Full wwPDB EM Validation Report (i)

Sep 16, 2026 – 05:56 PM EDT

PDB ID	:	9C4G / pdb_00009c4g
EMDB ID	:	EMD-45185
Title	:	Cutibacterium acnes 50S ribosomal subunit with Clindamycin bound
Authors	:	Lomakin, I.B.; Devarkar, S.C.; Bunick, C.G.
Deposited on	:	2024-06-04
Resolution	:	2.53 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

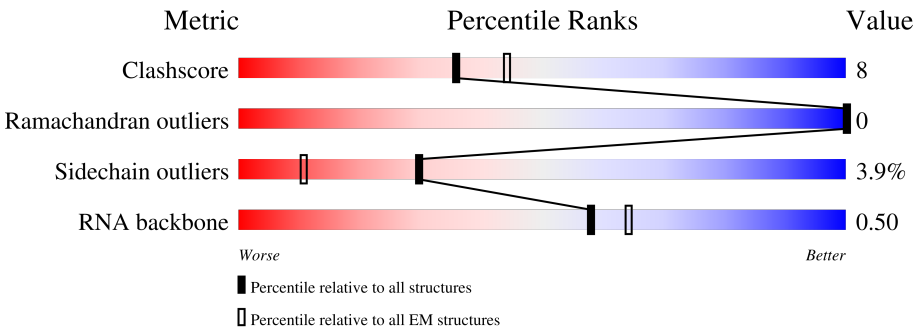
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)	:	2.50

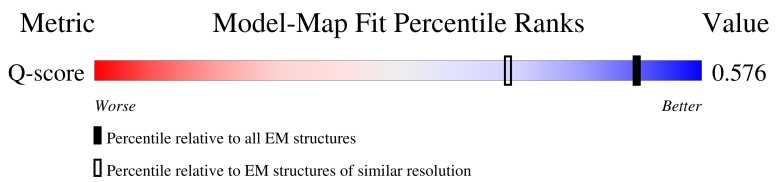
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.53 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	7309 (2.03 - 3.03)

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	c	278	82% 15%
2	d	223	77% 18%
3	e	301	8% 50% 19% 30%

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Mol	Chain	Length	Quality of chain
4	f	210	67% 54% 34% 12%
5	g	180	65% 63% 34%
6	i	147	88% 10%
7	j	122	11% 71% 26%
8	k	146	9% 73% 24%
9	l	139	9% 78% 19%
10	m	187	49% 14% 36%
11	n	127	17% 79% 19%
12	o	117	26% 70% 26%
13	p	123	85% 11%
14	q	102	15% 85% 15%
15	r	153	8% 67% 16% 14%
16	s	102	13% 76% 17% 7%
17	t	122	20% 71% 14% 13%
18	u	205	52% 70% 16% 13%
19	v	89	9% 78% 9% 12%
20	w	61	80% 18%
21	x	77	12% 73% 17% 10%
22	y	60	7% 65% 32%
23	z	63	5% 84% 14%
24	0	56	12% 68% 21% 11%
25	1	44	5% 93% 7%
26	2	68	79% 19%
27	4	69	96% 62% 33%
28	a	3086	10% 53% 34% 7% 6%

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Mol	Chain	Length	Quality of chain
29	b	120	66% 32%
30	V	24	92%
31	3	37	8% 84% 16%

2 Entry composition (i)

There are 35 unique types of molecules in this entry. The entry contains 91105 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 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	c	274	2091	1289	425	372	5	0	0

- Molecule 2 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	d	214	1586	984	304	291	7	0	0

- Molecule 3 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	e	210	1577	979	301	295	2	0	0

- Molecule 4 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	f	184	1468	924	269	266	9	0	0

- Molecule 5 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	g	177	1376	867	250	258	1	0	0

- Molecule 6 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	i	146	1139	718	213	205	3	0	0

- Molecule 7 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	j	122	946	596	177	169	4	0	0

- Molecule 8 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	k	144	1072	675	196	199	2	0	0

- Molecule 9 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	l	136	1082	685	210	181	6	0	0

- Molecule 10 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	m	120	936	583	188	163	2	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
m	124	ALA	THR	conflict	UNP A0A8B2VJI7
m	185	PRO	SER	conflict	UNP A0A8B2VJI7

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	n	126	952	583	190	176	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	o	114	896	559	174	162	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	p	119	958	589	196	171	2	0	0

- Molecule 14 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	q	102	778	487	140	150	1	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
q	52	ALA	VAL	conflict	UNP Q6A9I3

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	r	132	1017	624	204	182	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	s	95	751	474	138	138	1	0	0

- Molecule 17 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	t	106	829	514	162	152	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	u	179	1376	865	240	268	3	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
19	v	78	591	355	127	109	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	w	60	474	290	102	77	5	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
21	x	69	564	348	108	108	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	y	58	467	290	91	83	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	z	62	477	287	102	83	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	0	50	423	253	91	73	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	1	44	362	213	91	56	2	0	0

- Molecule 26 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	2	67	513	315	110	87	1	0	0

- Molecule 27 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	4	66	512	313	97	97	5	0	0

- Molecule 28 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
28	a	2903	62406	27794	11385	20324	2903	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	63	A	G	conflict	GB CP012350
a	524	C	G	conflict	GB CP012350
a	1038	PSU	G	conflict	GB CP012350

- Molecule 29 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
29	b	120	2567	1145	466	836	120	0	0

- Molecule 30 is a protein called 50S ribosomal protein bL37.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
30	V	23	183	106	50	27	0	0

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	3	37	302	184	66	47	5	0	0

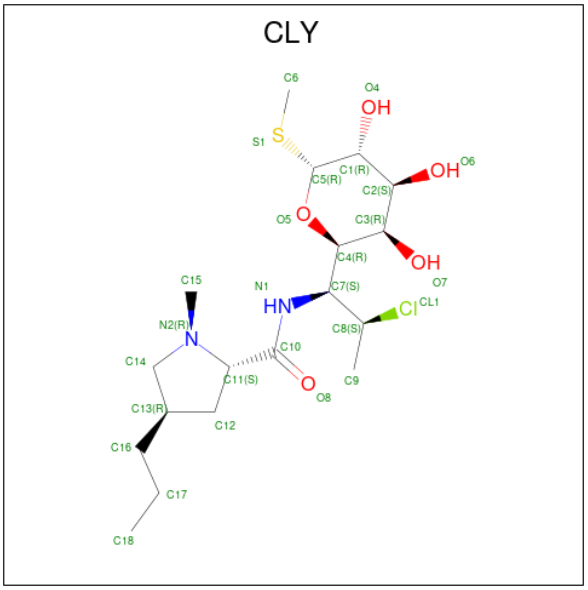
- Molecule 32 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
32	c	1	Total 1	Mg 1	0
32	d	1	Total 1	Mg 1	0
32	k	1	Total 1	Mg 1	0
32	a	241	Total 241	Mg 241	0
32	b	3	Total 3	Mg 3	0

- Molecule 33 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
33	w	1	Total 1	Zn 1	0
33	z	1	Total 1	Zn 1	0
33	0	1	Total 1	Zn 1	0
33	4	1	Total 1	Zn 1	0

- Molecule 34 is CLINDAMYCIN (CCD ID: CLY) (formula: $C_{18}H_{33}ClN_2O_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	Cl	N	O	S	
34	a	1	27	18	1	2	5	1	0

- Molecule 35 is water.

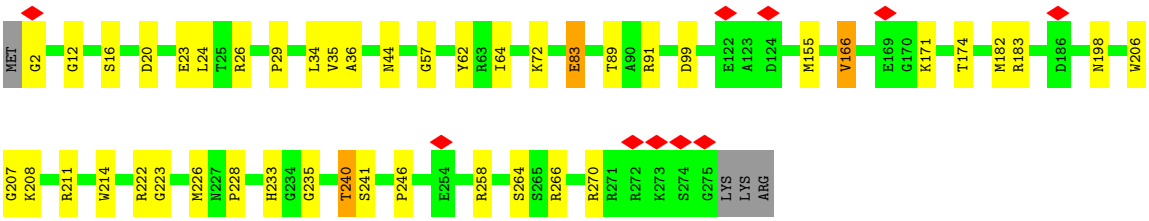
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
35	c	1	1	1	0
35	d	1	1	1	0
35	e	2	2	2	0
35	i	1	1	1	0
35	m	1	1	1	0
35	o	1	1	1	0
35	p	1	1	1	0
35	r	2	2	2	0
35	z	1	1	1	0
35	a	141	141	141	0
35	b	4	4	4	0

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.

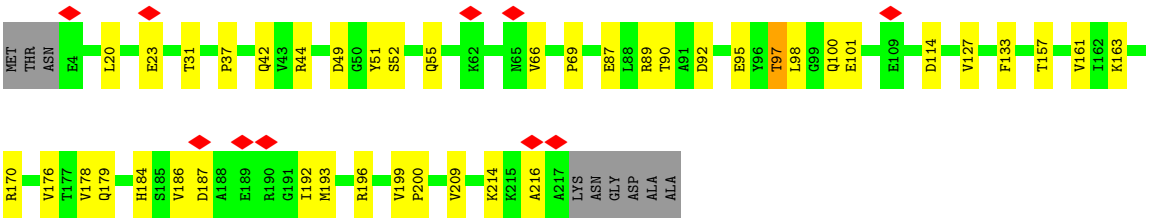
- Molecule 1: 50S ribosomal protein L2

Chain c:



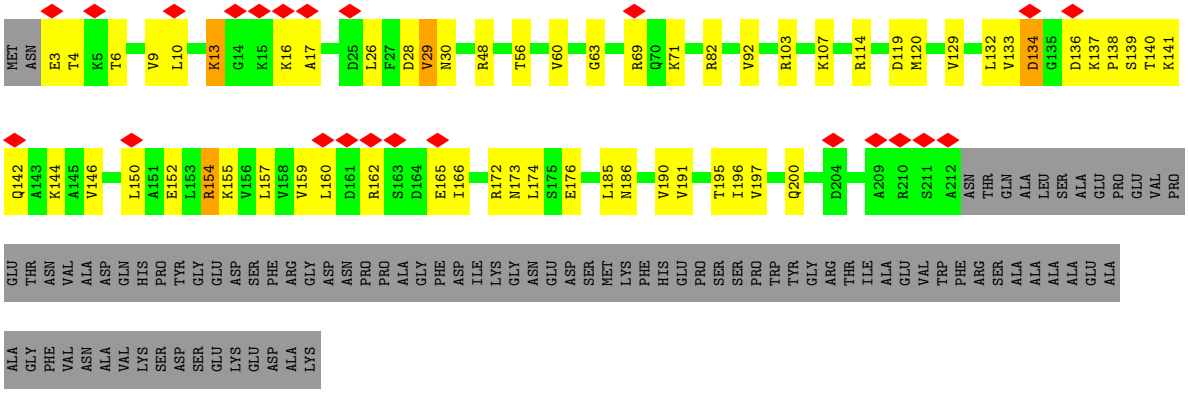
- Molecule 2: 50S ribosomal protein L3

Chain d:



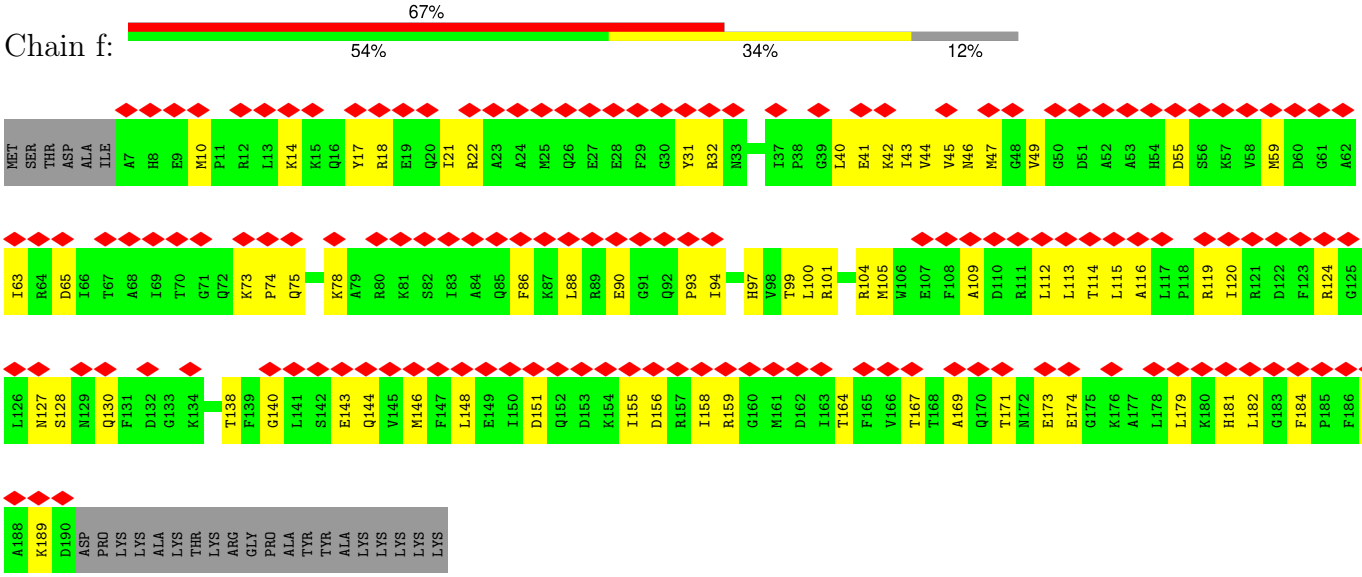
- Molecule 3: 50S ribosomal protein L4

Chain e:



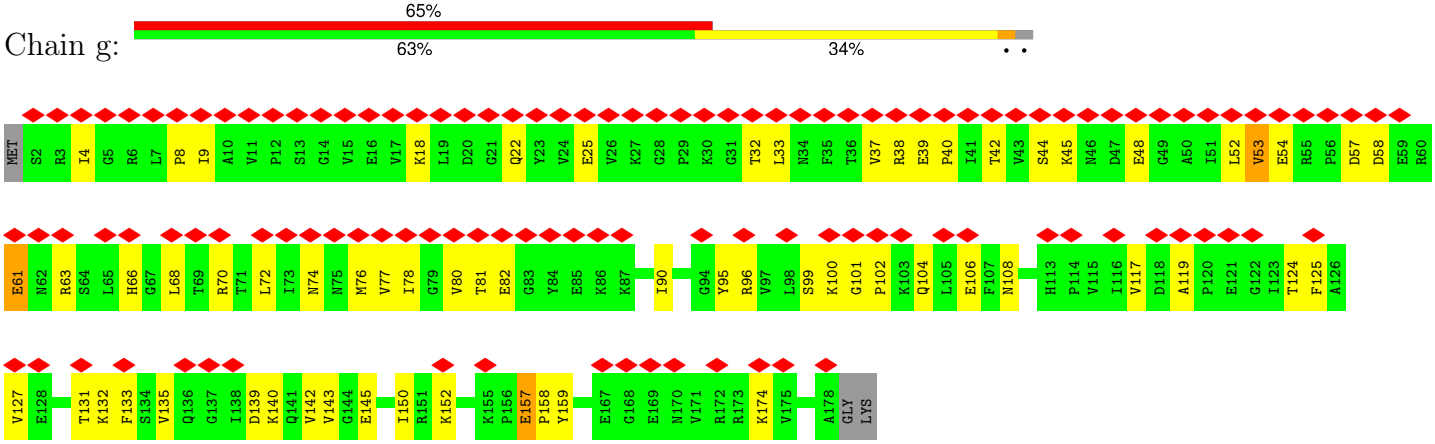
- Molecule 4: 50S ribosomal protein L5

Chain f:



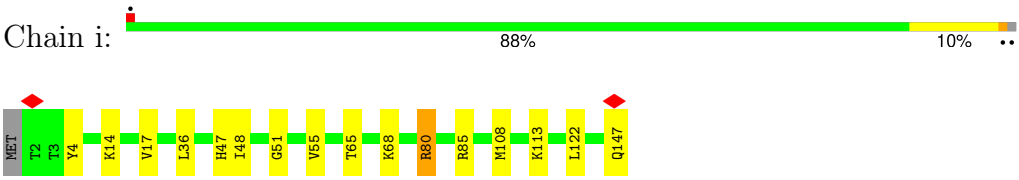
- Molecule 5: 50S ribosomal protein L6

Chain g:



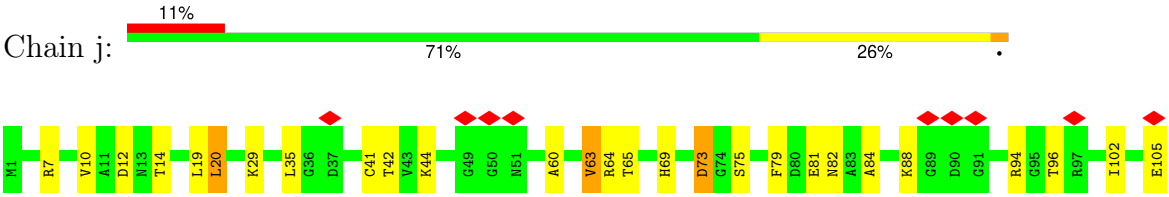
- Molecule 6: 50S ribosomal protein L13

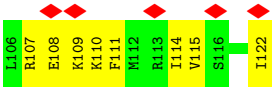
Chain i:



- Molecule 7: 50S ribosomal protein L14

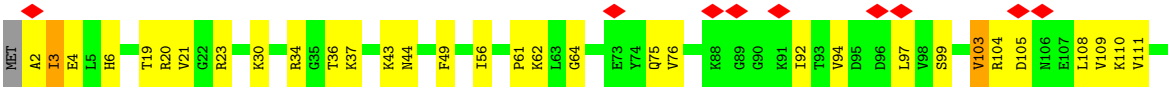
Chain j:

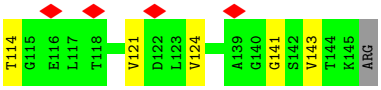




- Molecule 8: 50S ribosomal protein L15

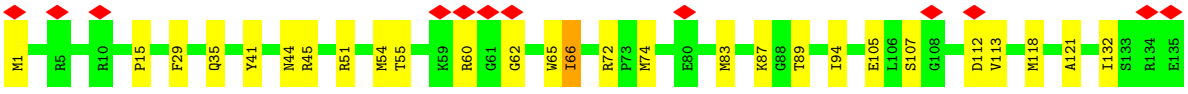
Chain k:





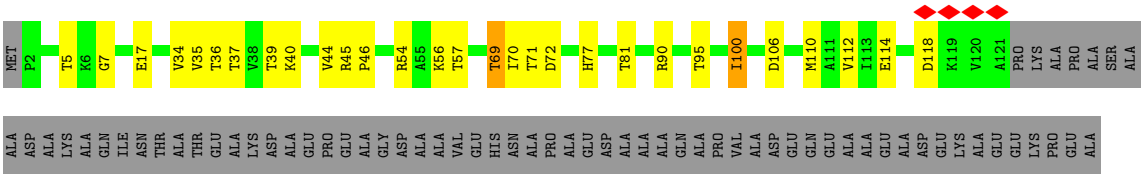
- Molecule 9: 50S ribosomal protein L16

Chain l:



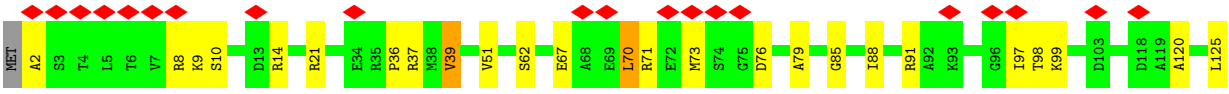
- Molecule 10: Large ribosomal subunit protein bL17

Chain m:



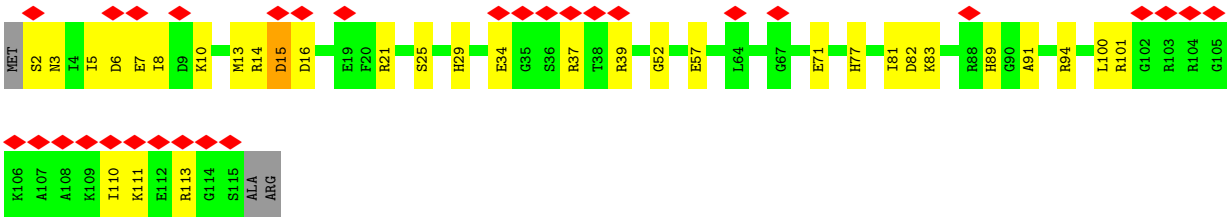
- Molecule 11: 50S ribosomal protein L18

Chain n:



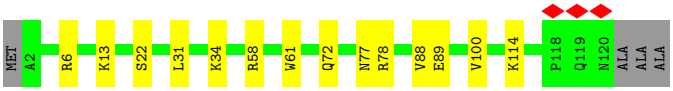
- Molecule 12: 50S ribosomal protein L19

Chain o:



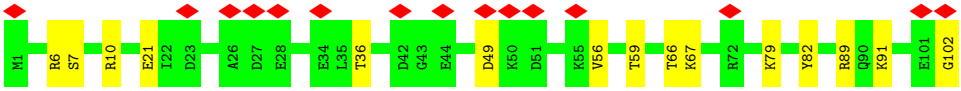
• Molecule 13: 50S ribosomal protein L20

Chain p:



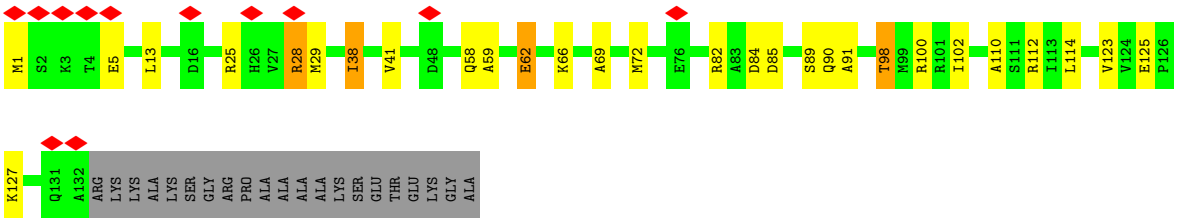
• Molecule 14: Large ribosomal subunit protein bL21

Chain q:



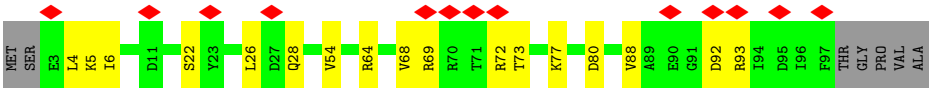
• Molecule 15: 50S ribosomal protein L22

Chain r:



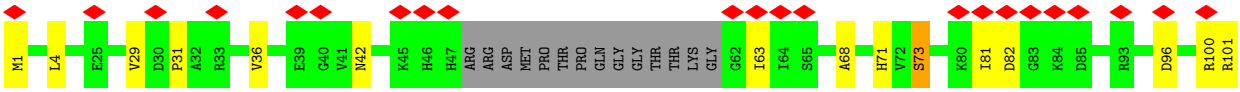
• Molecule 16: 50S ribosomal protein L23

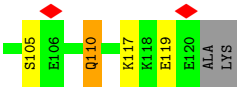
Chain s:



• Molecule 17: Large ribosomal subunit protein uL24

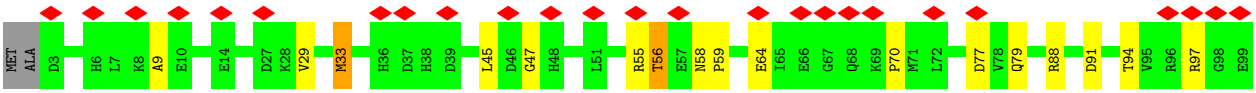
Chain t:

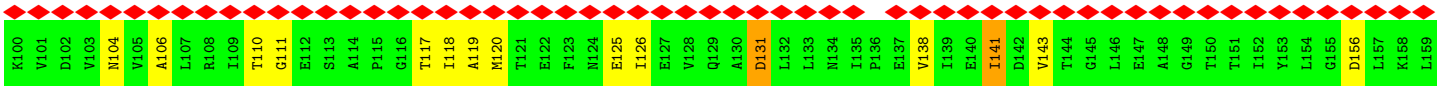


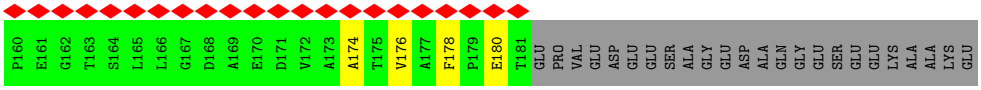


- Molecule 18: 50S ribosomal protein L25

Chain u:

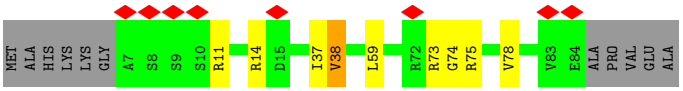






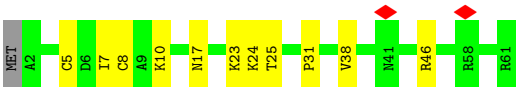
- Molecule 19: 50S ribosomal protein L27

Chain v:



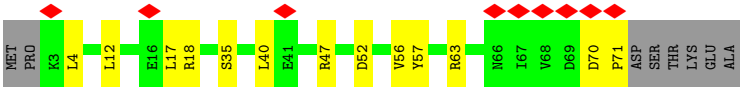
- Molecule 20: 50S ribosomal protein L28

Chain w:



- Molecule 21: 50S ribosomal protein L29

Chain x:

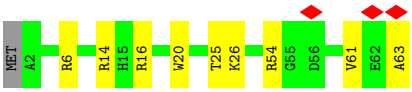


- Molecule 22: 50S ribosomal protein L30

Chain y:

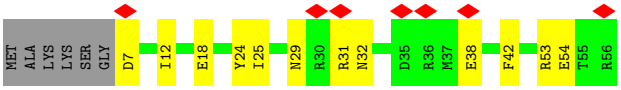
- Molecule 23: 50S ribosomal protein L32

Chain z:



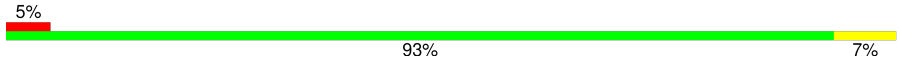
• Molecule 24: 50S ribosomal protein L33

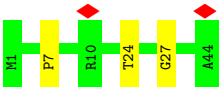
Chain 0:



• Molecule 25: 50S ribosomal protein L34

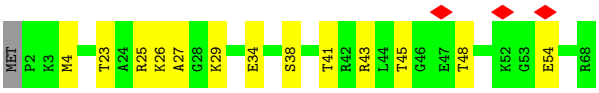
Chain 1:





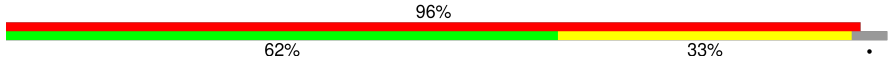
• Molecule 26: Large ribosomal subunit protein bL35

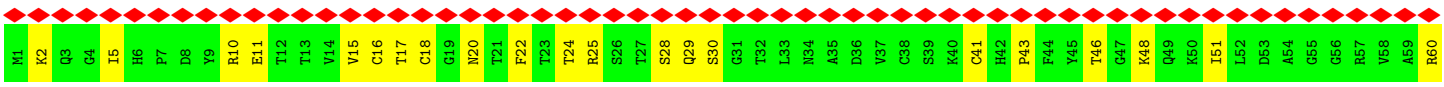
Chain 2:

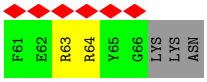


• Molecule 27: 50S ribosomal protein L31

Chain 4:

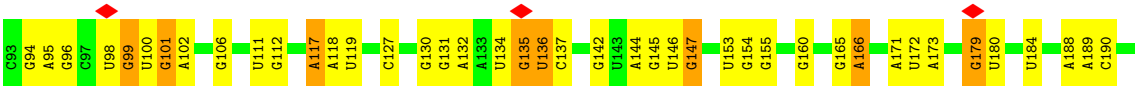


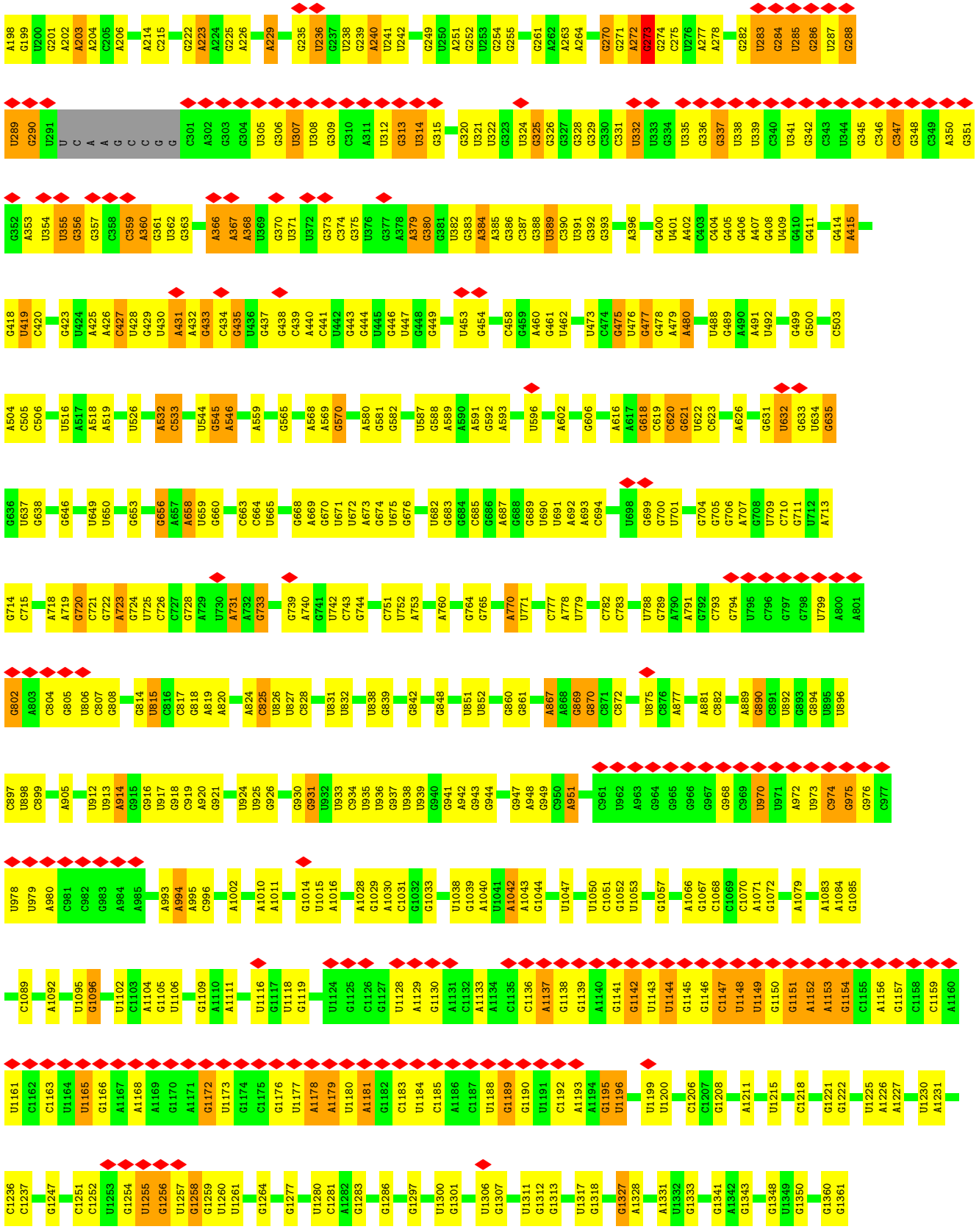




• Molecule 28: 23S rRNA

Chain a:

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U289 G290 U291 U C A A G C C G G C301 A302 G303 G304 U305 G306 U307 U308 G309 C310 A311 U312 G313 U314 G315 G320 U321 U322 G323 U324 G325 G326 G327 G328 G329 C330 C331 U332 U333 G334 U335 G336 G337 U338 U339 C340 U341 G342 C343 U344 G345 C346 C347 G348 C349 A350 G351
G352 A353 U354 U355 G356 G357 C358 C359 A360 G361 U362 G363 A366 A367 A368 U369 G370 U371 U372 G373 C374 G375 U376 G377 A378 A379 G380 G381 U382 G383 A384 A385 G386 C387 G388 U389 C390 U391 G392 G393 A396 G400 U401 A402 C403 C404 G405 G406 A407 G408 U409 G410 G411 G414 A415
G418 U419 C420 G423 U424 A425 A426 C427 U428 G429 U430 A431 A432 G433 C434 G435 U436 G437 G438 C439 A440 C441 U442 G443 G444 U445 G446 U447 G448 G449 U453 G454 C458 G459 A460 G461 U462 U473 C474 G475 U476 G477 G478 A479 A480 U488 G489 A490 A491 U492 G499 G500 C503
A504 C505 C506 U516 A517 A518 A519 U526 A532 C533 U544 G545 A546 A559 G565 A568 A569 G570 A580 G581 G582 U587 G588 A589 A590 A591 G592 A593 U596 A602 G606 A616 A617 G618 C619 C620 G621 U622 C623 A626 G631 U632 G633 U634 G635
G636 U637 G638 G646 U649 U650 G653 G656 A657 A658 U659 G660 C663 C664 U665 G668 A669 G670 U671 U672 A673 G674 U675 G676 U682 G683 G684 C685 G686 A687 G688 G689 U690 U691 A692 A693 C694 U698 G699 G700 U701 G704 G705 G706 A707 G708 U709 C710 G711 U712 A713
G714 C715 A718 A719 G720 C721 G722 A723 G724 U725 C726 C727 G728 A729 U730 A731 A732 G733 G739 A740 G741 U742 C743 G744 C751 U752 A753 A760 G764 G765 A770 U771 C777 A778 U779 C782 C783 U788 G789 A790 A791 G792 C793 G794 U795 C796 G797 G798 U799 A800 A801
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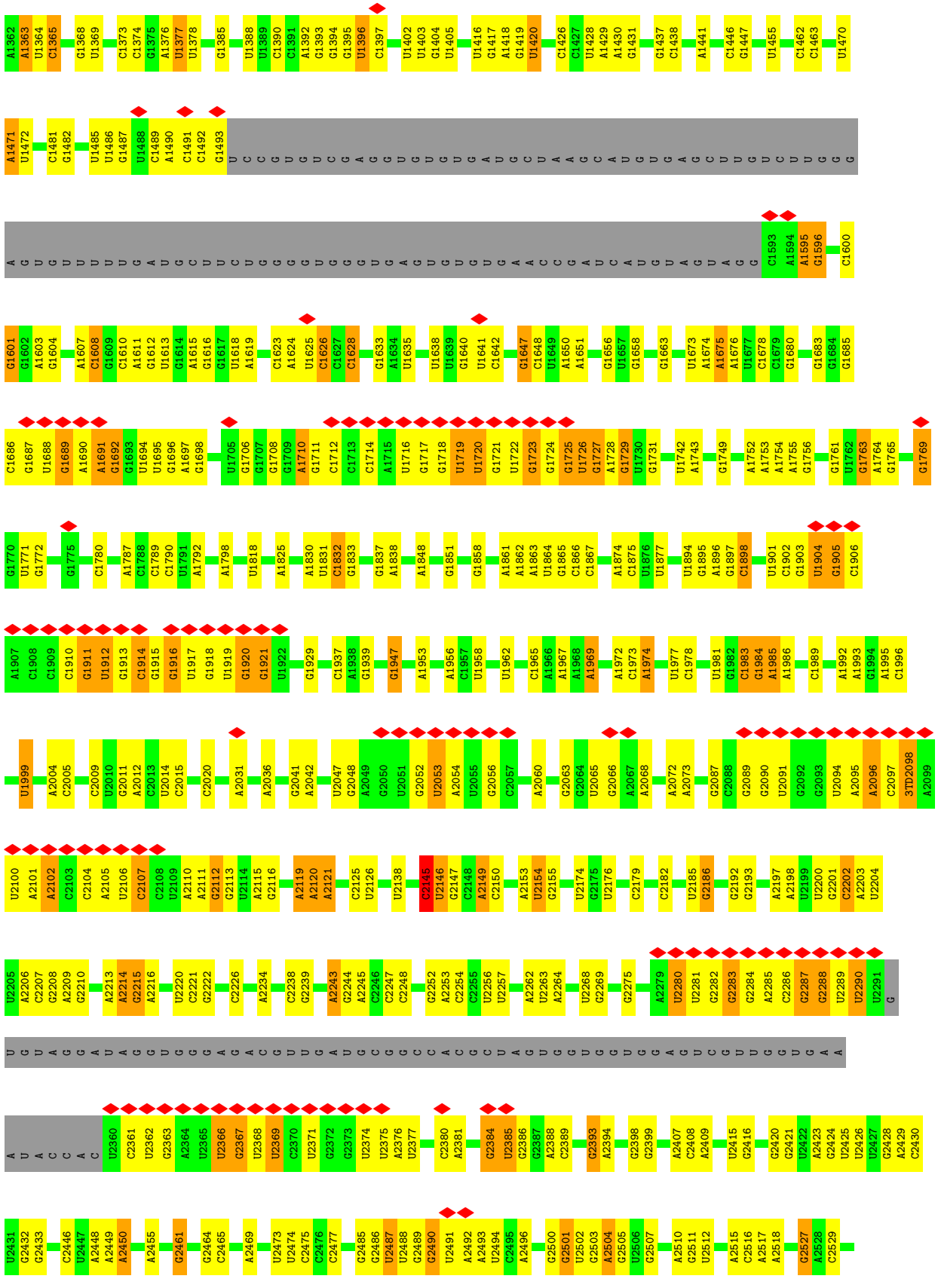
C897 U898 C899 A905 U912 U913 A914 G915 G916 U917 G918 C919 A920 G921 U924 U925 G926 G930 G931 U932 U933 C934 U935 U936 G937 U938 U939 G940 G941 A942 G943 G944 G947 A948 G949 C950 A951 C961 U962 A963 G964 G965 G966 G967 G968 C969 U970 U971 A972 U973 C974 G975 G976 C977
U978 U979 A980 C981 C982 G983 A984 A985 A993 A994 A995 C996 A1002 A1010 A1011 G1014 U1015 A1016 A1028 G1029 A1030 C1031 G1032 G1033 U1038 G1039 A1040 U1041 A1042 A1043 G1044 U1047 U1050 C1051 G1052 U1053 G1057 A1066 G1067 C1068 C1069 C1070 A1071 G1072 A1079 A1083 A1084 G1085
C1089 A1092 U1095 G1096 U1102 C1103 A1104 G1105 U1106 G1109 A1110 A1111 U1116 G1117 U1118 G1119 U1124 G1125 C1126 G1127 U1128 A1129 G1130 A1131 C1132 A1133 A1134 C1135 C1136 A1137 G1138 G1139 A1140 G1141 G1142 U1143 U1144 G1145 G1146 C1147 U1148 U1149 G1150 G1151 A1152 A1153 G1154 C1155 A1156 G1157 C1158 C1159 A1160
U1161 C1162 C1163 U1164 U1165 G1166 A1167 A1168 A1169 G1170 A1171 G1172 U1173 G1174 C1175 G1176 U1177 A1178 A1179 U1180 A1181 G1182 C1183 U1184 C1185 A1186 C1187 U1188 G1189 G1190 U1191 C1192 A1193 A1194 G1195 U1196 U1199 U1200 C1206 C1207 G1208 A1211 U1215 C1218 G1221 G1222 U1225 A1226 A1227 U1230 A1231
C1236 C1237 G1247 C1251 C1252 U1253 G1254 U1255 G1256 U1257 G1258 G1259 U1260 U1261 G1264 G1277 U1280 C1281 A1282 G1283 G1286 G1297 U1300 G1301 U1306 G1307 U1311 G1312 G1313 U1317 G1318 G1327 A1328 A1331 U1332 G1333 G1341 A1342 G1343 G1348 U1349 G1350 G1360 G1361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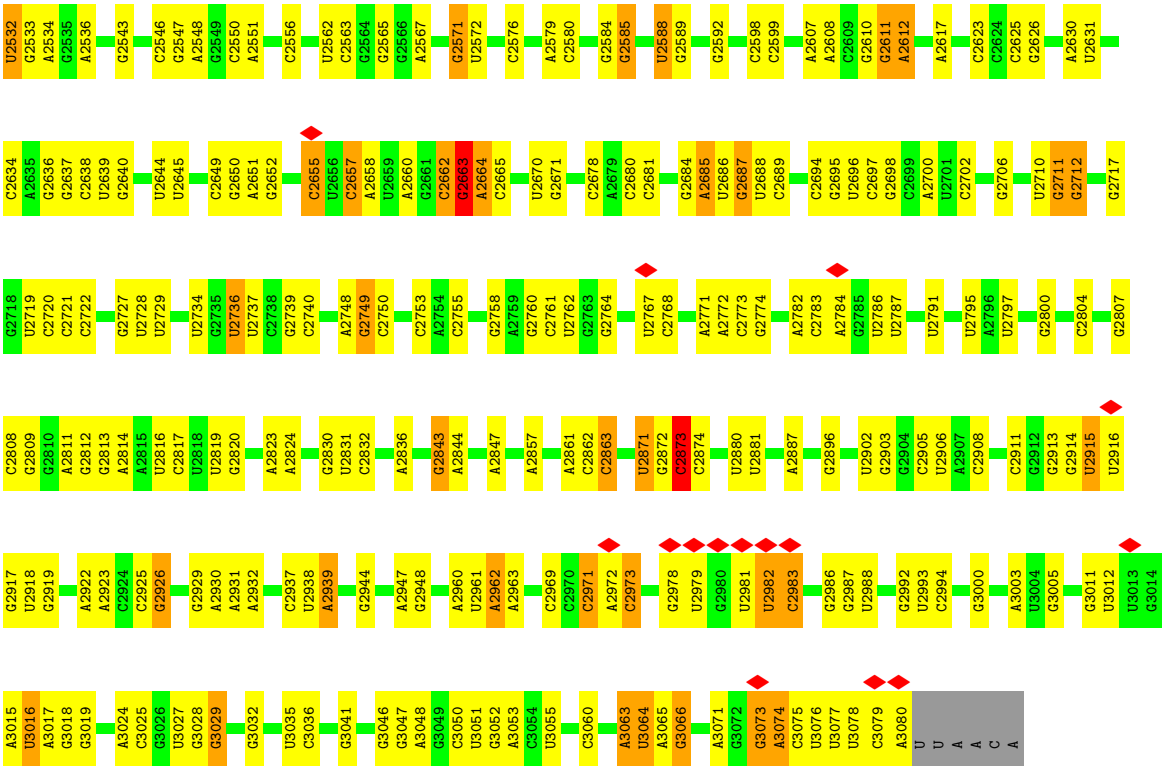
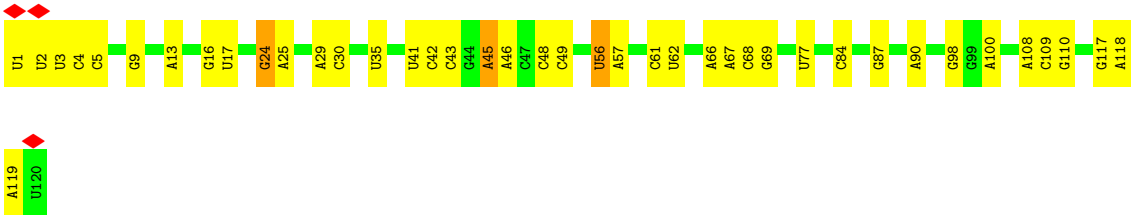
A1471 U1472 C1481 G1482 U1485 U1486 G1487 U1488 C1489 A1490 C1491 C1492 G1493
C1593 A1594 A1595 G1596 C1600
G1601 G1602 A1603 G1604 A1607 C1608 G1609 C1610 A1611 G1612 U1613 G1614 A1615 G1616 G1617 U1618 A1619 C1623 A1624 U1625 C1626 C1627 C1628 G1633 A1634 U1635 U1638 U1639 G1640 U1641 C1642 G1647 C1648 U1649 A1650 A1651 G1656 U1657 G1658 G1663 U1673 A1674 A1675 A1676 U1677 C1678 C1679 G1680 G1683 G1684 G1685
C1686 G1687 U1688 G1689 A1690 A1691 G1692 G1693 U1694 U1695 G1696 A1697 G1698 U1705 G1706 G1707 G1708 G1709 A1710 G1711 C1712 C1713 C1714 A1715 U1716 G1717 G1718 U1719 U1720 G1721 U1722 G1723 G1724 G1725 U1726 G1727 A1728 G1729 U1730 G1731 U1742 A1743 G1749 A1752 A1753 A1754 A1755 G1756 G1761 U1762 G1763 A1764 G1765 G1769
G1770 U1771 G1772 G1775 C1780 A1787 C1788 C1789 C1790 U1791 A1792 A1798 U1818 A1825 A1830 U1831 C1832 G1833 G1837 A1838 A1848 G1851 G1858 A1861 A1862 A1863 U1864 G1865 C1866 C1867 A1874 C1875 U1876 U1877 U1894 G1895 A1896 G1897 C1898 U1901 C1902 G1903 U1904 G1905 C1906
A1907 C1908 C1909 G1910 G1911 U1912 G1913 C1914 G1915 G1916 U1917 G1918 U1919 G1920 G1921 U1922 G1929 C1937 A1938 G1939 G1947 A1953 A1956 C1957 U1958 U1962 C1965 A1966 A1967 A1968 A1969 A1972 C1973 A1974 U1977 C1978 U1981 G1982 C1983 G1984 A1985 A1986 C1989 A1992 A1993 G1994 A1995 C1996
U1999 A2004 C2005 C2009 U2010 G2011 A2012 C2013 U2014 C2015 C2020 A2031 A2036 G2041 A2042 U2047 G2048 A2049 G2050 U2051 G2052 U2053 A2054 U2055 G2056 C2057 A2060 G2063 G2064 U2065 G2066 A2067 A2068 A2072 A2073 G2087 C2088 G2089 G2090 U2091 G2092 G2093 U2094 A2095 A2096 C2097 3TD2098 A2099
U2100 A2101 A2102 C2103 C2104 A2105 U2106 C2107 C2108 U2109 A2110 A2111 G2112 G2113 U2114 A2115 G2116 A2119 A2120 A2121 C2125 U2126 U2138 C2145 U2146 G2147 C2148 A2149 C2150 A2153 U2154 G2155 U2174 G2175 U2176 C2179 C2182 U2185 G2186 G2192 G2193 A2197 A2198 U2199 U2200 G2201 G2202 A2203 U2204
U2205 A2206 C2207 G2208 A2209 G2210 A2213 A2214 G2215 A2216 U2220 C2221 G2222 C2226 A2234 C2238 G2239 A2243 G2244 A2245 C2246 C2247 C2248 G2252 A2253 C2254 C2255 U2256 U2257 A2262 U2263 A2264 U2268 G2269 G2275 A2279 U2280 U2281 G2282 G2283 G2284 A2285 C2286 G2287 G2288 U2289 U2290 U2291 G
U G U A G G A U A G G U G G A G A C G G U U G A U G G C G G A G C U U G U C U U G G G A A
A U A C C A C U2360 C2361 U2362 G2363 A2364 U2365 U2366 G2367 U2368 U2369 C2370 U2371 G2372 G2373 U2374 U2375 A2376 U2377 C2380 A2381 G2384 U2385 G2386 G2387 A2388 C2389 G2393 A2394 G2398 G2399 A2407 C2408 A2409 U2415 G2416 G2420 G2421 U2422 A2423 A2424 U2425 U2426 U2427 G2428 A2429 C2430
U2431 G2432 G2433 C2446 U2447 A2448 A2449 A2450 A2455 G2461 G2464 C2465 A2469 U2473 U2474 C2475 C2476 C2477 G2485 G2486 U2487 U2488 G2489 G2490 U2491 A2492 A2493 U2494 C2495 A2496 G2500 G2501 U2502 G2503 A2504 G2505 U2506 G2507 A2510 G2511 U2512 A2515 C2516 A2517 A2518 G2527 A2528 C2529



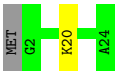
- Molecule 29: 5S rRNA

Chain b:



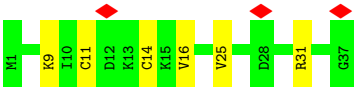
- Molecule 30: 50S ribosomal protein bL37

Chain V:



- Molecule 31: 50S ribosomal protein L36

Chain 3:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	283291	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	38.58	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.109	Depositor
Minimum map value	-0.351	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.051	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	347.19998, 347.19998, 347.19998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.868, 0.868, 0.868	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 5MU, CLY, OMC, PSU, 5MC, OMG, H2U, 3TD, 2MG, 2MA, OMU, ZN

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	c	0.18	0/2132	0.40	0/2871
2	d	0.18	0/1611	0.35	0/2172
3	e	0.20	0/1600	0.44	0/2165
4	f	0.17	0/1493	0.42	0/2001
5	g	0.18	0/1398	0.42	0/1884
6	i	0.18	0/1164	0.32	0/1574
7	j	0.17	0/957	0.36	0/1282
8	k	0.18	0/1090	0.45	0/1465
9	l	0.17	0/1108	0.34	0/1488
10	m	0.18	0/949	0.37	0/1277
11	n	0.13	0/959	0.31	0/1281
12	o	0.15	0/909	0.36	0/1216
13	p	0.18	0/969	0.30	0/1292
14	q	0.18	0/785	0.37	0/1050
15	r	0.26	0/1028	0.39	0/1379
16	s	0.18	0/759	0.40	0/1022
17	t	0.21	0/836	0.41	0/1118
18	u	0.14	0/1396	0.36	0/1896
19	v	0.16	0/598	0.35	0/800
20	w	0.20	0/483	0.38	0/648
21	x	0.14	0/567	0.30	0/759
22	y	0.15	0/471	0.30	0/627
23	z	0.17	0/487	0.32	0/654
24	0	0.15	0/429	0.33	0/569
25	1	0.19	0/365	0.30	0/478
26	2	0.17	0/519	0.34	0/682
27	4	0.14	0/521	0.39	0/700
28	a	0.20	0/69440	0.34	12/108351 (0.0%)
29	b	0.15	0/2871	0.27	0/4475
30	V	0.16	0/184	0.31	0/236
31	3	0.17	0/305	0.36	0/401
All	All	0.20	0/98383	0.34	12/147813 (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
15	r	0	1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	a	274	G	P-O3'-C3'	-8.17	107.94	120.20
28	a	270	G	P-O3'-C3'	-8.11	108.03	120.20
28	a	2664	A	P-O3'-C3'	-7.81	108.49	120.20
28	a	2662	C	P-O3'-C3'	-7.40	109.11	120.20
28	a	2663	G	P-O3'-C3'	-7.38	109.12	120.20
28	a	2686	PSU	P-O3'-C3'	-7.27	109.29	120.20
28	a	273	G	P-O3'-C3'	-7.09	109.56	120.20
28	a	2873	C	P-O3'-C3'	-6.96	109.76	120.20
28	a	621	G	P-O3'-C3'	-6.27	110.79	120.20
28	a	831	U	P-O3'-C3'	-6.21	110.88	120.20
28	a	620	C	P-O3'-C3'	-5.31	112.23	120.20
28	a	618	G	P-O3'-C3'	-5.15	112.47	120.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	r	28	ARG	Sidechain

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	c	2091	0	2150	33	0
2	d	1586	0	1634	29	0
3	e	1577	0	1619	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	f	1468	0	1487	56	0
5	g	1376	0	1421	37	0
6	i	1139	0	1163	14	0
7	j	946	0	1011	22	0
8	k	1072	0	1106	28	0
9	l	1082	0	1117	17	0
10	m	936	0	997	17	0
11	n	952	0	995	19	0
12	o	896	0	928	20	0
13	p	958	0	986	11	0
14	q	778	0	824	7	0
15	r	1017	0	1070	22	0
16	s	751	0	803	11	0
17	t	829	0	880	11	0
18	u	1376	0	1397	22	0
19	v	591	0	581	6	0
20	w	474	0	487	6	0
21	x	564	0	582	9	0
22	y	467	0	504	10	0
23	z	477	0	479	6	0
24	0	423	0	429	7	0
25	1	362	0	388	2	0
26	2	513	0	565	7	0
27	4	512	0	498	15	0
28	a	62406	0	31295	739	0
29	b	2567	0	1297	30	0
30	V	183	0	202	2	0
31	3	302	0	330	7	0
32	a	241	0	0	0	0
32	b	3	0	0	0	0
32	c	1	0	0	0	0
32	d	1	0	0	0	0
32	k	1	0	0	0	0
33	0	1	0	0	0	0
33	4	1	0	0	0	0
33	w	1	0	0	0	0
33	z	1	0	0	0	0
34	a	27	0	32	4	0
35	a	141	0	0	0	0
35	b	4	0	0	0	0
35	c	1	0	0	0	0
35	d	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	e	2	0	0	0	0
35	i	1	0	0	0	0
35	m	1	0	0	0	0
35	o	1	0	0	0	0
35	p	1	0	0	0	0
35	r	2	0	0	0	0
35	z	1	0	0	0	0
All	All	91105	0	59257	1140	0

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

All (1140) 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)
28:a:2042:A:H61	28:a:2066:G:H1	1.12	0.94
28:a:1490:A:H2	28:a:1772:G:H1	1.10	0.94
28:a:2090:G:H1	28:a:2106:U:H3	1.05	0.91
8:k:20:ARG:NH2	28:a:1327:G:N7	2.21	0.89
28:a:1490:A:C2	28:a:1772:G:N1	2.41	0.88
28:a:1142:G:N2	28:a:1163:C:O2	2.07	0.87
28:a:500:G:OP1	28:a:2589:G:OP1	1.92	0.86
28:a:2626:G:O2'	28:a:2626:G:O4'	1.88	0.85
20:w:5:CYS:SG	20:w:7:ILE:O	2.34	0.85
28:a:669:A:H62	28:a:1328:A:H2	1.21	0.84
8:k:36:THR:HG22	8:k:37:LYS:HG2	1.59	0.83
31:3:11:CYS:N	31:3:14:CYS:SG	2.51	0.82
28:a:1492:C:H2'	28:a:1493:G:C8	2.16	0.80
6:i:68:LYS:NZ	28:a:1105:G:O6	2.14	0.80
28:a:2284:G:H1	28:a:2369:U:H3	1.26	0.80
8:k:34:ARG:HD2	28:a:670:G:H1	1.46	0.80
28:a:2706:G:H1	28:a:2721:C:H5	1.31	0.79
28:a:85:U:H3	28:a:95:A:H61	1.29	0.79
3:e:159:VAL:HG22	3:e:160:LEU:HG	1.63	0.79
28:a:3073:G:H4'	28:a:3074:A:H5'	1.64	0.79
21:x:47:ARG:NH2	28:a:73:A:OP1	2.18	0.77
28:a:1281:C:H5	28:a:1318:G:H1	1.32	0.77
28:a:1490:A:H2	28:a:1772:G:N1	1.81	0.77
28:a:1493:G:H1'	28:a:1769:G:H22	1.50	0.76
9:l:1:MET:HE1	9:l:45:ARG:HG2	1.67	0.76
28:a:283:U:O2	28:a:315:G:O6	2.03	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:225:G:H22	28:a:242:U:H4'	1.50	0.76
4:f:144:GLN:HG2	4:f:159:ARG:HG3	1.66	0.75
28:a:2973:C:N3	28:a:2986:G:N1	2.31	0.75
28:a:127:C:C4	28:a:127:C:C2	2.74	0.74
28:a:60:G:H22	28:a:92:G:H1	1.34	0.74
28:a:1628:C:O2'	28:a:1727:G:N3	2.19	0.74
28:a:86:U:H3	28:a:94:G:H1	1.35	0.74
28:a:332:U:H3	28:a:449:G:H1	1.36	0.74
3:e:132:LEU:HB3	3:e:142:GLN:HB2	1.70	0.73
28:a:2510:A:H2'	28:a:2511:G:C8	2.22	0.73
28:a:2282:G:H1	28:a:2371:U:H3	1.35	0.73
29:b:87:G:H21	29:b:90:A:H2	1.37	0.73
2:d:170:ARG:NH1	28:a:3005:G:O6	2.21	0.73
27:4:11:GLU:HA	27:4:25:ARG:HG2	1.71	0.73
28:a:130:G:H22	28:a:154:G:H1	1.37	0.72
28:a:142:G:H22	28:a:147:G:H22	1.36	0.72
28:a:360:A:H2	28:a:444:G:H22	1.35	0.72
28:a:1647:G:H5"	28:a:1648:C:H5'	1.70	0.72
28:a:2973:C:O2	28:a:2986:G:N2	2.14	0.72
27:4:43:PRO:HB3	27:4:48:LYS:HB3	1.72	0.71
4:f:113:LEU:HD11	4:f:184:PHE:HE1	1.55	0.71
28:a:2533:G:O2'	28:a:2548:A:N6	2.23	0.71
31:3:16:VAL:HG22	31:3:25:VAL:HG22	1.73	0.71
28:a:1985:A:H2'	28:a:1986:A:C8	2.26	0.70
29:b:5:C:OP1	29:b:61:C:O2'	2.08	0.70
28:a:660:G:O2'	28:a:1331:A:OP1	2.08	0.70
28:a:1139:G:H22	28:a:1185:C:H5"	1.57	0.70
10:m:35:VAL:HG22	10:m:112:VAL:HG22	1.74	0.70
1:c:183:ARG:NH2	28:a:1983:C:OP2	2.24	0.69
28:a:142:G:H21	28:a:147:G:H1	1.38	0.69
4:f:100:LEU:HD23	4:f:104:ARG:HG2	1.74	0.69
18:u:106:ALA:HB3	18:u:138:VAL:HG12	1.75	0.69
15:r:98:THR:O	15:r:100:ARG:NH1	2.26	0.69
28:a:50:G:O2'	28:a:117:A:N6	2.26	0.69
28:a:941:G:H2'	28:a:942:A:C8	2.28	0.69
5:g:22:GLN:O	5:g:37:VAL:N	2.25	0.69
28:a:1142:G:N1	28:a:1163:C:N3	2.38	0.69
28:a:1650:A:H2'	28:a:1651:A:C8	2.28	0.68
24:0:29:ASN:ND2	24:0:32:ASN:OD1	2.25	0.68
28:a:6:G:H1	28:a:3076:U:H3	1.42	0.68
28:a:285:U:N3	28:a:313:G:N1	2.41	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1:24:THR:HG23	25:1:27:GLY:H	1.58	0.68
28:a:1623:C:H5	28:a:1731:G:H1	1.39	0.68
1:c:16:SER:HB3	1:c:207:GLY:HA3	1.74	0.68
28:a:1656:G:O2'	28:a:1696:G:N1	2.26	0.68
27:4:15:VAL:HG22	27:4:17:THR:H	1.59	0.68
28:a:2720:C:O2'	28:a:2721:C:O2	2.08	0.68
28:a:2009:C:O2'	28:a:2154:U:OP2	2.12	0.67
28:a:565:G:N1	28:a:568:A:OP2	2.24	0.67
4:f:46:ASN:ND2	28:a:2494:U:O2	2.27	0.67
28:a:106:G:H4'	28:a:379:A:H5"	1.76	0.67
28:a:2887:A:O2'	28:a:3032:G:OP1	2.12	0.67
17:t:100:ARG:NE	28:a:101:G:OP2	2.25	0.67
28:a:392:G:H21	28:a:415:A:H62	1.43	0.67
28:a:1974:A:N6	28:a:2011:G:O2'	2.28	0.67
11:n:67:GLU:OE1	11:n:91:ARG:NH2	2.26	0.66
1:c:44:ASN:ND2	28:a:1989:C:O2	2.28	0.66
10:m:37:THR:HA	10:m:110:MET:HA	1.78	0.66
28:a:379:A:O2'	28:a:380:G:O4'	2.12	0.66
28:a:804:C:H2'	28:a:805:G:H8	1.61	0.66
5:g:58:ASP:O	5:g:63:ARG:NH2	2.29	0.66
13:p:89:GLU:OE1	14:q:6:ARG:NH2	2.29	0.66
1:c:270:ARG:NH2	28:a:1981:U:OP2	2.29	0.66
28:a:1138:G:H21	28:a:1168:A:H1'	1.59	0.66
11:n:8:ARG:NH1	29:b:17:U:OP2	2.29	0.65
10:m:36:THR:O	10:m:37:THR:HG22	1.97	0.65
4:f:119:ARG:NH1	4:f:146:MET:O	2.28	0.65
8:k:103:VAL:HG21	8:k:109:VAL:HG13	1.79	0.65
4:f:40:LEU:HD21	4:f:43:ILE:HD11	1.79	0.65
28:a:2090:G:N2	28:a:2106:U:O2	2.22	0.65
15:r:38:ILE:HD12	15:r:91:ALA:HB1	1.79	0.65
16:s:72:ARG:O	16:s:73:THR:OG1	2.13	0.64
17:t:96:ASP:OD1	17:t:110:GLN:NE2	2.29	0.64
28:a:91:A:H2'	28:a:92:G:C8	2.32	0.64
28:a:153:U:H2'	28:a:154:G:C8	2.31	0.64
28:a:2711:G:N7	31:3:31:ARG:NH2	2.46	0.64
28:a:84:G:H22	28:a:96:G:N2	1.94	0.64
28:a:367:A:H61	28:a:444:G:H21	1.43	0.64
3:e:107:LYS:NZ	28:a:690:U:OP2	2.31	0.64
28:a:204:A:N6	28:a:2612:A:O2'	2.30	0.64
28:a:1149:U:H3	28:a:1152:A:H5"	1.62	0.64
28:a:1896:A:N6	28:a:1929:G:O2'	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:y:4:LYS:NZ	22:y:39:GLU:OE1	2.30	0.64
28:a:1083:A:H2'	28:a:1084:A:C8	2.33	0.64
5:g:100:LYS:HB2	5:g:104:GLN:HG2	1.80	0.63
28:a:1726:U:H4'	28:a:1727:G:H5'	1.80	0.63
28:a:285:U:O4	28:a:313:G:O6	2.15	0.63
28:a:1489:C:H2'	28:a:1490:A:C8	2.33	0.63
28:a:2584:G:OP2	28:a:2584:G:N2	2.23	0.63
19:v:75:ARG:NH2	28:a:2515:A:OP1	2.30	0.63
24:0:38:GLU:OE2	24:0:53:ARG:NH1	2.30	0.63
28:a:503:C:H2'	28:a:504:A:H8	1.64	0.63
27:4:60:ARG:HA	27:4:63:ARG:HG2	1.80	0.63
28:a:1906:C:H42	28:a:1920:G:H1'	1.62	0.63
3:e:162:ARG:HA	3:e:165:GLU:HG3	1.80	0.63
28:a:917:U:H2'	28:a:918:G:H8	1.63	0.63
28:a:1092:A:N3	28:a:1237:C:O2'	2.30	0.63
3:e:103:ARG:NH1	28:a:744:G:OP1	2.32	0.62
12:o:2:SER:HA	28:a:3055:U:H4'	1.81	0.62
31:3:11:CYS:SG	31:3:14:CYS:N	2.72	0.62
28:a:2473:U:H2'	28:a:2474:U:C6	2.35	0.62
8:k:114:THR:HB	28:a:723:A:H5"	1.82	0.62
11:n:8:ARG:NH2	29:b:16:G:OP1	2.33	0.62
28:a:1724:G:H3'	28:a:1725:G:C8	2.35	0.62
14:q:56:VAL:HG22	14:q:102:GLY:HA2	1.82	0.62
17:t:101:ARG:NH1	17:t:105:SER:OG	2.32	0.62
4:f:115:LEU:HD12	4:f:148:LEU:HD21	1.80	0.62
28:a:142:G:N2	28:a:147:G:H1	1.98	0.62
28:a:637:U:H2'	28:a:638:G:O4'	1.99	0.62
28:a:1490:A:N1	28:a:1772:G:O6	2.32	0.62
28:a:430:U:O2'	28:a:431:A:N7	2.33	0.61
28:a:500:G:OP2	28:a:2588:U:O2'	2.18	0.61
8:k:94:VAL:HG22	8:k:97:LEU:HG	1.81	0.61
3:e:119:ASP:OD2	8:k:2:ALA:N	2.33	0.61
15:r:25:ARG:NH1	28:a:582:G:OP1	2.32	0.61
28:a:1656:G:HO2'	28:a:1696:G:H1	1.46	0.61
28:a:2104:C:H2'	28:a:2105:A:H8	1.64	0.61
28:a:917:U:H2'	28:a:918:G:C8	2.35	0.61
21:x:17:LEU:HD22	21:x:56:VAL:HG13	1.82	0.61
27:4:18:CYS:CB	27:4:41:CYS:SG	2.88	0.61
28:a:725:U:H2'	28:a:726:C:C6	2.36	0.61
7:j:73:ASP:OD1	7:j:75:SER:OG	2.19	0.61
10:m:69:THR:O	10:m:71:THR:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:503:C:H2'	28:a:504:A:C8	2.35	0.61
12:o:15:ASP:N	12:o:15:ASP:OD1	2.33	0.61
28:a:130:G:N2	28:a:154:G:H22	1.99	0.61
28:a:827:U:H2'	28:a:828:C:C6	2.36	0.61
12:o:37:ARG:HH22	12:o:39:ARG:HG3	1.66	0.60
4:f:138:THR:HG22	4:f:164:THR:HG23	1.83	0.60
25:1:7:PRO:HB2	28:a:1385:G:H4'	1.82	0.60
28:a:249:G:O2'	28:a:261:G:O6	2.19	0.60
10:m:56:LYS:NZ	10:m:90:ARG:O	2.33	0.60
16:s:77:LYS:NZ	16:s:80:ASP:OD1	2.34	0.60
31:3:9:LYS:HB3	31:3:14:CYS:HB2	1.83	0.60
27:4:10:ARG:HH21	27:4:30:SER:H	1.49	0.60
28:a:357:G:N2	28:a:446:G:O6	2.33	0.60
28:a:1716:U:H3	28:a:1722:U:H3	1.49	0.60
28:a:1771:U:H2'	28:a:1772:G:C8	2.35	0.60
12:o:2:SER:OG	12:o:3:ASN:N	2.32	0.60
4:f:21:ILE:HD12	4:f:181:HIS:HB3	1.83	0.60
4:f:144:GLN:HE21	4:f:155:ILE:HD12	1.67	0.60
7:j:108:GLU:HB2	7:j:110:LYS:HE2	1.84	0.60
8:k:6:HIS:HB3	28:a:1280:U:O2	2.02	0.60
28:a:2612:A:H2'	28:a:2612:A:N3	2.17	0.60
28:a:634:U:HO2'	28:a:635:G:H8	1.50	0.60
28:a:1901:U:H2'	28:a:1902:C:C6	2.37	0.60
28:a:672:U:H2'	28:a:673:A:H8	1.67	0.59
28:a:2104:C:H2'	28:a:2105:A:C8	2.37	0.59
14:q:67:LYS:HG2	14:q:91:LYS:HE3	1.84	0.59
28:a:804:C:H2'	28:a:805:G:C8	2.38	0.59
28:a:2685:2MA:H8	34:a:3342:CLY:O8	2.03	0.59
4:f:14:LYS:HE3	4:f:18:ARG:HH21	1.67	0.59
15:r:84:ASP:O	15:r:127:LYS:NZ	2.28	0.59
28:a:2145:5MC:H4'	28:a:2146:U:OP1	2.02	0.59
3:e:157:LEU:HD11	3:e:185:LEU:HG	1.85	0.59
28:a:198:A:H2'	28:a:199:G:C8	2.38	0.59
28:a:2208:G:H2'	28:a:2209:A:C8	2.38	0.59
28:a:899:C:H1'	28:a:1301:G:H21	1.68	0.59
28:a:477:G:O2'	28:a:479:A:OP2	2.20	0.58
28:a:658:A:OP2	28:a:2681:C:O2'	2.21	0.58
28:a:898:U:H2'	28:a:899:C:C6	2.38	0.58
28:a:2290:U:O2'	28:a:2363:G:N2	2.33	0.58
28:a:337:G:H22	28:a:355:U:H2'	1.69	0.58
18:u:131:ASP:OD1	18:u:131:ASP:N	2.31	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:222:ARG:NH2	28:a:1972:A:OP2	2.33	0.58
7:j:35:LEU:HD21	7:j:65:THR:H	1.68	0.58
28:a:359:C:H2'	28:a:360:A:H8	1.68	0.58
12:o:71:GLU:OE2	12:o:101:ARG:NH1	2.35	0.58
23:z:6:ARG:NH1	28:a:2202:C:H41	2.02	0.58
28:a:970:U:H3	28:a:975:G:H1	1.50	0.58
4:f:40:LEU:HD12	4:f:167:THR:HG22	1.86	0.58
8:k:4:GLU:OE1	8:k:6:HIS:NE2	2.37	0.58
28:a:672:U:H2'	28:a:673:A:C8	2.39	0.58
28:a:1719:U:O2'	28:a:1720:U:OP1	2.22	0.58
28:a:306:G:H4'	28:a:307:U:O5'	2.03	0.57
28:a:1600:C:O2'	28:a:2393:G:N1	2.30	0.57
3:e:191:VAL:HG13	8:k:3:ILE:HG13	1.86	0.57
4:f:43:ILE:HG12	4:f:105:MET:HG3	1.85	0.57
28:a:2268:U:H2'	28:a:2269:G:C8	2.39	0.57
28:a:2971:C:H1'	28:a:3071:A:H2	1.69	0.57
19:v:14:ARG:NH2	28:a:2461:G:N7	2.44	0.57
21:x:35:SER:HB2	21:x:40:LEU:HD22	1.85	0.57
28:a:1257:U:C4	28:a:1258:G:H1'	2.40	0.57
2:d:163:LYS:HB3	6:i:80:ARG:HB2	1.86	0.57
7:j:63:VAL:HG11	7:j:102:ILE:HG23	1.87	0.57
28:a:2247:C:H2'	28:a:2248:C:C6	2.40	0.57
12:o:94:ARG:NH1	28:a:1937:C:OP1	2.37	0.57
20:w:10:LYS:HD2	20:w:31:PRO:HB3	1.87	0.57
28:a:1904:U:H5	28:a:1921:G:H21	1.52	0.57
1:c:240:THR:OG1	1:c:241:SER:O	2.20	0.57
28:a:263:A:H2'	28:a:264:A:C8	2.40	0.57
27:4:18:CYS:HB3	27:4:41:CYS:SG	2.45	0.57
28:a:2042:A:N6	28:a:2066:G:H1	1.93	0.57
1:c:29:PRO:HG2	1:c:34:LEU:HD11	1.86	0.57
3:e:140:THR:O	3:e:144:LYS:HG2	2.05	0.57
28:a:1490:A:N1	28:a:1772:G:C6	2.73	0.57
11:n:37:ARG:HG2	11:n:39:VAL:HG22	1.86	0.56
28:a:235:G:H22	28:a:506:C:HO2'	1.53	0.56
28:a:1650:A:H2'	28:a:1651:A:H8	1.69	0.56
29:b:29:A:H2'	29:b:30:C:C6	2.39	0.56
29:b:117:G:H2'	29:b:118:A:C8	2.41	0.56
4:f:124:ARG:HH21	27:4:51:ILE:HG21	1.71	0.56
12:o:21:ARG:NH1	28:a:3029:G:O6	2.36	0.56
18:u:88:ARG:HH21	29:b:77:U:H5"	1.71	0.56
28:a:1727:G:H2'	28:a:1728:A:C8	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:e:134:ASP:N	3:e:134:ASP:OD1	2.36	0.56
28:a:1716:U:O2'	28:a:1721:G:N2	2.38	0.56
29:b:2:U:H2'	29:b:3:U:C6	2.39	0.56
5:g:117:VAL:HG11	5:g:150:ILE:HD11	1.87	0.56
8:k:56:ILE:HG21	26:2:54:GLU:HG3	1.86	0.56
28:a:2423:A:H2'	28:a:2424:G:C8	2.41	0.56
5:g:45:LYS:HB3	5:g:48:GLU:HA	1.87	0.56
7:j:10:VAL:HG12	7:j:12:ASP:H	1.69	0.56
10:m:36:THR:O	10:m:36:THR:OG1	2.20	0.56
28:a:1137:A:N6	28:a:1189:G:O6	2.39	0.56
28:a:1708:G:H22	28:a:1729:G:H1	1.54	0.56
28:a:1095:U:H5'	28:a:1096:G:H5"	1.88	0.56
28:a:1638:U:O2'	28:a:1640:G:N2	2.34	0.56
28:a:2425:U:H2'	28:a:2426:U:C6	2.41	0.56
28:a:283:U:O2	28:a:315:G:C6	2.59	0.56
28:a:1698:G:H22	28:a:1915:G:N2	2.04	0.56
28:a:172:U:H2'	28:a:173:A:H8	1.71	0.55
28:a:1489:C:H2'	28:a:1490:A:H8	1.72	0.55
3:e:137:LYS:HE3	3:e:166:ILE:HD13	1.87	0.55
6:i:108:MET:O	28:a:1089:C:O2'	2.24	0.55
9:l:112:ASP:OD1	9:l:112:ASP:N	2.37	0.55
10:m:106:ASP:OD2	28:a:1833:G:O2'	2.18	0.55
20:w:7:ILE:O	20:w:8:CYS:SG	2.64	0.55
1:c:206:TRP:O	1:c:211:ARG:HD3	2.07	0.55
9:l:60:ARG:HD3	9:l:60:ARG:H	1.71	0.55
17:t:42:ASN:HB3	17:t:68:ALA:HB3	1.88	0.55
28:a:84:G:H1	28:a:96:G:H1	1.54	0.55
7:j:64:ARG:O	7:j:82:ASN:HA	2.06	0.55
28:a:663:C:H2'	28:a:664:C:C6	2.40	0.55
28:a:222:G:H4'	28:a:223:A:H4'	1.88	0.55
28:a:225:G:N2	28:a:242:U:H4'	2.19	0.55
28:a:2651:A:H2'	28:a:2652:G:O4'	2.06	0.55
12:o:16:ASP:OD1	12:o:16:ASP:N	2.35	0.55
28:a:2256:U:H2'	28:a:2257:U:C6	2.41	0.55
3:e:139:SER:N	28:a:406:G:OP2	2.39	0.55
9:l:51:ARG:HG3	9:l:66:ILE:HD11	1.87	0.55
28:a:892:U:O2'	28:a:2243:A:N1	2.37	0.55
28:a:1042:A:H2'	28:a:1043:A:C8	2.41	0.55
28:a:1896:A:H2'	28:a:1897:G:H5'	1.89	0.55
28:a:2880:U:H2'	28:a:2881:U:C6	2.42	0.55
2:d:193:MET:HE1	2:d:209:VAL:HG11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:g:99:SER:OG	5:g:101:GLY:O	2.25	0.55
12:o:91:ALA:HB3	12:o:111:LYS:HB2	1.89	0.55
28:a:130:G:H22	28:a:154:G:H22	1.55	0.55
28:a:134:U:O2'	28:a:135:G:O3'	2.20	0.55
28:a:949:G:H21	28:a:951:A:H62	1.55	0.55
28:a:2710:U:H5'	31:3:31:ARG:HE	1.72	0.55
28:a:2773:C:H2'	28:a:2774:G:C8	2.42	0.55
6:i:36:LEU:HD11	6:i:122:LEU:HB2	1.89	0.55
9:l:72:ARG:HB2	9:l:94:ILE:HG13	1.89	0.55
1:c:24:LEU:HD21	1:c:91:ARG:HD2	1.89	0.55
6:i:147:GLN:HG3	13:p:78:ARG:HG3	1.89	0.55
18:u:104:ASN:HB3	18:u:125:GLU:HB3	1.88	0.55
28:a:63:A:H2'	28:a:64:C:C6	2.41	0.55
28:a:806:U:H2'	28:a:807:C:C6	2.42	0.55
5:g:78:ILE:HA	5:g:81:THR:HG22	1.89	0.54
15:r:89:SER:CB	15:r:125:GLU:HG3	2.38	0.54
23:z:16:ARG:NH2	28:a:1341:G:OP1	2.29	0.54
28:a:1437:G:H2'	28:a:1438:C:C6	2.42	0.54
28:a:2428:G:H2'	28:a:2429:A:C8	2.43	0.54
28:a:2922:A:H2'	28:a:2923:A:C8	2.42	0.54
5:g:139:ASP:OD1	5:g:140:LYS:N	2.39	0.54
28:a:332:U:H3	28:a:449:G:H22	1.55	0.54
28:a:1848:A:H61	28:a:2179:C:H42	1.54	0.54
28:a:2488:U:OP2	28:a:2489:G:O2'	2.19	0.54
28:a:3011:G:N2	28:a:3064:U:OP2	2.39	0.54
2:d:161:VAL:HG21	28:a:2800:G:H21	1.72	0.54
3:e:10:LEU:HG	3:e:16:LYS:HE2	1.89	0.54
24:0:7:ASP:OD1	24:0:7:ASP:N	2.40	0.54
28:a:2655:C:OP1	28:a:2657:C:N4	2.40	0.54
1:c:99:ASP:O	28:a:1680:G:N2	2.37	0.54
28:a:43:A:H2'	28:a:44:G:O4'	2.07	0.54
4:f:86:PHE:HE2	28:a:2492:A:N1	2.05	0.54
5:g:77:VAL:O	5:g:80:VAL:HG22	2.08	0.54
28:a:78:U:H2'	28:a:79:G:C8	2.43	0.54
28:a:499:G:O2'	28:a:2589:G:OP2	2.23	0.54
28:a:1142:G:C8	28:a:1143:U:H2'	2.43	0.54
28:a:1977:U:H2'	28:a:1978:C:H6	1.73	0.54
28:a:2111:A:H2'	28:a:2112:G:O4'	2.08	0.54
3:e:3:GLU:OE1	3:e:3:GLU:N	2.41	0.54
9:l:65:TRP:HB2	9:l:105:GLU:HB2	1.89	0.54
15:r:102:ILE:HG23	15:r:110:ALA:HB1	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:t:42:ASN:O	17:t:68:ALA:N	2.41	0.54
28:a:1984:G:N1	28:a:2384:G:OP1	2.38	0.54
13:p:31:LEU:HD13	28:a:663:C:H4'	1.90	0.54
16:s:68:VAL:HG22	16:s:77:LYS:HG2	1.89	0.54
22:y:18:PRO:O	22:y:22:GLU:HG2	2.07	0.54
28:a:82:G:N2	28:a:102:A:OP2	2.41	0.54
28:a:2651:A:N6	28:a:2663:G:H1'	2.22	0.54
28:a:3016:U:H2'	28:a:3017:A:C8	2.43	0.54
4:f:75:GLN:HB2	29:b:42:C:C6	2.42	0.53
28:a:1481:C:H2'	28:a:1482:G:H8	1.73	0.53
28:a:2415:U:H2'	28:a:2416:G:C8	2.43	0.53
10:m:54:ARG:HH22	28:a:3050:C:H5"	1.73	0.53
28:a:325:G:H2'	28:a:326:G:C8	2.43	0.53
28:a:1153:A:C5	28:a:1180:U:H4'	2.43	0.53
10:m:5:THR:HG21	10:m:17:GLU:OE2	2.08	0.53
28:a:288:G:N2	28:a:308:U:OP2	2.41	0.53
28:a:2773:C:H2'	28:a:2774:G:H8	1.74	0.53
28:a:1711:G:N1	28:a:1725:G:O2'	2.34	0.53
22:y:16:THR:O	22:y:21:ARG:NH1	2.42	0.53
28:a:172:U:H2'	28:a:173:A:C8	2.43	0.53
28:a:235:G:N2	28:a:506:C:O2'	2.31	0.53
28:a:1010:A:H2'	28:a:1011:A:C8	2.44	0.53
7:j:88:LYS:HG2	7:j:94:ARG:HG2	1.91	0.53
15:r:82:ARG:NH2	15:r:84:ASP:OD2	2.42	0.53
28:a:1258:G:H2'	28:a:1259:G:C8	2.42	0.53
2:d:51:TYR:OH	2:d:87:GLU:OE2	2.22	0.53
16:s:64:ARG:NH2	28:a:1416:U:OP2	2.42	0.53
28:a:359:C:H2'	28:a:360:A:C8	2.44	0.53
28:a:1462:C:H2'	28:a:1463:C:C6	2.43	0.53
4:f:78:LYS:HA	4:f:93:PRO:HA	1.90	0.53
28:a:1199:U:H2'	28:a:1200:U:H6	1.74	0.53
5:g:53:VAL:O	5:g:66:HIS:NE2	2.40	0.53
13:p:22:SER:O	13:p:22:SER:OG	2.17	0.53
28:a:949:G:O2'	28:a:951:A:N1	2.36	0.53
28:a:2220:U:H2'	28:a:2221:C:C6	2.44	0.53
1:c:26:ARG:HD3	1:c:83:GLU:OE1	2.09	0.52
4:f:17:TYR:HA	4:f:21:ILE:HG12	1.90	0.52
28:a:84:G:N2	28:a:96:G:H22	2.06	0.52
28:a:1255:U:O2'	28:a:1256:G:OP2	2.26	0.52
28:a:1490:A:H2'	28:a:1491:C:O2	2.09	0.52
28:a:2096:A:H4'	28:a:2097:C:H5"	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:i:80:ARG:HD2	28:a:2824:A:H5"	1.90	0.52
24:0:25:ILE:HG12	26:2:34:GLU:HG3	1.92	0.52
27:4:2:LYS:HE3	27:4:5:ILE:HD13	1.91	0.52
28:a:814:G:O2'	28:a:848:G:H4'	2.09	0.52
28:a:994:A:H2'	28:a:995:A:C8	2.44	0.52
1:c:258:ARG:HH22	1:c:264:SER:HB2	1.73	0.52
5:g:8:PRO:O	5:g:70:ARG:NH2	2.41	0.52
28:a:51:A:H2'	28:a:52:A:C8	2.44	0.52
28:a:2473:U:H2'	28:a:2474:U:H6	1.73	0.52
4:f:59:MET:HE1	4:f:93:PRO:HB2	1.92	0.52
28:a:3:A:H61	28:a:3079:C:H42	1.57	0.52
28:a:83:A:H62	28:a:101:G:H8	1.58	0.52
28:a:350:A:H2'	28:a:351:G:H8	1.75	0.52
28:a:415:A:H2	28:a:1286:G:HO2'	1.55	0.52
28:a:1199:U:H2'	28:a:1200:U:C6	2.45	0.52
28:a:142:G:N2	28:a:147:G:H22	2.06	0.52
28:a:2500:G:H5"	28:a:2501:G:OP2	2.09	0.52
4:f:112:LEU:HD12	4:f:116:ALA:HB3	1.92	0.52
18:u:33:MET:HG2	18:u:94:THR:HG22	1.92	0.52
28:a:1977:U:H2'	28:a:1978:C:C6	2.43	0.52
28:a:2253:A:H2'	28:a:2254:C:C6	2.44	0.52
28:a:2982:U:H3'	28:a:2983:C:C6	2.44	0.52
28:a:2986:G:H2'	28:a:2987:G:C8	2.44	0.52
4:f:140:GLY:HA3	28:a:2487:U:H5"	1.91	0.52
28:a:1866:C:H2'	28:a:1867:C:C6	2.44	0.52
28:a:433:G:H2'	28:a:435:G:O4'	2.10	0.52
28:a:733:G:O2'	28:a:2533:G:H4'	2.10	0.52
28:a:1962:U:OP2	28:a:1967:A:N6	2.33	0.52
7:j:64:ARG:HA	7:j:79:PHE:CD1	2.45	0.52
28:a:2072:A:H2'	28:a:2073:A:C8	2.44	0.52
28:a:2486:G:H22	28:a:2494:U:H3	1.58	0.52
2:d:178:VAL:HG23	2:d:200:PRO:HD3	1.92	0.51
28:a:1148:U:H2'	28:a:1149:U:C6	2.45	0.51
28:a:2871:U:O2	28:a:2871:U:H5'	2.10	0.51
2:d:87:GLU:OE1	28:a:2817:C:O2'	2.19	0.51
5:g:18:LYS:HB2	5:g:25:GLU:HB2	1.93	0.51
7:j:42:THR:HG23	7:j:44:LYS:HD3	1.92	0.51
15:r:13:LEU:O	15:r:90:GLN:NE2	2.42	0.51
28:a:325:G:H2'	28:a:326:G:H8	1.76	0.51
28:a:390:C:H2'	28:a:391:U:C6	2.45	0.51
28:a:2197:A:H2'	28:a:2198:A:C8	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:d:97:THR:HG22	2:d:100:GLN:HB2	1.92	0.51
9:l:54:MET:HG3	9:l:121:ALA:HB2	1.92	0.51
22:y:12:SER:HB2	22:y:32:ILE:HD11	1.92	0.51
28:a:2252:G:H2'	28:a:2253:A:C8	2.45	0.51
29:b:3:U:H2'	29:b:4:C:C6	2.45	0.51
4:f:59:MET:CE	4:f:93:PRO:HB2	2.40	0.51
14:q:49:ASP:OD1	14:q:49:ASP:N	2.34	0.51
28:a:60:G:N2	28:a:92:G:H1	2.07	0.51
28:a:664:C:H2'	28:a:665:U:C6	2.45	0.51
28:a:938:U:H2'	28:a:939:U:C6	2.45	0.51
5:g:57:ASP:OD1	5:g:58:ASP:N	2.42	0.51
28:a:1691:A:HO2'	28:a:1692:G:H8	1.57	0.51
28:a:1995:A:H2'	28:a:1996:C:C6	2.46	0.51
5:g:9:ILE:HD12	5:g:74:ASN:HB2	1.92	0.51
28:a:2287:G:O2'	28:a:2288:G:O5'	2.28	0.51
28:a:2381:A:N1	28:a:2408:C:N4	2.58	0.51
28:a:2929:G:O6	28:a:2937:C:H5"	2.11	0.51
1:c:23:GLU:HG3	1:c:91:ARG:HG3	1.93	0.51
28:a:235:G:H4'	28:a:236:U:C6	2.46	0.51
28:a:491:A:H2'	28:a:492:U:O4'	2.11	0.51
28:a:824:A:H1'	28:a:825:C:H5	1.76	0.51
5:g:158:PRO:HB2	5:g:174:LYS:HG2	1.92	0.51
16:s:28:GLN:OE1	16:s:28:GLN:N	2.44	0.51
27:4:16:CYS:HB3	27:4:20:ASN:HB2	1.93	0.51
28:a:1897:G:O2'	28:a:1898:C:H6	1.94	0.51
3:e:136:ASP:O	3:e:138:PRO:HD3	2.12	0.50
18:u:9:ALA:HB2	18:u:45:LEU:HD23	1.92	0.50
23:z:61:VAL:HG12	23:z:63:ALA:H	1.77	0.50
28:a:480:A:H1'	28:a:500:G:O4'	2.11	0.50
28:a:3046:G:C2	28:a:3048:A:H1'	2.45	0.50
5:g:68:LEU:O	5:g:72:LEU:HB2	2.11	0.50
28:a:899:C:H1'	28:a:1301:G:N2	2.26	0.50
28:a:3077:U:H2'	28:a:3078:U:C6	2.46	0.50
3:e:150:LEU:O	3:e:154:ARG:NH1	2.44	0.50
15:r:112:ARG:HD2	15:r:114:LEU:HD21	1.92	0.50
28:a:84:G:N2	28:a:96:G:N2	2.59	0.50
28:a:1176:G:O2'	28:a:1181:A:N6	2.45	0.50
28:a:1897:G:O2'	28:a:1898:C:O5'	2.28	0.50
4:f:114:THR:HB	4:f:115:LEU:HD22	1.93	0.50
28:a:1363:A:N1	28:a:1832:C:O2'	2.41	0.50
2:d:69:PRO:HG3	28:a:2969:C:H1'	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:d:192:ILE:HG21	12:o:8:ILE:HD11	1.93	0.50
13:p:34:LYS:HE3	28:a:2201:G:O2'	2.11	0.50
28:a:814:G:H5'	28:a:815:U:H5"	1.93	0.50
28:a:924:U:H2'	28:a:925:U:C6	2.47	0.50
28:a:1183:C:H2'	28:a:1184:U:O4'	2.10	0.50
28:a:1647:G:H4'	28:a:1729:G:H21	1.76	0.50
5:g:119:ALA:HB2	5:g:125:PHE:CE2	2.46	0.50
26:2:25:ARG:NH2	28:a:2599:C:OP1	2.43	0.50
28:a:1429:A:H2'	28:a:1430:A:C8	2.46	0.50
8:k:30:LYS:HE3	28:a:649:U:H5"	1.94	0.50
28:a:341:U:H2'	28:a:342:G:H8	1.77	0.50
28:a:580:A:H2'	28:a:581:G:O4'	2.11	0.50
28:a:777:C:H2'	28:a:778:A:C8	2.46	0.50
28:a:1317:U:H2'	28:a:1318:G:C8	2.47	0.50
3:e:69:ARG:NH1	3:e:71:LYS:O	2.44	0.50
9:l:15:PRO:O	9:l:41:TYR:OH	2.30	0.50
28:a:374:C:H2'	28:a:375:G:C8	2.46	0.50
28:a:1368:G:H2'	28:a:1369:U:C6	2.47	0.50
28:a:2048:G:H1'	28:a:2060:A:N6	2.27	0.50
1:c:99:ASP:C	28:a:1680:G:H21	2.20	0.50
4:f:169:ALA:HB1	4:f:174:GLU:HG3	1.93	0.50
12:o:13:MET:HG3	12:o:77:HIS:CE1	2.46	0.50
16:s:73:THR:HG22	28:a:545:G:H5"	1.94	0.50
27:4:43:PRO:HA	27:4:46:THR:HG22	1.94	0.50
28:a:2993:U:H2'	28:a:2994:C:H6	1.76	0.50
2:d:31:THR:HG21	2:d:199:VAL:HG22	1.95	0.49
2:d:44:ARG:O	2:d:52:SER:HA	2.11	0.49
17:t:81:ILE:HG13	17:t:82:ASP:H	1.77	0.49
28:a:993:A:H2'	28:a:996:C:H5	1.77	0.49
28:a:2106:U:H2'	28:a:2107:C:C6	2.47	0.49
28:a:2644:U:H2'	28:a:2645:U:C6	2.46	0.49
7:j:7:ARG:HG3	7:j:20:LEU:HD12	1.94	0.49
28:a:361:G:H1	28:a:443:G:H1	1.58	0.49
28:a:405:G:H4'	28:a:407:A:N7	2.27	0.49
28:a:692:A:H2'	28:a:693:A:C8	2.47	0.49
28:a:725:U:H2'	28:a:726:C:H6	1.75	0.49
28:a:254:G:H4'	28:a:475:G:C5	2.47	0.49
28:a:935:U:H2'	28:a:936:U:C6	2.47	0.49
28:a:2550:C:H2'	28:a:2551:A:H8	1.76	0.49
15:r:62:GLU:O	15:r:66:LYS:HG3	2.13	0.49
28:a:993:A:H2'	28:a:996:C:C5	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:1610:C:H2'	28:a:1611:A:C8	2.48	0.49
4:f:10:MET:HG3	4:f:14:LYS:HD3	1.94	0.49
7:j:107:ARG:HD3	7:j:115:VAL:HG11	1.95	0.49
13:p:6:ARG:NH1	28:a:668:G:N7	2.53	0.49
28:a:135:G:H3'	28:a:135:G:N3	2.27	0.49
28:a:682:U:H2'	28:a:683:G:C8	2.48	0.49
3:e:172:ARG:NH2	28:a:425:A:O2'	2.46	0.49
4:f:41:GLU:OE2	4:f:42:LYS:NZ	2.44	0.49
28:a:130:G:H22	28:a:154:G:N2	2.10	0.49
3:e:142:GLN:O	3:e:146:VAL:HG22	2.12	0.49
5:g:4:ILE:HG22	5:g:70:ARG:HD2	1.93	0.49
28:a:1317:U:H2'	28:a:1318:G:H8	1.77	0.49
1:c:223:GLY:HA2	1:c:226:MET:SD	2.53	0.49
9:l:62:GLY:HA2	18:u:120:MET:HE1	1.94	0.49
17:t:29:VAL:HG13	17:t:36:VAL:HG12	1.94	0.49
18:u:64:GLU:OE1	18:u:70:PRO:HB3	2.13	0.49
28:a:272:A:H2'	28:a:273:G:H1'	1.94	0.49
28:a:1914:C:H2'	28:a:1914:C:O2	2.13	0.49
7:j:60:ALA:HB1	7:j:84:ALA:HB1	1.94	0.49
11:n:2:ALA:N	29:b:9:G:O6	2.46	0.49
13:p:13:LYS:NZ	28:a:1328:A:OP1	2.33	0.49
24:0:24:TYR:OH	24:0:42:PHE:O	2.30	0.49
28:a:2047:U:OP1	28:a:2592:G:O2'	2.21	0.49
28:a:2527:G:N3	28:a:2563:C:H2'	2.28	0.49
29:b:2:U:H2'	29:b:3:U:H6	1.78	0.49
2:d:214:LYS:HD3	28:a:2915:U:N3	2.28	0.49
5:g:42:THR:OG1	5:g:54:GLU:OE1	2.19	0.49
28:a:918:G:H2'	28:a:919:C:C6	2.48	0.49
28:a:974:C:H3'	28:a:975:G:H8	1.78	0.49
28:a:1710:A:N6	28:a:1726:U:O4'	2.45	0.49
28:a:1717:G:N1	28:a:1721:G:O6	2.46	0.49
2:d:184:HIS:HB2	2:d:196:ARG:HG3	1.95	0.48
28:a:189:A:H2'	28:a:190:C:H6	1.78	0.48
28:a:669:A:N1	28:a:894:G:O2'	2.35	0.48
28:a:777:C:H2'	28:a:778:A:H8	1.78	0.48
28:a:2004:A:H2'	28:a:2005:C:C6	2.48	0.48
4:f:55:ASP:OD1	4:f:55:ASP:N	2.44	0.48
5:g:70:ARG:HH12	5:g:74:ASN:HD22	1.61	0.48
5:g:96:ARG:HG2	5:g:108:ASN:HB2	1.95	0.48
16:s:22:SER:O	16:s:26:LEU:HG	2.12	0.48
1:c:2:GLY:N	1:c:20:ASP:OD1	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:f:101:ARG:NH1	29:b:43:C:O2	2.40	0.48
10:m:5:THR:O	10:m:7:GLY:N	2.46	0.48
28:a:277:A:C2	28:a:458:C:H4'	2.47	0.48
28:a:1030:A:H2'	28:a:1031:C:C6	2.47	0.48
28:a:1258:G:H2'	28:a:1259:G:H8	1.77	0.48
28:a:1364:U:H5	28:a:1402:U:O2	1.96	0.48
28:a:1618:U:H2'	28:a:1619:A:H8	1.77	0.48
28:a:1910:C:H2'	28:a:1912:U:C2	2.48	0.48
28:a:1985:A:H2'	28:a:1986:A:H8	1.78	0.48
29:b:66:A:N6	29:b:108:A:H2'	2.28	0.48
4:f:46:ASN:OD1	4:f:47:MET:N	2.46	0.48
13:p:72:GLN:O	13:p:114:LYS:NZ	2.44	0.48
28:a:382:U:H2'	28:a:383:G:O4'	2.14	0.48
28:a:2207:C:H2'	28:a:2208:G:H8	1.78	0.48
29:b:66:A:H61	29:b:109:C:H5'	1.79	0.48
1:c:174:THR:HA	1:c:183:ARG:O	2.13	0.48
6:i:4:TYR:CG	13:p:100:VAL:HG11	2.49	0.48
12:o:29:HIS:CG	12:o:83:LYS:HE3	2.48	0.48
20:w:46:ARG:HD3	28:a:2399:G:OP1	2.14	0.48
28:a:913:U:H2'	28:a:914:A:C8	2.48	0.48
2:d:90:THR:OG1	2:d:92:ASP:OD1	2.30	0.48
20:w:23:LYS:HE2	28:a:2262:A:H1'	1.95	0.48
28:a:2809:G:O2'	28:a:2963:A:N1	2.41	0.48
4:f:65:ASP:OD2	4:f:159:ARG:NH1	2.47	0.48
8:k:99:SER:OG	8:k:105:ASP:HB3	2.13	0.48
28:a:663:C:H2'	28:a:664:C:H6	1.79	0.48
28:a:1753:A:H2'	28:a:1754:A:C8	2.49	0.48
28:a:2739:G:H2'	28:a:2740:C:C6	2.49	0.48
29:b:67:A:H2'	29:b:68:C:C6	2.48	0.48
28:a:1084:A:H2'	28:a:1085:G:O4'	2.13	0.48
28:a:1491:C:H2'	28:a:1492:C:H6	1.78	0.48
28:a:1861:A:H2'	28:a:1862:A:C8	2.48	0.48
28:a:742:U:H2'	28:a:743:C:C6	2.48	0.48
28:a:1612:G:H2'	28:a:1613:U:C6	2.48	0.48
3:e:29:VAL:HG21	3:e:114:ARG:HB3	1.95	0.47
7:j:7:ARG:HA	7:j:19:LEU:O	2.14	0.47
18:u:58:ASN:N	18:u:59:PRO:HD3	2.29	0.47
28:a:373:G:H2'	28:a:373:G:N3	2.29	0.47
28:a:653:G:H2'	28:a:2213:A:N7	2.29	0.47
28:a:1437:G:H2'	28:a:1438:C:H6	1.78	0.47
28:a:2125:C:OP2	28:a:2126:U:O2'	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:2214:A:N3	28:a:2637:G:O2'	2.43	0.47
28:a:63:A:H2'	28:a:64:C:H6	1.79	0.47
28:a:1230:U:H2'	28:a:1231:A:C8	2.49	0.47
29:b:117:G:H2'	29:b:118:A:H8	1.77	0.47
3:e:155:LYS:HZ3	3:e:196:ILE:HG12	1.79	0.47
4:f:21:ILE:HG13	4:f:182:LEU:HD23	1.96	0.47
5:g:142:VAL:O	5:g:145:GLU:HG3	2.15	0.47
19:v:37:ILE:HG21	19:v:78:VAL:HG11	1.94	0.47
28:a:2048:G:H1'	28:a:2060:A:H61	1.78	0.47
28:a:2428:G:H2'	28:a:2429:A:H8	1.78	0.47
18:u:156:ASP:N	18:u:156:ASP:OD1	2.47	0.47
28:a:341:U:H2'	28:a:342:G:C8	2.50	0.47
28:a:347:C:H3'	28:a:348:G:H8	1.78	0.47
28:a:728:G:N2	28:a:731:A:H5"	2.29	0.47
28:a:1916:G:H2'	28:a:1917:U:C6	2.49	0.47
28:a:2634:C:C2	34:a:3342:CLY:H162	2.49	0.47
4:f:187:LYS:HD3	4:f:189:LYS:HB3	1.97	0.47
8:k:121:VAL:O	8:k:141:GLY:HA3	2.15	0.47
15:r:112:ARG:HE	15:r:112:ARG:HB3	1.55	0.47
28:a:1139:G:N1	28:a:1185:C:OP2	2.42	0.47
28:a:1491:C:H2'	28:a:1492:C:C6	2.49	0.47
28:a:2534:A:N6	28:a:2547:G:O2'	2.46	0.47
12:o:52:GLY:HA2	12:o:57:GLU:CD	2.38	0.47
28:a:350:A:H2'	28:a:351:G:C8	2.49	0.47
28:a:400:G:H2'	28:a:401:U:O4'	2.15	0.47
28:a:1118:U:H2'	28:a:1119:G:C8	2.50	0.47
28:a:1481:C:H2'	28:a:1482:G:C8	2.49	0.47
3:e:92:VAL:HG21	28:a:669:A:H5'	1.96	0.47
9:l:62:GLY:H	18:u:118:ILE:HG13	1.80	0.47
10:m:70:ILE:HG22	10:m:72:ASP:H	1.80	0.47
19:v:11:ARG:NH2	28:a:2461:G:OP2	2.46	0.47
28:a:4:A:H2'	28:a:5:A:C8	2.49	0.47
28:a:724:G:H2'	28:a:725:U:C6	2.49	0.47
28:a:2182:C:OP1	28:a:2905:C:O2'	2.28	0.47
28:a:2474:U:H2'	28:a:2475:C:C6	2.49	0.47
28:a:2710:U:H2'	28:a:2712:G:H5"	1.96	0.47
28:a:2973:C:N4	28:a:2986:G:O6	2.37	0.47
28:a:3035:U:H2'	28:a:3036:C:C6	2.49	0.47
29:b:87:G:N2	29:b:90:A:OP2	2.39	0.47
7:j:29:LYS:HB3	28:a:2857:A:H4'	1.97	0.47
8:k:49:PHE:HZ	28:a:203:A:C2	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:o:82:ASP:OD2	12:o:83:LYS:HE2	2.14	0.47
28:a:1147:C:O5'	28:a:1147:C:H6	1.98	0.47
28:a:1958:U:O4	28:a:1972:A:H2	1.98	0.47
28:a:2579:A:H2'	28:a:2580:C:C6	2.49	0.47
28:a:2649:C:H2'	28:a:2650:G:O4'	2.14	0.47
28:a:2816:U:H2'	28:a:2817:C:C6	2.50	0.47
28:a:3079:C:H3'	28:a:3080:A:H8	1.80	0.47
9:l:83:MET:HE1	28:a:1039:G:H1'	1.97	0.47
28:a:1470:U:H2'	28:a:1471:A:O4'	2.15	0.47
28:a:2020:C:O2'	28:a:2110:A:N3	2.41	0.47
29:b:48:C:H2'	29:b:49:C:H6	1.79	0.47
5:g:135:VAL:HG23	5:g:143:VAL:HG13	1.97	0.47
11:n:67:GLU:O	11:n:71:ARG:HG2	2.15	0.47
11:n:99:LYS:HB3	11:n:126:ASP:HB3	1.97	0.47
28:a:285:U:O2	28:a:313:G:N2	2.48	0.47
28:a:881:A:H2'	28:a:882:C:C6	2.50	0.47
28:a:1601:G:H1'	28:a:1763:G:O6	2.15	0.47
28:a:2366:U:H2'	28:a:2367:G:C8	2.50	0.47
28:a:2862:C:O2'	28:a:2863:C:H5'	2.15	0.47
11:n:36:PRO:HB2	11:n:51:VAL:HG12	1.97	0.46
15:r:84:ASP:OD1	15:r:84:ASP:N	2.46	0.46
16:s:5:LYS:HA	21:x:57:TYR:CZ	2.50	0.46
28:a:1361:G:N2	28:a:1404:G:H5"	2.31	0.46
28:a:2200:U:O2'	28:a:2202:C:OP2	2.24	0.46
28:a:2510:A:H2'	28:a:2511:G:H8	1.76	0.46
4:f:109:ALA:O	4:f:113:LEU:HD13	2.15	0.46
22:y:6:LYS:HG3	22:y:37:ILE:HD13	1.96	0.46
28:a:82:G:N2	28:a:101:G:H2'	2.30	0.46
28:a:328:G:C4	28:a:329:G:C8	3.03	0.46
28:a:488:U:H2'	28:a:489:G:O4'	2.14	0.46
28:a:1102:U:OP1	28:a:1118:U:O2'	2.22	0.46
28:a:1595:A:H2'	28:a:1596:G:O4'	2.15	0.46
1:c:57:GLY:HA2	1:c:214:TRP:HA	1.98	0.46
4:f:119:ARG:HD3	4:f:146:MET:O	2.16	0.46
28:a:581:G:H2'	28:a:582:G:O4'	2.15	0.46
28:a:1395:G:O2'	28:a:1396:U:H5'	2.15	0.46
28:a:1917:U:H2'	28:a:1918:G:H8	1.79	0.46
28:a:1969:A:H1'	28:a:2121:A:N6	2.30	0.46
28:a:270:G:O2'	28:a:518:A:N3	2.48	0.46
28:a:948:A:H2'	28:a:949:G:C8	2.50	0.46
4:f:18:ARG:O	4:f:22:ARG:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:l:87:LYS:NZ	28:a:1039:G:OP2	2.49	0.46
28:a:384:A:N3	28:a:404:C:O2'	2.41	0.46
28:a:1139:G:N2	28:a:1185:C:H5"	2.28	0.46
28:a:2384:G:N2	28:a:2398:G:OP1	2.48	0.46
28:a:2432:G:O2'	28:a:2678:C:OP1	2.31	0.46
2:d:37:PRO:HB3	2:d:101:GLU:OE2	2.16	0.46
10:m:36:THR:O	10:m:40:LYS:HB2	2.15	0.46
17:t:71:HIS:ND1	17:t:73:SER:HB3	2.31	0.46
28:a:214:A:H2'	28:a:215:C:O4'	2.16	0.46
28:a:671:U:H2'	28:a:672:U:C6	2.51	0.46
28:a:2749:G:H2'	28:a:2750:C:C6	2.51	0.46
3:e:129:VAL:O	3:e:200:GLN:N	2.49	0.46
5:g:78:ILE:O	5:g:82:GLU:HG2	2.16	0.46
5:g:133:PHE:HE1	5:g:150:ILE:HG21	1.80	0.46
28:a:405:G:H4'	28:a:407:A:C8	2.51	0.46
28:a:764:G:H2'	28:a:765:G:H8	1.81	0.46
28:a:1403:U:H2'	28:a:1404:G:O4'	2.16	0.46
28:a:2915:U:H2'	28:a:2916:U:C6	2.51	0.46
28:a:3027:U:H2'	28:a:3028:G:O4'	2.16	0.46
2:d:214:LYS:O	2:d:216:ALA:N	2.48	0.46
4:f:179:LEU:HB3	4:f:184:PHE:CD2	2.51	0.46
11:n:9:LYS:HG2	11:n:10:SER:H	1.80	0.46
14:q:79:LYS:NZ	28:a:656:G:OP2	2.42	0.46
28:a:76:C:H2'	28:a:77:C:H6	1.81	0.46
28:a:367:A:H2'	28:a:368:A:C8	2.51	0.46
28:a:1050:U:H2'	28:a:1051:C:C6	2.50	0.46
28:a:3016:U:H2'	28:a:3017:A:H8	1.79	0.46
12:o:10:LYS:HD2	12:o:13:MET:HE2	1.98	0.46
28:a:626:A:N6	28:a:638:G:O2'	2.48	0.46
28:a:913:U:H4'	28:a:916:G:N1	2.31	0.46
28:a:1897:G:HO2'	28:a:1898:C:C5'	2.28	0.46
28:a:2694:C:H2'	28:a:2695:G:O4'	2.16	0.46
28:a:3024:A:H2'	28:a:3025:C:O4'	2.16	0.46
1:c:226:MET:HG2	28:a:867:A:C2	2.51	0.46
18:u:141:ILE:HD12	18:u:174:ALA:HB2	1.98	0.46
28:a:948:A:H2'	28:a:949:G:H8	1.80	0.46
28:a:1894:U:H2'	28:a:1895:G:O4'	2.15	0.46
6:i:14:LYS:HE3	6:i:14:LYS:HB2	1.74	0.45
11:n:14:ARG:HD3	29:b:30:C:OP1	2.16	0.45
27:4:28:SER:OG	27:4:29:GLN:N	2.49	0.45
28:a:2830:G:H2'	28:a:2831:U:C6	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:263:A:H2'	28:a:264:A:H8	1.79	0.45
28:a:277:A:OP2	28:a:320:G:N1	2.44	0.45
3:e:48:ARG:NH2	28:a:533:C:OP2	2.49	0.45
28:a:83:A:O2'	28:a:99:G:O6	2.23	0.45
28:a:2546:C:H2'	28:a:2547:G:O4'	2.15	0.45
6:i:65:THR:O	6:i:68:LYS:HG3	2.17	0.45
19:v:73:ARG:HB3	19:v:74:GLY:H	1.61	0.45
28:a:925:U:H2'	28:a:926:G:H8	1.80	0.45
28:a:1104:A:O2'	28:a:1206:C:OP1	2.27	0.45
28:a:1429:A:H2'	28:a:1430:A:H8	1.82	0.45
28:a:1992:A:H2'	28:a:1993:A:C8	2.50	0.45
28:a:2706:G:N1	28:a:2721:C:H5	2.07	0.45
3:e:63:GLY:HA3	3:e:82:ARG:HG2	1.99	0.45
4:f:45:VAL:O	4:f:97:HIS:HA	2.16	0.45
8:k:43:LYS:NZ	28:a:889:A:OP1	2.31	0.45
8:k:43:LYS:HG3	8:k:44:ASN:H	1.82	0.45
11:n:97:ILE:O	11:n:98:THR:OG1	2.30	0.45
15:r:110:ALA:HB2	28:a:1798:A:C2	2.51	0.45
28:a:29:G:H2'	28:a:30:C:C6	2.51	0.45
28:a:373:G:N3	28:a:438:G:N2	2.65	0.45
28:a:622:U:H2'	28:a:623:C:C6	2.52	0.45
28:a:693:A:H2'	28:a:694:C:O4'	2.17	0.45
28:a:1866:C:H2'	28:a:1867:C:H6	1.81	0.45
28:a:2285:A:H2'	28:a:2286:C:O4'	2.17	0.45
28:a:2758:G:O2'	28:a:2761:C:OP2	2.28	0.45
4:f:179:LEU:HB3	4:f:184:PHE:CE2	2.52	0.45
28:a:764:G:H2'	28:a:765:G:C8	2.52	0.45
28:a:2384:G:H4'	28:a:2385:U:OP2	2.17	0.45
3:e:152:GLU:O	3:e:154:ARG:NE	2.47	0.45
4:f:120:ILE:HD11	4:f:146:MET:SD	2.56	0.45
11:n:8:ARG:HG3	11:n:9:LYS:O	2.16	0.45
28:a:155:G:O6	28:a:184:U:H5	2.00	0.45
28:a:1624:A:H2'	28:a:1626:C:C5	2.52	0.45
30:V:20:LYS:HE3	30:V:20:LYS:HB2	1.68	0.45
18:u:180:GLU:OE1	18:u:180:GLU:N	2.36	0.45
28:a:1393:G:H2'	28:a:1394:G:C8	2.52	0.45
28:a:2247:C:H2'	28:a:2248:C:H6	1.80	0.45
28:a:2433:OMG:H1'	28:a:2433:OMG:HM23	1.67	0.45
28:a:2449:A:H5"	28:a:2450:A:H5'	1.97	0.45
28:a:2836:A:N1	28:a:2847:A:H5"	2.31	0.45
4:f:75:GLN:HB2	29:b:42:C:C5	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:m:118:ASP:OD1	10:m:118:ASP:N	2.41	0.45
16:s:4:LEU:HG	16:s:5:LYS:H	1.82	0.45
18:u:77:ASP:HB3	18:u:91:ASP:HB2	1.99	0.45
18:u:79:GLN:O	18:u:88:ARG:N	2.35	0.45
28:a:1002:A:H5"	29:b:98:G:O2'	2.17	0.45
28:a:1675:A:H2'	28:a:1676:A:C8	2.52	0.45
29:b:66:A:O2'	29:b:108:A:N6	2.42	0.45
4:f:151:ASP:OD1	4:f:151:ASP:N	2.48	0.45
7:j:109:LYS:HE3	7:j:109:LYS:HB3	1.69	0.45
22:y:2:MET:HA	22:y:40:ASP:HB3	1.98	0.45
27:4:63:ARG:HG3	27:4:64:ARG:N	2.31	0.45
28:a:1485:U:H2'	28:a:1486:U:C6	2.52	0.45
28:a:1698:G:N2	28:a:1915:G:N2	2.64	0.45
28:a:1896:A:C2'	28:a:1897:G:H5'	2.47	0.45
28:a:2532:U:H2'	28:a:2533:G:O4'	2.16	0.45
28:a:189:A:H2'	28:a:190:C:C6	2.51	0.44
28:a:1722:U:H2'	28:a:1723:G:C8	2.52	0.44
1:c:155:MET:HE3	1:c:155:MET:HB2	1.87	0.44
2:d:186:VAL:HG22	2:d:193:MET:HG3	1.99	0.44
5:g:39:GLU:HG3	5:g:40:PRO:HD3	1.98	0.44
5:g:61:GLU:CD	5:g:61:GLU:H	2.23	0.44
6:i:85:ARG:HD3	28:a:2823:A:OP1	2.17	0.44
18:u:117:THR:HG22	18:u:178:PHE:HA	1.99	0.44
21:x:4:LEU:HD12	21:x:52:ASP:HB3	1.99	0.44
28:a:480:A:O2'	28:a:499:G:OP1	2.20	0.44
28:a:1052:G:H2'	28:a:1053:U:C6	2.52	0.44
28:a:1754:A:H2'	28:a:1755:A:C8	2.52	0.44
28:a:2804:C:O2'	28:a:3005:G:N7	2.49	0.44
28:a:2807:G:H2'	28:a:2808:C:C6	2.52	0.44
3:e:16:LYS:HD2	3:e:17:ALA:H	1.81	0.44
23:z:26:LYS:HA	23:z:26:LYS:HD3	1.62	0.44
28:a:229:A:N6	28:a:239:G:H1'	2.32	0.44
28:a:388:G:H2'	28:a:389:U:C6	2.52	0.44
28:a:426:A:H2'	28:a:427:C:O4'	2.17	0.44
28:a:2014:U:H2'	28:a:2015:C:C6	2.52	0.44
28:a:2098:3TD:H6	28:a:2098:3TD:OP2	2.17	0.44
28:a:2115:A:H2'	28:a:2116:G:O4'	2.16	0.44
1:c:166:VAL:HG21	1:c:182:MET:HE1	1.99	0.44
4:f:86:PHE:CE2	28:a:2492:A:C2	3.05	0.44
28:a:286:G:N7	28:a:313:G:N2	2.65	0.44
28:a:826:U:H2'	28:a:827:U:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:943:G:N3	28:a:2450:A:H2'	2.32	0.44
28:a:2004:A:H2'	28:a:2005:C:H6	1.83	0.44
3:e:154:ARG:HD3	3:e:195:THR:OG1	2.18	0.44
4:f:32:ARG:H	4:f:32:ARG:HD3	1.83	0.44
15:r:1:MET:HB2	28:a:1311:U:OP2	2.17	0.44
16:s:54:VAL:HG13	16:s:92:ASP:HB3	1.99	0.44
18:u:111:GLY:HA3	18:u:143:VAL:H	1.82	0.44
18:u:119:ALA:HB2	18:u:176:VAL:HG12	2.00	0.44
28:a:285:U:C4	28:a:313:G:O6	2.71	0.44
28:a:568:A:N3	28:a:570:G:H5"	2.32	0.44
28:a:2913:G:H2'	28:a:2914:G:C8	2.53	0.44
3:e:4:THR:HG22	3:e:4:THR:O	2.18	0.44
28:a:289:U:OP1	28:a:290:G:N1	2.51	0.44
28:a:418:G:O2'	28:a:419:U:OP1	2.35	0.44
28:a:931:G:N2	28:a:1015:U:O2	2.38	0.44
28:a:1603:A:H2'	28:a:1604:G:C8	2.53	0.44
28:a:2695:G:H2'	28:a:2696:U:C6	2.52	0.44
28:a:2961:U:H5"	28:a:2962:A:H2'	2.00	0.44
28:a:2971:C:H2'	28:a:3073:G:N7	2.33	0.44
7:j:107:ARG:O	7:j:107:ARG:HG3	2.18	0.44
11:n:76:ASP:H	11:n:79:ALA:HB3	1.83	0.44
21:x:12:LEU:O	21:x:63:ARG:NH2	2.45	0.44
22:y:46:GLY:HA3	28:a:937:G:H5'	2.00	0.44
28:a:817:C:H2'	28:a:818:G:O4'	2.16	0.44
28:a:1178:A:H5'	28:a:1179:A:N7	2.33	0.44
28:a:1771:U:H2'	28:a:1772:G:H8	1.79	0.44
28:a:1973:C:H2'	28:a:1974:A:C5	2.52	0.44
28:a:2670:U:H2'	28:a:2671:G:C8	2.53	0.44
28:a:3065:A:H2'	28:a:3066:G:O4'	2.18	0.44
1:c:72:LYS:HE3	1:c:72:LYS:HB3	1.75	0.44
2:d:98:LEU:HD12	2:d:98:LEU:HA	1.84	0.44
12:o:6:ASP:O	12:o:10:LYS:HG2	2.18	0.44
15:r:89:SER:HB3	15:r:125:GLU:HG3	2.00	0.44
17:t:1:MET:SD	17:t:1:MET:N	2.80	0.44
21:x:52:ASP:O	21:x:56:VAL:HG23	2.17	0.44
28:a:201:G:H2'	28:a:202:A:O4'	2.17	0.44
28:a:705:G:OP2	28:a:706:G:N2	2.46	0.44
28:a:1610:C:H2'	28:a:1611:A:H8	1.83	0.44
28:a:1910:C:H4'	28:a:1911:G:C5	2.53	0.44
28:a:2185:U:H2'	28:a:2186:G:C8	2.53	0.44
28:a:2282:G:O2'	28:a:2283:G:H8	2.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:2961:U:H4'	28:a:2962:A:O5'	2.18	0.44
2:d:44:ARG:NH2	28:a:2817:C:O2	2.50	0.44
4:f:127:ASN:OD1	4:f:128:SER:N	2.51	0.44
4:f:189:LYS:HB3	4:f:189:LYS:HE3	1.76	0.44
26:2:29:LYS:HD2	26:2:41:THR:HG23	2.00	0.44
28:a:649:U:H2'	28:a:650:U:O4'	2.18	0.44
28:a:2263:U:H2'	28:a:2264:A:H8	1.83	0.44
28:a:2284:G:H2'	28:a:2285:A:C8	2.53	0.44
28:a:2473:U:O2'	28:a:2556:C:O2	2.36	0.44
28:a:2660:A:H5'	31:3:31:ARG:HD3	1.99	0.44
28:a:2925:C:H2'	28:a:2926:G:O4'	2.17	0.44
1:c:211:ARG:HG2	1:c:214:TRP:CZ2	2.53	0.43
2:d:42:GLN:HB3	2:d:55:GLN:HB3	2.00	0.43
10:m:77:HIS:O	10:m:81:THR:HB	2.17	0.43
28:a:532:A:H8	28:a:1277:G:H21	1.66	0.43
28:a:1040:A:N1	28:a:2640:G:H4'	2.32	0.43
6:i:113:LYS:HD3	28:a:616:A:H5'	1.99	0.43
14:q:89:ARG:HD2	14:q:89:ARG:HA	1.75	0.43
24:0:12:ILE:HB	24:0:54:GLU:HG3	1.99	0.43
28:a:76:C:H2'	28:a:77:C:C6	2.53	0.43
28:a:373:G:N2	28:a:437:G:H22	2.16	0.43
28:a:728:G:O2'	28:a:731:A:N7	2.50	0.43
28:a:1138:G:N2	28:a:1168:A:H1'	2.31	0.43
28:a:2584:G:H1'	28:a:2585:G:N7	2.33	0.43
1:c:62:TYR:CE1	28:a:1999:U:H3'	2.53	0.43
4:f:49:VAL:HG12	4:f:49:VAL:O	2.18	0.43
5:g:76:MET:O	5:g:80:VAL:HG13	2.19	0.43
7:j:29:LYS:HD3	28:a:2729:U:H4'	2.00	0.43
12:o:14:ARG:NH1	12:o:81:ILE:O	2.41	0.43
28:a:18:G:H2'	28:a:19:A:C8	2.53	0.43
28:a:111:U:H2'	28:a:112:G:O4'	2.19	0.43
28:a:1165:U:C4	28:a:1166:G:H1'	2.54	0.43
28:a:2511:G:H2'	28:a:2512:U:C6	2.53	0.43
2:d:157:THR:O	28:a:2753:C:O2'	2.36	0.43
8:k:34:ARG:NH1	28:a:670:G:H22	2.17	0.43
28:a:51:A:H2'	28:a:52:A:H8	1.83	0.43
28:a:226:A:N3	28:a:241:U:O2'	2.37	0.43
28:a:1111:A:N6	28:a:1208:G:H2'	2.33	0.43
28:a:2065:U:H2'	28:a:2066:G:C8	2.54	0.43
28:a:238:U:H2'	28:a:239:G:O4'	2.17	0.43
28:a:1901:U:H2'	28:a:1902:C:H6	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:f:130:GLN:O	28:a:2485:G:O2'	2.36	0.43
10:m:100:ILE:HD12	10:m:100:ILE:HA	1.73	0.43
23:z:14:ARG:HB3	28:a:15:U:H5"	2.00	0.43
28:a:307:U:O2	28:a:307:U:H2'	2.18	0.43
28:a:659:U:H2'	28:a:660:G:C8	2.53	0.43
28:a:760:A:N3	28:a:2625:C:O2'	2.42	0.43
2:d:114:ASP:OD2	2:d:179:GLN:HA	2.19	0.43
3:e:141:LYS:HB3	3:e:141:LYS:NZ	2.33	0.43
28:a:1159:C:N4	28:a:1172:G:OP2	2.51	0.43
28:a:1176:G:H1'	28:a:1181:A:H61	1.84	0.43
28:a:2101:A:O2'	28:a:2102:A:N7	2.47	0.43
28:a:2819:U:H2'	28:a:2820:G:O4'	2.19	0.43
28:a:2938:U:H1'	28:a:2939:A:H5"	2.00	0.43
3:e:139:SER:HA	3:e:142:GLN:OE1	2.19	0.43
5:g:38:ARG:HA	5:g:38:ARG:HD3	1.72	0.43
28:a:602:A:N3	28:a:664:C:O2'	2.44	0.43
28:a:975:G:H2'	28:a:976:G:C8	2.53	0.43
28:a:1070:C:H2'	28:a:1071:A:O4'	2.19	0.43
28:a:1221:G:H2'	28:a:1222:G:O4'	2.19	0.43
28:a:1716:U:O2	28:a:1721:G:N2	2.52	0.43
28:a:2119:A:OP1	28:a:2120:A:H5'	2.19	0.43
28:a:2719:U:O2'	28:a:2720:C:H5'	2.18	0.43
3:e:174:LEU:HD23	3:e:174:LEU:HA	1.83	0.43
8:k:75:GLN:N	8:k:108:LEU:O	2.42	0.43
8:k:109:VAL:HG12	8:k:109:VAL:O	2.19	0.43
17:t:4:LEU:HD11	17:t:31:PRO:HA	2.00	0.43
26:2:4:MET:HG3	28:a:751:C:O2'	2.18	0.43
28:a:419:U:OP2	28:a:420:C:N4	2.51	0.43
28:a:461:G:H1'	28:a:462:U:H5	1.83	0.43
28:a:631:G:H4'	28:a:632:U:H3'	1.99	0.43
28:a:1686:C:H2'	28:a:1687:G:O4'	2.19	0.43
28:a:1848:A:H61	28:a:2179:C:N4	2.17	0.43
28:a:2448:A:H4'	28:a:2449:A:N3	2.34	0.43
28:a:2736:U:C2	28:a:2737:U:C5	3.07	0.43
5:g:95:TYR:HA	5:g:108:ASN:O	2.19	0.43
8:k:23:ARG:HA	28:a:896:U:H2'	2.00	0.43
9:l:54:MET:HE3	9:l:54:MET:HB2	1.85	0.43
26:2:26:LYS:HE2	26:2:43:ARG:O	2.19	0.43
28:a:685:C:O2'	28:a:689:G:OP1	2.35	0.43
28:a:838:U:H2'	28:a:839:G:H8	1.84	0.43
28:a:1047:U:O2'	28:a:2455:A:N3	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:1195:G:O2'	28:a:1196:U:OP1	2.35	0.43
28:a:2376:A:H2'	28:a:2377:U:C6	2.54	0.43
28:a:2918:U:H2'	28:a:2919:G:C8	2.54	0.43
28:a:2931:A:OP2	28:a:2932:A:O2'	2.33	0.43
6:i:36:LEU:O	6:i:51:GLY:HA3	2.19	0.42
15:r:59:ALA:HB2	28:a:2193:G:H5"	1.99	0.42
28:a:64:C:H2'	28:a:65:C:H6	1.83	0.42
28:a:135:G:H2'	28:a:136:U:C6	2.54	0.42
28:a:1789:C:H2'	28:a:1790:C:O4'	2.19	0.42
28:a:1863:A:H2	28:a:1947:G:C8	2.37	0.42
28:a:2263:U:H2'	28:a:2264:A:C8	2.53	0.42
28:a:60:G:O2'	28:a:61:U:H5'	2.19	0.42
28:a:165:G:HO2'	28:a:166:A:P	2.42	0.42
28:a:918:G:H2'	28:a:919:C:H6	1.83	0.42
28:a:2149:A:N3	28:a:2774:G:O2'	2.38	0.42
28:a:2550:C:H2'	28:a:2551:A:C8	2.53	0.42
28:a:3018:G:C4	28:a:3019:G:C8	3.07	0.42
4:f:44:VAL:HG11	28:a:2496:A:H5'	2.01	0.42
8:k:76:VAL:HG11	28:a:722:G:N1	2.35	0.42
8:k:104:ARG:NH2	28:a:711:G:N7	2.64	0.42
15:r:29:MET:HE2	15:r:29:MET:HB3	1.73	0.42
28:a:82:G:H22	28:a:101:G:H2'	1.84	0.42
28:a:356:G:O2'	28:a:357:G:O5'	2.26	0.42
28:a:634:U:O2'	28:a:635:G:H8	2.01	0.42
28:a:1486:U:H2'	28:a:1487:G:C8	2.54	0.42
28:a:2429:A:H2'	28:a:2430:C:H6	1.84	0.42
5:g:33:LEU:HD13	5:g:76:MET:HE3	2.01	0.42
11:n:9:LYS:O	11:n:10:SER:OG	2.29	0.42
28:a:95:A:H2'	28:a:96:G:C8	2.54	0.42
28:a:1377:U:H5	28:a:1825:A:N1	2.17	0.42
28:a:1393:G:H2'	28:a:1394:G:H8	1.84	0.42
28:a:1716:U:H2'	28:a:1717:G:N7	2.34	0.42
28:a:2376:A:H2'	28:a:2377:U:H6	1.84	0.42
28:a:2474:U:H2'	28:a:2475:C:H6	1.85	0.42
28:a:2637:G:H2'	28:a:2638:C:H6	1.84	0.42
7:j:107:ARG:HB2	7:j:115:VAL:HG21	2.02	0.42
8:k:61:PRO:HD3	26:2:27:ALA:HB2	2.01	0.42
27:4:22:PHE:HD2	27:4:24:THR:HB	1.85	0.42
28:a:165:G:O2'	28:a:166:A:O5'	2.35	0.42
28:a:782:C:H2'	28:a:783:C:C6	2.54	0.42
28:a:1603:A:H2'	28:a:1604:G:H8	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:233:HIS:NE2	1:c:246:PRO:HA	2.35	0.42
9:l:74:MET:HE3	9:l:74:MET:HB3	1.98	0.42
22:y:25:ARG:HD2	28:a:1014:G:H1'	2.01	0.42
28:a:718:A:H2'	28:a:719:A:C8	2.54	0.42
28:a:905:A:H4'	28:a:921:G:N2	2.35	0.42
6:i:47:HIS:CD2	6:i:48:ILE:HG12	2.55	0.42
8:k:62:LYS:HE2	28:a:2576:C:H5"	2.01	0.42
11:n:62:SER:O	11:n:91:ARG:NH1	2.47	0.42
13:p:58:ARG:HA	13:p:61:TRP:CE3	2.54	0.42
28:a:145:G:H2'	28:a:146:U:C6	2.55	0.42
28:a:1395:G:H2'	28:a:1396:U:C6	2.54	0.42
28:a:1864:U:H2'	28:a:1865:G:O4'	2.19	0.42
29:b:24:G:O6	29:b:56:U:O2'	2.27	0.42
2:d:214:LYS:HD3	28:a:2915:U:H3	1.84	0.42
18:u:180:GLU:H	18:u:180:GLU:CD	2.23	0.42
22:y:15:ALA:HA	28:a:1052:G:O3'	2.19	0.42
28:a:3079:C:H3'	28:a:3080:A:C8	2.54	0.42
1:c:35:VAL:HG13	1:c:64:ILE:HD11	2.01	0.42
3:e:155:LYS:HE3	3:e:190:VAL:HG22	2.00	0.42
3:e:155:LYS:NZ	3:e:196:ILE:HG12	2.34	0.42
4:f:99:THR:HG21	4:f:101:ARG:NH1	2.35	0.42
9:l:29:PHE:HB3	9:l:65:TRP:CE2	2.55	0.42
28:a:240:A:H2'	28:a:241:U:O4'	2.20	0.42
28:a:284:G:C6	28:a:314:U:C4	3.08	0.42
28:a:546:A:N1	28:a:559:A:H5"	2.34	0.42
28:a:1446:C:H2'	28:a:1447:G:O4'	2.20	0.42
28:a:1973:C:H2'	28:a:1974:A:C8	2.55	0.42
9:l:44:ASN:OD1	9:l:44:ASN:N	2.52	0.42
28:a:272:A:O2'	28:a:273:G:H4'	2.20	0.42
28:a:1033:G:H5'	30:V:20:LYS:HG2	2.01	0.42
28:a:2215:G:OP1	28:a:2636:G:O2'	2.23	0.42
28:a:2374:U:H2'	28:a:2375:U:O4'	2.20	0.42
1:c:36:ALA:HB2	28:a:1753:A:H5'	2.02	0.41
9:l:35:GLN:HB2	9:l:132:ILE:HD13	2.00	0.41
28:a:366:A:H5'	28:a:367:A:OP2	2.20	0.41
28:a:443:G:O5'	28:a:443:G:H8	2.03	0.41
28:a:587:U:H2'	28:a:588:G:O4'	2.19	0.41
28:a:1136:C:N4	28:a:1137:A:H62	2.18	0.41
28:a:1418:A:O2'	28:a:1420:U:OP1	2.38	0.41
28:a:1607:A:H4'	28:a:1608:C:O4'	2.20	0.41
28:a:1688:U:H2'	28:a:1689:G:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:2489:G:H4'	28:a:2490:G:C4	2.55	0.41
28:a:2727:G:H2'	28:a:2728:U:O4'	2.20	0.41
2:d:176:VAL:HG11	28:a:2861:A:H4'	2.01	0.41
3:e:185:LEU:HD23	3:e:185:LEU:HA	1.79	0.41
17:t:117:LYS:C	17:t:119:GLU:H	2.29	0.41
28:a:1105:G:N2	28:a:1106:U:O4	2.40	0.41
28:a:1676:A:H2'	28:a:1678:C:C5	2.55	0.41
28:a:2087:G:O2'	28:a:2111:A:N1	2.47	0.41
28:a:2464:G:H4'	28:a:2571:G:O2'	2.20	0.41
5:g:44:SER:OG	5:g:52:LEU:HB2	2.20	0.41
5:g:152:LYS:HB2	5:g:152:LYS:HE3	1.81	0.41
7:j:69:HIS:CE1	7:j:105:GLU:HG2	2.55	0.41
27:4:60:ARG:O	27:4:64:ARG:HG2	2.20	0.41
28:a:1143:U:H4'	28:a:1144:U:H3'	2.01	0.41
28:a:1260:U:H2'	28:a:1261:U:O4'	2.20	0.41
28:a:1470:U:H4'	28:a:1787:A:H4'	2.03	0.41
28:a:1691:A:O2'	28:a:1692:G:H8	2.04	0.41
28:a:2207:C:H2'	28:a:2208:G:C8	2.54	0.41
28:a:2473:U:OP1	28:a:2562:U:O2'	2.37	0.41
28:a:2571:G:H5"	28:a:2572:U:O4'	2.20	0.41
28:a:2687:G:H4'	34:a:3342:CLY:H11	2.03	0.41
28:a:2771:A:H2'	28:a:2772:A:C8	2.55	0.41
28:a:2982:U:H3'	28:a:2983:C:H6	1.84	0.41
1:c:89:THR:O	1:c:198:ASN:ND2	2.51	0.41
3:e:138:PRO:HG2	3:e:141:LYS:HB2	2.02	0.41
4:f:88:LEU:HD11	4:f:94:ILE:HD13	2.00	0.41
5:g:102:PRO:O	5:g:124:THR:OG1	2.34	0.41
10:m:45:ARG:HB3	10:m:46:PRO:HD3	2.02	0.41
12:o:89:HIS:HB3	12:o:113:ARG:HH21	1.86	0.41
22:y:43:GLU:HG2	22:y:44:PHE:N	2.35	0.41
28:a:144:A:H2'	28:a:145:G:C8	2.55	0.41
28:a:890:G:N2	28:a:914:A:OP1	2.53	0.41
28:a:1151:G:H21	28:a:1178:A:H2'	1.86	0.41
28:a:1192:C:H2'	28:a:1193:A:O4'	2.21	0.41
28:a:1874:A:H2'	28:a:1875:C:O4'	2.21	0.41
28:a:2361:C:H2'	28:a:2362:U:C5	2.55	0.41
28:a:2902:U:C2	28:a:2903:G:C8	3.08	0.41
3:e:13:LYS:HA	3:e:13:LYS:HD2	1.69	0.41
15:r:1:MET:HE3	28:a:1312:G:O6	2.21	0.41
20:w:17:ASN:O	20:w:24:LYS:HA	2.20	0.41
28:a:147:G:H1'	28:a:1780:C:O2'	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:439:C:H2'	28:a:440:A:H8	1.86	0.41
28:a:1364:U:H5"	28:a:1365:C:OP2	2.20	0.41
28:a:1848:A:N6	28:a:2179:C:H42	2.19	0.41
28:a:2052:G:H3'	28:a:2053:U:C5'	2.51	0.41
28:a:2388:A:H2'	28:a:2389:C:C6	2.55	0.41
28:a:2831:U:H2'	28:a:2832:C:C6	2.55	0.41
29:b:45:A:C4	29:b:46:A:C8	3.09	0.41
1:c:171:LYS:O	1:c:171:LYS:HG2	2.20	0.41
4:f:31:TYR:OH	4:f:174:GLU:OE1	2.23	0.41
7:j:111:PHE:HB3	7:j:114:ILE:HD12	2.03	0.41
28:a:1300:U:H2'	28:a:1301:G:C8	2.55	0.41
28:a:1490:A:H2	28:a:1772:G:C2	2.38	0.41
28:a:2918:U:H2'	28:a:2919:G:H8	1.86	0.41
29:b:1:U:H2'	29:b:2:U:C6	2.55	0.41
3:e:173:ASN:HB2	28:a:407:A:OP2	2.20	0.41
11:n:70:LEU:HD23	11:n:70:LEU:O	2.21	0.41
14:q:82:TYR:CE1	28:a:1264:G:H5"	2.56	0.41
19:v:38:VAL:HG13	19:v:59:LEU:HB2	2.02	0.41
28:a:160:G:O6	28:a:179:G:N2	2.54	0.41
28:a:270:G:H1'	28:a:519:A:N3	2.35	0.41
28:a:504:A:H2'	28:a:505:C:C6	2.55	0.41
28:a:799:U:H1'	28:a:802:G:C8	2.55	0.41
28:a:1373:C:H2'	28:a:1374:C:H6	1.86	0.41
28:a:1710:A:H61	28:a:1726:U:C5'	2.33	0.41
28:a:1903:G:H2'	28:a:1904:U:C5	2.55	0.41
28:a:1953:A:H4'	28:a:2121:A:OP1	2.20	0.41
28:a:2047:U:H2'	28:a:2048:G:O4'	2.21	0.41
28:a:2812:G:H2'	28:a:2813:G:C8	2.56	0.41
6:i:17:VAL:HA	6:i:55:VAL:O	2.21	0.41
8:k:76:VAL:HA	8:k:110:LYS:O	2.20	0.41
15:r:82:ARG:HB2	15:r:85:ASP:OD1	2.20	0.41
18:u:56:THR:HG23	18:u:59:PRO:HG3	2.01	0.41
28:a:588:G:N1	28:a:591:A:OP2	2.52	0.41
28:a:664:C:H2'	28:a:665:U:H6	1.85	0.41
28:a:714:G:H2'	28:a:715:C:C6	2.56	0.41
28:a:778:A:H2'	28:a:779:U:C6	2.56	0.41
28:a:793:C:H2'	28:a:794:G:C8	2.56	0.41
28:a:807:C:H2'	28:a:808:G:O4'	2.20	0.41
28:a:933:U:H2'	28:a:934:C:H6	1.86	0.41
28:a:1392:A:H2'	28:a:1393:G:C8	2.56	0.41
28:a:1430:A:H2'	28:a:1431:G:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:1618:U:H2'	28:a:1619:A:C8	2.54	0.41
28:a:2490:G:H2'	28:a:2490:G:N3	2.36	0.41
28:a:2687:G:O5'	34:a:3342:CLY:H3	2.20	0.41
1:c:12:GLY:O	1:c:208:LYS:HB2	2.21	0.41
2:d:127:VAL:HB	2:d:133:PHE:CD2	2.55	0.41
4:f:73:LYS:HA	4:f:74:PRO:HD3	1.80	0.41
4:f:173:GLU:HG2	4:f:174:GLU:N	2.35	0.41
5:g:90:ILE:O	5:g:131:THR:OG1	2.39	0.41
7:j:19:LEU:HB3	7:j:41:CYS:HB3	2.03	0.41
10:m:45:ARG:HG3	10:m:95:THR:OG1	2.21	0.41
15:r:58:GLN:NE2	28:a:2192:G:OP1	2.54	0.41
18:u:29:VAL:HG23	18:u:47:GLY:HA2	2.03	0.41
21:x:70:ASP:HA	21:x:71:PRO:HD2	1.96	0.41
28:a:392:G:N2	28:a:415:A:H62	2.14	0.41
28:a:568:A:H4'	28:a:569:A:OP1	2.21	0.41
28:a:720:G:H2'	28:a:721:C:C6	2.55	0.41
28:a:751:C:H2'	28:a:752:U:C6	2.56	0.41
28:a:919:C:C2	28:a:920:A:C8	3.09	0.41
28:a:994:A:H2	28:a:2446:C:O2	2.04	0.41
28:a:1154:G:H21	28:a:1172:G:N2	2.19	0.41
28:a:1755:A:H2'	28:a:1756:G:H8	1.86	0.41
28:a:1904:U:H2'	28:a:1905:G:O4'	2.21	0.41
28:a:2234:A:OP2	28:a:2234:A:H8	2.03	0.41
28:a:2280:U:H2'	28:a:2281:U:C6	2.55	0.41
28:a:2843:G:H2'	28:a:2844:A:C8	2.55	0.41
2:d:49:ASP:OD1	2:d:49:ASP:N	2.54	0.41
4:f:143:GLU:OE2	4:f:158:ILE:HD12	2.21	0.41
7:j:107:ARG:HH12	12:o:34:GLU:HG3	1.85	0.41
8:k:34:ARG:HH11	28:a:670:G:H1	1.69	0.41
11:n:21:ARG:NH1	28:a:2477:C:OP1	2.54	0.41
11:n:85:GLY:HA2	11:n:88:ILE:HG22	2.03	0.41
28:a:251:A:H2'	28:a:252:G:O4'	2.20	0.41
28:a:1694:U:H2'	28:a:1695:U:O4'	2.20	0.41
29:b:3:U:H2'	29:b:4:C:H6	1.85	0.41
29:b:118:A:H2'	29:b:119:A:C8	2.56	0.41
1:c:266:ARG:HD2	1:c:266:ARG:N	2.36	0.40
3:e:3:GLU:O	3:e:3:GLU:HG2	2.20	0.40
5:g:157:GLU:CG	5:g:159:TYR:H	2.34	0.40
16:s:6:ILE:HD11	21:x:18:ARG:HG2	2.04	0.40
24:0:29:ASN:C	24:0:31:ARG:H	2.28	0.40
28:a:709:U:H2'	28:a:710:C:C6	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:788:U:H2'	28:a:789:G:O4'	2.21	0.40
28:a:1251:C:H2'	28:a:1252:C:C6	2.56	0.40
28:a:2036:A:N3	28:a:2415:U:O2'	2.48	0.40
28:a:2408:C:H2'	28:a:2409:A:O4'	2.20	0.40
28:a:2637:G:H2'	28:a:2638:C:C6	2.56	0.40
28:a:2905:C:H2'	28:a:2906:U:O4'	2.22	0.40
28:a:3012:U:O4	28:a:3063:A:H5"	2.21	0.40
2:d:89:ARG:NH1	28:a:2819:U:H5"	2.36	0.40
5:g:38:ARG:HG3	5:g:40:PRO:CD	2.51	0.40
18:u:104:ASN:HA	18:u:126:ILE:O	2.20	0.40
28:a:235:G:O2'	28:a:236:U:OP2	2.38	0.40
28:a:428:U:H2'	28:a:429:G:C8	2.56	0.40
28:a:1764:A:H2'	28:a:1765:G:O4'	2.21	0.40
3:e:56:THR:O	3:e:60:VAL:HG23	2.21	0.40
11:n:120:ALA:HB1	11:n:125:LEU:HD12	2.02	0.40
15:r:13:LEU:HB3	15:r:123:VAL:HG21	2.04	0.40
28:a:440:A:H2'	28:a:441:C:C6	2.57	0.40
28:a:819:A:C4	28:a:820:A:C8	3.10	0.40
28:a:869:G:H5'	28:a:870:G:OP1	2.20	0.40
28:a:1151:G:H1'	28:a:1179:A:H4'	2.03	0.40
28:a:1615:A:H2'	28:a:1616:G:C8	2.56	0.40
28:a:1916:G:C6	28:a:1917:U:O4	2.75	0.40
28:a:2610:G:H5"	28:a:2611:G:O5'	2.21	0.40
28:a:2697:C:H2'	28:a:2698:G:H8	1.86	0.40
1:c:258:ARG:NH2	1:c:264:SER:HB2	2.35	0.40
8:k:64:GLY:HA3	28:a:2598:C:OP1	2.21	0.40
12:o:100:LEU:HD11	12:o:110:ILE:HD11	2.02	0.40
28:a:947:G:H2'	28:a:948:A:O4'	2.22	0.40
28:a:1146:G:C2	28:a:1147:C:C4	3.10	0.40
28:a:1984:G:H3'	28:a:1985:A:H5'	2.03	0.40
28:a:2873:C:H2'	28:a:2874:C:C6	2.57	0.40
29:b:5:C:OP1	29:b:62:U:H5'	2.21	0.40
1:c:228:PRO:HD3	1:c:235:GLY:CA	2.52	0.40
2:d:23:GLU:H	2:d:23:GLU:HG3	1.58	0.40
4:f:47:MET:HE3	4:f:47:MET:HB3	1.78	0.40
4:f:156:ASP:OD1	4:f:159:ARG:NH1	2.45	0.40
13:p:77:ASN:HA	28:a:1236:C:H4'	2.03	0.40
15:r:69:ALA:HA	15:r:72:MET:HE2	2.03	0.40
23:z:20:TRP:CE2	28:a:1343:G:H2'	2.55	0.40
28:a:285:U:N3	28:a:313:G:C6	2.88	0.40
28:a:691:U:N3	28:a:692:A:N7	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:770:A:C2	28:a:872:C:H1'	2.56	0.40
28:a:851:U:H2'	28:a:852:U:C6	2.56	0.40
28:a:2504:A:H2'	28:a:2505:G:O4'	2.21	0.40
28:a:2782:A:O2'	28:a:2783:C:H5'	2.20	0.40
28:a:2902:U:H4'	28:a:3025:C:O2'	2.21	0.40
28:a:3050:C:H2'	28:a:3051:U:O4'	2.22	0.40
29:b:13:A:N1	29:b:69:G:O2'	2.46	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	c	272/278 (98%)	255 (94%)	17 (6%)	0	100	100
2	d	212/223 (95%)	200 (94%)	12 (6%)	0	100	100
3	e	208/301 (69%)	190 (91%)	18 (9%)	0	100	100
4	f	182/210 (87%)	169 (93%)	13 (7%)	0	100	100
5	g	175/180 (97%)	162 (93%)	13 (7%)	0	100	100
6	i	144/147 (98%)	143 (99%)	1 (1%)	0	100	100
7	j	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
8	k	142/146 (97%)	120 (84%)	22 (16%)	0	100	100
9	l	134/139 (96%)	131 (98%)	3 (2%)	0	100	100
10	m	118/187 (63%)	114 (97%)	4 (3%)	0	100	100
11	n	124/127 (98%)	119 (96%)	5 (4%)	0	100	100
12	o	112/117 (96%)	110 (98%)	2 (2%)	0	100	100
13	p	117/123 (95%)	114 (97%)	3 (3%)	0	100	100
14	q	100/102 (98%)	97 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	r	130/153 (85%)	126 (97%)	4 (3%)	0	100	100
16	s	93/102 (91%)	86 (92%)	7 (8%)	0	100	100
17	t	102/122 (84%)	99 (97%)	3 (3%)	0	100	100
18	u	177/205 (86%)	167 (94%)	10 (6%)	0	100	100
19	v	76/89 (85%)	73 (96%)	3 (4%)	0	100	100
20	w	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
21	x	67/77 (87%)	65 (97%)	2 (3%)	0	100	100
22	y	56/60 (93%)	54 (96%)	2 (4%)	0	100	100
23	z	60/63 (95%)	58 (97%)	2 (3%)	0	100	100
24	0	48/56 (86%)	45 (94%)	3 (6%)	0	100	100
25	1	42/44 (96%)	42 (100%)	0	0	100	100
26	2	65/68 (96%)	63 (97%)	2 (3%)	0	100	100
27	4	64/69 (93%)	61 (95%)	3 (5%)	0	100	100
30	V	21/24 (88%)	21 (100%)	0	0	100	100
31	3	35/37 (95%)	35 (100%)	0	0	100	100
All	All	3254/3632 (90%)	3087 (95%)	167 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	c	216/220 (98%)	213 (99%)	3 (1%)	59	80
2	d	166/172 (96%)	161 (97%)	5 (3%)	36	62
3	e	165/237 (70%)	151 (92%)	14 (8%)	10	20
4	f	154/175 (88%)	151 (98%)	3 (2%)	50	74
5	g	150/152 (99%)	143 (95%)	7 (5%)	23	44
6	i	118/120 (98%)	117 (99%)	1 (1%)	73	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	j	101/101 (100%)	94 (93%)	7 (7%)	14	28
8	k	111/113 (98%)	103 (93%)	8 (7%)	13	26
9	l	108/110 (98%)	102 (94%)	6 (6%)	19	37
10	m	100/142 (70%)	93 (93%)	7 (7%)	14	27
11	n	95/96 (99%)	92 (97%)	3 (3%)	34	60
12	o	97/99 (98%)	93 (96%)	4 (4%)	27	50
13	p	98/99 (99%)	97 (99%)	1 (1%)	68	85
14	q	84/84 (100%)	78 (93%)	6 (7%)	13	27
15	r	105/118 (89%)	99 (94%)	6 (6%)	18	36
16	s	84/89 (94%)	81 (96%)	3 (4%)	31	55
17	t	91/103 (88%)	88 (97%)	3 (3%)	33	58
18	u	149/168 (89%)	142 (95%)	7 (5%)	23	44
19	v	60/67 (90%)	59 (98%)	1 (2%)	53	77
20	w	52/53 (98%)	50 (96%)	2 (4%)	29	53
21	x	61/68 (90%)	61 (100%)	0	100	100
22	y	53/55 (96%)	51 (96%)	2 (4%)	29	53
23	z	51/52 (98%)	49 (96%)	2 (4%)	28	52
24	0	47/51 (92%)	46 (98%)	1 (2%)	47	72
25	1	36/36 (100%)	36 (100%)	0	100	100
26	2	54/55 (98%)	50 (93%)	4 (7%)	13	25
27	4	56/59 (95%)	56 (100%)	0	100	100
30	V	16/17 (94%)	16 (100%)	0	100	100
31	3	35/35 (100%)	35 (100%)	0	100	100
All	All	2713/2946 (92%)	2607 (96%)	106 (4%)	30	52

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

Mol	Chain	Res	Type
1	c	83	GLU
1	c	166	VAL
1	c	240	THR
2	d	20	LEU
2	d	66	VAL
2	d	95	GLU

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Mol	Chain	Res	Type
2	d	97	THR
2	d	187	ASP
3	e	6	THR
3	e	9	VAL
3	e	13	LYS
3	e	26	LEU
3	e	28	ASP
3	e	29	VAL
3	e	30	ASN
3	e	120	MET
3	e	133	VAL
3	e	134	ASP
3	e	154	ARG
3	e	176	GLU
3	e	186	ASN
3	e	197	VAL
4	f	63	ILE
4	f	90	GLU
4	f	171	THR
5	g	32	THR
5	g	53	VAL
5	g	61	GLU
5	g	106	GLU
5	g	127	VAL
5	g	132	LYS
5	g	157	GLU
6	i	80	ARG
7	j	14	THR
7	j	20	LEU
7	j	63	VAL
7	j	73	ASP
7	j	81	GLU
7	j	96	THR
7	j	122	ILE
8	k	3	ILE
8	k	19	THR
8	k	21	VAL
8	k	92	ILE
8	k	103	VAL
8	k	111	VAL
8	k	124	VAL
8	k	143	VAL

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Mol	Chain	Res	Type
9	l	55	THR
9	l	66	ILE
9	l	89	THR
9	l	107	SER
9	l	113	VAL
9	l	118	MET
10	m	34	VAL
10	m	39	THR
10	m	44	VAL
10	m	57	THR
10	m	69	THR
10	m	100	ILE
10	m	114	GLU
11	n	39	VAL
11	n	70	LEU
11	n	73	MET
12	o	5	ILE
12	o	7	GLU
12	o	15	ASP
12	o	25	SER
13	p	88	VAL
14	q	7	SER
14	q	10	ARG
14	q	21	GLU
14	q	36	THR
14	q	59	THR
14	q	66	THR
15	r	5	GLU
15	r	28	ARG
15	r	38	ILE
15	r	41	VAL
15	r	62	GLU
15	r	98	THR
16	s	69	ARG
16	s	88	VAL
16	s	93	ARG
17	t	63	ILE
17	t	73	SER
17	t	110	GLN
18	u	33	MET
18	u	55	ARG
18	u	56	THR

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Mol	Chain	Res	Type
18	u	97	ARG
18	u	110	THR
18	u	131	ASP
18	u	141	ILE
19	v	38	VAL
20	w	25	THR
20	w	38	VAL
22	y	8	THR
22	y	30	LYS
23	z	25	THR
23	z	54	ARG
24	0	18	GLU
26	2	23	THR
26	2	38	SER
26	2	45	THR
26	2	48	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	c	135	ASN
2	d	25	ASN
2	d	84	HIS
3	e	43	GLN
3	e	186	ASN
4	f	92	GLN
4	f	170	GLN
5	g	74	ASN
5	g	136	GLN
6	i	47	HIS
9	l	14	HIS
9	l	123	HIS
11	n	58	ASN
13	p	81	ASN
13	p	120	ASN
14	q	12	HIS
16	s	63	ASN
17	t	47	HIS
18	u	104	ASN
23	z	19	GLN
27	4	20	ASN
31	3	4	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
28	a	2892/3086 (93%)	531 (18%)	0
29	b	117/120 (97%)	10 (8%)	0
All	All	3009/3206 (93%)	541 (17%)	0

All (541) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
28	a	11	G
28	a	12	U
28	a	26	G
28	a	31	C
28	a	33	U
28	a	34	G
28	a	42	G
28	a	44	G
28	a	50	G
28	a	57	G
28	a	59	U
28	a	62	G
28	a	70	A
28	a	73	A
28	a	74	G
28	a	82	G
28	a	91	A
28	a	92	G
28	a	98	U
28	a	99	G
28	a	100	U
28	a	101	G
28	a	117	A
28	a	118	A
28	a	119	U
28	a	131	G
28	a	132	A
28	a	135	G
28	a	136	U
28	a	137	C
28	a	147	G
28	a	166	A
28	a	171	A
28	a	179	G

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Mol	Chain	Res	Type
28	a	180	U
28	a	188	A
28	a	203	A
28	a	206	A
28	a	223	A
28	a	229	A
28	a	236	U
28	a	240	A
28	a	255	G
28	a	271	G
28	a	272	A
28	a	273	G
28	a	275	C
28	a	278	A
28	a	282	G
28	a	283	U
28	a	284	G
28	a	285	U
28	a	286	G
28	a	287	U
28	a	288	G
28	a	289	U
28	a	290	G
28	a	305	U
28	a	307	U
28	a	309	G
28	a	312	U
28	a	313	G
28	a	314	U
28	a	321	U
28	a	322	U
28	a	324	U
28	a	325	G
28	a	331	C
28	a	332	U
28	a	335	U
28	a	336	G
28	a	337	G
28	a	338	U
28	a	339	U
28	a	345	G
28	a	346	C

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Mol	Chain	Res	Type
28	a	347	C
28	a	353	A
28	a	354	U
28	a	355	U
28	a	356	G
28	a	359	C
28	a	360	A
28	a	362	U
28	a	363	G
28	a	366	A
28	a	367	A
28	a	368	A
28	a	370	G
28	a	371	U
28	a	379	A
28	a	380	G
28	a	384	A
28	a	385	A
28	a	386	G
28	a	387	C
28	a	389	U
28	a	393	G
28	a	396	A
28	a	402	A
28	a	408	G
28	a	409	U
28	a	411	G
28	a	414	G
28	a	415	A
28	a	419	U
28	a	423	G
28	a	427	C
28	a	431	A
28	a	432	A
28	a	433	G
28	a	434	C
28	a	435	G
28	a	447	U
28	a	453	U
28	a	454	G
28	a	460	A
28	a	473	U

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Mol	Chain	Res	Type
28	a	475	G
28	a	476	U
28	a	477	G
28	a	478	G
28	a	480	A
28	a	516	U
28	a	526	U
28	a	532	A
28	a	533	C
28	a	544	U
28	a	545	G
28	a	546	A
28	a	570	G
28	a	589	A
28	a	592	G
28	a	593	A
28	a	596	U
28	a	606	G
28	a	618	G
28	a	619	C
28	a	620	C
28	a	621	G
28	a	632	U
28	a	633	G
28	a	635	G
28	a	646	G
28	a	656	G
28	a	658	A
28	a	674	G
28	a	675	U
28	a	676	G
28	a	687	A
28	a	699	G
28	a	700	G
28	a	701	U
28	a	704	G
28	a	707	A
28	a	713	A
28	a	720	G
28	a	723	A
28	a	731	A
28	a	733	G

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Mol	Chain	Res	Type
28	a	739	G
28	a	740	A
28	a	753	A
28	a	770	A
28	a	771	U
28	a	791	A
28	a	802	G
28	a	815	U
28	a	825	C
28	a	832	U
28	a	842	G
28	a	860	G
28	a	861	G
28	a	867	A
28	a	869	G
28	a	870	G
28	a	875	U
28	a	877	A
28	a	890	G
28	a	897	C
28	a	912	U
28	a	914	A
28	a	930	G
28	a	931	G
28	a	944	G
28	a	951	A
28	a	968	G
28	a	970	U
28	a	972	A
28	a	973	U
28	a	974	C
28	a	975	G
28	a	978	U
28	a	979	U
28	a	980	A
28	a	994	A
28	a	1016	A
28	a	1028	A
28	a	1029	G
28	a	1042	A
28	a	1044	G
28	a	1057	G

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Mol	Chain	Res	Type
28	a	1066	A
28	a	1067	G
28	a	1068	C
28	a	1072	G
28	a	1079	A
28	a	1096	G
28	a	1109	G
28	a	1116	U
28	a	1128	U
28	a	1129	A
28	a	1130	G
28	a	1133	A
28	a	1137	A
28	a	1141	G
28	a	1142	G
28	a	1144	U
28	a	1145	G
28	a	1147	C
28	a	1148	U
28	a	1149	U
28	a	1150	G
28	a	1151	G
28	a	1152	A
28	a	1153	A
28	a	1154	G
28	a	1156	A
28	a	1157	G
28	a	1161	U
28	a	1165	U
28	a	1172	G
28	a	1173	U
28	a	1177	U
28	a	1178	A
28	a	1179	A
28	a	1181	A
28	a	1188	U
28	a	1189	G
28	a	1190	G
28	a	1195	G
28	a	1196	U
28	a	1211	A
28	a	1215	U

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Mol	Chain	Res	Type
28	a	1218	C
28	a	1225	U
28	a	1226	A
28	a	1227	A
28	a	1247	G
28	a	1254	G
28	a	1255	U
28	a	1256	G
28	a	1258	G
28	a	1283	G
28	a	1297	G
28	a	1306	U
28	a	1307	G
28	a	1313	G
28	a	1327	G
28	a	1333	G
28	a	1348	G
28	a	1350	G
28	a	1360	G
28	a	1363	A
28	a	1365	C
28	a	1376	A
28	a	1377	U
28	a	1378	U
28	a	1388	U
28	a	1390	C
28	a	1396	U
28	a	1397	C
28	a	1405	U
28	a	1417	G
28	a	1419	G
28	a	1420	U
28	a	1426	C
28	a	1428	U
28	a	1441	A
28	a	1455	U
28	a	1471	A
28	a	1472	U
28	a	1595	A
28	a	1596	G
28	a	1601	G
28	a	1608	C

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Mol	Chain	Res	Type
28	a	1625	U
28	a	1626	C
28	a	1628	C
28	a	1633	G
28	a	1635	U
28	a	1641	U
28	a	1642	C
28	a	1647	G
28	a	1658	G
28	a	1663	G
28	a	1673	U
28	a	1674	A
28	a	1675	A
28	a	1683	G
28	a	1685	G
28	a	1689	G
28	a	1690	A
28	a	1691	A
28	a	1692	G
28	a	1697	A
28	a	1706	G
28	a	1710	A
28	a	1712	C
28	a	1714	C
28	a	1718	G
28	a	1719	U
28	a	1720	U
28	a	1723	G
28	a	1725	G
28	a	1726	U
28	a	1727	G
28	a	1729	G
28	a	1742	U
28	a	1743	A
28	a	1749	G
28	a	1752	A
28	a	1761	G
28	a	1763	G
28	a	1769	G
28	a	1792	A
28	a	1818	U
28	a	1830	A

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Mol	Chain	Res	Type
28	a	1831	U
28	a	1832	C
28	a	1837	G
28	a	1838	A
28	a	1851	G
28	a	1858	G
28	a	1877	U
28	a	1898	C
28	a	1904	U
28	a	1905	G
28	a	1911	G
28	a	1912	U
28	a	1913	G
28	a	1914	C
28	a	1916	G
28	a	1919	U
28	a	1920	G
28	a	1921	G
28	a	1939	G
28	a	1947	G
28	a	1956	A
28	a	1965	C
28	a	1969	A
28	a	1974	A
28	a	1983	C
28	a	1984	G
28	a	1985	A
28	a	1999	U
28	a	2012	A
28	a	2031	A
28	a	2041	G
28	a	2053	U
28	a	2054	A
28	a	2056	G
28	a	2063	G
28	a	2068	A
28	a	2089	G
28	a	2091	U
28	a	2095	A
28	a	2096	A
28	a	2102	A
28	a	2107	C

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Mol	Chain	Res	Type
28	a	2112	G
28	a	2113	G
28	a	2119	A
28	a	2120	A
28	a	2121	A
28	a	2138	U
28	a	2145	5MC
28	a	2146	U
28	a	2147	G
28	a	2149	A
28	a	2150	C
28	a	2153	A
28	a	2154	U
28	a	2155	G
28	a	2174	U
28	a	2176	U
28	a	2186	G
28	a	2202	C
28	a	2203	A
28	a	2204	U
28	a	2206	A
28	a	2210	G
28	a	2214	A
28	a	2215	G
28	a	2216	A
28	a	2222	G
28	a	2226	C
28	a	2238	C
28	a	2239	G
28	a	2243	A
28	a	2244	G
28	a	2245	A
28	a	2275	G
28	a	2280	U
28	a	2283	G
28	a	2287	G
28	a	2288	G
28	a	2289	U
28	a	2290	U
28	a	2366	U
28	a	2367	G
28	a	2368	U

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Mol	Chain	Res	Type
28	a	2369	U
28	a	2380	C
28	a	2384	G
28	a	2385	U
28	a	2386	G
28	a	2393	G
28	a	2394	A
28	a	2407	A
28	a	2420	G
28	a	2421	G
28	a	2450	A
28	a	2461	G
28	a	2465	C
28	a	2469	A
28	a	2487	U
28	a	2490	G
28	a	2491	U
28	a	2493	A
28	a	2501	G
28	a	2502	U
28	a	2503	G
28	a	2504	A
28	a	2507	G
28	a	2516	C
28	a	2517	A
28	a	2518	A
28	a	2527	G
28	a	2529	C
28	a	2532	U
28	a	2536	A
28	a	2543	G
28	a	2565	G
28	a	2567	A
28	a	2571	G
28	a	2585	G
28	a	2588	U
28	a	2607	A
28	a	2608	A
28	a	2611	G
28	a	2612	A
28	a	2617	A
28	a	2623	C

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Mol	Chain	Res	Type
28	a	2630	A
28	a	2655	C
28	a	2657	C
28	a	2658	A
28	a	2662	C
28	a	2663	G
28	a	2664	A
28	a	2665	C
28	a	2680	OMC
28	a	2684	G
28	a	2687	G
28	a	2688	U
28	a	2689	C
28	a	2700	A
28	a	2702	C
28	a	2711	G
28	a	2712	G
28	a	2717	G
28	a	2722	C
28	a	2736	U
28	a	2748	A
28	a	2749	G
28	a	2755	C
28	a	2760	G
28	a	2764	G
28	a	2767	U
28	a	2768	C
28	a	2784	A
28	a	2791	U
28	a	2795	U
28	a	2797	U
28	a	2811	A
28	a	2814	A
28	a	2843	G
28	a	2863	C
28	a	2871	U
28	a	2872	G
28	a	2873	C
28	a	2896	G
28	a	2908	C
28	a	2911	C
28	a	2915	U

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Mol	Chain	Res	Type
28	a	2917	G
28	a	2926	G
28	a	2930	A
28	a	2939	A
28	a	2944	G
28	a	2947	A
28	a	2948	G
28	a	2960	A
28	a	2962	A
28	a	2971	C
28	a	2972	A
28	a	2973	C
28	a	2978	G
28	a	2979	U
28	a	2981	U
28	a	2982	U
28	a	2983	C
28	a	2988	U
28	a	2992	G
28	a	3000	G
28	a	3003	A
28	a	3015	A
28	a	3016	U
28	a	3029	G
28	a	3041	G
28	a	3047	G
28	a	3052	G
28	a	3053	A
28	a	3060	C
28	a	3063	A
28	a	3064	U
28	a	3066	G
28	a	3073	G
28	a	3074	A
28	a	3075	C
29	b	24	G
29	b	25	A
29	b	35	U
29	b	41	U
29	b	45	A
29	b	56	U
29	b	57	A

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Mol	Chain	Res	Type
29	b	84	C
29	b	100	A
29	b	110	G

There are no RNA pucker outliers to report.

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

18 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	2094	28	18,21,22	1.15	1 (5%)	21,30,33	1.89	5 (23%)
28	PSU	a	2786	28	18,21,22	1.06	1 (5%)	21,30,33	1.86	4 (19%)
28	OMC	a	2680	32,28	19,22,23	0.54	0	25,31,34	0.72	0
28	2MA	a	2685	32,28	22,25,26	0.87	1 (4%)	32,37,40	1.17	4 (12%)
28	PSU	a	2762	28	18,21,22	1.12	1 (5%)	21,30,33	1.94	5 (23%)
28	H2U	a	2631	28	18,21,22	0.67	1 (5%)	19,30,33	0.63	0
28	OMG	a	2433	32,28	23,26,27	0.52	0	32,38,41	0.46	0
28	2MG	a	2627	28	23,26,27	0.52	0	33,38,41	0.53	0
28	PSU	a	2639	28	18,21,22	1.06	1 (5%)	21,30,33	2.02	6 (28%)
28	PSU	a	1038	28	18,21,22	1.01	1 (5%)	21,30,33	1.96	3 (14%)
28	PSU	a	2686	28	18,21,22	0.93	1 (5%)	21,30,33	0.71	0
28	OMU	a	2734	28	19,22,23	2.92	7 (36%)	25,31,34	1.84	5 (20%)
28	PSU	a	2100	28	18,21,22	1.13	1 (5%)	21,30,33	1.93	5 (23%)
28	3TD	a	2098	28	19,22,23	4.25	6 (31%)	23,32,35	1.77	4 (17%)
28	PSU	a	2787	28	18,21,22	1.10	1 (5%)	21,30,33	1.89	4 (19%)
28	2MG	a	2018	28	23,26,27	0.48	0	33,38,41	0.52	0
28	5MC	a	2145	28	19,22,23	0.56	0	26,32,35	1.05	2 (7%)
28	5MU	a	2122	28	19,22,23	0.48	0	27,32,35	0.49	0

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	2094	28	-	2/7/25/26	0/2/2/2
28	PSU	a	2786	28	-	1/7/25/26	0/2/2/2
28	OMC	a	2680	32,28	-	1/9/27/28	0/2/2/2
28	2MA	a	2685	32,28	-	3/7/25/26	0/3/3/3
28	PSU	a	2762	28	-	0/7/25/26	0/2/2/2
28	H2U	a	2631	28	-	0/7/38/39	0/2/2/2
28	OMG	a	2433	32,28	-	1/9/27/28	0/3/3/3
28	2MG	a	2627	28	-	2/9/27/28	0/3/3/3
28	PSU	a	2639	28	-	0/7/25/26	0/2/2/2
28	PSU	a	1038	28	-	0/7/25/26	0/2/2/2
28	PSU	a	2686	28	-	1/7/25/26	0/2/2/2
28	OMU	a	2734	28	-	0/9/27/28	0/2/2/2
28	PSU	a	2100	28	-	0/7/25/26	0/2/2/2
28	3TD	a	2098	28	-	2/7/25/26	0/2/2/2
28	PSU	a	2787	28	-	0/7/25/26	0/2/2/2
28	2MG	a	2018	28	-	0/9/27/28	0/3/3/3
28	5MC	a	2145	28	-	0/7/25/26	0/2/2/2
28	5MU	a	2122	28	-	0/7/25/26	0/2/2/2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	2098	3TD	C6-C5	12.97	1.49	1.35
28	a	2098	3TD	C2-N1	9.57	1.49	1.37
28	a	2734	OMU	C2-N1	7.07	1.49	1.38
28	a	2734	OMU	C2-N3	6.54	1.49	1.38
28	a	2098	3TD	C6-N1	6.08	1.46	1.36
28	a	2734	OMU	C6-C5	5.78	1.48	1.35
28	a	2098	3TD	C2-N3	4.84	1.48	1.38
28	a	2094	PSU	C6-C5	3.85	1.39	1.35
28	a	2100	PSU	C6-C5	3.69	1.39	1.35
28	a	2686	PSU	C6-C5	3.52	1.39	1.35
28	a	2787	PSU	C6-C5	3.48	1.39	1.35
28	a	2734	OMU	C4-N3	3.42	1.44	1.38
28	a	2786	PSU	C6-C5	3.40	1.39	1.35
28	a	2762	PSU	C6-C5	3.38	1.39	1.35
28	a	1038	PSU	C6-C5	3.31	1.39	1.35
28	a	2639	PSU	C6-C5	3.25	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	2098	3TD	C4-N3	3.07	1.46	1.40
28	a	2734	OMU	O2-C2	-2.88	1.18	1.23
28	a	2734	OMU	O4-C4	-2.68	1.19	1.24
28	a	2685	2MA	C6-N6	-2.46	1.27	1.34
28	a	2098	3TD	O4-C4	-2.15	1.18	1.23
28	a	2631	H2U	C2-N3	-2.14	1.34	1.38
28	a	2734	OMU	C6-N1	2.07	1.43	1.38

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	a	2734	OMU	C4-N3-C2	-5.64	119.61	126.61
28	a	2098	3TD	N1-C2-N3	5.43	120.08	116.13
28	a	1038	PSU	C4-N3-C2	-5.33	119.03	126.37
28	a	2639	PSU	N1-C2-N3	5.19	120.64	115.17
28	a	2639	PSU	C4-N3-C2	-4.97	119.53	126.37
28	a	1038	PSU	N1-C2-N3	4.91	120.34	115.17
28	a	2787	PSU	N1-C2-N3	4.79	120.22	115.17
28	a	2094	PSU	C4-N3-C2	-4.78	119.78	126.37
28	a	2762	PSU	N1-C2-N3	4.76	120.19	115.17
28	a	2094	PSU	N1-C2-N3	4.74	120.17	115.17
28	a	2786	PSU	N1-C2-N3	4.72	120.15	115.17
28	a	2787	PSU	C4-N3-C2	-4.71	119.89	126.37
28	a	2100	PSU	N1-C2-N3	4.70	120.13	115.17
28	a	2762	PSU	C4-N3-C2	-4.67	119.93	126.37
28	a	2100	PSU	C4-N3-C2	-4.65	119.96	126.37
28	a	2786	PSU	C4-N3-C2	-4.57	120.07	126.37
28	a	2098	3TD	C4-N3-C2	-4.19	120.18	124.61
28	a	2734	OMU	N3-C2-N1	4.07	120.19	114.89
28	a	2734	OMU	C5-C4-N3	3.65	119.91	114.80
28	a	2100	PSU	O2-C2-N1	-3.44	119.25	122.79
28	a	2685	2MA	C5-C4-N3	-3.13	123.88	127.18
28	a	2734	OMU	O4-C4-C5	-2.82	120.31	125.16
28	a	2639	PSU	O2-C2-N1	-2.76	119.94	122.79
28	a	2100	PSU	C6-N1-C2	-2.72	120.17	122.69
28	a	2786	PSU	O2-C2-N1	-2.71	120.00	122.79
28	a	2762	PSU	O2-C2-N1	-2.70	120.01	122.79
28	a	2685	2MA	N3-C2-N1	-2.66	121.07	125.77
28	a	2639	PSU	C6-N1-C2	-2.66	120.23	122.69
28	a	2145	5MC	C1'-N1-C6	-2.62	116.83	121.15
28	a	2762	PSU	C6-N1-C2	-2.62	120.26	122.69
28	a	2685	2MA	CM2-C2-N1	2.61	121.03	117.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	a	2787	PSU	C6-N1-C2	-2.61	120.27	122.69
28	a	2786	PSU	C6-N1-C2	-2.56	120.31	122.69
28	a	2787	PSU	O2-C2-N1	-2.49	120.22	122.79
28	a	2094	PSU	O2-C2-N1	-2.45	120.27	122.79
28	a	2762	PSU	O4'-C1'-C2'	2.43	108.51	105.15
28	a	2094	PSU	C6-N1-C2	-2.36	120.50	122.69
28	a	2145	5MC	C1'-N1-C2	2.31	123.55	118.44
28	a	2685	2MA	C2-N1-C6	2.20	121.48	118.10
28	a	2098	3TD	C1'-C5-C4	2.17	120.90	117.61
28	a	1038	PSU	O2-C2-N1	-2.17	120.55	122.79
28	a	2639	PSU	C6-C5-C4	2.11	119.60	118.17
28	a	2100	PSU	O4'-C1'-C2'	2.10	108.06	105.15
28	a	2094	PSU	C6-C5-C4	2.06	119.56	118.17
28	a	2639	PSU	O4'-C1'-C2'	2.05	107.98	105.15
28	a	2098	3TD	C6-C5-C4	2.03	119.55	118.19
28	a	2734	OMU	O2-C2-N1	-2.01	120.18	122.80

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	a	2433	OMG	C1'-C2'-O2'-CM2
28	a	2098	3TD	C3'-C4'-C5'-O5'
28	a	2627	2MG	C3'-C4'-C5'-O5'
28	a	2685	2MA	O4'-C4'-C5'-O5'
28	a	2685	2MA	C3'-C4'-C5'-O5'
28	a	2098	3TD	O4'-C4'-C5'-O5'
28	a	2094	PSU	O4'-C4'-C5'-O5'
28	a	2627	2MG	O4'-C4'-C5'-O5'
28	a	2686	PSU	O4'-C4'-C5'-O5'
28	a	2786	PSU	O4'-C4'-C5'-O5'
28	a	2685	2MA	C4'-C5'-O5'-P
28	a	2094	PSU	C3'-C4'-C5'-O5'
28	a	2680	OMC	C4'-C5'-O5'-P

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	a	2685	2MA	1	0
28	a	2433	OMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	a	2098	3TD	1	0
28	a	2145	5MC	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 252 ligands modelled in this entry, 251 are monoatomic - leaving 1 for Mogul analysis.

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	$\#\|Z\| > 2$
34	CLY	a	3342	-	26,28,28	0.30	0	31,40,40	0.68	1 (3%)

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
34	CLY	a	3342	-	-	2/21/53/53	0/2/2/2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	a	3342	CLY	C14-N2-C11	2.04	107.86	104.81

There are no chirality outliers.

All (2) torsion outliers are listed below:

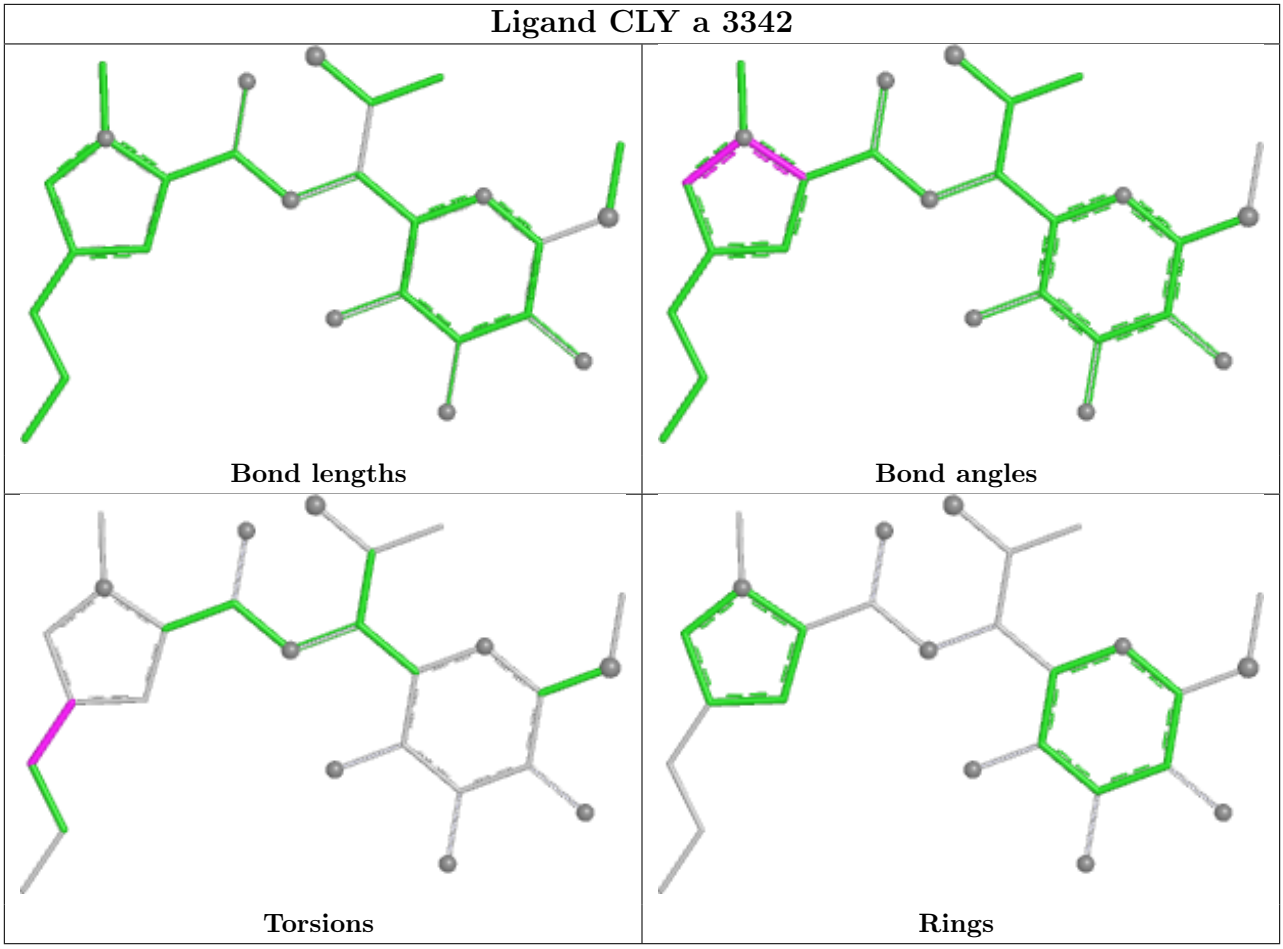
Mol	Chain	Res	Type	Atoms
34	a	3342	CLY	C14-C13-C16-C17
34	a	3342	CLY	C12-C13-C16-C17

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	a	3342	CLY	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

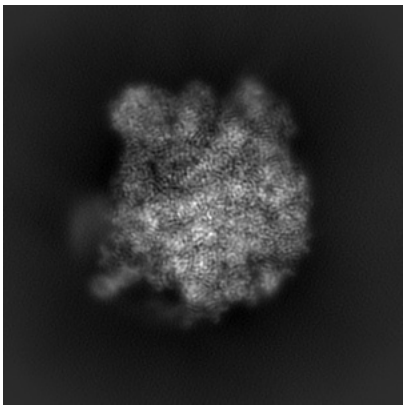
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-45185. These allow visual inspection of the internal detail of the map and identification of artifacts.

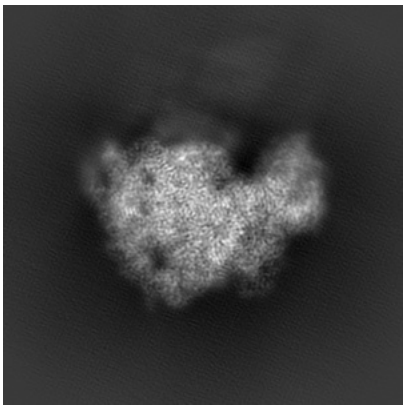
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

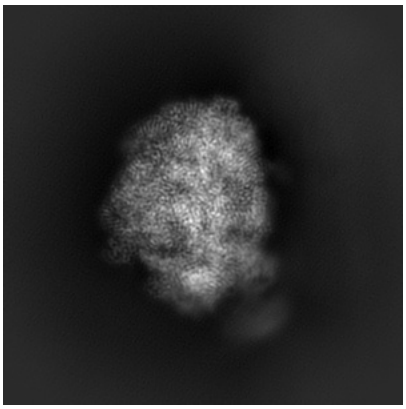
6.1.1 Primary map



X

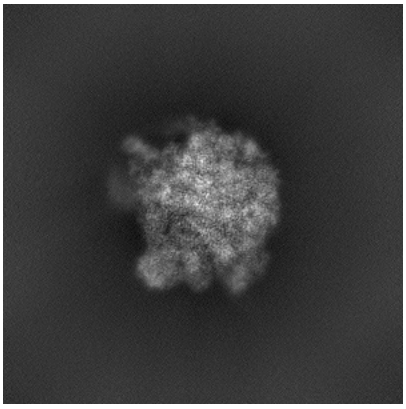


Y

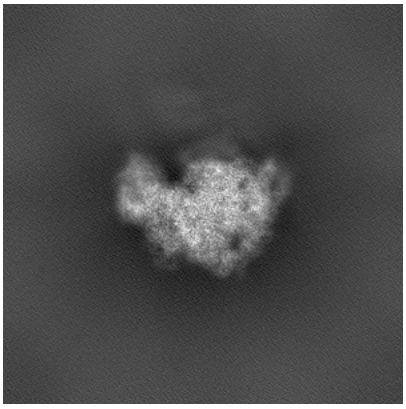


Z

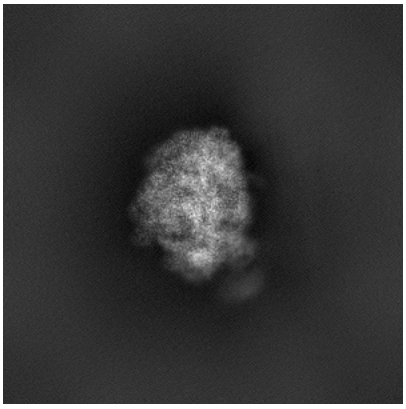
6.1.2 Raw map



X



Y

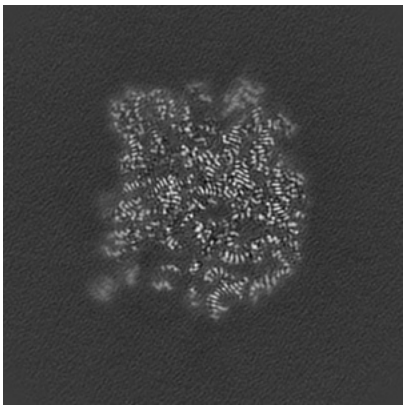


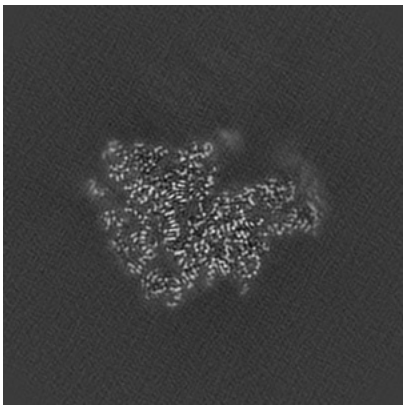
Z

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

6.2 Central slices (i)

6.2.1 Primary map


X Index: 200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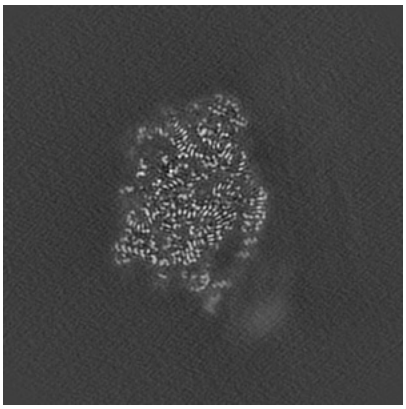
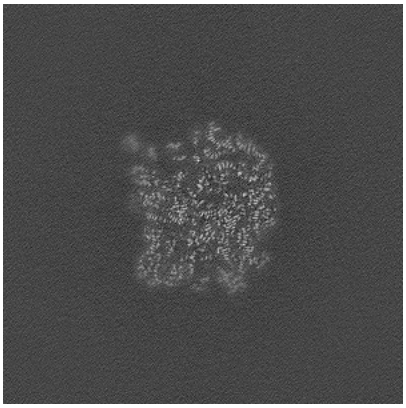

Z Index: 200

6.2.2 Raw map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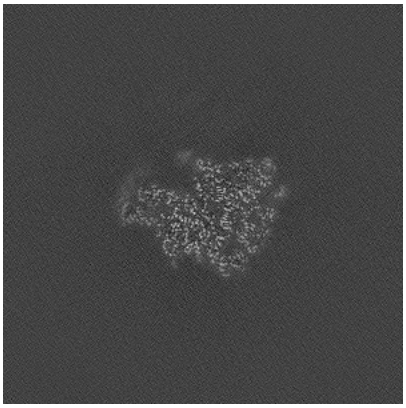
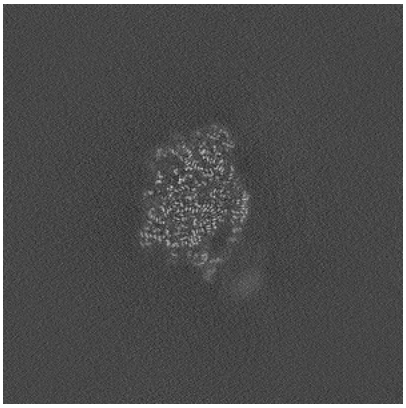
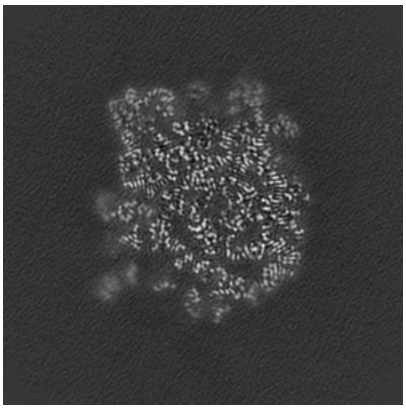

Y Index: 280


Z Index: 280

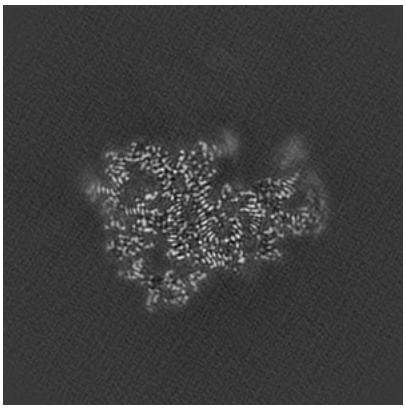
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

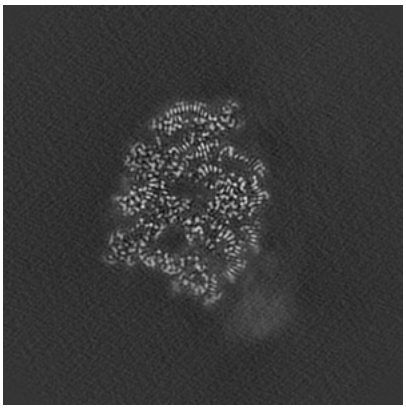
6.3.1 Primary map



X Index: 204

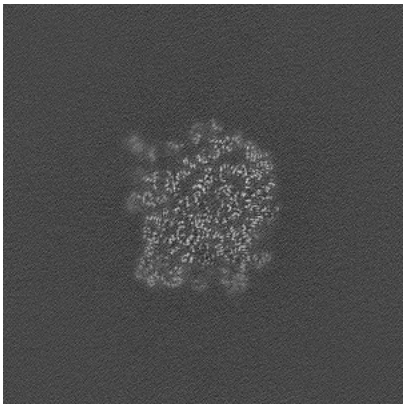


Y Index: 192

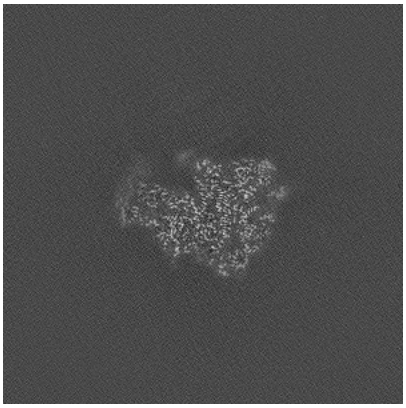


Z Index: 187

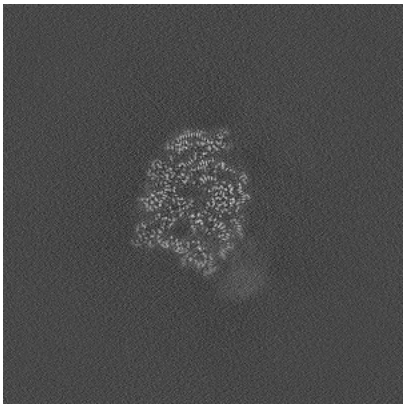
6.3.2 Raw map



X Index: 284



Y Index: 278

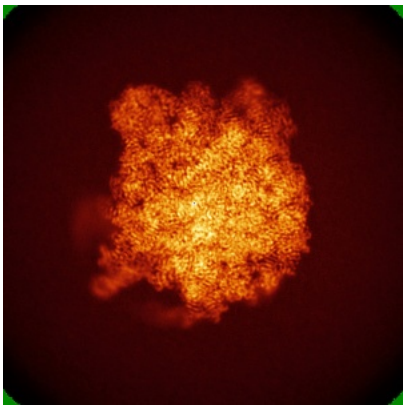


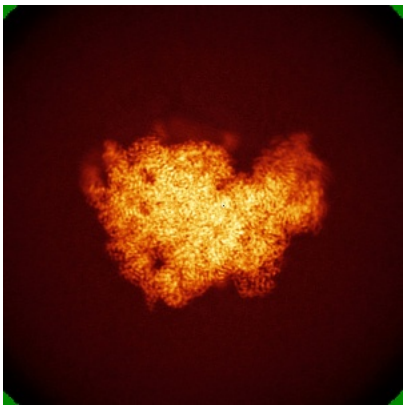
Z Index: 293

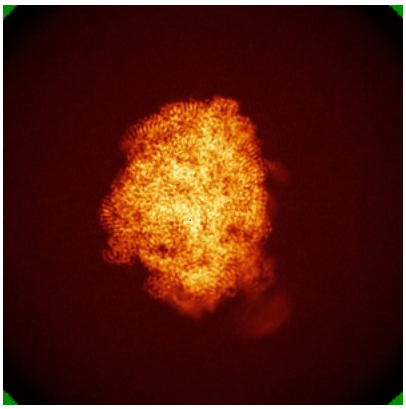
The images above show the largest variance slices of the map in three orthogonal directions.

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

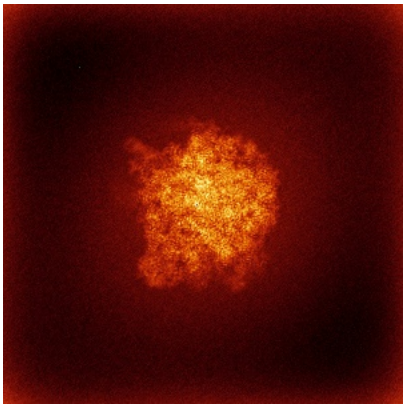
6.4.1 Primary map

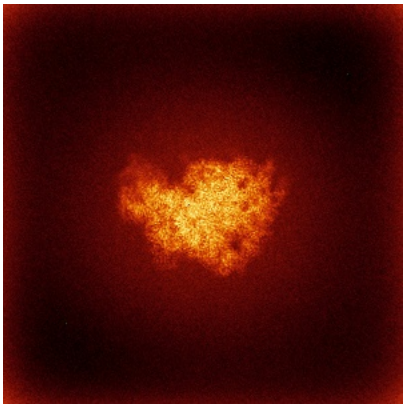

X

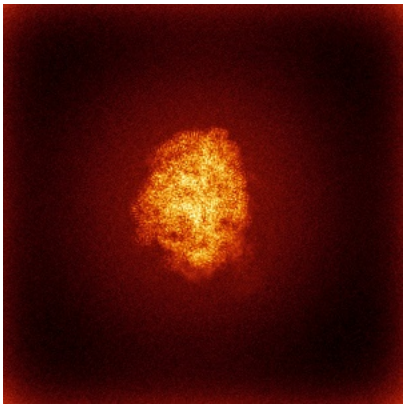

Y


Z

6.4.2 Raw map


X

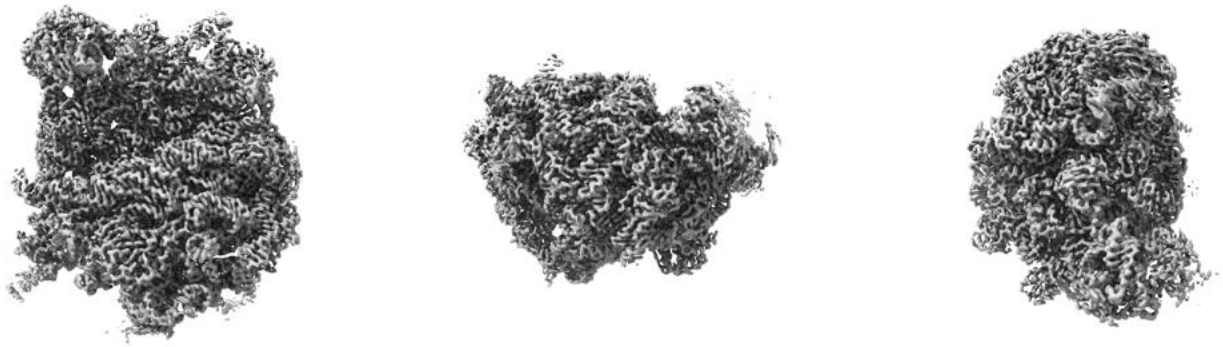

Y


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 0.25. 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.

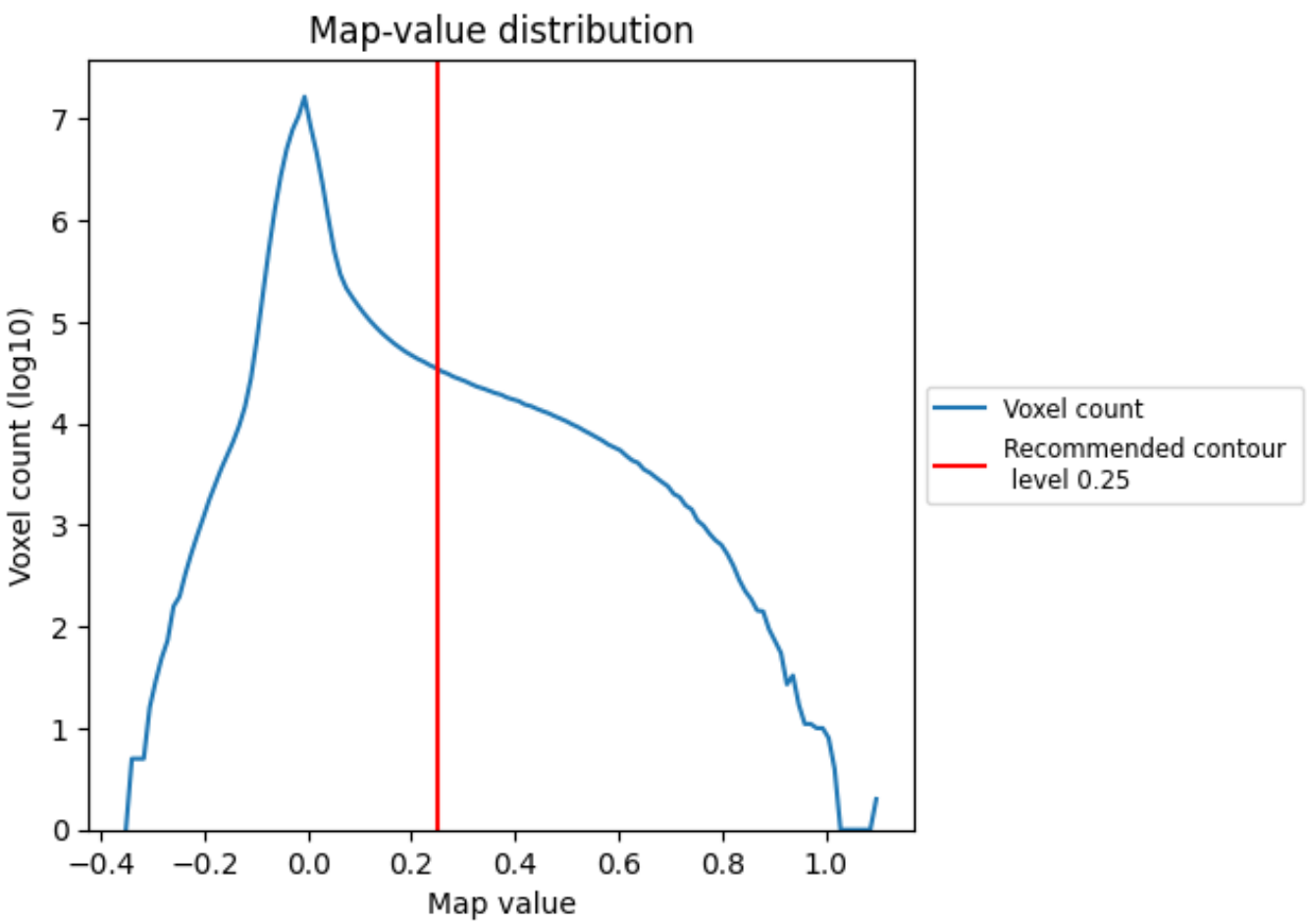
6.6 Mask visualisation (i)

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

7 Map analysis (i)

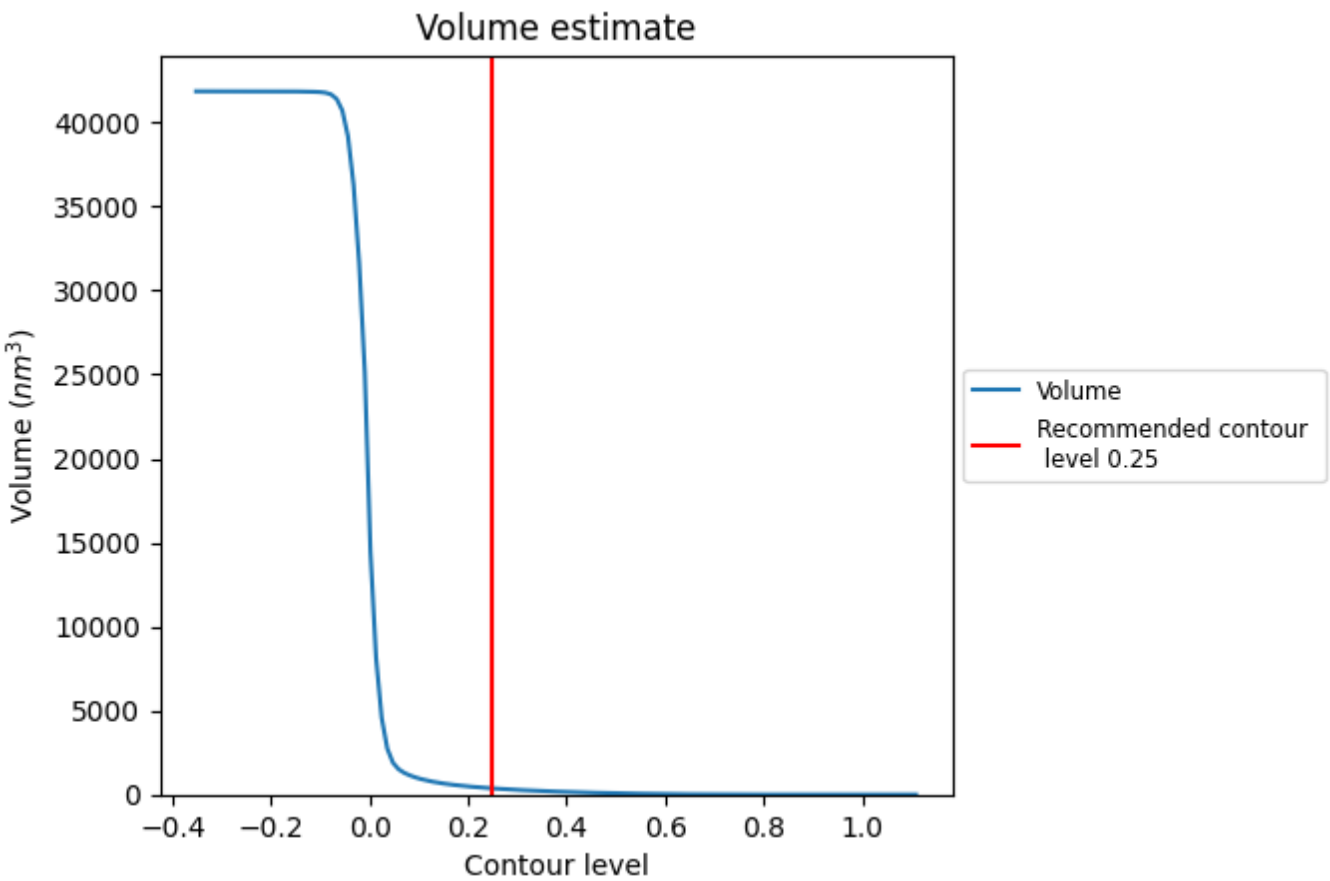
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

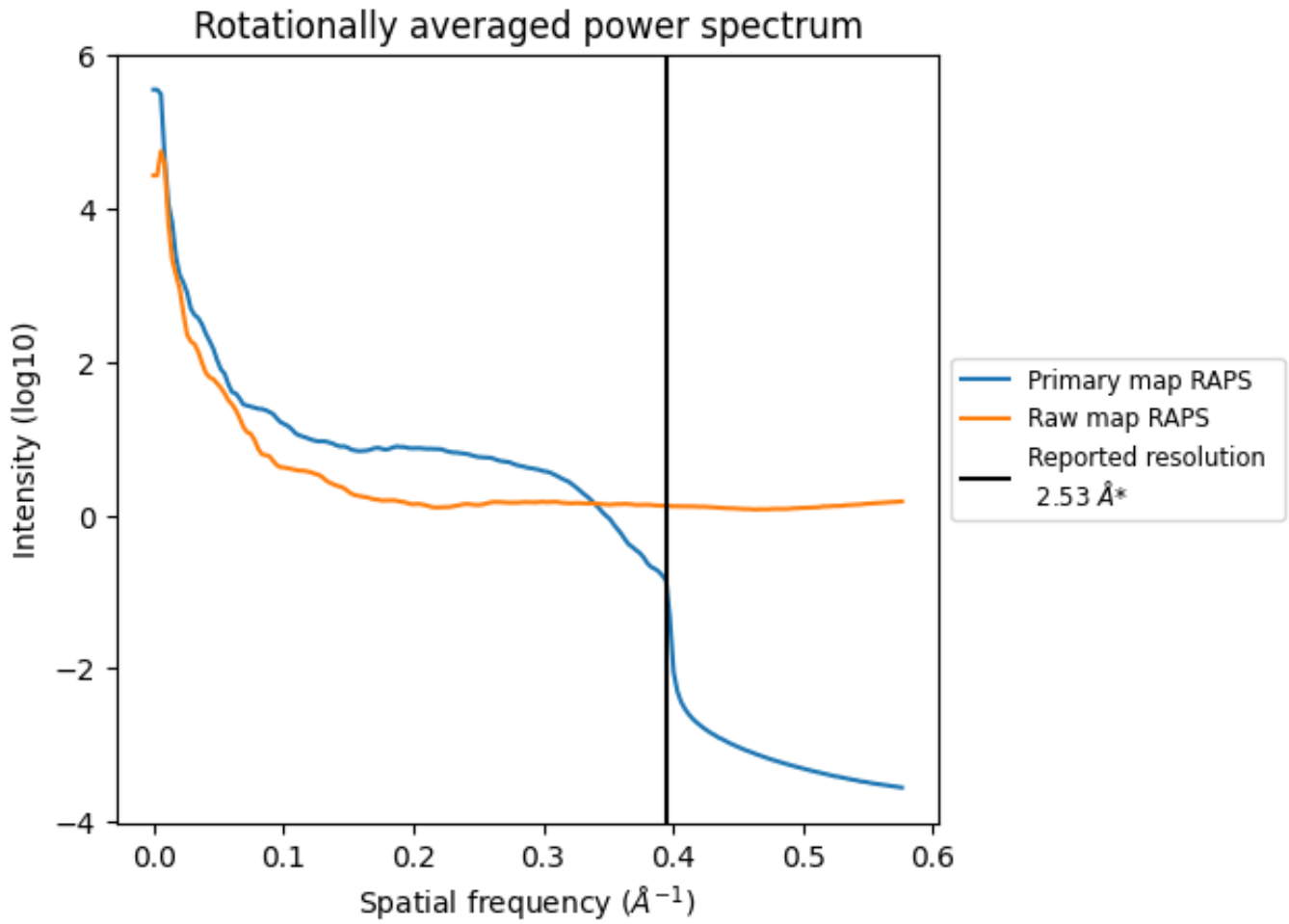
7.2 Volume estimate (i)



The volume at the recommended contour level is 369 nm^3; this corresponds to an approximate mass of 333 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)

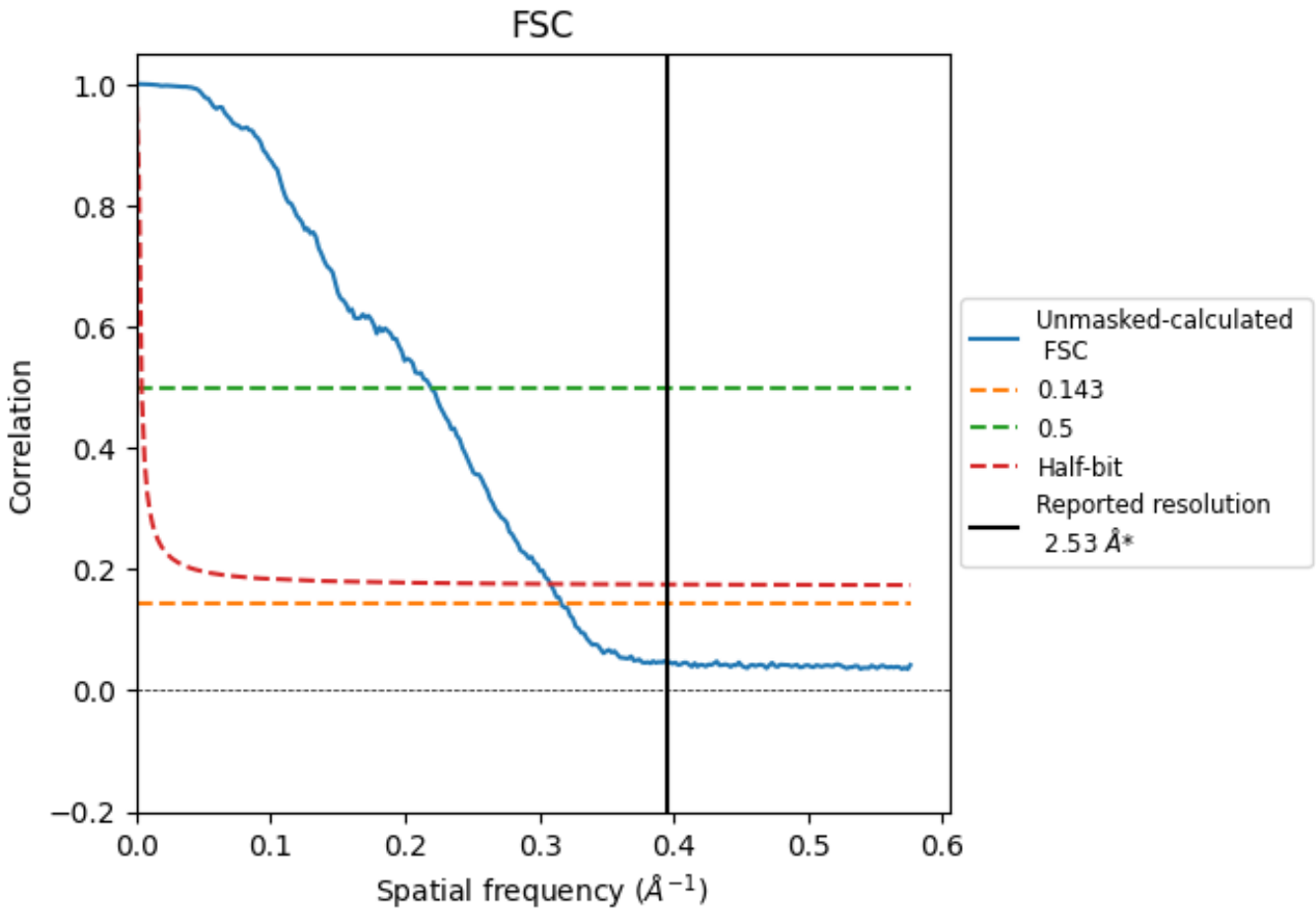


*Reported resolution corresponds to spatial frequency of 0.395 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.395 Å^{-1}

8.2 Resolution estimates (i)

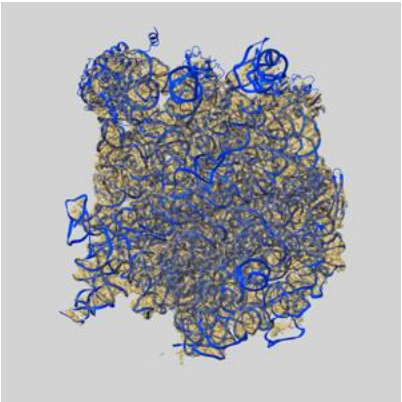
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.53	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.16	4.56	3.24

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.16 differs from the reported value 2.53 by more than 10 %

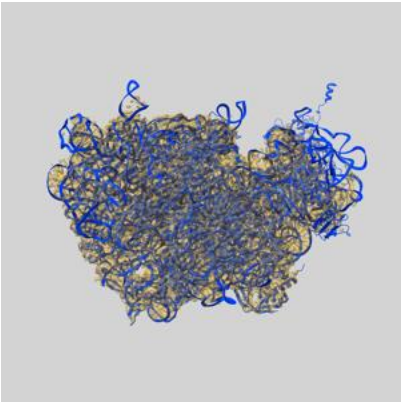
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-45185 and PDB model 9C4G. Per-residue inclusion information can be found in section 3 on page 12.

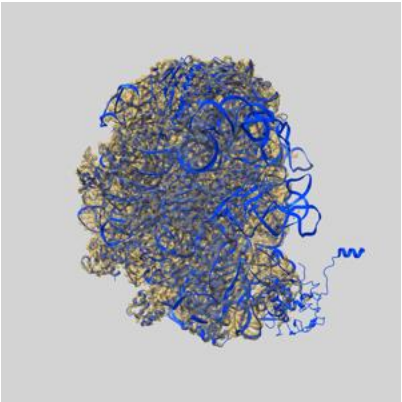
9.1 Map-model overlay (i)



X



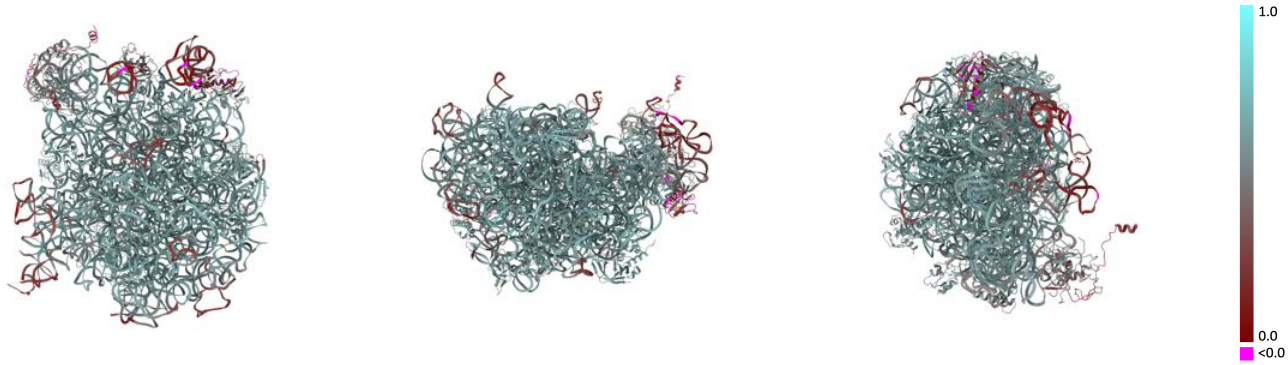
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.25 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.

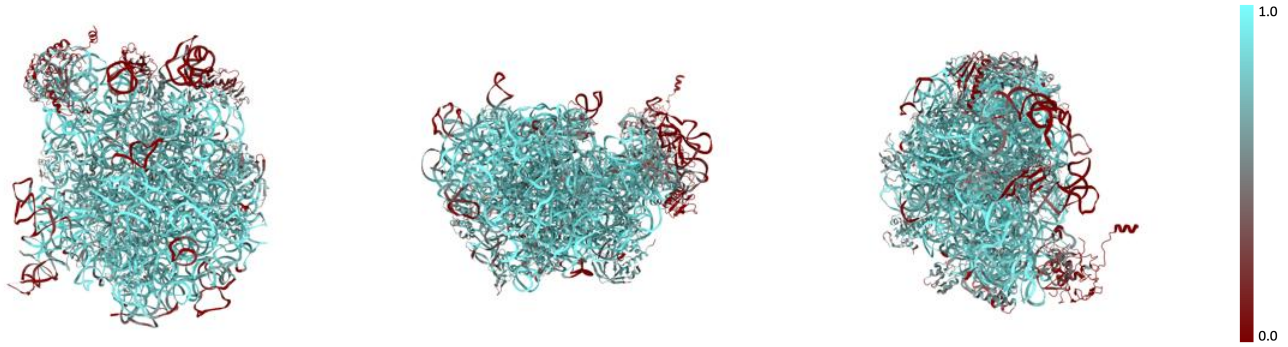
9.2 Q-score mapped to coordinate model (i)



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.

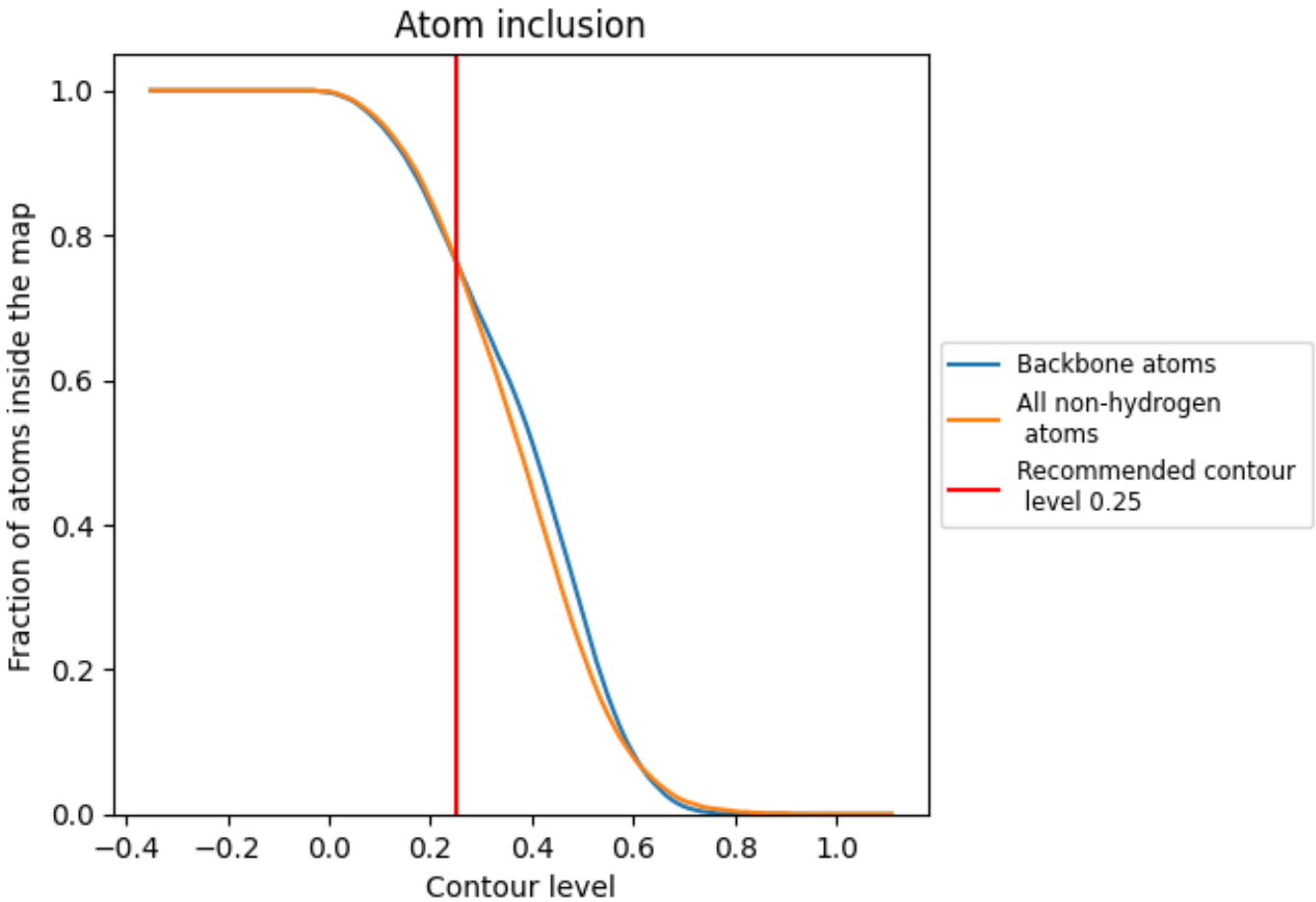
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.25).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7650	0.5760
0	0.6620	0.6030
1	0.8010	0.6370
2	0.7300	0.6290
3	0.6920	0.6130
4	0.0040	0.2200
V	0.8190	0.6400
a	0.8220	0.5780
b	0.8380	0.5750
c	0.7890	0.6250
d	0.7610	0.6200
e	0.6990	0.5830
f	0.2360	0.4560
g	0.2840	0.3450
i	0.7730	0.6300
j	0.6570	0.6030
k	0.6850	0.5980
l	0.6870	0.6100
m	0.7720	0.6160
n	0.6140	0.5610
o	0.5920	0.5670
p	0.7900	0.6210
q	0.6670	0.6100
r	0.7110	0.6060
s	0.6580	0.5970
t	0.5810	0.5710
u	0.3150	0.4740
v	0.7550	0.6210
w	0.7990	0.6300
x	0.6130	0.5870
y	0.7110	0.6150
z	0.7720	0.6280