17	L	89	D2T	SB-CB-CG-OD2
31	d	150	MEQ	NE2-CD-CG-CB
28	a	736	PSU	O4'-C1'-C5-C6
28	a	2436	H2U	C4'-C5'-O5'-P
28	a	2490	2MA	C4'-C5'-O5'-P
28	a	1902	3TD	O4'-C4'-C5'-O5'
39	l	83	MS6	CA-CB-CG-SD
28	a	2485	OMC	C4'-C5'-O5'-P
16	K	119	IAS	CA-CB-CG-OD1
6	A	1396	4OC	O4'-C4'-C5'-O5'
28	a	2567	PSU	O4'-C4'-C5'-O5'

There are no ring outliers.

11 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	a	2017	6MZ	1	0
6	A	960	2MG	2	0
31	d	150	MEQ	1	0
28	a	735	1MG	1	0
6	A	510	PSU	1	0
6	A	1396	4OC	2	0
28	a	2490	2MA	1	0
6	A	961	5MC	1	0
6	A	1201	2MG	2	0
28	a	2238	OMG	1	0
16	K	119	IAS	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 525 ligands modelled in this entry, 525 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)

There are no chain breaks in this entry.

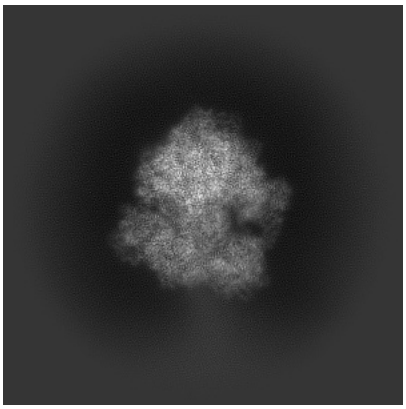
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-55712. These allow visual inspection of the internal detail of the map and identification of artifacts.

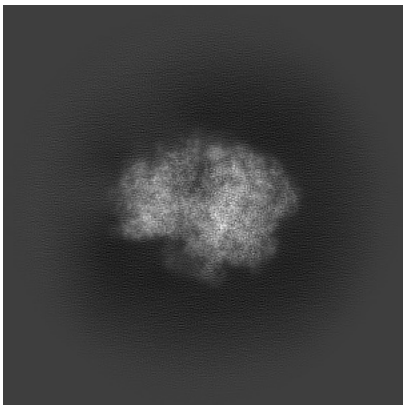
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

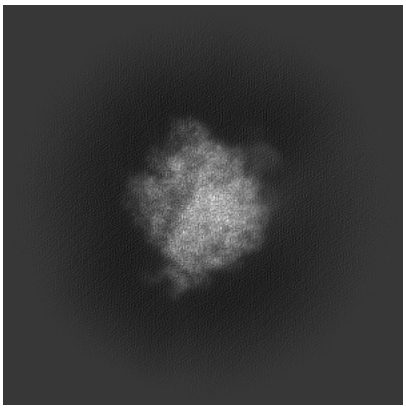
6.1.1 Primary map



X

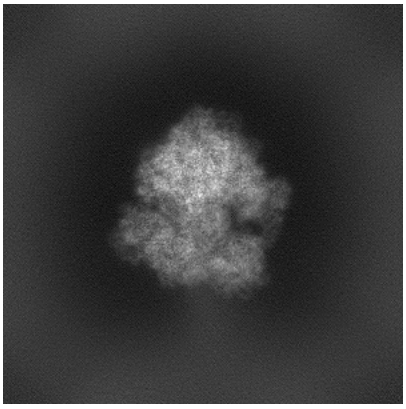


Y

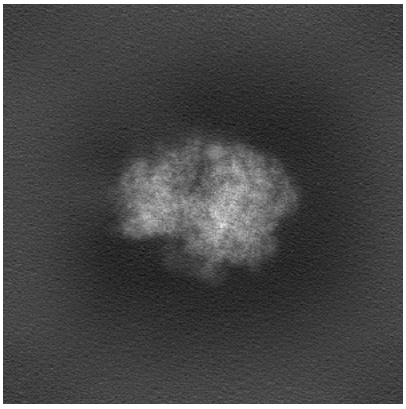


Z

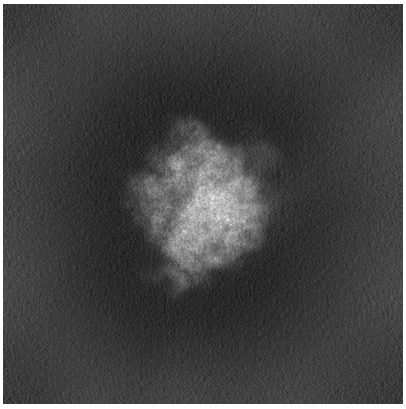
6.1.2 Raw map



X



Y

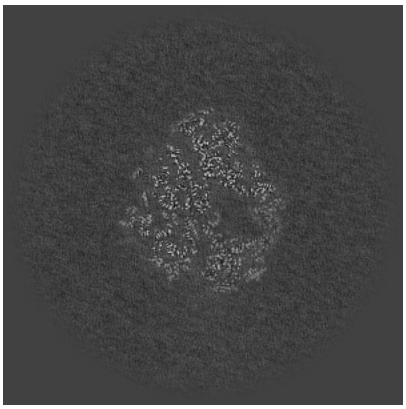


Z

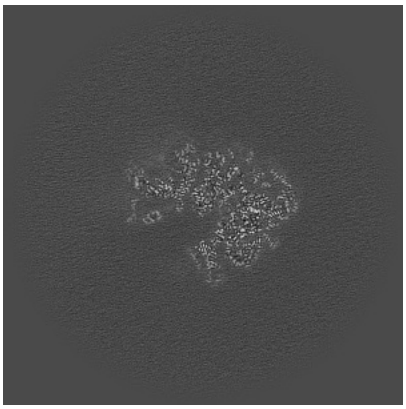
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

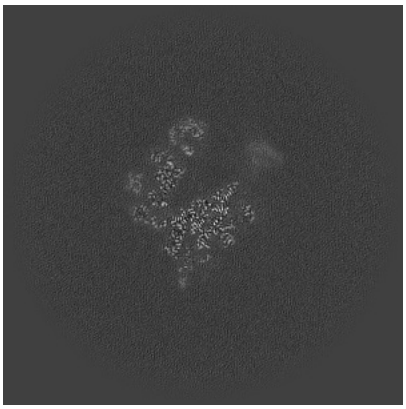
6.2.1 Primary map



X Index: 256

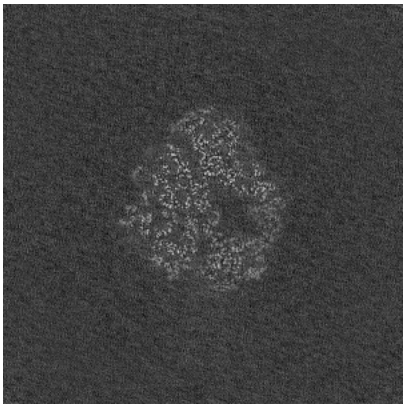


Y Index: 256

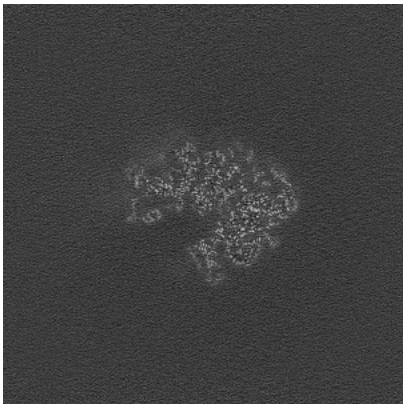


Z Index: 256

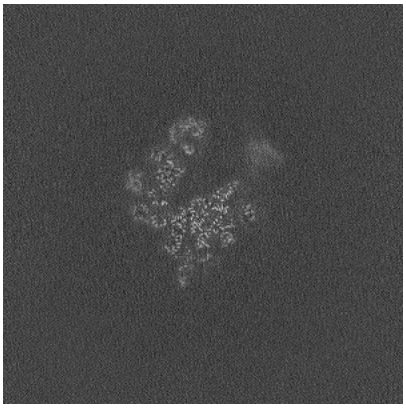
6.2.2 Raw map



X Index: 256



Y Index: 256

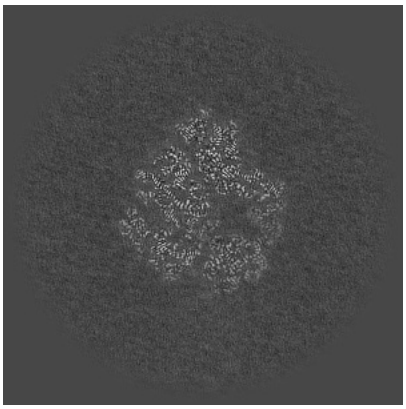


Z Index: 256

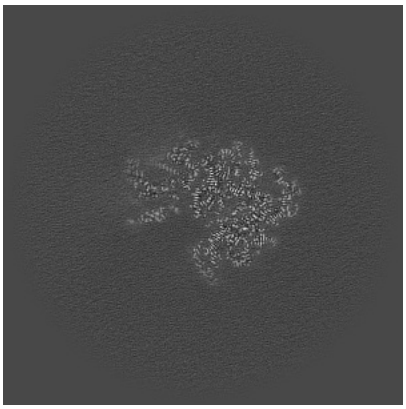
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

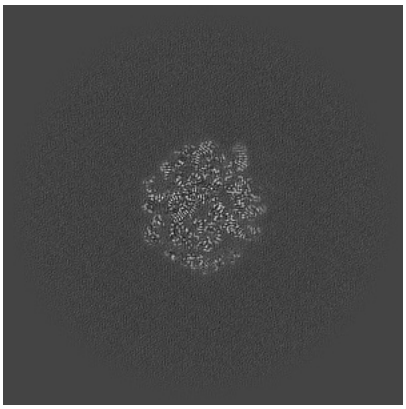
6.3.1 Primary map



X Index: 252

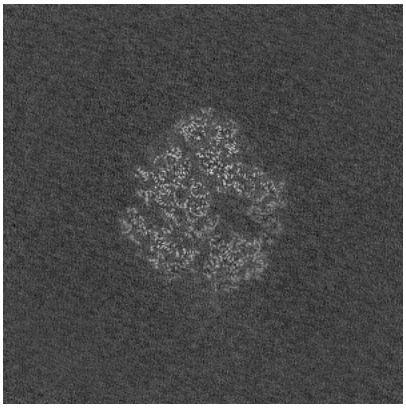


Y Index: 252

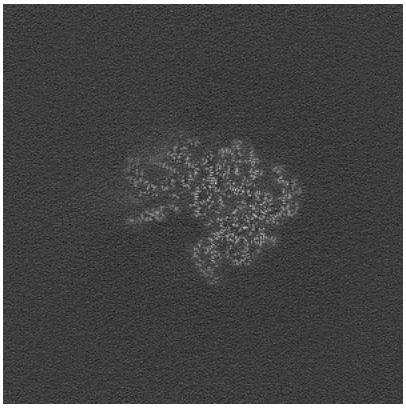


Z Index: 295

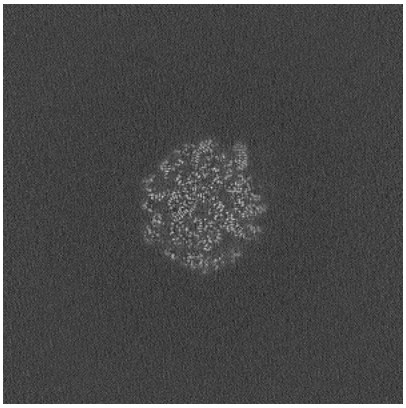
6.3.2 Raw map



X Index: 253



Y Index: 252

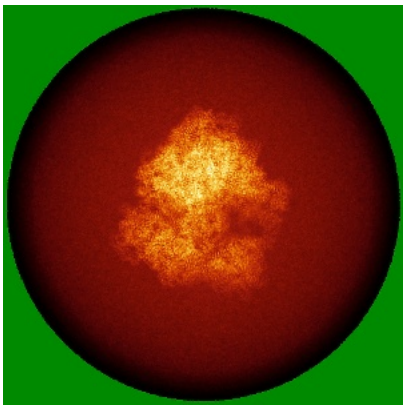


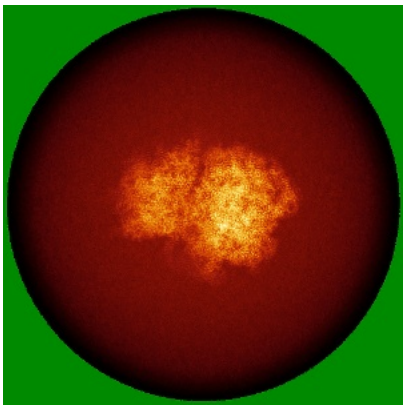
Z Index: 295

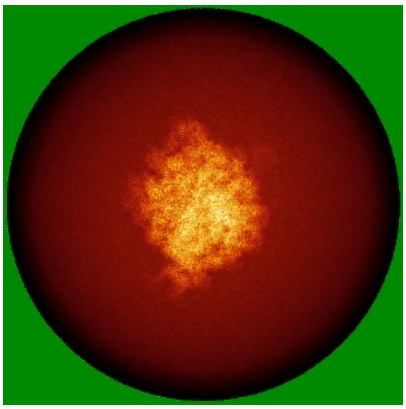
The images above show the largest variance slices of the map in three orthogonal directions.

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

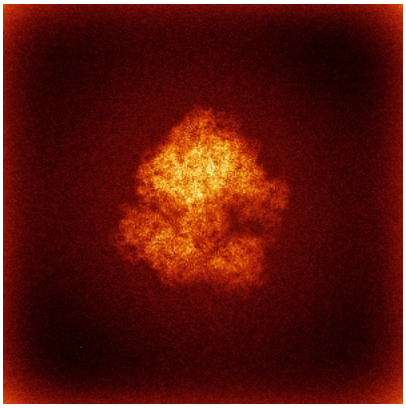
6.4.1 Primary map

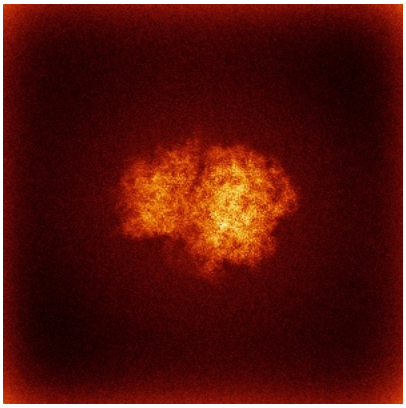

X

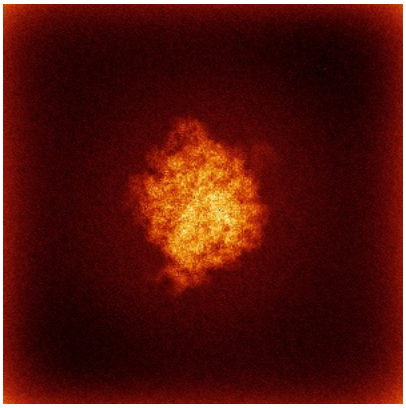

Y


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 0.55. 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.

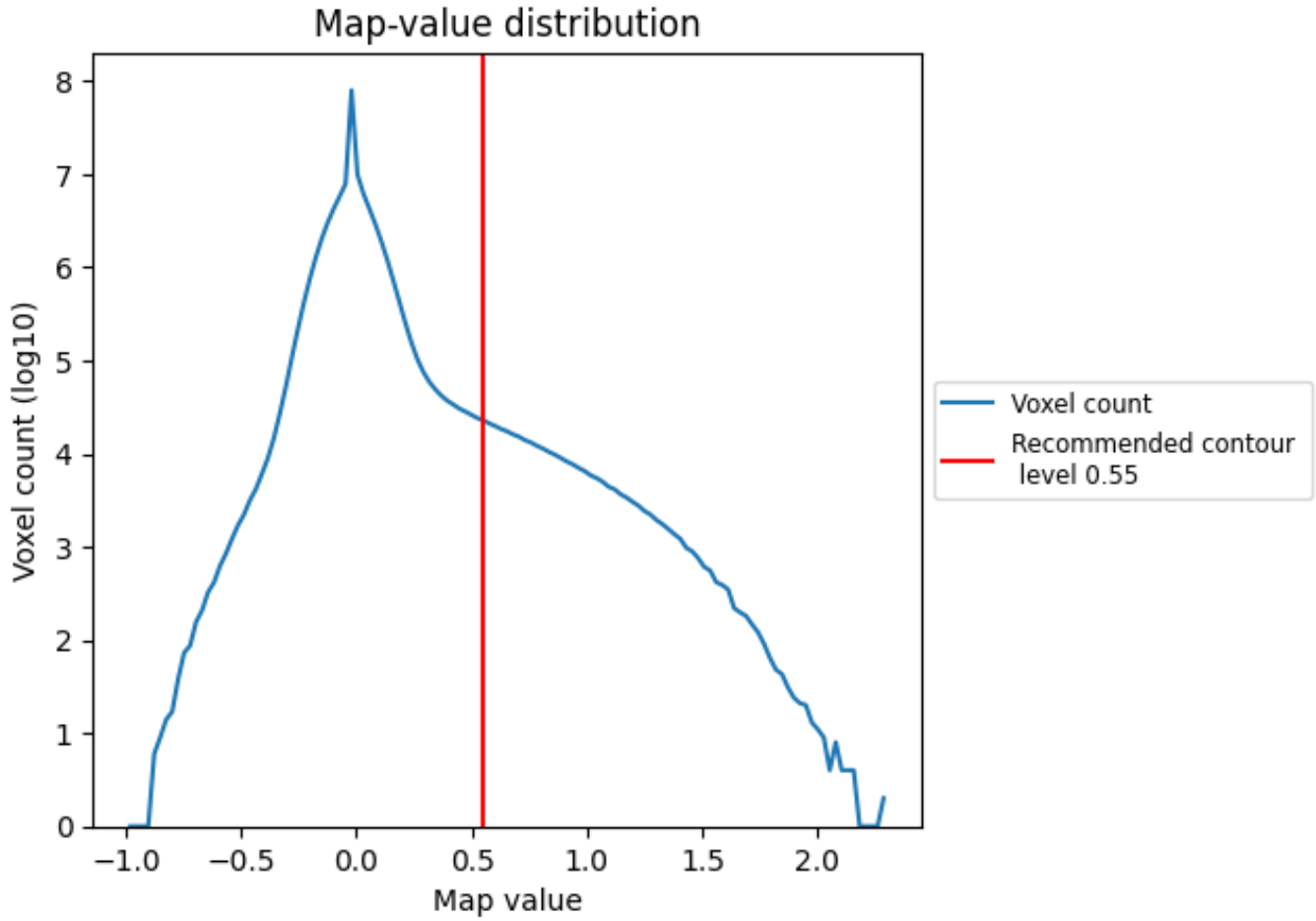
6.6 Mask visualisation (i)

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

7 Map analysis

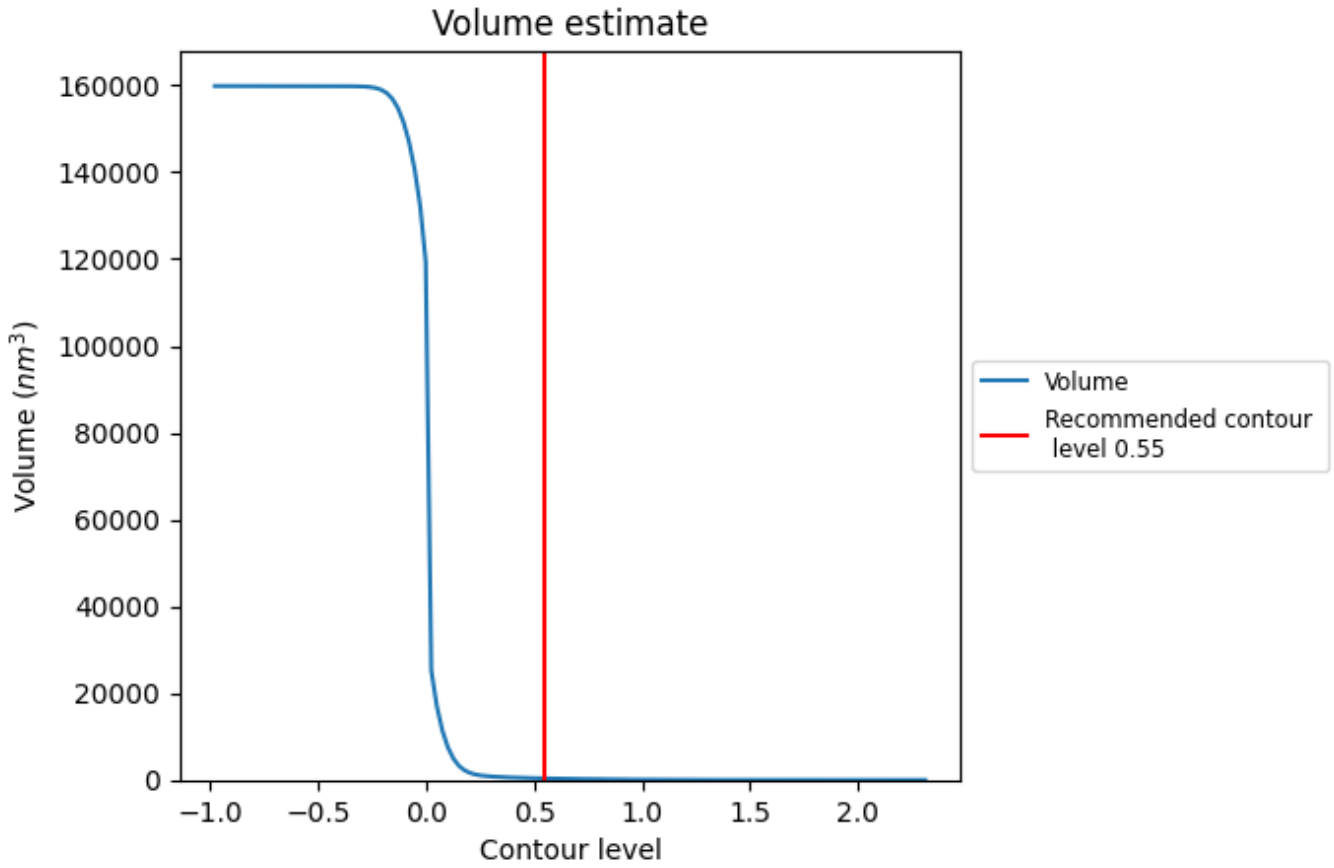
This section contains the results of statistical analysis of the map.

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.

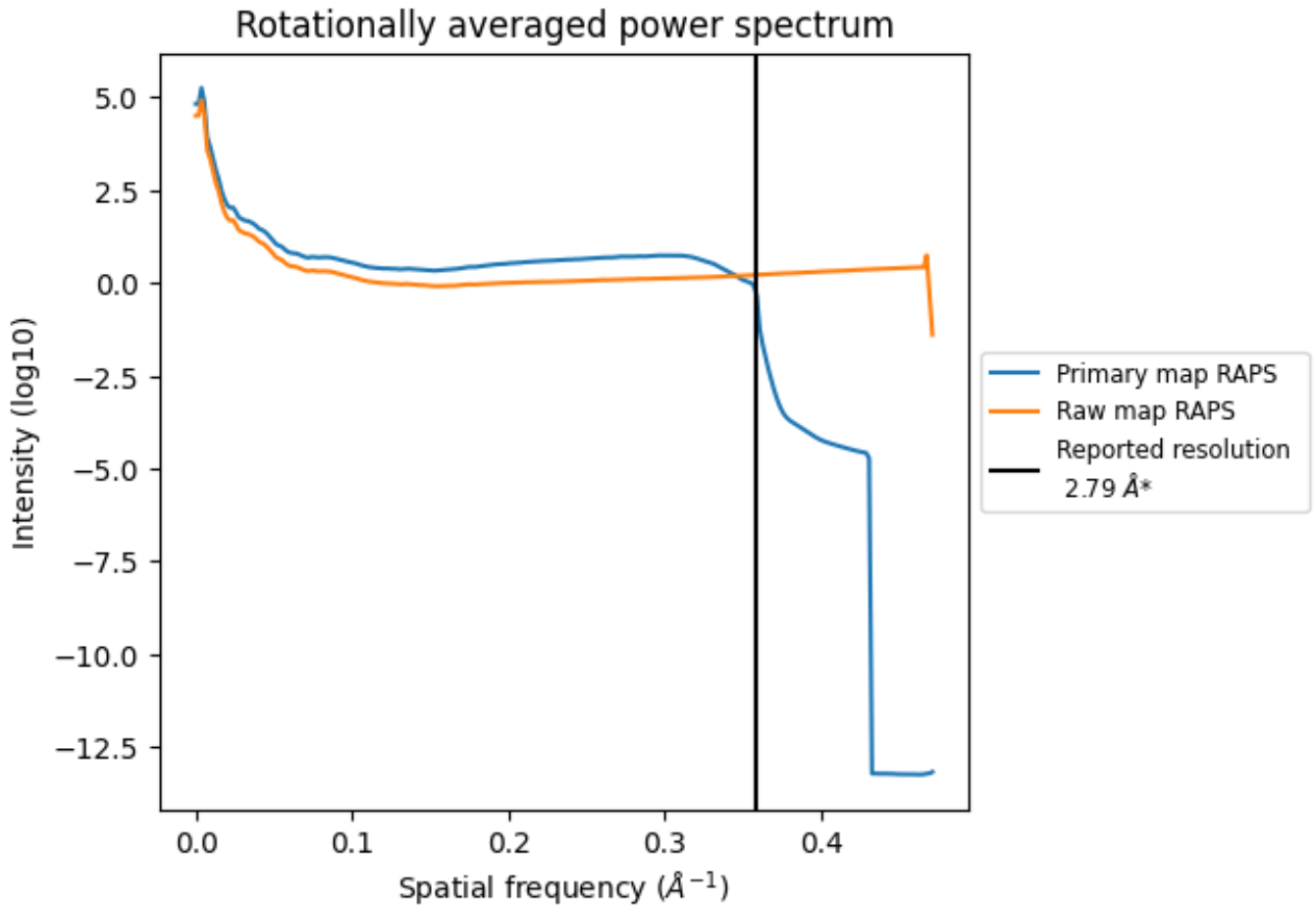
7.2 Volume estimate



The volume at the recommended contour level is 353 nm^3; this corresponds to an approximate mass of 319 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)

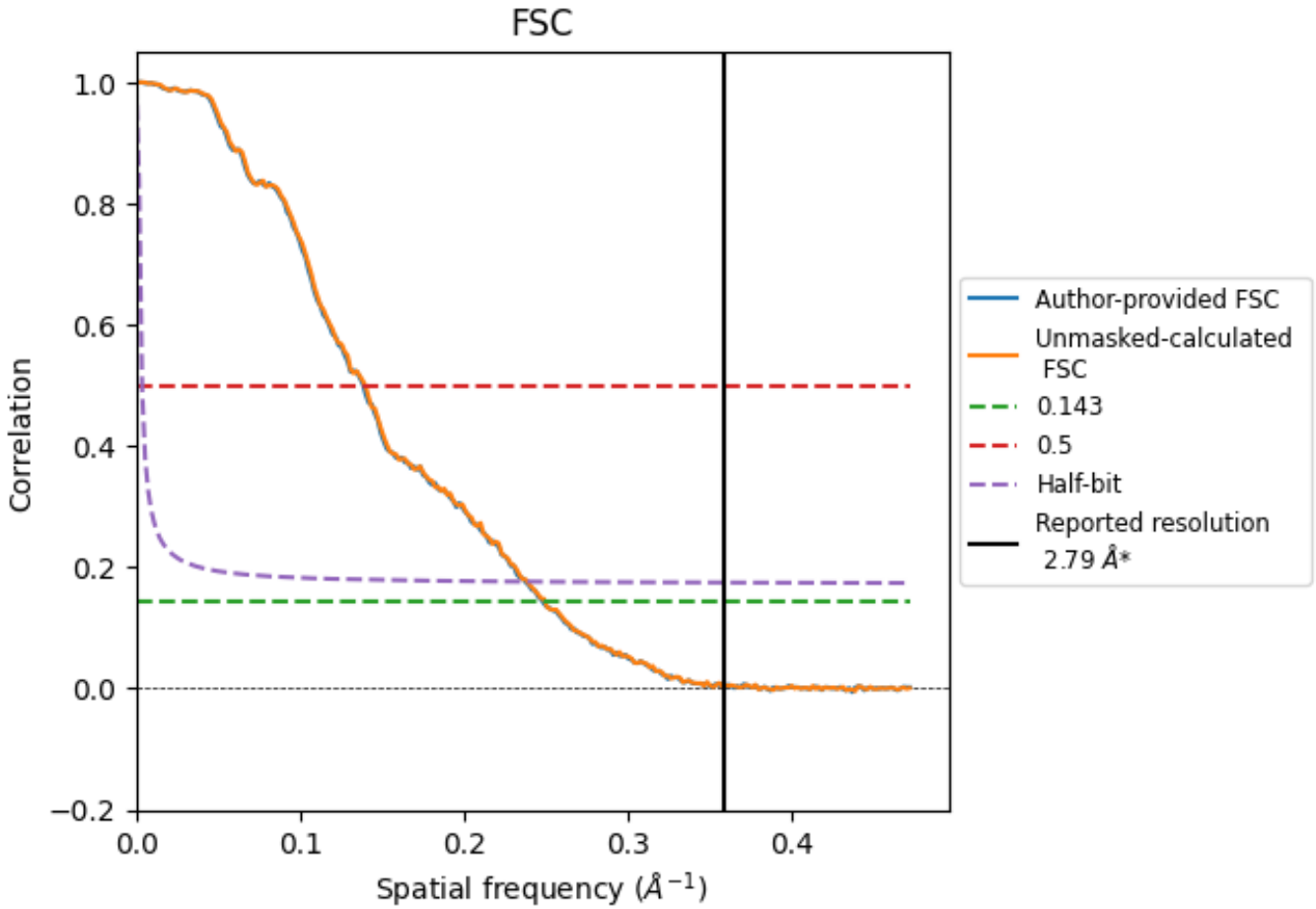


*Reported resolution corresponds to spatial frequency of 0.358 $Å^{-1}$

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 0.358 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.79	-	-
Author-provided FSC curve	4.03	7.22	4.21
Unmasked-calculated*	4.01	7.16	4.19

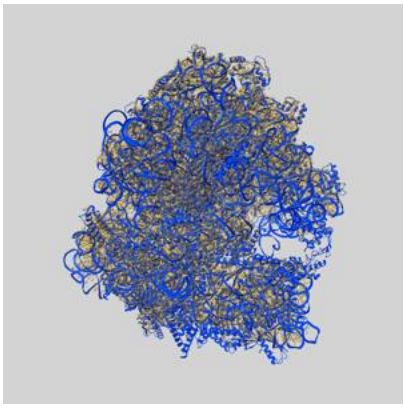
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.03 differs from the reported value 2.79 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.01 differs from the reported value 2.79 by more than 10 %

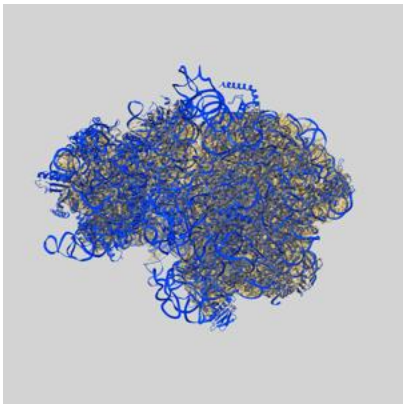
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-55712 and PDB model 9T8U. Per-residue inclusion information can be found in section 3 on page 14.

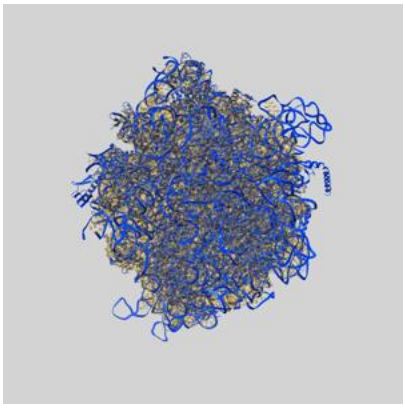
9.1 Map-model overlay



X



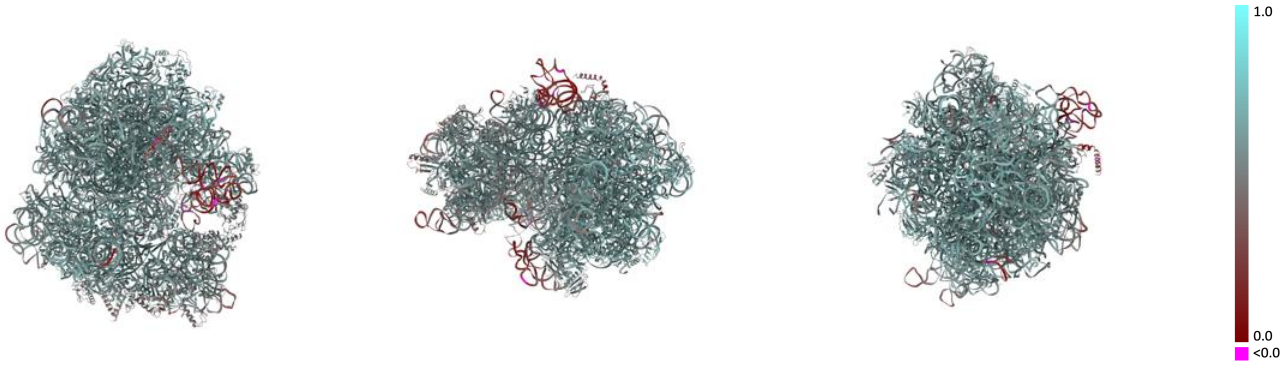
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.55 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.

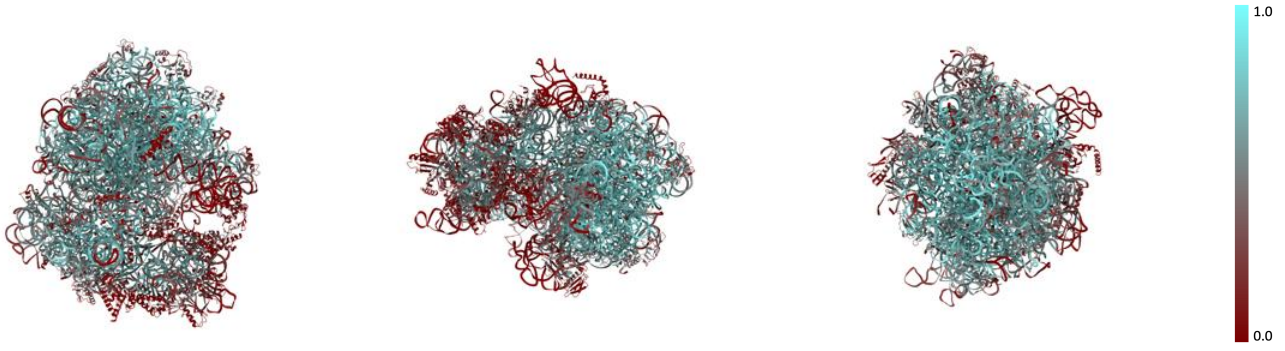
9.2 Q-score mapped to coordinate model (i)



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.

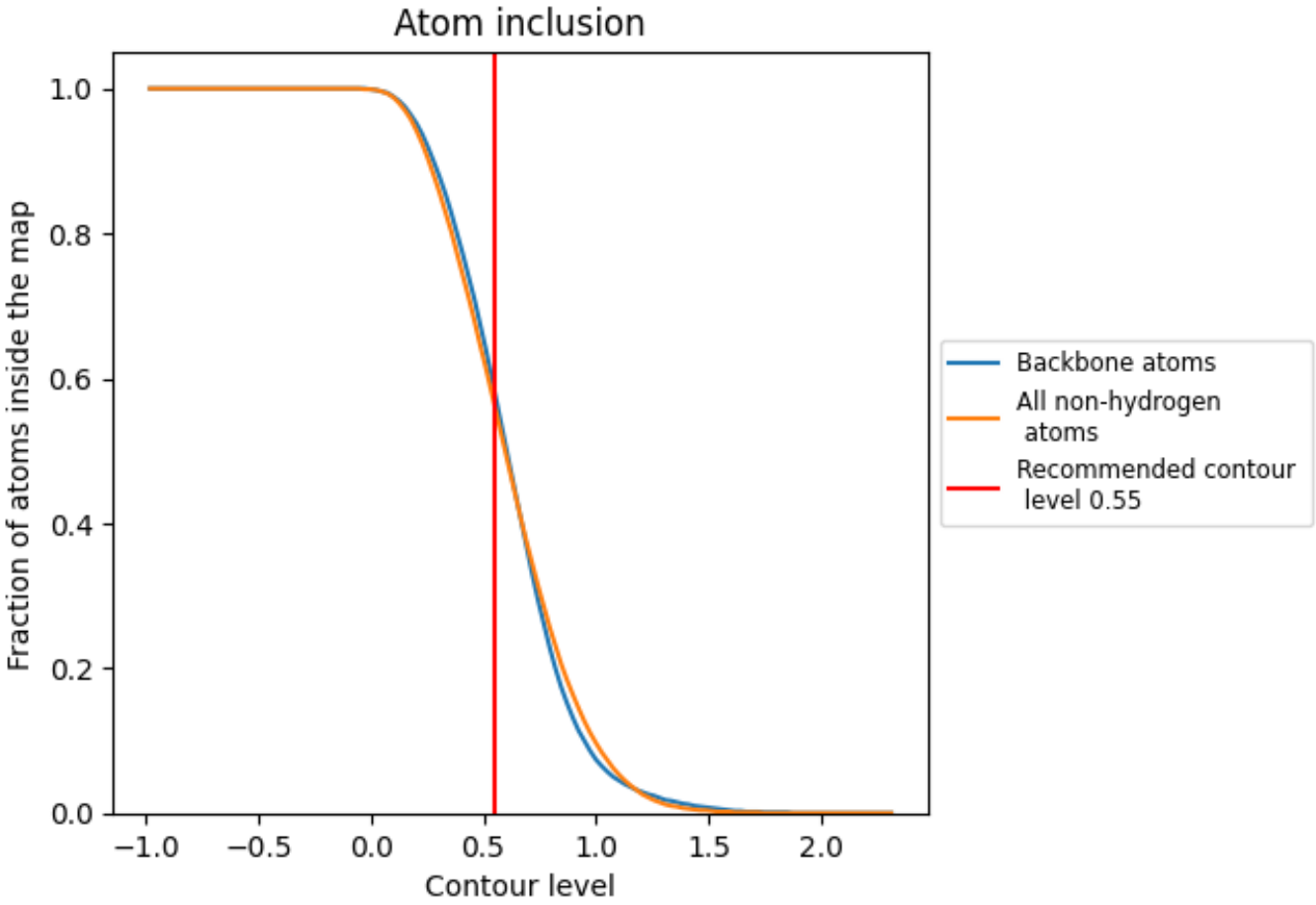
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.55).

9.4 Atom inclusion (i)



At the recommended contour level, 58% of all backbone atoms, 56% 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 (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5620	0.5800
0	0.3470	0.5950
1	0.7230	0.6320
2	0.6350	0.6330
3	0.5310	0.6130
4	0.0170	0.4300
A	0.5750	0.5760
B	0.0580	0.4920
C	0.3120	0.5660
D	0.3050	0.5650
E	0.4670	0.5900
F	0.2430	0.5590
G	0.1120	0.5130
H	0.4750	0.6020
I	0.1930	0.5430
J	0.1970	0.5040
K	0.3500	0.5710
L	0.4640	0.6020
M	0.1280	0.5250
N	0.3040	0.5560
O	0.4080	0.5840
P	0.5390	0.6060
Q	0.4050	0.5840
R	0.3910	0.5560
S	0.1350	0.5190
T	0.4500	0.5950
U	0.1460	0.5210
X	0.2520	0.5680
a	0.6790	0.5860
b	0.4850	0.5740
c	0.6350	0.6290
d	0.6320	0.6200
e	0.5320	0.6050
f	0.0730	0.5050
g	0.1620	0.5450



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Chain	Atom inclusion	Q-score
h	0.0000	0.3550
i	0.6140	0.6160
j	0.5280	0.6160
k	0.5720	0.6170
l	0.5320	0.6130
m	0.6600	0.6210
n	0.3310	0.5710
o	0.5280	0.6200
p	0.6570	0.6260
q	0.5110	0.6130
r	0.5850	0.6190
s	0.4610	0.5920
t	0.3500	0.5530
u	0.2500	0.5710
v	0.6100	0.6210
w	0.5270	0.6150
x	0.4060	0.5890
y	0.5590	0.6150
z	0.5730	0.6120