wwPDB EM Map/Model Validation Report (i)

Sep 20, 2016 – 08:43 PM EDT

PDB ID	:	5L3P
EMDB ID:	:	EMD-4001
Title	:	Cryo-EM structure of stringent response factor RelA bound to ErmCL-stalled ribosome complex
Authors	:	Arenz, S.; Wilson, D.N.
Deposited on	:	2016-05-24
Resolution	:	3.70 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

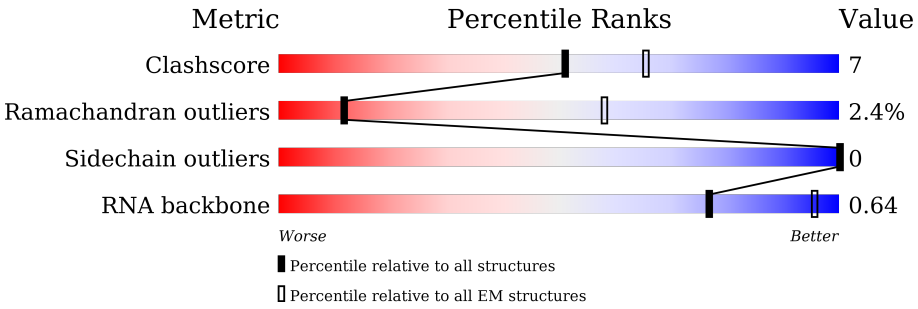
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 3.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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%

Mol	Chain	Length	Quality of chain
1	A	2903	63% 32% 5%
2	B	120	68% 27% 5%
3	D	273	73% 26% .
4	E	209	78% 22%
5	F	201	76% 24%
6	G	179	75% 24% .
7	H	177	83% 16% .
8	I	149	79% 19% .

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Mol	Chain	Length	Quality of chain
9	N	142	74% 25%
10	O	123	65% 32%
11	P	144	66% 33%
12	Q	136	81% 18%
13	R	127	67% 28% 6%
14	S	117	86% 13%
15	T	115	76% 23%
16	U	118	80% 19%
17	V	103	70% 30%
18	W	110	77% 23%
19	X	100	69% 24% 7%
20	Y	104	73% 24%
21	Z	94	74% 26%
22	0	85	65% 22% 12%
23	1	78	81% 18%
24	2	63	76% 24%
25	3	59	69% 29%
26	4	70	80% 13% 6%
27	5	57	79% 19%
28	6	55	67% 22% 9%
29	7	46	67% 33%
30	8	65	72% 26%
31	9	38	79% 21%
32	a	1539	88% 11%
33	b	240	89% 9%

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Mol	Chain	Length	Quality of chain
34	c	233	88% 12%
35	d	206	98%
36	e	167	90% 6%
37	f	135	71% 26%
38	g	179	81% 16%
39	h	130	98%
40	i	130	94%
41	j	103	89% 6% 5%
42	k	129	87% 10%
43	l	124	93% 6%
44	m	118	95%
45	o	89	93% 6%
46	p	82	98%
47	q	84	90% 5% 5%
48	r	75	83% 13%
49	t	87	98%
50	u	71	85% 7% 8%
51	v	6	100%
52	x	77	82% 14%
53	J	165	50% 27% 21%
54	K	142	75% 23%
55	n	102	95%
56	s	92	85% 14%
57	z	819	65% 33%
58	y	73	60% 37%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	2MG	A	1835	X	-	-	-
1	PSU	A	1911	X	-	-	-
1	3TD	A	1915	X	-	-	-
1	PSU	A	1917	X	-	-	-
1	5MU	A	1939	X	-	-	-
1	7MG	A	2069	X	-	-	-
1	OMG	A	2251	X	-	-	-
1	2MG	A	2445	X	-	-	-
1	H2U	A	2449	X	-	-	-
1	PSU	A	2457	X	-	-	-
1	OMC	A	2498	X	-	-	-
1	2MA	A	2503	X	-	-	-
1	PSU	A	2504	X	-	-	-
1	OMU	A	2552	X	-	-	-
1	PSU	A	2580	X	-	-	-
1	PSU	A	2604	X	-	-	-
1	PSU	A	2605	X	-	-	-
1	PSU	A	746	X	-	-	-
1	PSU	A	955	X	-	-	-
32	2MG	a	1207	X	-	-	-
32	4OC	a	1402	X	-	-	-
32	UR3	a	1498	X	-	-	-
32	2MG	a	1516	X	-	-	-
32	MA6	a	1518	X	-	-	-
32	MA6	a	1519	X	-	-	-
32	PSU	a	516	X	-	-	-
32	7MG	a	527	X	-	-	-
32	2MG	a	966	X	-	-	-
52	H2U	x	20	X	-	-	-
52	5MU	x	54	X	-	-	-
52	PSU	x	55	X	-	-	-
52	4SU	x	8	X	-	-	-
58	H2U	y	16	X	-	-	-
58	H2U	y	17	X	-	-	-
58	H2U	y	20	X	-	-	-
58	7MG	y	46	X	-	-	-
58	5MU	y	54	X	-	-	-
58	PSU	y	55	X	-	-	-

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 149606 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	2890	62057	27688	11422	20057	2890	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1847	G	A	conflict	GB 802133627

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	120	2572	1145	471	836	120	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	120	A	U	conflict	GB 999944586

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	271	2082	1288	423	364	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	209	1565	979	288	294	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

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

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

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 8 is a protein called 50S ribosomal protein L9.

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

- Molecule 9 is a protein called 50S ribosomal protein L13.

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

- Molecule 10 is a protein called 50S ribosomal protein L14.

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

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	P	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Q	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	R	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 14 is a protein called 50S ribosomal protein L18.

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

- Molecule 15 is a protein called 50S ribosomal protein L19.

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

- Molecule 16 is a protein called 50S ribosomal protein L20.

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

- Molecule 17 is a protein called 50S ribosomal protein L21.

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

- Molecule 18 is a protein called 50S ribosomal protein L22.

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

- Molecule 19 is a protein called 50S ribosomal protein L23.

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

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	Y	102	Total	C	N	O	0	0
			779	492	146	141		

- Molecule 21 is a protein called 50S ribosomal protein L25.

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

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	0	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	1	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	2	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	3	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	4	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	5	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	6	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	7	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	8	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	9	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 32 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	1539	Total	C	N	O	P	0	0
			33029	14738	6052	10700	1539		

- Molecule 33 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 34 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	c	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 35 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	d	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 36 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	e	157	Total	C	N	O	S	0	0
			1141	709	218	208	6		

- Molecule 37 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	f	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 38 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	g	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 39 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	h	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 40 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	i	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 41 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	j	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 42 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	k	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 43 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	l	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 44 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	m	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 45 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	o	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 46 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	p	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 47 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 48 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	r	65	Total	C	N	O	0	0
			504	317	96	91		

- Molecule 49 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	t	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 50 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	u	65	Total	C	N	O	S	0	0
			495	307	100	87	1		

- Molecule 51 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	v	6	Total	C	N	O	P	0	0
			129	58	24	41	6		

- Molecule 52 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	x	77	Total	C	N	O	P	S	0	0
			1644	733	297	536	77	1		

- Molecule 53 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	J	131	Total	C	N	O	S	0	0
			988	625	175	183	5		

- Molecule 54 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	K	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 55 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	n	101	Total	C	N	O	S	0	0
			799	498	165	133	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	35	ALA	-	insertion	UNP P0AG59

- Molecule 56 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	s	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 57 is a protein called GTP pyrophosphokinase,GTP pyrophosphokinase,GTP pyrophosphokinase.

Mol	Chain	Residues	Atoms				AltConf	Trace
57	z	545	Total	C	N	O	0	0
			2255	1165	545	545		

- Molecule 58 is a RNA chain called deacylated A/R-tRNA.

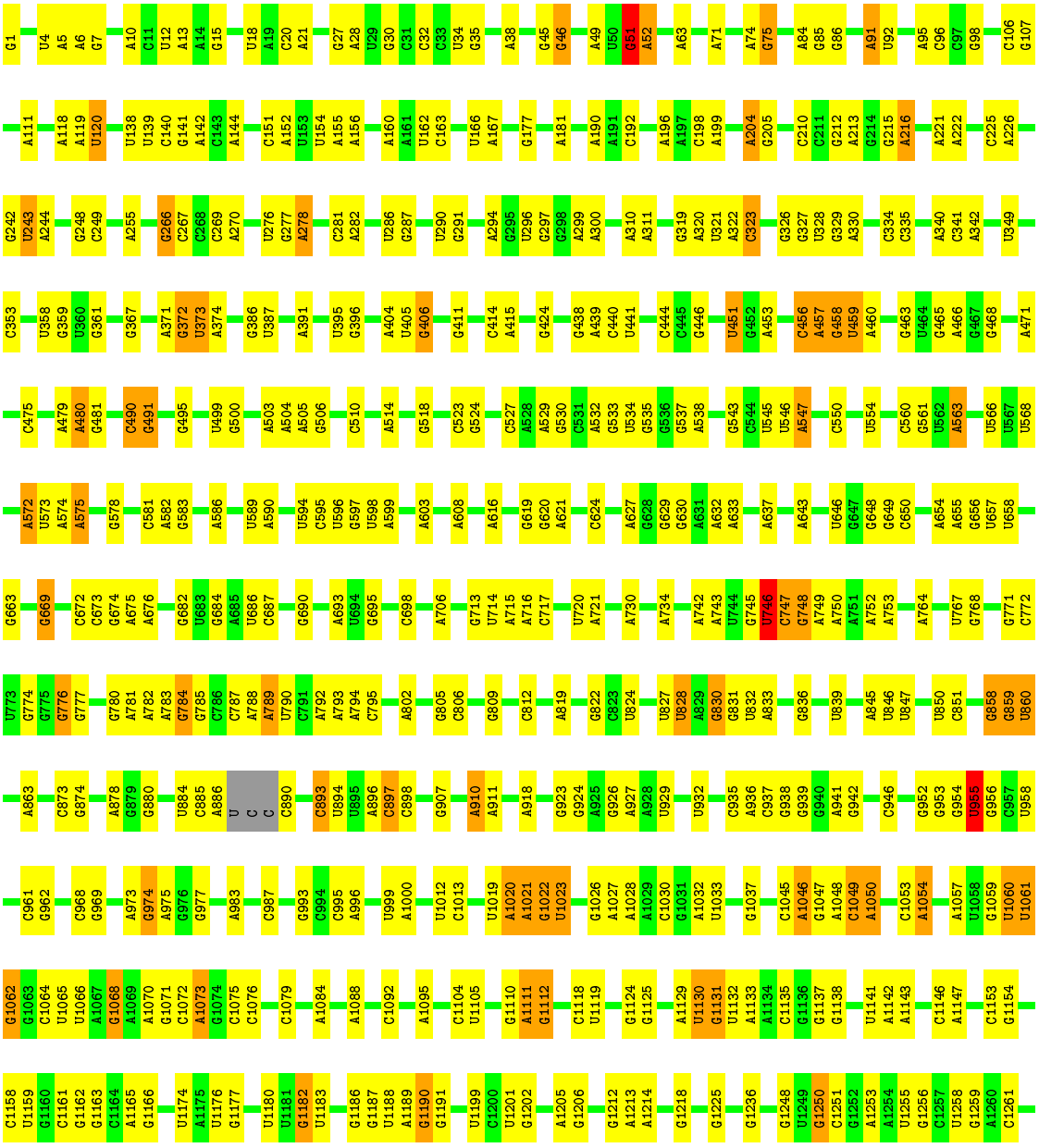
Mol	Chain	Residues	Atoms					AltConf	Trace
58	y	73	Total	C	N	O	P	0	0
			1581	709	280	519	73		

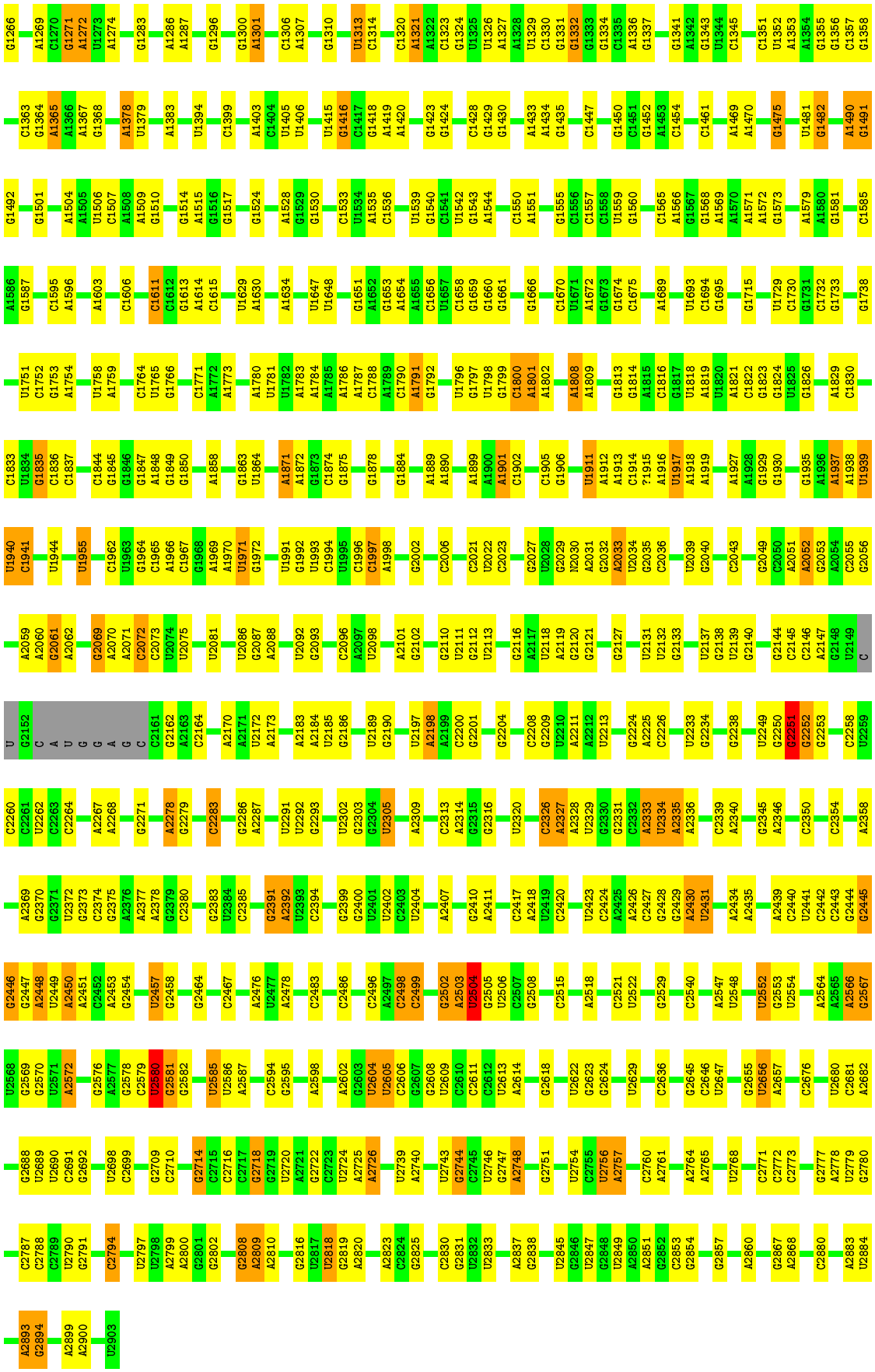
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 23S ribosomal RNA

Chain A: 63% 32% 5%




G1266 A1269 C1270 G1271 A1272 U1273 A1274 G1283 A1286 A1287 G1296 G1300 A1301 C1306 A1307 G1310 U1313 C1314 C1320 A1321 A1322 C1323 G1324 U1325 U1326 A1327 A1328 U1329 C1330 G1331 G1332 G1333 G1334 C1335 A1336 G1337 G1341 A1342 G1343 U1344 C1345 C1351 U1352 A1353 A1354 G1355 G1356 C1357 G1358
C1363 G1364 A1365 A1366 A1367 G1368 A1378 U1379 A1383 U1394 C1399 A1403 C1404 U1405 U1406 U1415 G1416 C1417 G1418 A1419 A1420 G1423 G1424 C1428 G1429 G1430 C1447 G1450 C1451 A1452 A1453 C1454 C1461 A1469 A1470 G1475 U1481 G1482 A1490 G1491
G1492 G1501 A1504 A1505 U1506 C1507 A1508 A1509 G1510 G1514 A1515 G1516 G1517 G1524 A1528 G1529 G1530 C1533 U1534 A1535 C1536 U1539 G1540 C1541 U1542 G1543 A1544 C1550 A1551 G1555 C1556 C1557 C1558 U1559 G1560 C1565 A1566 G1567 G1568 A1569 A1570 A1571 A1572 G1573 A1579 A1580 G1581 C1585
A1586 G1587 C1595 A1596 A1603 C1606 C1611 C1612 G1613 A1614 C1615 U1629 A1630 A1634 A1528 G1529 U1647 U1648 G1651 A1652 G1653 A1654 A1655 C1656 U1657 C1658 G1659 G1660 G1661 G1666 C1670 U1671 A1672 G1673 G1674 C1675 A1689 U1693 C1694 G1695 A1715 U1729 C1730 G1731 C1732 G1733 G1738
U1751 C1752 G1753 A1754 U1758 A1759 C1764 U1765 G1766 C1771 A1772 A1773 A1780 U1781 U1782 A1783 A1784 A1785 A1786 A1787 C1788 A1789 C1790 A1791 G1792 U1796 G1797 U1798 G1799 C1800 A1801 A1802 A1808 A1809 G1813 G1814 A1815 C1816 G1817 U1818 A1819 U1820 A1821 C1822 G1823 G1824 U1825 G1826 A1829 C1830
C1833 U1834 G1835 C1836 C1837 C1844 G1845 G1846 G1847 A1848 G1849 G1850 A1858 G1863 U1864 A1871 A1872 G1873 C1874 G1875 G1878 G1884 A1889 A1890 A1899 A1900 A1901 C1902 C1905 G1906 U1911 A1912 A1913 C1914 ?1915 A1916 U1917 A1918 A1919 A1927 A1928 G1929 G1930 G1935 A1936 A1937 A1938 U1939
U1940 C1941 U1944 U1955 C1962 U1963 G1964 C1965 A1966 C1967 G1968 A1969 A1970 U1971 G1972 U1991 G1992 U1993 C1994 U1995 C1996 C1997 A1998 G2002 C2006 C2021 U2022 C2023 G2027 U2028 G2029 N2030 A2031 G2032 A2033 U2034 G2035 C2036 U2039 G2040 C2043 G2049 C2050 A2051 A2052 G2053 A2054 C2055 G2056
A2059 A2060 G2061 A2062 G2069 A2070 A2071 C2072 C2073 U2074 U2075 U2081 U2086 G2087 A2088 U2092 G2093 C2096 A2097 U2098 A2101 G2102 G2110 U2111 G2112 U2113 G2116 A2117 U2118 A2119 G2120 G2121 G2127 U2131 U2132 G2133 U2137 G2138 U2139 G2140 G2144 C2145 C2146 A2147 G2148 U2149 C
U G2152 C A U G A G C C2161 G2162 A2163 C2164 A2170 A2171 U2172 A2173 A2183 A2184 U2185 G2186 U2189 G2190 U2197 A2198 A2199 C2200 G2201 G2204 C2208 G2209 U2210 A2211 A2212 U2213 G2224 A2225 C2226 U2233 G2234 G2238 U2249 G2250 G2251 A2252 G2253 C2258 U2259
C2260 C2261 U2262 C2263 C2264 A2267 A2268 G2271 A2278 G2279 C2283 G2286 A2287 U2291 U2292 G2293 U2302 G2303 G2304 U2305 A2309 C2313 A2314 G2315 G2316 U2320 C2326 A2327 A2328 U2329 G2330 G2331 C2332 A2333 U2334 A2335 A2336 C2339 A2340 G2345 A2346 C2350 C2354 A2358
A2369 G2370 G2371 U2372 G2373 C2374 G2375 A2376 A2377 A2378 G2379 C2380 G2383 U2384 C2385 G2391 A2392 U2393 C2394 G2399 G2400 U2401 U2402 C2403 U2404 A2407 G2410 A2411 C2417 A2418 U2419 C2420 U2423 C2424 A2425 A2426 C2427 G2428 G2429 A2430 U2431 A2434 A2435 A2439 C2440 U2441 C2442 C2443 G2444 G2445
G2446 G2447 A2448 U2449 A2450 A2451 C2452 A2453 G2454 C2457 G2458 G2464 C2467 A2476 U2477 A2478 C2483 C2486 C2496 A2497 C2498 C2499 G2502 A2503 U2504 G2505 U2506 C2507 G2508 C2515 A2518 C2521 U2522 G2529 C2540 A2547 U2548 U2552 G2553 U2554 A2564 A2565 A2566 G2567
U2568 G2569 G2570 U2571 A2572 G2576 A2577 G2578 C2579 U2580 G2581 G2582 U2585 U2586 A2587 C2594 G2595 A2698 A2602 G2603 U2604 U2605 C2606 G2607 G2608 U2609 C2610 C2611 C2612 U2613 A2614 G2618 U2622 G2623 G2624 U2629 C2636 G2645 C2646 U2647 G2655 U2656 A2657 C2676 U2680 C2681 A2682
G2688 U2689 U2690 C2691 G2692 U2698 C2699 G2709 C2710 G2714 C2715 C2716 C2717 G2718 G2719 U2720 A2721 G2722 C2723 U2724 A2725 A2726 U2739 A2740 U2743 G2744 C2745 U2746 G2747 A2748 G2751 U2754 C2755 U2756 A2757 C2760 A2761 A2764 A2765 U2768 C2771 C2772 C2773 G2777 A2778 U2779 G2780
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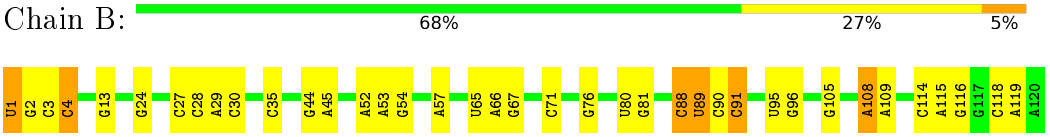
A2893 G2894 A2899 A2900 U2903

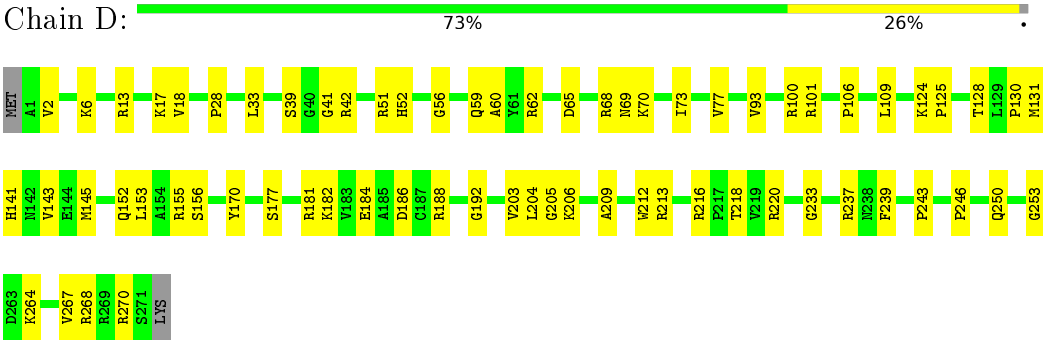
- Molecule 2: 5S ribosomal RNA

Chain B:



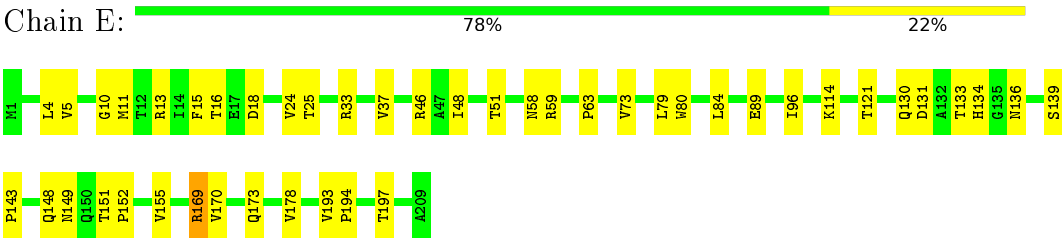
- Molecule 3: 50S ribosomal protein L2

Chain D:



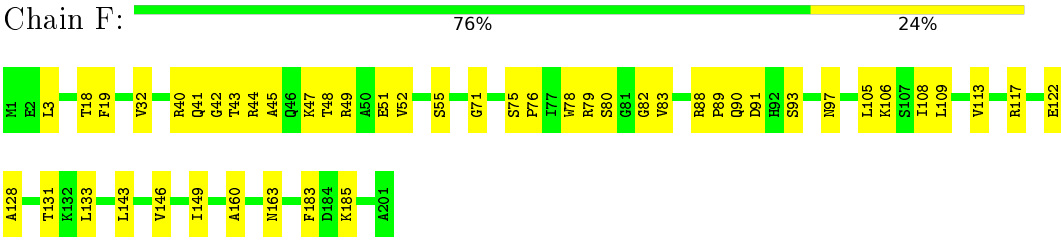
- Molecule 4: 50S ribosomal protein L3

Chain E:



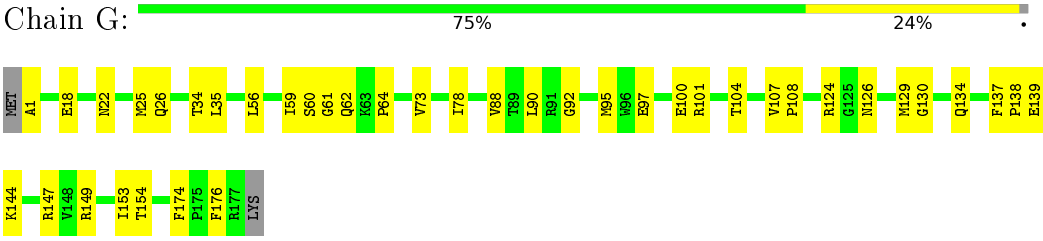
- Molecule 5: 50S ribosomal protein L4

Chain F:



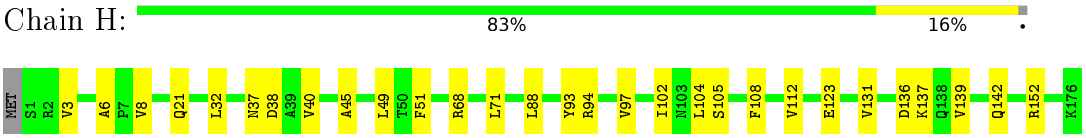
- Molecule 6: 50S ribosomal protein L5

Chain G:



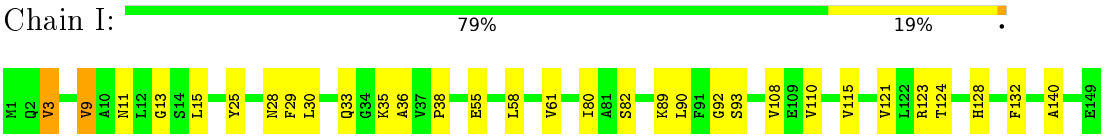
- Molecule 7: 50S ribosomal protein L6

Chain H:



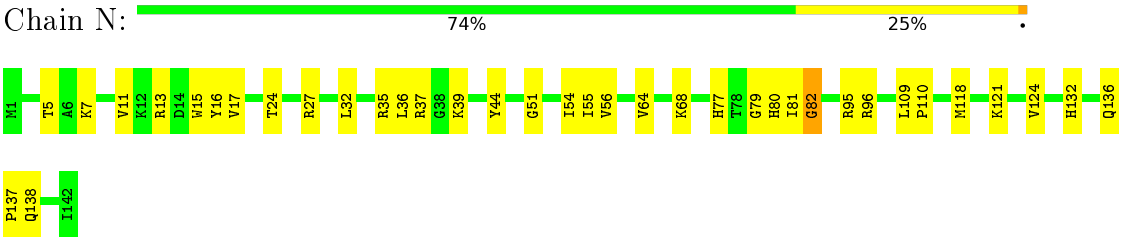
• Molecule 8: 50S ribosomal protein L9

Chain I:



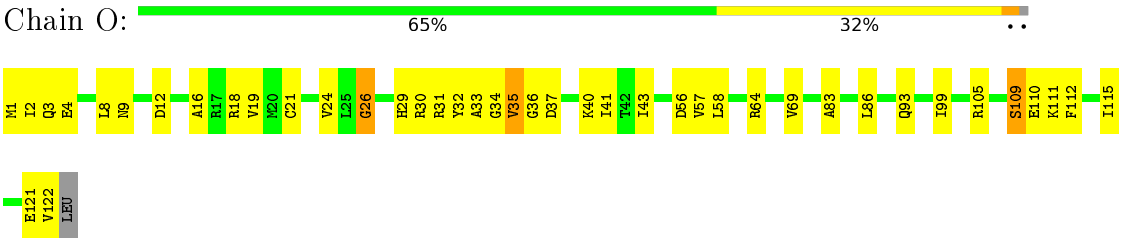
• Molecule 9: 50S ribosomal protein L13

Chain N:



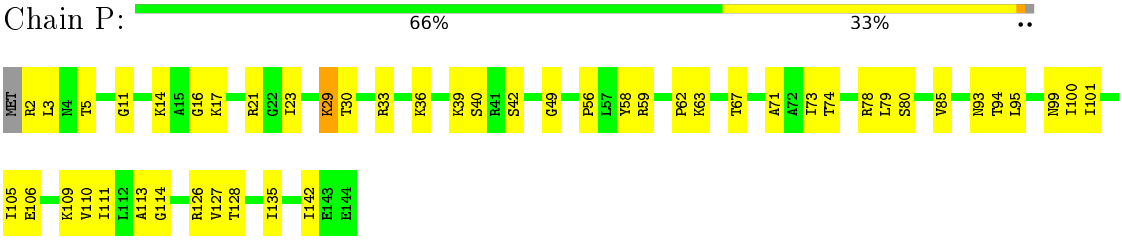
• Molecule 10: 50S ribosomal protein L14

Chain O:



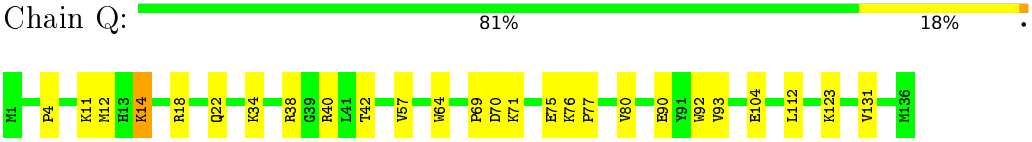
• Molecule 11: 50S ribosomal protein L15

Chain P:



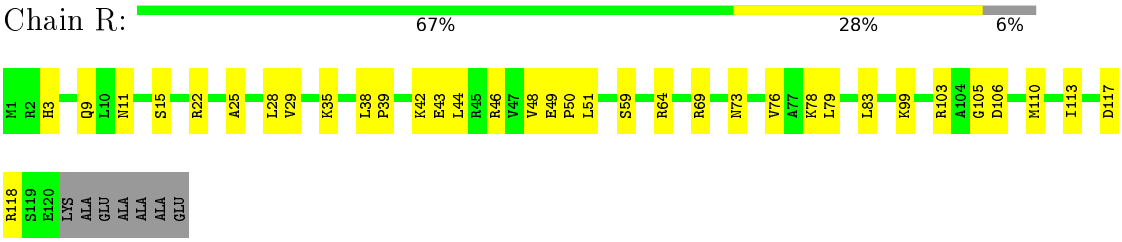
• Molecule 12: 50S ribosomal protein L16

Chain Q:



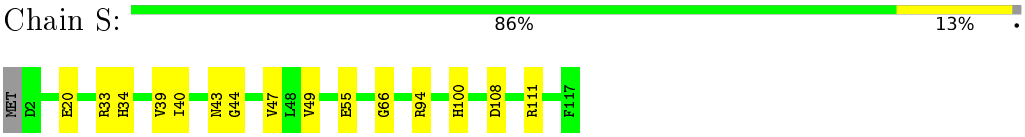
• Molecule 13: 50S ribosomal protein L17

Chain R:



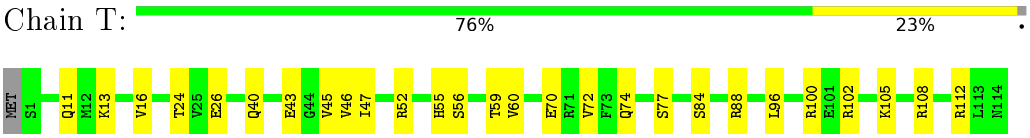
• Molecule 14: 50S ribosomal protein L18

Chain S:



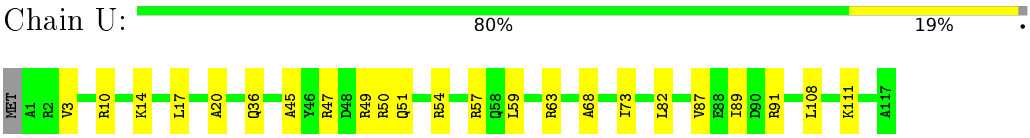
• Molecule 15: 50S ribosomal protein L19

Chain T:



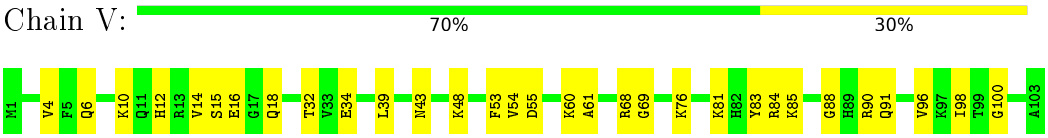
• Molecule 16: 50S ribosomal protein L20

Chain U:



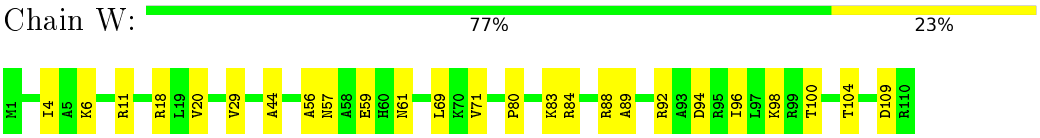
• Molecule 17: 50S ribosomal protein L21

Chain V:



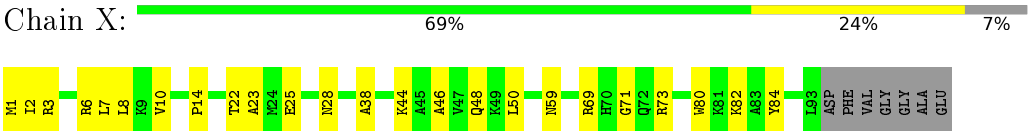
• Molecule 18: 50S ribosomal protein L22

Chain W:



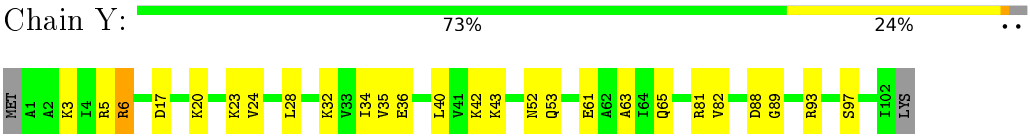
• Molecule 19: 50S ribosomal protein L23

Chain X:



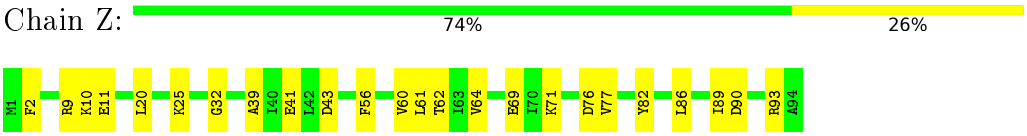
• Molecule 20: 50S ribosomal protein L24

Chain Y:



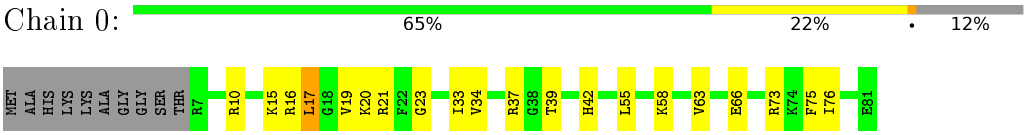
- Molecule 21: 50S ribosomal protein L25

Chain Z:



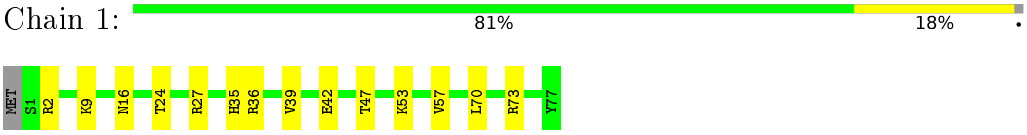
- Molecule 22: 50S ribosomal protein L27

Chain 0:



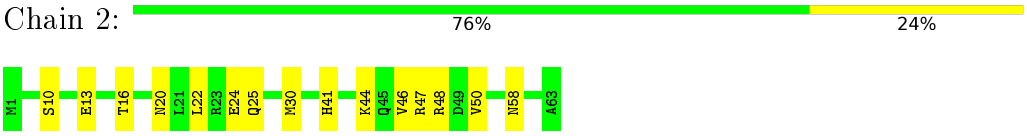
- Molecule 23: 50S ribosomal protein L28

Chain 1:



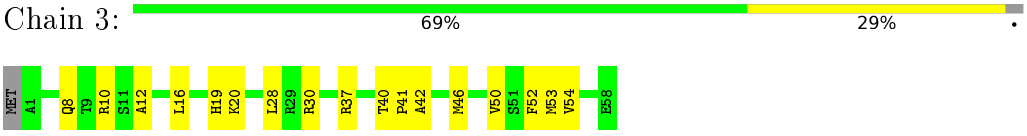
- Molecule 24: 50S ribosomal protein L29

Chain 2:



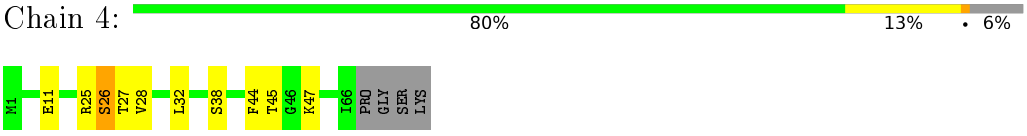
- Molecule 25: 50S ribosomal protein L30

Chain 3:



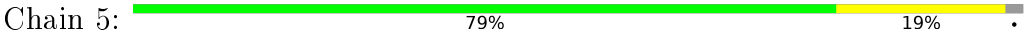
- Molecule 26: 50S ribosomal protein L31

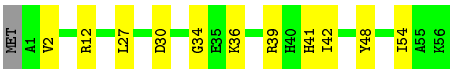
Chain 4:



- Molecule 27: 50S ribosomal protein L32

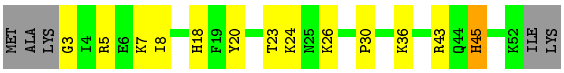
Chain 5:





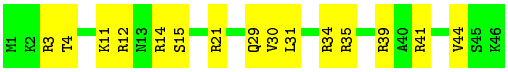
• Molecule 28: 50S ribosomal protein L33

Chain 6:



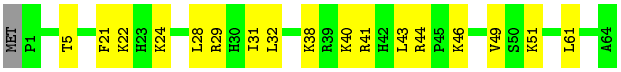
• Molecule 29: 50S ribosomal protein L34

Chain 7:



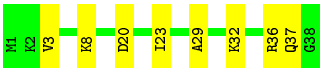
• Molecule 30: 50S ribosomal protein L35

Chain 8:



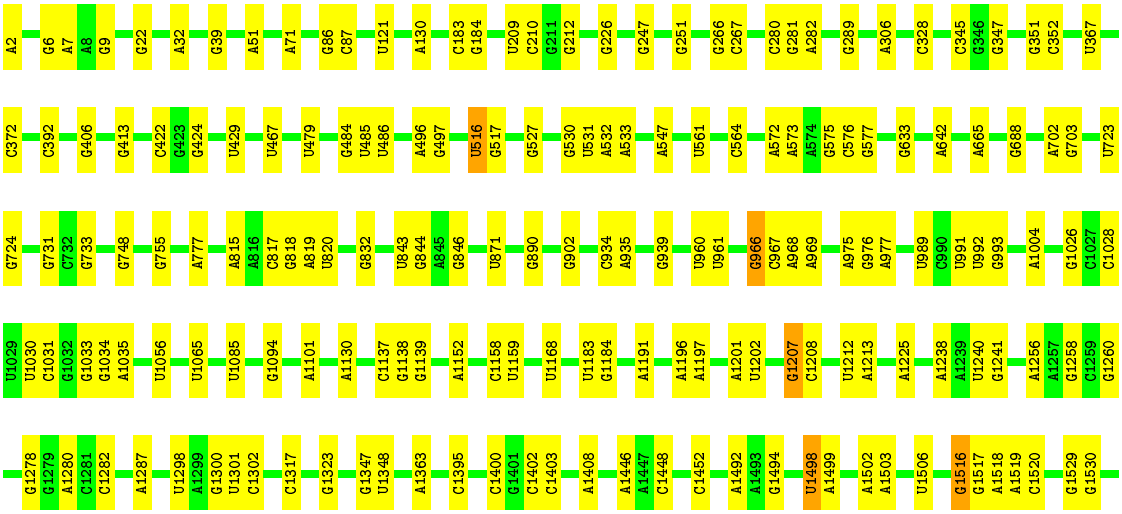
• Molecule 31: 50S ribosomal protein L36

Chain 9:



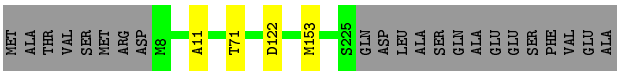
• Molecule 32: 16S ribosomal RNA

Chain a:



- Molecule 33: 30S ribosomal protein S2

Chain b:

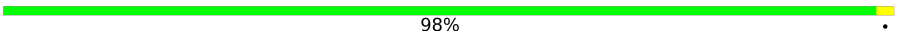


- Molecule 34: 30S ribosomal protein S3

Chain c:

- Molecule 35: 30S ribosomal protein S4

Chain d:



- Molecule 36: 30S ribosomal protein S5

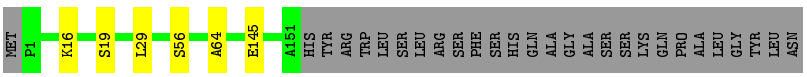
Chain e:

- Molecule 37: 30S ribosomal protein S6

Chain f:

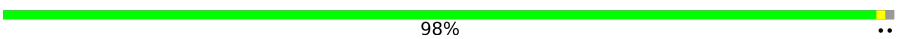
- Molecule 38: 30S ribosomal protein S7

Chain g:



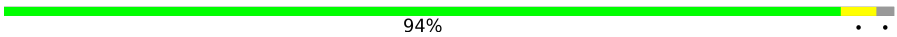
- Molecule 39: 30S ribosomal protein S8

Chain h:



- Molecule 40: 30S ribosomal protein S9

Chain i:

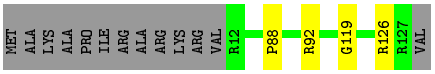


- Molecule 41: 30S ribosomal protein S10

Chain j:

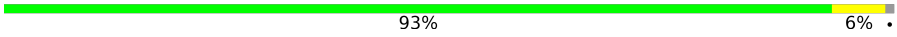
- Molecule 42: 30S ribosomal protein S11

Chain k:



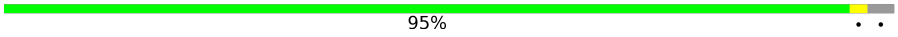
- Molecule 43: 30S ribosomal protein S12

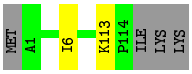
Chain l:



- Molecule 44: 30S ribosomal protein S13

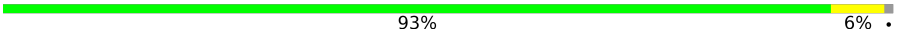
Chain m:

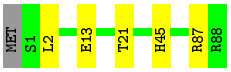




- Molecule 45: 30S ribosomal protein S15

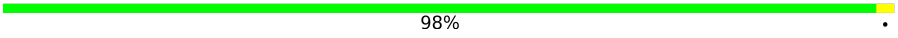
Chain o:





- Molecule 46: 30S ribosomal protein S16

Chain p:

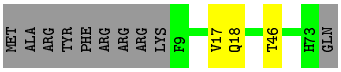


- Molecule 47: 30S ribosomal protein S17

Chain q:

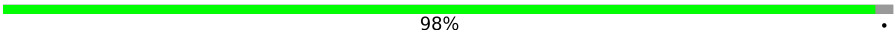
• Molecule 48: 30S ribosomal protein S18

Chain r:



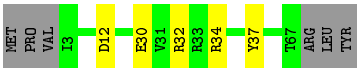
• Molecule 49: 30S ribosomal protein S20

Chain t:



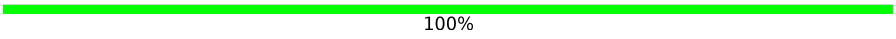
• Molecule 50: 30S ribosomal protein S21

Chain u:



• Molecule 51: mRNA

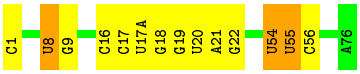
Chain v:



There are no outlier residues recorded for this chain.

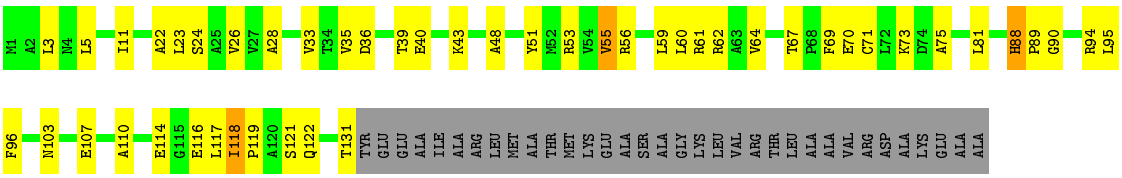
• Molecule 52: P-site tRNA

Chain x:



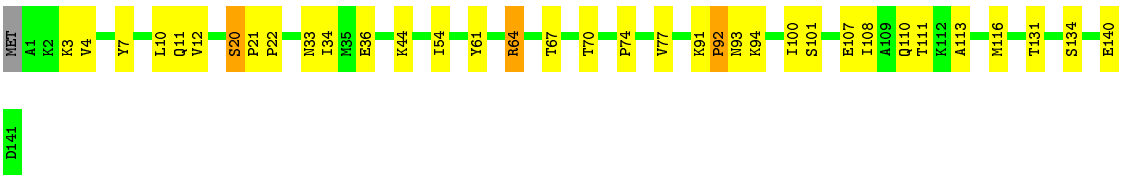
• Molecule 53: 50S ribosomal protein L10

Chain J:



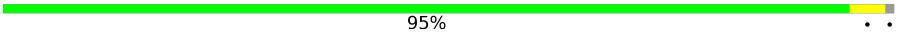
• Molecule 54: 50S ribosomal protein L11

Chain K:



• Molecule 55: 30S ribosomal protein S14

Chain n:

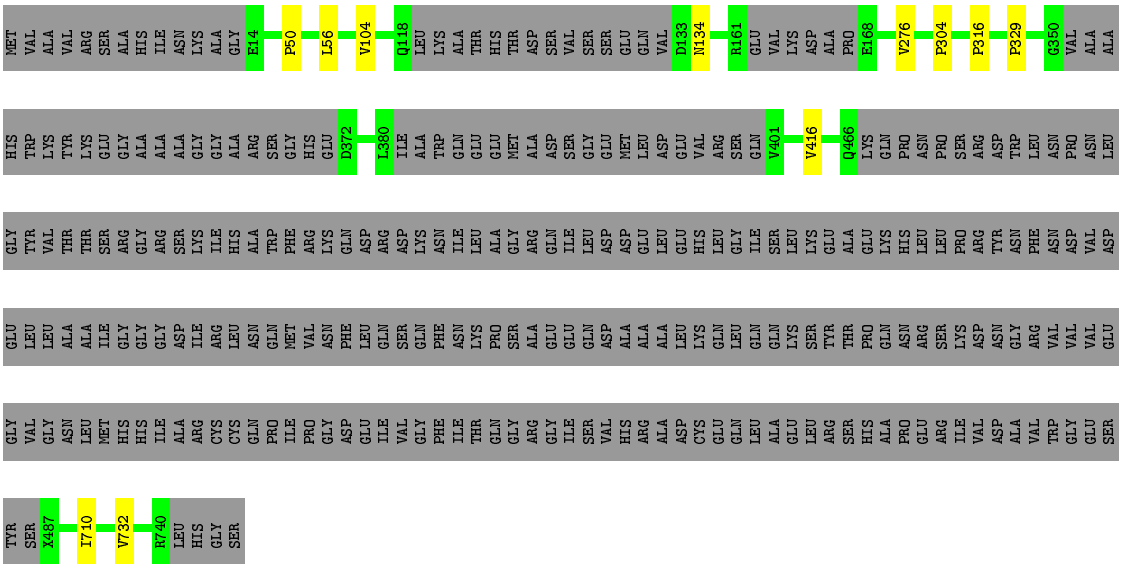


• Molecule 56: 30S ribosomal protein S19

Chain s:

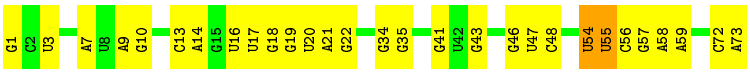
• Molecule 57: GTP pyrophosphokinase,GTP pyrophosphokinase,GTP pyrophosphokinase

Chain z:



• Molecule 58: deacylated A/R-tRNA

Chain y:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	24749	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3TD, OMC, OMG, OMU, MA6, H2U, YG, 2MA, 6MZ, 2MG, 5MC, UR3, 4OC, 4SU, 7MG, 5MU, 1MG, PSU

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	#$\|Z\|$ >2	RMSZ	#$\|Z\|$ >2
1	A	0.12	1/68920 (0.0%)	0.67	20/107498 (0.0%)
10	O	0.20	0/947	0.40	0/1268
11	P	0.20	0/1054	0.39	0/1403
12	Q	0.21	0/1093	0.41	0/1460
13	R	0.21	0/973	0.39	0/1301
14	S	0.20	0/902	0.35	0/1209
15	T	0.20	0/929	0.41	0/1242
16	U	0.21	0/960	0.35	0/1278
17	V	0.21	0/829	0.38	0/1107
18	W	0.19	0/864	0.39	0/1156
19	X	0.20	0/744	0.39	0/994
2	B	0.23	1/2876 (0.0%)	0.65	0/4483
20	Y	0.21	0/787	0.37	0/1051
21	Z	0.20	0/766	0.36	0/1025
22	0	0.20	0/582	0.35	0/769
23	1	0.19	0/635	0.36	0/848
24	2	0.21	0/510	0.36	0/677
25	3	0.21	0/453	0.41	0/605
26	4	0.21	0/531	0.40	0/709
27	5	0.19	0/450	0.36	0/599
28	6	0.21	0/416	0.41	0/554
29	7	0.20	0/380	0.36	0/498
3	D	0.20	0/2121	0.39	0/2852
30	8	0.21	0/513	0.42	0/676
31	9	0.19	0/303	0.38	0/397
32	a	0.13	1/36701 (0.0%)	0.66	5/57246 (0.0%)
33	b	0.21	0/1735	0.39	0/2338
34	c	0.21	0/1651	0.41	0/2225
35	d	0.21	0/1665	0.38	0/2227
36	e	0.22	0/1154	0.41	0/1554
37	f	0.21	0/835	0.39	0/1128

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >2	RMSZ	#|Z| >2
38	g	0.20	0/1195	0.39	0/1602
39	h	0.21	0/989	0.40	0/1326
4	E	0.21	0/1586	0.38	0/2134
40	i	0.21	0/1034	0.40	0/1375
41	j	0.21	0/796	0.42	0/1077
42	k	0.20	0/885	0.39	0/1195
43	l	0.21	0/969	0.42	0/1300
44	m	0.20	0/892	0.41	0/1193
45	o	0.20	0/722	0.35	0/964
46	p	0.20	0/659	0.35	0/884
47	q	0.22	0/657	0.43	0/881
48	r	0.20	0/511	0.40	0/689
49	t	0.20	0/671	0.34	0/888
5	F	0.20	0/1571	0.37	0/2113
50	u	0.21	0/500	0.38	0/668
51	v	0.10	0/144	0.64	0/222
52	x	0.27	1/1747 (0.1%)	0.64	0/2721
53	J	0.22	0/1001	0.43	0/1350
54	K	0.21	0/1046	0.41	0/1410
55	n	0.20	0/811	0.37	0/1081
56	s	0.20	0/652	0.37	0/877
57	z	0.16	0/1874	0.32	0/2332
58	y	0.29	1/1585 (0.1%)	0.66	0/2469
6	G	0.21	0/1434	0.40	0/1926
7	H	0.20	0/1343	0.37	0/1816
8	I	0.21	0/1122	0.38	0/1515
9	N	0.21	0/1152	0.39	0/1551
All	All	0.16	5/160827 (0.0%)	0.60	25/239936 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	35	0
32	a	17	0
52	x	9	0
58	y	9	0
All	All	70	0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	U	OP3-P	-10.62	1.48	1.61
58	y	1	G	OP3-P	-10.62	1.48	1.61
52	x	1	C	OP3-P	-10.58	1.48	1.61
32	a	2	A	OP3-P	-10.57	1.48	1.61
1	A	1	G	OP3-P	-10.54	1.48	1.61

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1049	C	C2-N3-C4	18.01	128.91	119.90
1	A	1050	A	N1-C2-N3	16.54	137.57	129.30
1	A	1073	A	N1-C2-N3	16.48	137.54	129.30
1	A	1050	A	C2-N3-C4	12.07	116.63	110.60
1	A	1073	A	C2-N3-C4	11.70	116.45	110.60
1	A	1049	C	N3-C4-C5	10.61	126.14	121.90
1	A	1073	A	C6-N1-C2	10.21	124.72	118.60
1	A	1050	A	C6-N1-C2	10.07	124.64	118.60
32	a	1158	C	N1-C2-O2	8.98	124.29	118.90
32	a	1158	C	C2-N1-C1'	8.38	128.02	118.80
1	A	1313	U	C2-N1-C1'	7.96	127.25	117.70
1	A	2884	U	C2-N1-C1'	7.82	127.09	117.70
32	a	1158	C	N3-C2-O2	-7.38	116.73	121.90
1	A	2884	U	N1-C2-O2	7.29	127.90	122.80
1	A	1313	U	N1-C2-O2	7.25	127.88	122.80
1	A	2884	U	N3-C2-O2	-6.77	117.46	122.20
1	A	1313	U	N3-C2-O2	-6.54	117.62	122.20
32	a	1158	C	C6-N1-C2	-5.82	117.97	120.30
1	A	51	G	OP2-P-O3'	5.76	117.88	105.20
1	A	1049	C	N1-C2-N3	5.75	123.22	119.20
32	a	1158	C	C6-N1-C1'	-5.73	113.93	120.80
1	A	893	C	P-O3'-C3'	5.42	126.20	119.70
1	A	1313	U	C6-N1-C1'	-5.19	113.94	121.20
1	A	51	G	P-O3'-C3'	5.14	125.87	119.70
1	A	2884	U	C6-N1-C1'	-5.01	114.19	121.20

All (70) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	746	PSU	C4',C2'
1	A	955	PSU	C4',C2'
1	A	1835	2MG	C2',C3'
1	A	1911	PSU	C4',C2'
1	A	1915	3TD	C4'

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Mol	Chain	Res	Type	Atom
1	A	1917	PSU	C4',C2'
1	A	1939	5MU	C4',C2',C3'
1	A	2069	7MG	C1'
1	A	2251	OMG	C3',C1'
1	A	2445	2MG	C2',C3'
1	A	2449	H2U	C1'
1	A	2457	PSU	C4',C2'
1	A	2498	OMC	C4',C2'
1	A	2503	2MA	C2',C1'
1	A	2504	PSU	C4',C2'
1	A	2552	OMU	C4'
1	A	2580	PSU	C4',C2'
1	A	2604	PSU	C4',C2'
1	A	2605	PSU	C4',C2'
32	a	516	PSU	C4',C2'
32	a	527	7MG	C1'
32	a	966	2MG	C2',C3'
32	a	1207	2MG	C2',C3'
32	a	1402	4OC	C2',C1'
32	a	1498	UR3	C2',C3'
32	a	1516	2MG	C2',C3'
32	a	1518	MA6	C2',C3'
32	a	1519	MA6	C2',C3'
52	x	8	4SU	C4',C2',C3'
52	x	20	H2U	C1'
52	x	54	5MU	C4',C2',C3'
52	x	55	PSU	C4',C2'
58	y	16	H2U	C1'
58	y	17	H2U	C1'
58	y	20	H2U	C1'
58	y	46	7MG	C1'
58	y	54	5MU	C4',C2',C3'
58	y	55	PSU	C4',C2'

There are no planarity outliers.

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	A	62057	0	31229	578	0
2	B	2572	0	1302	21	0
3	D	2082	0	2157	57	0
4	E	1565	0	1616	36	0
5	F	1552	0	1619	34	0
6	G	1410	0	1447	27	0
7	H	1323	0	1374	17	0
8	I	1111	0	1148	19	0
9	N	1129	0	1162	28	0
10	O	938	0	1012	26	0
11	P	1045	0	1117	32	0
12	Q	1074	0	1157	18	0
13	R	960	0	1000	25	0
14	S	892	0	923	10	0
15	T	917	0	965	20	0
16	U	947	0	1022	18	0
17	V	816	0	839	20	0
18	W	857	0	922	19	0
19	X	738	0	807	15	0
20	Y	779	0	834	16	0
21	Z	753	0	780	17	0
22	0	575	0	592	16	0
23	1	625	0	655	10	0
24	2	509	0	543	11	0
25	3	449	0	491	13	0
26	4	522	0	522	9	0
27	5	444	0	461	6	0
28	6	409	0	440	10	0
29	7	377	0	418	16	0
30	8	504	0	574	11	0
31	9	302	0	343	6	0
32	a	33029	0	16645	0	0
33	b	1704	0	1732	0	0
34	c	1624	0	1699	0	0
35	d	1643	0	1710	0	0
36	e	1141	0	1170	0	0
37	f	817	0	808	0	0
38	g	1181	0	1240	0	0
39	h	979	0	1034	0	0
40	i	1022	0	1070	0	0
41	j	786	0	828	0	0
42	k	869	0	878	0	0
43	l	955	0	1019	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	m	883	0	944	0	0
45	o	714	0	737	0	0
46	p	649	0	666	0	0
47	q	648	0	691	0	0
48	r	504	0	502	0	0
49	t	665	0	714	0	0
50	u	495	0	486	0	0
51	v	129	0	65	0	0
52	x	1644	0	840	0	0
53	J	988	0	1025	26	0
54	K	1032	0	1088	19	0
55	n	799	0	841	0	0
56	s	637	0	665	0	0
57	z	2255	0	592	0	0
58	y	1581	0	813	0	0
All	All	149606	0	99973	1013	0

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

All (1013) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:140:ILE:HG22	6:G:142:TYR:H	1.46	0.80
21:Z:9:ARG:HD3	21:Z:39:ALA:HB1	1.65	0.77
1:A:2279:G:HO2'	1:A:2327:A:HO2'	1.31	0.77
17:V:98:ILE:HG22	17:V:100:GLY:H	1.50	0.77
7:H:94:ARG:HB2	7:H:105:SER:HB2	1.68	0.76
5:F:146:VAL:HG12	5:F:185:LYS:HB2	1.69	0.75
22:0:33:ILE:HG22	22:0:34:VAL:HG23	1.69	0.74
11:P:23:ILE:HD13	17:V:84:ARG:HH22	1.52	0.73
53:J:73:LYS:HB3	53:J:117:LEU:HD11	1.69	0.73
1:A:38:A:H4'	5:F:45:ALA:HB3	1.71	0.73
1:A:2746:U:H5"	7:H:137:LYS:HE2	1.71	0.72
1:A:910:A:H62	12:Q:12:MET:HA	1.54	0.72
10:O:121:GLU:HG2	10:O:122:VAL:HG23	1.72	0.72
28:6:36:LYS:HE2	28:6:45:HIS:HD2	1.55	0.71
1:A:1060:U:H5'	1:A:1062:G:H5'	1.72	0.70
1:A:1759:A:HO2'	1:A:2714:G:HO2'	1.37	0.70
22:0:15:LYS:HG3	22:0:37:ARG:HH22	1.56	0.70
25:3:8:GLN:HB2	25:3:28:LEU:HD13	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2417:C:H5"	30:8:44:ARG:HE	1.56	0.70
5:F:75:SER:HB3	5:F:78:TRP:HD1	1.55	0.69
1:A:1046:A:H4'	53:J:61:ARG:HB3	1.74	0.69
1:A:210:C:OP1	29:7:29:GLN:NE2	2.24	0.68
1:A:2478:A:H5'	31:9:32:LYS:HE3	1.75	0.68
2:B:30:C:H1'	2:B:57:A:H61	1.58	0.68
1:A:45:G:H5"	1:A:46:G:H5'	1.75	0.68
13:R:28:LEU:HD23	13:R:48:VAL:HG21	1.75	0.67
3:D:143:VAL:HB	3:D:153:LEU:HB2	1.77	0.67
1:A:776:G:H22	1:A:2072:C:H5'	1.59	0.67
1:A:1363:C:O2'	1:A:1809:A:N3	2.27	0.67
1:A:910:A:N3	1:A:2264:C:O2'	2.28	0.67
1:A:51:G:H4'	1:A:52:A:H5'	1.77	0.67
10:O:105:ARG:NH2	15:T:40:GLN:OE1	2.28	0.66
7:H:104:LEU:HB2	7:H:112:VAL:HB	1.77	0.66
1:A:1320:C:N4	1:A:1330:C:OP2	2.28	0.66
1:A:2394:C:H5"	11:P:63:LYS:HE3	1.76	0.66
6:G:35:LEU:HB2	6:G:88:VAL:HB	1.76	0.66
1:A:747:5MC:O2'	18:W:88:ARG:NH1	2.29	0.65
5:F:117:ARG:NH2	5:F:183:PHE:O	2.27	0.65
15:T:59:THR:HG22	15:T:72:VAL:HG12	1.77	0.65
23:1:39:VAL:HG12	23:1:42:GLU:H	1.61	0.65
1:A:560:C:O2'	16:U:47:ARG:NH2	2.29	0.65
1:A:177:G:N2	1:A:177:G:OP2	2.28	0.65
14:S:108:ASP:OD1	14:S:111:ARG:NH1	2.30	0.65
1:A:1799:G:N2	1:A:1819:A:OP2	2.25	0.65
1:A:673:C:OP1	5:F:49:ARG:NH2	2.30	0.65
54:K:11:GLN:NE2	54:K:54:ILE:O	2.30	0.65
1:A:621:A:OP2	11:P:99:ASN:ND2	2.30	0.64
1:A:2032:G:N2	4:E:151:THR:OG1	2.30	0.64
24:2:16:THR:O	24:2:20:ASN:ND2	2.29	0.64
18:W:57:ASN:OD1	18:W:61:ASN:ND2	2.30	0.64
1:A:1054:A:H61	1:A:1105:U:H3	1.42	0.64
6:G:134:GLN:NE2	6:G:149:ARG:O	2.30	0.64
9:N:80:HIS:O	9:N:82:GLY:N	2.27	0.64
9:N:32:LEU:HD22	9:N:54:ILE:HG21	1.80	0.64
21:Z:77:VAL:HG23	21:Z:89:ILE:HG12	1.77	0.64
1:A:772:C:O2	3:D:42:ARG:NH1	2.31	0.64
6:G:62:GLN:HE22	6:G:90:LEU:HB3	1.62	0.64
11:P:33:ARG:NH2	11:P:39:LYS:O	2.31	0.64
1:A:572:A:H61	1:A:2029:G:H21	1.44	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:W:88:ARG:NH2	18:W:94:ASP:OD2	2.32	0.63
1:A:1992:G:N2	1:A:1996:C:O2'	2.31	0.63
1:A:291:G:H1	1:A:349:U:H3	1.46	0.63
1:A:466:A:OP1	29:7:34:ARG:NH1	2.31	0.63
1:A:444:C:OP2	5:F:44:ARG:NH2	2.32	0.63
1:A:672:C:OP2	11:P:42:SER:OG	2.17	0.63
21:Z:25:LYS:HG2	21:Z:43:ASP:HA	1.80	0.63
53:J:33:VAL:HG12	53:J:35:VAL:H	1.62	0.63
29:7:34:ARG:NH2	29:7:41:ARG:O	2.32	0.63
4:E:15:PHE:H	15:T:11:GLN:HE22	1.46	0.63
4:E:121:THR:HG21	4:E:143:PRO:HB3	1.81	0.63
1:A:684:G:O2'	1:A:788:A:N7	2.32	0.62
1:A:281:C:N3	1:A:359:G:N2	2.46	0.62
1:A:514:A:N3	1:A:581:C:O2'	2.31	0.62
1:A:1798:U:H5"	3:D:257:ARG:HB2	1.82	0.62
11:P:33:ARG:HD2	11:P:40:SER:HA	1.82	0.62
17:V:76:LYS:HB2	17:V:85:LYS:HB3	1.80	0.62
1:A:499:U:H5"	20:Y:42:LYS:HE2	1.82	0.62
26:4:28:VAL:HG11	26:4:32:LEU:HD13	1.82	0.62
1:A:1394:U:H4'	1:A:1603:A:H4'	1.82	0.62
6:G:147:ARG:HG3	6:G:149:ARG:H	1.64	0.62
1:A:144:A:H4'	19:X:2:ILE:HD11	1.82	0.62
1:A:2688:G:N1	1:A:2720:U:OP2	2.31	0.62
1:A:886:A:H2'	1:A:890:C:H42	1.65	0.61
10:O:19:VAL:HG12	10:O:43:ILE:HA	1.81	0.61
10:O:21:CYS:HA	10:O:41:ILE:HG22	1.82	0.61
1:A:2893:A:H5"	1:A:2894:G:H5'	1.81	0.61
11:P:49:GLY:HA3	11:P:58:TYR:HE2	1.64	0.61
1:A:1022:G:N2	1:A:1023:U:O4	2.31	0.61
1:A:563:A:N3	16:U:36:GLN:NE2	2.45	0.61
28:6:36:LYS:HE2	28:6:45:HIS:CD2	2.36	0.61
1:A:1072:C:N3	1:A:1092:C:N4	2.48	0.61
1:A:468:G:O6	29:7:39:ARG:NH2	2.33	0.61
1:A:574:A:N6	1:A:2034:U:OP1	2.33	0.61
25:3:12:ALA:HB1	25:3:20:LYS:HG2	1.82	0.61
1:A:453:A:N3	1:A:457:A:O2'	2.33	0.61
7:H:8:VAL:HB	7:H:49:LEU:HB2	1.83	0.61
8:I:108:VAL:HG12	8:I:110:VAL:H	1.66	0.61
1:A:1858:A:N6	1:A:1884:G:O2'	2.34	0.60
1:A:828:U:O4	1:A:858:G:N2	40.70	0.60
3:D:51:ARG:HH12	3:D:246:PRO:HG2	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:P:62:PRO:HB2	30:8:29:ARG:HH11	1.66	0.60
1:A:297:G:N2	1:A:300:A:OP2	13.06	0.60
1:A:674:G:H5"	5:F:71:GLY:H	1.65	0.60
1:A:1899:A:H4'	1:A:1901:A:H5"	1.82	0.60
1:A:1992:G:O2'	1:A:1997:C:N4	2.34	0.60
3:D:106:PRO:HG2	3:D:109:LEU:HB2	1.83	0.60
5:F:75:SER:HB3	5:F:78:TRP:CD1	2.36	0.60
13:R:38:LEU:HG	13:R:42:LYS:HE2	1.84	0.60
4:E:131:ASP:O	4:E:136:ASN:ND2	2.34	0.60
5:F:41:GLN:NE2	5:F:43:THR:OG1	2.34	0.60
53:J:26:VAL:HG21	53:J:114:GLU:HG2	1.83	0.60
9:N:17:VAL:HG23	9:N:137:PRO:HB2	1.84	0.60
11:P:78:ARG:NH2	11:P:80:SER:OG	2.35	0.60
11:P:101:ILE:HB	11:P:105:ILE:HG13	1.83	0.59
14:S:40:ILE:HG12	14:S:47:VAL:HG12	1.83	0.59
29:7:15:SER:O	29:7:21:ARG:NH2	2.35	0.59
1:A:2743:U:O2'	7:H:152:ARG:NH1	2.35	0.59
10:O:43:ILE:HD12	10:O:56:ASP:HB2	1.84	0.59
12:Q:42:THR:HA	12:Q:93:VAL:HG12	1.84	0.59
21:Z:86:LEU:HD13	21:Z:89:ILE:HD11	1.82	0.59
1:A:2262:U:OP1	22:0:37:ARG:NH2	2.36	0.59
1:A:1801:A:N6	1:A:2201:G:O2'	2.35	0.59
1:A:1416:G:O2'	1:A:1587:G:N2	2.35	0.59
6:G:176:PHE:O	26:4:47:LYS:NZ	2.36	0.59
53:J:88:HIS:HB2	53:J:89:PRO:HD3	1.83	0.59
10:O:29:HIS:CE1	10:O:31:ARG:HH12	2.20	0.59
11:P:93:ASN:O	11:P:95:LEU:N	2.34	0.59
1:A:977:G:H5'	16:U:54:ARG:HH22	1.68	0.59
24:2:25:GLN:HE21	24:2:50:VAL:HG21	1.66	0.59
9:N:35:ARG:HB2	9:N:54:ILE:HD11	1.84	0.59
17:V:34:GLU:HG2	17:V:60:LYS:HG2	1.84	0.59
15:T:52:ARG:H	15:T:56:SER:HB3	1.68	0.58
20:Y:17:ASP:HB3	20:Y:20:LYS:HD2	1.84	0.58
19:X:3:ARG:HH12	19:X:7:LEU:HD21	1.68	0.58
1:A:743:A:O2'	1:A:1659:G:OP1	2.20	0.58
25:3:10:ARG:NH2	25:3:52:PHE:O	2.37	0.58
2:B:3:C:H3'	2:B:4:C:H5"	1.85	0.58
13:R:43:GLU:OE2	13:R:46:ARG:NH2	2.36	0.58
1:A:527:C:N4	1:A:2777:G:O2'	2.37	0.58
19:X:1:MET:HG3	19:X:3:ARG:H	1.66	0.58
1:A:1818:U:H5'	3:D:156:SER:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:37:VAL:HG22	4:E:48:ILE:HG22	1.86	0.58
1:A:1199:U:H1'	16:U:3:VAL:HG22	1.85	0.58
1:A:2075:U:OP2	1:A:2238:G:O2'	2.22	0.58
21:Z:64:VAL:HG22	21:Z:69:GLU:HG2	1.85	0.58
1:A:2581:G:N2	1:A:2581:G:OP2	2.36	0.57
1:A:973:A:H5'	1:A:1188:U:H1'	1.85	0.57
1:A:2748:A:H5'	7:H:3:VAL:HG21	1.86	0.57
12:Q:64:TRP:HB2	12:Q:104:GLU:HB2	1.84	0.57
27:5:27:LEU:HD23	27:5:36:LYS:HB3	1.86	0.57
1:A:192:C:O2'	1:A:802:A:N3	2.32	0.57
7:H:32:LEU:HD21	7:H:136:ASP:HB2	1.85	0.57
1:A:2451:A:N6	1:A:2504:PSU:O2	2.38	0.57
1:A:771:G:OP2	29:7:11:LYS:NZ	2.38	0.57
11:P:29:LYS:HG2	11:P:30:THR:HG23	1.85	0.57
1:A:1406:U:O2	1:A:1517:G:N2	33.55	0.57
1:A:955:PSU:HN3	1:A:962:G:H1	1.53	0.57
6:G:104:THR:HA	26:4:38:SER:HB3	1.86	0.57
1:A:880:G:H1	1:A:897:C:H42	1.52	0.57
53:J:53:ARG:HB3	53:J:55:VAL:HG13	1.86	0.57
25:3:10:ARG:HD2	25:3:53:MET:HA	1.85	0.57
1:A:1062:G:N2	54:K:134:SER:OG	2.38	0.57
1:A:1343:G:O6	1:A:1403:A:N6	2.37	0.57
1:A:2291:U:OP1	1:A:2380:C:O2'	2.23	0.57
1:A:2420:C:H5"	28:6:7:LYS:HD2	1.87	0.57
1:A:643:A:N1	1:A:2369:A:O2'	2.38	0.57
1:A:63:A:N6	1:A:91:A:N1	2.47	0.57
54:K:61:TYR:HE2	54:K:67:THR:HG22	1.69	0.57
21:Z:76:ASP:HB3	21:Z:90:ASP:HB2	1.86	0.57
23:1:36:ARG:HA	23:1:47:THR:HA	1.86	0.57
1:A:1250:G:OP2	11:P:21:ARG:NH2	2.37	0.57
11:P:73:ILE:HD12	11:P:106:GLU:HB2	1.87	0.57
20:Y:28:LEU:HD12	20:Y:32:LYS:HB2	1.85	0.57
1:A:698:C:O2'	1:A:734:A:N6	2.37	0.56
5:F:48:THR:OG1	5:F:51:GLU:OE1	2.16	0.56
1:A:1218:G:OP2	16:U:14:LYS:NZ	2.36	0.56
18:W:6:LYS:HA	18:W:104:THR:HA	1.86	0.56
1:A:2331:G:H4'	22:0:39:THR:H	1.69	0.56
1:A:1323:C:OP1	18:W:98:LYS:NZ	2.38	0.56
5:F:45:ALA:HB2	5:F:89:PRO:HD3	1.87	0.56
22:0:15:LYS:HG3	22:0:37:ARG:NH2	2.20	0.56
6:G:59:ILE:O	6:G:101:ARG:NH1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:J:3:LEU:HD12	53:J:5:LEU:H	1.69	0.56
1:A:952:G:OP1	12:Q:18:ARG:NH2	2.38	0.56
13:R:78:LYS:HE2	13:R:83:LEU:HD21	1.86	0.56
1:A:1796:U:H2'	1:A:1797:G:H8	1.71	0.56
1:A:747:5MC:H3'	1:A:748:G:H5'	1.88	0.56
5:F:40:ARG:HG2	5:F:42:GLY:H	1.69	0.56
9:N:64:VAL:HB	9:N:68:LYS:HE3	1.86	0.56
18:W:20:VAL:HG11	18:W:44:ALA:HA	1.87	0.56
1:A:198:C:H1'	1:A:2434:A:H61	1.71	0.56
1:A:962:G:HO2'	1:A:2496:C:HO2'	1.51	0.56
18:W:80:PRO:O	18:W:100:THR:OG1	2.20	0.56
1:A:1187:G:N2	1:A:1188:U:O4	2.39	0.56
1:A:2576:G:O2'	1:A:2579:C:OP2	2.24	0.56
10:O:112:PHE:HD1	10:O:115:ILE:HD12	1.71	0.56
1:A:1528:A:N6	1:A:1543:G:O2'	2.40	0.55
1:A:451:U:O2	1:A:453:A:N6	2.38	0.55
1:A:824:U:O2'	1:A:2358:A:N6	2.37	0.55
1:A:597:G:O2'	11:P:11:GLY:O	2.22	0.55
1:A:911:A:N6	12:Q:11:LYS:O	2.29	0.55
1:A:684:G:OP1	29:7:21:ARG:NH1	2.39	0.55
1:A:2618:G:H21	4:E:155:VAL:HG21	1.71	0.55
1:A:1073:A:C6	1:A:1073:A:C4	2.95	0.55
1:A:1323:C:N4	1:A:1324:G:O6	2.39	0.55
2:B:24:G:N2	2:B:27:C:N3	2.54	0.55
2:B:54:G:N2	6:G:25:MET:SD	2.78	0.55
18:W:4:ILE:HD12	18:W:6:LYS:HE3	1.87	0.55
1:A:2061:G:H5"	1:A:2503:2MA:HM22	1.88	0.55
17:V:61:ALA:HB1	17:V:96:VAL:HB	1.89	0.55
1:A:1296:G:OP1	1:A:2709:G:O2'	2.21	0.55
1:A:463:G:N2	1:A:466:A:OP2	2.30	0.55
1:A:2831:G:OP2	4:E:59:ARG:NH1	2.40	0.55
54:K:44:LYS:HE2	54:K:70:THR:HG21	1.89	0.55
1:A:1355:G:H2'	1:A:1356:G:H8	1.72	0.55
1:A:1818:U:C5	3:D:155:ARG:HD3	2.41	0.55
5:F:76:PRO:HA	5:F:82:GLY:HA3	1.87	0.55
1:A:1613:G:H4'	29:7:3:ARG:HE	1.72	0.55
1:A:1154:G:OP2	16:U:57:ARG:NH1	2.34	0.55
1:A:1998:A:OP2	4:E:141:ARG:NH1	2.35	0.55
1:A:2709:G:H5'	13:R:22:ARG:HH22	1.71	0.55
7:H:6:ALA:O	7:H:68:ARG:NE	2.38	0.55
1:A:1050:A:C6	1:A:1050:A:C4	2.95	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:G:OP1	1:A:1255:U:O2'	2.21	0.54
1:A:793:A:OP2	1:A:2071:A:O2'	2.20	0.54
53:J:48:ALA:HB3	53:J:51:TYR:HE2	1.72	0.54
9:N:95:ARG:HG2	9:N:96:ARG:HG2	1.88	0.54
22:0:21:ARG:HB2	22:0:33:ILE:HG23	1.89	0.54
19:X:14:PRO:HD3	24:2:30:MET:HG3	1.89	0.54
11:P:127:VAL:HG21	11:P:142:ILE:HG21	1.88	0.54
30:8:32:LEU:HB3	30:8:40:LYS:HD3	1.89	0.54
1:A:1826:G:O2'	1:A:1971:U:OP2	2.20	0.54
14:S:20:GLU:OE2	22:0:58:LYS:NZ	2.41	0.54
16:U:87:VAL:HG12	16:U:89:ILE:H	1.71	0.54
5:F:91:ASP:OD2	5:F:93:SER:OG	2.25	0.54
6:G:1:ALA:N	6:G:100:GLU:OE1	2.39	0.54
17:V:16:GLU:HG3	17:V:100:GLY:HA2	1.89	0.54
1:A:111:A:O2'	24:2:58:ASN:ND2	2.41	0.54
1:A:2069:7MG:H2'	1:A:2070:A:H8	1.73	0.54
1:A:806:C:O2	1:A:2444:G:O2'	2.25	0.54
29:7:12:ARG:HE	29:7:44:VAL:HG21	1.72	0.54
1:A:2857:G:N2	1:A:2860:A:OP2	2.33	0.54
12:Q:34:LYS:HE3	12:Q:131:VAL:HG11	1.90	0.54
30:8:22:LYS:HB2	30:8:46:LYS:HB3	1.89	0.53
1:A:2788:C:O2'	1:A:2809:A:N3	2.38	0.53
1:A:1020:A:H4'	1:A:1021:A:O5'	2.07	0.53
1:A:1824:G:H5"	3:D:51:ARG:HH21	1.72	0.53
1:A:2249:U:N3	1:A:2253:G:OP2	2.39	0.53
1:A:2059:A:N6	1:A:2503:2MA:H1'	2.23	0.53
1:A:321:U:H5"	5:F:131:THR:HG23	1.89	0.53
3:D:69:ASN:HA	3:D:188:ARG:HH12	1.73	0.53
8:I:28:ASN:OD1	23:1:35:HIS:NE2	2.37	0.53
23:1:16:ASN:N	23:1:24:THR:O	2.38	0.53
1:A:2744:G:N2	7:H:142:GLN:OE1	2.34	0.53
18:W:56:ALA:HA	18:W:59:GLU:HG2	1.91	0.53
1:A:1266:G:N2	1:A:1269:A:OP2	13.06	0.53
2:B:95:U:H2'	2:B:96:G:H8	1.74	0.53
1:A:682:G:O6	1:A:794:A:N6	2.42	0.53
1:A:2676:C:OP1	10:O:31:ARG:NH2	2.42	0.53
13:R:76:VAL:HA	13:R:79:LEU:HD12	1.90	0.53
1:A:1182:G:H5'	1:A:1183:U:OP1	5.97	0.52
1:A:575:A:OP2	1:A:2499:C:O2'	2.27	0.52
4:E:46:ARG:NH2	4:E:89:GLU:OE1	2.42	0.52
53:J:94:ARG:HD3	53:J:131:THR:HG22	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:R:103:ARG:HG2	13:R:105:GLY:H	1.72	0.52
3:D:184:GLU:HG3	3:D:186:ASP:H	1.74	0.52
1:A:1864:U:OP1	1:A:2410:G:O2'	2.28	0.52
1:A:693:A:O2'	1:A:1353:A:N3	2.42	0.52
27:5:39:ARG:O	27:5:41:HIS:ND1	2.35	0.52
1:A:320:A:N3	5:F:163:ASN:ND2	2.57	0.52
1:A:1272:A:O2'	1:A:1274:A:OP1	2.23	0.52
15:T:105:LYS:HB3	15:T:108:ARG:HH22	1.73	0.52
1:A:1905:C:N4	1:A:1969:A:OP2	2.42	0.52
1:A:2267:A:H5"	1:A:2268:A:H5'	1.91	0.52
1:A:2278:A:OP1	12:Q:11:LYS:NZ	2.34	0.52
1:A:538:A:H4'	9:N:7:LYS:HG2	1.90	0.52
1:A:781:A:OP1	3:D:216:ARG:NH2	2.36	0.52
3:D:130:PRO:HA	3:D:188:ARG:HA	1.91	0.52
54:K:91:LYS:HG3	54:K:94:LYS:HE2	1.92	0.52
17:V:68:ARG:HH11	17:V:90:ARG:HB2	1.74	0.52
1:A:1792:G:O2'	1:A:1830:C:OP1	2.27	0.52
1:A:28:A:O2'	1:A:296:U:OP1	48.98	0.52
1:A:767:U:H2'	1:A:768:G:H8	1.75	0.52
9:N:17:VAL:HG22	9:N:55:ILE:HB	1.90	0.52
10:O:8:LEU:HB2	10:O:19:VAL:HG23	1.91	0.52
1:A:328:U:H4'	20:Y:65:GLN:HG3	1.91	0.52
1:A:244:A:H5"	11:P:67:THR:HG21	1.91	0.52
1:A:619:G:H3'	1:A:620:G:H21	1.75	0.52
1:A:2002:G:H5"	13:R:9:GLN:HE21	1.75	0.52
1:A:2258:C:O2'	1:A:2427:C:OP2	2.24	0.52
54:K:107:GLU:O	54:K:110:GLN:NE2	2.43	0.52
1:A:1693:U:O2'	3:D:13:ARG:NH1	2.43	0.51
1:A:2092:U:OP2	8:I:28:ASN:ND2	2.41	0.51
1:A:2440:C:H5"	1:A:2587:A:H4'	1.91	0.51
1:A:568:U:H1'	1:A:2030:6MZ:H9C1	1.92	0.51
26:4:26:SER:OG	26:4:27:THR:N	2.43	0.51
1:A:690:G:H1	1:A:772:C:H42	1.57	0.51
1:A:830:G:H22	1:A:2446:G:H5'	1.76	0.51
1:A:2039:U:H2'	1:A:2040:G:C8	2.45	0.51
3:D:2:VAL:HG22	3:D:18:VAL:HG13	1.92	0.51
20:Y:40:LEU:HD23	20:Y:61:GLU:HG3	1.92	0.51
1:A:676:A:H62	1:A:802:A:H61	1.58	0.51
4:E:24:VAL:HG12	4:E:178:VAL:HG21	1.91	0.51
1:A:518:G:OP2	27:5:12:ARG:NH2	2.40	0.51
1:A:2006:C:O2'	1:A:2823:A:N3	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1571:A:H2'	1:A:1572:A:C8	2.46	0.51
27:5:30:ASP:HB3	27:5:34:GLY:H	1.75	0.51
1:A:968:C:H2'	1:A:969:G:C8	2.46	0.51
10:O:64:ARG:HB2	10:O:83:ALA:HB3	1.93	0.51
7:H:88:LEU:HD23	7:H:93:TYR:HB3	1.93	0.51
12:Q:4:PRO:HG2	12:Q:92:TRP:CZ3	2.46	0.51
1:A:2283:C:OP1	28:6:3:GLY:N	2.44	0.51
1:A:1450:G:H21	1:A:1452:G:H1	1.57	0.51
1:A:2039:U:H2'	1:A:2040:G:H8	1.75	0.51
22:0:42:HIS:CD2	22:0:73:ARG:HD3	2.46	0.50
1:A:1158:C:O2	1:A:1158:C:H2'	2.94	0.50
1:A:2144:G:O2'	1:A:2147:A:N1	2.43	0.50
1:A:2645:G:N2	1:A:2645:G:OP2	2.32	0.50
1:A:2794:C:H42	1:A:2802:G:H1	1.59	0.50
6:G:92:GLY:O	6:G:95:MET:HG2	2.11	0.50
8:I:80:ILE:HG22	8:I:82:SER:H	1.75	0.50
1:A:1187:G:H5"	17:V:83:TYR:CZ	2.46	0.50
1:A:2370:G:H4'	28:6:43:ARG:HH11	1.76	0.50
1:A:714:U:N3	1:A:717:C:OP2	2.40	0.50
1:A:918:A:N3	2:B:80:U:O2'	2.39	0.50
3:D:243:PRO:O	3:D:250:GLN:NE2	2.44	0.50
3:D:77:VAL:HG22	3:D:93:VAL:HG22	1.92	0.50
4:E:130:GLN:OE1	4:E:139:SER:OG	2.24	0.50
15:T:26:GLU:HA	15:T:43:GLU:HA	1.92	0.50
1:A:1261:C:OP2	18:W:83:LYS:NZ	2.34	0.50
15:T:47:ILE:HA	15:T:96:LEU:HD12	1.94	0.50
1:A:1287:A:OP2	13:R:103:ARG:NH1	2.38	0.50
1:A:2595:G:N2	1:A:2598:A:OP2	2.35	0.50
1:A:863:A:OP1	12:Q:22:GLN:NE2	2.44	0.50
1:A:1656:C:P	4:E:141:ARG:HE	2.35	0.50
8:I:30:LEU:HB3	8:I:36:ALA:HB3	1.92	0.50
1:A:1153:C:OP1	16:U:91:ARG:NH2	2.44	0.50
22:0:17:LEU:O	22:0:20:LYS:NZ	2.45	0.50
1:A:1863:G:H4'	1:A:2411:A:H4'	1.94	0.50
1:A:2787:C:H1'	4:E:63:PRO:HG3	1.93	0.50
1:A:790:U:H3	1:A:795:C:H5'	1.76	0.50
4:E:10:GLY:H	4:E:197:THR:HG23	1.77	0.50
1:A:1940:U:H4'	1:A:1941:C:O5'	2.11	0.50
1:A:2598:A:H5"	3:D:233:GLY:HA3	1.94	0.50
1:A:1162:G:H2'	1:A:1163:G:H8	1.77	0.50
1:A:322:A:H5'	1:A:340:A:H1'	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:W:29:VAL:HG22	18:W:71:VAL:HG23	1.94	0.50
29:7:39:ARG:HG2	29:7:41:ARG:H	1.76	0.50
1:A:1255:U:O4'	1:A:2502:G:N2	2.44	0.50
1:A:780:G:O2'	1:A:783:A:N6	2.44	0.50
4:E:48:ILE:HG23	4:E:84:LEU:HD21	1.94	0.50
29:7:30:VAL:O	29:7:34:ARG:HG2	2.11	0.50
1:A:1378:A:OP1	29:7:14:ARG:NH1	2.44	0.50
1:A:299:A:N3	1:A:319:G:O2'	2.38	0.50
1:A:518:G:OP1	18:W:18:ARG:NH1	2.30	0.50
1:A:1283:G:N1	1:A:1286:A:OP2	2.44	0.49
8:I:9:VAL:HB	8:I:13:GLY:HA3	1.94	0.49
1:A:958:U:H5	12:Q:40:ARG:HH21	1.59	0.49
1:A:2680:U:O2'	4:E:11:MET:SD	2.70	0.49
1:A:372:G:O2'	1:A:373:U:O5'	2.28	0.49
6:G:97:GLU:OE2	26:4:25:ARG:N	2.43	0.49
1:A:190:A:H5"	1:A:204:A:H61	1.76	0.49
3:D:106:PRO:HD2	3:D:109:LEU:HD22	1.93	0.49
8:I:115:VAL:HG21	53:J:62:ARG:HB2	190.85	0.49
1:A:495:G:O2'	18:W:61:ASN:ND2	2.45	0.49
1:A:674:G:H5"	5:F:71:GLY:N	2.26	0.49
1:A:746:PSU:H1'	1:A:748:G:H21	1.77	0.49
1:A:747:5MC:H3'	1:A:748:G:C5'	2.43	0.49
3:D:204:LEU:HD21	3:D:213:ARG:HH21	1.77	0.49
3:D:206:LYS:HD3	3:D:212:TRP:HH2	1.76	0.49
53:J:23:LEU:HD21	53:J:96:PHE:HB2	1.94	0.49
1:A:1937:A:H62	1:A:1940:U:H5	1.59	0.49
1:A:471:A:OP1	5:F:79:ARG:NH1	2.42	0.49
6:G:56:LEU:HB2	6:G:64:PRO:HG3	1.94	0.49
10:O:12:ASP:HB3	10:O:99:ILE:HG12	1.94	0.49
1:A:1026:G:H2'	1:A:1027:A:H8	1.77	0.49
1:A:942:G:OP2	11:P:39:LYS:NZ	2.46	0.49
1:A:1798:U:OP2	3:D:270:ARG:NH2	2.40	0.49
1:A:783:A:H2'	1:A:784:G:H4'	1.95	0.49
1:A:774:G:N2	1:A:787:C:O2'	2.46	0.49
9:N:77:HIS:HD1	9:N:79:GLY:H	1.60	0.49
11:P:79:LEU:H	11:P:113:ALA:HB3	1.78	0.49
15:T:74:GLN:HB2	15:T:77:SER:HB2	1.94	0.49
15:T:88:ARG:HH11	15:T:112:ARG:NH1	2.11	0.49
1:A:1048:A:OP2	1:A:1110:G:N2	2.45	0.49
1:A:676:A:HO2'	1:A:2442:C:HO2'	1.56	0.49
1:A:993:G:OP2	16:U:50:ARG:NH2	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:133:THR:OG1	4:E:134:HIS:N	2.45	0.49
54:K:33:ASN:OD1	54:K:34:ILE:N	2.46	0.49
10:O:2:ILE:HD12	10:O:8:LEU:HD21	1.95	0.49
1:A:663:G:H5"	11:P:17:LYS:HD3	1.94	0.49
29:7:34:ARG:HH21	29:7:39:ARG:HD2	1.78	0.49
1:A:1509:A:H2'	1:A:1510:G:C8	2.48	0.49
1:A:2069:7MG:H2'	1:A:2070:A:C8	2.48	0.49
1:A:2540:C:O2'	1:A:2740:A:N3	2.45	0.49
16:U:47:ARG:NH2	16:U:51:GLN:OE1	2.46	0.49
1:A:1225:G:H5'	17:V:88:GLY:H	1.77	0.49
1:A:1787:A:OP1	3:D:237:ARG:NH2	2.46	0.48
1:A:1915:3TD:H3'	1:A:1916:A:H8	1.76	0.48
1:A:2081:U:H5"	23:1:16:ASN:HD22	1.78	0.48
53:J:67:THR:HG21	53:J:75:ALA:HB2	1.95	0.48
11:P:95:LEU:HB3	11:P:100:ILE:HD11	1.94	0.48
1:A:1528:A:OP2	1:A:1543:G:N2	2.47	0.48
9:N:24:THR:HB	9:N:27:ARG:HB2	1.95	0.48
19:X:23:ALA:O	19:X:28:ASN:N	2.46	0.48
22:0:55:LEU:HD12	22:0:76:ILE:HD12	1.95	0.48
28:6:3:GLY:O	28:6:5:ARG:N	2.43	0.48
1:A:1447:C:O2'	1:A:1544:A:N3	2.43	0.48
1:A:1818:U:H4'	1:A:1821:A:H1'	1.94	0.48
1:A:2086:U:H2'	1:A:2087:G:C8	2.48	0.48
1:A:2508:G:H1	1:A:2580:PSU:HN3	1.61	0.48
28:6:8:ILE:HD13	28:6:24:LYS:HE3	1.96	0.48
1:A:942:G:O2'	1:A:1189:A:N3	2.44	0.48
22:0:19:VAL:HG13	22:0:34:VAL:HG22	1.95	0.48
1:A:1364:G:N2	1:A:1367:A:OP2	2.42	0.48
1:A:2391:G:O2'	1:A:2392:A:O5'	2.23	0.48
1:A:2771:C:O2'	4:E:173:GLN:NE2	2.45	0.48
1:A:648:G:H2'	1:A:649:G:H8	1.78	0.48
3:D:141:HIS:ND1	3:D:192:GLY:O	2.46	0.48
1:A:2305:U:H5"	6:G:130:GLY:HA3	1.96	0.48
10:O:30:ARG:NH2	10:O:37:ASP:OD2	2.29	0.48
1:A:742:A:H2'	1:A:743:A:C8	2.49	0.48
1:A:953:G:H2'	1:A:954:G:C8	2.49	0.48
2:B:1:U:H2'	2:B:2:G:C8	2.49	0.48
1:A:973:A:H5"	17:V:81:LYS:HD2	1.96	0.48
9:N:56:VAL:HB	9:N:124:VAL:HA	1.96	0.48
10:O:9:ASN:OD1	10:O:18:ARG:NH1	2.47	0.48
1:A:1068:G:N2	1:A:1095:A:O2'	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1321:A:O2'	18:W:11:ARG:NH2	2.36	0.48
5:F:18:THR:HG23	5:F:106:LYS:HG2	1.96	0.48
9:N:37:ARG:HH22	9:N:110:PRO:HG3	1.79	0.48
14:S:33:ARG:HG2	14:S:34:HIS:CD2	2.49	0.48
2:B:116:G:H5'	14:S:55:GLU:HG2	1.96	0.48
1:A:1364:G:H5'	1:A:1809:A:H1'	1.96	0.48
53:J:59:LEU:HB3	53:J:62:ARG:HB3	1.96	0.48
9:N:55:ILE:HD11	9:N:132:HIS:HB2	1.95	0.48
17:V:69:GLY:N	17:V:91:GLN:O	2.39	0.48
1:A:1514:G:O2'	1:A:1557:C:O2'	2.32	0.47
1:A:2271:G:H5'	22:0:16:ARG:HD3	1.95	0.47
2:B:88:C:O2'	2:B:89:U:O5'	2.23	0.47
7:H:97:VAL:HG22	7:H:102:ILE:HG23	1.95	0.47
54:K:108:ILE:O	54:K:111:THR:OG1	2.26	0.47
1:A:1137:G:H2'	1:A:1138:G:H8	1.79	0.47
1:A:1201:U:H2'	1:A:1202:G:H8	1.78	0.47
1:A:2313:C:H2'	1:A:2314:A:C8	2.49	0.47
5:F:18:THR:HA	5:F:106:LYS:HE3	1.95	0.47
1:A:2548:U:O2'	10:O:4:GLU:OE2	2.31	0.47
17:V:14:VAL:HG21	17:V:98:ILE:HG13	1.95	0.47
19:X:59:ASN:OD1	19:X:84:TYR:HB2	2.14	0.47
25:3:16:LEU:HB2	25:3:19:HIS:HD2	1.79	0.47
1:A:1000:A:OP2	1:A:1154:G:N1	2.36	0.47
1:A:830:G:N3	1:A:2448:A:N6	2.63	0.47
1:A:290:U:H2'	1:A:291:G:C8	2.50	0.47
1:A:326:G:H2'	1:A:327:G:H8	1.80	0.47
1:A:395:U:H2'	1:A:396:G:C8	2.49	0.47
1:A:546:U:H2'	1:A:547:A:H4'	1.95	0.47
3:D:56:GLY:HA2	3:D:212:TRP:HA	1.95	0.47
2:B:91:C:OP1	12:Q:38:ARG:NH2	2.47	0.47
1:A:1032:A:H1'	31:9:23:ILE:HD13	1.95	0.47
1:A:2069:7MG:O6	1:A:2443:C:N4	2.48	0.47
1:A:2316:G:H4'	6:G:124:ARG:HH21	1.79	0.47
6:G:129:MET:HG2	6:G:153:ILE:HB	1.96	0.47
53:J:36:ASP:O	53:J:39:THR:OG1	2.23	0.47
1:A:95:A:O2'	24:2:41:HIS:ND1	2.42	0.47
26:4:11:GLU:HA	26:4:25:ARG:HA	1.97	0.47
1:A:1800:C:N4	1:A:1818:U:O2'	2.48	0.47
1:A:2439:A:H61	1:A:2585:U:H4'	1.80	0.47
1:A:500:G:N1	1:A:503:A:OP2	2.47	0.47
9:N:36:LEU:HD22	9:N:121:LYS:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1158:C:H5"	25:3:30:ARG:HD2	1.97	0.47
1:A:2144:G:H1'	1:A:2147:A:H61	1.79	0.47
53:J:103:ASN:HA	53:J:107:GLU:HB3	1.95	0.47
53:J:24:SER:HB2	53:J:116:GLU:HG3	1.96	0.47
15:T:70:GLU:OE2	15:T:100:ARG:NH1	2.47	0.47
17:V:14:VAL:HG22	17:V:15:SER:O	2.14	0.47
1:A:851:C:O2'	25:3:42:ALA:O	2.33	0.47
25:3:53:MET:HG3	25:3:54:VAL:HG13	1.97	0.47
27:5:42:ILE:HG22	27:5:48:TYR:HB2	1.95	0.47
1:A:1019:U:H3	1:A:1142:A:H62	1.63	0.47
1:A:749:A:H5'	1:A:1271:G:H1'	1.97	0.47
3:D:28:PRO:HB2	3:D:33:LEU:HD11	1.96	0.47
53:J:121:SER:OG	53:J:122:GLN:N	2.45	0.47
1:A:2899:A:H4'	9:N:136:GLN:HE22	1.80	0.47
12:Q:14:LYS:O	12:Q:71:LYS:NZ	2.42	0.47
16:U:68:ALA:HB1	16:U:73:ILE:HG23	1.96	0.47
1:A:669:G:N2	1:A:672:C:OP1	2.40	0.47
1:A:676:A:O2'	1:A:2442:C:O2'	2.28	0.47
1:A:1307:A:N6	1:A:1606:C:O2'	2.48	0.47
1:A:1935:G:N2	1:A:1964:G:O4'	2.47	0.47
1:A:2372:U:H2'	1:A:2373:G:H8	1.80	0.47
1:A:581:C:H2'	1:A:582:A:C8	2.50	0.47
1:A:586:A:N1	1:A:809:G:O2'	2.42	0.47
25:3:16:LEU:HB2	25:3:19:HIS:CD2	2.50	0.47
1:A:2339:C:H2'	1:A:2340:A:C8	2.50	0.47
1:A:2830:C:O2'	1:A:2883:A:N1	2.44	0.47
4:E:16:THR:OG1	4:E:18:ASP:OD1	2.33	0.47
11:P:56:PRO:HD2	11:P:59:ARG:HD3	1.96	0.47
1:A:468:G:H5"	5:F:55:SER:HB3	1.97	0.47
1:A:1754:A:N1	1:A:2716:C:O2'	2.46	0.46
1:A:2399:G:H2'	1:A:2400:G:H8	1.80	0.46
1:A:968:C:H2'	1:A:969:G:H8	1.80	0.46
10:O:40:LYS:HE3	10:O:57:VAL:HG12	1.97	0.46
13:R:35:LYS:NZ	13:R:110:MET:SD	2.78	0.46
1:A:1849:G:H2'	1:A:1850:G:H8	1.80	0.46
53:J:39:THR:OG1	53:J:40:GLU:OE1	2.34	0.46
1:A:1022:G:H4'	1:A:1023:U:O5'	2.16	0.46
1:A:2326:C:O2'	1:A:2327:A:OP1	2.30	0.46
1:A:993:G:O6	1:A:1045:C:N4	82.65	0.46
10:O:34:GLY:O	10:O:36:GLY:N	2.48	0.46
16:U:17:LEU:HA	16:U:20:ALA:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Y:52:ASN:OD1	20:Y:53:GLN:N	2.48	0.46
12:Q:34:LYS:HD3	21:Z:82:TYR:HA	1.97	0.46
13:R:78:LYS:HG2	13:R:83:LEU:HG	1.97	0.46
20:Y:5:ARG:HG2	20:Y:93:ARG:HH22	1.81	0.46
1:A:1037:G:N2	1:A:1118:C:O2	2.39	0.46
3:D:65:ASP:HB2	3:D:101:ARG:HB3	1.97	0.46
7:H:21:GLN:NE2	7:H:37:ASN:O	2.48	0.46
7:H:37:ASN:OD1	7:H:38:ASP:N	2.48	0.46
10:O:1:MET:HG3	10:O:32:TYR:CG	2.50	0.46
25:3:46:MET:O	25:3:50:VAL:HG22	2.16	0.46
1:A:1165:A:H2'	1:A:1166:G:H8	1.79	0.46
1:A:2120:G:H2'	1:A:2121:G:C8	2.50	0.46
1:A:2189:U:H2'	1:A:2190:G:C8	2.51	0.46
1:A:1915:3TD:H3'	1:A:1916:A:C8	2.51	0.46
1:A:266:G:O6	1:A:270:A:N6	13.02	0.46
54:K:4:VAL:HA	54:K:7:TYR:HE2	1.80	0.46
28:6:26:LYS:NZ	28:6:30:PRO:O	2.49	0.46
1:A:1415:U:H2'	1:A:1416:G:H4'	1.98	0.46
1:A:225:C:H2'	1:A:226:A:O4'	2.16	0.46
9:N:15:TRP:HB3	9:N:137:PRO:HB3	1.98	0.46
1:A:1258:U:H2'	1:A:1259:G:C8	2.51	0.46
1:A:2087:G:H2'	1:A:2088:A:C8	2.51	0.46
1:A:2623:G:H2'	1:A:2624:G:C8	2.51	0.46
1:A:953:G:H2'	1:A:954:G:H8	1.80	0.46
2:B:76:G:OP1	21:Z:9:ARG:NH2	2.46	0.46
5:F:131:THR:HG22	5:F:160:ALA:HA	1.97	0.46
15:T:47:ILE:HB	15:T:96:LEU:HB2	1.98	0.46
1:A:1992:G:HO2'	1:A:1997:C:H42	1.64	0.46
6:G:137:PHE:HA	6:G:138:PRO:HD3	1.85	0.46
1:A:2816:G:H5"	13:R:99:LYS:HE2	1.97	0.46
20:Y:34:ILE:HG12	20:Y:63:ALA:HA	1.98	0.46
21:Z:32:GLY:O	21:Z:93:ARG:NH1	2.49	0.46
1:A:1837:C:O2'	1:A:1927:A:N3	2.42	0.45
1:A:2830:C:H3'	4:E:59:ARG:HH11	1.81	0.45
1:A:538:A:H5"	9:N:7:LYS:HE3	1.97	0.45
6:G:1:ALA:N	6:G:97:GLU:OE1	2.46	0.45
54:K:74:PRO:HG2	54:K:77:VAL:HG22	1.97	0.45
1:A:1566:A:O2'	1:A:1568:G:N2	2.49	0.45
1:A:2681:C:OP2	4:E:114:LYS:NZ	2.49	0.45
1:A:534:U:H2'	1:A:535:G:H8	1.81	0.45
8:I:124:THR:O	8:I:128:HIS:NE2	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:N:51:GLY:O	9:N:121:LYS:NZ	2.40	0.45
17:V:32:THR:OG1	17:V:61:ALA:O	2.27	0.45
1:A:1213:A:N6	1:A:1236:G:H1'	2.32	0.45
1:A:13:A:O2'	1:A:15:G:N7	2.48	0.45
1:A:106:C:H2'	1:A:107:G:C8	2.66	0.45
1:A:2033:A:O2'	1:A:2035:G:OP1	2.34	0.45
1:A:1129:A:O2'	1:A:2515:C:O2	2.32	0.45
4:E:51:THR:HB	4:E:79:LEU:HD23	1.98	0.45
19:X:80:TRP:HZ3	19:X:82:LYS:HB3	1.80	0.45
1:A:789:A:H5'	29:7:4:THR:HG21	1.98	0.45
1:A:215:G:H4'	1:A:216:A:H4'	1.99	0.45
1:A:2772:C:H5'	4:E:173:GLN:HE21	1.81	0.45
1:A:326:G:H2'	1:A:327:G:C8	2.52	0.45
1:A:405:U:H3'	1:A:406:G:H5'	3.72	0.45
1:A:598:U:H2'	1:A:599:A:C8	2.52	0.45
1:A:1022:G:H1'	1:A:1023:U:OP2	2.16	0.45
1:A:1363:C:H2'	1:A:1364:G:H8	1.81	0.45
1:A:1902:C:H5"	3:D:239:PHE:HE2	1.81	0.45
1:A:2453:A:H2'	1:A:2454:G:C8	2.52	0.45
1:A:334:C:OP1	1:A:335:C:N4	2.47	0.45
11:P:71:ALA:O	11:P:74:THR:HG22	2.17	0.45
1:A:85:G:OP1	20:Y:6:ARG:N	2.50	0.45
22:0:66:GLU:HB2	22:0:75:PHE:HB2	1.98	0.45
23:1:9:LYS:HE3	23:1:53:LYS:HD3	1.99	0.45
28:6:5:ARG:HG2	28:6:23:THR:HB	1.99	0.45
1:A:1130:U:O2'	1:A:1131:G:OP1	2.32	0.45
1:A:154:U:H2'	1:A:155:A:C8	2.52	0.45
1:A:1871:A:H8	1:A:1872:A:C8	2.35	0.45
1:A:2443:C:H2'	1:A:2444:G:C8	2.51	0.45
1:A:2656:U:H2'	1:A:2657:A:H8	1.81	0.45
2:B:114:C:H2'	2:B:115:A:C8	2.52	0.45
4:E:25:THR:HG21	4:E:193:VAL:HG21	1.99	0.45
1:A:1808:A:H3'	1:A:1809:A:C8	2.52	0.45
1:A:2374:C:N4	1:A:2375:G:O6	2.50	0.45
1:A:750:A:OP1	1:A:1615:C:N4	2.33	0.45
3:D:70:LYS:HB3	3:D:73:ILE:HD12	1.98	0.45
11:P:14:LYS:O	11:P:16:GLY:N	2.50	0.45
1:A:2200:C:H2'	1:A:2201:G:H8	1.82	0.45
1:A:414:C:H2'	1:A:415:A:C8	2.52	0.45
2:B:65:U:H3'	2:B:108:A:H61	1.81	0.45
53:J:56:ARG:HD3	53:J:81:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:N:13:ARG:HE	9:N:121:LYS:HZ1	1.65	0.45
13:R:79:LEU:HD23	13:R:83:LEU:HD12	1.99	0.45
1:A:1059:G:H5'	1:A:1060:U:OP2	2.17	0.45
1:A:2851:A:O3'	13:R:64:ARG:NH2	2.50	0.45
1:A:937:C:OP2	30:8:51:LYS:NZ	2.49	0.45
3:D:204:LEU:HD22	3:D:209:ALA:HB1	1.99	0.45
3:D:60:ALA:HB3	3:D:62:ARG:HH12	1.82	0.45
53:J:69:PHE:CD2	53:J:70:GLU:HG2	2.52	0.45
1:A:2566:A:H4'	1:A:2567:G:O5'	2.16	0.44
1:A:873:C:H2'	1:A:874:G:C8	2.53	0.44
3:D:52:HIS:CE1	3:D:218:THR:HA	2.52	0.44
4:E:5:VAL:HG21	4:E:80:TRP:CD2	2.52	0.44
5:F:128:ALA:HB3	5:F:133:LEU:HD12	1.99	0.44
53:J:11:ILE:HD11	53:J:62:ARG:HG2	1.99	0.44
1:A:582:A:H4'	16:U:10:ARG:HH22	1.81	0.44
1:A:2029:G:N1	1:A:2033:A:OP2	2.37	0.44
1:A:2291:U:H2'	1:A:2292:U:C6	2.51	0.44
1:A:2751:G:OP1	1:A:2751:G:N2	2.31	0.44
54:K:10:LEU:O	54:K:10:LEU:HD12	2.17	0.44
54:K:36:GLU:OE2	54:K:64:ARG:NH2	2.51	0.44
13:R:51:LEU:HD21	13:R:69:ARG:HD2	1.99	0.44
19:X:8:LEU:HD11	24:2:22:LEU:HD12	1.99	0.44
21:Z:2:PHE:O	21:Z:62:THR:OG1	2.26	0.44
1:A:1365:A:P	23:1:27:ARG:HH22	2.40	0.44
1:A:1629:U:O4	1:A:1630:A:N6	2.50	0.44
3:D:257:ARG:NH2	3:D:262:THR:OG1	2.47	0.44
1:A:1813:G:O2'	3:D:41:GLY:O	2.35	0.44
1:A:1046:A:O2'	53:J:61:ARG:O	2.24	0.44
10:O:29:HIS:ND1	10:O:29:HIS:O	2.50	0.44
4:E:13:ARG:HH11	15:T:55:HIS:HA	1.81	0.44
19:X:44:LYS:O	19:X:48:GLN:HG2	2.17	0.44
13:R:118:ARG:NH1	27:5:54:ILE:O	2.44	0.44
1:A:1955:U:C4	1:A:2552:OMU:H6	2.51	0.44
1:A:1965:C:H5"	1:A:1966:A:H2'	1.99	0.44
1:A:2853:C:H2'	1:A:2854:G:C8	2.53	0.44
1:A:935:C:H2'	1:A:936:A:H8	1.82	0.44
4:E:133:THR:HG23	4:E:134:HIS:CD2	2.52	0.44
53:J:118:ILE:HB	53:J:119:PRO:HD3	2.00	0.44
54:K:92:PRO:HB2	54:K:93:ASN:H	1.68	0.44
9:N:44:TYR:O	16:U:63:ARG:NE	2.51	0.44
17:V:68:ARG:NH1	17:V:90:ARG:HB2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:C:H2'	19:X:73:ARG:HH22	1.82	0.44
1:A:1190:G:H2'	1:A:1191:G:C8	2.53	0.44
1:A:1656:C:OP1	4:E:141:ARG:NE	2.44	0.44
1:A:475:C:H4'	1:A:510:C:H5'	1.99	0.44
3:D:267:VAL:HG12	3:D:268:ARG:HG2	1.98	0.44
6:G:141:ASP:HB2	6:G:144:LYS:HD3	1.99	0.44
10:O:58:LEU:HD11	10:O:86:LEU:HD22	1.99	0.44
21:Z:9:ARG:HG2	21:Z:41:GLU:HB2	2.00	0.44
1:A:106:C:H2'	1:A:107:G:H8	1.97	0.44
1:A:30:G:O2'	1:A:1214:A:N3	2.49	0.44
5:F:47:LYS:HB2	5:F:51:GLU:HB2	2.00	0.44
1:A:2335:A:HO2'	1:A:2336:A:H8	1.65	0.44
1:A:2399:G:H2'	1:A:2400:G:C8	2.53	0.44
1:A:2724:U:H2'	1:A:2725:A:C8	2.53	0.44
1:A:2757:A:OP1	31:9:20:ASP:N	2.49	0.44
1:A:720:U:H2'	1:A:721:A:C8	2.52	0.44
2:B:118:C:H2'	2:B:119:A:H8	1.83	0.44
1:A:566:U:H5"	11:P:29:LYS:HE3	2.00	0.44
30:8:5:THR:HG23	30:8:61:LEU:HA	1.99	0.44
1:A:20:C:H2'	1:A:21:A:C8	2.53	0.44
1:A:2101:A:H2'	1:A:2102:G:H8	1.82	0.44
1:A:534:U:H2'	1:A:535:G:C8	2.53	0.44
3:D:203:VAL:O	3:D:205:GLY:N	2.50	0.44
4:E:33:ARG:HD3	4:E:73:VAL:HB	2.00	0.44
5:F:109:LEU:O	5:F:113:VAL:HG23	2.18	0.44
5:F:32:VAL:HG21	11:P:3:LEU:HD11	1.99	0.44
9:N:16:TYR:HE1	9:N:138:GLN:HE21	1.66	0.44
13:R:25:ALA:O	13:R:29:VAL:HG23	2.18	0.44
30:8:38:LYS:HA	30:8:41:ARG:HE	1.83	0.44
1:A:160:A:N3	1:A:2208:C:O2'	2.40	0.44
1:A:1844:C:H2'	1:A:1845:G:C8	2.52	0.44
1:A:414:C:O3'	1:A:1878:G:N2	2.51	0.44
8:I:121:VAL:HG23	8:I:123:ARG:HG3	2.00	0.44
54:K:4:VAL:HA	54:K:7:TYR:CE2	2.53	0.44
24:2:24:GLU:HB3	24:2:46:VAL:HG21	2.00	0.43
1:A:1248:G:OP1	5:F:44:ARG:NH1	2.51	0.43
1:A:1752:C:H2'	1:A:1753:G:C8	2.53	0.43
1:A:2809:A:H2'	1:A:2810:A:C8	2.53	0.43
1:A:457:A:H2	1:A:458:G:H21	1.66	0.43
1:A:18:U:O2'	1:A:554:U:OP1	2.36	0.43
10:O:26:GLY:HA3	10:O:30:ARG:HH11	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:P:62:PRO:HG2	30:8:24:LYS:HB3	1.99	0.43
15:T:24:THR:HA	15:T:45:VAL:HA	1.99	0.43
21:Z:20:LEU:HD11	21:Z:41:GLU:HG3	1.99	0.43
1:A:1915:3TD:O4	1:A:1915:3TD:O4'	2.36	0.43
1:A:2893:A:H4'	1:A:2894:G:C4	2.52	0.43
1:A:839:U:H3	1:A:939:G:H1	1.66	0.43
2:B:80:U:H2'	2:B:81:G:H8	1.83	0.43
3:D:132:ARG:HH12	8:I:93:SER:H	1.66	0.43
7:H:123:GLU:HB2	7:H:131:VAL:HB	2.00	0.43
17:V:4:VAL:HA	17:V:12:HIS:O	2.18	0.43
20:Y:3:LYS:HB3	20:Y:82:VAL:HG21	2.00	0.43
25:3:8:GLN:HA	25:3:54:VAL:HG12	2.00	0.43
1:A:1475:G:O2'	1:A:1732:C:N4	2.51	0.43
1:A:1844:C:H2'	1:A:1845:G:H8	1.82	0.43
1:A:633:A:O2'	1:A:2404:U:OP1	2.32	0.43
3:D:68:ARG:O	3:D:188:ARG:NH1	2.51	0.43
8:I:132:PHE:HB2	8:I:140:ALA:HB3	2.00	0.43
20:Y:24:VAL:HA	20:Y:35:VAL:HG22	1.99	0.43
1:A:1423:G:H2'	1:A:1424:G:H8	1.83	0.43
1:A:2224:G:OP1	3:D:264:LYS:NZ	2.39	0.43
1:A:2464:G:H1	1:A:2486:C:H42	1.65	0.43
1:A:2521:C:O2'	1:A:2564:A:N3	2.48	0.43
1:A:2768:U:O2'	9:N:95:ARG:NH2	2.51	0.43
1:A:2718:G:O2'	1:A:2847:U:OP1	2.25	0.43
54:K:101:SER:HA	54:K:140:GLU:H	1.83	0.43
9:N:37:ARG:HD3	9:N:39:LYS:HD2	2.00	0.43
15:T:13:LYS:HG3	15:T:16:VAL:HG23	2.00	0.43
21:Z:76:ASP:OD1	21:Z:77:VAL:N	2.52	0.43
24:2:44:LYS:HG3	24:2:47:ARG:HH12	1.82	0.43
1:A:119:A:H4'	1:A:120:U:H5'	1.99	0.43
1:A:589:U:H2'	1:A:590:A:C8	2.54	0.43
1:A:624:C:O2'	1:A:657:U:OP1	2.36	0.43
1:A:674:G:H2'	1:A:675:A:C8	4.94	0.43
1:A:1501:G:P	3:D:100:ARG:HH22	2.41	0.43
5:F:88:ARG:O	5:F:90:GLN:N	2.47	0.43
53:J:43:LYS:HE3	53:J:95:LEU:HD22	2.00	0.43
18:W:89:ALA:O	18:W:92:ARG:HG2	2.19	0.43
18:W:88:ARG:HB2	18:W:92:ARG:HG3	2.01	0.43
24:2:10:SER:HA	24:2:13:GLU:HG2	1.99	0.43
1:A:1653:G:O6	13:R:11:ASN:N	2.46	0.43
1:A:2622:U:O2'	1:A:2825:G:N7	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:C:H2'	1:A:270:A:H8	1.84	0.43
1:A:290:U:H2'	1:A:291:G:H8	1.84	0.43
1:A:459:U:H2'	1:A:460:A:C8	2.54	0.43
7:H:21:GLN:NE2	7:H:40:VAL:O	2.43	0.43
17:V:6:GLN:HG3	17:V:39:LEU:HD11	2.00	0.43
1:A:2260:C:N4	22:0:10:ARG:HD2	2.34	0.43
1:A:1506:U:H2'	1:A:1507:C:C6	2.54	0.43
1:A:2443:C:H2'	1:A:2444:G:H8	1.83	0.43
1:A:2725:A:H2'	1:A:2726:A:H2'	2.00	0.43
1:A:745:1MG:O2'	1:A:748:G:H1'	2.19	0.43
4:E:170:VAL:HG23	4:E:194:PRO:HB3	2.01	0.43
9:N:109:LEU:HD13	9:N:118:MET:HG3	2.00	0.43
12:Q:77:PRO:HB2	12:Q:80:VAL:HG21	2.00	0.43
30:8:40:LYS:HA	30:8:43:LEU:HD12	2.00	0.43
1:A:2185:U:H2'	1:A:2186:G:C8	2.53	0.43
1:A:2790:U:OP2	1:A:2893:A:N6	2.52	0.43
5:F:105:LEU:HA	5:F:108:ILE:HG12	2.01	0.43
1:A:1165:A:H2'	1:A:1166:G:C8	2.53	0.43
1:A:1418:G:N1	1:A:1579:A:OP2	2.39	0.43
1:A:2818:U:H2'	1:A:2819:G:C8	2.54	0.43
1:A:563:A:H61	1:A:884:U:H3	106.07	0.43
2:B:28:C:H2'	2:B:29:A:C8	2.54	0.43
53:J:28:ALA:H	53:J:110:ALA:HA	1.83	0.43
11:P:110:VAL:HG11	11:P:135:ILE:HD11	2.01	0.43
22:0:23:GLY:HA2	22:0:63:VAL:HB	2.00	0.43
23:1:70:LEU:HD23	23:1:73:ARG:HH21	1.84	0.43
1:A:1124:G:O2'	31:9:37:GLN:OE1	2.26	0.43
1:A:1469:A:H2'	1:A:1470:A:C8	2.54	0.43
1:A:2137:U:H2'	1:A:2138:G:C8	2.54	0.43
1:A:2522:U:O2'	1:A:2647:U:OP1	2.21	0.43
1:A:286:U:H2'	1:A:287:G:C8	2.54	0.43
1:A:373:U:H2'	1:A:374:A:H8	1.83	0.43
1:A:75:G:OP1	24:2:48:ARG:NH2	2.52	0.43
1:A:926:G:H2'	1:A:927:A:C8	2.53	0.43
3:D:145:MET:HG2	3:D:152:GLN:HG3	2.01	0.43
4:E:151:THR:HB	4:E:152:PRO:HD3	2.01	0.43
6:G:138:PRO:HB3	26:4:32:LEU:HD11	2.01	0.43
22:0:42:HIS:CD2	22:0:73:ARG:HB2	2.54	0.42
6:G:139:GLU:HA	26:4:28:VAL:HG22	2.01	0.42
28:6:18:HIS:HE1	28:6:20:TYR:CZ	2.36	0.42
31:9:3:VAL:HG12	31:9:36:ARG:HE	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2233:U:H2'	1:A:2234:G:C8	2.54	0.42
1:A:648:G:H2'	1:A:649:G:C8	2.54	0.42
1:A:832:U:H2'	1:A:833:A:C8	2.54	0.42
6:G:60:SER:HA	6:G:101:ARG:HH12	1.83	0.42
8:I:58:LEU:HA	8:I:61:VAL:HG22	2.01	0.42
8:I:55:GLU:HA	8:I:58:LEU:HD12	2.01	0.42
25:3:40:THR:OG1	25:3:41:PRO:HD2	2.19	0.42
29:7:31:LEU:HB3	29:7:35:ARG:HH12	1.83	0.42
1:A:1310:G:H1'	1:A:1611:C:H5"	2.01	0.42
1:A:1336:A:H2'	1:A:1337:G:C8	2.54	0.42
1:A:1814:G:OP1	3:D:39:SER:OG	2.33	0.42
1:A:2417:C:H2'	1:A:2418:A:C8	2.54	0.42
1:A:2747:G:H1	1:A:2754:U:H2'	1.84	0.42
1:A:2760:C:H2'	1:A:2761:A:H8	1.83	0.42
1:A:32:C:N4	1:A:446:G:O2'	2.52	0.42
1:A:608:A:N7	1:A:619:G:N2	2.67	0.42
1:A:672:C:H5	11:P:42:SER:HB2	1.84	0.42
2:B:71:C:H42	2:B:105:G:H1	1.68	0.42
10:O:16:ALA:HB3	10:O:86:LEU:HD11	2.01	0.42
21:Z:25:LYS:HD3	21:Z:41:GLU:OE2	2.19	0.42
1:A:2233:U:H2'	1:A:2234:G:H8	1.85	0.42
1:A:2073:C:O2'	1:A:2598:A:O2'	2.33	0.42
1:A:2808:G:O2'	1:A:2809:A:H8	2.02	0.42
1:A:323:C:H2'	1:A:1205:A:N1	2.35	0.42
1:A:629:G:H5"	1:A:650:C:O2'	2.20	0.42
1:A:655:A:H4'	1:A:656:G:H5'	2.00	0.42
1:A:918:A:O2'	2:B:96:G:N2	2.52	0.42
2:B:52:A:N6	14:S:33:ARG:HB2	2.33	0.42
3:D:77:VAL:HA	3:D:93:VAL:HA	2.00	0.42
1:A:658:U:O2'	5:F:97:ASN:OD1	2.34	0.42
54:K:113:ALA:HA	54:K:116:MET:HB2	2.00	0.42
15:T:26:GLU:OE1	15:T:84:SER:OG	2.33	0.42
1:A:987:C:O2'	1:A:1000:A:N3	2.48	0.42
1:A:1313:U:H2'	1:A:1313:U:O2	2.17	0.42
1:A:1331:G:O2'	1:A:1332:G:N2	2.51	0.42
1:A:1334:G:H5"	19:X:69:ARG:NH2	2.34	0.42
1:A:1550:C:H2'	1:A:1551:A:H8	1.85	0.42
1:A:1658:C:H2'	1:A:1659:G:H8	1.84	0.42
1:A:1799:G:O5'	1:A:1819:A:N6	2.52	0.42
1:A:2200:C:H2'	1:A:2201:G:C8	2.55	0.42
1:A:440:C:H2'	1:A:441:U:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:C:H2'	1:A:524:G:C8	2.54	0.42
1:A:594:U:H2'	1:A:595:C:C6	2.54	0.42
7:H:136:ASP:OD2	7:H:139:VAL:HG23	2.20	0.42
21:Z:10:LYS:HG3	21:Z:11:GLU:HG3	2.01	0.42
1:A:1363:C:H2'	1:A:1364:G:C8	2.54	0.42
1:A:2146:C:H4'	1:A:2147:A:C5	2.54	0.42
4:E:13:ARG:HG2	15:T:55:HIS:CE1	2.55	0.42
8:I:33:GLN:HB2	8:I:35:LYS:HG2	2.01	0.42
8:I:9:VAL:HG12	8:I:11:ASN:H	1.84	0.42
19:X:22:THR:HA	19:X:25:GLU:HG2	2.01	0.42
26:4:44:PHE:CE1	26:4:45:THR:HG23	2.53	0.42
1:A:1137:G:H2'	1:A:1138:G:C8	2.53	0.42
1:A:1190:G:H2'	1:A:1191:G:H8	1.84	0.42
1:A:1434:A:H2'	1:A:1435:G:C8	2.53	0.42
1:A:1491:G:H2'	1:A:1492:G:C8	2.54	0.42
1:A:2580:PSU:H3'	1:A:2581:G:C2	2.55	0.42
1:A:341:C:H2'	1:A:342:A:C8	2.55	0.42
1:A:859:G:H1'	1:A:860:U:H5	1.85	0.42
1:A:935:C:H2'	1:A:936:A:C8	2.54	0.42
4:E:4:LEU:HD21	4:E:96:ILE:HG22	2.00	0.42
12:Q:57:VAL:HA	12:Q:112:LEU:HD21	2.01	0.42
18:W:84:ARG:HB2	18:W:96:ILE:HG13	2.02	0.42
21:Z:56:PHE:CE1	21:Z:61:LEU:HD21	2.55	0.42
1:A:1162:G:H2'	1:A:1163:G:C8	2.53	0.42
1:A:1491:G:H2'	1:A:1492:G:H8	1.84	0.42
1:A:1572:A:H2'	1:A:1573:G:H8	1.85	0.42
1:A:1475:G:H4'	1:A:1689:A:H4'	68.78	0.42
1:A:2139:U:H2'	1:A:2140:G:C8	2.54	0.42
1:A:2183:A:H2'	1:A:2184:A:C8	2.55	0.42
5:F:52:VAL:HG21	5:F:82:GLY:H	1.85	0.42
8:I:3:VAL:HA	8:I:38:PRO:HA	2.00	0.42
11:P:79:LEU:HD12	11:P:114:GLY:H	1.84	0.42
1:A:1429:G:H2'	1:A:1430:G:H8	1.85	0.42
1:A:2197:U:H1'	1:A:2198:A:C8	2.55	0.42
1:A:2853:C:H2'	1:A:2854:G:H8	1.84	0.42
2:B:115:A:H2'	2:B:116:G:C8	2.54	0.42
5:F:143:LEU:HB3	5:F:146:VAL:HG11	2.02	0.42
6:G:73:VAL:HG22	6:G:78:ILE:HD11	2.01	0.42
10:O:109:SER:O	10:O:111:LYS:N	2.51	0.42
13:R:49:GLU:HB2	13:R:50:PRO:HD3	2.01	0.42
1:A:480:A:O3'	20:Y:43:LYS:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Y:88:ASP:CG	20:Y:89:GLY:H	2.24	0.42
1:A:1030:C:H42	1:A:1124:G:H1	1.68	0.42
1:A:1429:G:H2'	1:A:1430:G:C8	2.55	0.42
1:A:1666:G:H1	1:A:1994:C:H42	1.68	0.42
1:A:1822:C:H2'	1:A:1823:G:H8	1.84	0.42
1:A:2698:U:H2'	1:A:2699:C:C6	2.55	0.42
1:A:2845:U:O3'	15:T:52:ARG:NH1	2.52	0.42
1:A:537:G:H4'	9:N:5:THR:HG21	2.02	0.42
1:A:767:U:H2'	1:A:768:G:C8	2.55	0.42
20:Y:36:GLU:HA	20:Y:61:GLU:HG2	2.01	0.42
1:A:1481:U:H2'	1:A:1482:G:C8	7.01	0.42
1:A:1651:G:H5'	13:R:39:PRO:HG2	2.02	0.42
1:A:1751:U:H2'	1:A:1752:C:C6	2.55	0.42
1:A:2483:C:N3	12:Q:123:LYS:NZ	2.65	0.42
1:A:2710:C:OP1	13:R:15:SER:OG	2.25	0.42
1:A:690:G:H21	3:D:42:ARG:HH22	1.68	0.42
1:A:715:A:H2'	1:A:716:A:C8	2.92	0.42
3:D:124:LYS:HA	3:D:125:PRO:HD3	1.86	0.42
5:F:3:LEU:HD21	5:F:19:PHE:CZ	2.55	0.42
13:R:73:ASN:HA	13:R:76:VAL:HG12	2.00	0.42
1:A:1614:A:H61	18:W:88:ARG:H	1.68	0.42
1:A:2345:G:H4'	1:A:2346:A:H3'	2.02	0.41
1:A:438:G:H2'	1:A:439:A:C8	2.55	0.41
1:A:674:G:H1	1:A:806:C:H42	1.69	0.41
19:X:6:ARG:O	19:X:10:VAL:HG23	2.19	0.41
1:A:1186:G:H2'	1:A:1187:G:C8	3.03	0.41
1:A:1326:U:H2'	1:A:1327:A:C8	2.54	0.41
1:A:1790:C:H2'	1:A:1791:A:C5	2.54	0.41
1:A:2120:G:H2'	1:A:2121:G:H8	1.85	0.41
1:A:459:U:H2'	1:A:460:A:H8	1.85	0.41
1:A:630:G:N2	1:A:633:A:OP2	2.36	0.41
1:A:836:G:H1	1:A:850:U:H3	29.43	0.41
1:A:923:G:H2'	1:A:924:G:H8	1.84	0.41
1:A:974:G:H1'	1:A:975:A:C8	2.55	0.41
13:R:44:LEU:HD23	13:R:113:ILE:HD13	2.01	0.41
14:S:43:ASN:OD1	14:S:44:GLY:N	2.53	0.41
21:Z:60:VAL:HG11	21:Z:71:LYS:HE3	2.01	0.41
1:A:358:U:H2'	1:A:359:G:C8	3.34	0.41
3:D:177:SER:O	3:D:270:ARG:HG3	2.21	0.41
1:A:1568:G:H5'	3:D:59:GLN:HA	2.03	0.41
2:B:27:C:OP2	14:S:33:ARG:NH1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1061:U:N3	54:K:11:GLN:O	2.53	0.41
1:A:1141:U:H4'	1:A:1142:A:O4'	2.19	0.41
1:A:1357:C:H2'	1:A:1358:G:O4'	2.20	0.41
1:A:1660:G:H2'	1:A:1661:G:H8	1.85	0.41
1:A:2430:A:H5'	1:A:2431:U:OP2	2.20	0.41
1:A:632:A:H2'	1:A:633:A:C8	2.56	0.41
16:U:59:LEU:O	16:U:63:ARG:HG2	2.20	0.41
1:A:1565:C:H5'	3:D:17:LYS:HE3	2.02	0.41
1:A:1595:C:H2'	1:A:1596:A:C8	2.55	0.41
1:A:1675:C:O2	4:E:133:THR:OG1	2.33	0.41
1:A:1787:A:H5"	3:D:237:ARG:HH21	1.85	0.41
1:A:2101:A:H2'	1:A:2102:G:C8	2.55	0.41
1:A:690:G:H21	3:D:42:ARG:HH12	1.68	0.41
6:G:22:ASN:N	6:G:26:GLN:OE1	2.53	0.41
1:A:7:G:H5'	9:N:132:HIS:HE1	1.86	0.41
1:A:1754:A:HO2'	15:T:102:ARG:HH22	1.64	0.41
17:V:10:LYS:HE2	17:V:12:HIS:CE1	2.55	0.41
1:A:999:U:H2'	1:A:1000:A:H8	1.86	0.41
1:A:1501:G:OP1	3:D:100:ARG:NH2	2.52	0.41
1:A:1783:A:N1	1:A:2587:A:H2'	2.35	0.41
1:A:1962:5MC:O2'	1:A:1964:G:OP2	2.30	0.41
1:A:243:U:H2'	1:A:244:A:H8	1.86	0.41
1:A:2453:A:H2'	1:A:2454:G:H8	1.85	0.41
1:A:2837:A:H2'	1:A:2838:G:C8	2.56	0.41
1:A:2899:A:H2'	1:A:2900:A:C8	2.55	0.41
1:A:490:C:O2'	1:A:491:G:OP2	2.35	0.41
3:D:131:MET:HA	3:D:134:ILE:HD12	2.02	0.41
11:P:109:LYS:HD2	11:P:126:ARG:HH11	1.86	0.41
12:Q:75:GLU:HB3	12:Q:90:GLU:HG3	2.01	0.41
19:X:7:LEU:HD22	19:X:46:ALA:HB2	2.03	0.41
1:A:1530:G:H22	1:A:1542:U:H1'	1.86	0.41
1:A:2051:A:H2'	1:A:2578:G:OP1	2.21	0.41
1:A:2302:U:H2'	1:A:2303:G:H8	1.86	0.41
1:A:372:G:H8	23:1:57:VAL:HG22	1.85	0.41
1:A:5:A:H2'	1:A:6:A:C8	2.55	0.41
1:A:746:PSU:O2'	1:A:2611:C:H4'	2.21	0.41
1:A:774:G:H1'	1:A:777:G:H21	1.86	0.41
6:G:107:VAL:HB	6:G:108:PRO:HD3	2.02	0.41
1:A:2198:A:C2	8:I:29:PHE:HB2	2.55	0.41
54:K:20:SER:HB3	54:K:21:PRO:HD3	2.03	0.41
9:N:36:LEU:O	9:N:51:GLY:HA3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:S:39:VAL:N	14:S:49:VAL:O	2.51	0.41
1:A:929:U:H4'	25:3:37:ARG:NH2	2.36	0.41
1:A:1028:A:N6	1:A:1125:G:H2'	2.36	0.41
1:A:1158:C:H2'	1:A:1159:U:H4'	4.13	0.41
1:A:1365:A:OP1	23:1:2:ARG:NH1	2.41	0.41
1:A:1672:A:C2	1:A:2582:G:H5'	2.55	0.41
1:A:1765:U:H2'	1:A:1766:G:C8	2.56	0.41
1:A:1783:A:H5'	1:A:2608:G:H4'	2.03	0.41
1:A:676:A:N6	1:A:713:G:O6	92.47	0.41
3:D:170:TYR:HB3	3:D:182:LYS:HD3	2.02	0.41
11:P:2:ARG:O	11:P:5:THR:OG1	2.26	0.41
17:V:15:SER:O	17:V:18:GLN:HG2	2.21	0.41
1:A:212:G:H2'	1:A:213:A:C8	2.56	0.41
1:A:2293:G:OP1	14:S:94:ARG:NH1	2.54	0.41
3:D:68:ARG:NH1	3:D:128:THR:OG1	2.54	0.41
6:G:34:THR:HB	6:G:154:THR:HB	2.02	0.41
8:I:25:TYR:O	8:I:29:PHE:HB3	2.21	0.41
13:R:38:LEU:HB3	13:R:39:PRO:HD3	2.02	0.41
15:T:105:LYS:HE3	15:T:108:ARG:NH2	2.35	0.41
19:X:8:LEU:HD23	19:X:50:LEU:HD21	2.03	0.41
30:8:28:LEU:HA	30:8:32:LEU:HD21	2.03	0.41
1:A:1539:U:H2'	1:A:1540:G:C8	2.55	0.41
1:A:1771:C:O2'	1:A:1786:A:O4'	2.38	0.41
1:A:1788:C:OP1	3:D:220:ARG:NH2	2.52	0.41
1:A:2328:A:H2'	1:A:2329:U:C6	2.56	0.41
1:A:2691:C:H2'	1:A:2692:G:C8	2.56	0.41
1:A:2773:C:OP1	4:E:169:ARG:NH2	2.54	0.41
3:D:153:LEU:HD11	3:D:181:ARG:NH2	2.35	0.41
5:F:126:VAL:HG22	5:F:128:ALA:H	1.86	0.41
1:A:2208:C:H2'	1:A:2209:G:C8	2.55	0.41
1:A:2251:OMG:H2'	1:A:2252:G:O5'	2.21	0.41
1:A:2467:C:OP1	31:9:8:LYS:NZ	2.48	0.41
1:A:2569:G:H2'	1:A:2570:G:H8	1.86	0.41
1:A:706:A:OP1	3:D:6:LYS:NZ	2.54	0.41
53:J:60:LEU:O	53:J:64:VAL:HB	2.21	0.41
54:K:131:THR:O	54:K:134:SER:OG	2.28	0.41
9:N:7:LYS:O	9:N:11:VAL:HG23	2.21	0.41
10:O:24:VAL:HG13	10:O:33:ALA:HB2	2.03	0.41
30:8:21:PHE:O	30:8:49:VAL:HG23	2.21	0.40
1:A:1020:A:H1'	1:A:1021:A:OP2	2.21	0.40
1:A:1111:A:H2'	1:A:1112:G:H4'	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1255:U:H5'	1:A:2502:G:H22	1.86	0.40
1:A:1351:C:H2'	1:A:1352:U:C6	2.56	0.40
1:A:1405:U:H2'	1:A:1406:U:C6	2.56	0.40
1:A:4:U:H2'	1:A:5:A:C8	2.55	0.40
6:G:124:ARG:HB3	6:G:126:ASN:HD22	1.86	0.40
15:T:46:VAL:HG22	15:T:60:VAL:HG22	2.02	0.40
16:U:82:LEU:HD21	16:U:108:LEU:HD21	2.03	0.40
20:Y:23:LYS:O	20:Y:35:VAL:HG13	2.21	0.40
1:A:300:A:P	20:Y:81:ARG:HH12	2.43	0.40
1:A:465:G:P	29:7:12:ARG:HH12	2.45	0.40
1:A:1490:A:N6	3:D:73:ILE:HG23	2.37	0.40
1:A:155:A:H2'	1:A:156:A:C8	2.57	0.40
1:A:1666:G:N3	10:O:3:GLN:NE2	2.70	0.40
1:A:1847:G:O2'	1:A:1848:A:H8	2.05	0.40
1:A:1874:C:H2'	1:A:1875:G:O4'	2.21	0.40
1:A:2447:G:H21	1:A:2450:A:P	2.43	0.40
1:A:2572:A:OP2	4:E:149:ASN:HB3	2.21	0.40
1:A:2594:C:N4	1:A:2595:G:O6	2.55	0.40
1:A:923:G:H2'	1:A:924:G:C8	2.56	0.40
1:A:938:G:H2'	1:A:939:G:H8	1.86	0.40
10:O:35:VAL:HA	10:O:69:VAL:HG11	2.03	0.40
1:A:2722:G:O2'	13:R:3:HIS:O	2.35	0.40
1:A:1161:C:H2'	1:A:1162:G:C8	2.57	0.40
1:A:1301:A:H2'	1:A:1301:A:N3	2.37	0.40
1:A:1320:C:O2'	1:A:1321:A:H8	2.04	0.40
1:A:1433:A:H2'	1:A:1434:A:C8	2.56	0.40
1:A:151:C:H2'	1:A:152:A:C8	2.56	0.40
1:A:1889:A:H2'	1:A:1890:A:C8	2.57	0.40
1:A:2333:A:H4'	1:A:2334:U:O5'	2.22	0.40
1:A:277:G:H4'	1:A:278:A:N7	2.37	0.40
1:A:745:1MG:HM11	1:A:745:1MG:HN21	1.63	0.40
16:U:111:LYS:HB2	17:V:48:LYS:HD2	2.04	0.40
1:A:1550:C:H2'	1:A:1551:A:C8	2.56	0.40
1:A:2027:G:H1	1:A:2036:C:H42	1.69	0.40
1:A:2137:U:H2'	1:A:2138:G:H8	1.86	0.40
1:A:2377:A:H2'	1:A:2378:A:C8	2.56	0.40
1:A:281:C:H2'	1:A:282:A:C8	2.56	0.40
1:A:341:C:H2'	1:A:342:A:H8	1.86	0.40
1:A:582:A:H2'	1:A:583:G:C8	2.57	0.40
8:I:90:LEU:HG	8:I:92:GLY:H	1.87	0.40
12:Q:76:LYS:HA	12:Q:77:PRO:HD3	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:C:H4'	24:2:41:HIS:CD2	2.56	0.40
1:A:1049:C:C5	1:A:1049:C:N1	2.89	0.40
1:A:1146:C:H2'	1:A:1147:A:C8	2.56	0.40
1:A:166:U:H2'	1:A:167:A:C8	2.84	0.40
1:A:2052:A:H2'	1:A:2053:G:H8	1.85	0.40
1:A:2756:U:H1'	1:A:2757:A:H5"	2.04	0.40
1:A:560:C:H2'	1:A:561:G:C8	2.57	0.40
1:A:596:U:H2'	1:A:597:G:C8	2.57	0.40
7:H:51:PHE:CZ	7:H:71:LEU:HD22	2.56	0.40
16:U:45:ALA:O	16:U:49:ARG:HG3	2.20	0.40
18:W:69:LEU:HA	18:W:109:ASP:HA	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	D	269/273 (98%)	243 (90%)	25 (9%)	1 (0%)	39 80
4	E	207/209 (99%)	187 (90%)	17 (8%)	3 (1%)	14 60
5	F	199/201 (99%)	184 (92%)	11 (6%)	4 (2%)	9 55
6	G	175/179 (98%)	154 (88%)	18 (10%)	3 (2%)	11 57
7	H	174/177 (98%)	149 (86%)	23 (13%)	2 (1%)	17 65
8	I	147/149 (99%)	129 (88%)	14 (10%)	4 (3%)	6 48
9	N	140/142 (99%)	130 (93%)	8 (6%)	2 (1%)	14 60
10	O	120/123 (98%)	108 (90%)	7 (6%)	5 (4%)	3 36
11	P	141/144 (98%)	122 (86%)	13 (9%)	6 (4%)	3 35
12	Q	134/136 (98%)	123 (92%)	8 (6%)	3 (2%)	8 52
13	R	118/127 (93%)	103 (87%)	12 (10%)	3 (2%)	7 49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
14	S	114/117 (97%)	106 (93%)	6 (5%)	2 (2%)	11 56
15	T	112/115 (97%)	105 (94%)	7 (6%)	0	100 100
16	U	115/118 (98%)	113 (98%)	2 (2%)	0	100 100
17	V	101/103 (98%)	91 (90%)	6 (6%)	4 (4%)	4 38
18	W	108/110 (98%)	94 (87%)	14 (13%)	0	100 100
19	X	91/100 (91%)	81 (89%)	8 (9%)	2 (2%)	8 52
20	Y	100/104 (96%)	87 (87%)	11 (11%)	2 (2%)	9 55
21	Z	92/94 (98%)	88 (96%)	4 (4%)	0	100 100
22	0	73/85 (86%)	68 (93%)	4 (6%)	1 (1%)	14 60
23	1	75/78 (96%)	71 (95%)	4 (5%)	0	100 100
24	2	61/63 (97%)	59 (97%)	2 (3%)	0	100 100
25	3	56/59 (95%)	54 (96%)	2 (4%)	0	100 100
26	4	64/70 (91%)	56 (88%)	7 (11%)	1 (2%)	12 58
27	5	54/57 (95%)	51 (94%)	2 (4%)	1 (2%)	10 55
28	6	48/55 (87%)	43 (90%)	4 (8%)	1 (2%)	9 53
29	7	44/46 (96%)	42 (96%)	2 (4%)	0	100 100
30	8	62/65 (95%)	58 (94%)	3 (5%)	1 (2%)	12 58
31	9	36/38 (95%)	32 (89%)	3 (8%)	1 (3%)	6 47
33	b	216/240 (90%)	187 (87%)	25 (12%)	4 (2%)	10 55
34	c	204/233 (88%)	188 (92%)	14 (7%)	2 (1%)	19 66
35	d	203/206 (98%)	180 (89%)	19 (9%)	4 (2%)	9 55
36	e	155/167 (93%)	132 (85%)	17 (11%)	6 (4%)	4 38
37	f	98/135 (73%)	85 (87%)	9 (9%)	4 (4%)	3 37
38	g	149/179 (83%)	130 (87%)	13 (9%)	6 (4%)	4 38
39	h	127/130 (98%)	115 (91%)	11 (9%)	1 (1%)	24 70
40	i	125/130 (96%)	107 (86%)	13 (10%)	5 (4%)	4 38
41	j	96/103 (93%)	79 (82%)	11 (12%)	6 (6%)	2 26
42	k	114/129 (88%)	99 (87%)	11 (10%)	4 (4%)	4 43
43	l	121/124 (98%)	104 (86%)	9 (7%)	8 (7%)	1 24
44	m	112/118 (95%)	103 (92%)	7 (6%)	2 (2%)	11 56
45	o	86/89 (97%)	76 (88%)	5 (6%)	5 (6%)	2 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
46	p	80/82 (98%)	71 (89%)	7 (9%)	2 (2%)	7 49
47	q	78/84 (93%)	65 (83%)	9 (12%)	4 (5%)	2 31
48	r	63/75 (84%)	56 (89%)	4 (6%)	3 (5%)	3 32
49	t	83/87 (95%)	80 (96%)	3 (4%)	0	100 100
50	u	63/71 (89%)	48 (76%)	10 (16%)	5 (8%)	1 18
53	J	129/165 (78%)	102 (79%)	21 (16%)	6 (5%)	3 33
54	K	139/142 (98%)	118 (85%)	14 (10%)	7 (5%)	3 31
55	n	99/102 (97%)	87 (88%)	8 (8%)	4 (4%)	4 38
56	s	77/92 (84%)	71 (92%)	5 (6%)	1 (1%)	15 62
57	z	458/819 (56%)	423 (92%)	24 (5%)	11 (2%)	7 51
All	All	6305/7039 (90%)	5637 (89%)	516 (8%)	152 (2%)	12 51

All (152) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	N	81	ILE
11	P	128	THR
34	c	96	VAL
34	c	156	LEU
36	e	122	VAL
48	r	17	VAL
54	K	22	PRO
54	K	92	PRO
55	n	38	ASP
57	z	50	PRO
57	z	104	VAL
57	z	304	PRO
57	z	316	PRO
57	z	329	PRO
57	z	732	VAL
7	H	108	PHE
8	I	9	VAL
9	N	82	GLY
11	P	85	VAL
11	P	111	ILE
17	V	55	ASP
20	Y	97	SER
28	6	45	HIS

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Mol	Chain	Res	Type
31	9	29	ALA
35	d	26	ALA
35	d	191	SER
37	f	92	THR
38	g	16	LYS
38	g	29	LEU
38	g	56	SER
39	h	74	ILE
40	i	90	ASP
41	j	57	VAL
42	k	88	PRO
43	l	42	LYS
44	m	6	ILE
46	p	8	ARG
50	u	30	GLU
50	u	37	TYR
53	J	55	VAL
53	J	90	GLY
54	K	12	VAL
55	n	54	ASP
57	z	56	LEU
4	E	169	ARG
5	F	122	GLU
6	G	18	GLU
7	H	45	ALA
8	I	15	LEU
11	P	29	LYS
11	P	94	THR
13	R	59	SER
17	V	43	ASN
20	Y	6	ARG
22	0	17	LEU
33	b	11	ALA
35	d	152	SER
36	e	23	THR
36	e	98	ALA
37	f	54	LEU
37	f	63	ASN
37	f	86	ARG
38	g	64	ALA
38	g	145	GLU
40	i	57	VAL

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Mol	Chain	Res	Type
40	i	107	ALA
40	i	125	GLN
42	k	92	ARG
43	l	2	THR
43	l	23	LEU
43	l	33	CYS
44	m	113	LYS
45	o	2	LEU
47	q	17	GLU
47	q	49	ASN
48	r	18	GLN
50	u	12	ASP
54	K	20	SER
54	K	64	ARG
54	K	100	ILE
55	n	2	LYS
4	E	58	ASN
4	E	148	GLN
5	F	80	SER
10	O	109	SER
12	Q	14	LYS
12	Q	70	ASP
14	S	100	HIS
19	X	38	ALA
26	4	26	SER
33	b	71	THR
33	b	153	MET
35	d	166	LYS
36	e	102	THR
41	j	29	ALA
41	j	35	GLN
43	l	46	SER
45	o	13	GLU
45	o	45	HIS
47	q	16	MET
50	u	34	ARG
53	J	22	ALA
53	J	88	HIS
55	n	22	LYS
57	z	134	ASN
57	z	276	VAL
57	z	416	VAL

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Mol	Chain	Res	Type
5	F	83	VAL
8	I	3	VAL
8	I	89	LYS
10	O	35	VAL
10	O	93	GLN
10	O	110	GLU
11	P	36	LYS
13	R	117	ASP
14	S	66	GLY
17	V	53	PHE
27	5	2	VAL
33	b	122	ASP
41	j	33	GLY
41	j	75	ASP
42	k	126	ARG
43	l	75	GLU
43	l	77	SER
45	o	21	THR
45	o	87	ARG
50	u	32	ARG
53	J	71	CYS
53	J	118	ILE
54	K	3	LYS
6	G	61	GLY
13	R	106	ASP
38	g	19	SER
40	i	9	GLY
41	j	41	PRO
47	q	79	GLU
48	r	46	THR
57	z	710	ILE
3	D	253	GLY
19	X	71	GLY
42	k	119	GLY
30	8	31	ILE
43	l	21	PRO
56	s	7	GLY
5	F	149	ILE
6	G	174	PHE
12	Q	69	PRO
46	p	36	VAL
10	O	26	GLY

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Mol	Chain	Res	Type
17	V	54	VAL
36	e	24	VAL
36	e	93	VAL

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	
3	D	216/218 (99%)	216 (100%)	0	100	100
4	E	164/164 (100%)	164 (100%)	0	100	100
5	F	165/165 (100%)	165 (100%)	0	100	100
6	G	148/150 (99%)	148 (100%)	0	100	100
7	H	137/138 (99%)	137 (100%)	0	100	100
8	I	114/114 (100%)	114 (100%)	0	100	100
9	N	116/116 (100%)	116 (100%)	0	100	100
10	O	103/104 (99%)	103 (100%)	0	100	100
11	P	102/103 (99%)	102 (100%)	0	100	100
12	Q	109/109 (100%)	109 (100%)	0	100	100
13	R	100/103 (97%)	100 (100%)	0	100	100
14	S	86/87 (99%)	86 (100%)	0	100	100
15	T	99/100 (99%)	99 (100%)	0	100	100
16	U	89/90 (99%)	89 (100%)	0	100	100
17	V	84/84 (100%)	84 (100%)	0	100	100
18	W	93/93 (100%)	93 (100%)	0	100	100
19	X	80/84 (95%)	80 (100%)	0	100	100
20	Y	83/85 (98%)	83 (100%)	0	100	100
21	Z	78/78 (100%)	78 (100%)	0	100	100
22	0	57/63 (90%)	57 (100%)	0	100	100
23	1	67/68 (98%)	67 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	2	55/55 (100%)	55 (100%)	0	100	100
25	3	48/49 (98%)	48 (100%)	0	100	100
26	4	59/62 (95%)	59 (100%)	0	100	100
27	5	47/48 (98%)	47 (100%)	0	100	100
28	6	45/49 (92%)	45 (100%)	0	100	100
29	7	38/38 (100%)	38 (100%)	0	100	100
30	8	51/52 (98%)	51 (100%)	0	100	100
31	9	34/34 (100%)	34 (100%)	0	100	100
33	b	180/198 (91%)	180 (100%)	0	100	100
34	c	170/190 (90%)	170 (100%)	0	100	100
35	d	172/173 (99%)	172 (100%)	0	100	100
36	e	114/126 (90%)	114 (100%)	0	100	100
37	f	87/116 (75%)	87 (100%)	0	100	100
38	g	124/147 (84%)	124 (100%)	0	100	100
39	h	104/105 (99%)	104 (100%)	0	100	100
40	i	105/107 (98%)	105 (100%)	0	100	100
41	j	86/90 (96%)	86 (100%)	0	100	100
42	k	89/99 (90%)	89 (100%)	0	100	100
43	l	103/104 (99%)	103 (100%)	0	100	100
44	m	92/96 (96%)	92 (100%)	0	100	100
45	o	76/77 (99%)	76 (100%)	0	100	100
46	p	65/65 (100%)	65 (100%)	0	100	100
47	q	74/78 (95%)	74 (100%)	0	100	100
48	r	48/65 (74%)	48 (100%)	0	100	100
49	t	65/66 (98%)	65 (100%)	0	100	100
50	u	44/61 (72%)	44 (100%)	0	100	100
53	J	100/123 (81%)	100 (100%)	0	100	100
54	K	109/110 (99%)	109 (100%)	0	100	100
55	n	79/84 (94%)	79 (100%)	0	100	100
56	s	70/79 (89%)	70 (100%)	0	100	100
All	All	4823/5062 (95%)	4823 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	225	ASN
4	E	32	ASN
4	E	173	GLN
5	F	41	GLN
5	F	165	HIS
6	G	4	HIS
7	H	138	GLN
10	O	3	GLN
11	P	99	ASN
12	Q	13	HIS
13	R	9	GLN
15	T	2	ASN
15	T	11	GLN
17	V	18	GLN
18	W	7	HIS
18	W	40	ASN
18	W	61	ASN
20	Y	73	ASN
21	Z	87	GLN
22	0	42	HIS
23	1	16	ASN
24	2	25	GLN
24	2	58	ASN
25	3	19	HIS
28	6	18	HIS
28	6	45	HIS
31	9	35	GLN
33	b	18	GLN
33	b	41	ASN
35	d	119	HIS
35	d	125	ASN
36	e	145	ASN
37	f	11	HIS
37	f	58	HIS
38	g	141	HIS
39	h	3	GLN
40	i	4	GLN
41	j	70	HIS
42	k	27	ASN

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Mol	Chain	Res	Type
43	l	4	ASN
44	m	11	HIS
44	m	90	HIS
45	o	39	GLN
46	p	9	HIS
46	p	63	GLN
46	p	79	ASN
47	q	30	HIS
49	t	2	ASN
49	t	74	HIS
53	J	4	ASN
53	J	88	HIS
56	s	55	GLN
56	s	68	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2881/2903 (99%)	415 (14%)	43 (1%)
2	B	119/120 (99%)	13 (10%)	2 (1%)
32	a	1535/1539 (99%)	176 (11%)	0
51	v	5/6 (83%)	0	0
52	x	76/77 (98%)	13 (17%)	0
58	y	72/73 (98%)	28 (38%)	0
All	All	4688/4718 (99%)	645 (13%)	45 (0%)

All (645) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	A
1	A	12	U
1	A	27	G
1	A	34	U
1	A	35	G
1	A	46	G
1	A	49	A
1	A	51	G
1	A	52	A
1	A	71	A
1	A	74	A
1	A	75	G

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Mol	Chain	Res	Type
1	A	84	A
1	A	91	A
1	A	92	U
1	A	98	G
1	A	118	A
1	A	120	U
1	A	138	U
1	A	139	U
1	A	140	C
1	A	141	G
1	A	142	A
1	A	162	U
1	A	163	C
1	A	181	A
1	A	196	A
1	A	199	A
1	A	205	G
1	A	216	A
1	A	221	A
1	A	222	A
1	A	242	G
1	A	243	U
1	A	248	G
1	A	249	C
1	A	255	A
1	A	266	G
1	A	267	C
1	A	276	U
1	A	278	A
1	A	294	A
1	A	310	A
1	A	311	A
1	A	323	C
1	A	329	G
1	A	330	A
1	A	353	C
1	A	361	G
1	A	367	G
1	A	371	A
1	A	373	U
1	A	386	G
1	A	387	U

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Mol	Chain	Res	Type
1	A	391	A
1	A	404	A
1	A	406	G
1	A	411	G
1	A	424	G
1	A	451	U
1	A	456	C
1	A	457	A
1	A	458	G
1	A	459	U
1	A	480	A
1	A	481	G
1	A	491	G
1	A	504	A
1	A	505	A
1	A	506	G
1	A	529	A
1	A	530	G
1	A	532	A
1	A	533	G
1	A	543	G
1	A	545	U
1	A	547	A
1	A	550	C
1	A	563	A
1	A	572	A
1	A	573	U
1	A	575	A
1	A	603	A
1	A	616	A
1	A	627	A
1	A	637	A
1	A	646	U
1	A	654	A
1	A	669	G
1	A	686	U
1	A	687	C
1	A	695	G
1	A	730	A
1	A	746	PSU
1	A	747	5MC
1	A	748	G

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Mol	Chain	Res	Type
1	A	752	A
1	A	753	A
1	A	764	A
1	A	776	G
1	A	782	A
1	A	784	G
1	A	785	G
1	A	789	A
1	A	792	A
1	A	805	G
1	A	812	C
1	A	819	A
1	A	822	G
1	A	827	U
1	A	828	U
1	A	830	G
1	A	831	G
1	A	845	A
1	A	846	U
1	A	847	U
1	A	858	G
1	A	859	G
1	A	860	U
1	A	878	A
1	A	885	C
1	A	894	U
1	A	896	A
1	A	897	C
1	A	898	C
1	A	907	G
1	A	910	A
1	A	932	U
1	A	941	A
1	A	946	C
1	A	955	PSU
1	A	956	G
1	A	961	C
1	A	974	G
1	A	983	A
1	A	995	C
1	A	996	A
1	A	1012	U

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Mol	Chain	Res	Type
1	A	1013	C
1	A	1021	A
1	A	1022	G
1	A	1023	U
1	A	1033	U
1	A	1046	A
1	A	1047	G
1	A	1053	C
1	A	1054	A
1	A	1057	A
1	A	1060	U
1	A	1061	U
1	A	1062	G
1	A	1064	C
1	A	1065	U
1	A	1066	U
1	A	1068	G
1	A	1070	A
1	A	1071	G
1	A	1075	C
1	A	1076	C
1	A	1079	C
1	A	1084	A
1	A	1088	A
1	A	1104	C
1	A	1111	A
1	A	1112	G
1	A	1119	U
1	A	1130	U
1	A	1131	G
1	A	1132	U
1	A	1133	A
1	A	1135	C
1	A	1143	A
1	A	1174	U
1	A	1176	U
1	A	1177	G
1	A	1180	U
1	A	1206	G
1	A	1212	G
1	A	1250	G
1	A	1251	C

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Mol	Chain	Res	Type
1	A	1253	A
1	A	1256	G
1	A	1271	G
1	A	1272	A
1	A	1300	G
1	A	1301	A
1	A	1306	C
1	A	1314	C
1	A	1321	A
1	A	1329	U
1	A	1332	G
1	A	1341	G
1	A	1345	C
1	A	1365	A
1	A	1368	G
1	A	1378	A
1	A	1379	U
1	A	1383	A
1	A	1416	G
1	A	1419	A
1	A	1420	A
1	A	1428	C
1	A	1454	C
1	A	1461	C
1	A	1475	G
1	A	1482	G
1	A	1490	A
1	A	1491	G
1	A	1504	A
1	A	1515	A
1	A	1524	G
1	A	1533	C
1	A	1535	A
1	A	1536	C
1	A	1555	G
1	A	1559	U
1	A	1560	G
1	A	1569	A
1	A	1581	G
1	A	1585	C
1	A	1611	C
1	A	1634	A

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Mol	Chain	Res	Type
1	A	1647	U
1	A	1648	U
1	A	1654	A
1	A	1670	C
1	A	1674	G
1	A	1694	C
1	A	1695	G
1	A	1715	G
1	A	1729	U
1	A	1730	C
1	A	1733	G
1	A	1738	G
1	A	1758	U
1	A	1764	C
1	A	1773	A
1	A	1780	A
1	A	1781	U
1	A	1784	A
1	A	1791	A
1	A	1800	C
1	A	1801	A
1	A	1802	A
1	A	1808	A
1	A	1816	C
1	A	1829	A
1	A	1833	C
1	A	1835	2MG
1	A	1836	C
1	A	1871	A
1	A	1901	A
1	A	1906	G
1	A	1911	PSU
1	A	1912	A
1	A	1913	A
1	A	1914	C
1	A	1917	PSU
1	A	1918	A
1	A	1919	A
1	A	1929	G
1	A	1930	G
1	A	1937	A
1	A	1938	A

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Mol	Chain	Res	Type
1	A	1939	5MU
1	A	1940	U
1	A	1941	C
1	A	1944	U
1	A	1955	U
1	A	1967	C
1	A	1970	A
1	A	1971	U
1	A	1972	G
1	A	1991	U
1	A	1993	U
1	A	1997	C
1	A	2021	C
1	A	2022	U
1	A	2023	C
1	A	2031	A
1	A	2033	A
1	A	2043	C
1	A	2049	G
1	A	2052	A
1	A	2055	C
1	A	2056	G
1	A	2060	A
1	A	2061	G
1	A	2062	A
1	A	2069	7MG
1	A	2072	C
1	A	2093	G
1	A	2096	C
1	A	2098	U
1	A	2110	G
1	A	2111	U
1	A	2112	G
1	A	2113	U
1	A	2116	G
1	A	2118	U
1	A	2119	A
1	A	2127	G
1	A	2131	U
1	A	2132	U
1	A	2133	G
1	A	2145	C

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Mol	Chain	Res	Type
1	A	2162	G
1	A	2164	C
1	A	2170	A
1	A	2172	U
1	A	2173	A
1	A	2198	A
1	A	2204	G
1	A	2211	A
1	A	2213	U
1	A	2225	A
1	A	2226	C
1	A	2250	G
1	A	2251	OMG
1	A	2252	G
1	A	2278	A
1	A	2283	C
1	A	2286	G
1	A	2287	A
1	A	2305	U
1	A	2309	A
1	A	2320	U
1	A	2327	A
1	A	2334	U
1	A	2335	A
1	A	2350	C
1	A	2354	C
1	A	2383	G
1	A	2385	C
1	A	2392	A
1	A	2402	U
1	A	2407	A
1	A	2423	U
1	A	2424	C
1	A	2426	A
1	A	2428	G
1	A	2429	G
1	A	2430	A
1	A	2431	U
1	A	2435	A
1	A	2441	U
1	A	2445	2MG
1	A	2446	G

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Mol	Chain	Res	Type
1	A	2448	A
1	A	2449	H2U
1	A	2450	A
1	A	2457	PSU
1	A	2458	G
1	A	2476	A
1	A	2498	OMC
1	A	2499	C
1	A	2502	G
1	A	2504	PSU
1	A	2505	G
1	A	2506	U
1	A	2518	A
1	A	2529	G
1	A	2547	A
1	A	2552	OMU
1	A	2553	G
1	A	2554	U
1	A	2567	G
1	A	2572	A
1	A	2580	PSU
1	A	2581	G
1	A	2585	U
1	A	2586	U
1	A	2602	A
1	A	2604	PSU
1	A	2605	PSU
1	A	2606	C
1	A	2609	U
1	A	2613	U
1	A	2614	A
1	A	2629	U
1	A	2636	C
1	A	2646	C
1	A	2655	G
1	A	2656	U
1	A	2682	A
1	A	2689	U
1	A	2690	U
1	A	2714	G
1	A	2718	G
1	A	2726	A

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Mol	Chain	Res	Type
1	A	2739	U
1	A	2744	G
1	A	2748	A
1	A	2757	A
1	A	2764	A
1	A	2765	A
1	A	2778	A
1	A	2779	U
1	A	2780	G
1	A	2791	G
1	A	2794	C
1	A	2797	U
1	A	2799	A
1	A	2800	A
1	A	2808	G
1	A	2809	A
1	A	2818	U
1	A	2820	A
1	A	2833	U
1	A	2849	U
1	A	2867	G
1	A	2868	A
1	A	2880	C
1	A	2893	A
1	A	2894	G
2	B	4	C
2	B	13	G
2	B	35	C
2	B	44	G
2	B	45	A
2	B	53	A
2	B	67	G
2	B	88	C
2	B	89	U
2	B	90	C
2	B	91	C
2	B	108	A
2	B	109	A
32	a	6	G
32	a	7	A
32	a	9	G
32	a	22	G

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Mol	Chain	Res	Type
32	a	32	A
32	a	39	G
32	a	51	A
32	a	71	A
32	a	86	G
32	a	87	C
32	a	121	U
32	a	130	A
32	a	183	C
32	a	184	G
32	a	209	U
32	a	210	C
32	a	212	G
32	a	226	G
32	a	247	G
32	a	251	G
32	a	266	G
32	a	267	C
32	a	280	C
32	a	281	G
32	a	282	A
32	a	289	G
32	a	306	A
32	a	328	C
32	a	345	C
32	a	347	G
32	a	351	G
32	a	352	C
32	a	367	U
32	a	372	C
32	a	392	C
32	a	406	G
32	a	413	G
32	a	422	C
32	a	424	G
32	a	429	U
32	a	467	U
32	a	479	U
32	a	484	G
32	a	485	U
32	a	486	U
32	a	496	A

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Mol	Chain	Res	Type
32	a	497	G
32	a	516	PSU
32	a	517	G
32	a	527	7MG
32	a	530	G
32	a	531	U
32	a	532	A
32	a	533	A
32	a	547	A
32	a	561	U
32	a	564	C
32	a	572	A
32	a	573	A
32	a	575	G
32	a	576	C
32	a	577	G
32	a	633	G
32	a	642	A
32	a	665	A
32	a	688	G
32	a	702	A
32	a	703	G
32	a	723	U
32	a	724	G
32	a	731	G
32	a	733	G
32	a	748	G
32	a	755	G
32	a	777	A
32	a	815	A
32	a	817	C
32	a	818	G
32	a	819	A
32	a	820	U
32	a	832	G
32	a	843	U
32	a	844	G
32	a	846	G
32	a	871	U
32	a	890	G
32	a	902	G
32	a	934	C

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Mol	Chain	Res	Type
32	a	935	A
32	a	939	G
32	a	960	U
32	a	961	U
32	a	966	2MG
32	a	967	5MC
32	a	968	A
32	a	969	A
32	a	975	A
32	a	976	G
32	a	977	A
32	a	989	U
32	a	991	U
32	a	992	U
32	a	993	G
32	a	1004	A
32	a	1026	G
32	a	1028	C
32	a	1030	U
32	a	1031	C
32	a	1033	G
32	a	1034	G
32	a	1035	A
32	a	1056	U
32	a	1065	U
32	a	1085	U
32	a	1094	G
32	a	1101	A
32	a	1130	A
32	a	1137	C
32	a	1138	G
32	a	1139	G
32	a	1152	A
32	a	1159	U
32	a	1168	U
32	a	1183	U
32	a	1184	G
32	a	1191	A
32	a	1196	A
32	a	1197	A
32	a	1201	A
32	a	1202	U

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Mol	Chain	Res	Type
32	a	1207	2MG
32	a	1208	C
32	a	1212	U
32	a	1213	A
32	a	1225	A
32	a	1238	A
32	a	1240	U
32	a	1241	G
32	a	1256	A
32	a	1258	G
32	a	1260	G
32	a	1278	G
32	a	1280	A
32	a	1282	C
32	a	1287	A
32	a	1298	U
32	a	1300	G
32	a	1301	U
32	a	1302	C
32	a	1317	C
32	a	1323	G
32	a	1347	G
32	a	1348	U
32	a	1363	A
32	a	1395	C
32	a	1400	C
32	a	1403	C
32	a	1408	A
32	a	1446	A
32	a	1448	C
32	a	1452	C
32	a	1492	A
32	a	1494	G
32	a	1498	UR3
32	a	1499	A
32	a	1502	A
32	a	1503	A
32	a	1506	U
32	a	1516	2MG
32	a	1517	G
32	a	1520	C
32	a	1529	G

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Mol	Chain	Res	Type
32	a	1530	G
32	a	1534	A
32	a	1535	C
32	a	1536	C
52	x	8	4SU
52	x	9	G
52	x	16	C
52	x	17	C
52	x	17(A)	U
52	x	18	G
52	x	19	G
52	x	20	H2U
52	x	21	A
52	x	22	G
52	x	54	5MU
52	x	55	PSU
52	x	56	C
58	y	3	U
58	y	7	A
58	y	9	A
58	y	10	G
58	y	13	C
58	y	14	A
58	y	16	H2U
58	y	17	H2U
58	y	18	G
58	y	19	G
58	y	20	H2U
58	y	21	A
58	y	22	G
58	y	34	G
58	y	35	G
58	y	41	G
58	y	43	G
58	y	46	7MG
58	y	47	U
58	y	48	C
58	y	54	5MU
58	y	55	PSU
58	y	56	C
58	y	57	G
58	y	58	A

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Mol	Chain	Res	Type
58	y	59	A
58	y	72	C
58	y	73	A

All (45) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	51	G
1	A	86	G
1	A	204	A
1	A	242	G
1	A	372	G
1	A	458	G
1	A	479	A
1	A	490	C
1	A	746	PSU
1	A	752	A
1	A	858	G
1	A	859	G
1	A	893	C
1	A	955	PSU
1	A	1020	A
1	A	1022	G
1	A	1070	A
1	A	1130	U
1	A	1182	G
1	A	1190	G
1	A	1300	G
1	A	1399	C
1	A	1835	2MG
1	A	1911	PSU
1	A	1917	PSU
1	A	1939	5MU
1	A	1940	U
1	A	2251	OMG
1	A	2286	G
1	A	2326	C
1	A	2333	A
1	A	2391	G
1	A	2445	2MG
1	A	2449	H2U
1	A	2457	PSU

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Mol	Chain	Res	Type
1	A	2498	OMC
1	A	2504	PSU
1	A	2566	A
1	A	2580	PSU
1	A	2605	PSU
1	A	2655	G
1	A	2756	U
1	A	2808	G
2	B	66	A
2	B	88	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	6MZ	A	1618	1	17,25,26	0.77	1 (5%)	15,36,39	3.16	2 (13%)
1	2MG	A	1835	1	18,26,27	2.80	2 (11%)	21,38,41	2.40	8 (38%)
1	PSU	A	1911	1	15,21,22	1.33	3 (20%)	16,30,33	2.02	3 (18%)
1	3TD	A	1915	1	15,22,23	2.19	3 (20%)	17,32,35	1.38	3 (17%)
1	PSU	A	1917	1	15,21,22	1.45	3 (20%)	16,30,33	2.08	3 (18%)
1	5MU	A	1939	1	13,22,23	1.36	1 (7%)	16,32,35	2.36	3 (18%)
1	5MC	A	1962	1	14,22,23	1.24	2 (14%)	17,32,35	0.83	1 (5%)
1	6MZ	A	2030	1	17,25,26	0.75	1 (5%)	15,36,39	3.15	2 (13%)
1	7MG	A	2069	1	20,26,27	2.74	5 (25%)	23,39,42	2.70	6 (26%)
1	OMG	A	2251	1,52	18,26,27	2.34	2 (11%)	21,38,41	1.53	4 (19%)
1	2MG	A	2445	1	18,26,27	2.80	2 (11%)	21,38,41	2.25	7 (33%)
1	H2U	A	2449	1	17,21,22	3.63	5 (29%)	23,30,33	2.61	5 (21%)
1	PSU	A	2457	1	15,21,22	1.36	3 (20%)	16,30,33	2.04	3 (18%)
1	OMC	A	2498	1	15,22,23	1.04	1 (6%)	20,31,34	0.87	1 (5%)
1	2MA	A	2503	1	17,25,26	2.03	1 (5%)	18,37,40	2.99	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	PSU	A	2504	1	15,21,22	1.31	2 (13%)	16,30,33	2.02	3 (18%)
1	OMU	A	2552	1	14,22,23	2.06	3 (21%)	19,31,34	1.66	1 (5%)
1	PSU	A	2580	1	15,21,22	1.44	4 (26%)	16,30,33	2.12	3 (18%)
1	PSU	A	2604	1	15,21,22	1.29	2 (13%)	16,30,33	2.09	3 (18%)
1	PSU	A	2605	1	15,21,22	1.43	3 (20%)	16,30,33	2.01	2 (12%)
1	1MG	A	745	1	17,26,27	2.44	3 (17%)	19,39,42	1.07	1 (5%)
1	PSU	A	746	1	15,21,22	1.28	2 (13%)	16,30,33	2.17	4 (25%)
1	5MC	A	747	1	14,22,23	1.24	2 (14%)	17,32,35	0.84	1 (5%)
1	PSU	A	955	1	15,21,22	1.38	3 (20%)	16,30,33	2.03	3 (18%)
32	2MG	a	1207	32	18,26,27	2.81	2 (11%)	21,38,41	2.26	7 (33%)
32	4OC	a	1402	32	15,23,24	0.91	1 (6%)	21,32,35	1.51	3 (14%)
32	5MC	a	1407	32	14,22,23	1.26	2 (14%)	17,32,35	0.83	1 (5%)
32	UR3	a	1498	32	13,22,23	1.64	2 (15%)	18,32,35	0.62	0
32	2MG	a	1516	32	18,26,27	2.82	2 (11%)	21,38,41	2.23	6 (28%)
32	MA6	a	1518	32	18,26,27	0.61	0	15,38,41	1.87	2 (13%)
32	MA6	a	1519	32	18,26,27	0.56	0	15,38,41	2.09	2 (13%)
32	PSU	a	516	32	15,21,22	1.34	3 (20%)	16,30,33	2.05	3 (18%)
32	7MG	a	527	32	20,26,27	2.70	4 (20%)	23,39,42	2.47	4 (17%)
32	2MG	a	966	32	18,26,27	2.80	2 (11%)	21,38,41	2.33	8 (38%)
32	5MC	a	967	32	14,22,23	1.30	2 (14%)	17,32,35	0.89	1 (5%)
52	H2U	x	20	52	17,21,22	3.63	5 (29%)	23,30,33	2.60	5 (21%)
52	5MU	x	54	52	13,22,23	1.31	1 (7%)	16,32,35	2.36	3 (18%)
52	PSU	x	55	52	15,21,22	1.41	4 (26%)	16,30,33	2.16	3 (18%)
52	4SU	x	8	52	12,21,22	1.62	2 (16%)	15,30,33	1.04	1 (6%)
58	H2U	y	16	58	17,21,22	3.65	5 (29%)	23,30,33	2.51	5 (21%)
58	H2U	y	17	58	17,21,22	3.63	5 (29%)	23,30,33	2.57	5 (21%)
58	H2U	y	20	58	17,21,22	3.62	5 (29%)	23,30,33	2.59	5 (21%)
58	YG	y	37	58	28,42,43	1.54	2 (7%)	28,62,65	1.92	8 (28%)
58	7MG	y	46	58	20,26,27	2.69	4 (20%)	23,39,42	2.27	5 (21%)
58	5MU	y	54	58	13,22,23	1.33	1 (7%)	16,32,35	2.35	3 (18%)
58	PSU	y	55	58	15,21,22	1.45	3 (20%)	16,30,33	2.25	4 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	6MZ	A	1618	1	-	0/5/27/28	0/3/3/3
1	2MG	A	1835	1	2/2/5/6	0/5/27/28	0/3/3/3
1	PSU	A	1911	1	2/2/5/5	0/7/25/26	0/2/2/2
1	3TD	A	1915	1	1/1/5/5	0/7/25/26	0/2/2/2
1	PSU	A	1917	1	2/2/5/5	0/7/25/26	0/2/2/2
1	5MU	A	1939	1	3/3/5/5	0/3/25/26	0/2/2/2
1	5MC	A	1962	1	-	0/3/25/26	0/2/2/2
1	6MZ	A	2030	1	-	0/5/27/28	0/3/3/3
1	7MG	A	2069	1	1/1/7/7	0/7/37/38	0/3/3/3
1	OMG	A	2251	1,52	2/2/5/5	0/5/27/28	0/3/3/3
1	2MG	A	2445	1	2/2/5/6	0/5/27/28	0/3/3/3
1	H2U	A	2449	1	1/1/8/9	0/7/38/39	0/2/2/2
1	PSU	A	2457	1	2/2/5/5	0/7/25/26	0/2/2/2
1	OMC	A	2498	1	2/2/5/5	0/5/27/28	0/2/2/2
1	2MA	A	2503	1	2/2/5/5	0/3/25/26	0/3/3/3
1	PSU	A	2504	1	2/2/5/5	0/7/25/26	0/2/2/2
1	OMU	A	2552	1	1/1/5/5	0/5/27/28	0/2/2/2
1	PSU	A	2580	1	2/2/5/5	0/7/25/26	0/2/2/2
1	PSU	A	2604	1	2/2/5/5	0/7/25/26	0/2/2/2
1	PSU	A	2605	1	2/2/5/5	0/7/25/26	0/2/2/2
1	1MG	A	745	1	-	0/3/25/26	0/3/3/3
1	PSU	A	746	1	2/2/5/5	0/7/25/26	0/2/2/2
1	5MC	A	747	1	-	0/3/25/26	0/2/2/2
1	PSU	A	955	1	2/2/5/5	0/7/25/26	0/2/2/2
32	2MG	a	1207	32	2/2/5/6	0/5/27/28	0/3/3/3
32	4OC	a	1402	32	2/2/5/6	0/7/29/30	0/2/2/2
32	5MC	a	1407	32	-	0/3/25/26	0/2/2/2
32	UR3	a	1498	32	2/2/5/5	0/3/25/26	0/2/2/2
32	2MG	a	1516	32	2/2/5/6	0/5/27/28	0/3/3/3
32	MA6	a	1518	32	2/2/6/6	0/7/29/30	0/3/3/3
32	MA6	a	1519	32	2/2/6/6	0/7/29/30	0/3/3/3
32	PSU	a	516	32	2/2/5/5	0/7/25/26	0/2/2/2
32	7MG	a	527	32	1/1/7/7	0/7/37/38	0/3/3/3
32	2MG	a	966	32	2/2/5/6	0/5/27/28	0/3/3/3
32	5MC	a	967	32	-	0/3/25/26	0/2/2/2
52	H2U	x	20	52	1/1/8/9	0/7/38/39	0/2/2/2
52	5MU	x	54	52	3/3/5/5	0/3/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	PSU	x	55	52	2/2/5/5	0/7/25/26	0/2/2/2
52	4SU	x	8	52	3/3/5/5	0/3/25/26	0/2/2/2
58	H2U	y	16	58	1/1/8/9	0/7/38/39	0/2/2/2
58	H2U	y	17	58	1/1/8/9	0/7/38/39	0/2/2/2
58	H2U	y	20	58	1/1/8/9	0/7/38/39	0/2/2/2
58	YG	y	37	58	-	0/20/42/43	0/4/4/4
58	7MG	y	46	58	1/1/7/7	0/7/37/38	0/3/3/3
58	5MU	y	54	58	3/3/5/5	0/3/25/26	0/2/2/2
58	PSU	y	55	58	2/2/5/5	0/7/25/26	0/2/2/2

All (116) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	y	16	H2U	C6-N1	-9.23	1.35	1.47
1	A	2449	H2U	C6-N1	-9.09	1.35	1.47
52	x	20	H2U	C6-N1	-9.05	1.35	1.47
58	y	17	H2U	C6-N1	-9.05	1.35	1.47
58	y	20	H2U	C6-N1	-9.02	1.35	1.47
58	y	46	7MG	C8-N9	-7.44	1.34	1.45
1	A	2069	7MG	C8-N9	-7.43	1.34	1.45
32	a	527	7MG	C8-N9	-7.41	1.34	1.45
58	y	37	YG	O23-C21	-6.58	1.25	1.34
58	y	20	H2U	C6-C5	-5.92	1.42	1.52
1	A	2449	H2U	C6-C5	-5.92	1.42	1.52
52	x	20	H2U	C6-C5	-5.91	1.42	1.52
58	y	16	H2U	C6-C5	-5.90	1.42	1.52
58	y	17	H2U	C6-C5	-5.88	1.42	1.52
58	y	54	5MU	C2-N3	-4.10	1.29	1.38
1	A	1939	5MU	C2-N3	-4.10	1.29	1.38
52	x	54	5MU	C2-N3	-4.04	1.29	1.38
52	x	20	H2U	C5-C4	-3.92	1.40	1.50
58	y	16	H2U	C5-C4	-3.90	1.40	1.50
58	y	20	H2U	C5-C4	-3.90	1.40	1.50
1	A	2449	H2U	C5-C4	-3.88	1.40	1.50
58	y	17	H2U	C5-C4	-3.88	1.40	1.50
1	A	745	1MG	CM1-N1	-3.70	1.39	1.47
1	A	955	PSU	C2-N1	-3.14	1.31	1.38
32	a	516	PSU	C2-N1	-3.13	1.31	1.38
58	y	55	PSU	C2-N1	-3.11	1.31	1.38
1	A	1911	PSU	C2-N1	-3.11	1.31	1.38
52	x	55	PSU	C2-N1	-3.10	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1917	PSU	C2-N1	-3.10	1.31	1.38
1	A	2605	PSU	C2-N1	-3.10	1.31	1.38
1	A	2580	PSU	C2-N1	-3.07	1.31	1.38
1	A	2504	PSU	C2-N1	-3.07	1.31	1.38
1	A	2457	PSU	C2-N1	-3.06	1.31	1.38
1	A	746	PSU	C2-N1	-3.04	1.31	1.38
1	A	2604	PSU	C2-N1	-3.03	1.31	1.38
58	y	37	YG	O18-C16	-2.96	1.25	1.33
52	x	20	H2U	C2-N3	-2.91	1.32	1.38
58	y	17	H2U	C2-N3	-2.90	1.32	1.38
58	y	16	H2U	C2-N3	-2.89	1.32	1.38
58	y	20	H2U	C2-N3	-2.89	1.32	1.38
1	A	2449	H2U	C2-N3	-2.87	1.32	1.38
1	A	1917	PSU	O4'-C1'	-2.83	1.40	1.44
1	A	2580	PSU	O4'-C1'	-2.82	1.40	1.44
1	A	1915	3TD	C10-N3	-2.75	1.41	1.47
52	x	8	4SU	C2-N3	-2.68	1.32	1.38
32	a	1402	4OC	C2-N3	-2.66	1.32	1.38
58	y	55	PSU	O4'-C1'	-2.53	1.40	1.44
1	A	2605	PSU	O4'-C1'	-2.52	1.40	1.44
32	a	1407	5MC	C2-N3	-2.51	1.33	1.38
32	a	967	5MC	C2-N3	-2.50	1.33	1.38
1	A	747	5MC	C2-N3	-2.48	1.33	1.38
1	A	1962	5MC	C2-N3	-2.47	1.33	1.38
1	A	2552	OMU	C6-N1	-2.39	1.32	1.35
58	y	55	PSU	C2-N3	-2.37	1.33	1.38
52	x	55	PSU	C2-N3	-2.34	1.33	1.38
1	A	2457	PSU	O4'-C1'	-2.33	1.40	1.44
1	A	955	PSU	O4'-C1'	-2.33	1.40	1.44
1	A	2552	OMU	C2-N3	-2.31	1.33	1.38
1	A	2580	PSU	C2-N3	-2.26	1.33	1.38
1	A	2605	PSU	C2-N3	-2.19	1.33	1.38
1	A	1911	PSU	C2-N3	-2.18	1.33	1.38
1	A	2457	PSU	C2-N3	-2.18	1.33	1.38
1	A	1917	PSU	C2-N3	-2.17	1.33	1.38
52	x	55	PSU	O4'-C1'	-2.17	1.41	1.44
1	A	2504	PSU	C2-N3	-2.16	1.33	1.38
1	A	2604	PSU	C2-N3	-2.16	1.33	1.38
32	a	516	PSU	C2-N3	-2.15	1.33	1.38
1	A	955	PSU	C2-N3	-2.14	1.33	1.38
1	A	746	PSU	C2-N3	-2.13	1.33	1.38
32	a	516	PSU	O4'-C1'	-2.10	1.41	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1911	PSU	O4'-C1'	-2.03	1.41	1.44
1	A	2580	PSU	C6-C5	2.03	1.41	1.38
1	A	2069	7MG	C1'-N9	2.06	1.49	1.44
52	x	55	PSU	C6-C5	2.07	1.41	1.38
32	a	1498	UR3	C6-C5	2.18	1.42	1.38
1	A	2030	6MZ	C6-N6	2.19	1.38	1.35
58	y	46	7MG	C4-N3	2.20	1.37	1.34
1	A	1618	6MZ	C6-N6	2.29	1.39	1.35
1	A	2069	7MG	C4-N3	2.39	1.37	1.34
32	a	527	7MG	C4-N3	2.50	1.37	1.34
1	A	2498	OMC	C4-N4	2.66	1.42	1.35
1	A	1915	3TD	C6-C5	2.92	1.42	1.38
1	A	1962	5MC	C4-N4	3.55	1.43	1.34
1	A	747	5MC	C4-N4	3.57	1.43	1.34
32	a	1407	5MC	C4-N4	3.58	1.43	1.34
32	a	967	5MC	C4-N4	3.59	1.43	1.34
52	x	8	4SU	C5-C4	4.72	1.44	1.38
32	a	527	7MG	C2-N2	4.80	1.44	1.34
1	A	2069	7MG	C2-N2	4.83	1.44	1.34
58	y	46	7MG	C2-N2	4.84	1.44	1.34
32	a	1498	UR3	O4-C4	5.26	1.37	1.24
1	A	745	1MG	C2-N2	5.31	1.44	1.33
1	A	2251	OMG	C2-N2	5.78	1.46	1.34
1	A	1835	2MG	O6-C6	6.67	1.41	1.24
32	a	527	7MG	O6-C6	6.67	1.41	1.24
1	A	1915	3TD	O4-C4	6.67	1.41	1.24
1	A	2552	OMU	O4-C4	6.68	1.41	1.24
1	A	2445	2MG	O6-C6	6.70	1.41	1.24
32	a	966	2MG	O6-C6	6.73	1.41	1.24
32	a	1516	2MG	O6-C6	6.74	1.41	1.24
32	a	1207	2MG	O6-C6	6.74	1.41	1.24
58	y	46	7MG	O6-C6	6.79	1.41	1.24
1	A	2069	7MG	O6-C6	6.80	1.41	1.24
1	A	745	1MG	O6-C6	7.10	1.42	1.24
1	A	2251	OMG	O6-C6	7.68	1.44	1.24
1	A	2503	2MA	C6-N6	8.11	1.43	1.29
58	y	16	H2U	O4-C4	8.95	1.42	1.23
52	x	20	H2U	O4-C4	8.96	1.42	1.23
58	y	20	H2U	O4-C4	8.97	1.42	1.23
1	A	2449	H2U	O4-C4	8.98	1.42	1.23
58	y	17	H2U	O4-C4	8.99	1.42	1.23
32	a	966	2MG	C2-N2	9.46	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1835	2MG	C2-N2	9.47	1.45	1.34
32	a	1207	2MG	C2-N2	9.50	1.45	1.34
1	A	2445	2MG	C2-N2	9.50	1.45	1.34
32	a	1516	2MG	C2-N2	9.52	1.45	1.34

All (157) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1618	6MZ	N3-C2-N1	-10.08	120.95	128.87
1	A	2030	6MZ	N3-C2-N1	-10.02	121.00	128.87
1	A	2069	7MG	C5-C4-N3	-8.83	117.75	126.74
32	a	527	7MG	C5-C4-N3	-8.15	118.44	126.74
58	y	46	7MG	C5-C4-N3	-7.36	119.24	126.74
32	a	1519	MA6	N3-C2-N1	-6.43	123.82	128.87
32	a	1518	MA6	N3-C2-N1	-6.00	124.16	128.87
58	y	16	H2U	C4-N3-C2	-4.83	121.39	125.77
58	y	17	H2U	C4-N3-C2	-4.70	121.51	125.77
1	A	2449	H2U	C4-N3-C2	-4.40	121.78	125.77
52	x	20	H2U	C4-N3-C2	-4.40	121.78	125.77
1	A	1939	5MU	C5-C4-N3	-4.35	121.69	125.35
58	y	20	H2U	C4-N3-C2	-4.31	121.86	125.77
52	x	54	5MU	C5-C4-N3	-4.12	121.89	125.35
58	y	54	5MU	C5-C4-N3	-3.93	122.05	125.35
58	y	37	YG	O23-C21-O22	-3.92	119.11	124.61
58	y	37	YG	C13-C12-C11	-3.88	125.58	131.05
1	A	1835	2MG	C1'-N9-C4	-3.62	122.77	126.81
32	a	1402	4OC	CM4-N4-C4	-3.59	119.84	122.87
1	A	1835	2MG	C6-C5-C4	-3.54	116.82	120.86
1	A	745	1MG	C6-C5-C4	-3.53	117.40	119.93
1	A	1915	3TD	C5-C6-N1	-3.53	119.46	124.38
52	x	8	4SU	C5-C4-N3	-3.38	119.98	123.56
32	a	966	2MG	C6-C5-C4	-3.36	117.02	120.86
1	A	2251	OMG	C5-C6-N1	-3.34	119.16	123.52
32	a	1207	2MG	C6-C5-C4	-3.26	117.13	120.86
1	A	2445	2MG	C6-C5-C4	-3.22	117.18	120.86
32	a	966	2MG	N3-C2-N1	-3.21	121.39	126.19
1	A	1835	2MG	N3-C2-N1	-3.15	121.47	126.19
1	A	1835	2MG	CM2-N2-C2	-3.14	119.50	123.03
1	A	2251	OMG	N3-C2-N1	-3.13	123.30	127.56
32	a	1207	2MG	N3-C2-N1	-3.12	121.53	126.19
1	A	746	PSU	C5-C1'-C2'	-3.08	110.20	115.44
1	A	2604	PSU	C5-C6-N1	-3.08	120.09	124.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2445	2MG	N3-C2-N1	-3.07	121.59	126.19
32	a	1516	2MG	C6-C5-C4	-3.06	117.36	120.86
58	y	17	H2U	O2-C2-N1	-3.06	119.17	123.17
32	a	1516	2MG	N3-C2-N1	-3.04	121.64	126.19
1	A	2445	2MG	CM2-N2-C2	-3.00	119.66	123.03
1	A	746	PSU	C5-C6-N1	-2.97	120.24	124.38
32	a	1207	2MG	CM2-N2-C2	-2.94	119.72	123.03
32	a	966	2MG	CM2-N2-C2	-2.93	119.73	123.03
1	A	2457	PSU	C5-C6-N1	-2.91	120.32	124.38
32	a	516	PSU	C5-C6-N1	-2.88	120.37	124.38
1	A	2504	PSU	C5-C6-N1	-2.87	120.37	124.38
1	A	1911	PSU	C5-C6-N1	-2.85	120.41	124.38
32	a	1516	2MG	CM2-N2-C2	-2.79	119.90	123.03
1	A	2580	PSU	C5-C6-N1	-2.77	120.52	124.38
32	a	966	2MG	C1'-N9-C4	-2.77	123.72	126.81
1	A	955	PSU	C5-C6-N1	-2.76	120.53	124.38
1	A	1917	PSU	C5-C6-N1	-2.71	120.60	124.38
58	y	16	H2U	O2-C2-N1	-2.67	119.68	123.17
1	A	2605	PSU	C5-C6-N1	-2.57	120.79	124.38
1	A	2251	OMG	C6-C5-C4	-2.53	117.96	120.86
32	a	1207	2MG	C5-C6-N1	-2.47	120.29	123.52
32	a	1516	2MG	C5-C6-N1	-2.47	120.30	123.52
1	A	2445	2MG	C5-C6-N1	-2.46	120.31	123.52
32	a	1402	4OC	C5-C4-N3	-2.45	118.80	123.22
52	x	55	PSU	C5-C6-N1	-2.44	120.98	124.38
32	a	966	2MG	C5-C6-N1	-2.41	120.37	123.52
58	y	55	PSU	C5-C6-N1	-2.41	121.02	124.38
1	A	1915	3TD	C5-C1'-C2'	-2.37	111.42	115.44
1	A	1939	5MU	C5M-C5-C6	-2.35	113.86	118.63
58	y	54	5MU	C5M-C5-C6	-2.32	113.91	118.63
52	x	54	5MU	C5M-C5-C6	-2.32	113.92	118.63
1	A	1835	2MG	C5-C6-N1	-2.26	120.57	123.52
58	y	46	7MG	C5-C6-N1	-2.24	120.06	123.39
58	y	37	YG	C3-N3-C2	-2.20	115.09	118.41
58	y	37	YG	O18-C16-O17	-2.17	119.20	123.77
1	A	2069	7MG	C5-C6-N1	-2.14	120.21	123.39
1	A	2445	2MG	N2-C2-N1	2.07	119.34	116.94
1	A	1917	PSU	O4'-C1'-C2'	2.10	106.96	104.69
52	x	55	PSU	O4'-C1'-C2'	2.15	107.02	104.69
32	a	1207	2MG	N2-C2-N1	2.17	119.46	116.94
1	A	955	PSU	O4'-C1'-C2'	2.23	107.10	104.69
58	y	46	7MG	C2-N3-C4	2.28	120.98	114.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	y	55	PSU	O4'-C1'-C2'	2.29	107.16	104.69
32	a	967	5MC	N4-C4-N3	2.31	120.31	116.92
1	A	1962	5MC	N4-C4-N3	2.32	120.32	116.92
1	A	2504	PSU	O4'-C1'-C2'	2.33	107.21	104.69
32	a	966	2MG	N2-C2-N1	2.33	119.64	116.94
1	A	1835	2MG	N2-C2-N1	2.34	119.65	116.94
32	a	1407	5MC	N4-C4-N3	2.35	120.36	116.92
1	A	747	5MC	N4-C4-N3	2.35	120.36	116.92
1	A	2580	PSU	O4'-C1'-C2'	2.37	107.25	104.69
1	A	746	PSU	O4'-C1'-C2'	2.38	107.27	104.69
1	A	1911	PSU	O4'-C1'-C2'	2.39	107.27	104.69
58	y	20	H2U	C5-C4-N3	2.42	119.18	116.62
32	a	516	PSU	O4'-C1'-C2'	2.45	107.34	104.69
1	A	2498	OMC	N4-C4-N3	2.46	120.79	116.50
52	x	20	H2U	C5-C4-N3	2.48	119.24	116.62
1	A	2449	H2U	C5-C4-N3	2.50	119.26	116.62
32	a	527	7MG	C2-N3-C4	2.50	121.61	114.50
1	A	2457	PSU	O4'-C1'-C2'	2.50	107.40	104.69
58	y	17	H2U	C5-C4-N3	2.57	119.34	116.62
1	A	2069	7MG	C2-N3-C4	2.59	121.86	114.50
58	y	16	H2U	C5-C4-N3	2.70	119.47	116.62
58	y	55	PSU	C4-C5-C1'	2.75	125.85	121.22
1	A	1915	3TD	O4'-C1'-C2'	3.03	107.97	104.69
1	A	2604	PSU	O4'-C1'-C2'	3.05	107.99	104.69
1	A	2069	7MG	C4-N9-C1'	3.09	133.97	126.65
1	A	2449	H2U	C1'-N1-C2	3.12	122.56	118.19
58	y	20	H2U	C1'-N1-C2	3.16	122.61	118.19
52	x	20	H2U	C1'-N1-C2	3.23	122.71	118.19
32	a	1518	MA6	C2-N1-C6	3.28	119.38	111.64
58	y	37	YG	O18-C16-C15	3.31	120.04	111.41
32	a	1519	MA6	C2-N1-C6	3.39	119.64	111.64
58	y	37	YG	O23-C21-N20	3.41	117.73	110.84
1	A	1835	2MG	C6-N1-C2	3.43	120.16	115.24
32	a	1516	2MG	C6-N1-C2	3.47	120.21	115.24
1	A	2445	2MG	C6-N1-C2	3.50	120.25	115.24
1	A	2069	7MG	C6-N1-C2	3.50	119.99	115.88
32	a	966	2MG	C6-N1-C2	3.53	120.29	115.24
32	a	1207	2MG	C6-N1-C2	3.55	120.32	115.24
32	a	527	7MG	C6-N1-C2	3.63	120.14	115.88
58	y	37	YG	C3-N3-C4	3.69	123.98	118.41
58	y	37	YG	C24-O23-C21	3.71	120.28	115.65
58	y	46	7MG	C6-N1-C2	3.82	120.36	115.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2251	OMG	C6-N1-C2	3.90	120.46	115.88
32	a	1402	4OC	C2-N3-C4	4.72	121.44	115.43
58	y	16	H2U	N3-C2-N1	5.29	121.54	116.64
58	y	20	H2U	N3-C2-N1	5.30	121.55	116.64
1	A	2449	H2U	N3-C2-N1	5.30	121.55	116.64
52	x	20	H2U	N3-C2-N1	5.34	121.58	116.64
58	y	17	H2U	N3-C2-N1	5.56	121.79	116.64
58	y	46	7MG	N3-C4-N9	5.58	134.19	126.98
32	a	527	7MG	N3-C4-N9	6.18	134.97	126.98
1	A	2552	OMU	C4-N3-C2	6.61	121.17	114.21
1	A	2030	6MZ	C2-N1-C6	6.68	121.27	116.47
1	A	1618	6MZ	C2-N1-C6	6.71	121.29	116.47
32	a	1207	2MG	C2-N3-C4	6.73	122.37	114.99
1	A	2604	PSU	C4-N3-C2	6.74	120.78	115.16
1	A	2445	2MG	C2-N3-C4	6.76	122.41	114.99
32	a	1516	2MG	C2-N3-C4	6.77	122.41	114.99
1	A	2457	PSU	C4-N3-C2	6.78	120.81	115.16
1	A	1911	PSU	C4-N3-C2	6.79	120.82	115.16
1	A	2069	7MG	N3-C4-N9	6.80	135.78	126.98
1	A	2504	PSU	C4-N3-C2	6.81	120.83	115.16
32	a	966	2MG	C2-N3-C4	6.84	122.49	114.99
32	a	516	PSU	C4-N3-C2	6.85	120.88	115.16
1	A	1835	2MG	C2-N3-C4	6.87	122.53	114.99
1	A	746	PSU	C4-N3-C2	6.91	120.92	115.16
1	A	955	PSU	C4-N3-C2	6.92	120.93	115.16
1	A	2580	PSU	C4-N3-C2	7.01	121.00	115.16
1	A	2605	PSU	C4-N3-C2	7.08	121.07	115.16
1	A	1917	PSU	C4-N3-C2	7.14	121.11	115.16
58	y	55	PSU	C4-N3-C2	7.44	121.37	115.16
52	x	55	PSU	C4-N3-C2	7.50	121.41	115.16
1	A	1939	5MU	C5M-C5-C4	7.85	128.67	119.97
58	y	54	5MU	C5M-C5-C4	7.93	128.75	119.97
52	x	54	5MU	C5M-C5-C4	7.95	128.78	119.97
58	y	16	H2U	C5-C6-N1	8.38	119.94	110.76
58	y	17	H2U	C5-C6-N1	8.69	120.28	110.76
52	x	20	H2U	C5-C6-N1	8.87	120.48	110.76
1	A	2449	H2U	C5-C6-N1	8.91	120.52	110.76
58	y	20	H2U	C5-C6-N1	8.91	120.53	110.76
1	A	2503	2MA	C2-N3-C4	12.31	121.22	115.29

All (70) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
52	x	8	4SU	C4'
52	x	8	4SU	C2'
52	x	8	4SU	C3'
32	a	1498	UR3	C2'
32	a	1498	UR3	C3'
58	y	46	7MG	C1'
32	a	516	PSU	C4'
32	a	516	PSU	C2'
1	A	2457	PSU	C4'
1	A	2457	PSU	C2'
1	A	1835	2MG	C2'
1	A	1835	2MG	C3'
32	a	1402	4OC	C2'
32	a	1402	4OC	C1'
1	A	2449	H2U	C1'
1	A	955	PSU	C4'
1	A	955	PSU	C2'
32	a	1516	2MG	C2'
32	a	1516	2MG	C3'
58	y	16	H2U	C1'
1	A	746	PSU	C4'
1	A	746	PSU	C2'
52	x	55	PSU	C4'
52	x	55	PSU	C2'
32	a	527	7MG	C1'
32	a	1519	MA6	C2'
32	a	1519	MA6	C3'
1	A	2445	2MG	C2'
1	A	2445	2MG	C3'
58	y	17	H2U	C1'
1	A	2069	7MG	C1'
1	A	1917	PSU	C4'
1	A	1917	PSU	C2'
1	A	2580	PSU	C4'
1	A	2580	PSU	C2'
1	A	2498	OMC	C4'
1	A	2498	OMC	C2'
32	a	966	2MG	C2'
32	a	966	2MG	C3'
1	A	1915	3TD	C4'
58	y	55	PSU	C4'
58	y	55	PSU	C2'
1	A	2552	OMU	C4'

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Mol	Chain	Res	Type	Atom
52	x	20	H2U	C1'
1	A	2251	OMG	C3'
1	A	2251	OMG	C1'
1	A	2605	PSU	C4'
1	A	2605	PSU	C2'
1	A	1911	PSU	C4'
1	A	1911	PSU	C2'
52	x	54	5MU	C4'
52	x	54	5MU	C2'
52	x	54	5MU	C3'
58	y	54	5MU	C4'
58	y	54	5MU	C2'
58	y	54	5MU	C3'
32	a	1207	2MG	C2'
32	a	1207	2MG	C3'
1	A	1939	5MU	C4'
1	A	1939	5MU	C2'
1	A	1939	5MU	C3'
1	A	2503	2MA	C2'
1	A	2503	2MA	C1'
32	a	1518	MA6	C2'
32	a	1518	MA6	C3'
1	A	2604	PSU	C4'
1	A	2604	PSU	C2'
1	A	2504	PSU	C4'
1	A	2504	PSU	C2'
58	y	20	H2U	C1'

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1915	3TD	3	0
1	A	1962	5MC	1	0
1	A	2030	6MZ	1	0
1	A	2069	7MG	3	0
1	A	2251	OMG	1	0
1	A	2503	2MA	2	0
1	A	2504	PSU	1	0
1	A	2552	OMU	1	0
1	A	2580	PSU	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	745	1MG	2	0
1	A	746	PSU	2	0
1	A	747	5MC	3	0
1	A	955	PSU	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
57	z	6

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	z	517:UNK	C	518:UNK	N	39.33
1	z	561:UNK	C	663:ALA	N	37.34
1	z	493:UNK	C	494:UNK	N	34.24
1	z	547:UNK	C	548:UNK	N	30.19
1	z	526:UNK	C	527:UNK	N	18.32
1	z	535:UNK	C	536:UNK	N	8.04