



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 29, 2025 – 05:30 AM EDT

PDB ID : 4IOA / pdb_00004ioa
Title : Crystal structure of compound 4e bound to large ribosomal subunit (50S) from *Deinococcus radiodurans*
Authors : Han, S.; Marr, E.S.
Deposited on : 2013-01-07
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0rc1
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

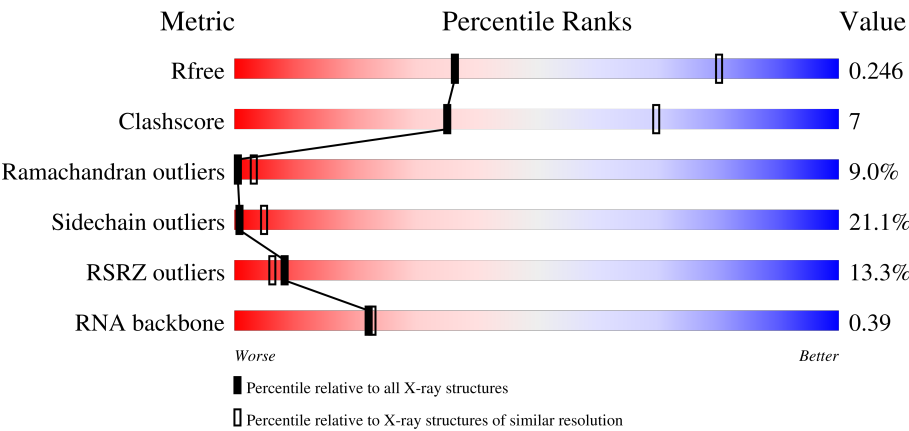
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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)	Similar resolution (#Entries, resolution range(Å))
R _{free}	164625	1370 (3.20-3.20)
Clashscore	180529	1497 (3.20-3.20)
Ramachandran outliers	177936	1479 (3.20-3.20)
Sidechain outliers	177891	1478 (3.20-3.20)
RSRZ outliers	164620	1371 (3.20-3.20)
RNA backbone	3690	1111 (3.50-2.90)

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

Mol	Chain	Length	Quality of chain
1	X	2880	<div><div>4%</div><div>50%</div><div>28%</div><div>12%</div><div>7%</div></div>
2	Y	123	<div><div>7%</div><div>61%</div><div>29%</div><div>8%</div><div></div></div>
3	A	274	<div><div>18%</div><div>43%</div><div>30%</div><div>12%</div><div>12%</div></div>
4	B	211	<div><div>5%</div><div>60%</div><div>23%</div><div>12%</div><div></div></div>

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Mol	Chain	Length	Quality of chain
5	C	205	
6	D	180	
7	E	185	
8	F	144	
9	G	174	
10	H	134	
11	I	156	
12	J	141	
13	K	116	
14	L	114	
15	M	166	
16	N	118	
17	O	100	
18	P	134	
19	Q	95	
20	R	115	
21	S	237	
22	T	91	
23	U	81	
24	V	67	
25	W	55	
26	Z	60	
27	1	55	
28	2	47	
29	3	66	

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Mol	Chain	Length	Quality of chain
30	4	37	<div> <div>84%</div> <div> <div></div> <div>68%</div> <div>27%</div> <div>5%</div> </div> </div>

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
31	MG	X	2904	-	-	-	X
31	MG	X	2922	-	-	-	X
31	MG	X	2930	-	-	-	X

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 83879 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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					ZeroOcc	AltConf	Trace
1	X	2686	Total	C	N	O	P	0	0	0
			57651	25718	10642	18606	2685			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	122	Total	C	N	O	P	0	0	0
			2598	1161	476	840	121			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	240	Total	C	N	O	S	0	0	0
			1826	1137	366	321	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	205	Total	C	N	O	S	0	0	0
			1539	965	295	271	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	197	Total	C	N	O	S	0	0	0
			1506	935	287	282	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	177	Total	C	N	O	S	0	0	0
			1400	892	247	254	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	171	Total	C	N	O	S	0	0	0
			1286	812	237	236	1			

- Molecule 8 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	71	Total	C	N	O	S	0	0	0
			503	310	91	99	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	G	142	Total	C	N	O	S	0	0	0
			1114	704	209	198	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	134	Total	C	N	O	S	0	0	0
			997	614	198	180	5			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	I	141	Total	C	N	O	0	0	0
			1067	655	216	196			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	J	136	Total	C	N	O	S	0	0	0
			1090	696	202	185	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	113	Total	C	N	O	S	0	0	0
			878	541	178	157	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	L	104	Total	C	N	O	0	0	0
			779	476	161	142			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	M	108	Total	C	N	O	0	0	0
			871	543	172	156			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	N	117	Total	C	N	O	S	0	0	0
			978	608	210	159	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	O	94	Total	C	N	O	0	0	0
			741	465	139	137			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	P	127	Total	C	N	O	S	0	0	0
			1014	639	199	174	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Q	93	Total	C	N	O	S	0	0	0
			726	458	136	130	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	110	Total	C	N	O	S	0	0	0
			825	513	160	151	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	S	175	Total	C	N	O	S	0	0	0
			1345	849	236	254	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	T	84	Total	C	N	O	S	0	0	0
			625	393	122	109	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	U	72	Total	C	N	O		0	0	0
			552	341	116	95				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	V	66	Total	C	N	O	S	0	0	0
			533	327	107	96	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	W	55	Total	C	N	O	S	0	0	0
			424	264	82	76	2			

- Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	58	Total	C	N	O	S	0	0	0
			457	281	94	77	5			

- Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
27	1	53	Total C	0	0	53
			53 53			

- Molecule 28 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
28	2	46	Total C 46 46	0	0	46

- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
29	3	63	Total C 63 63	0	0	63

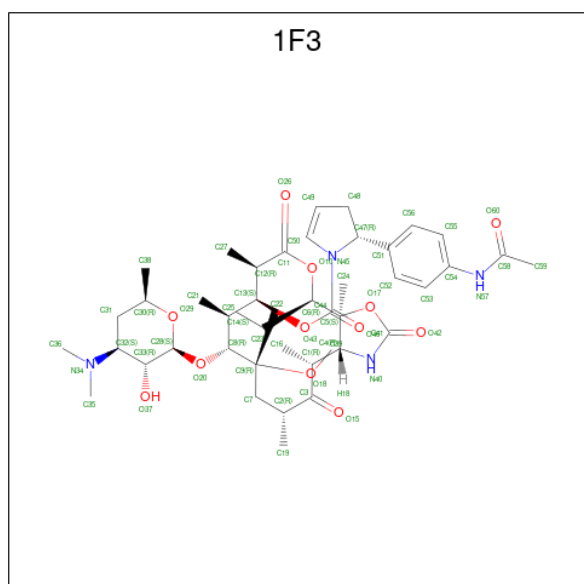
- Molecule 30 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
30	4	37	Total C N O S 297 179 66 47 5	0	0	0

- Molecule 31 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	X	30	Total Mg 30 30	0	0
31	Y	5	Total Mg 5 5	0	0

- Molecule 32 is (3aS,4R,7R,8S,9S,10R,11R,13R,15R,15aR)-4-ethyl-11-methoxy-3a,7,9,11,13,15-hexamethyl-2,6,14-trioxo-10-{[3,4,6-trideoxy-3-(dimethylamino)-beta-D-xylo-hexopyranosyl]oxy}tetradecahydro-2H-oxacyclotetradecino[4,3-d][1,3]oxazol-8-yl (2R)-2-[4-(acetylamino)phenyl]-2,3-dihydro-1H-pyrrole-1-carboxylate (CCD ID: 1F3) (formula: C₄₄H₆₆N₄O₁₂).

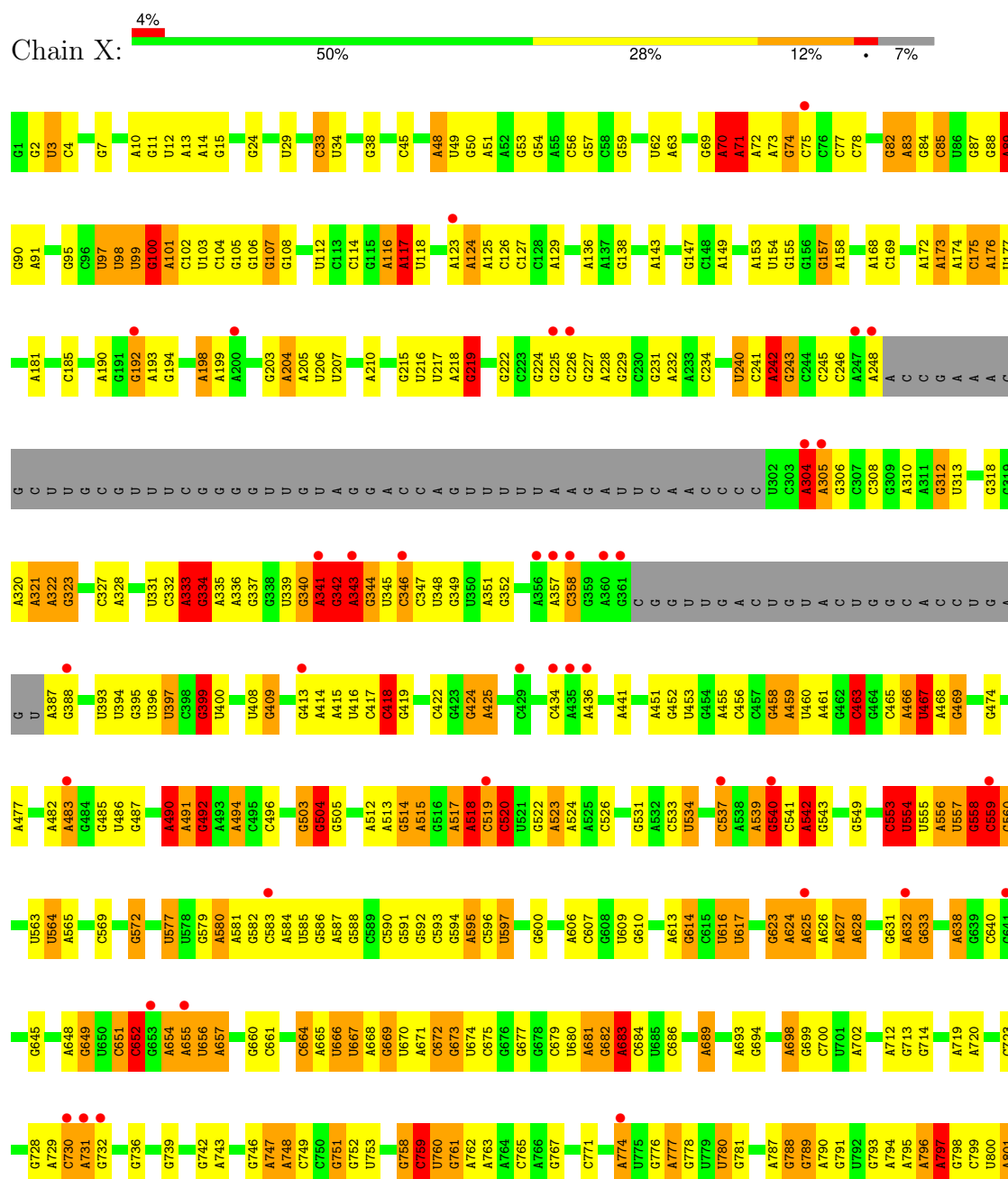


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	X	1	Total	C	N	O	0	0
			60	44	4	12		

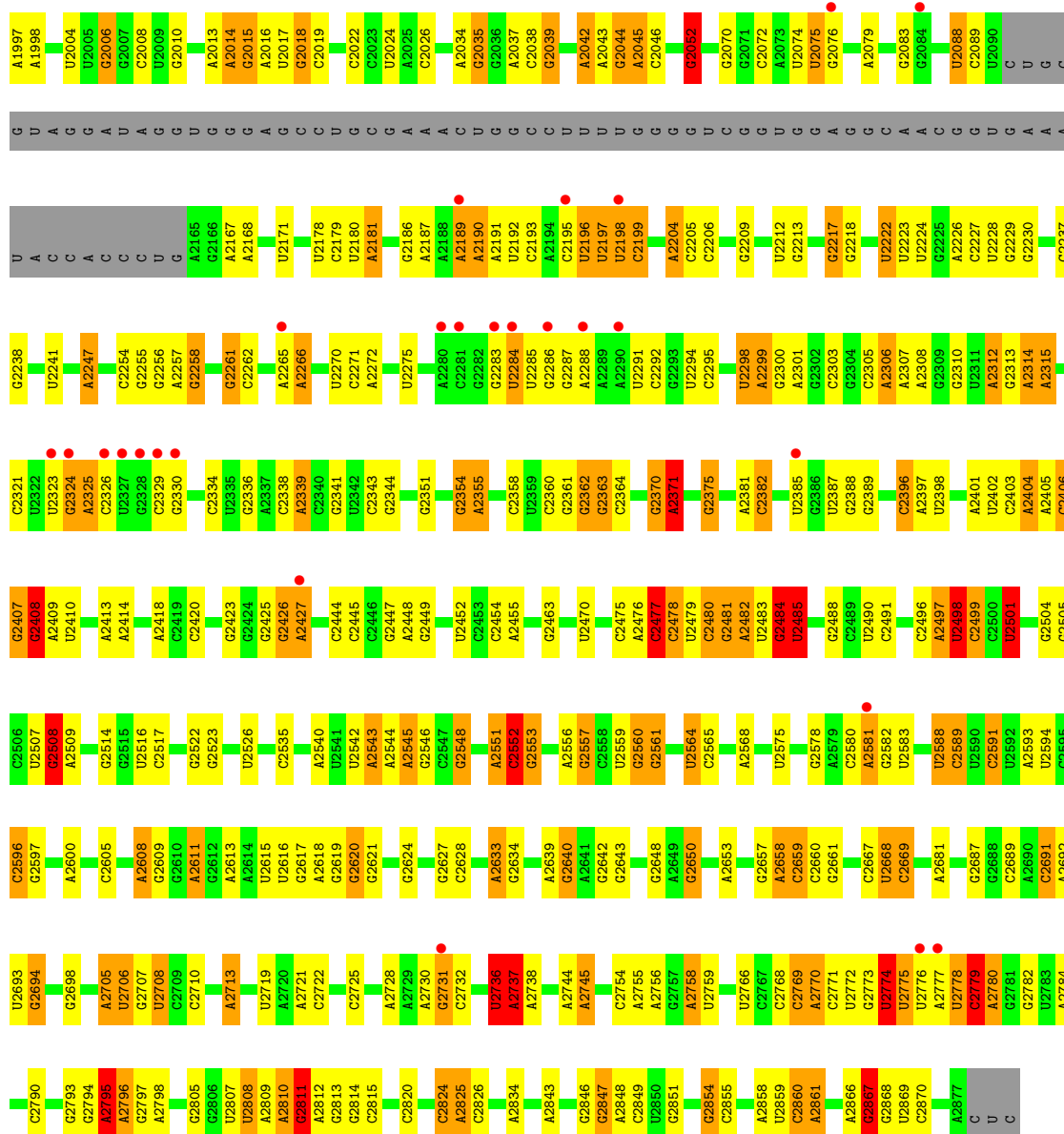
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

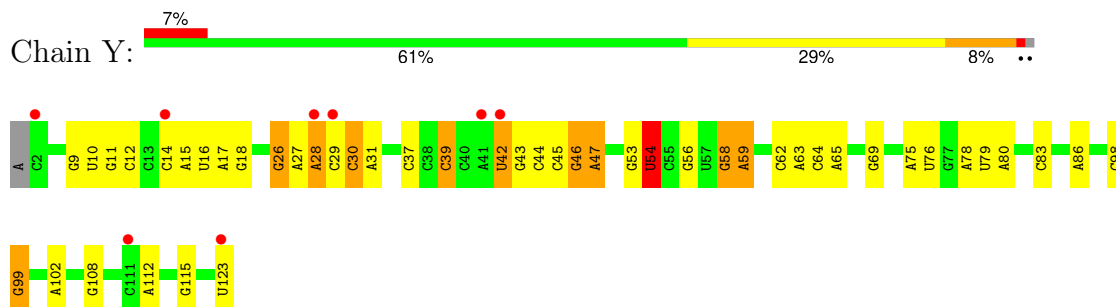
- Molecule 1: 23S ribosomal RNA



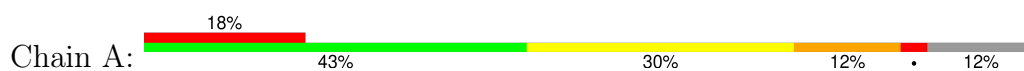
U1914	G1831	G1737	U1666	U1551	G1465	U1357	G1273	A1154	A1081	G1000	U	A802
G1918	G1832	G1742	U1657	C1552	C1466	C1388	C1274	G1155	G1082	A1001	A	C803
A1920	G1834	G1747	A1658	U1553	U1467	U1365	A1275	U1161	C1083	G0805	C	C804
A1921	A1240	G1753	G1660	G1554	U1469	A1366	U1276	C1169	G1085	A1004	A	A806
U1922	A1945	A1753	C1661	A1561	G1471	A1367	A1277	G1173	C1086	C1006	C	A807
U1923	A1850	G1754	G1662	U1562	C1472	G1368	G1278	G1173	A1087	A1007	U	G811
U1926	G1850	G1755	C1663	G1563	U1473	G1373	U1280	U1182	C1088	U1010	U	G812
U1927	G1854	C1756	G1664	U1564	A1474	A1378	A1281	C1183	C1091	A1011	A	A813
G1928	G1854	C1757	C1665	G1570	G1476	G1381	C1283	C1185	U1092	A1012	C	G814
A1935	A1859	A1764	G1666	G1571	U1481	G1384	A1285	G1186	C1094	G1014	A911	A815
U1938	A1860	C1765	A1689	A1574	U1482	G1385	U1286	A1187	A1095	U1015	A922	G818
U1939	C1862	A1771	A1670	C1575	G1483	U1392	A1287	A1188	A1096	C1016	A923	G822
A1943	U1863	G1772	C1673	G1576	U1490	U1403	A1289	G1189	A1097	U1019	C926	U823
U1946	G1864	A1774	C1674	C1581	A1493	A1404	A1290	G1191	A1099	G0825	C927	U824
U1947	C1865	A1775	U1675	A1582	G1494	A1405	G1291	A1192	G1100	A1022	G931	U826
G1947	G1866	A1776	G1677	A1583	G1495	U1406	A1297	G1193	G1104	U1023	G938	C828
U1950	A1872	U1778	U1679	G1584	C1496	A1407	A1300	U1194	U1108	G1024	G939	C829
G1951	A1873	C1779	U1680	A1586	G1498	A1408	U1301	U1195	A1109	C1028	G940	C830
A1952	G1874	G1787	G1683	A1587	U1505	A1409	C1302	C1218	U1112	C1031	G944	G831
A1953	U1881	C1788	G1684	A1588	C1506	U1410	U1307	C1219	C1113	A1032	U945	A840
G1955	A1882	G1789	A1685	G1589	A1507	U1411	A1313	G1220	C1114	G1033	U946	G841
G1958	G1883	G1790	A1686	U1600	G1508	C1412	A1314	U1195	C1115	U1034	C947	A842
U1959	C1884	C1791	G1687	U1601	A1509	U1413	A1315	A1233	U1116	G1035	C948	G843
A1960	C1885	C1792	U1688	G1602	A1510	U1414	A1316	C1234	G1117	U1037	G949	U852
G1961	G1886	U1793	U1689	A1603	U1513	U1421	C1319	C1235	U1119	U1038	G951	C853
A1962	U1887	A1800	U1690	U1607	C1514	C1422	G1324	A1238	G1121	U1044	U954	G858
G1963	C1888	G1803	A1693	U1608	A1516	G1428	C1328	G1240	A1122	G1050	G955	U859
U1964	G	U1804	A1699	G1613	G1519	A1429	U1329	G1248	C1127	U1051	A956	U868
U1965	C	U1805	C1702	U1618	G1520	U1431	G1330	G1249	G1128	C1052	A957	C869
U1974	C	G1806	C1702	U1618	U1521	U1432	G1333	A1250	A1129	G1053	U971	C870
G1975	U	A1807	C1702	C1623	C1522	A1433	A1334	G1251	U1130	C1054	A964	U871
U1976	A	C1808	U1710	A1624	A1523	U1434	A1335	C1252	U1134	A1055	G967	G872
C1979	C	G1809	C1711	A1625	C1524	A1437	A1336	G1253	U1135	U1056	C968	U873
A1980	U	U1810	G1712	A1626	A1525	U1438	G1337	G1254	G1136	A1057	U969	G874
G1983	A	A1811	G1713	C1627	C1528	A1441	U1338	U1257	C1137	G1058	A970	G875
A1984	A	U1812	G1716	G1628	C1531	C1442	C1340	U1257	A1138	C1060	A971	C878
G1985	C	A1813	A1717	G1629	A1532	G1443	G1341	A1259	U1140	G1067	C972	A879
G1986	C	G1816	U1723	A1630	G1533	U1444	U1342	G1261	A1143	A1068	U973	C880
G1987	C	U1817	C1724	A1632	G1533	U1448	C1343	G1261	U1144	G1069	U978	U890
A1988	G	G1820	C1725	C1633	G1541	U1448	U1344	G1264	A1143	G1070	A891	A891
C1989	U	A1821	C1726	A1634	G1542	U1448	C1344	G1264	U1144	U1071	G985	G
U1990	C	C1726	C1726	G1635	G1543	U1448	G1345	G1264	U1144	U1072	A986	G
C1991	C	C1726	C1726	G1636	G1543	U1448	G1345	G1264	U1144	U1073	A990	G
G1992	U1909	C1825	U1732	U1636	G1544	U1448	G1345	G1264	U1144	U1073	A991	G
G1993	A1910	U1826	U1733	G1644	G1545	U1448	A1353	G1266	U1145	U1077	A994	G
U1994	A1911	G1827	C1735	U1645	C1546	U1460	A1354	U1267	G1146	A1078	A995	G
G1995	G1912	G1827	G1735	U1646	C1547	U1460	A1355	U1268	C1152	A1078	A995	C
A1996	G1913	C1830	C1736	C1648	U1548	U1460	G1356	G1269	A1153	A1078	A995	C

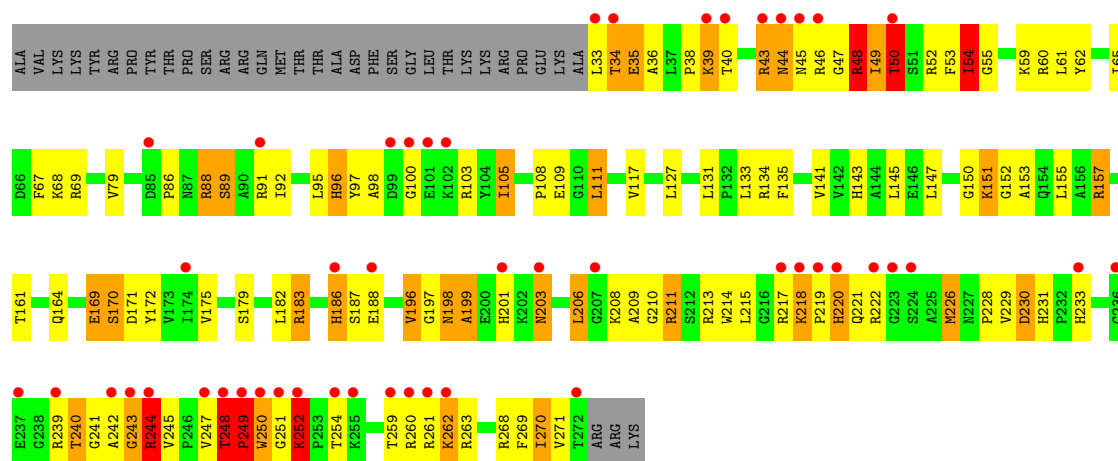


- Molecule 2: 5S ribosomal RNA

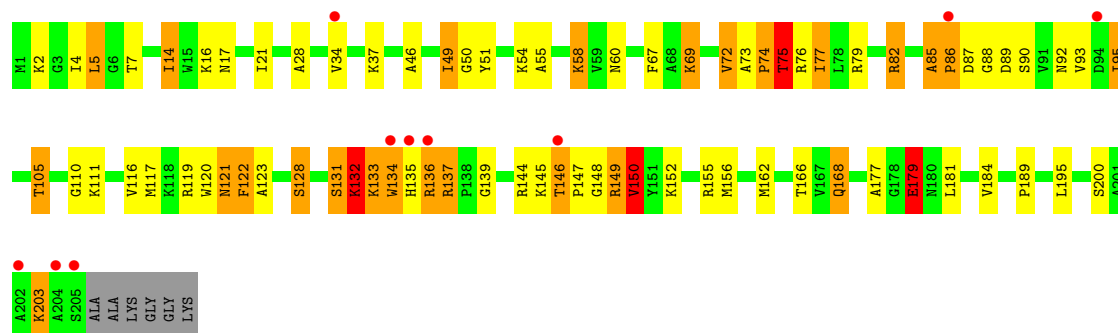


- Molecule 3: 50S ribosomal protein L2

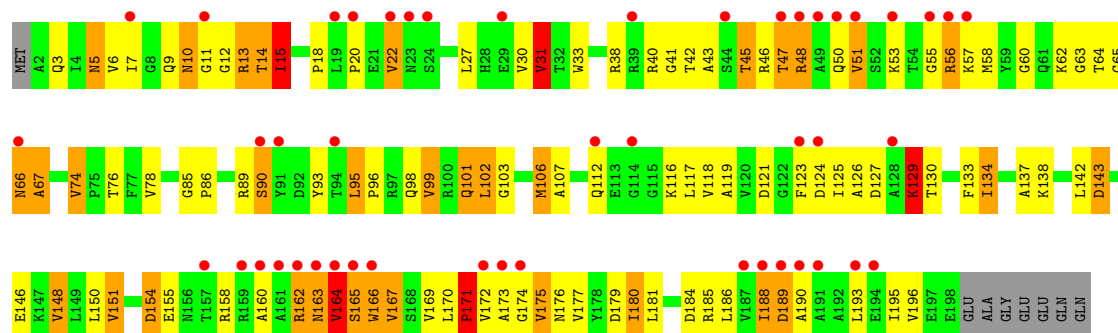
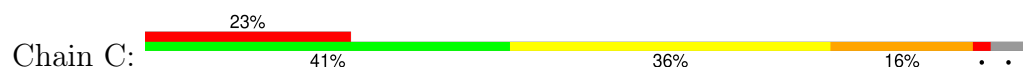




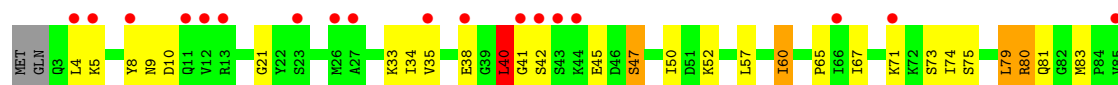
• Molecule 4: 50S ribosomal protein L3

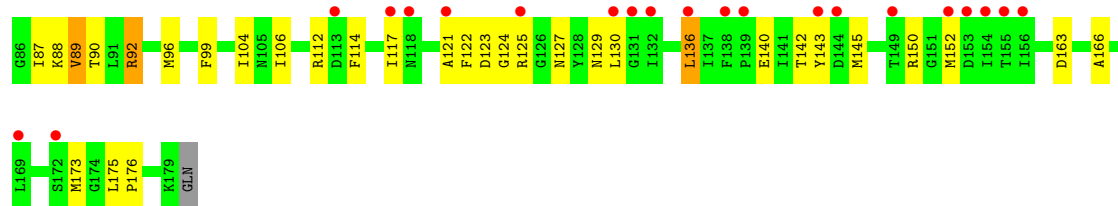


• Molecule 5: 50S ribosomal protein L4

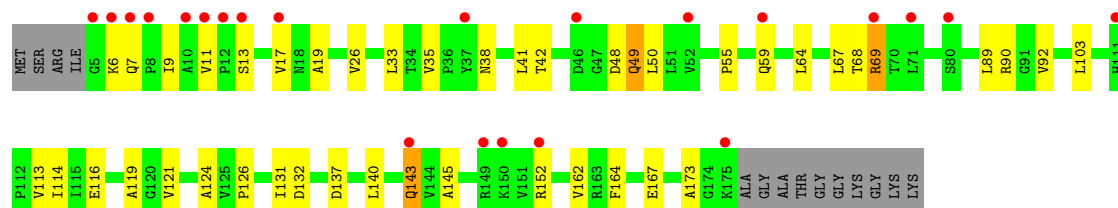


• Molecule 6: 50S ribosomal protein L5

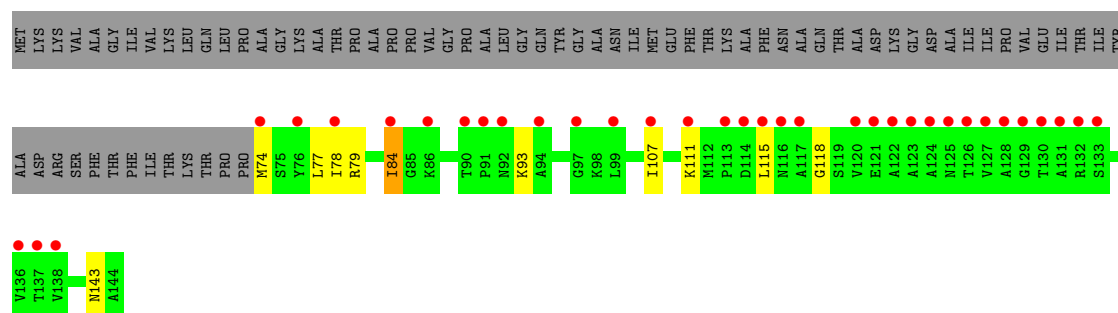
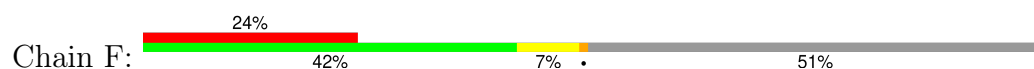




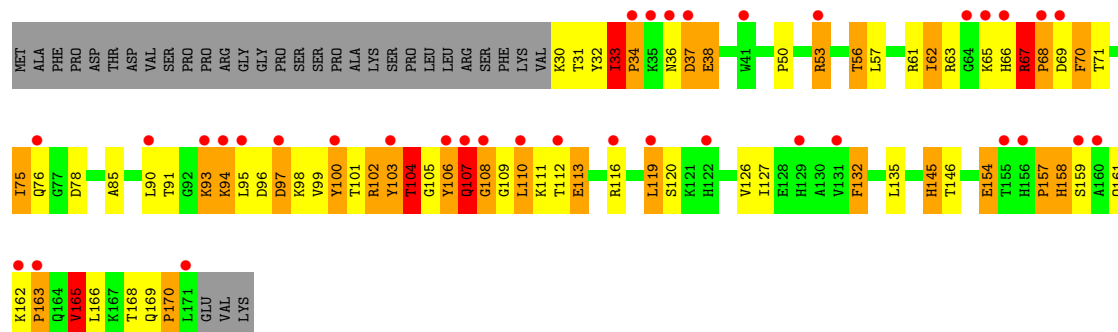
• Molecule 7: 50S ribosomal protein L6



• Molecule 8: 50S ribosomal protein L11

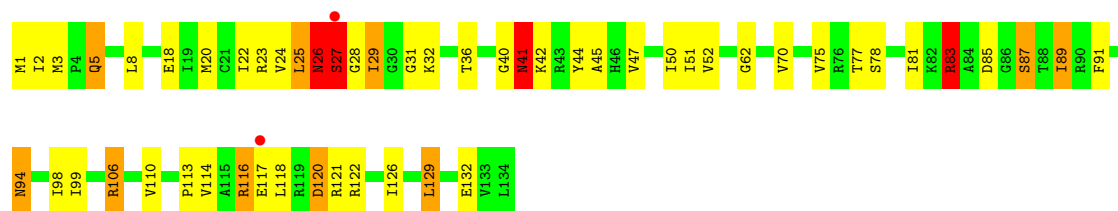


• Molecule 9: 50S ribosomal protein L13

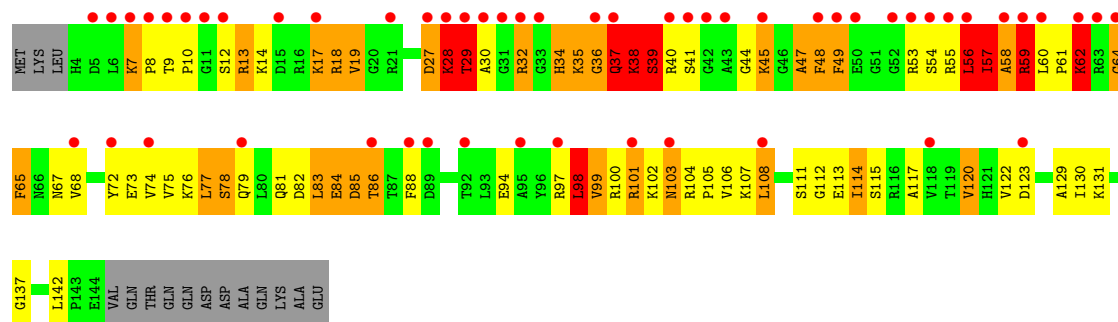


• Molecule 10: 50S ribosomal protein L14

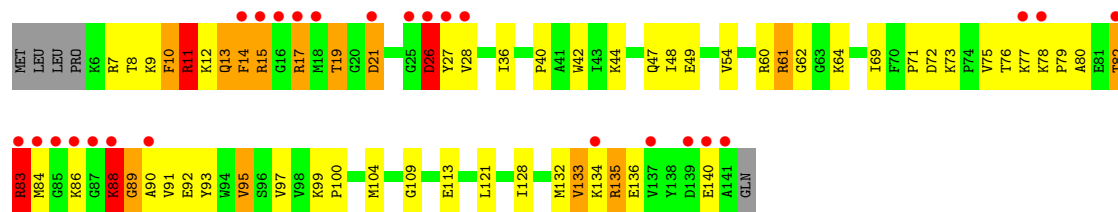




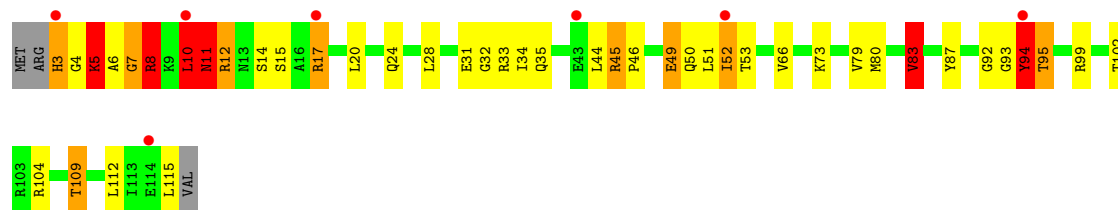
• Molecule 11: 50S ribosomal protein L15



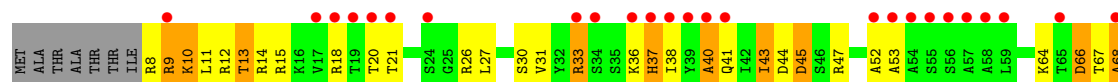
• Molecule 12: 50S ribosomal protein L16

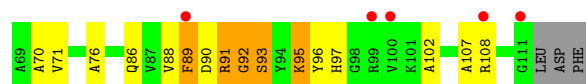


• Molecule 13: 50S ribosomal protein L17

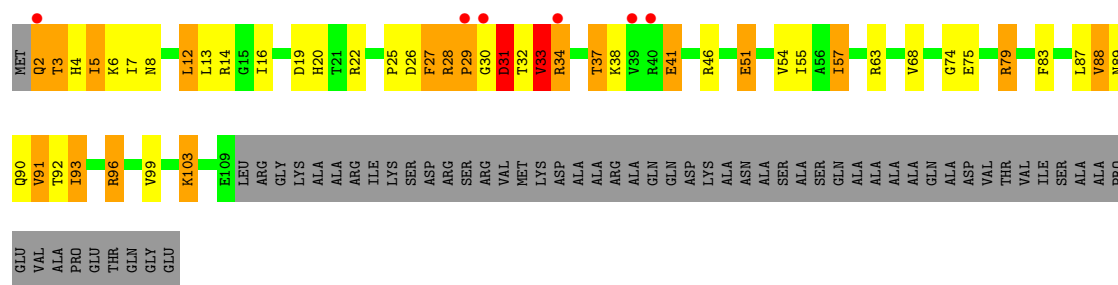
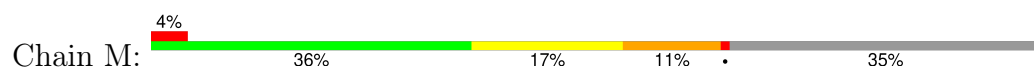


• Molecule 14: 50S ribosomal protein L18

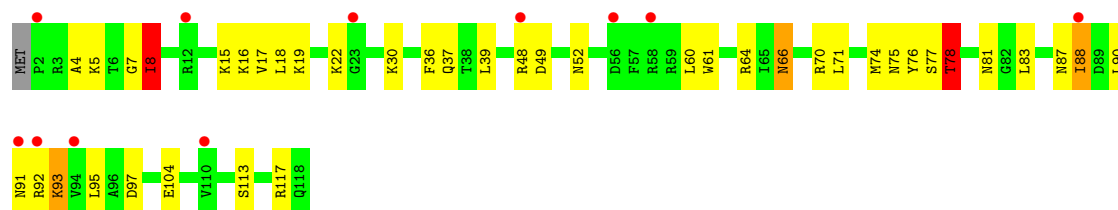




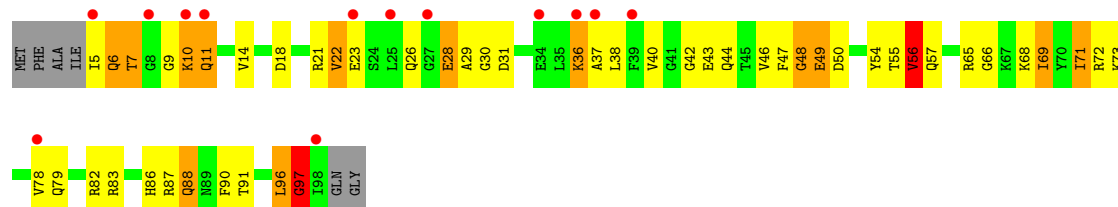
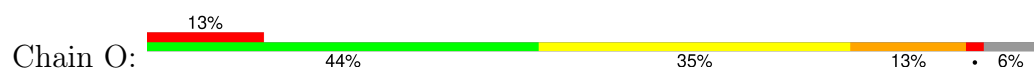
• Molecule 15: 50S ribosomal protein L19



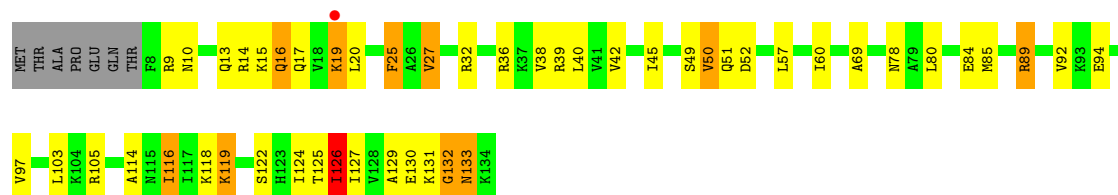
• Molecule 16: 50S ribosomal protein L20



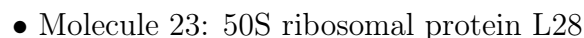
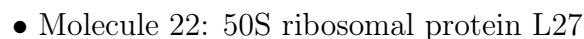
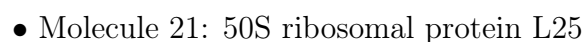
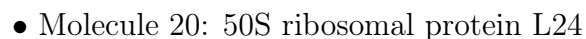
• Molecule 17: 50S ribosomal protein L21



• Molecule 18: 50S ribosomal protein L22

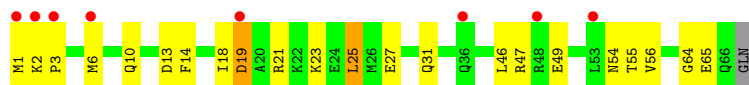


• Molecule 19: 50S ribosomal protein L23





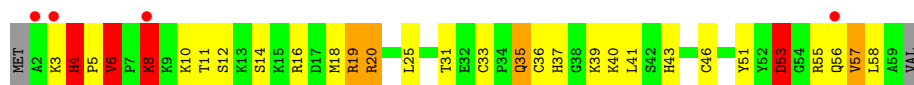
- Molecule 24: 50S ribosomal protein L29



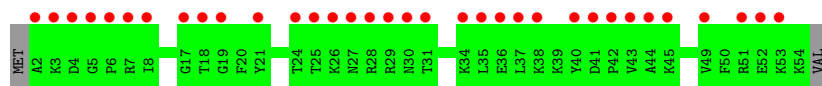
- Molecule 25: 50S ribosomal protein L30



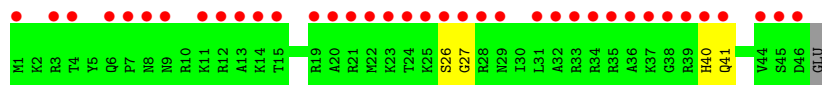
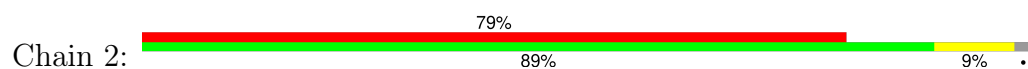
- Molecule 26: 50S ribosomal protein L32



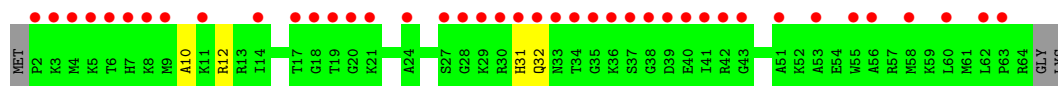
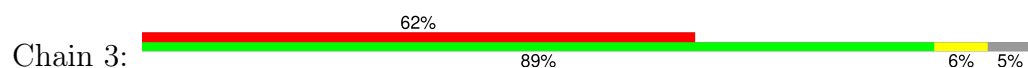
- Molecule 27: 50S ribosomal protein L33



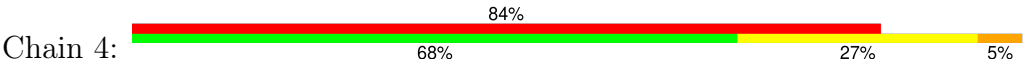
- Molecule 28: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L36



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	169.77Å 406.66Å 696.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.20 30.00 – 3.23	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.20) 89.7 (30.00-3.23)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.51 (at 3.24Å)	Xtriage
Refinement program	autoBUSTER	Depositor
R, R_{free}	0.197 , 0.230 0.210 , 0.246	Depositor DCC
R_{free} test set	17364 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	80.0	Xtriage
Anisotropy	0.713	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 84.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	83879	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 1F3

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	X	0.69	21/64561 (0.0%)	1.38	832/100708 (0.8%)
2	Y	0.69	0/2904	1.24	12/4525 (0.3%)
3	A	1.07	9/1862 (0.5%)	1.62	31/2510 (1.2%)
4	B	1.01	3/1567 (0.2%)	1.55	21/2105 (1.0%)
5	C	1.04	3/1529 (0.2%)	1.70	41/2070 (2.0%)
6	D	0.86	0/1419	1.31	4/1903 (0.2%)
7	E	0.82	0/1308	1.33	4/1771 (0.2%)
8	F	0.92	0/508	1.38	0/683
9	G	1.01	2/1138 (0.2%)	1.71	29/1539 (1.9%)
10	H	0.94	1/1007 (0.1%)	1.48	12/1352 (0.9%)
11	I	1.25	9/1081 (0.8%)	1.83	32/1448 (2.2%)
12	J	1.10	2/1113 (0.2%)	1.61	17/1486 (1.1%)
13	K	1.25	4/886 (0.5%)	1.76	21/1188 (1.8%)
14	L	0.97	0/785	1.75	12/1048 (1.1%)
15	M	1.06	5/884 (0.6%)	1.60	15/1186 (1.3%)
16	N	0.86	0/994	1.55	6/1323 (0.5%)
17	O	0.94	0/750	1.60	14/1000 (1.4%)
18	P	0.93	0/1027	1.47	10/1373 (0.7%)
19	Q	1.05	1/737 (0.1%)	1.70	18/988 (1.8%)
20	R	1.12	1/835 (0.1%)	1.68	23/1121 (2.1%)
21	S	0.92	0/1370	1.40	10/1862 (0.5%)
22	T	0.92	0/633	1.44	11/838 (1.3%)
23	U	1.33	3/556 (0.5%)	1.92	22/741 (3.0%)
24	V	0.83	0/537	1.56	5/714 (0.7%)
25	W	0.79	0/426	1.48	7/568 (1.2%)
26	Z	1.07	1/469 (0.2%)	1.69	11/629 (1.7%)
30	4	0.95	0/298	1.31	0/390
All	All	0.79	65/91184 (0.1%)	1.43	1220/137069 (0.9%)

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	X	0	6

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	I	38	LYS	CA-C	11.43	1.62	1.52
13	K	52	ILE	CG1-CD1	10.65	1.93	1.51
26	Z	53	ASP	CA-C	8.64	1.64	1.52
15	M	29	PRO	CA-C	8.60	1.64	1.52
11	I	29	THR	CA-C	8.14	1.63	1.52
13	K	3	HIS	CA-C	8.07	1.70	1.52
3	A	239	ARG	C-N	7.82	1.40	1.33
3	A	242	ALA	CA-C	7.63	1.63	1.52
11	I	28	LYS	CA-C	7.04	1.62	1.52
3	A	240	THR	CA-C	6.97	1.59	1.53
11	I	28	LYS	C-N	6.92	1.43	1.33
1	X	1946	U	C1'-N1	6.87	1.58	1.48
4	B	156	MET	SD-CE	-6.87	1.62	1.79
23	U	46	LEU	CA-C	6.70	1.61	1.52
1	X	434	C	C1'-N1	6.49	1.57	1.47
12	J	19	THR	CA-C	6.49	1.60	1.52
5	C	66	ASN	C-N	6.40	1.42	1.33
13	K	8	ARG	CA-C	6.29	1.61	1.52
4	B	136	ARG	CA-C	-6.18	1.44	1.52
11	I	39	SER	CA-C	6.16	1.61	1.52
9	G	33	ILE	CA-C	6.07	1.59	1.52
5	C	57	LYS	C-N	6.04	1.42	1.33
1	X	483	A	O5'-C5'	5.95	1.51	1.42
1	X	1467	U	C1'-N1	5.92	1.57	1.48
12	J	15	ARG	CA-C	5.89	1.60	1.52
23	U	46	LEU	C-N	5.89	1.42	1.33
4	B	89	ASP	CA-C	5.84	1.59	1.53
3	A	239	ARG	CA-C	5.84	1.60	1.52
11	I	41	SER	CA-C	5.74	1.60	1.52
19	Q	58	VAL	CA-C	5.67	1.57	1.52
15	M	57	ILE	CG1-CD1	5.64	1.73	1.51
3	A	241	GLY	C-N	5.63	1.41	1.33
3	A	242	ALA	N-CA	5.61	1.53	1.46
1	X	2321	C	C1'-N1	5.61	1.56	1.48
11	I	38	LYS	C-N	5.59	1.41	1.33
1	X	868	U	C1'-N1	5.53	1.56	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	M	33	VAL	CA-CB	5.52	1.60	1.53
5	C	47	THR	CA-CB	5.50	1.62	1.53
9	G	107	GLN	CA-C	5.49	1.60	1.52
1	X	327	C	C1'-N1	5.44	1.56	1.48
1	X	2485	U	C1'-N1	5.42	1.56	1.48
1	X	358	C	C1'-N1	5.42	1.56	1.48
1	X	78	C	C1'-N1	5.41	1.56	1.48
10	H	1	MET	SD-CE	-5.35	1.66	1.79
11	I	39	SER	N-CA	5.31	1.53	1.46
13	K	11	ASN	N-CA	5.30	1.53	1.46
1	X	1522	C	C1'-N1	5.29	1.56	1.48
23	U	47	HIS	C-N	5.24	1.41	1.33
1	X	2072	C	C1'-N1	5.23	1.56	1.48
3	A	245	VAL	CA-C	5.18	1.56	1.52
11	I	29	THR	N-CA	5.17	1.52	1.46
1	X	422	C	C1'-N1	5.17	1.56	1.48
1	X	1909	U	C1'-N1	5.15	1.55	1.47
1	X	661	C	C1'-N1	5.13	1.56	1.48
3	A	54	ILE	CA-C	5.12	1.59	1.52
1	X	346	C	C1'-N1	5.11	1.56	1.48
15	M	29	PRO	C-O	5.09	1.30	1.24
1	X	723	C	C1'-N1	5.08	1.56	1.48
1	X	927	C	C1'-N1	5.08	1.56	1.48
20	R	49	GLU	CA-C	5.05	1.59	1.52
1	X	1253	C	C1'-N1	5.03	1.55	1.48
3	A	203	ASN	C-N	5.03	1.38	1.33
1	X	540	G	C3'-O3'	5.03	1.49	1.42
1	X	2284	U	C1'-N1	5.02	1.55	1.48
15	M	93	ILE	CG1-CD1	-5.01	1.32	1.51

All (1220) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1288	A	C1'-O4'-C4'	-30.81	78.89	109.70
1	X	1288	A	C4'-C3'-C2'	-19.04	83.56	102.60
1	X	1288	A	C5'-C4'-O4'	16.75	134.22	109.10
11	I	64	GLY	N-CA-C	15.62	126.04	111.67
1	X	1716	G	P-O3'-C3'	14.94	142.60	120.20
1	X	1775	A	P-O3'-C3'	13.93	141.10	120.20
1	X	1975	G	C2'-C3'-O3'	13.71	130.07	109.50
1	X	540	G	P-O3'-C3'	13.16	139.94	120.20
1	X	1468	A	O4'-C1'-C2'	-12.97	94.63	107.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2497	A	P-O3'-C3'	12.19	138.49	120.20
1	X	1473	U	P-O3'-C3'	12.00	138.20	120.20
1	X	1631	C	P-O3'-C3'	11.89	138.03	120.20
1	X	2705	A	P-O3'-C3'	11.88	138.03	120.20
1	X	1475	U	P-O3'-C3'	11.59	137.59	120.20
1	X	994	A	P-O3'-C3'	11.57	137.56	120.20
1	X	1775	A	C2'-C3'-O3'	11.48	126.73	109.50
1	X	1288	A	O4'-C4'-C3'	-11.46	94.64	106.10
1	X	777	A	P-O3'-C3'	11.45	137.37	120.20
1	X	2014	A	P-O3'-C3'	11.44	137.36	120.20
1	X	2706	U	P-O3'-C3'	11.43	137.35	120.20
1	X	1812	U	C1'-O4'-C4'	-11.43	98.27	109.70
1	X	399	G	P-O3'-C3'	11.40	137.30	120.20
1	X	1141	U	C2'-C3'-O3'	11.20	126.31	109.50
1	X	1249	G	P-O3'-C3'	11.19	136.99	120.20
1	X	802	A	P-O3'-C3'	11.11	136.86	120.20
1	X	1574	A	C4'-C3'-C2'	-11.06	91.54	102.60
1	X	1963	G	C2'-C3'-O3'	11.05	126.08	109.50
1	X	2824	C	C2'-C3'-O3'	10.98	125.97	109.50
14	L	88	VAL	CA-C-N	10.83	136.08	120.82
14	L	88	VAL	C-N-CA	10.83	136.08	120.82
1	X	1669	A	O4'-C4'-C3'	-10.80	93.20	104.00
1	X	777	A	C2'-C3'-O3'	10.69	125.53	109.50
3	A	211	ARG	N-CA-C	-10.63	98.61	111.69
1	X	100	G	P-O3'-C3'	10.60	136.10	120.20
1	X	1409	U	P-O3'-C3'	10.47	135.91	120.20
1	X	176	A	P-O3'-C3'	10.44	135.86	120.20
1	X	2564	U	P-O3'-C3'	10.39	135.78	120.20
1	X	98	U	P-O3'-C3'	10.37	135.75	120.20
13	K	94	TYR	CA-C-N	10.29	141.19	121.54
13	K	94	TYR	C-N-CA	10.29	141.19	121.54
1	X	2736	U	P-O3'-C3'	10.25	135.58	120.20
1	X	1467	U	P-O3'-C3'	-10.16	104.96	120.20
1	X	1037	U	C1'-O4'-C4'	-10.07	99.63	109.70
19	Q	60	GLY	CA-C-N	10.03	140.70	121.54
19	Q	60	GLY	C-N-CA	10.03	140.70	121.54
1	X	1019	U	P-O3'-C3'	10.01	135.21	120.20
1	X	2404	A	P-O3'-C3'	10.00	135.20	120.20
1	X	1811	A	P-O3'-C3'	9.94	135.11	120.20
1	X	1820	G	P-O3'-C3'	9.94	135.11	120.20
1	X	1152	C	P-O3'-C3'	9.87	135.00	120.20
3	A	49	ILE	N-CA-CB	9.85	121.82	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	758	G	C2'-C3'-O3'	9.82	128.43	113.70
1	X	33	C	P-O3'-C3'	9.81	134.92	120.20
1	X	2018	G	P-O3'-C3'	9.80	134.91	120.20
1	X	788	G	C2'-C3'-O3'	9.79	124.19	109.50
1	X	1938	U	P-O3'-C3'	9.74	134.81	120.20
1	X	467	U	C1'-O4'-C4'	-9.74	100.16	109.90
1	X	1561	A	P-O3'-C3'	9.74	134.80	120.20
1	X	1811	A	C2'-C3'-O3'	9.68	124.01	109.50
1	X	2691	C	O4'-C1'-C2'	-9.66	96.14	105.80
1	X	1233	A	P-O3'-C3'	9.63	134.65	120.20
1	X	1249	G	C2'-C3'-O3'	9.63	123.95	109.50
1	X	2808	U	O4'-C1'-N1	9.55	122.53	108.20
1	X	334	G	P-O3'-C3'	9.55	134.52	120.20
3	A	203	ASN	CA-CB-CG	9.51	122.11	112.60
1	X	399	G	C2'-C3'-O3'	9.50	123.76	109.50
1	X	1467	U	C4'-C3'-O3'	9.49	127.24	113.00
1	X	1963	G	P-O3'-C3'	9.48	134.42	120.20
1	X	1055	A	P-O3'-C3'	9.41	134.31	120.20
1	X	1314	A	C4'-C3'-O3'	-9.38	95.33	109.40
1	X	1233	A	C2'-C3'-O3'	9.28	123.43	109.50
1	X	2705	A	C4'-C3'-O3'	9.29	123.33	109.40
1	X	1283	C	P-O3'-C3'	9.26	134.09	120.20
1	X	2770	A	P-O3'-C3'	9.25	134.07	120.20
1	X	683	A	P-O3'-C3'	9.22	134.03	120.20
1	X	2608	A	P-O3'-C3'	9.14	133.92	120.20
13	K	7	GLY	CA-C-N	9.09	138.91	121.54
13	K	7	GLY	C-N-CA	9.09	138.91	121.54
1	X	2204	A	P-O3'-C3'	9.07	133.81	120.20
1	X	99	U	P-O3'-C3'	9.07	133.80	120.20
1	X	2312	A	P-O3'-C3'	9.04	133.77	120.20
1	X	1031	C	P-O3'-C3'	9.04	133.76	120.20
20	R	28	LYS	N-CA-C	-8.99	97.56	110.59
1	X	48	A	P-O3'-C3'	8.97	133.66	120.20
1	X	559	C	N1-C1'-C2'	8.96	125.44	112.00
1	X	683	A	C2'-C3'-O3'	8.96	122.94	109.50
1	X	969	U	P-O3'-C3'	8.92	133.58	120.20
1	X	780	U	P-O3'-C3'	8.89	133.54	120.20
1	X	1953	A	P-O5'-C5'	-8.88	107.58	120.90
1	X	594	G	P-O3'-C3'	8.87	133.50	120.20
1	X	1790	G	P-O3'-C3'	8.85	133.48	120.20
1	X	2408	G	P-O5'-C5'	-8.85	107.62	120.90
1	X	631	G	P-O5'-C5'	-8.80	107.70	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	825	C	P-O3'-C3'	-8.79	107.01	120.20
1	X	2706	U	C4'-C3'-C2'	8.78	111.38	102.60
2	Y	16	U	P-O3'-C3'	8.78	133.37	120.20
3	A	53	PHE	CA-CB-CG	-8.78	105.02	113.80
1	X	2589	C	P-O3'-C3'	8.76	133.34	120.20
9	G	70	PHE	CA-CB-CG	8.73	122.53	113.80
1	X	1033	G	C2'-C3'-O3'	8.73	122.59	109.50
13	K	83	VAL	N-CA-C	8.64	118.54	110.42
26	Z	57	VAL	CA-C-N	8.62	133.38	121.05
26	Z	57	VAL	C-N-CA	8.62	133.38	121.05
1	X	1938	U	C4'-C3'-C2'	8.58	111.18	102.60
1	X	1469	U	N1-C1'-C2'	8.56	124.85	112.00
1	X	242	A	C4'-C3'-C2'	-8.55	94.05	102.60
1	X	2298	U	P-O3'-C3'	8.54	133.01	120.20
1	X	1561	A	C4'-C3'-O3'	8.54	125.81	113.00
1	X	1975	G	P-O3'-C3'	8.54	133.01	120.20
1	X	2088	U	P-O3'-C3'	8.53	133.00	120.20
1	X	2498	U	P-O3'-C3'	8.53	132.99	120.20
1	X	1333	G	O4'-C1'-N9	8.52	120.98	108.20
1	X	514	G	P-O3'-C3'	8.51	132.96	120.20
1	X	1790	G	C2'-C3'-O3'	8.48	122.22	109.50
9	G	120	SER	N-CA-C	-8.48	102.48	113.17
1	X	1631	C	O4'-C1'-N1	8.48	121.21	108.50
1	X	537	C	O4'-C1'-N1	8.45	121.18	108.50
1	X	2261	G	P-O3'-C3'	8.44	132.86	120.20
1	X	1096	A	P-O3'-C3'	8.41	132.82	120.20
1	X	1716	G	C4'-C3'-C2'	8.38	110.98	102.60
1	X	2706	U	C4'-C3'-O3'	8.38	121.97	109.40
1	X	1288	A	O4'-C1'-N9	8.37	120.75	108.20
23	U	18	VAL	CA-C-N	8.37	137.03	121.97
23	U	18	VAL	C-N-CA	8.37	137.03	121.97
4	B	95	ILE	N-CA-C	-8.35	102.72	110.82
1	X	2018	G	C5'-C4'-C3'	-8.34	102.69	115.20
11	I	28	LYS	CA-C-N	8.34	137.47	121.54
11	I	28	LYS	C-N-CA	8.34	137.47	121.54
1	X	1812	U	C1'-C2'-O2'	-8.34	99.29	111.80
1	X	540	G	C3'-C2'-C1'	8.32	109.62	101.30
9	G	94	LYS	N-CA-C	-8.31	100.98	112.12
1	X	2811	G	C3'-C2'-O2'	8.31	123.17	110.70
1	X	537	C	C1'-O4'-C4'	-8.29	101.61	109.90
1	X	1186	G	P-O3'-C3'	8.23	132.55	120.20
15	M	31	ASP	N-CA-C	8.23	121.84	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1775	A	C4'-C3'-O3'	-8.19	97.11	109.40
1	X	841	G	N9-C1'-C2'	8.19	124.28	112.00
1	X	3	U	C2'-C3'-O3'	8.17	125.95	113.70
4	B	179	GLU	N-CA-C	-8.16	103.32	113.28
1	X	2501	U	C5'-C4'-C3'	-8.14	103.80	116.00
1	X	1976	U	P-O5'-C5'	-8.11	108.73	120.90
1	X	1194	U	P-O3'-C3'	8.11	132.36	120.20
1	X	1975	G	C1'-C2'-O2'	-8.10	99.65	111.80
1	X	2769	C	C1'-O4'-C4'	-8.08	101.62	109.70
1	X	751	G	O4'-C4'-C3'	-8.08	95.92	104.00
1	X	597	U	O4'-C4'-C3'	-8.07	95.93	104.00
1	X	553	C	P-O3'-C3'	8.07	132.30	120.20
1	X	71	A	P-O3'-C3'	8.07	132.30	120.20
1	X	1850	G	P-O3'-C3'	8.05	132.28	120.20
9	G	103	TYR	CA-C-N	8.05	136.92	121.54
9	G	103	TYR	C-N-CA	8.05	136.92	121.54
1	X	664	C	P-O3'-C3'	8.04	132.27	120.20
11	I	36	GLY	CA-C-N	8.01	136.83	121.54
11	I	36	GLY	C-N-CA	8.01	136.83	121.54
1	X	74	G	O4'-C4'-C3'	-8.00	96.00	104.00
23	U	39	LYS	N-CA-C	7.98	120.81	108.12
1	X	2551	A	P-O3'-C3'	7.96	132.15	120.20
1	X	342	G	P-O3'-C3'	7.96	132.14	120.20
1	X	494	A	C3'-C2'-O2'	7.93	122.60	110.70
3	A	209	ALA	CA-C-N	-7.93	112.38	123.08
3	A	209	ALA	C-N-CA	-7.93	112.38	123.08
1	X	2560	G	C2'-C3'-O3'	7.92	121.38	109.50
1	X	1496	G	P-O3'-C3'	7.92	132.07	120.20
11	I	38	LYS	CA-C-N	7.90	136.63	121.54
11	I	38	LYS	C-N-CA	7.90	136.63	121.54
1	X	1139	A	C1'-O4'-C4'	-7.90	101.80	109.70
1	X	458	G	P-O3'-C3'	7.90	132.05	120.20
1	X	467	U	C4'-C3'-C2'	-7.89	94.71	102.60
5	C	167	VAL	N-CA-C	7.88	119.96	108.53
1	X	518	A	P-O3'-C3'	7.88	132.02	120.20
13	K	52	ILE	N-CA-CB	7.87	119.75	110.55
1	X	1033	G	P-O3'-C3'	7.86	132.00	120.20
1	X	1278	A	O4'-C1'-N9	7.86	120.00	108.20
1	X	1265	G	P-O5'-C5'	7.83	132.64	120.90
1	X	1770	U	O4'-C4'-C3'	-7.83	96.17	104.00
1	X	1053	G	P-O3'-C3'	7.82	131.93	120.20
19	Q	61	LYS	N-CA-C	7.82	127.45	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1482	U	C1'-O4'-C4'	-7.80	102.09	109.90
1	X	672	C	O4'-C4'-C3'	-7.80	96.20	104.00
3	A	248	THR	CB-CA-C	7.78	125.50	110.17
1	X	939	C	C5'-C4'-O4'	7.76	121.45	109.80
1	X	346	C	N1-C1'-C2'	7.76	123.63	112.00
1	X	803	C	P-O3'-C3'	7.74	131.81	120.20
1	X	83	A	P-O3'-C3'	7.73	131.79	120.20
1	X	2426	G	P-O3'-C3'	7.72	131.78	120.20
1	X	554	U	P-O3'-C3'	7.71	131.76	120.20
1	X	2408	G	C5'-C4'-C3'	-7.68	104.47	116.00
1	X	2018	G	N9-C1'-C2'	7.68	125.52	114.00
11	I	41	SER	N-CA-C	7.68	127.16	110.80
1	X	343	A	O4'-C1'-N9	7.68	120.02	108.50
1	X	1632	A	P-O3'-C3'	7.68	131.71	120.20
13	K	3	HIS	CA-CB-CG	7.67	121.47	113.80
5	C	66	ASN	CA-CB-CG	7.67	120.27	112.60
1	X	841	G	O4'-C4'-C3'	-7.66	96.34	104.00
1	X	2795	A	P-O3'-C3'	7.65	131.67	120.20
1	X	175	C	P-O3'-C3'	7.64	131.66	120.20
1	X	542	A	C3'-C2'-C1'	7.64	109.14	101.50
1	X	1613	G	C1'-O4'-C4'	-7.63	102.27	109.90
11	I	32	ARG	N-CA-C	-7.63	97.14	109.96
4	B	132	LYS	CA-C-N	7.58	134.46	122.86
4	B	132	LYS	C-N-CA	7.58	134.46	122.86
1	X	1552	C	P-O3'-C3'	7.58	131.56	120.20
1	X	1812	U	N1-C1'-C2'	7.56	125.34	114.00
1	X	655	A	P-O3'-C3'	7.54	131.52	120.20
1	X	1288	A	C3'-C2'-C1'	-7.52	93.98	101.50
25	W	47	VAL	CA-C-N	7.52	130.69	120.54
25	W	47	VAL	C-N-CA	7.52	130.69	120.54
1	X	483	A	P-O3'-C3'	-7.50	108.96	120.20
1	X	2418	A	P-O3'-C3'	7.49	131.43	120.20
1	X	554	U	C1'-O4'-C4'	-7.48	102.22	109.70
1	X	1466	C	C4'-C3'-C2'	-7.48	95.12	102.60
10	H	70	VAL	N-CA-CB	-7.48	102.94	112.60
1	X	1482	U	O4'-C1'-N1	7.47	119.71	108.50
1	X	814	G	P-O3'-C3'	7.47	131.40	120.20
1	X	2330	G	P-O3'-C3'	7.45	131.38	120.20
1	X	2559	U	C4'-C3'-O3'	-7.45	101.83	113.00
3	A	50	THR	CB-CA-C	7.45	122.16	109.65
1	X	1442	C	P-O3'-C3'	7.44	131.36	120.20
1	X	661	C	C4'-C3'-C2'	-7.44	95.16	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2633	A	P-O3'-C3'	7.44	131.35	120.20
1	X	304	A	P-O5'-C5'	7.41	132.01	120.90
1	X	558	G	P-O3'-C3'	7.40	131.30	120.20
1	X	73	A	P-O3'-C3'	7.39	131.29	120.20
1	X	503	G	O4'-C4'-C3'	-7.39	96.61	104.00
1	X	1182	U	P-O3'-C3'	7.39	131.29	120.20
5	C	123	PHE	CA-C-N	7.39	130.92	120.28
5	C	123	PHE	C-N-CA	7.39	130.92	120.28
1	X	751	G	C2'-C3'-O3'	7.38	124.78	113.70
9	G	106	TYR	N-CA-CB	7.36	122.94	110.49
1	X	308	C	P-O5'-C5'	7.36	131.94	120.90
1	X	2018	G	P-O5'-C5'	-7.36	109.87	120.90
10	H	22	ILE	N-CA-C	-7.35	105.94	111.90
1	X	1984	A	P-O5'-C5'	-7.35	109.87	120.90
3	A	240	THR	N-CA-C	7.35	116.94	108.49
19	Q	62	ARG	CA-C-N	7.34	135.55	121.54
19	Q	62	ARG	C-N-CA	7.34	135.55	121.54
1	X	1575	C	P-O3'-C3'	7.33	131.19	120.20
1	X	3	U	P-O3'-C3'	7.31	131.16	120.20
5	C	58	MET	CA-C-N	7.25	133.16	122.86
5	C	58	MET	C-N-CA	7.25	133.16	122.86
1	X	2330	G	C4'-C3'-O3'	-7.25	102.12	113.00
1	X	1334	A	O4'-C4'-C3'	-7.25	96.75	104.00
1	X	1574	A	C1'-O4'-C4'	-7.25	102.66	109.90
1	X	1412	C	C3'-C2'-C1'	-7.22	94.08	101.30
23	U	53	GLU	N-CA-C	7.22	119.90	109.14
1	X	1010	U	P-O5'-C5'	7.21	131.72	120.90
2	Y	26	G	P-O3'-C3'	7.21	131.02	120.20
1	X	1680	U	O4'-C4'-C3'	-7.21	96.79	104.00
1	X	666	U	C1'-O4'-C4'	-7.21	102.69	109.90
1	X	1664	G	P-O5'-C5'	7.17	131.66	120.90
1	X	2229	G	P-O3'-C3'	7.17	130.96	120.20
1	X	1601	U	P-O3'-C3'	7.14	130.92	120.20
1	X	702	A	O3'-P-O5'	-7.14	93.29	104.00
4	B	72	VAL	N-CA-C	7.14	118.46	111.67
1	X	242	A	O4'-C4'-C3'	-7.14	96.86	104.00
1	X	557	U	C2'-C3'-O3'	7.14	120.20	109.50
1	X	2481	G	O3'-P-O5'	-7.13	93.30	104.00
1	X	1570	C	O4'-C1'-N1	7.13	118.90	108.20
1	X	714	G	O4'-C4'-C3'	-7.13	96.87	104.00
1	X	1288	A	C5'-C4'-C3'	7.12	125.89	115.20
1	X	1031	C	C2'-C3'-O3'	7.12	120.18	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1679	U	O4'-C4'-C3'	-7.12	96.88	104.00
1	X	2408	G	C4'-C3'-C2'	7.12	109.72	102.60
1	X	343	A	N9-C1'-C2'	7.10	122.65	112.00
3	A	44	ASN	CA-CB-CG	7.08	119.68	112.60
1	X	1496	G	C4'-C3'-O3'	7.04	123.57	113.00
1	X	126	C	C4'-C3'-O3'	-7.04	102.44	113.00
1	X	1086	C	P-O3'-C3'	7.04	130.76	120.20
1	X	3	U	C3'-C2'-C1'	-7.03	94.27	101.30
1	X	1410	U	C2'-C3'-O3'	7.01	120.02	109.50
1	X	1469	U	O3'-P-O5'	7.01	114.51	104.00
1	X	418	C	C1'-O4'-C4'	-7.00	102.90	109.90
1	X	2669	C	O4'-C1'-C2'	-7.00	98.81	105.80
12	J	76	THR	N-CA-C	6.99	120.02	109.95
1	X	1630	A	O3'-P-O5'	-6.99	93.52	104.00
1	X	1716	G	C2'-C3'-O3'	6.99	119.98	109.50
1	X	955	G	N9-C1'-C2'	6.98	122.47	112.00
1	X	1412	C	C2'-C3'-O3'	6.98	124.17	113.70
1	X	1799	A	C1'-O4'-C4'	-6.98	102.72	109.70
12	J	19	THR	N-CA-C	6.98	119.94	108.99
1	X	638	A	P-O3'-C3'	6.97	130.66	120.20
23	U	35	THR	CB-CA-C	6.97	122.36	111.77
1	X	1345	G	P-O3'-C3'	6.96	130.64	120.20
1	X	2698	G	C4'-C3'-C2'	-6.96	95.64	102.60
13	K	11	ASN	CA-C-N	6.95	134.81	121.54
13	K	11	ASN	C-N-CA	6.95	134.81	121.54
2	Y	54	U	P-O5'-C5'	6.92	131.29	120.90
1	X	1278	A	C3'-C2'-C1'	-6.92	94.58	101.50
1	X	763	A	P-O3'-C3'	6.92	130.58	120.20
1	X	1754	G	P-O3'-C3'	6.92	130.58	120.20
23	U	17	SER	N-CA-C	6.92	119.59	109.07
1	X	1459	U	P-O3'-C3'	6.92	130.58	120.20
1	X	789	G	P-O3'-C3'	6.91	130.57	120.20
11	I	58	ALA	N-CA-C	-6.91	99.59	109.96
1	X	243	G	P-O5'-C5'	6.90	131.25	120.90
4	B	51	TYR	N-CA-C	6.90	121.62	111.34
1	X	2710	C	P-O3'-C3'	-6.89	109.86	120.20
1	X	759	C	C5'-C4'-C3'	-6.88	105.68	116.00
12	J	10	PHE	CA-CB-CG	6.88	120.68	113.80
5	C	163	ASN	CA-C-N	6.88	134.34	121.97
5	C	163	ASN	C-N-CA	6.88	134.34	121.97
1	X	1333	G	C1'-C2'-O2'	-6.86	101.50	111.80
1	X	198	A	P-O3'-C3'	6.86	130.48	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1249	G	C4'-C3'-C2'	6.84	109.44	102.60
23	U	33	LYS	N-CA-C	-6.83	103.59	112.68
1	X	1154	A	P-O3'-C3'	6.83	130.45	120.20
1	X	334	G	C2'-C3'-O3'	6.81	119.72	109.50
1	X	1223	G	C3'-C2'-C1'	6.81	108.31	101.50
18	P	36	ARG	CA-C-N	6.81	129.30	120.44
18	P	36	ARG	C-N-CA	6.81	129.30	120.44
1	X	2591	C	C2'-C3'-O3'	-6.81	103.49	113.70
1	X	554	U	N1-C1'-C2'	6.79	124.19	114.00
1	X	1184	G	P-O3'-C3'	6.79	130.39	120.20
1	X	1407	G	N9-C1'-C2'	6.79	122.18	112.00
1	X	515	A	P-O3'-C3'	6.78	130.37	120.20
1	X	1137	A	P-O3'-C3'	6.78	130.37	120.20
1	X	2854	G	N9-C1'-C2'	6.78	124.16	114.00
1	X	467	U	N1-C1'-C2'	6.77	122.16	112.00
10	H	26	ASN	CA-C-N	6.77	134.47	121.54
10	H	26	ASN	C-N-CA	6.77	134.47	121.54
1	X	1820	G	C2'-C3'-O3'	6.77	119.65	109.50
1	X	2261	G	C2'-C3'-O3'	6.75	119.62	109.50
1	X	759	C	C4'-C3'-C2'	6.75	109.34	102.60
1	X	973	U	O3'-P-O5'	-6.74	93.89	104.00
1	X	341	A	P-O3'-C3'	6.74	130.31	120.20
1	X	939	C	C1'-O4'-C4'	-6.74	103.16	109.90
1	X	483	A	O5'-C5'-C4'	6.74	121.60	111.50
1	X	656	U	P-O5'-C5'	6.72	130.98	120.90
1	X	1830	C	P-O3'-C3'	6.72	130.28	120.20
1	X	1248	G	O3'-P-O5'	-6.72	93.93	104.00
1	X	1958	G	O4'-C4'-C3'	-6.71	97.29	104.00
15	M	28	ARG	N-CA-C	-6.71	94.98	109.81
1	X	1575	C	C2'-C3'-O3'	6.71	119.56	109.50
1	X	418	C	C4'-C3'-C2'	-6.70	95.90	102.60
1	X	1441	A	C2'-C3'-O3'	6.70	119.54	109.50
1	X	2689	C	P-O3'-C3'	6.69	130.24	120.20
1	X	1467	U	N1-C1'-C2'	6.68	122.03	112.00
23	U	14	VAL	CA-C-N	6.68	134.00	121.97
23	U	14	VAL	C-N-CA	6.68	134.00	121.97
1	X	2611	A	C3'-C2'-O2'	6.68	120.72	110.70
1	X	1037	U	O4'-C1'-N1	6.68	118.22	108.20
20	R	109	ALA	N-CA-C	-6.68	105.89	112.97
1	X	2706	U	O4'-C1'-N1	6.67	118.21	108.20
1	X	2204	A	C2'-C3'-O3'	6.67	119.50	109.50
1	X	559	C	C2'-C3'-O3'	6.66	123.69	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	558	G	C2'-C3'-O3'	6.66	119.49	109.50
13	K	11	ASN	CA-CB-CG	-6.65	105.95	112.60
23	U	32	ARG	N-CA-C	-6.64	96.65	110.80
1	X	1468	A	N9-C1'-C2'	6.64	121.95	112.00
1	X	1663	C	O3'-P-O5'	-6.63	94.05	104.00
1	X	1669	A	P-O5'-C5'	6.62	130.83	120.90
1	X	677	G	C4'-C3'-C2'	-6.61	95.99	102.60
9	G	106	TYR	CA-C-N	6.61	134.16	121.54
9	G	106	TYR	C-N-CA	6.61	134.16	121.54
1	X	776	G	N9-C1'-C2'	6.60	121.90	112.00
4	B	88	GLY	CA-C-N	6.60	130.57	121.33
4	B	88	GLY	C-N-CA	6.60	130.57	121.33
1	X	1467	U	C4'-C3'-C2'	6.59	109.19	102.60
2	Y	11	G	C3'-C2'-O2'	6.59	120.59	110.70
1	X	2770	A	C2'-C3'-O3'	6.58	119.38	109.50
1	X	625	A	P-O3'-C3'	6.58	130.07	120.20
11	I	48	PHE	CA-C-N	6.58	134.11	121.54
11	I	48	PHE	C-N-CA	6.58	134.11	121.54
1	X	780	U	C2'-C3'-O3'	6.58	123.57	113.70
1	X	323	G	P-O5'-C5'	-6.58	111.03	120.90
1	X	759	C	O5'-C5'-C4'	6.58	121.37	111.50
15	M	93	ILE	N-CA-CB	6.58	118.40	110.31
1	X	1154	A	C2'-C3'-O3'	6.57	119.36	109.50
1	X	467	U	O4'-C4'-C3'	-6.57	97.43	104.00
12	J	88	LYS	N-CA-C	6.57	124.80	110.80
1	X	1468	A	P-O3'-C3'	6.56	130.04	120.20
1	X	879	A	C1'-C2'-O2'	6.55	118.22	108.40
4	B	150	VAL	N-CA-CB	6.54	120.15	111.25
1	X	1278	A	C1'-O4'-C4'	-6.54	103.16	109.70
3	A	242	ALA	N-CA-C	6.54	124.73	110.80
1	X	1496	G	C2'-C3'-O3'	6.54	123.50	113.70
1	X	2691	C	P-O3'-C3'	6.53	130.00	120.20
1	X	656	U	P-O3'-C3'	6.53	130.00	120.20
11	I	61	PRO	CA-C-N	6.53	134.00	121.54
11	I	61	PRO	C-N-CA	6.53	134.00	121.54
1	X	2593	A	O3'-P-O5'	-6.52	94.21	104.00
1	X	2867	G	C1'-C2'-O2'	6.52	118.18	108.40
1	X	467	U	P-O3'-C3'	6.52	129.98	120.20
9	G	113	GLU	N-CA-C	6.52	119.34	108.13
1	X	469	G	O4'-C1'-N9	6.51	117.97	108.20
1	X	204	A	P-O3'-C3'	6.50	129.96	120.20
1	X	358	C	P-O5'-C5'	6.49	130.64	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	596	C	P-O5'-C5'	-6.49	111.17	120.90
1	X	788	G	P-O3'-C3'	6.49	129.93	120.20
17	O	6	GLN	CA-C-N	6.49	133.94	121.54
17	O	6	GLN	C-N-CA	6.49	133.94	121.54
1	X	2414	A	P-O5'-C5'	6.48	130.61	120.90
1	X	540	G	C4'-C3'-C2'	-6.47	96.13	102.60
1	X	774	A	O4'-C1'-C2'	-6.47	101.13	107.60
1	X	181	A	P-O3'-C3'	6.47	129.90	120.20
1	X	2795	A	C4'-C3'-O3'	-6.47	103.30	113.00
1	X	2477	C	C5'-C4'-O4'	-6.47	100.10	109.80
1	X	343	A	O4'-C1'-C2'	-6.46	101.14	107.60
1	X	1340	C	O3'-P-O5'	-6.46	94.32	104.00
5	C	130	THR	CA-C-N	6.45	129.80	120.38
5	C	130	THR	C-N-CA	6.45	129.80	120.38
12	J	88	LYS	CA-C-N	6.44	134.04	121.41
12	J	88	LYS	C-N-CA	6.44	134.04	121.41
15	M	37	THR	CB-CA-C	6.44	120.76	110.19
1	X	1182	U	C2'-C3'-O3'	6.43	123.35	113.70
1	X	33	C	C2'-C3'-O3'	6.43	119.15	109.50
1	X	606	A	O4'-C4'-C3'	-6.43	97.57	104.00
15	M	29	PRO	N-CA-C	6.43	125.72	112.47
1	X	554	U	O4'-C1'-N1	6.43	117.84	108.20
1	X	1602	G	P-O3'-C3'	6.43	129.84	120.20
3	A	88	ARG	N-CA-C	6.42	124.48	110.80
1	X	1581	C	P-O3'-C3'	6.40	129.80	120.20
1	X	1943	A	C4'-C3'-C2'	6.40	109.00	102.60
1	X	71	A	C4'-C3'-C2'	6.40	109.00	102.60
5	C	67	ALA	CA-C-N	6.39	133.75	121.54
5	C	67	ALA	C-N-CA	6.39	133.75	121.54
11	I	55	ARG	CA-C-N	6.38	133.72	121.54
11	I	55	ARG	C-N-CA	6.38	133.72	121.54
1	X	2691	C	O3'-P-O5'	-6.37	94.44	104.00
1	X	1441	A	P-O3'-C3'	6.37	129.75	120.20
1	X	71	A	C4'-C3'-O3'	6.36	118.94	109.40
1	X	2778	U	P-O3'-C3'	6.36	129.74	120.20
1	X	483	A	C4'-C3'-C2'	6.36	108.96	102.60
1	X	504	G	O4'-C4'-C3'	-6.36	97.64	104.00
1	X	2371	A	O4'-C1'-N9	6.36	118.04	108.50
23	U	47	HIS	CA-C-N	6.35	133.67	121.54
23	U	47	HIS	C-N-CA	6.35	133.67	121.54
1	X	610	G	O3'-P-O5'	-6.34	94.48	104.00
1	X	2189	A	P-O3'-C3'	6.33	129.69	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Q	90	ALA	N-CA-C	-6.33	105.33	114.12
9	G	78	ASP	CA-CB-CG	6.32	118.92	112.60
12	J	83	ARG	CA-C-N	6.32	133.61	121.54
12	J	83	ARG	C-N-CA	6.32	133.61	121.54
14	L	89	PHE	CA-CB-CG	-6.31	107.49	113.80
1	X	2257	A	P-O5'-C5'	6.31	130.37	120.90
13	K	15	SER	CA-C-N	6.31	129.03	120.44
13	K	15	SER	C-N-CA	6.31	129.03	120.44
1	X	242	A	P-O5'-C5'	6.31	130.36	120.90
1	X	2426	G	C5'-C4'-C3'	-6.31	105.74	115.20
4	B	162	MET	CB-CA-C	6.31	120.84	111.89
1	X	1754	G	P-O5'-C5'	6.30	130.35	120.90
1	X	2406	C	P-O5'-C5'	6.30	130.35	120.90
1	X	2745	A	P-O3'-C3'	6.30	129.65	120.20
1	X	825	C	P-O5'-C5'	6.30	130.35	120.90
1	X	2578	G	P-O5'-C5'	6.30	130.35	120.90
1	X	2258	G	C1'-O4'-C4'	-6.29	103.61	109.90
4	B	128	SER	N-CA-C	6.29	121.79	114.62
3	A	261	ARG	N-CA-C	6.28	119.75	110.46
1	X	466	A	P-O5'-C5'	6.28	130.31	120.90
1	X	322	A	N9-C1'-C2'	6.27	121.41	112.00
1	X	1662	G	N9-C1'-C2'	6.27	121.41	112.00
1	X	1631	C	N1-C1'-C2'	6.27	121.40	112.00
1	X	2813	G	C3'-C2'-O2'	6.26	120.10	110.70
26	Z	35	GLN	N-CA-C	6.26	120.20	111.56
1	X	2736	U	C2'-C3'-O3'	6.26	118.89	109.50
1	X	1467	U	O4'-C1'-C2'	-6.25	101.35	107.60
1	X	2552	C	N1-C1'-C2'	6.25	121.38	112.00
1	X	2658	A	C3'-C2'-O2'	6.25	120.08	110.70
1	X	758	G	C3'-C2'-C1'	-6.25	95.05	101.30
1	X	2705	A	C4'-C3'-C2'	6.25	108.85	102.60
19	Q	19	ALA	CA-C-N	6.24	128.56	120.44
19	Q	19	ALA	C-N-CA	6.24	128.56	120.44
1	X	879	A	C4'-C3'-C2'	6.24	108.84	102.60
1	X	1962	C	C3'-C2'-C1'	-6.24	95.06	101.30
1	X	2551	A	O3'-P-O5'	-6.24	94.64	104.00
12	J	82	THR	CA-C-N	6.24	133.46	121.54
12	J	82	THR	C-N-CA	6.24	133.46	121.54
4	B	60	ASN	CA-CB-CG	6.24	118.84	112.60
9	G	119	LEU	CA-C-N	6.24	132.83	122.54
9	G	119	LEU	C-N-CA	6.24	132.83	122.54
1	X	490	A	P-O3'-C3'	6.23	129.55	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	O	22	VAL	N-CA-CB	6.23	120.18	110.14
1	X	518	A	N9-C1'-C2'	6.23	123.35	114.00
1	X	1468	A	O4'-C1'-N9	6.23	117.84	108.50
1	X	731	A	P-O3'-C3'	6.23	129.54	120.20
1	X	1087	C	P-O5'-C5'	6.22	130.23	120.90
1	X	1523	A	P-O3'-C3'	6.22	129.53	120.20
1	X	2018	G	C2'-C3'-O3'	6.22	118.83	109.50
1	X	99	U	C2'-C3'-O3'	6.22	118.83	109.50
1	X	176	A	C2'-C3'-O3'	6.22	118.83	109.50
1	X	595	A	O3'-P-O5'	-6.21	94.69	104.00
1	X	2824	C	P-O3'-C3'	6.21	129.51	120.20
1	X	824	U	N1-C1'-C2'	6.21	123.31	114.00
1	X	1574	A	C5'-C4'-O4'	6.21	119.11	109.80
4	B	90	SER	N-CA-C	6.21	124.02	110.80
1	X	540	G	O4'-C1'-C2'	-6.21	101.39	107.60
1	X	2793	G	C3'-C2'-O2'	6.20	120.00	110.70
9	G	32	TYR	CA-C-N	6.19	133.57	122.13
9	G	32	TYR	C-N-CA	6.19	133.57	122.13
1	X	242	A	C1'-O4'-C4'	-6.18	103.72	109.90
1	X	564	U	C3'-C2'-O2'	6.18	119.97	110.70
15	M	83	PHE	CA-CB-CG	6.18	119.98	113.80
1	X	1286	U	P-O5'-C5'	6.17	130.15	120.90
1	X	1680	U	C2'-C3'-O3'	6.17	122.95	113.70
1	X	2315	A	P-O5'-C5'	6.17	130.15	120.90
1	X	2854	G	C1'-O4'-C4'	-6.17	103.53	109.70
5	C	143	ASP	CA-CB-CG	6.17	118.77	112.60
1	X	952	A	P-O5'-C5'	6.16	130.15	120.90
1	X	504	G	C3'-C2'-O2'	6.16	119.94	110.70
1	X	469	G	P-O3'-C3'	6.16	129.44	120.20
1	X	2034	A	P-O3'-C3'	6.16	129.44	120.20
1	X	1470	G	P-O3'-C3'	-6.16	110.97	120.20
13	K	94	TYR	N-CA-C	6.15	119.52	110.30
3	A	228	PRO	CA-C-N	6.15	128.30	120.56
3	A	228	PRO	C-N-CA	6.15	128.30	120.56
1	X	1314	A	O3'-P-O5'	-6.14	94.78	104.00
1	X	1467	U	C1'-C2'-O2'	6.14	117.62	108.40
1	X	2730	A	P-O3'-C3'	6.14	129.42	120.20
20	R	75	ALA	N-CA-C	6.14	118.22	110.24
1	X	1188	A	P-O3'-C3'	6.14	129.41	120.20
3	A	220	HIS	CA-CB-CG	6.14	119.94	113.80
21	S	141	MET	N-CA-C	6.13	119.51	109.76
1	X	1710	U	C2'-C3'-O3'	6.11	118.67	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2199	C	N1-C1'-C2'	6.11	121.17	112.00
1	X	1716	G	O3'-P-O5'	-6.11	94.84	104.00
1	X	813	A	P-O3'-C3'	6.11	129.36	120.20
1	X	1882	G	C3'-C2'-O2'	6.11	119.86	110.70
1	X	580	A	P-O3'-C3'	6.10	129.35	120.20
20	R	93	ARG	N-CA-C	6.10	123.79	110.80
1	X	2535	C	C5'-C4'-C3'	-6.09	106.86	116.00
1	X	797	A	C4'-C3'-O3'	-6.08	103.87	113.00
1	X	399	G	C4'-C3'-C2'	6.08	108.68	102.60
1	X	858	G	C3'-C2'-O2'	6.08	119.82	110.70
1	X	1524	C	P-O3'-C3'	6.08	129.32	120.20
1	X	2667	C	P-O3'-C3'	6.08	129.32	120.20
1	X	1142	G	O4'-C1'-C2'	-6.08	99.72	105.80
10	H	83	ARG	CA-C-N	6.08	129.26	120.38
10	H	83	ARG	C-N-CA	6.08	129.26	120.38
1	X	824	U	O3'-P-O5'	-6.08	94.88	104.00
9	G	108	GLY	N-CA-C	-6.08	98.78	113.18
1	X	1412	C	C4'-C3'-O3'	6.08	122.11	113.00
1	X	344	G	N9-C1'-C2'	6.07	121.10	112.00
1	X	112	U	N1-C1'-C2'	6.06	121.09	112.00
1	X	1710	U	P-O3'-C3'	6.06	129.29	120.20
3	A	48	ARG	N-CA-C	6.06	119.05	110.14
12	J	9	LYS	N-CA-C	6.06	117.97	111.36
1	X	117	A	P-O3'-C3'	6.05	129.28	120.20
16	N	78	THR	CB-CA-C	6.05	120.39	110.88
19	Q	74	ASP	N-CA-C	6.05	123.69	110.80
20	R	6	ALA	N-CA-C	6.05	123.68	110.80
19	Q	64	ARG	CA-C-N	6.04	132.85	121.97
19	Q	64	ARG	C-N-CA	6.04	132.85	121.97
20	R	90	LYS	N-CA-C	6.04	117.38	108.86
1	X	2578	G	O5'-C5'-C4'	-6.03	102.45	111.50
1	X	2854	G	P-O3'-C3'	6.03	129.25	120.20
5	C	171	PRO	CA-C-N	6.03	132.82	121.97
5	C	171	PRO	C-N-CA	6.03	132.82	121.97
1	X	1689	U	C3'-C2'-O2'	6.03	119.74	110.70
2	Y	54	U	C4'-C3'-C2'	-6.02	96.58	102.60
1	X	1994	U	C4'-C3'-O3'	6.02	122.03	113.00
1	X	2548	G	O4'-C4'-C3'	-6.02	97.98	104.00
1	X	1314	A	P-O3'-C3'	6.01	129.22	120.20
1	X	1683	G	C3'-C2'-O2'	6.01	119.72	110.70
1	X	1496	G	C3'-C2'-C1'	-6.01	95.29	101.30
1	X	1475	U	C2'-C3'-O3'	6.01	118.51	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	674	U	C1'-C2'-O2'	6.00	117.41	108.40
23	U	45	ASN	CA-CB-CG	6.00	118.60	112.60
1	X	1469	U	P-O3'-C3'	6.00	129.19	120.20
1	X	1774	A	C4'-C3'-O3'	-6.00	104.00	113.00
1	X	1820	G	C4'-C3'-O3'	6.00	118.39	109.40
1	X	2526	U	C3'-C2'-O2'	5.99	119.69	110.70
1	X	2640	G	C3'-C2'-O2'	5.99	119.68	110.70
18	P	52	ASP	N-CA-C	-5.99	104.67	111.14
1	X	1938	U	O4'-C1'-C2'	5.99	111.79	105.80
1	X	1541	G	C4'-C3'-C2'	-5.99	96.61	102.60
1	X	827	C	P-O5'-C5'	5.98	129.87	120.90
1	X	631	G	P-O3'-C3'	5.98	129.17	120.20
23	U	19	ILE	N-CA-C	5.98	121.78	109.34
1	X	526	C	C3'-C2'-C1'	-5.98	95.32	101.30
1	X	879	A	C5'-C4'-C3'	-5.98	107.03	116.00
1	X	1341	G	P-O5'-C5'	5.97	129.86	120.90
1	X	2193	C	O4'-C4'-C3'	-5.97	98.03	104.00
1	X	2691	C	C1'-C2'-O2'	5.97	120.76	111.80
1	X	1742	G	P-O3'-C3'	-5.97	111.24	120.20
1	X	1986	G	P-O3'-C3'	-5.97	111.25	120.20
1	X	540	G	O5'-C5'-C4'	-5.97	102.55	111.50
1	X	1882	G	P-O5'-C5'	5.96	129.85	120.90
5	C	154	ASP	CA-C-N	5.96	129.09	120.38
5	C	154	ASP	C-N-CA	5.96	129.09	120.38
20	R	8	SER	CA-C-N	5.96	129.09	120.38
20	R	8	SER	C-N-CA	5.96	129.09	120.38
1	X	822	G	C4'-C3'-C2'	-5.96	96.64	102.60
17	O	6	GLN	N-CA-C	-5.96	105.32	112.59
1	X	956	A	O3'-P-O5'	-5.96	95.07	104.00
1	X	2303	C	C4'-C3'-O3'	-5.95	104.08	113.00
1	X	2258	G	C4'-C3'-C2'	-5.94	96.66	102.60
23	U	60	VAL	N-CA-C	5.94	121.70	109.34
1	X	2810	A	P-O3'-C3'	5.94	129.11	120.20
1	X	1019	U	O3'-P-O5'	-5.94	95.09	104.00
1	X	2255	G	C3'-C2'-O2'	5.94	119.61	110.70
1	X	1561	A	C3'-C2'-C1'	-5.93	95.37	101.30
1	X	681	A	C1'-C2'-O2'	5.93	117.29	108.40
1	X	2552	C	C4'-C3'-C2'	-5.93	96.67	102.60
13	K	5	LYS	N-CA-C	5.93	120.03	113.21
1	X	780	U	C4'-C3'-O3'	5.92	121.89	113.00
1	X	520	C	C4'-C3'-C2'	-5.92	96.68	102.60
1	X	418	C	C5'-C4'-C3'	5.92	124.88	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1429	A	C1'-O4'-C4'	-5.92	103.98	109.90
1	X	2354	G	O4'-C4'-C3'	-5.92	98.08	104.00
1	X	2229	G	P-O5'-C5'	-5.91	112.03	120.90
1	X	747	A	O3'-P-O5'	-5.91	95.14	104.00
1	X	1412	C	O4'-C4'-C3'	-5.91	98.09	104.00
1	X	2854	G	O4'-C1'-C2'	-5.90	99.90	105.80
5	C	18	PRO	N-CA-C	5.90	120.51	110.95
16	N	8	ILE	N-CA-CB	5.90	120.96	111.23
1	X	85	C	C3'-C2'-O2'	5.90	119.55	110.70
1	X	2708	U	C5'-C4'-C3'	-5.89	107.16	116.00
1	X	342	G	C2'-C3'-O3'	5.89	118.33	109.50
1	X	823	U	C2'-C3'-O3'	5.89	122.53	113.70
1	X	1409	U	O3'-P-O5'	-5.88	95.17	104.00
11	I	39	SER	CA-C-N	5.88	132.78	121.54
11	I	39	SER	C-N-CA	5.88	132.78	121.54
20	R	12	ASP	N-CA-C	-5.88	103.80	111.74
1	X	2190	A	C5'-C4'-C3'	5.88	124.82	116.00
1	X	2275	U	P-O3'-C3'	5.88	129.02	120.20
1	X	652	C	P-O5'-C5'	-5.88	112.08	120.90
23	U	49	LYS	N-CA-C	5.88	117.79	108.79
1	X	2299	A	P-O3'-C3'	5.88	129.02	120.20
1	X	1468	A	C3'-C2'-C1'	-5.87	95.43	101.30
1	X	1288	A	C2'-C3'-O3'	5.87	118.31	109.50
14	L	20	THR	CA-C-N	5.87	132.75	121.54
14	L	20	THR	C-N-CA	5.87	132.75	121.54
21	S	79	ILE	CB-CA-C	5.87	116.96	110.62
1	X	2860	C	C3'-C2'-O2'	5.87	119.50	110.70
1	X	2045	A	C2'-C3'-O3'	5.87	118.30	109.50
2	Y	30	C	P-O5'-C5'	5.87	129.70	120.90
1	X	2808	U	C1'-O4'-C4'	-5.86	103.84	109.70
1	X	2826	C	C4'-C3'-C2'	-5.86	96.75	102.60
1	X	7	G	C5'-C4'-C3'	-5.85	107.22	116.00
1	X	2341	G	C3'-C2'-O2'	5.85	119.48	110.70
1	X	1992	G	C3'-C2'-O2'	5.85	119.48	110.70
1	X	2669	C	C2'-C3'-O3'	5.85	118.28	109.50
1	X	2758	A	C2'-C3'-O3'	5.85	118.27	109.50
1	X	312	G	P-O3'-C3'	5.84	128.97	120.20
1	X	2808	U	P-O5'-C5'	5.84	129.66	120.90
1	X	1747	G	N9-C1'-C2'	5.84	120.75	112.00
26	Z	39	LYS	N-CA-C	5.83	118.52	110.35
23	U	25	ARG	CA-C-N	5.83	132.68	121.54
23	U	25	ARG	C-N-CA	5.83	132.68	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	312	G	C1'-O4'-C4'	-5.83	103.87	109.70
1	X	761	G	P-O5'-C5'	-5.83	112.16	120.90
1	X	1713	G	P-O5'-C5'	5.83	129.64	120.90
1	X	1946	U	O4'-C1'-C2'	-5.83	101.77	107.60
1	X	2476	A	C2'-C3'-O3'	5.83	118.24	109.50
1	X	1943	A	C5'-C4'-C3'	-5.82	107.27	116.00
1	X	321	A	C2'-C3'-O3'	5.82	118.22	109.50
1	X	1466	C	O4'-C1'-C2'	-5.81	101.79	107.60
2	Y	16	U	N1-C1'-C2'	5.81	122.72	114.00
1	X	477	A	C3'-C2'-O2'	5.81	119.41	110.70
1	X	1947	G	P-O3'-C3'	5.80	128.91	120.20
13	K	104	ARG	N-CA-C	5.80	118.48	111.40
9	G	99	VAL	CA-C-N	5.80	129.11	120.87
9	G	99	VAL	C-N-CA	5.80	129.11	120.87
1	X	1938	U	P-O5'-C5'	5.80	129.60	120.90
1	X	1935	A	P-O5'-C5'	-5.80	112.20	120.90
1	X	318	G	C1'-C2'-O2'	5.79	117.09	108.40
1	X	1429	A	N9-C1'-C2'	5.79	120.68	112.00
17	O	97	GLY	N-CA-C	5.79	126.90	113.18
1	X	2589	C	O3'-P-O5'	-5.79	95.32	104.00
1	X	242	A	C5'-C4'-C3'	5.79	124.68	116.00
1	X	2370	G	C1'-O4'-C4'	-5.78	103.92	109.70
5	C	193	LEU	N-CA-C	-5.78	104.58	111.69
1	X	2484	G	P-O5'-C5'	5.78	129.57	120.90
9	G	97	ASP	CA-CB-CG	5.78	118.38	112.60
1	X	2013	A	C4'-C3'-O3'	-5.78	104.34	113.00
23	U	47	HIS	N-CA-C	5.78	123.10	110.80
11	I	64	GLY	CA-C-N	5.77	132.56	121.54
11	I	64	GLY	C-N-CA	5.77	132.56	121.54
1	X	1717	A	O5'-C5'-C4'	5.77	120.15	111.50
1	X	2756	A	P-O3'-C3'	5.76	128.85	120.20
1	X	2618	A	O3'-P-O5'	-5.76	95.36	104.00
5	C	63	GLY	CA-C-N	5.76	132.54	121.54
5	C	63	GLY	C-N-CA	5.76	132.54	121.54
15	M	57	ILE	N-CA-C	-5.76	99.82	108.12
1	X	537	C	P-O3'-C3'	5.76	128.83	120.20
1	X	2261	G	C4'-C3'-O3'	5.75	118.03	109.40
1	X	157	G	C5'-C4'-C3'	-5.75	107.38	116.00
1	X	1264	C	C2'-C3'-O3'	5.75	118.12	109.50
19	Q	60	GLY	N-CA-C	5.75	126.80	113.18
19	Q	73	ASN	CA-C-N	5.75	132.52	121.54
19	Q	73	ASN	C-N-CA	5.75	132.52	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	3	U	O4'-C4'-C3'	-5.74	98.26	104.00
1	X	523	A	N9-C1'-C2'	5.74	120.62	112.00
5	C	46	ARG	CA-C-N	5.74	129.44	120.82
5	C	46	ARG	C-N-CA	5.74	129.44	120.82
1	X	1392	U	P-O3'-C3'	5.74	128.81	120.20
1	X	1938	U	N1-C1'-C2'	5.74	122.60	114.00
1	X	1561	A	O4'-C4'-C3'	-5.73	98.27	104.00
1	X	1685	A	P-O5'-C5'	5.73	129.50	120.90
12	J	135	ARG	CA-C-N	5.73	132.49	121.54
12	J	135	ARG	C-N-CA	5.73	132.49	121.54
1	X	1264	C	O3'-P-O5'	-5.73	95.41	104.00
20	R	81	VAL	N-CA-C	5.73	117.58	108.87
1	X	467	U	C5'-C4'-C3'	5.73	124.59	116.00
1	X	1012	A	O3'-P-O5'	-5.72	95.41	104.00
1	X	1575	C	C4'-C3'-C2'	5.72	108.32	102.60
1	X	2016	A	P-O3'-C3'	5.72	128.78	120.20
5	C	90	SER	N-CA-C	5.72	122.98	110.80
18	P	116	ILE	N-CA-C	5.72	116.37	107.28
1	X	1544	A	C3'-C2'-O2'	5.72	119.28	110.70
1	X	1607	A	P-O3'-C3'	5.71	128.77	120.20
1	X	777	A	C4'-C3'-C2'	5.71	108.31	102.60
3	A	245	VAL	N-CA-C	5.70	115.29	108.45
1	X	1938	U	C2'-C3'-O3'	5.70	118.05	109.50
1	X	1072	U	P-O3'-C3'	5.70	128.75	120.20
17	O	96	LEU	CA-C-N	5.70	132.58	121.41
17	O	96	LEU	C-N-CA	5.70	132.58	121.41
14	L	37	HIS	CA-CB-CG	5.70	119.50	113.80
1	X	70	A	P-O5'-C5'	-5.68	112.38	120.90
11	I	40	ARG	CA-C-N	5.68	132.40	121.54
11	I	40	ARG	C-N-CA	5.68	132.40	121.54
1	X	948	C	P-O3'-C3'	-5.68	111.68	120.20
1	X	463	C	C1'-C2'-O2'	5.67	116.91	108.40
1	X	2808	U	C3'-C2'-C1'	-5.67	95.83	101.50
15	M	4	HIS	N-CA-C	5.67	119.98	111.81
3	A	261	ARG	CA-C-N	5.67	128.68	120.79
3	A	261	ARG	C-N-CA	5.67	128.68	120.79
1	X	520	C	P-O3'-C3'	5.67	128.71	120.20
1	X	1280	U	N1-C1'-C2'	5.67	120.51	112.00
14	L	9	ARG	CA-C-N	5.67	128.45	120.28
14	L	9	ARG	C-N-CA	5.67	128.45	120.28
14	L	90	ASP	CA-CB-CG	5.67	118.27	112.60
1	X	467	U	C4'-C3'-O3'	5.67	121.50	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1339	U	O5'-C5'-C4'	5.66	119.99	111.50
1	X	2275	U	P-O5'-C5'	5.66	129.39	120.90
5	C	57	LYS	CA-C-O	-5.66	114.77	120.77
1	X	2722	C	C3'-C2'-O2'	5.66	119.18	110.70
5	C	89	ARG	N-CA-C	5.66	115.70	108.24
15	M	30	GLY	CA-C-N	5.66	128.87	120.90
15	M	30	GLY	C-N-CA	5.66	128.87	120.90
1	X	418	C	P-O5'-C5'	5.65	129.37	120.90
1	X	1820	G	C4'-C3'-C2'	5.65	108.25	102.60
5	C	78	VAL	N-CA-C	-5.65	102.24	109.30
1	X	2808	U	C5'-C4'-O4'	5.65	117.57	109.10
1	X	153	A	O3'-P-O5'	-5.64	95.53	104.00
1	X	1341	G	C3'-C2'-O2'	5.64	119.16	110.70
1	X	2847	G	N9-C1'-C2'	5.63	120.45	112.00
17	O	56	VAL	N-CA-CB	5.63	116.86	110.72
1	X	2706	U	O4'-C1'-C2'	5.63	111.43	105.80
1	X	1128	G	P-O3'-C3'	5.63	128.64	120.20
20	R	74	LEU	CA-C-N	5.63	129.09	120.82
20	R	74	LEU	C-N-CA	5.63	129.09	120.82
1	X	1960	A	C3'-C2'-O2'	5.63	119.14	110.70
1	X	219	G	O4'-C1'-C2'	-5.62	100.17	105.80
1	X	774	A	N9-C1'-C2'	5.62	120.44	112.00
1	X	2479	U	C4'-C3'-C2'	-5.62	96.98	102.60
1	X	352	G	P-O5'-C5'	5.62	129.33	120.90
1	X	33	C	C4'-C3'-C2'	5.62	108.22	102.60
1	X	408	U	P-O3'-C3'	5.61	128.62	120.20
1	X	2024	U	C3'-C2'-O2'	5.61	119.12	110.70
1	X	1194	U	C2'-C3'-O3'	5.61	122.11	113.70
1	X	218	A	P-O3'-C3'	5.61	128.61	120.20
1	X	1983	G	C4'-C3'-C2'	-5.61	97.00	102.60
1	X	458	G	C4'-C3'-O3'	5.60	117.81	109.40
1	X	2508	G	N9-C1'-C2'	5.60	120.40	112.00
1	X	492	G	C2'-C3'-O3'	5.60	117.90	109.50
1	X	807	A	C3'-C2'-O2'	5.60	119.09	110.70
13	K	99	ARG	CA-C-N	5.59	127.71	120.88
13	K	99	ARG	C-N-CA	5.59	127.71	120.88
1	X	1344	C	O4'-C4'-C3'	-5.59	98.41	104.00
11	I	44	GLY	N-CA-C	5.59	126.42	113.18
16	N	66	ASN	CA-CB-CG	5.59	118.19	112.60
1	X	15	G	C3'-C2'-O2'	5.58	119.08	110.70
1	X	2774	U	N1-C1'-C2'	5.58	120.38	112.00
12	J	14	PHE	N-CA-C	5.58	118.35	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1988	A	P-O3'-C3'	5.58	128.57	120.20
13	K	31	GLU	N-CA-C	5.58	118.55	111.69
1	X	967	G	P-O5'-C5'	5.57	129.25	120.90
1	X	1152	C	C2'-C3'-O3'	5.57	117.85	109.50
1	X	607	C	O4'-C4'-C3'	-5.56	98.44	104.00
20	R	78	ALA	N-CA-C	-5.56	104.03	111.87
1	X	1574	A	O4'-C1'-N9	5.56	116.84	108.50
1	X	2708	U	P-O3'-C3'	-5.56	111.86	120.20
1	X	3	U	C4'-C3'-O3'	5.56	121.34	113.00
1	X	1031	C	C4'-C3'-C2'	5.56	108.16	102.60
1	X	1434	U	C1'-O4'-C4'	-5.56	104.34	109.90
1	X	321	A	O3'-P-O5'	-5.55	95.67	104.00
1	X	357	A	P-O3'-C3'	5.55	128.53	120.20
10	H	70	VAL	N-CA-C	5.55	116.85	108.96
11	I	35	LYS	N-CA-C	-5.55	97.02	108.18
10	H	44	TYR	N-CA-C	5.55	118.60	109.72
1	X	593	C	P-O5'-C5'	5.55	129.22	120.90
1	X	2596	C	O4'-C1'-N1	5.55	116.83	108.50
1	X	2224	U	C4'-C3'-O3'	-5.55	104.68	113.00
1	X	2408	G	C2'-C3'-O3'	5.54	122.02	113.70
11	I	37	GLN	CA-C-N	5.54	128.88	121.90
11	I	37	GLN	C-N-CA	5.54	128.88	121.90
1	X	349	G	P-O5'-C5'	5.54	129.21	120.90
1	X	638	A	C5'-C4'-C3'	5.54	123.51	115.20
1	X	2854	G	P-O5'-C5'	5.54	129.21	120.90
1	X	1220	G	O4'-C1'-C2'	-5.54	102.06	107.60
1	X	1656	U	P-O3'-C3'	5.54	128.50	120.20
2	Y	28	A	N9-C1'-C2'	5.54	120.30	112.00
1	X	1411	C	C3'-C2'-O2'	5.53	119.00	110.70
1	X	97	U	C5'-C4'-C3'	-5.53	107.70	116.00
1	X	192	G	P-O3'-C3'	5.53	128.50	120.20
1	X	969	U	O3'-P-O5'	-5.53	95.70	104.00
5	C	58	MET	N-CA-C	5.53	122.58	110.80
12	J	140	GLU	N-CA-C	5.53	117.36	107.80
1	X	33	C	C4'-C3'-O3'	5.53	117.69	109.40
1	X	89	A	P-O3'-C3'	5.53	128.49	120.20
1	X	990	A	O4'-C4'-C3'	-5.53	98.47	104.00
1	X	765	C	P-O3'-C3'	5.52	128.48	120.20
1	X	2858	A	P-O5'-C5'	5.52	129.19	120.90
1	X	174	A	P-O3'-C3'	5.52	128.48	120.20
15	M	3	THR	CA-C-N	-5.52	112.06	122.27
15	M	3	THR	C-N-CA	-5.52	112.06	122.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	494	A	C3'-C2'-C1'	5.51	106.81	101.30
18	P	133	ASN	N-CA-C	-5.51	104.91	111.69
20	R	109	ALA	CA-C-N	5.51	132.07	121.54
20	R	109	ALA	C-N-CA	5.51	132.07	121.54
1	X	762	A	C1'-C2'-O2'	5.51	116.66	108.40
1	X	1570	C	C1'-O4'-C4'	-5.51	104.19	109.70
1	X	1711	C	P-O5'-C5'	5.50	129.16	120.90
1	X	569	C	P-O3'-C3'	-5.50	111.94	120.20
1	X	1442	C	C4'-C3'-C2'	5.50	108.10	102.60
4	B	136	ARG	N-CA-CB	5.50	118.01	109.48
1	X	2039	G	O4'-C1'-C2'	-5.50	102.10	107.60
1	X	418	C	C5'-C4'-O4'	5.50	118.05	109.80
1	X	1068	A	P-O3'-C3'	5.49	128.44	120.20
1	X	1044	U	P-O3'-C3'	5.48	128.43	120.20
2	Y	29	C	N1-C1'-C2'	5.48	120.23	112.00
1	X	2540	A	O4'-C4'-C3'	-5.48	98.52	104.00
1	X	1629	G	C4'-C3'-C2'	-5.48	97.12	102.60
1	X	2668	U	O4'-C1'-C2'	5.48	111.28	105.80
1	X	496	C	P-O3'-C3'	-5.47	111.99	120.20
1	X	669	G	O4'-C4'-C3'	-5.47	98.53	104.00
1	X	1951	G	O3'-P-O5'	-5.47	95.79	104.00
1	X	814	G	O4'-C1'-N9	-5.47	100.00	108.20
23	U	18	VAL	N-CA-C	5.47	117.98	108.95
1	X	656	U	O4'-C1'-N1	5.46	116.69	108.50
1	X	2619	G	C5'-C4'-C3'	-5.46	107.81	116.00
10	H	28	GLY	N-CA-C	5.46	118.21	111.93
17	O	90	PHE	N-CA-C	5.46	116.55	108.86
1	X	802	A	C4'-C3'-C2'	5.46	108.06	102.60
1	X	341	A	C2'-C3'-O3'	5.45	117.68	109.50
1	X	59	G	P-O3'-C3'	5.45	128.37	120.20
3	A	171	ASP	N-CA-C	-5.45	106.41	112.57
1	X	1278	A	N9-C1'-C2'	5.45	122.17	114.00
1	X	2605	C	C3'-C2'-O2'	5.45	118.87	110.70
1	X	742	G	P-O3'-C3'	5.45	128.37	120.20
1	X	1670	G	P-O3'-C3'	5.45	128.37	120.20
21	S	173	PRO	N-CA-C	5.45	117.34	110.70
1	X	1882	G	C3'-C2'-C1'	5.44	106.74	101.30
22	T	18	PRO	CA-C-N	5.44	131.93	121.54
22	T	18	PRO	C-N-CA	5.44	131.93	121.54
4	B	150	VAL	N-CA-C	-5.44	100.56	108.17
1	X	2659	C	P-O5'-C5'	5.43	129.05	120.90
5	C	134	ILE	CA-C-N	5.43	127.82	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	134	ILE	C-N-CA	5.43	127.82	120.65
1	X	485	G	P-O5'-C5'	5.43	129.04	120.90
1	X	1314	A	N9-C1'-C2'	5.43	122.14	114.00
1	X	2396	C	P-O5'-C5'	-5.43	112.76	120.90
3	A	230	ASP	CA-CB-CG	5.43	118.03	112.60
1	X	345	U	P-O5'-C5'	5.43	129.04	120.90
1	X	1660	G	C4'-C3'-C2'	-5.43	97.17	102.60
1	X	2794	G	P-O5'-C5'	-5.42	112.76	120.90
1	X	843	G	P-O3'-C3'	5.42	128.34	120.20
1	X	2779	C	N1-C1'-C2'	5.42	120.13	112.00
1	X	761	G	C1'-O4'-C4'	-5.42	104.28	109.70
1	X	1821	A	O4'-C4'-C3'	-5.42	98.58	104.00
1	X	2314	A	P-O5'-C5'	5.42	129.03	120.90
1	X	673	G	C4'-C3'-C2'	5.42	108.02	102.60
1	X	2687	G	O3'-P-O5'	-5.41	95.88	104.00
1	X	71	A	P-O5'-C5'	5.41	129.02	120.90
1	X	2199	C	C4'-C3'-O3'	-5.41	104.89	113.00
1	X	505	G	N9-C1'-C2'	5.41	120.11	112.00
1	X	1474	A	P-O3'-C3'	5.41	128.31	120.20
1	X	1509	A	P-O5'-C5'	5.41	129.01	120.90
1	X	2042	A	C4'-C3'-C2'	-5.41	97.19	102.60
4	B	75	THR	CB-CA-C	5.41	121.18	110.42
20	R	86	PRO	CA-C-N	5.41	131.87	121.54
20	R	86	PRO	C-N-CA	5.41	131.87	121.54
22	T	54	GLY	CA-C-N	5.41	127.78	120.38
22	T	54	GLY	C-N-CA	5.41	127.78	120.38
1	X	1812	U	P-O3'-C3'	5.40	128.31	120.20
1	X	387	A	P-O3'-C3'	5.40	128.31	120.20
11	I	67	ASN	N-CA-C	5.40	119.23	111.02
1	X	98	U	C4'-C3'-O3'	5.40	117.50	109.40
1	X	1774	A	C3'-C2'-O2'	5.40	118.79	110.70
1	X	1928	G	P-O5'-C5'	5.40	128.99	120.90
1	X	2548	G	O4'-C1'-C2'	-5.39	102.21	107.60
1	X	1909	U	N1-C1'-C2'	5.39	122.08	114.00
25	W	48	LYS	CA-C-N	5.39	129.72	120.72
25	W	48	LYS	C-N-CA	5.39	129.72	120.72
1	X	1281	A	O3'-P-O5'	-5.39	95.92	104.00
1	X	2745	A	O5'-C5'-C4'	-5.39	103.42	111.50
19	Q	56	MET	N-CA-C	5.39	117.28	108.55
1	X	1636	G	C3'-C2'-O2'	5.38	118.78	110.70
1	X	1408	A	C4'-C3'-O3'	-5.38	104.93	113.00
1	X	1601	U	C2'-C3'-O3'	5.38	117.57	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2731	G	P-O3'-C3'	5.38	128.27	120.20
1	X	683	A	N9-C1'-C2'	5.38	122.07	114.00
1	X	1282	A	C5'-C4'-C3'	-5.38	107.93	116.00
3	A	249	PRO	CA-C-N	5.38	131.81	121.54
3	A	249	PRO	C-N-CA	5.38	131.81	121.54
1	X	517	A	P-O3'-C3'	5.38	128.26	120.20
18	P	27	VAL	N-CA-C	5.38	115.64	108.27
1	X	117	A	C1'-O4'-C4'	-5.37	104.33	109.70
1	X	1139	A	O4'-C1'-C2'	-5.37	100.43	105.80
1	X	1467	U	O4'-C4'-C3'	-5.37	98.63	104.00
1	X	1702	C	C3'-C2'-O2'	5.37	118.76	110.70
1	X	107	G	C5'-C4'-C3'	-5.37	107.94	116.00
1	X	2217	G	P-O3'-C3'	5.37	128.25	120.20
1	X	801	A	P-O3'-C3'	5.37	128.25	120.20
5	C	162	ARG	CA-C-N	5.37	131.79	121.54
5	C	162	ARG	C-N-CA	5.37	131.79	121.54
1	X	1288	A	N9-C1'-C2'	5.37	122.05	114.00
23	U	59	THR	CA-C-N	5.37	131.63	121.97
23	U	59	THR	C-N-CA	5.37	131.63	121.97
1	X	465	C	P-O5'-C5'	-5.37	112.85	120.90
22	T	19	LYS	N-CA-C	5.37	122.23	110.80
1	X	1266	G	P-O3'-C3'	5.36	128.25	120.20
1	X	616	U	C5'-C4'-C3'	-5.36	107.96	116.00
1	X	633	G	P-O5'-C5'	5.36	128.94	120.90
1	X	1290	A	C3'-C2'-O2'	5.36	118.74	110.70
1	X	1355	A	P-O3'-C3'	5.36	128.24	120.20
1	X	1812	U	P-O5'-C5'	5.36	128.94	120.90
18	P	10	ASN	CA-CB-CG	5.36	117.96	112.60
1	X	767	G	P-O5'-C5'	5.36	128.94	120.90
1	X	2737	A	C5'-C4'-C3'	-5.36	107.97	116.00
1	X	2825	A	C4'-C3'-O3'	-5.36	104.97	113.00
1	X	232	A	P-O5'-C5'	5.35	128.93	120.90
1	X	1442	C	C4'-C3'-O3'	5.35	117.43	109.40
7	E	137	ASP	CA-C-N	5.35	127.71	120.38
7	E	137	ASP	C-N-CA	5.35	127.71	120.38
22	T	71	ASN	CA-CB-CG	5.35	117.95	112.60
1	X	2404	A	C4'-C3'-O3'	5.34	117.42	109.40
1	X	2298	U	C4'-C3'-O3'	5.34	117.41	109.40
22	T	18	PRO	N-CA-C	5.34	122.43	113.78
1	X	2639	A	P-O3'-C3'	-5.34	112.19	120.20
1	X	15	G	O5'-C5'-C4'	-5.33	103.50	111.50
1	X	853	C	C3'-C2'-O2'	5.33	118.69	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	10	U	O4'-C4'-C3'	-5.33	98.67	104.00
20	R	88	THR	CA-C-N	5.33	125.16	120.10
20	R	88	THR	C-N-CA	5.33	125.16	120.10
1	X	413	G	O4'-C1'-C2'	-5.33	102.27	107.60
1	X	1664	G	C2'-C3'-O3'	5.33	117.49	109.50
2	Y	12	C	O4'-C4'-C3'	-5.33	98.67	104.00
1	X	1037	U	O4'-C4'-C3'	-5.32	100.78	106.10
1	X	2454	C	N1-C1'-C2'	5.32	119.98	112.00
11	I	100	ARG	N-CA-C	5.32	118.16	109.59
1	X	1627	C	C3'-C2'-O2'	5.32	118.68	110.70
1	X	978	U	C3'-C2'-O2'	5.32	118.68	110.70
12	J	77	LYS	N-CA-C	5.32	117.15	109.07
1	X	2375	G	O4'-C4'-C3'	-5.32	98.69	104.00
1	X	2769	C	C5'-C4'-C3'	-5.32	107.23	115.20
1	X	698	A	O3'-P-O5'	-5.31	96.03	104.00
2	Y	99	G	C1'-C2'-O2'	5.31	116.37	108.40
17	O	68	LYS	CA-C-N	5.31	130.10	122.45
17	O	68	LYS	C-N-CA	5.31	130.10	122.45
1	X	805	G	O4'-C1'-N9	-5.31	100.23	108.20
1	X	1410	U	C3'-C2'-O2'	5.31	122.57	114.60
21	S	172	LEU	N-CA-C	5.31	117.64	110.31
1	X	524	A	O4'-C4'-C3'	-5.31	98.69	104.00
4	B	74	PRO	N-CA-C	5.31	123.40	112.47
1	X	666	U	P-O3'-C3'	5.30	128.16	120.20
1	X	1341	G	P-O3'-C3'	-5.30	112.25	120.20
12	J	11	ARG	N-CA-C	5.30	122.10	110.80
15	M	103	LYS	N-CA-C	5.30	120.62	114.04
1	X	1324	G	O3'-P-O5'	-5.30	96.05	104.00
1	X	2507	U	C3'-C2'-O2'	5.30	118.65	110.70
5	C	163	ASN	N-CA-C	5.30	122.09	110.80
1	X	689	A	C1'-O4'-C4'	-5.30	104.60	109.90
1	X	2768	C	O3'-P-O5'	-5.30	96.05	104.00
1	X	1481	U	O3'-P-O5'	-5.30	96.06	104.00
1	X	1634	A	P-O3'-C3'	5.30	128.15	120.20
1	X	1661	C	C4'-C3'-C2'	-5.30	97.30	102.60
1	X	1935	A	P-O3'-C3'	5.30	128.15	120.20
1	X	2815	C	P-O5'-C5'	5.30	128.85	120.90
4	B	139	GLY	CA-C-N	5.29	129.45	122.30
4	B	139	GLY	C-N-CA	5.29	129.45	122.30
1	X	2017	U	N1-C1'-C2'	5.29	119.94	112.00
1	X	1991	C	P-O3'-C3'	-5.29	112.26	120.20
1	X	675	C	C3'-C2'-O2'	5.29	118.64	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2814	G	N9-C1'-C2'	5.29	119.93	112.00
1	X	2382	C	O4'-C1'-C2'	-5.29	102.31	107.60
1	X	1154	A	C4'-C3'-C2'	5.29	107.89	102.60
25	W	10	ILE	N-CA-CB	5.29	117.21	110.13
1	X	964	A	C3'-C2'-O2'	5.28	118.62	110.70
3	A	243	GLY	CA-C-N	5.28	131.63	121.54
3	A	243	GLY	C-N-CA	5.28	131.63	121.54
1	X	469	G	C1'-O4'-C4'	-5.28	104.42	109.70
1	X	969	U	C4'-C3'-C2'	5.28	107.88	102.60
1	X	2444	C	P-O5'-C5'	5.28	128.82	120.90
1	X	2769	C	O4'-C1'-N1	5.28	116.12	108.20
1	X	2181	A	C1'-O4'-C4'	-5.28	104.62	109.90
1	X	1071	U	P-O3'-C3'	5.27	128.11	120.20
1	X	108	G	P-O5'-C5'	5.27	128.81	120.90
1	X	342	G	C4'-C3'-O3'	5.27	117.31	109.40
1	X	2044	G	C2'-C3'-O3'	5.27	117.41	109.50
1	X	2861	A	O4'-C1'-C2'	-5.27	102.33	107.60
1	X	2826	C	C4'-C3'-O3'	-5.27	105.09	113.00
1	X	334	G	C1'-O4'-C4'	-5.27	104.43	109.70
1	X	1831	G	O4'-C1'-C2'	-5.27	102.33	107.60
1	X	2008	C	O3'-P-O5'	-5.27	96.10	104.00
1	X	2408	G	P-O3'-C3'	-5.27	112.30	120.20
5	C	56	ARG	N-CA-C	5.27	121.25	114.56
13	K	109	THR	CB-CA-C	5.27	118.68	110.67
1	X	2568	A	O4'-C4'-C3'	-5.27	98.73	104.00
1	X	1129	A	P-O5'-C5'	5.27	128.80	120.90
1	X	1776	A	P-O3'-C3'	5.27	128.10	120.20
5	C	181	LEU	CA-C-N	5.26	127.76	120.29
5	C	181	LEU	C-N-CA	5.26	127.76	120.29
26	Z	6	VAL	N-CA-CB	-5.26	106.01	111.64
1	X	1434	U	P-O3'-C3'	5.26	128.09	120.20
1	X	1582	A	C4'-C3'-O3'	-5.26	101.52	109.40
1	X	1943	A	C1'-C2'-O2'	5.26	116.29	108.40
9	G	112	THR	CB-CA-C	5.25	118.40	109.53
18	P	19	LYS	N-CA-C	5.25	119.38	112.92
9	G	100	TYR	N-CA-C	-5.25	102.51	110.28
1	X	1006	C	N1-C1'-C2'	5.25	121.87	114.00
1	X	1974	U	C3'-C2'-O2'	5.24	118.56	110.70
1	X	748	A	C5'-C4'-C3'	-5.24	108.14	116.00
1	X	666	U	P-O5'-C5'	5.24	128.76	120.90
1	X	2721	A	C3'-C2'-O2'	5.24	118.56	110.70
1	X	219	G	N9-C1'-C2'	5.24	121.85	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	485	G	P-O3'-C3'	5.24	128.06	120.20
1	X	1055	A	C4'-C3'-O3'	5.24	120.85	113.00
1	X	2014	A	C4'-C3'-C2'	5.24	107.84	102.60
1	X	1811	A	C4'-C3'-C2'	5.23	107.83	102.60
5	C	31	VAL	N-CA-CB	5.23	117.66	110.54
26	Z	12	SER	CA-C-N	5.23	127.82	120.28
26	Z	12	SER	C-N-CA	5.23	127.82	120.28
1	X	539	A	C1'-O4'-C4'	-5.23	104.47	109.70
16	N	4	ALA	CA-C-N	5.23	129.71	120.87
16	N	4	ALA	C-N-CA	5.23	129.71	120.87
1	X	12	U	C1'-C2'-O2'	5.23	116.24	108.40
1	X	459	A	P-O3'-C3'	5.23	128.04	120.20
1	X	491	A	C5'-C4'-C3'	-5.23	108.16	116.00
3	A	252	LYS	N-CA-C	5.23	121.36	109.81
17	O	50	ASP	N-CA-C	-5.23	106.16	112.54
11	I	27	ASP	CA-CB-CG	5.23	117.83	112.60
1	X	534	U	C3'-C2'-O2'	5.22	118.54	110.70
1	X	588	G	C3'-C2'-O2'	5.22	118.53	110.70
1	X	2820	C	C3'-C2'-O2'	5.22	118.53	110.70
1	X	2824	C	C3'-C2'-O2'	5.22	122.43	114.60
1	X	1989	C	C1'-O4'-C4'	5.22	115.12	109.90
1	X	1812	U	O4'-C1'-N1	5.22	116.03	108.20
1	X	2190	A	C4'-C3'-C2'	-5.21	97.39	102.60
19	Q	75	ARG	CA-C-N	5.21	130.50	121.64
19	Q	75	ARG	C-N-CA	5.21	130.50	121.64
1	X	1467	U	C5'-C4'-C3'	5.21	123.82	116.00
1	X	2230	G	C3'-C2'-O2'	5.21	118.52	110.70
21	S	29	ASN	CA-C-N	5.21	128.36	120.13
21	S	29	ASN	C-N-CA	5.21	128.36	120.13
9	G	101	THR	N-CA-C	5.21	116.68	109.54
1	X	2425	G	C3'-C2'-O2'	5.21	118.51	110.70
4	B	92	ASN	N-CA-C	5.21	118.89	112.54
1	X	1412	C	P-O3'-C3'	5.20	128.00	120.20
1	X	1631	C	C4'-C3'-C2'	-5.20	97.40	102.60
1	X	2482	A	C5'-C4'-O4'	5.20	116.90	109.10
4	B	168	GLN	N-CA-C	5.20	118.18	110.48
1	X	2018	G	O4'-C1'-C2'	-5.20	100.60	105.80
6	D	47	SER	CA-C-N	5.20	127.67	120.29
6	D	47	SER	C-N-CA	5.20	127.67	120.29
1	X	2581	A	P-O3'-C3'	5.19	127.99	120.20
20	R	4	PRO	CA-C-N	5.19	131.46	121.54
20	R	4	PRO	C-N-CA	5.19	131.46	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	494	A	N9-C1'-C2'	-5.19	104.21	112.00
1	X	1140	A	C5'-C4'-C3'	-5.19	108.21	116.00
1	X	2488	G	C3'-C2'-O2'	5.19	118.49	110.70
1	X	549	G	P-O5'-C5'	5.19	128.68	120.90
1	X	823	U	C3'-C2'-O2'	5.19	118.48	110.70
1	X	2860	C	P-O5'-C5'	5.18	128.67	120.90
26	Z	4	HIS	CA-C-O	-5.18	113.06	120.16
17	O	18	ASP	CA-CB-CG	5.18	117.78	112.60
1	X	537	C	C5'-C4'-O4'	5.18	117.57	109.80
1	X	2805	G	P-O5'-C5'	-5.18	113.13	120.90
1	X	185	C	C3'-C2'-O2'	5.18	118.47	110.70
18	P	126	ILE	N-CA-CB	5.18	119.08	111.52
1	X	24	G	O5'-C5'-C4'	-5.17	103.74	111.50
1	X	1299	A	P-O5'-C5'	5.17	128.66	120.90
1	X	799	C	P-O5'-C5'	-5.17	113.14	120.90
1	X	2043	A	P-O3'-C3'	5.17	127.95	120.20
1	X	2496	C	O3'-P-O5'	-5.17	96.25	104.00
1	X	1522	C	C3'-C2'-C1'	-5.16	96.14	101.30
1	X	1669	A	N9-C1'-C2'	5.16	119.75	112.00
11	I	39	SER	CA-CB-OG	5.16	121.42	111.10
1	X	2575	U	C3'-C2'-O2'	5.16	118.44	110.70
1	X	53	G	C3'-C2'-O2'	5.16	118.44	110.70
1	X	825	C	C5'-C4'-C3'	-5.16	108.26	116.00
1	X	2650	G	C4'-C3'-C2'	5.16	107.76	102.60
20	R	7	GLY	CA-C-N	5.16	129.45	120.68
20	R	7	GLY	C-N-CA	5.16	129.45	120.68
1	X	1269	G	C3'-C2'-O2'	5.16	118.43	110.70
1	X	1680	U	C3'-C2'-O2'	5.16	118.43	110.70
1	X	2336	G	C1'-C2'-O2'	5.16	116.13	108.40
17	O	78	VAL	N-CA-C	-5.16	107.27	112.17
1	X	951	G	O4'-C4'-C3'	-5.15	98.85	104.00
1	X	1261	G	P-O5'-C5'	5.15	128.63	120.90
1	X	1469	U	P-O5'-C5'	5.15	128.63	120.90
11	I	62	LYS	CA-C-N	5.15	132.61	121.64
11	I	62	LYS	C-N-CA	5.15	132.61	121.64
1	X	2075	U	P-O3'-C3'	5.15	127.92	120.20
1	X	951	G	C3'-C2'-C1'	-5.15	96.15	101.30
25	W	34	VAL	N-CA-C	5.15	117.25	108.86
22	T	15	ASP	CA-C-N	5.14	131.60	122.45
22	T	15	ASP	C-N-CA	5.14	131.60	122.45
24	V	19	ASP	CA-CB-CG	5.14	117.74	112.60
1	X	537	C	O4'-C1'-C2'	-5.14	102.46	107.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1790	G	C4'-C3'-C2'	5.14	107.74	102.60
1	X	2413	A	N9-C1'-C2'	5.14	119.71	112.00
1	X	1259	A	O3'-P-O5'	-5.14	96.30	104.00
24	V	55	THR	CA-C-N	5.13	127.13	120.56
24	V	55	THR	C-N-CA	5.13	127.13	120.56
26	Z	14	SER	CA-C-N	5.13	128.52	120.82
26	Z	14	SER	C-N-CA	5.13	128.52	120.82
1	X	1629	G	C4'-C3'-O3'	-5.13	105.30	113.00
1	X	2407	G	P-O3'-C3'	5.13	127.90	120.20
1	X	2298	U	C4'-C3'-C2'	5.13	107.73	102.60
15	M	14	ARG	CA-C-N	5.13	125.63	119.94
15	M	14	ARG	C-N-CA	5.13	125.63	119.94
1	X	2022	C	C2'-C3'-O3'	-5.13	106.01	113.70
22	T	32	LYS	N-CA-C	-5.13	102.93	110.52
1	X	240	U	O4'-C4'-C3'	-5.12	98.88	104.00
3	A	186	HIS	CA-C-N	5.12	131.32	121.54
3	A	186	HIS	C-N-CA	5.12	131.32	121.54
1	X	1677	C	C1'-C2'-O2'	5.12	116.08	108.40
1	X	2681	A	C4'-C3'-C2'	-5.12	97.48	102.60
1	X	949	G	C3'-C2'-O2'	5.12	118.37	110.70
19	Q	65	VAL	N-CA-CB	5.12	119.67	111.23
9	G	85	ALA	CA-C-N	5.11	127.64	120.28
9	G	85	ALA	C-N-CA	5.11	127.64	120.28
5	C	164	VAL	N-CA-C	5.11	119.97	109.34
1	X	1965	U	C3'-C2'-O2'	5.11	118.36	110.70
1	X	1630	A	C4'-C3'-O3'	-5.11	105.34	113.00
1	X	2338	C	N1-C1'-C2'	5.11	119.66	112.00
3	A	34	THR	N-CA-C	5.11	116.95	109.24
9	G	106	TYR	CA-C-O	5.11	127.81	120.51
22	T	21	LEU	N-CA-C	5.11	121.67	110.80
9	G	110	LEU	CA-C-N	5.10	129.87	123.03
9	G	110	LEU	C-N-CA	5.10	129.87	123.03
1	X	1975	G	O3'-P-O5'	5.10	111.65	104.00
1	X	2608	A	C4'-C3'-O3'	5.10	117.05	109.40
1	X	1656	U	C3'-C2'-O2'	5.10	118.35	110.70
1	X	2298	U	C2'-C3'-O3'	5.10	117.15	109.50
1	X	1732	U	N1-C1'-C2'	5.10	119.64	112.00
1	X	1770	U	C1'-O4'-C4'	-5.10	104.80	109.90
1	X	556	A	P-O3'-C3'	5.10	127.84	120.20
1	X	1991	C	O3'-P-O5'	-5.09	96.36	104.00
1	X	2476	A	P-O5'-C5'	5.09	128.54	120.90
1	X	632	A	O4'-C1'-N9	5.09	116.14	108.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	794	A	C4'-C3'-O3'	-5.09	105.36	113.00
1	X	841	G	C1'-O4'-C4'	-5.09	104.81	109.90
9	G	70	PHE	CA-C-N	5.09	127.72	120.49
9	G	70	PHE	C-N-CA	5.09	127.72	120.49
1	X	1988	A	C3'-C2'-O2'	5.09	118.33	110.70
18	P	122	SER	N-CA-C	5.09	117.86	109.72
1	X	1771	A	P-O3'-C3'	5.08	127.83	120.20
1	X	455	A	O3'-P-O5'	-5.08	96.38	104.00
1	X	503	G	P-O5'-C5'	5.08	128.52	120.90
1	X	1403	U	C4'-C3'-O3'	-5.08	105.38	113.00
25	W	28	ILE	N-CA-C	-5.08	103.03	109.58
1	X	1122	A	N9-C1'-C2'	5.07	119.61	112.00
1	X	1473	U	C2'-C3'-O3'	5.07	117.11	109.50
1	X	2719	U	P-O5'-C5'	5.07	128.51	120.90
1	X	2769	C	P-O5'-C5'	-5.07	113.29	120.90
5	C	174	GLY	CA-C-N	5.07	128.16	120.75
5	C	174	GLY	C-N-CA	5.07	128.16	120.75
1	X	2564	U	C4'-C3'-O3'	5.07	117.01	109.40
1	X	333	A	P-O3'-C3'	5.07	127.80	120.20
21	S	128	ARG	CA-C-N	5.07	130.73	122.67
21	S	128	ARG	C-N-CA	5.07	130.73	122.67
1	X	483	A	C2'-C3'-O3'	5.07	121.30	113.70
3	A	96	HIS	CA-CB-CG	-5.07	108.73	113.80
1	X	2861	A	N9-C1'-C2'	5.06	119.60	112.00
24	V	18	ILE	CA-C-N	5.06	127.32	120.38
24	V	18	ILE	C-N-CA	5.06	127.32	120.38
1	X	730	C	P-O3'-C3'	5.06	127.79	120.20
1	X	2052	G	O5'-C5'-C4'	-5.05	103.92	111.50
1	X	1291	G	C3'-C2'-O2'	5.05	118.28	110.70
1	X	1666	G	O4'-C4'-C3'	-5.05	98.95	104.00
1	X	1922	U	P-O3'-C3'	5.05	127.77	120.20
1	X	2669	C	P-O5'-C5'	5.05	128.47	120.90
16	N	95	LEU	N-CA-C	-5.05	107.12	113.28
9	G	32	TYR	N-CA-C	5.04	117.66	110.24
1	X	1194	U	C4'-C3'-O3'	-5.04	105.44	113.00
1	X	1476	G	C3'-C2'-O2'	5.04	118.26	110.70
1	X	469	G	C1'-C2'-O2'	-5.04	104.24	111.80
1	X	1467	U	C5'-C4'-O4'	-5.04	102.24	109.80
14	L	93	SER	N-CA-C	-5.04	106.28	114.09
1	X	2477	C	P-O5'-C5'	5.04	128.46	120.90
1	X	1872	A	C4'-C3'-C2'	-5.04	97.56	102.60
1	X	2480	C	N1-C1'-C2'	5.03	119.55	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1291	G	O4'-C4'-C3'	-5.03	98.97	104.00
10	H	62	GLY	CA-C-N	5.03	128.37	120.82
10	H	62	GLY	C-N-CA	5.03	128.37	120.82
1	X	2694	G	C5'-C4'-O4'	-5.03	102.25	109.80
1	X	2798	A	P-O5'-C5'	5.03	128.44	120.90
1	X	560	G	C4'-C3'-C2'	5.03	107.63	102.60
1	X	2620	G	C4'-C3'-C2'	-5.03	97.57	102.60
13	K	49	GLU	CA-C-N	5.03	127.01	120.28
13	K	49	GLU	C-N-CA	5.03	127.01	120.28
1	X	519	C	C5'-C4'-O4'	-5.02	102.26	109.80
1	X	1368	G	C3'-C2'-O2'	5.02	118.23	110.70
1	X	1757	C	C3'-C2'-O2'	5.02	118.23	110.70
6	D	166	ALA	CA-C-N	5.02	127.26	120.38
6	D	166	ALA	C-N-CA	5.02	127.26	120.38
21	S	87	THR	CA-C-N	5.02	131.13	121.54
21	S	87	THR	C-N-CA	5.02	131.13	121.54
1	X	632	A	P-O3'-C3'	5.02	127.73	120.20
14	L	13	THR	CA-C-N	5.02	127.28	120.65
14	L	13	THR	C-N-CA	5.02	127.28	120.65
1	X	1662	G	P-O3'-C3'	5.02	127.72	120.20
1	X	1282	A	C4'-C3'-O3'	-5.01	105.48	113.00
1	X	1724	C	C3'-C2'-O2'	5.01	118.22	110.70
1	X	2628	C	C3'-C2'-C1'	-5.01	96.29	101.30
1	X	927	C	P-O5'-C5'	5.01	128.42	120.90
1	X	2261	G	C4'-C3'-C2'	5.01	107.61	102.60
1	X	2648	G	O3'-P-O5'	-5.01	96.48	104.00
7	E	145	ALA	CA-C-N	5.01	126.95	120.44
7	E	145	ALA	C-N-CA	5.01	126.95	120.44
1	X	652	C	C5'-C4'-C3'	-5.01	108.49	116.00
1	X	2396	C	O5'-C5'-C4'	5.01	119.01	111.50
1	X	2478	C	P-O3'-C3'	-5.01	112.69	120.20
10	H	120	ASP	CA-CB-CG	5.01	117.61	112.60
26	Z	8	LYS	N-CA-C	5.00	119.10	112.89
1	X	531	G	C1'-C2'-O2'	5.00	115.91	108.40
5	C	129	LYS	N-CA-C	5.00	121.45	110.80

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	1288	A	Sidechain
1	X	1684	G	Sidechain

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Mol	Chain	Res	Type	Group
1	X	219	G	Sidechain
1	X	474	G	Sidechain
1	X	683	A	Sidechain
1	X	739	G	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	57651	0	29049	437	0
2	Y	2598	0	1328	17	0
3	A	1826	0	1885	63	0
4	B	1539	0	1600	67	0
5	C	1506	0	1525	58	0
6	D	1400	0	1481	23	0
7	E	1286	0	1336	9	0
8	F	503	0	520	3	0
9	G	1114	0	1144	64	0
10	H	997	0	1046	23	0
11	I	1067	0	1103	48	0
12	J	1090	0	1125	32	0
13	K	878	0	930	29	0
14	L	779	0	820	17	0
15	M	871	0	894	30	0
16	N	978	0	1020	26	0
17	O	741	0	756	31	0
18	P	1014	0	1096	22	0
19	Q	726	0	753	23	0
20	R	825	0	881	29	0
21	S	1345	0	1372	23	0
22	T	625	0	655	11	0
23	U	552	0	604	28	0
24	V	533	0	558	5	0
25	W	424	0	470	9	0
26	Z	457	0	462	16	0
27	1	53	0	0	0	0
28	2	46	0	0	2	0
29	3	63	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	4	297	0	330	6	0
31	X	30	0	0	0	0
31	Y	5	0	0	0	0
32	X	60	0	66	2	0
All	All	83879	0	54809	994	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 (994) 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)
13:K:52:ILE:CD1	13:K:52:ILE:CG1	1.93	1.47
11:I:62:LYS:NZ	11:I:64:GLY:HA2	1.60	1.15
1:X:1333:G:N2	1:X:1344:C:H41	1.44	1.12
15:M:79:ARG:HG3	15:M:79:ARG:HH11	1.03	1.10
19:Q:29:VAL:HG11	19:Q:38:ILE:HD11	1.35	1.09
1:X:759:C:H6	1:X:759:C:H5''	1.07	1.09
1:X:542:A:C2	1:X:2004:U:H2'	1.93	1.03
11:I:62:LYS:HZ1	11:I:64:GLY:HA2	1.24	1.02
1:X:542:A:H2	1:X:2004:U:H2'	1.24	1.00
4:B:152:LYS:HB2	9:G:106:TYR:HB3	1.39	1.00
1:X:759:C:H5''	1:X:759:C:C6	1.98	0.98
1:X:617:U:H5	1:X:632:A:C2	1.82	0.96
1:X:1919:A:H2	1:X:1926:U:H3	0.99	0.95
1:X:1333:G:H22	1:X:1344:C:N4	1.62	0.95
1:X:1448:A:H61	1:X:1574:A:H61	0.97	0.94
1:X:1466:C:H2'	1:X:1467:U:O4'	1.69	0.91
16:N:93:LYS:HE3	17:O:5:ILE:HD13	1.52	0.91
1:X:2042:A:H5''	5:C:65:GLY:HA2	1.53	0.91
1:X:1333:G:H22	1:X:1344:C:H41	0.94	0.91
1:X:2371:A:H2	1:X:2403:C:H42	1.15	0.91
15:M:79:ARG:HG3	15:M:79:ARG:NH1	1.80	0.91
9:G:33:ILE:HB	9:G:34:PRO:HD3	1.53	0.89
1:X:617:U:H5	1:X:632:A:H2	1.16	0.89
1:X:1277:G:OP1	26:Z:19:ARG:NH2	2.04	0.89
17:O:5:ILE:HD12	17:O:6:GLN:H	1.35	0.88
1:X:1468:A:H5'	1:X:1472:C:N4	1.87	0.88
1:X:1919:A:H2	1:X:1926:U:N3	1.70	0.88
1:X:1542:G:H22	1:X:1562:G:H1	1.15	0.88
1:X:1770:U:H5	1:X:1775:A:N7	1.73	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:4:HIS:HB3	26:Z:5:PRO:HD3	1.56	0.86
1:X:617:U:C5	1:X:632:A:C2	2.64	0.86
4:B:152:LYS:CB	9:G:106:TYR:HB3	2.07	0.85
9:G:67:ARG:HG2	9:G:70:PHE:HA	1.56	0.85
1:X:542:A:H2	1:X:2004:U:C2'	1.88	0.85
5:C:43:ALA:HB1	5:C:86:PRO:HB2	1.59	0.83
1:X:787:A:H2	1:X:800:U:HO2'	1.23	0.82
23:U:48:LYS:HG2	23:U:49:LYS:H	1.42	0.82
1:X:1882:G:N2	1:X:1885:C:H41	1.77	0.82
4:B:131:SER:O	4:B:132:LYS:HG3	1.78	0.81
4:B:54:LYS:HB2	4:B:75:THR:O	1.81	0.81
1:X:971:A:H61	12:J:83:ARG:HH22	1.27	0.81
1:X:1266:G:N7	11:I:32:ARG:NH1	2.29	0.81
1:X:1811:A:H4'	1:X:1812:U:H5''	1.62	0.80
11:I:62:LYS:HZ3	11:I:64:GLY:HA2	1.45	0.80
1:X:1173:G:H21	17:O:88:GLN:HE22	1.29	0.80
9:G:132:PHE:CZ	9:G:145:HIS:HB2	2.16	0.80
1:X:70:A:H5'	1:X:71:A:H3'	1.63	0.79
5:C:137:ALA:HB1	5:C:142:LEU:HB2	1.63	0.79
1:X:689:A:H8	1:X:2052:G:H21	1.31	0.79
11:I:58:ALA:O	11:I:59:ARG:HB2	1.80	0.79
1:X:482:A:H2'	1:X:483:A:O4'	1.83	0.78
1:X:320:A:N3	1:X:340:G:O2'	2.15	0.78
9:G:33:ILE:HB	9:G:34:PRO:CD	2.13	0.78
1:X:215:G:H21	1:X:632:A:H8	1.33	0.77
23:U:22:GLY:HA3	23:U:39:LYS:HD2	1.66	0.77
9:G:100:TYR:HB2	9:G:116:ARG:NH1	1.99	0.77
19:Q:61:LYS:H	19:Q:72:ARG:HA	1.50	0.77
1:X:1448:A:N6	1:X:1574:A:H61	1.79	0.76
1:X:1673:C:H5''	4:B:136:ARG:CD	2.15	0.76
1:X:1333:G:N2	1:X:1344:C:N4	2.25	0.76
1:X:463:C:H42	1:X:467:U:H5	1.30	0.76
1:X:1963:G:O2'	1:X:1965:U:OP2	2.03	0.76
4:B:116:VAL:HG22	4:B:136:ARG:HE	1.50	0.76
4:B:50:GLY:HA3	4:B:75:THR:HG21	1.67	0.75
16:N:66:ASN:ND2	16:N:70:ARG:HH12	1.84	0.75
15:M:79:ARG:HH11	15:M:79:ARG:CG	1.92	0.75
5:C:48:ARG:HB2	5:C:51:VAL:HG22	1.69	0.75
1:X:2617:G:P	4:B:82:ARG:HH22	2.10	0.74
2:Y:46:G:H5'	6:D:92:ARG:HH12	1.53	0.74
13:K:17:ARG:NH1	13:K:20:LEU:HD23	2.01	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2551:A:N7	4:B:145:LYS:HB2	2.04	0.73
1:X:1054:C:H42	1:X:1123:G:H1	1.37	0.73
17:O:10:LYS:HG3	17:O:11:GLN:HG2	1.70	0.72
1:X:1811:A:H5''	3:A:161:THR:HG21	1.71	0.72
3:A:210:GLY:HA2	3:A:213:ARG:HB2	1.71	0.72
3:A:231:HIS:HD2	3:A:233:HIS:H	1.35	0.72
1:X:759:C:H6	1:X:759:C:C5'	1.95	0.71
1:X:1673:C:C5'	4:B:136:ARG:HD2	2.19	0.71
1:X:2042:A:H5''	5:C:65:GLY:CA	2.19	0.71
1:X:2266:A:H2	1:X:2325:A:H62	1.38	0.71
25:W:12:ARG:CG	25:W:12:ARG:HH11	2.02	0.71
25:W:12:ARG:HH11	25:W:12:ARG:HG2	1.56	0.71
3:A:231:HIS:CD2	3:A:233:HIS:H	2.08	0.71
1:X:1675:C:OP1	4:B:134:TRP:NE1	2.24	0.71
1:X:2653:A:O2'	10:H:41:ASN:ND2	2.24	0.71
4:B:116:VAL:HG22	4:B:136:ARG:NE	2.05	0.70
1:X:304:A:H2'	1:X:305:A:H5''	1.71	0.70
18:P:92:VAL:HG13	18:P:126:ILE:HD13	1.73	0.70
23:U:17:SER:HB2	23:U:44:ALA:HA	1.74	0.70
23:U:48:LYS:CG	23:U:49:LYS:H	2.04	0.70
13:K:79:VAL:HA	13:K:83:VAL:HG13	1.74	0.70
1:X:640:C:H4'	1:X:660:G:H21	1.54	0.70
1:X:1030:U:H3	1:X:1153:A:H62	1.38	0.70
1:X:2772:U:H3	1:X:2780:A:H61	1.39	0.70
5:C:38:ARG:HH12	5:C:176:ASN:HD21	1.40	0.69
4:B:16:LYS:HB2	4:B:21:ILE:HD11	1.73	0.69
3:A:36:ALA:HB1	3:A:62:TYR:O	1.91	0.69
9:G:100:TYR:HB2	9:G:116:ARG:HH11	1.58	0.69
1:X:1673:C:H5''	4:B:136:ARG:HD2	1.75	0.69
17:O:66:GLY:O	17:O:87:ARG:NH1	2.26	0.69
23:U:32:ARG:H	23:U:32:ARG:HE	1.41	0.69
1:X:2779:C:H2'	1:X:2780:A:C8	2.28	0.69
1:X:415:A:H61	1:X:436:A:H61	1.41	0.68
1:X:797:A:C5	3:A:229:VAL:HG21	2.28	0.68
4:B:7:THR:HG21	15:M:5:ILE:HD11	1.75	0.68
13:K:11:ASN:OD1	13:K:11:ASN:N	2.26	0.68
1:X:1753:A:O5'	1:X:1753:A:H8	1.76	0.68
1:X:1238:A:H4'	17:O:83:ARG:HG2	1.76	0.68
1:X:1675:C:OP1	4:B:134:TRP:CE2	2.47	0.68
15:M:34:ARG:NH2	15:M:88:VAL:HG13	2.09	0.68
1:X:797:A:N7	3:A:229:VAL:HG21	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2501:U:H5''	1:X:2501:U:H6	1.59	0.67
15:M:27:PHE:HA	15:M:96:ARG:HH21	1.59	0.67
10:H:98:ILE:HG22	10:H:106:ARG:HG3	1.76	0.67
11:I:76:LYS:HB2	11:I:79:GLN:HG2	1.76	0.67
16:N:83:LEU:HD12	16:N:113:SER:HB2	1.77	0.67
16:N:88:ILE:HG13	17:O:49:GLU:HB2	1.76	0.67
1:X:841:G:H2'	1:X:842:A:C8	2.30	0.66
23:U:47:HIS:CD2	23:U:48:LYS:H	2.13	0.66
1:X:38:G:H1	1:X:453:U:H3	1.43	0.66
1:X:652:C:H42	1:X:657:A:H61	1.42	0.66
23:U:48:LYS:HG2	23:U:49:LYS:N	2.10	0.66
1:X:1586:A:H5'	3:A:38:PRO:HG3	1.76	0.66
20:R:22:VAL:HG11	20:R:80:LYS:HZ3	1.60	0.66
1:X:1816:G:O2'	3:A:252:LYS:HG2	1.95	0.66
1:X:1468:A:H5'	1:X:1472:C:H41	1.56	0.66
3:A:89:SER:HB2	3:A:201:HIS:CE1	2.30	0.66
5:C:164:VAL:C	5:C:166:TRP:H	2.04	0.65
12:J:14:PHE:HE1	12:J:90:ALA:HA	1.59	0.65
1:X:219:G:N2	1:X:231:G:H2'	2.12	0.65
1:X:1467:U:H2'	1:X:1468:A:OP1	1.94	0.65
26:Z:4:HIS:HB3	26:Z:5:PRO:CD	2.24	0.65
1:X:1770:U:C5	1:X:1775:A:N7	2.61	0.65
9:G:70:PHE:CB	16:N:64:ARG:HG2	2.27	0.65
1:X:2266:A:H62	1:X:2323:U:H3	1.43	0.65
1:X:1466:C:C2'	1:X:1467:U:O4'	2.44	0.65
6:D:80:ARG:HD3	6:D:83:MET:HB2	1.78	0.65
11:I:28:LYS:HE3	11:I:36:GLY:HA3	1.79	0.65
12:J:40:PRO:HB3	12:J:99:LYS:HD2	1.78	0.65
11:I:28:LYS:HZ1	11:I:37:GLN:H	1.45	0.64
19:Q:60:GLY:H	19:Q:72:ARG:HD3	1.62	0.64
20:R:92:THR:HB	20:R:95:ARG:HH22	1.60	0.64
2:Y:45:C:H2'	6:D:92:ARG:NH1	2.12	0.64
3:A:183:ARG:HH11	3:A:183:ARG:HB3	1.62	0.64
23:U:22:GLY:HA3	23:U:39:LYS:CD	2.27	0.64
3:A:96:HIS:HE1	3:A:100:GLY:HA2	1.62	0.64
11:I:30:ALA:HB3	11:I:34:HIS:CE1	2.32	0.64
1:X:1584:G:H4'	3:A:59:LYS:HB3	1.80	0.64
1:X:2222:U:H2'	1:X:2223:U:C6	2.32	0.64
3:A:172:TYR:HA	3:A:186:HIS:HA	1.80	0.64
1:X:1033:G:N2	1:X:1153:A:C2	2.66	0.63
20:R:105:ARG:HH12	20:R:112:LYS:HA	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:17:ARG:HH11	13:K:20:LEU:HD23	1.60	0.63
9:G:61:ARG:HH11	9:G:66:HIS:H	1.44	0.63
1:X:1673:C:H5''	4:B:136:ARG:HD3	1.79	0.63
1:X:2545:A:H61	10:H:40:GLY:HA3	1.63	0.63
9:G:70:PHE:HB3	16:N:64:ARG:HG2	1.81	0.63
1:X:203:G:H1'	1:X:205:A:H61	1.64	0.63
1:X:1803:G:H21	3:A:46:ARG:HD2	1.64	0.63
15:M:25:PRO:HD2	15:M:91:VAL:HG12	1.81	0.63
5:C:133:PHE:HB2	5:C:160:ALA:HB1	1.81	0.62
9:G:161:GLN:HG2	9:G:165:VAL:HG11	1.80	0.62
1:X:564:U:H2'	1:X:565:A:C8	2.33	0.62
3:A:244:ARG:HB3	3:A:252:LYS:NZ	2.13	0.62
4:B:55:ALA:HB3	4:B:58:LYS:HG3	1.81	0.62
5:C:48:ARG:C	5:C:50:GLN:H	2.07	0.62
1:X:2790:C:O2'	26:Z:43:HIS:HD2	1.82	0.62
11:I:73:GLU:OE1	11:I:101:ARG:HB2	1.98	0.62
1:X:1007:A:H4'	16:N:93:LYS:HB3	1.81	0.62
16:N:66:ASN:HB3	16:N:76:TYR:H	1.64	0.62
1:X:82:G:H1	1:X:100:G:H2'	1.64	0.62
13:K:24:GLN:HB3	13:K:44:LEU:HD22	1.82	0.62
1:X:1033:G:H4'	1:X:1034:U:H5'	1.82	0.62
32:X:2931:1F3:H20	32:X:2931:1F3:H61	1.81	0.61
11:I:32:ARG:HD2	17:O:79:GLN:NE2	2.15	0.61
20:R:46:VAL:HG11	20:R:80:LYS:HD3	1.81	0.61
1:X:617:U:C5	1:X:632:A:H2	2.06	0.61
20:R:92:THR:HB	20:R:95:ARG:NH2	2.16	0.61
1:X:346:C:H2'	1:X:347:C:C6	2.36	0.61
1:X:224:G:OP2	1:X:226:C:N4	2.31	0.60
1:X:2037:A:H2'	26:Z:8:LYS:HE3	1.82	0.60
1:X:971:A:N6	12:J:83:ARG:HH22	1.99	0.60
1:X:774:A:O5'	1:X:774:A:H8	1.85	0.60
1:X:649:G:H1	1:X:660:G:H1	1.49	0.60
1:X:2197:U:H2'	1:X:2198:U:C6	2.37	0.60
4:B:116:VAL:H	4:B:136:ARG:HE	1.49	0.60
1:X:540:G:O6	1:X:2006:G:OP1	2.18	0.60
5:C:48:ARG:C	5:C:50:GLN:N	2.58	0.60
10:H:85:ASP:HB3	15:M:87:LEU:HD12	1.83	0.60
9:G:62:ILE:HG22	9:G:135:LEU:HD21	1.84	0.60
9:G:67:ARG:CG	9:G:70:PHE:HA	2.29	0.60
13:K:11:ASN:OD1	13:K:17:ARG:NH2	2.33	0.60
16:N:66:ASN:HD22	16:N:70:ARG:HH12	1.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2334:C:H1'	22:T:39:ARG:HH21	1.65	0.60
17:O:5:ILE:HD12	17:O:6:GLN:N	2.12	0.60
1:X:2551:A:C8	4:B:144:ARG:HD3	2.37	0.60
1:X:946:U:H2'	1:X:947:C:H6	1.67	0.59
1:X:2362:G:H2'	1:X:2363:G:C8	2.37	0.59
17:O:11:GLN:HE22	17:O:38:LEU:HB3	1.65	0.59
16:N:66:ASN:HB3	16:N:76:TYR:N	2.18	0.59
1:X:2597:G:H21	4:B:150:VAL:HG11	1.66	0.59
5:C:3:GLN:HG2	5:C:116:LYS:HD2	1.84	0.59
20:R:10:HIS:O	20:R:11:ASN:HB2	2.02	0.59
1:X:504:G:H21	18:P:78:ASN:HD21	1.51	0.59
1:X:2713:A:H61	4:B:203:LYS:HG2	1.68	0.59
3:A:244:ARG:HB3	3:A:252:LYS:HZ2	1.68	0.59
1:X:760:U:C6	26:Z:3:LYS:HG3	2.38	0.59
9:G:105:GLY:O	9:G:106:TYR:C	2.42	0.59
1:X:512:A:H4'	18:P:15:LYS:HB3	1.84	0.59
4:B:147:PRO:C	4:B:149:ARG:H	2.11	0.59
4:B:152:LYS:HD2	9:G:106:TYR:H	1.68	0.59
4:B:134:TRP:H	4:B:134:TRP:CD1	2.20	0.58
12:J:92:GLU:HG3	12:J:93:TYR:HD2	1.67	0.58
1:X:827:C:H2'	1:X:828:C:H6	1.68	0.58
1:X:597:U:O4	1:X:683:A:H1'	2.03	0.58
25:W:4:LYS:HG2	25:W:52:GLU:HB3	1.85	0.58
1:X:946:U:H2'	1:X:947:C:C6	2.38	0.58
10:H:78:SER:HA	10:H:91:PHE:O	2.04	0.58
1:X:2371:A:H8	11:I:59:ARG:HG3	1.69	0.58
11:I:81:GLN:HG2	11:I:114:ILE:HG22	1.86	0.58
18:P:13:GLN:O	18:P:16:GLN:HG2	2.02	0.58
29:3:10:ALA:CA	29:3:12:ARG:CA	2.82	0.58
1:X:1050:G:H1	1:X:1127:C:H42	1.51	0.58
1:X:2617:G:P	4:B:82:ARG:NH2	2.76	0.58
1:X:451:A:H2'	1:X:452:G:C8	2.39	0.58
1:X:1468:A:H5'	1:X:1472:C:H42	1.68	0.58
3:A:91:ARG:HG3	3:A:198:ASN:H	1.69	0.58
9:G:61:ARG:NH1	9:G:66:HIS:H	2.02	0.58
3:A:39:LYS:HB2	3:A:62:TYR:HB2	1.86	0.58
4:B:120:TRP:HB3	4:B:155:ARG:HH11	1.69	0.58
20:R:16:PHE:HZ	20:R:46:VAL:HG22	1.69	0.58
1:X:623:G:H3'	1:X:624:A:H5''	1.86	0.57
1:X:1773:C:H1'	1:X:2588:U:H5''	1.85	0.57
1:X:1962:C:H2'	1:X:1963:G:H5'	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:43:ALA:CB	5:C:86:PRO:HB2	2.32	0.57
9:G:158:HIS:HA	9:G:161:GLN:CD	2.29	0.57
5:C:27:LEU:O	5:C:31:VAL:HG23	2.05	0.57
15:M:32:THR:CG2	15:M:91:VAL:HG22	2.34	0.57
18:P:40:LEU:HB3	26:Z:25:LEU:HD13	1.86	0.57
1:X:759:C:C6	1:X:759:C:C5'	2.78	0.57
1:X:1287:A:H2'	1:X:1288:A:H5''	1.86	0.57
12:J:99:LYS:HG3	12:J:100:PRO:HD2	1.87	0.57
1:X:1918:G:H1'	1:X:1947:G:N2	2.20	0.57
9:G:102:ARG:HH11	9:G:102:ARG:HB3	1.70	0.57
11:I:17:LYS:O	11:I:18:ARG:HB2	2.03	0.57
16:N:88:ILE:HG23	17:O:48:GLY:HA3	1.86	0.57
18:P:85:MET:HE2	18:P:130:GLU:HG3	1.87	0.57
1:X:787:A:H2	1:X:800:U:O2'	1.84	0.57
1:X:1811:A:H4'	1:X:1812:U:C5'	2.32	0.57
4:B:131:SER:O	4:B:132:LYS:CG	2.52	0.57
1:X:558:G:O3'	1:X:559:C:H4'	2.03	0.57
1:X:504:G:H4'	18:P:27:VAL:HG13	1.87	0.57
1:X:1882:G:H22	1:X:1885:C:H41	1.49	0.57
18:P:105:ARG:HD3	18:P:119:LYS:HE3	1.86	0.57
19:Q:66:GLY:C	19:Q:68:PHE:H	2.13	0.57
9:G:69:ASP:H	9:G:76:GLN:HE21	1.51	0.56
13:K:10:LEU:HA	13:K:17:ARG:HG2	1.86	0.56
1:X:670:U:H2'	1:X:671:A:C8	2.40	0.56
1:X:954:U:OP2	11:I:38:LYS:HG2	2.04	0.56
2:Y:45:C:H2'	6:D:92:ARG:HH11	1.69	0.56
4:B:16:LYS:HB2	4:B:21:ILE:CD1	2.35	0.56
1:X:673:G:H5'	5:C:93:TYR:CD1	2.41	0.56
6:D:47:SER:HA	6:D:50:ILE:HD12	1.87	0.56
13:K:3:HIS:CG	13:K:5:LYS:HZ3	2.23	0.56
15:M:31:ASP:OD2	15:M:31:ASP:N	2.31	0.56
1:X:1030:U:HO2'	1:X:1032:A:H2	1.52	0.56
1:X:1033:G:H22	1:X:1153:A:H2	1.49	0.56
12:J:15:ARG:HB3	12:J:73:LYS:HZ2	1.70	0.56
17:O:36:LYS:HZ1	17:O:54:TYR:HB3	1.70	0.56
1:X:1113:C:H2'	1:X:1114:A:H8	1.70	0.56
17:O:10:LYS:HD2	17:O:37:ALA:HB3	1.88	0.56
1:X:760:U:O2	1:X:1997:A:H1'	2.06	0.56
5:C:176:ASN:HD22	5:C:179:ASP:H	1.54	0.56
16:N:66:ASN:HB3	16:N:76:TYR:HB2	1.87	0.56
1:X:172:A:H61	1:X:175:C:H3'	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:334:G:H3'	5:C:162:ARG:HE	1.70	0.56
11:I:32:ARG:HD2	17:O:79:GLN:HE22	1.70	0.56
5:C:30:VAL:HG11	5:C:177:VAL:HG21	1.88	0.55
21:S:149:ALA:HA	21:S:152:ILE:HD12	1.87	0.55
4:B:134:TRP:H	4:B:134:TRP:HD1	1.53	0.55
9:G:116:ARG:HD2	9:G:119:LEU:HD12	1.89	0.55
11:I:75:VAL:HG22	11:I:99:VAL:HG11	1.88	0.55
13:K:87:TYR:HE1	13:K:94:TYR:HD2	1.54	0.55
18:P:85:MET:HE1	18:P:129:ALA:HA	1.89	0.55
1:X:1032:A:H8	1:X:1033:G:H5''	1.71	0.55
5:C:95:LEU:HD23	5:C:96:PRO:HD2	1.88	0.55
1:X:1673:C:H5'	4:B:136:ARG:HD2	1.88	0.55
11:I:94:GLU:HA	11:I:97:ARG:HE	1.71	0.55
13:K:7:GLY:O	13:K:8:ARG:HG2	2.06	0.55
13:K:33:ARG:HD3	13:K:112:LEU:HD22	1.89	0.55
20:R:90:LYS:HB2	20:R:108:VAL:HG11	1.88	0.55
23:U:48:LYS:CG	23:U:49:LYS:N	2.70	0.55
1:X:1278:A:H2	1:X:1997:A:H62	1.54	0.55
7:E:164:PHE:HB2	7:E:167:GLU:HB2	1.88	0.55
1:X:2387:U:H2'	1:X:2388:G:H8	1.71	0.55
3:A:218:LYS:HE3	3:A:221:GLN:HB2	1.89	0.55
12:J:44:LYS:HD3	12:J:47:GLN:HE22	1.71	0.55
1:X:1373:G:H22	1:X:2192:U:H3	1.54	0.55
1:X:1448:A:H61	1:X:1574:A:N6	1.82	0.55
1:X:746:G:N7	1:X:774:A:C6	2.75	0.54
18:P:14:ARG:HA	18:P:17:GLN:HG2	1.88	0.54
1:X:1473:U:OP2	1:X:1473:U:H6	1.90	0.54
1:X:2797:G:OP2	13:K:3:HIS:NE2	2.40	0.54
3:A:89:SER:HB2	3:A:201:HIS:HE1	1.72	0.54
3:A:96:HIS:HE1	3:A:100:GLY:CA	2.20	0.54
9:G:104:THR:OG1	9:G:110:LEU:HB3	2.07	0.54
19:Q:38:ILE:O	19:Q:42:ILE:HG22	2.07	0.54
21:S:25:ASN:HB3	21:S:85:MET:HB2	1.88	0.54
1:X:2617:G:OP2	4:B:82:ARG:NH2	2.40	0.54
23:U:29:GLY:C	23:U:31:GLY:H	2.16	0.54
12:J:109:GLY:HA3	21:S:112:LEU:HD21	1.90	0.54
18:P:57:LEU:HA	18:P:60:ILE:HD12	1.89	0.54
2:Y:62:C:H2'	2:Y:63:A:C8	2.42	0.54
12:J:12:LYS:O	12:J:13:GLN:HB2	2.08	0.54
16:N:81:ASN:HD22	16:N:117:ARG:HH21	1.56	0.54
1:X:1790:G:H5'	1:X:1811:A:H61	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:146:GLU:HG3	5:C:185:ARG:HH11	1.72	0.54
1:X:2371:A:C8	11:I:59:ARG:HG3	2.41	0.54
11:I:10:PRO:HA	11:I:14:LYS:HB2	1.89	0.54
1:X:1810:U:H2'	3:A:157:ARG:HD3	1.90	0.54
1:X:2790:C:O2'	26:Z:43:HIS:CD2	2.61	0.53
6:D:92:ARG:HH21	6:D:92:ARG:HB2	1.72	0.53
13:K:3:HIS:HB3	13:K:5:LYS:CE	2.39	0.53
1:X:346:C:H2'	1:X:347:C:H6	1.73	0.53
11:I:117:ALA:HA	11:I:137:GLY:O	2.08	0.53
18:P:57:LEU:HD13	18:P:69:ALA:HA	1.91	0.53
1:X:748:A:H3'	1:X:749:C:H6	1.73	0.53
1:X:2196:U:H2'	1:X:2197:U:O4'	2.08	0.53
2:Y:42:U:H1'	2:Y:47:A:H61	1.73	0.53
25:W:1:MET:HB3	25:W:34:VAL:HG12	1.90	0.53
1:X:1976:U:H4'	4:B:128:SER:OG	2.08	0.53
2:Y:9:G:O2'	14:L:41:GLN:NE2	2.41	0.53
5:C:98:GLN:HA	5:C:101:GLN:HG3	1.90	0.53
10:H:116:ARG:HG3	15:M:38:LYS:NZ	2.22	0.53
15:M:28:ARG:H	15:M:96:ARG:NH2	2.06	0.53
1:X:2306:A:H2'	1:X:2307:A:C8	2.43	0.53
1:X:1467:U:H6	1:X:1467:U:H3'	1.74	0.53
6:D:75:SER:HB2	6:D:79:LEU:HD13	1.90	0.53
1:X:77:C:H42	1:X:106:G:H1	1.55	0.53
1:X:490:A:N3	1:X:492:G:H5''	2.24	0.53
3:A:206:LEU:HA	3:A:211:ARG:HG2	1.90	0.53
4:B:147:PRO:C	4:B:149:ARG:N	2.65	0.53
23:U:49:LYS:HB2	23:U:61:TRP:HA	1.91	0.53
1:X:2766:U:OP1	4:B:69:LYS:HE2	2.09	0.53
2:Y:83:C:N4	2:Y:98:C:N3	2.57	0.53
5:C:148:VAL:HG13	5:C:185:ARG:HB2	1.91	0.53
1:X:172:A:H5''	1:X:173:A:OP2	2.09	0.53
4:B:149:ARG:CZ	9:G:106:TYR:HD1	2.22	0.53
6:D:38:GLU:HB3	6:D:87:ILE:HB	1.91	0.53
7:E:89:LEU:HD23	7:E:162:VAL:HG22	1.91	0.53
9:G:61:ARG:HH11	9:G:65:LYS:HB3	1.73	0.53
9:G:67:ARG:NE	9:G:70:PHE:O	2.40	0.53
15:M:27:PHE:HB3	15:M:93:ILE:HD12	1.89	0.53
1:X:870:C:H4'	22:T:23:VAL:HG21	1.90	0.52
1:X:1519:G:H2'	1:X:1520:G:H8	1.73	0.52
1:X:1943:A:H8	1:X:1943:A:H5''	1.74	0.52
1:X:2272:A:H5''	14:L:15:ARG:HH21	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2811:G:H2'	1:X:2812:A:C8	2.45	0.52
5:C:14:THR:HG22	5:C:15:ILE:H	1.74	0.52
13:K:32:GLY:HA2	13:K:115:LEU:HD12	1.91	0.52
20:R:22:VAL:HG11	20:R:80:LYS:HD2	1.91	0.52
1:X:2241:U:H5	22:T:17:ASN:OD1	1.92	0.52
1:X:2659:C:H5'	4:B:189:PRO:HA	1.91	0.52
3:A:145:LEU:HD23	3:A:155:LEU:HD12	1.92	0.52
9:G:67:ARG:HB3	9:G:70:PHE:HA	1.90	0.52
9:G:103:TYR:CE2	9:G:111:LYS:HB2	2.44	0.52
1:X:793:G:H21	1:X:796:A:H62	1.57	0.52
1:X:823:U:OP1	11:I:32:ARG:NH1	2.42	0.52
20:R:16:PHE:CE2	20:R:80:LYS:HE2	2.43	0.52
1:X:2505:G:H1'	30:4:1:MET:HB2	1.91	0.52
9:G:68:PRO:HD2	9:G:76:GLN:HB3	1.92	0.52
12:J:62:GLY:H	21:S:175:ARG:H	1.57	0.52
21:S:3:LEU:HD11	21:S:33:ALA:H	1.75	0.52
1:X:2484:G:C2	32:X:2931:1F3:H7	2.45	0.52
19:Q:68:PHE:O	19:Q:70:GLY:N	2.42	0.52
20:R:60:PRO:HD2	20:R:62:MET:HB2	1.91	0.52
21:S:3:LEU:HD22	21:S:34:LEU:HB3	1.92	0.52
1:X:666:U:O2'	1:X:667:U:H5''	2.10	0.52
1:X:760:U:C5	26:Z:3:LYS:HG3	2.44	0.52
3:A:226:MET:HG2	3:A:230:ASP:HB2	1.92	0.52
1:X:553:C:H42	1:X:559:C:N4	2.08	0.52
1:X:1850:G:H1'	1:X:1867:A:N6	2.25	0.52
1:X:1909:U:H5'	1:X:1911:A:OP2	2.09	0.52
3:A:108:PRO:HB3	3:A:143:HIS:CE1	2.45	0.51
11:I:97:ARG:O	11:I:98:LEU:HB2	2.10	0.51
23:U:41:VAL:HG23	23:U:42:GLN:H	1.74	0.51
12:J:79:PRO:HD2	12:J:88:LYS:HD2	1.90	0.51
15:M:34:ARG:HB2	15:M:91:VAL:HG23	1.91	0.51
1:X:2387:U:H2'	1:X:2388:G:C8	2.46	0.51
11:I:28:LYS:CE	11:I:36:GLY:HA3	2.40	0.51
26:Z:16:ARG:HD3	26:Z:20:ARG:CZ	2.40	0.51
1:X:1805:G:H1'	3:A:50:THR:HG21	1.92	0.51
1:X:1673:C:C5'	4:B:136:ARG:CD	2.80	0.51
1:X:1071:U:H4'	1:X:1072:U:H3'	1.92	0.51
23:U:49:LYS:HB3	23:U:61:TRP:CE3	2.46	0.51
3:A:243:GLY:C	3:A:244:ARG:HD3	2.36	0.51
4:B:46:ALA:HB2	4:B:82:ARG:HG2	1.92	0.51
4:B:110:GLY:O	13:K:3:HIS:CD2	2.64	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Q:31:PRO:HA	19:Q:76:LYS:HD2	1.92	0.51
1:X:168:A:H2'	1:X:169:C:C6	2.45	0.51
7:E:6:LYS:HB3	7:E:69:ARG:HD2	1.92	0.51
19:Q:12:ILE:HG12	19:Q:13:SER:H	1.74	0.51
1:X:2867:G:O5'	1:X:2867:G:H8	1.93	0.51
10:H:41:ASN:ND2	10:H:41:ASN:H	2.07	0.51
11:I:108:LEU:HD23	11:I:129:ALA:HB1	1.93	0.51
14:L:76:ALA:HB2	14:L:107:ALA:HA	1.91	0.51
1:X:686:C:H5''	5:C:74:VAL:HB	1.93	0.51
1:X:2725:C:H1'	7:E:143:GLN:HG3	1.91	0.51
9:G:100:TYR:CB	9:G:116:ARG:NH1	2.72	0.51
13:K:45:ARG:HB3	13:K:46:PRO:HD3	1.91	0.51
14:L:66:ASP:C	14:L:68:ALA:H	2.19	0.51
1:X:1134:C:H2'	1:X:1135:C:H6	1.76	0.50
1:X:1685:A:H5''	10:H:5:GLN:HG2	1.92	0.50
17:O:57:GLN:H	17:O:97:GLY:CA	2.25	0.50
21:S:3:LEU:HD21	21:S:32:PHE:HB3	1.93	0.50
12:J:78:LYS:HA	12:J:88:LYS:NZ	2.26	0.50
1:X:553:C:H42	1:X:559:C:H42	1.58	0.50
24:V:23:LYS:O	24:V:27:GLU:HG2	2.10	0.50
1:X:2406:C:H5''	1:X:2408:G:OP1	2.11	0.50
1:X:2542:U:O2	1:X:2544:A:H8	1.95	0.50
13:K:49:GLU:O	13:K:52:ILE:HG12	2.12	0.50
21:S:127:PRO:C	21:S:129:ARG:H	2.19	0.50
1:X:1142:G:H5''	9:G:111:LYS:HD2	1.93	0.50
1:X:2355:A:H61	14:L:91:ARG:CZ	2.25	0.50
1:X:2543:A:H5'	1:X:2627:G:H4'	1.93	0.50
9:G:103:TYR:CG	9:G:111:LYS:HA	2.46	0.50
1:X:1699:A:H61	1:X:1723:U:H3	1.58	0.50
3:A:79:VAL:HG21	3:A:111:LEU:HD22	1.94	0.50
13:K:10:LEU:CD2	13:K:17:ARG:HB2	2.42	0.50
17:O:88:GLN:HE21	17:O:88:GLN:HA	1.76	0.50
1:X:1467:U:C2'	1:X:1468:A:OP1	2.58	0.50
1:X:1827:G:H1'	1:X:1914:U:C2	2.47	0.50
2:Y:62:C:H2'	2:Y:63:A:H8	1.76	0.50
4:B:116:VAL:HG13	4:B:136:ARG:HH21	1.75	0.50
5:C:96:PRO:HB2	5:C:99:VAL:HG23	1.93	0.50
5:C:151:VAL:HG11	5:C:175:VAL:HG22	1.93	0.50
10:H:75:VAL:HG12	10:H:118:LEU:HD11	1.94	0.50
1:X:2006:G:H5'	1:X:2596:C:H4'	1.93	0.50
9:G:154:GLU:O	9:G:157:PRO:HD2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1006:C:O2	16:N:61:TRP:HZ2	1.95	0.50
1:X:1032:A:C8	1:X:1033:G:H5''	2.47	0.50
9:G:103:TYR:CZ	9:G:111:LYS:HB2	2.46	0.50
9:G:104:THR:OG1	9:G:105:GLY:N	2.44	0.50
1:X:347:C:H4'	20:R:15:HIS:CD2	2.48	0.49
9:G:157:PRO:C	9:G:159:SER:H	2.20	0.49
11:I:108:LEU:HD13	11:I:120:VAL:HG11	1.94	0.49
1:X:2423:G:P	5:C:62:LYS:HD2	2.52	0.49
11:I:77:LEU:HB2	11:I:111:SER:H	1.77	0.49
1:X:341:A:H2	1:X:1223:G:H2'	1.77	0.49
1:X:1033:G:H5'	9:G:93:LYS:NZ	2.26	0.49
1:X:1805:G:H1'	3:A:50:THR:CG2	2.43	0.49
6:D:33:LYS:HB3	6:D:92:ARG:HG2	1.94	0.49
18:P:103:LEU:HB2	18:P:119:LYS:HB2	1.95	0.49
1:X:494:A:C8	20:R:56:LYS:HD2	2.48	0.49
1:X:1443:G:H2'	1:X:1444:C:C6	2.47	0.49
1:X:2657:G:H2'	1:X:2658:A:O4'	2.13	0.49
18:P:49:SER:O	18:P:51:GLN:N	2.45	0.49
1:X:1219:C:H5''	11:I:7:LYS:HE2	1.93	0.49
1:X:2490:U:H2'	1:X:2491:C:O4'	2.13	0.49
5:C:22:VAL:HG13	5:C:106:MET:HG2	1.93	0.49
9:G:106:TYR:O	9:G:110:LEU:HD12	2.12	0.49
11:I:47:ALA:O	11:I:49:PHE:N	2.41	0.49
16:N:17:VAL:HG11	16:N:36:PHE:HB2	1.94	0.49
17:O:38:LEU:HD23	17:O:47:PHE:HB3	1.95	0.49
26:Z:16:ARG:HD3	26:Z:20:ARG:NH1	2.28	0.49
1:X:418:C:H4'	1:X:418:C:OP2	2.13	0.49
1:X:746:G:N7	1:X:774:A:C5	2.81	0.49
1:X:2178:U:H2'	1:X:2179:C:C6	2.48	0.49
11:I:62:LYS:HZ3	11:I:64:GLY:CA	2.21	0.49
13:K:3:HIS:CG	13:K:5:LYS:NZ	2.80	0.49
16:N:75:ASN:ND2	16:N:78:THR:H	2.10	0.49
1:X:1674:C:H2'	1:X:1675:C:H6	1.78	0.49
3:A:150:GLY:O	3:A:152:GLY:N	2.46	0.49
3:A:161:THR:O	3:A:196:VAL:HG23	2.13	0.49
10:H:83:ARG:NE	10:H:89:ILE:HD11	2.28	0.49
13:K:10:LEU:HD23	13:K:17:ARG:HB2	1.95	0.49
18:P:38:VAL:HG12	18:P:97:VAL:HG21	1.95	0.49
19:Q:71:GLN:HG2	19:Q:72:ARG:N	2.27	0.49
1:X:827:C:H2'	1:X:828:C:C6	2.48	0.48
1:X:969:U:C4	12:J:17:ARG:HB2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:2:LYS:HB2	4:B:200:SER:HB3	1.95	0.48
5:C:45:THR:HG21	5:C:85:GLY:HA3	1.94	0.48
24:V:6:MET:HE3	24:V:56:VAL:HG21	1.94	0.48
1:X:2212:U:H2'	1:X:2213:G:C8	2.48	0.48
14:L:27:LEU:HD23	14:L:44:ASP:HA	1.95	0.48
1:X:224:G:H4'	1:X:399:G:C5	2.48	0.48
12:J:78:LYS:HA	12:J:88:LYS:HZ2	1.77	0.48
14:L:8:ARG:HG3	14:L:9:ARG:H	1.77	0.48
14:L:68:ALA:HB1	14:L:102:ALA:HB3	1.95	0.48
16:N:49:ASP:HA	16:N:52:ASN:HB2	1.95	0.48
24:V:25:LEU:HD21	24:V:47:ARG:HG2	1.95	0.48
1:X:609:U:H5'	11:I:18:ARG:HD3	1.94	0.48
1:X:1329:U:H2'	1:X:1330:G:C8	2.48	0.48
21:S:132:GLN:HE21	21:S:132:GLN:H	1.61	0.48
1:X:791:G:H5'	3:A:48:ARG:HH21	1.77	0.48
10:H:110:VAL:HG23	10:H:129:LEU:HD12	1.94	0.48
15:M:5:ILE:HB	15:M:7:ILE:HG12	1.95	0.48
1:X:517:A:H5''	1:X:518:A:H5'	1.96	0.48
1:X:1833:U:H2'	1:X:1834:G:C8	2.48	0.48
1:X:2362:G:H2'	1:X:2363:G:H8	1.77	0.48
6:D:123:ASP:HB3	6:D:127:ASN:HB2	1.96	0.48
7:E:9:ILE:HD11	7:E:69:ARG:HG2	1.95	0.48
14:L:30:SER:O	14:L:40:ALA:HA	2.13	0.48
14:L:30:SER:HB2	14:L:43:ILE:HD11	1.96	0.48
1:X:2209:G:H4'	23:U:46:LEU:HB2	1.96	0.48
9:G:70:PHE:HB2	16:N:64:ARG:HG2	1.94	0.48
9:G:96:ASP:O	9:G:98:LYS:N	2.46	0.48
11:I:13:ARG:H	11:I:13:ARG:HE	1.62	0.48
14:L:8:ARG:HG3	14:L:9:ARG:N	2.29	0.48
1:X:879:A:H2'	1:X:879:A:N3	2.29	0.48
1:X:1922:U:OP1	1:X:2583:U:O2'	2.29	0.48
20:R:95:ARG:HH12	20:R:107:ALA:H	1.61	0.48
1:X:2307:A:H2'	1:X:2308:A:C8	2.49	0.48
1:X:572:G:N3	16:N:37:GLN:NE2	2.60	0.48
1:X:1753:A:O5'	1:X:1753:A:C8	2.63	0.48
1:X:1777:A:H1'	1:X:1921:A:N6	2.29	0.48
1:X:2522:G:H2'	1:X:2523:G:C8	2.49	0.48
21:S:91:PRO:HG2	21:S:125:PRO:HD2	1.96	0.48
1:X:1169:C:H4'	25:W:28:ILE:O	2.14	0.47
1:X:1468:A:O5'	1:X:1468:A:H8	1.97	0.47
1:X:2774:U:O2'	1:X:2775:U:H5''	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:3:HIS:HB3	13:K:5:LYS:HE2	1.96	0.47
20:R:25:LEU:HD12	20:R:81:VAL:HB	1.96	0.47
23:U:64:ALA:C	23:U:66:ALA:H	2.21	0.47
1:X:88:G:OP2	1:X:89:A:H3'	2.14	0.47
14:L:12:ARG:HA	14:L:92:GLY:O	2.14	0.47
21:S:117:VAL:HB	21:S:168:VAL:HG13	1.97	0.47
1:X:1257:U:H5''	11:I:17:LYS:HG3	1.95	0.47
1:X:1582:A:OP1	3:A:211:ARG:NE	2.43	0.47
1:X:1685:A:N6	1:X:1693:A:H61	2.12	0.47
1:X:2516:U:H2'	1:X:2517:C:C6	2.49	0.47
21:S:3:LEU:HD13	21:S:4:THR:H	1.78	0.47
1:X:1998:A:N3	26:Z:6:VAL:HG23	2.29	0.47
1:X:2779:C:H2'	1:X:2780:A:H8	1.79	0.47
21:S:71:MET:H	21:S:71:MET:HE2	1.79	0.47
23:U:43:ARG:HG2	23:U:44:ALA:N	2.30	0.47
3:A:43:ARG:HH21	3:A:54:ILE:HG13	1.80	0.47
5:C:186:LEU:HG	5:C:188:ILE:HG12	1.95	0.47
9:G:132:PHE:HB2	9:G:145:HIS:CE1	2.49	0.47
17:O:11:GLN:NE2	17:O:38:LEU:HB3	2.30	0.47
1:X:503:G:H2'	1:X:504:G:O4'	2.15	0.47
1:X:681:A:H5''	1:X:681:A:H8	1.79	0.47
5:C:3:GLN:O	5:C:12:GLY:HA3	2.15	0.47
11:I:78:SER:HB3	11:I:112:GLY:HA3	1.96	0.47
1:X:1173:G:H1'	17:O:21:ARG:HD2	1.97	0.47
1:X:2860:C:H2'	1:X:2861:A:O4'	2.14	0.47
2:Y:64:C:H2'	2:Y:65:A:H8	1.79	0.47
20:R:105:ARG:HH22	20:R:112:LYS:CA	2.28	0.47
1:X:922:A:H2'	1:X:923:A:C8	2.50	0.47
1:X:1662:G:H5''	1:X:1663:C:H5'	1.96	0.47
1:X:1787:U:H2'	1:X:1788:C:C6	2.50	0.47
1:X:1854:G:H1	1:X:1863:U:H3	1.62	0.47
1:X:2498:U:H4'	1:X:2499:C:OP1	2.14	0.47
9:G:107:GLN:C	9:G:109:GLY:H	2.23	0.47
13:K:11:ASN:ND2	13:K:12:ARG:HE	2.12	0.47
26:Z:16:ARG:O	26:Z:20:ARG:HD2	2.14	0.47
1:X:203:G:H5'	1:X:234:C:H4'	1.97	0.47
1:X:241:C:H2'	1:X:242:A:H5''	1.96	0.47
1:X:1287:A:C2'	1:X:1288:A:H5''	2.45	0.47
1:X:1342:U:H5''	1:X:1343:C:H5	1.80	0.47
1:X:2343:C:H2'	1:X:2344:G:O4'	2.15	0.47
5:C:112:GLN:HA	5:C:116:LYS:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:57:GLN:H	17:O:97:GLY:HA2	1.79	0.47
20:R:22:VAL:HG13	20:R:81:VAL:O	2.14	0.47
22:T:14:ARG:HG3	22:T:15:ASP:H	1.80	0.47
30:4:2:LYS:HA	30:4:2:LYS:HE2	1.97	0.47
9:G:75:ILE:H	9:G:75:ILE:HG13	1.58	0.47
1:X:341:A:C2	1:X:1223:G:H2'	2.50	0.46
1:X:1367:A:H2'	1:X:1368:G:O4'	2.16	0.46
1:X:1509:A:H8	1:X:1510:A:C8	2.33	0.46
1:X:1788:C:H2'	1:X:1789:U:H6	1.81	0.46
4:B:195:LEU:H	15:M:2:GLN:HG2	1.79	0.46
7:E:17:VAL:HG13	7:E:26:VAL:HG22	1.97	0.46
8:F:77:LEU:HD13	8:F:107:ILE:HG23	1.96	0.46
3:A:67:PHE:HD2	3:A:153:ALA:HB3	1.79	0.46
5:C:158:ARG:HA	5:C:169:VAL:HG21	1.96	0.46
12:J:69:ILE:HG23	12:J:104:MET:HA	1.97	0.46
23:U:47:HIS:HD2	23:U:48:LYS:O	1.97	0.46
4:B:120:TRP:O	4:B:121:ASN:HB2	2.14	0.46
9:G:107:GLN:C	9:G:109:GLY:N	2.72	0.46
20:R:15:HIS:O	20:R:16:PHE:HB3	2.15	0.46
1:X:651:C:H2'	1:X:652:C:H5''	1.98	0.46
1:X:1278:A:H61	1:X:1996:A:H5''	1.80	0.46
1:X:2661:G:O6	1:X:2708:U:H1'	2.16	0.46
14:L:10:LYS:O	14:L:14:ARG:HB2	2.16	0.46
1:X:240:U:H2'	1:X:241:C:O4'	2.15	0.46
1:X:956:A:C4	1:X:2427:A:C2	3.03	0.46
3:A:43:ARG:N	3:A:43:ARG:HD2	2.31	0.46
4:B:131:SER:O	4:B:132:LYS:CB	2.64	0.46
4:B:133:LYS:HB3	4:B:133:LYS:HE2	1.61	0.46
5:C:176:ASN:HB3	5:C:179:ASP:HB2	1.96	0.46
7:E:124:ALA:HB3	7:E:132:ASP:HB2	1.97	0.46
9:G:108:GLY:H	9:G:110:LEU:HG	1.79	0.46
26:Z:33:CYS:SG	26:Z:46:CYS:SG	3.11	0.46
30:4:19:ARG:HB2	30:4:24:LEU:HD13	1.98	0.46
1:X:590:C:H2'	1:X:591:G:C8	2.51	0.46
3:A:252:LYS:HE3	3:A:252:LYS:H	1.80	0.46
5:C:5:ASN:HB2	5:C:10:ASN:HA	1.98	0.46
9:G:36:ASN:O	9:G:38:GLU:N	2.34	0.46
15:M:27:PHE:HB3	15:M:93:ILE:CD1	2.45	0.46
21:S:87:THR:O	21:S:88:TYR:HB3	2.16	0.46
1:X:1845:A:N1	1:X:2070:G:H1'	2.30	0.46
1:X:2266:A:N6	1:X:2323:U:H3	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:90:LEU:HD23	9:G:94:LYS:HA	1.98	0.46
16:N:74:MET:HB3	16:N:75:ASN:H	1.63	0.46
16:N:74:MET:HE2	16:N:78:THR:HG23	1.98	0.46
19:Q:68:PHE:C	19:Q:70:GLY:H	2.21	0.46
1:X:627:A:H2'	1:X:628:A:C8	2.50	0.46
1:X:1882:G:H21	1:X:1885:C:H41	1.62	0.46
3:A:67:PHE:HB3	3:A:153:ALA:H	1.81	0.46
4:B:132:LYS:H	4:B:134:TRP:CD1	2.33	0.46
9:G:162:LYS:N	9:G:163:PRO:HD2	2.31	0.46
10:H:24:VAL:HA	10:H:51:ILE:HG22	1.98	0.46
10:H:27:SER:HB2	10:H:121:ARG:HH22	1.81	0.46
12:J:73:LYS:HB3	12:J:95:VAL:HG12	1.97	0.46
20:R:25:LEU:H	20:R:80:LYS:HA	1.81	0.46
23:U:10:LYS:HD3	23:U:60:VAL:HG21	1.97	0.46
1:X:331:U:H1'	5:C:162:ARG:NH1	2.31	0.46
1:X:1630:A:C2	18:P:114:ALA:HB2	2.51	0.46
1:X:2167:A:H2'	1:X:2168:A:H8	1.80	0.46
5:C:164:VAL:C	5:C:166:TRP:N	2.72	0.46
11:I:57:ILE:HD13	11:I:57:ILE:HA	1.93	0.46
4:B:181:LEU:HD11	15:M:12:LEU:HD23	1.98	0.46
11:I:30:ALA:HB3	11:I:34:HIS:HE1	1.78	0.46
30:4:19:ARG:HD2	30:4:24:LEU:HD22	1.98	0.46
1:X:2795:A:H4'	13:K:5:LYS:HG2	1.97	0.45
4:B:177:ALA:C	4:B:179:GLU:H	2.24	0.45
5:C:45:THR:HB	5:C:86:PRO:O	2.15	0.45
5:C:119:ALA:H	5:C:189:ASP:HA	1.81	0.45
9:G:57:LEU:HD22	9:G:170:PRO:HA	1.98	0.45
12:J:14:PHE:CE1	12:J:90:ALA:HA	2.46	0.45
18:P:25:PHE:C	18:P:25:PHE:CD2	2.94	0.45
1:X:2324:G:N3	1:X:2360:C:H2'	2.32	0.45
1:X:2754:C:H2'	1:X:2755:A:O4'	2.17	0.45
3:A:95:LEU:HD12	3:A:105:ILE:HD13	1.98	0.45
3:A:108:PRO:HB3	3:A:143:HIS:HE1	1.81	0.45
10:H:26:ASN:HD22	10:H:26:ASN:HA	1.41	0.45
1:X:1142:G:OP1	9:G:107:GLN:HB3	2.16	0.45
1:X:1466:C:H2'	1:X:1467:U:C1'	2.46	0.45
1:X:1817:U:O4'	3:A:252:LYS:HD3	2.16	0.45
1:X:2477:C:H6	1:X:2477:C:H5'	1.81	0.45
2:Y:54:U:H4'	2:Y:54:U:OP1	2.17	0.45
5:C:164:VAL:HB	5:C:165:SER:H	1.57	0.45
9:G:67:ARG:CB	9:G:70:PHE:HA	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:28:VAL:HG21	12:J:135:ARG:HA	1.98	0.45
18:P:94:GLU:HG3	18:P:127:ILE:HB	1.99	0.45
1:X:29:U:O5'	1:X:29:U:H6	2.00	0.45
1:X:1468:A:O5'	1:X:1468:A:C8	2.70	0.45
1:X:2397:A:H2'	1:X:2398:U:O4'	2.17	0.45
1:X:2772:U:H2'	1:X:2773:G:C8	2.52	0.45
4:B:14:ILE:HG13	15:M:20:HIS:CE1	2.52	0.45
5:C:102:LEU:O	5:C:106:MET:HB2	2.17	0.45
6:D:40:LEU:HD21	6:D:87:ILE:HD12	1.98	0.45
11:I:108:LEU:HB2	11:I:122:VAL:HG11	1.98	0.45
19:Q:11:VAL:HB	19:Q:26:SER:HB2	1.99	0.45
1:X:227:G:H2'	1:X:228:A:C8	2.52	0.45
1:X:336:A:H2'	1:X:337:G:C8	2.52	0.45
1:X:1467:U:C6	1:X:1467:U:C5'	3.00	0.45
1:X:2074:U:H1'	23:U:48:LYS:HE3	1.97	0.45
19:Q:68:PHE:C	19:Q:70:GLY:N	2.75	0.45
20:R:48:VAL:HG12	20:R:50:GLY:H	1.80	0.45
1:X:1187:A:H2'	1:X:1188:A:C8	2.52	0.45
1:X:1268:U:C2	5:C:66:ASN:HA	2.52	0.45
9:G:132:PHE:CE2	9:G:145:HIS:HB2	2.51	0.45
1:X:1218:C:O4'	11:I:13:ARG:HD3	2.16	0.45
1:X:1467:U:H5	1:X:1468:A:O4'	2.00	0.45
5:C:43:ALA:HB1	5:C:86:PRO:CB	2.41	0.45
6:D:136:LEU:HD11	6:D:143:TYR:HB2	1.99	0.45
8:F:93:LYS:HA	21:S:109:GLN:HG3	1.98	0.45
10:H:2:ILE:HB	10:H:45:ALA:HB3	1.99	0.45
13:K:17:ARG:NH1	13:K:20:LEU:CD2	2.77	0.45
17:O:69:ILE:HG22	17:O:86:HIS:HB3	1.98	0.45
1:X:231:G:H4'	1:X:397:U:H5''	1.98	0.45
1:X:1373:G:H1	1:X:2192:U:H3	1.64	0.45
1:X:2797:G:OP2	13:K:3:HIS:CD2	2.69	0.45
3:A:250:TRP:HB3	3:A:251:GLY:H	1.54	0.45
4:B:146:THR:OG1	4:B:147:PRO:HD3	2.17	0.45
5:C:45:THR:HG22	5:C:47:THR:OG1	2.17	0.45
1:X:1467:U:C5	1:X:1468:A:O4'	2.70	0.45
1:X:1919:A:C2	1:X:1926:U:N3	2.62	0.45
1:X:1022:A:H5''	16:N:77:SER:HB2	2.00	0.44
1:X:1234:C:H2'	1:X:1235:C:H6	1.82	0.44
1:X:1437:A:H2'	1:X:1438:G:H8	1.82	0.44
25:W:3:ILE:HD12	25:W:51:LEU:HD13	1.99	0.44
5:C:146:GLU:HG3	5:C:185:ARG:NH1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:79:ARG:HG2	8:F:84:ILE:HB	1.99	0.44
20:R:30:LYS:C	20:R:32:GLN:H	2.25	0.44
1:X:424:G:H4'	1:X:425:A:O5'	2.18	0.44
1:X:800:U:H5''	1:X:801:A:H5'	1.99	0.44
1:X:814:G:OP1	5:C:50:GLN:HB2	2.18	0.44
1:X:1675:C:OP1	4:B:134:TRP:CD1	2.69	0.44
3:A:147:LEU:HD22	3:A:183:ARG:HH22	1.81	0.44
10:H:116:ARG:HG3	15:M:38:LYS:CE	2.47	0.44
19:Q:29:VAL:HG21	19:Q:38:ILE:HG13	1.98	0.44
23:U:22:GLY:N	23:U:39:LYS:HB2	2.32	0.44
1:X:114:C:O2'	1:X:124:A:N3	2.50	0.44
9:G:132:PHE:CE1	9:G:145:HIS:HB2	2.52	0.44
13:K:66:VAL:HG21	13:K:80:MET:HE1	1.99	0.44
15:M:28:ARG:O	15:M:96:ARG:NH2	2.50	0.44
20:R:45:LYS:HA	20:R:76:LEU:O	2.16	0.44
1:X:2545:A:N6	10:H:40:GLY:HA3	2.31	0.44
7:E:103:LEU:HD11	7:E:131:ILE:HG12	1.99	0.44
12:J:61:ARG:HG2	21:S:175:ARG:HG3	2.00	0.44
13:K:3:HIS:CE1	13:K:5:LYS:HZ3	2.34	0.44
1:X:341:A:O2'	1:X:342:G:H8	2.01	0.44
1:X:553:C:H4'	1:X:554:U:OP1	2.17	0.44
1:X:1190:C:H2'	1:X:1191:G:H8	1.82	0.44
3:A:248:THR:HB	3:A:249:PRO:HD2	2.00	0.44
5:C:74:VAL:HG23	5:C:76:THR:H	1.83	0.44
12:J:11:ARG:HH12	12:J:72:ASP:HB2	1.83	0.44
12:J:92:GLU:HG3	12:J:93:TYR:CD2	2.51	0.44
13:K:46:PRO:O	13:K:50:GLN:HG3	2.18	0.44
1:X:689:A:H8	1:X:2052:G:N2	2.06	0.44
1:X:1030:U:O2'	1:X:1032:A:H2	1.99	0.44
1:X:585:U:H2'	1:X:586:G:C8	2.52	0.44
1:X:673:G:H5'	5:C:93:TYR:CE1	2.52	0.44
1:X:712:A:H2'	1:X:713:G:O4'	2.18	0.44
1:X:1012:A:H2'	1:X:1013:G:O4'	2.17	0.44
1:X:1255:A:H2'	1:X:1256:C:C6	2.53	0.44
17:O:23:GLU:HB2	17:O:91:THR:HG21	1.99	0.44
17:O:72:ARG:HD2	17:O:83:ARG:HH11	1.82	0.44
19:Q:60:GLY:H	19:Q:72:ARG:HH11	1.66	0.44
28:2:26:SER:CA	28:2:27:GLY:CA	2.95	0.44
1:X:649:G:H22	1:X:660:G:N2	2.16	0.44
1:X:1273:G:H2'	1:X:1274:C:O4'	2.18	0.44
1:X:1405:A:N6	19:Q:14:GLU:HG2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2339:A:H4'	11:I:56:LEU:HD21	2.00	0.44
11:I:45:LYS:HD3	11:I:45:LYS:H	1.82	0.44
1:X:1421:U:H2'	1:X:1422:C:O4'	2.18	0.43
1:X:1547:U:H2'	1:X:1548:U:C6	2.53	0.43
1:X:1674:C:H2'	1:X:1675:C:C6	2.53	0.43
1:X:1979:C:H4'	1:X:1980:A:OP1	2.18	0.43
15:M:41:GLU:HG3	15:M:46:ARG:HD2	2.00	0.43
16:N:17:VAL:HG13	16:N:39:LEU:HD12	1.98	0.43
19:Q:62:ARG:O	19:Q:70:GLY:HA3	2.18	0.43
24:V:21:ARG:HG3	24:V:46:LEU:HD22	2.00	0.43
1:X:38:G:H21	5:C:42:THR:HG21	1.83	0.43
1:X:116:A:C8	1:X:117:A:C8	3.06	0.43
1:X:875:G:O2'	2:Y:80:A:N3	2.44	0.43
1:X:1328:C:O2'	1:X:1405:A:N3	2.49	0.43
2:Y:39:C:H2'	14:L:97:HIS:HE1	1.83	0.43
3:A:97:TYR:HE2	3:A:103:ARG:HB2	1.83	0.43
15:M:33:VAL:HG22	15:M:51:GLU:HB2	2.00	0.43
23:U:25:ARG:O	23:U:32:ARG:HD2	2.18	0.43
1:X:748:A:H5''	1:X:749:C:H5	1.84	0.43
1:X:748:A:H5'	1:X:749:C:OP2	2.19	0.43
1:X:1307:U:H5''	1:X:1307:U:H6	1.83	0.43
1:X:2485:U:O2	1:X:2485:U:H2'	2.17	0.43
5:C:6:VAL:HG12	5:C:7:ILE:HG12	1.99	0.43
6:D:35:VAL:HG22	6:D:90:THR:HG23	1.99	0.43
22:T:25:LYS:HB2	22:T:37:LEU:HB3	2.00	0.43
1:X:2310:G:H4'	22:T:43:THR:H	1.83	0.43
18:P:39:ARG:HG3	18:P:97:VAL:HB	2.00	0.43
3:A:188:GLU:H	3:A:188:GLU:HG2	1.54	0.43
4:B:85:ALA:O	4:B:86:PRO:C	2.61	0.43
5:C:118:VAL:HG22	5:C:188:ILE:HD12	2.00	0.43
9:G:103:TYR:O	9:G:107:GLN:NE2	2.51	0.43
1:X:336:A:H2'	1:X:337:G:H8	1.83	0.43
1:X:1765:C:H6	1:X:1765:C:O5'	2.01	0.43
6:D:60:ILE:HB	6:D:99:PHE:HE1	1.83	0.43
1:X:577:U:O5'	1:X:956:A:N6	2.52	0.43
1:X:1574:A:O2'	1:X:1575:C:H3'	2.18	0.43
1:X:2186:G:H2'	1:X:2187:A:C8	2.54	0.43
1:X:2556:A:H5''	1:X:2557:G:H5'	2.00	0.43
11:I:28:LYS:NZ	11:I:36:GLY:CA	2.81	0.43
19:Q:35:LYS:HA	19:Q:38:ILE:HG22	2.00	0.43
1:X:517:A:C5'	1:X:518:A:H5'	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1859:A:H2'	1:X:1860:A:C8	2.54	0.43
1:X:2270:U:H2'	1:X:2271:C:C6	2.53	0.43
1:X:2634:G:O2'	1:X:2643:G:O6	2.32	0.43
2:Y:30:C:H2'	2:Y:31:A:H8	1.84	0.43
4:B:77:ILE:HD13	15:M:3:THR:HG22	2.00	0.43
6:D:65:PRO:HA	6:D:89:VAL:HG13	2.01	0.43
19:Q:28:TRP:CZ3	19:Q:77:LYS:HB2	2.53	0.43
28:2:40:HIS:CA	28:2:41:GLN:CA	2.97	0.43
1:X:890:U:H2'	1:X:891:A:H3'	2.00	0.43
1:X:1329:U:H2'	1:X:1330:G:H8	1.84	0.43
4:B:105:THR:HB	4:B:166:THR:HA	2.01	0.43
10:H:116:ARG:HG3	15:M:38:LYS:HE2	2.01	0.43
15:M:26:ASP:CG	15:M:27:PHE:N	2.76	0.43
20:R:9:HIS:CD2	20:R:9:HIS:H	2.37	0.43
21:S:51:LEU:HD13	21:S:86:VAL:HG21	2.00	0.43
1:X:169:C:O2'	1:X:815:A:N3	2.50	0.43
1:X:460:U:O4	1:X:592:G:H1'	2.18	0.43
1:X:651:C:C2'	1:X:652:C:H5''	2.49	0.43
1:X:1726:C:O2'	1:X:2834:A:N3	2.51	0.43
3:A:108:PRO:HD2	3:A:111:LEU:HB2	2.01	0.43
10:H:113:PRO:HB3	10:H:132:GLU:HB3	2.01	0.43
11:I:102:LYS:O	11:I:104:ARG:N	2.52	0.43
23:U:51:ILE:HG12	23:U:59:THR:HB	2.00	0.43
1:X:577:U:O2'	1:X:579:G:N7	2.48	0.42
1:X:590:C:H2'	1:X:591:G:H8	1.84	0.42
1:X:614:G:C8	11:I:98:LEU:HD21	2.53	0.42
1:X:719:A:H2'	1:X:720:A:O4'	2.18	0.42
2:Y:46:G:H4'	6:D:92:ARG:HH12	1.84	0.42
5:C:170:LEU:HA	5:C:171:PRO:HD3	1.84	0.42
1:X:748:A:H3'	1:X:749:C:C6	2.53	0.42
1:X:1583:A:H3'	3:A:86:PRO:HG3	2.01	0.42
6:D:73:SER:O	6:D:79:LEU:HB3	2.19	0.42
23:U:78:ILE:HG12	23:U:79:GLU:H	1.85	0.42
1:X:216:U:H2'	1:X:217:U:C6	2.55	0.42
1:X:333:A:O4'	1:X:351:A:H1'	2.19	0.42
1:X:533:C:H1'	1:X:563:U:O2'	2.19	0.42
1:X:873:U:H1'	1:X:2247:A:H5''	2.00	0.42
1:X:1193:G:H2'	1:X:1194:U:C6	2.54	0.42
11:I:83:LEU:HD23	11:I:84:GLU:H	1.84	0.42
12:J:26:ASP:HB3	12:J:27:TYR:H	1.61	0.42
17:O:36:LYS:NZ	17:O:54:TYR:HB3	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:103:U:H2'	1:X:104:C:H6	1.82	0.42
1:X:394:U:H2'	1:X:395:G:C8	2.54	0.42
1:X:771:C:O2	1:X:1964:A:H2	2.03	0.42
1:X:1336:G:OP1	18:P:105:ARG:HD2	2.20	0.42
1:X:1483:G:N2	1:X:1541:G:H1'	2.35	0.42
1:X:1779:C:OP1	3:A:222:ARG:NH1	2.52	0.42
1:X:1790:G:H5'	1:X:1811:A:N6	2.34	0.42
1:X:1974:U:H2'	1:X:1975:G:H5''	2.00	0.42
2:Y:78:A:H2'	2:Y:79:U:O4'	2.18	0.42
3:A:231:HIS:HD2	3:A:233:HIS:N	2.11	0.42
19:Q:66:GLY:O	19:Q:68:PHE:N	2.52	0.42
1:X:409:G:H1'	23:U:45:ASN:HD22	1.83	0.42
1:X:1339:U:H5''	1:X:1994:U:H1'	2.01	0.42
1:X:1493:A:H2'	1:X:1494:G:O4'	2.19	0.42
1:X:2015:G:O2'	4:B:145:LYS:HE2	2.20	0.42
5:C:107:ALA:C	5:C:180:ILE:HD11	2.44	0.42
10:H:77:THR:HA	10:H:94:ASN:HB3	2.00	0.42
22:T:23:VAL:HA	22:T:38:VAL:HG23	2.01	0.42
30:4:4:ARG:C	30:4:6:SER:H	2.28	0.42
1:X:1384:G:N2	1:X:1385:C:H41	2.17	0.42
1:X:1687:C:O5'	1:X:1687:C:H6	2.01	0.42
1:X:2784:A:C6	1:X:2866:A:C8	3.07	0.42
3:A:182:LEU:HB2	3:A:268:ARG:O	2.19	0.42
4:B:93:VAL:C	4:B:95:ILE:H	2.27	0.42
1:X:954:U:P	11:I:38:LYS:HG2	2.59	0.42
9:G:98:LYS:HB3	9:G:116:ARG:HB2	2.01	0.42
15:M:33:VAL:HA	15:M:51:GLU:HB2	2.01	0.42
18:P:89:ARG:CZ	18:P:132:GLY:H	2.32	0.42
19:Q:53:ILE:HD13	19:Q:80:VAL:HG13	2.01	0.42
1:X:520:C:O2	1:X:520:C:H2'	2.18	0.42
1:X:542:A:H2	1:X:2004:U:O2'	2.01	0.42
1:X:852:U:H2'	1:X:853:C:C6	2.55	0.42
1:X:1563:U:H2'	1:X:1564:U:C6	2.54	0.42
1:X:1736:C:H2'	1:X:1737:G:H8	1.84	0.42
1:X:2238:G:O4'	1:X:2406:C:H2'	2.20	0.42
3:A:96:HIS:CE1	3:A:100:GLY:HA2	2.47	0.42
10:H:85:ASP:OD2	10:H:87:SER:HB3	2.20	0.42
16:N:88:ILE:CG1	17:O:49:GLU:HB2	2.48	0.42
21:S:3:LEU:HB3	21:S:56:VAL:HA	2.02	0.42
21:S:23:ALA:HA	21:S:83:PHE:O	2.19	0.42
1:X:56:C:H2'	1:X:57:G:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:347:C:H2'	1:X:348:U:C6	2.54	0.42
1:X:616:U:H5'	1:X:617:U:OP2	2.20	0.42
1:X:689:A:H2	1:X:815:A:H61	1.64	0.42
1:X:693:A:H2'	1:X:694:G:C8	2.54	0.42
1:X:830:C:O2'	1:X:852:U:H5''	2.19	0.42
1:X:1441:A:H4'	1:X:1442:C:O5'	2.20	0.42
1:X:2237:C:O2'	1:X:2406:C:OP2	2.37	0.42
12:J:48:ILE:HD12	12:J:71:PRO:HG3	2.01	0.42
23:U:52:ARG:HD3	23:U:62:LEU:HD22	2.01	0.42
1:X:101:A:H5''	1:X:102:C:H5	1.85	0.42
1:X:487:G:H4'	1:X:512:A:N1	2.34	0.42
1:X:1033:G:N2	1:X:1153:A:H2	2.10	0.42
1:X:1128:G:H3'	1:X:1129:A:H5''	2.01	0.42
3:A:43:ARG:N	3:A:43:ARG:CD	2.83	0.42
9:G:33:ILE:O	9:G:69:ASP:OD1	2.38	0.42
12:J:82:THR:HB	12:J:83:ARG:H	1.76	0.42
12:J:88:LYS:HB3	12:J:89:GLY:H	1.59	0.42
19:Q:35:LYS:O	19:Q:38:ILE:HG22	2.20	0.42
1:X:339:U:O4	1:X:343:A:C8	2.73	0.41
1:X:649:G:N2	1:X:660:G:N2	2.68	0.41
1:X:1219:C:H2'	1:X:1220:G:O4'	2.20	0.41
1:X:1644:G:H2'	1:X:1645:U:H6	1.85	0.41
1:X:2445:C:H5''	30:4:6:SER:HB3	2.01	0.41
1:X:2621:G:OP1	9:G:110:LEU:HD22	2.20	0.41
4:B:85:ALA:H	4:B:86:PRO:HD2	1.85	0.41
9:G:36:ASN:C	9:G:38:GLU:H	2.23	0.41
9:G:106:TYR:O	9:G:108:GLY:N	2.48	0.41
10:H:25:LEU:HD11	10:H:52:VAL:HG23	2.01	0.41
1:X:534:U:H4'	1:X:564:U:H4'	2.01	0.41
1:X:679:C:H2'	1:X:680:U:C6	2.55	0.41
3:A:88:ARG:O	3:A:89:SER:CB	2.68	0.41
4:B:5:LEU:HG	4:B:195:LEU:HD11	2.02	0.41
5:C:33:TRP:CD1	5:C:95:LEU:HB2	2.55	0.41
6:D:40:LEU:HB2	6:D:41:GLY:H	1.70	0.41
20:R:10:HIS:O	20:R:11:ASN:CB	2.68	0.41
1:X:1276:U:H1'	26:Z:10:LYS:HG3	2.03	0.41
1:X:2226:A:H2'	1:X:2227:C:C6	2.55	0.41
1:X:2851:G:H4'	15:M:8:ASN:ND2	2.35	0.41
6:D:34:ILE:HG12	6:D:96:MET:HG3	2.02	0.41
21:S:25:ASN:O	21:S:26:LYS:HB3	2.20	0.41
29:3:31:HIS:CA	29:3:32:GLN:CA	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:85:C:H5''	20:R:42:ARG:HH21	1.85	0.41
1:X:1117:G:H2'	1:X:1118:G:H8	1.85	0.41
1:X:1437:A:H2'	1:X:1438:G:C8	2.55	0.41
1:X:1542:G:N2	1:X:1562:G:H1	1.99	0.41
1:X:1790:G:N7	3:A:179:SER:OG	2.50	0.41
1:X:2796:A:H2'	1:X:2797:G:C8	2.55	0.41
3:A:67:PHE:CD2	3:A:153:ALA:HB3	2.56	0.41
6:D:8:TYR:HB2	6:D:173:MET:HE1	2.01	0.41
15:M:55:ILE:O	15:M:103:LYS:O	2.38	0.41
17:O:56:VAL:HG12	17:O:97:GLY:HA3	2.02	0.41
25:W:45:LYS:O	25:W:48:LYS:HB2	2.19	0.41
1:X:71:A:C5	24:V:54:ASN:HB3	2.55	0.41
1:X:922:A:N1	1:X:2256:G:H1'	2.34	0.41
1:X:1658:A:H2'	1:X:1659:G:O4'	2.21	0.41
1:X:1672:A:H3'	1:X:1673:C:C6	2.55	0.41
1:X:2266:A:C2	1:X:2325:A:N6	2.81	0.41
1:X:2736:U:H1'	1:X:2737:A:H5''	2.02	0.41
6:D:114:PHE:HZ	6:D:176:PRO:HG2	1.84	0.41
9:G:50:PRO:HG2	9:G:53:ARG:HG3	2.02	0.41
11:I:62:LYS:CE	11:I:64:GLY:HA2	2.45	0.41
12:J:42:TRP:CD1	12:J:97:VAL:HG12	2.56	0.41
14:L:26:ARG:HG2	14:L:86:GLN:HB3	2.02	0.41
16:N:93:LYS:CE	17:O:5:ILE:HD13	2.37	0.41
17:O:73:LYS:HB2	17:O:82:ARG:HB2	2.03	0.41
1:X:203:G:H1'	1:X:205:A:N6	2.32	0.41
1:X:572:G:H22	1:X:587:A:H2	1.68	0.41
1:X:2292:C:H5''	6:D:88:LYS:HD3	2.01	0.41
4:B:4:ILE:HD13	4:B:28:ALA:HB1	2.02	0.41
4:B:149:ARG:CZ	9:G:106:TYR:CD1	3.02	0.41
21:S:1:MET:HE2	21:S:52:PHE:HB3	2.02	0.41
1:X:829:C:H2'	1:X:830:C:H6	1.86	0.41
1:X:2035:G:N2	4:B:148:GLY:O	2.48	0.41
3:A:169:GLU:HB3	3:A:170:SER:H	1.63	0.41
12:J:36:ILE:HD12	12:J:133:VAL:HG21	2.02	0.41
17:O:5:ILE:CD1	17:O:6:GLN:H	2.19	0.41
1:X:2508:G:H5''	1:X:2509:A:H5''	2.01	0.41
3:A:134:ARG:HG3	3:A:135:PHE:HD2	1.86	0.41
6:D:92:ARG:HB2	6:D:92:ARG:NH2	2.36	0.41
12:J:14:PHE:HE1	12:J:90:ALA:CA	2.28	0.41
20:R:84:VAL:HG23	20:R:88:THR:O	2.20	0.41
20:R:110:SER:OG	20:R:111:GLY:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:59:LEU:HD12	22:T:79:ILE:HD12	2.02	0.41
25:W:12:ARG:HG3	25:W:50:LEU:HD21	2.03	0.41
1:X:1378:A:H2'	1:X:1378:A:N3	2.36	0.41
1:X:2206:C:H1'	3:A:262:LYS:HE3	2.02	0.41
1:X:2552:C:H5''	1:X:2553:G:H5''	2.03	0.41
4:B:5:LEU:HD22	4:B:49:ILE:HG22	2.02	0.41
4:B:121:ASN:O	4:B:122:PHE:C	2.64	0.41
4:B:149:ARG:NH1	9:G:106:TYR:HB2	2.36	0.41
7:E:48:ASP:HB3	7:E:49:GLN:HE21	1.86	0.41
9:G:102:ARG:O	9:G:102:ARG:HG2	2.19	0.41
19:Q:12:ILE:O	19:Q:16:ALA:HB3	2.20	0.41
20:R:7:GLY:HA3	20:R:42:ARG:O	2.20	0.41
21:S:13:LYS:HB2	21:S:18:MET:HB2	2.03	0.41
22:T:14:ARG:HG3	22:T:15:ASP:N	2.36	0.41
22:T:48:GLY:H	22:T:51:VAL:HB	1.86	0.41
23:U:22:GLY:H	23:U:39:LYS:HB2	1.85	0.41
1:X:986:A:O3'	16:N:48:ARG:NH1	2.54	0.41
1:X:1443:G:H2'	1:X:1444:C:H6	1.86	0.41
1:X:1582:A:OP1	3:A:211:ARG:NH2	2.48	0.41
1:X:1997:A:H2'	1:X:1998:A:C8	2.56	0.41
1:X:2407:G:H5''	1:X:2408:G:OP1	2.21	0.41
1:X:2869:U:H2'	1:X:2870:C:C6	2.56	0.41
4:B:67:PHE:CE1	4:B:75:THR:HG22	2.56	0.41
5:C:3:GLN:CG	5:C:116:LYS:HD2	2.51	0.41
5:C:146:GLU:HB3	5:C:184:ASP:HB2	2.03	0.41
10:H:27:SER:HA	10:H:50:ILE:HD12	2.02	0.41
11:I:85:ASP:O	11:I:86:THR:C	2.64	0.41
1:X:654:A:H2'	1:X:654:A:N3	2.36	0.40
4:B:14:ILE:HG22	4:B:21:ILE:HB	2.04	0.40
26:Z:51:TYR:HA	26:Z:55:ARG:HA	2.03	0.40
1:X:88:G:H3'	1:X:89:A:H5''	2.04	0.40
1:X:1623:C:H4'	1:X:1624:A:O5'	2.21	0.40
1:X:2561:G:H5'	1:X:2561:G:H8	1.86	0.40
5:C:166:TRP:HB3	5:C:167:VAL:H	1.63	0.40
15:M:34:ARG:NH2	15:M:90:GLN:C	2.80	0.40
22:T:14:ARG:CG	22:T:15:ASP:H	2.34	0.40
23:U:14:VAL:O	23:U:15:VAL:HG22	2.21	0.40
1:X:10:A:H2'	1:X:11:G:C8	2.56	0.40
1:X:70:A:H5'	1:X:71:A:C3'	2.44	0.40
1:X:1337:G:OP2	18:P:105:ARG:NH1	2.54	0.40
2:Y:58:G:H4'	2:Y:59:A:H5''	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:64:C:H2'	2:Y:65:A:C8	2.56	0.40
3:A:198:ASN:O	3:A:199:ALA:C	2.63	0.40
9:G:162:LYS:N	9:G:163:PRO:CD	2.85	0.40
12:J:79:PRO:CD	12:J:88:LYS:HD2	2.50	0.40
19:Q:89:GLU:HB3	19:Q:90:ALA:H	1.51	0.40
20:R:108:VAL:HB	20:R:109:ALA:H	1.49	0.40
21:S:95:SER:HB3	21:S:119:ASN:HD22	1.86	0.40
23:U:21:ARG:HG2	23:U:40:ARG:HG2	2.04	0.40
1:X:463:C:N4	1:X:467:U:H5	2.08	0.40
1:X:923:A:C5	12:J:12:LYS:HE3	2.57	0.40
5:C:188:ILE:H	5:C:188:ILE:HG13	1.42	0.40
17:O:42:GLY:C	17:O:44:GLN:H	2.30	0.40
1:X:682:G:N3	1:X:682:G:C2'	2.83	0.40
1:X:811:G:OP2	5:C:56:ARG:HG3	2.21	0.40
1:X:1004:A:H5'	17:O:71:ILE:HD11	2.04	0.40
1:X:1016:C:O2'	9:G:56:THR:HG21	2.21	0.40
1:X:1467:U:H3'	1:X:1467:U:C6	2.54	0.40
11:I:72:TYR:CE2	11:I:105:PRO:HB2	2.57	0.40
12:J:54:VAL:CG1	12:J:121:LEU:HB3	2.52	0.40
14:L:15:ARG:HD3	14:L:15:ARG:HA	1.93	0.40
14:L:67:THR:O	14:L:70:ALA:HB3	2.22	0.40
25:W:3:ILE:O	25:W:31:SER:HA	2.22	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 X-ray entries followed by that with respect to entries of similar resolution.

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	A	238/274 (87%)	170 (71%)	39 (16%)	29 (12%)	0	1
4	B	203/211 (96%)	172 (85%)	17 (8%)	14 (7%)	1	7
5	C	195/205 (95%)	131 (67%)	37 (19%)	27 (14%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	D	175/180 (97%)	136 (78%)	26 (15%)	13 (7%)	1	6
7	E	169/185 (91%)	132 (78%)	29 (17%)	8 (5%)	2	14
8	F	69/144 (48%)	59 (86%)	8 (12%)	2 (3%)	3	24
9	G	140/174 (80%)	103 (74%)	23 (16%)	14 (10%)	0	2
10	H	132/134 (98%)	117 (89%)	9 (7%)	6 (4%)	2	15
11	I	139/156 (89%)	79 (57%)	34 (24%)	26 (19%)	0	0
12	J	134/141 (95%)	97 (72%)	26 (19%)	11 (8%)	1	4
13	K	111/116 (96%)	96 (86%)	7 (6%)	8 (7%)	1	6
14	L	102/114 (90%)	72 (71%)	20 (20%)	10 (10%)	0	3
15	M	106/166 (64%)	95 (90%)	7 (7%)	4 (4%)	2	18
16	N	115/118 (98%)	101 (88%)	10 (9%)	4 (4%)	3	20
17	O	92/100 (92%)	66 (72%)	13 (14%)	13 (14%)	0	1
18	P	125/134 (93%)	114 (91%)	5 (4%)	6 (5%)	2	14
19	Q	91/95 (96%)	59 (65%)	19 (21%)	13 (14%)	0	1
20	R	108/115 (94%)	66 (61%)	23 (21%)	19 (18%)	0	0
21	S	173/237 (73%)	145 (84%)	20 (12%)	8 (5%)	2	15
22	T	82/91 (90%)	64 (78%)	9 (11%)	9 (11%)	0	2
23	U	70/81 (86%)	39 (56%)	17 (24%)	14 (20%)	0	0
24	V	64/67 (96%)	57 (89%)	3 (5%)	4 (6%)	1	8
25	W	53/55 (96%)	49 (92%)	4 (8%)	0	100	100
26	Z	56/60 (93%)	47 (84%)	5 (9%)	4 (7%)	1	6
30	4	35/37 (95%)	28 (80%)	5 (14%)	2 (6%)	1	11
All	All	2977/3390 (88%)	2294 (77%)	415 (14%)	268 (9%)	0	3

All (268) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	60	ARG
3	A	151	LYS
3	A	170	SER
3	A	187	SER
3	A	199	ALA
3	A	248	THR
3	A	250	TRP

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Mol	Chain	Res	Type
3	A	271	VAL
4	B	76	ARG
4	B	86	PRO
4	B	122	PHE
5	C	20	PRO
5	C	64	THR
5	C	67	ALA
5	C	129	LYS
5	C	163	ASN
5	C	164	VAL
5	C	172	VAL
7	E	126	PRO
9	G	33	ILE
9	G	37	ASP
9	G	67	ARG
9	G	91	THR
9	G	97	ASP
9	G	104	THR
9	G	107	GLN
9	G	158	HIS
9	G	170	PRO
10	H	27	SER
10	H	29	ILE
11	I	17	LYS
11	I	18	ARG
11	I	37	GLN
11	I	39	SER
11	I	48	PHE
11	I	56	LEU
11	I	59	ARG
11	I	62	LYS
11	I	86	THR
11	I	98	LEU
11	I	103	ASN
12	J	13	GLN
12	J	26	ASP
12	J	83	ARG
12	J	89	GLY
12	J	136	GLU
13	K	6	ALA
13	K	8	ARG
13	K	95	THR

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Mol	Chain	Res	Type
14	L	21	THR
14	L	40	ALA
14	L	68	ALA
14	L	95	LYS
15	M	27	PHE
15	M	29	PRO
16	N	7	GLY
16	N	8	ILE
16	N	92	ARG
17	O	10	LYS
17	O	31	ASP
17	O	97	GLY
18	P	9	ARG
18	P	50	VAL
19	Q	12	ILE
19	Q	13	SER
19	Q	67	ARG
19	Q	69	ILE
19	Q	84	GLU
20	R	11	ASN
20	R	62	MET
20	R	66	GLN
20	R	82	ALA
20	R	98	ILE
20	R	108	VAL
21	S	26	LYS
21	S	156	GLU
22	T	15	ASP
22	T	19	LYS
23	U	15	VAL
23	U	27	ASP
23	U	47	HIS
23	U	48	LYS
23	U	60	VAL
24	V	2	LYS
26	Z	4	HIS
3	A	54	ILE
3	A	98	ALA
3	A	197	GLY
3	A	198	ASN
3	A	220	HIS
4	B	121	ASN

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Mol	Chain	Res	Type
4	B	123	ALA
4	B	132	LYS
4	B	135	HIS
4	B	146	THR
5	C	9	GLN
5	C	22	VAL
5	C	55	GLY
5	C	60	GLY
5	C	121	ASP
5	C	125	ILE
5	C	127	ASP
5	C	165	SER
5	C	195	ILE
6	D	4	LEU
6	D	9	ASN
6	D	121	ALA
6	D	124	GLY
7	E	19	ALA
10	H	31	GLY
11	I	19	VAL
11	I	47	ALA
11	I	49	PHE
12	J	17	ARG
12	J	21	ASP
12	J	60	ARG
12	J	80	ALA
13	K	14	SER
13	K	92	GLY
14	L	45	ASP
14	L	92	GLY
15	M	41	GLU
16	N	87	ASN
17	O	30	GLY
17	O	48	GLY
19	Q	6	ILE
19	Q	63	LYS
20	R	5	SER
20	R	6	ALA
20	R	7	GLY
20	R	60	PRO
21	S	57	GLU
21	S	88	TYR

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Mol	Chain	Res	Type
21	S	91	PRO
22	T	5	LYS
22	T	14	ARG
23	U	19	ILE
23	U	30	VAL
23	U	41	VAL
23	U	55	GLY
23	U	78	ILE
26	Z	36	CYS
26	Z	37	HIS
30	4	20	HIS
3	A	109	GLU
3	A	206	LEU
3	A	219	PRO
3	A	249	PRO
3	A	263	ARG
4	B	73	ALA
4	B	74	PRO
5	C	15	ILE
5	C	173	ALA
5	C	189	ASP
5	C	190	ALA
6	D	5	LYS
6	D	122	PHE
7	E	55	PRO
7	E	119	ALA
7	E	173	ALA
9	G	34	PRO
9	G	68	PRO
10	H	41	ASN
11	I	54	SER
11	I	65	PHE
11	I	82	ASP
13	K	93	GLY
14	L	52	ALA
14	L	96	TYR
17	O	43	GLU
18	P	20	LEU
18	P	80	LEU
18	P	131	LYS
19	Q	61	LYS
19	Q	86	GLN

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Mol	Chain	Res	Type
19	Q	87	SER
20	R	49	GLU
20	R	85	ASP
20	R	87	GLU
20	R	110	SER
24	V	3	PRO
24	V	10	GLN
26	Z	53	ASP
3	A	35	GLU
3	A	45	ASN
3	A	89	SER
3	A	127	LEU
3	A	254	THR
3	A	269	PHE
4	B	85	ALA
4	B	137	ARG
5	C	13	ARG
6	D	10	ASP
6	D	40	LEU
6	D	52	LYS
7	E	7	GLN
7	E	13	SER
10	H	5	GLN
11	I	28	LYS
11	I	88	PHE
11	I	115	SER
13	K	4	GLY
14	L	53	ALA
17	O	9	GLY
17	O	28	GLU
17	O	29	ALA
17	O	49	GLU
19	Q	3	HIS
19	Q	4	TYR
20	R	16	PHE
20	R	63	THR
21	S	58	GLY
21	S	125	PRO
22	T	74	LYS
23	U	34	THR
23	U	42	GLN
23	U	76	LYS

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Mol	Chain	Res	Type
3	A	55	GLY
3	A	244	ARG
3	A	270	ILE
5	C	196	VAL
6	D	21	GLY
6	D	42	SER
6	D	71	LYS
6	D	81	GLN
7	E	59	GLN
9	G	165	VAL
10	H	42	LYS
11	I	8	PRO
11	I	9	THR
11	I	131	LYS
12	J	11	ARG
12	J	84	MET
13	K	10	LEU
14	L	33	ARG
17	O	7	THR
17	O	36	LYS
19	Q	5	ASP
20	R	31	GLY
20	R	111	GLY
22	T	7	VAL
23	U	12	ASN
4	B	17	ASN
4	B	75	THR
5	C	11	GLY
5	C	126	ALA
8	F	143	ASN
11	I	29	THR
17	O	11	GLN
21	S	6	LYS
30	4	5	SER
9	G	163	PRO
11	I	68	VAL
24	V	64	GLY
3	A	47	GLY
3	A	252	LYS
5	C	41	GLY
5	C	103	GLY
8	F	118	GLY

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Mol	Chain	Res	Type
18	P	132	GLY
20	R	64	ASN
22	T	13	GLY
22	T	73	GLY
5	C	171	PRO
9	G	157	PRO
11	I	57	ILE
15	M	74	GLY
22	T	27	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	A	185/215 (86%)	139 (75%)	46 (25%)	0	2
4	B	155/157 (99%)	129 (83%)	26 (17%)	1	8
5	C	157/163 (96%)	123 (78%)	34 (22%)	1	4
6	D	153/156 (98%)	128 (84%)	25 (16%)	2	9
7	E	136/144 (94%)	115 (85%)	21 (15%)	2	11
8	F	51/107 (48%)	46 (90%)	5 (10%)	6	27
9	G	118/146 (81%)	92 (78%)	26 (22%)	1	4
10	H	103/103 (100%)	76 (74%)	27 (26%)	0	1
11	I	108/121 (89%)	71 (66%)	37 (34%)	0	0
12	J	110/115 (96%)	90 (82%)	20 (18%)	1	7
13	K	90/93 (97%)	73 (81%)	17 (19%)	1	6
14	L	74/82 (90%)	54 (73%)	20 (27%)	0	1
15	M	94/134 (70%)	69 (73%)	25 (27%)	0	1
16	N	96/97 (99%)	79 (82%)	17 (18%)	1	8
17	O	75/79 (95%)	61 (81%)	14 (19%)	1	6
18	P	109/115 (95%)	93 (85%)	16 (15%)	2	12
19	Q	75/76 (99%)	60 (80%)	15 (20%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	R	91/96 (95%)	70 (77%)	21 (23%)	0	3
21	S	149/192 (78%)	123 (83%)	26 (17%)	1	8
22	T	62/67 (92%)	54 (87%)	8 (13%)	3	17
23	U	57/66 (86%)	31 (54%)	26 (46%)	0	0
24	V	54/55 (98%)	46 (85%)	8 (15%)	2	12
25	W	48/48 (100%)	36 (75%)	12 (25%)	0	2
26	Z	51/53 (96%)	36 (71%)	15 (29%)	0	1
30	4	35/35 (100%)	29 (83%)	6 (17%)	1	8
All	All	2436/2715 (90%)	1923 (79%)	513 (21%)	1	5

All (513) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	33	LEU
3	A	34	THR
3	A	35	GLU
3	A	39	LYS
3	A	40	THR
3	A	43	ARG
3	A	44	ASN
3	A	48	ARG
3	A	49	ILE
3	A	50	THR
3	A	52	ARG
3	A	54	ILE
3	A	61	LEU
3	A	65	ILE
3	A	68	LYS
3	A	69	ARG
3	A	92	ILE
3	A	105	ILE
3	A	111	LEU
3	A	117	VAL
3	A	131	LEU
3	A	133	LEU
3	A	141	VAL
3	A	151	LYS
3	A	157	ARG
3	A	164	GLN

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Mol	Chain	Res	Type
3	A	169	GLU
3	A	175	VAL
3	A	183	ARG
3	A	196	VAL
3	A	203	ASN
3	A	208	LYS
3	A	214	TRP
3	A	215	LEU
3	A	217	ARG
3	A	218	LYS
3	A	226	MET
3	A	240	THR
3	A	244	ARG
3	A	247	VAL
3	A	248	THR
3	A	252	LYS
3	A	259	THR
3	A	260	ARG
3	A	262	LYS
3	A	270	ILE
4	B	5	LEU
4	B	14	ILE
4	B	34	VAL
4	B	37	LYS
4	B	49	ILE
4	B	58	LYS
4	B	69	LYS
4	B	72	VAL
4	B	77	ILE
4	B	79	ARG
4	B	82	ARG
4	B	87	ASP
4	B	105	THR
4	B	111	LYS
4	B	117	MET
4	B	119	ARG
4	B	131	SER
4	B	133	LYS
4	B	134	TRP
4	B	137	ARG
4	B	149	ARG
4	B	150	VAL

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Mol	Chain	Res	Type
4	B	168	GLN
4	B	179	GLU
4	B	184	VAL
4	B	203	LYS
5	C	5	ASN
5	C	10	ASN
5	C	13	ARG
5	C	14	THR
5	C	15	ILE
5	C	31	VAL
5	C	40	ARG
5	C	45	THR
5	C	48	ARG
5	C	51	VAL
5	C	53	LYS
5	C	74	VAL
5	C	90	SER
5	C	95	LEU
5	C	99	VAL
5	C	101	GLN
5	C	102	LEU
5	C	106	MET
5	C	117	LEU
5	C	124	ASP
5	C	129	LYS
5	C	134	ILE
5	C	138	LYS
5	C	143	ASP
5	C	148	VAL
5	C	150	LEU
5	C	151	VAL
5	C	154	ASP
5	C	155	GLU
5	C	164	VAL
5	C	166	TRP
5	C	175	VAL
5	C	180	ILE
5	C	188	ILE
6	D	40	LEU
6	D	45	GLU
6	D	57	LEU
6	D	60	ILE

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Mol	Chain	Res	Type
6	D	67	ILE
6	D	74	ILE
6	D	79	LEU
6	D	80	ARG
6	D	89	VAL
6	D	92	ARG
6	D	104	ILE
6	D	106	ILE
6	D	112	ARG
6	D	117	ILE
6	D	125	ARG
6	D	129	ASN
6	D	130	LEU
6	D	136	LEU
6	D	140	GLU
6	D	142	THR
6	D	145	MET
6	D	150	ARG
6	D	152	MET
6	D	163	ASP
6	D	175	LEU
7	E	11	VAL
7	E	33	LEU
7	E	35	VAL
7	E	38	ASN
7	E	41	LEU
7	E	42	THR
7	E	49	GLN
7	E	50	LEU
7	E	64	LEU
7	E	67	LEU
7	E	68	THR
7	E	69	ARG
7	E	90	ARG
7	E	92	VAL
7	E	113	VAL
7	E	114	ILE
7	E	116	GLU
7	E	121	VAL
7	E	140	LEU
7	E	143	GLN
7	E	152	ARG

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Mol	Chain	Res	Type
8	F	74	MET
8	F	78	ILE
8	F	84	ILE
8	F	111	LYS
8	F	115	LEU
9	G	30	LYS
9	G	31	THR
9	G	37	ASP
9	G	38	GLU
9	G	53	ARG
9	G	56	THR
9	G	62	ILE
9	G	63	ARG
9	G	67	ARG
9	G	71	THR
9	G	75	ILE
9	G	93	LYS
9	G	95	LEU
9	G	102	ARG
9	G	104	THR
9	G	113	GLU
9	G	126	VAL
9	G	127	ILE
9	G	132	PHE
9	G	145	HIS
9	G	146	THR
9	G	154	GLU
9	G	165	VAL
9	G	166	LEU
9	G	168	THR
9	G	169	GLN
10	H	3	MET
10	H	8	LEU
10	H	18	GLU
10	H	20	MET
10	H	23	ARG
10	H	25	LEU
10	H	26	ASN
10	H	27	SER
10	H	29	ILE
10	H	32	LYS
10	H	36	THR

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Mol	Chain	Res	Type
10	H	41	ASN
10	H	47	VAL
10	H	81	ILE
10	H	83	ARG
10	H	87	SER
10	H	89	ILE
10	H	94	ASN
10	H	99	ILE
10	H	106	ARG
10	H	114	VAL
10	H	116	ARG
10	H	117	GLU
10	H	120	ASP
10	H	122	ARG
10	H	126	ILE
10	H	129	LEU
11	I	7	LYS
11	I	12	SER
11	I	13	ARG
11	I	19	VAL
11	I	27	ASP
11	I	29	THR
11	I	34	HIS
11	I	35	LYS
11	I	38	LYS
11	I	39	SER
11	I	45	LYS
11	I	53	ARG
11	I	56	LEU
11	I	57	ILE
11	I	59	ARG
11	I	60	LEU
11	I	62	LYS
11	I	65	PHE
11	I	74	VAL
11	I	77	LEU
11	I	78	SER
11	I	83	LEU
11	I	84	GLU
11	I	85	ASP
11	I	98	LEU
11	I	99	VAL

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Mol	Chain	Res	Type
11	I	101	ARG
11	I	103	ASN
11	I	106	VAL
11	I	107	LYS
11	I	108	LEU
11	I	113	GLU
11	I	114	ILE
11	I	120	VAL
11	I	123	ASP
11	I	130	ILE
11	I	142	LEU
12	J	7	ARG
12	J	8	THR
12	J	10	PHE
12	J	11	ARG
12	J	19	THR
12	J	21	ASP
12	J	26	ASP
12	J	49	GLU
12	J	61	ARG
12	J	64	LYS
12	J	75	VAL
12	J	86	LYS
12	J	88	LYS
12	J	91	VAL
12	J	95	VAL
12	J	113	GLU
12	J	128	ILE
12	J	132	MET
12	J	133	VAL
12	J	134	LYS
13	K	5	LYS
13	K	10	LEU
13	K	11	ASN
13	K	12	ARG
13	K	17	ARG
13	K	28	LEU
13	K	34	ILE
13	K	35	GLN
13	K	45	ARG
13	K	51	LEU
13	K	53	THR

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Mol	Chain	Res	Type
13	K	73	LYS
13	K	83	VAL
13	K	94	TYR
13	K	95	THR
13	K	102	THR
13	K	109	THR
14	L	10	LYS
14	L	11	LEU
14	L	13	THR
14	L	18	ARG
14	L	31	VAL
14	L	33	ARG
14	L	36	LYS
14	L	37	HIS
14	L	38	ILE
14	L	43	ILE
14	L	45	ASP
14	L	47	ARG
14	L	64	LYS
14	L	66	ASP
14	L	71	VAL
14	L	89	PHE
14	L	91	ARG
14	L	93	SER
14	L	95	LYS
14	L	108	ARG
15	M	2	GLN
15	M	5	ILE
15	M	6	LYS
15	M	12	LEU
15	M	13	LEU
15	M	16	ILE
15	M	19	ASP
15	M	22	ARG
15	M	31	ASP
15	M	33	VAL
15	M	34	ARG
15	M	37	THR
15	M	51	GLU
15	M	54	VAL
15	M	57	ILE
15	M	63	ARG

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Mol	Chain	Res	Type
15	M	68	VAL
15	M	75	GLU
15	M	79	ARG
15	M	88	VAL
15	M	89	ASN
15	M	91	VAL
15	M	92	THR
15	M	96	ARG
15	M	99	VAL
16	N	5	LYS
16	N	8	ILE
16	N	15	LYS
16	N	16	LYS
16	N	18	LEU
16	N	19	LYS
16	N	22	LYS
16	N	30	LYS
16	N	60	LEU
16	N	71	LEU
16	N	78	THR
16	N	88	ILE
16	N	90	LEU
16	N	91	ASN
16	N	93	LYS
16	N	97	ASP
16	N	104	GLU
17	O	7	THR
17	O	14	VAL
17	O	22	VAL
17	O	26	GLN
17	O	28	GLU
17	O	40	VAL
17	O	46	VAL
17	O	55	THR
17	O	56	VAL
17	O	65	ARG
17	O	69	ILE
17	O	71	ILE
17	O	88	GLN
17	O	96	LEU
18	P	16	GLN
18	P	19	LYS

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Mol	Chain	Res	Type
18	P	25	PHE
18	P	32	ARG
18	P	42	VAL
18	P	45	ILE
18	P	50	VAL
18	P	84	GLU
18	P	89	ARG
18	P	116	ILE
18	P	118	LYS
18	P	119	LYS
18	P	124	ILE
18	P	125	THR
18	P	126	ILE
18	P	133	ASN
19	Q	6	ILE
19	Q	7	LEU
19	Q	12	ILE
19	Q	14	GLU
19	Q	15	LYS
19	Q	26	SER
19	Q	37	GLU
19	Q	38	ILE
19	Q	42	ILE
19	Q	61	LYS
19	Q	65	VAL
19	Q	69	ILE
19	Q	71	GLN
19	Q	79	ILE
19	Q	84	GLU
20	R	11	ASN
20	R	17	LYS
20	R	18	LYS
20	R	23	ILE
20	R	25	LEU
20	R	32	GLN
20	R	37	LEU
20	R	38	LEU
20	R	42	ARG
20	R	44	GLN
20	R	71	GLN
20	R	73	GLU
20	R	79	SER

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Mol	Chain	Res	Type
20	R	80	LYS
20	R	95	ARG
20	R	97	GLN
20	R	98	ILE
20	R	104	VAL
20	R	105	ARG
20	R	106	VAL
20	R	108	VAL
21	S	3	LEU
21	S	13	LYS
21	S	18	MET
21	S	22	VAL
21	S	26	LYS
21	S	29	ASN
21	S	51	LEU
21	S	60	GLU
21	S	67	LYS
21	S	71	MET
21	S	86	VAL
21	S	88	TYR
21	S	90	GLU
21	S	100	THR
21	S	120	LEU
21	S	122	ILE
21	S	123	VAL
21	S	128	ARG
21	S	132	GLN
21	S	134	LEU
21	S	135	VAL
21	S	154	LEU
21	S	159	THR
21	S	160	LEU
21	S	166	LEU
21	S	169	VAL
22	T	16	SER
22	T	17	ASN
22	T	37	LEU
22	T	38	VAL
22	T	62	LEU
22	T	63	SER
22	T	64	ASP
22	T	85	GLN

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Mol	Chain	Res	Type
23	U	8	THR
23	U	10	LYS
23	U	11	LYS
23	U	13	LEU
23	U	14	VAL
23	U	17	SER
23	U	19	ILE
23	U	20	ARG
23	U	21	ARG
23	U	23	LYS
23	U	32	ARG
23	U	34	THR
23	U	35	THR
23	U	37	ILE
23	U	42	GLN
23	U	43	ARG
23	U	46	LEU
23	U	49	LYS
23	U	54	ASN
23	U	56	GLN
23	U	62	LEU
23	U	63	SER
23	U	65	ASN
23	U	67	LEU
23	U	69	THR
23	U	76	LYS
24	V	1	MET
24	V	13	ASP
24	V	14	PHE
24	V	19	ASP
24	V	25	LEU
24	V	31	GLN
24	V	49	GLU
24	V	65	GLU
25	W	2	LYS
25	W	4	LYS
25	W	9	VAL
25	W	10	ILE
25	W	12	ARG
25	W	15	ASN
25	W	30	ASP
25	W	32	ARG

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Mol	Chain	Res	Type
25	W	34	VAL
25	W	36	ASP
25	W	45	LYS
25	W	46	THR
26	Z	4	HIS
26	Z	6	VAL
26	Z	8	LYS
26	Z	11	THR
26	Z	18	MET
26	Z	19	ARG
26	Z	20	ARG
26	Z	31	THR
26	Z	35	GLN
26	Z	40	LYS
26	Z	41	LEU
26	Z	53	ASP
26	Z	56	GLN
26	Z	57	VAL
26	Z	58	LEU
30	4	2	LYS
30	4	4	ARG
30	4	9	LYS
30	4	14	CYS
30	4	25	VAL
30	4	30	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	87	ASN
3	A	96	HIS
3	A	166	GLN
3	A	201	HIS
3	A	231	HIS
4	B	17	ASN
4	B	114	GLN
5	C	5	ASN
5	C	61	GLN
5	C	66	ASN
5	C	176	ASN
6	D	9	ASN
6	D	19	GLN

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Mol	Chain	Res	Type
6	D	37	ASN
6	D	135	GLN
7	E	38	ASN
7	E	49	GLN
7	E	143	GLN
8	F	92	ASN
9	G	40	ASN
9	G	73	ASN
9	G	76	GLN
9	G	87	GLN
9	G	164	GLN
10	H	26	ASN
10	H	41	ASN
10	H	101	ASN
11	I	37	GLN
11	I	66	ASN
11	I	79	GLN
12	J	46	ASN
14	L	41	GLN
14	L	86	GLN
14	L	97	HIS
15	M	20	HIS
15	M	48	GLN
15	M	58	ASN
16	N	31	GLN
16	N	41	ASN
16	N	52	ASN
16	N	66	ASN
16	N	75	ASN
16	N	81	ASN
16	N	91	ASN
17	O	79	GLN
17	O	88	GLN
18	P	13	GLN
18	P	16	GLN
18	P	17	GLN
18	P	78	ASN
18	P	81	HIS
19	Q	71	GLN
20	R	15	HIS
20	R	77	HIS
20	R	97	GLN

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Mol	Chain	Res	Type
21	S	80	HIS
21	S	99	HIS
21	S	105	GLN
21	S	119	ASN
21	S	132	GLN
22	T	35	ASN
22	T	71	ASN
23	U	42	GLN
23	U	47	HIS
24	V	31	GLN
25	W	15	ASN
25	W	49	HIS
26	Z	29	ASN
26	Z	43	HIS
26	Z	44	HIS
26	Z	56	GLN
30	4	13	ASN
30	4	36	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2681/2880 (93%)	664 (24%)	238 (8%)
2	Y	121/123 (98%)	28 (23%)	5 (4%)
All	All	2802/3003 (93%)	692 (24%)	243 (8%)

All (692) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	2	G
1	X	3	U
1	X	4	C
1	X	13	A
1	X	14	A
1	X	33	C
1	X	34	U
1	X	45	C
1	X	48	A
1	X	49	U
1	X	50	G
1	X	51	A

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Mol	Chain	Res	Type
1	X	54	G
1	X	62	U
1	X	63	A
1	X	69	G
1	X	70	A
1	X	71	A
1	X	72	A
1	X	74	G
1	X	75	C
1	X	82	G
1	X	83	A
1	X	84	G
1	X	87	G
1	X	89	A
1	X	90	G
1	X	91	A
1	X	95	G
1	X	97	U
1	X	98	U
1	X	99	U
1	X	100	G
1	X	101	A
1	X	105	G
1	X	107	G
1	X	116	A
1	X	117	A
1	X	118	U
1	X	123	A
1	X	124	A
1	X	125	A
1	X	127	C
1	X	129	A
1	X	136	A
1	X	138	G
1	X	143	A
1	X	147	G
1	X	149	A
1	X	154	U
1	X	155	G
1	X	157	G
1	X	158	A
1	X	173	A

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Mol	Chain	Res	Type
1	X	176	A
1	X	177	U
1	X	192	G
1	X	193	A
1	X	194	G
1	X	199	A
1	X	204	A
1	X	206	U
1	X	207	U
1	X	210	A
1	X	222	G
1	X	225	G
1	X	229	G
1	X	242	A
1	X	243	G
1	X	245	C
1	X	246	C
1	X	248	A
1	X	304	A
1	X	305	A
1	X	306	G
1	X	310	A
1	X	312	G
1	X	313	U
1	X	321	A
1	X	322	A
1	X	323	G
1	X	328	A
1	X	333	A
1	X	335	A
1	X	340	G
1	X	341	A
1	X	342	G
1	X	343	A
1	X	344	G
1	X	358	C
1	X	388	G
1	X	393	U
1	X	397	U
1	X	399	G
1	X	400	U
1	X	409	G

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Mol	Chain	Res	Type
1	X	414	A
1	X	417	C
1	X	418	C
1	X	419	G
1	X	424	G
1	X	425	A
1	X	441	A
1	X	456	C
1	X	458	G
1	X	459	A
1	X	461	A
1	X	463	C
1	X	466	A
1	X	467	U
1	X	468	A
1	X	469	G
1	X	486	U
1	X	491	A
1	X	492	G
1	X	504	G
1	X	513	A
1	X	514	G
1	X	515	A
1	X	518	A
1	X	519	C
1	X	520	C
1	X	522	G
1	X	523	A
1	X	539	A
1	X	540	G
1	X	541	C
1	X	542	A
1	X	543	G
1	X	554	U
1	X	555	U
1	X	556	A
1	X	557	U
1	X	558	G
1	X	559	C
1	X	560	G
1	X	572	G
1	X	577	U

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Mol	Chain	Res	Type
1	X	580	A
1	X	581	A
1	X	582	G
1	X	583	C
1	X	584	A
1	X	595	A
1	X	600	G
1	X	613	A
1	X	614	G
1	X	617	U
1	X	623	G
1	X	624	A
1	X	625	A
1	X	626	A
1	X	627	A
1	X	628	A
1	X	633	G
1	X	638	A
1	X	645	G
1	X	648	A
1	X	649	G
1	X	651	C
1	X	652	C
1	X	654	A
1	X	655	A
1	X	656	U
1	X	657	A
1	X	664	C
1	X	665	A
1	X	667	U
1	X	669	G
1	X	682	G
1	X	683	A
1	X	684	C
1	X	698	A
1	X	699	G
1	X	700	C
1	X	728	G
1	X	729	A
1	X	730	C
1	X	731	A
1	X	732	G

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Mol	Chain	Res	Type
1	X	736	G
1	X	743	A
1	X	747	A
1	X	751	G
1	X	752	G
1	X	753	U
1	X	758	G
1	X	759	C
1	X	760	U
1	X	777	A
1	X	778	G
1	X	780	U
1	X	781	G
1	X	788	G
1	X	789	G
1	X	790	A
1	X	795	A
1	X	797	A
1	X	798	G
1	X	802	A
1	X	803	C
1	X	804	C
1	X	805	G
1	X	806	A
1	X	814	G
1	X	815	A
1	X	818	G
1	X	825	C
1	X	832	A
1	X	840	U
1	X	841	G
1	X	842	A
1	X	843	G
1	X	858	G
1	X	859	U
1	X	872	G
1	X	879	A
1	X	880	C
1	X	922	A
1	X	926	C
1	X	931	G
1	X	938	G

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Mol	Chain	Res	Type
1	X	939	C
1	X	940	G
1	X	944	A
1	X	952	A
1	X	955	G
1	X	956	A
1	X	957	G
1	X	969	U
1	X	970	A
1	X	972	C
1	X	973	U
1	X	985	G
1	X	994	A
1	X	995	A
1	X	1000	G
1	X	1001	A
1	X	1006	C
1	X	1007	A
1	X	1014	G
1	X	1016	C
1	X	1022	A
1	X	1023	U
1	X	1024	G
1	X	1028	G
1	X	1031	C
1	X	1032	A
1	X	1033	G
1	X	1034	U
1	X	1036	G
1	X	1037	U
1	X	1038	U
1	X	1044	U
1	X	1051	U
1	X	1053	G
1	X	1054	C
1	X	1055	A
1	X	1056	U
1	X	1057	A
1	X	1058	G
1	X	1060	C
1	X	1068	A
1	X	1073	G

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Mol	Chain	Res	Type
1	X	1077	U
1	X	1078	A
1	X	1081	A
1	X	1082	G
1	X	1086	C
1	X	1087	C
1	X	1090	C
1	X	1094	C
1	X	1097	A
1	X	1098	G
1	X	1099	A
1	X	1100	G
1	X	1108	U
1	X	1115	C
1	X	1120	C
1	X	1121	G
1	X	1122	A
1	X	1123	G
1	X	1128	G
1	X	1129	A
1	X	1130	U
1	X	1139	A
1	X	1140	A
1	X	1141	U
1	X	1142	G
1	X	1143	A
1	X	1145	C
1	X	1146	G
1	X	1152	C
1	X	1153	A
1	X	1154	A
1	X	1155	G
1	X	1161	U
1	X	1183	C
1	X	1185	C
1	X	1187	A
1	X	1188	A
1	X	1189	G
1	X	1191	G
1	X	1192	A
1	X	1194	U
1	X	1195	U

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Mol	Chain	Res	Type
1	X	1223	G
1	X	1224	A
1	X	1233	A
1	X	1234	C
1	X	1240	G
1	X	1250	A
1	X	1251	G
1	X	1265	G
1	X	1266	G
1	X	1269	G
1	X	1275	A
1	X	1281	A
1	X	1284	G
1	X	1285	A
1	X	1286	U
1	X	1288	A
1	X	1289	A
1	X	1297	A
1	X	1299	A
1	X	1300	A
1	X	1302	C
1	X	1307	U
1	X	1313	U
1	X	1314	A
1	X	1315	A
1	X	1319	C
1	X	1334	A
1	X	1339	U
1	X	1341	G
1	X	1342	U
1	X	1353	A
1	X	1354	A
1	X	1357	U
1	X	1358	C
1	X	1365	U
1	X	1378	A
1	X	1381	G
1	X	1392	U
1	X	1399	C
1	X	1404	C
1	X	1410	U
1	X	1411	C

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Mol	Chain	Res	Type
1	X	1412	C
1	X	1413	U
1	X	1428	G
1	X	1429	A
1	X	1430	G
1	X	1432	G
1	X	1433	A
1	X	1434	U
1	X	1441	A
1	X	1442	C
1	X	1443	G
1	X	1451	C
1	X	1460	G
1	X	1465	G
1	X	1467	U
1	X	1468	A
1	X	1469	U
1	X	1470	G
1	X	1473	U
1	X	1474	A
1	X	1475	U
1	X	1476	G
1	X	1482	U
1	X	1490	U
1	X	1496	G
1	X	1497	C
1	X	1498	G
1	X	1505	U
1	X	1506	C
1	X	1508	G
1	X	1509	A
1	X	1513	U
1	X	1514	C
1	X	1523	A
1	X	1524	C
1	X	1525	A
1	X	1528	C
1	X	1531	C
1	X	1532	A
1	X	1533	G
1	X	1545	G
1	X	1551	U

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Mol	Chain	Res	Type
1	X	1552	C
1	X	1553	G
1	X	1554	G
1	X	1561	A
1	X	1562	G
1	X	1563	U
1	X	1571	G
1	X	1574	A
1	X	1575	C
1	X	1576	G
1	X	1581	C
1	X	1582	A
1	X	1583	A
1	X	1584	G
1	X	1585	A
1	X	1594	U
1	X	1600	U
1	X	1601	U
1	X	1602	G
1	X	1603	A
1	X	1607	A
1	X	1608	U
1	X	1613	G
1	X	1624	A
1	X	1625	A
1	X	1626	A
1	X	1631	C
1	X	1632	A
1	X	1634	A
1	X	1648	C
1	X	1657	A
1	X	1665	C
1	X	1669	A
1	X	1691	G
1	X	1710	U
1	X	1711	C
1	X	1712	G
1	X	1713	G
1	X	1716	G
1	X	1717	A
1	X	1732	U
1	X	1733	U

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Mol	Chain	Res	Type
1	X	1734	C
1	X	1747	G
1	X	1754	G
1	X	1755	G
1	X	1764	A
1	X	1773	C
1	X	1776	A
1	X	1790	G
1	X	1791	C
1	X	1792	C
1	X	1793	A
1	X	1799	A
1	X	1806	G
1	X	1807	A
1	X	1808	C
1	X	1812	U
1	X	1813	A
1	X	1820	G
1	X	1821	A
1	X	1825	C
1	X	1831	G
1	X	1840	A
1	X	1850	G
1	X	1861	G
1	X	1863	U
1	X	1867	A
1	X	1874	G
1	X	1882	G
1	X	1883	A
1	X	1884	A
1	X	1886	G
1	X	1910	A
1	X	1912	G
1	X	1913	G
1	X	1919	A
1	X	1920	A
1	X	1921	A
1	X	1923	U
1	X	1939	U
1	X	1943	A
1	X	1947	G
1	X	1950	C

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Mol	Chain	Res	Type
1	X	1953	A
1	X	1954	A
1	X	1955	G
1	X	1958	G
1	X	1963	G
1	X	1964	A
1	X	1965	U
1	X	1975	G
1	X	1976	U
1	X	1980	A
1	X	2006	G
1	X	2010	G
1	X	2014	A
1	X	2015	G
1	X	2018	G
1	X	2019	C
1	X	2026	C
1	X	2035	G
1	X	2038	C
1	X	2039	G
1	X	2044	G
1	X	2045	A
1	X	2046	C
1	X	2052	G
1	X	2076	G
1	X	2079	A
1	X	2088	U
1	X	2089	C
1	X	2171	U
1	X	2180	U
1	X	2181	A
1	X	2189	A
1	X	2190	A
1	X	2191	A
1	X	2195	C
1	X	2196	U
1	X	2197	U
1	X	2198	U
1	X	2199	C
1	X	2204	A
1	X	2205	C
1	X	2217	G

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Mol	Chain	Res	Type
1	X	2218	G
1	X	2222	U
1	X	2247	A
1	X	2262	C
1	X	2265	A
1	X	2266	A
1	X	2283	G
1	X	2284	U
1	X	2285	U
1	X	2286	G
1	X	2287	G
1	X	2288	A
1	X	2291	U
1	X	2294	U
1	X	2295	C
1	X	2298	U
1	X	2299	A
1	X	2300	G
1	X	2301	A
1	X	2305	C
1	X	2306	A
1	X	2313	G
1	X	2314	A
1	X	2315	A
1	X	2324	G
1	X	2325	A
1	X	2326	C
1	X	2329	C
1	X	2339	A
1	X	2351	G
1	X	2355	A
1	X	2358	C
1	X	2362	G
1	X	2363	G
1	X	2364	C
1	X	2370	G
1	X	2371	A
1	X	2375	G
1	X	2381	A
1	X	2382	C
1	X	2385	U
1	X	2389	G

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Mol	Chain	Res	Type
1	X	2396	C
1	X	2401	A
1	X	2402	U
1	X	2404	A
1	X	2405	A
1	X	2408	G
1	X	2409	A
1	X	2410	U
1	X	2420	C
1	X	2426	G
1	X	2427	A
1	X	2447	G
1	X	2448	A
1	X	2449	G
1	X	2452	U
1	X	2455	A
1	X	2463	G
1	X	2470	U
1	X	2475	C
1	X	2477	C
1	X	2478	C
1	X	2480	C
1	X	2481	G
1	X	2482	A
1	X	2483	U
1	X	2484	G
1	X	2485	U
1	X	2498	U
1	X	2499	C
1	X	2501	U
1	X	2504	G
1	X	2508	G
1	X	2514	G
1	X	2543	A
1	X	2545	A
1	X	2546	G
1	X	2548	G
1	X	2552	C
1	X	2553	G
1	X	2557	G
1	X	2561	G
1	X	2565	C

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Mol	Chain	Res	Type
1	X	2580	C
1	X	2581	A
1	X	2582	G
1	X	2588	U
1	X	2589	C
1	X	2591	C
1	X	2594	U
1	X	2600	A
1	X	2609	G
1	X	2611	A
1	X	2613	A
1	X	2615	U
1	X	2616	U
1	X	2620	G
1	X	2633	A
1	X	2640	G
1	X	2642	G
1	X	2650	G
1	X	2668	U
1	X	2692	A
1	X	2693	U
1	X	2694	G
1	X	2705	A
1	X	2706	U
1	X	2707	G
1	X	2713	A
1	X	2728	A
1	X	2731	G
1	X	2732	C
1	X	2736	U
1	X	2737	A
1	X	2738	A
1	X	2744	A
1	X	2745	A
1	X	2758	A
1	X	2759	U
1	X	2770	A
1	X	2771	C
1	X	2774	U
1	X	2775	U
1	X	2776	U
1	X	2777	A

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Mol	Chain	Res	Type
1	X	2778	U
1	X	2779	C
1	X	2780	A
1	X	2782	G
1	X	2795	A
1	X	2796	A
1	X	2807	U
1	X	2808	U
1	X	2809	A
1	X	2810	A
1	X	2811	G
1	X	2824	C
1	X	2825	A
1	X	2843	A
1	X	2846	G
1	X	2847	G
1	X	2848	A
1	X	2849	C
1	X	2854	G
1	X	2855	C
1	X	2859	U
1	X	2868	G
2	Y	14	C
2	Y	15	A
2	Y	17	A
2	Y	18	G
2	Y	26	G
2	Y	27	A
2	Y	28	A
2	Y	37	C
2	Y	39	C
2	Y	42	U
2	Y	43	G
2	Y	44	C
2	Y	46	G
2	Y	47	A
2	Y	53	G
2	Y	54	U
2	Y	56	G
2	Y	58	G
2	Y	59	A
2	Y	69	G

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Mol	Chain	Res	Type
2	Y	75	A
2	Y	76	U
2	Y	99	G
2	Y	102	A
2	Y	108	G
2	Y	112	A
2	Y	115	G
2	Y	123	U

All (243) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	3	U
1	X	13	A
1	X	33	C
1	X	48	A
1	X	50	G
1	X	62	U
1	X	70	A
1	X	71	A
1	X	74	G
1	X	82	G
1	X	83	A
1	X	89	A
1	X	98	U
1	X	99	U
1	X	100	G
1	X	117	A
1	X	124	A
1	X	154	U
1	X	176	A
1	X	190	A
1	X	198	A
1	X	199	A
1	X	242	A
1	X	312	G
1	X	321	A
1	X	322	A
1	X	328	A
1	X	332	C
1	X	334	G
1	X	341	A

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Mol	Chain	Res	Type
1	X	342	G
1	X	343	A
1	X	396	U
1	X	399	G
1	X	416	U
1	X	417	C
1	X	418	C
1	X	458	G
1	X	466	A
1	X	467	U
1	X	469	G
1	X	490	A
1	X	504	G
1	X	513	A
1	X	522	G
1	X	537	C
1	X	539	A
1	X	542	A
1	X	553	C
1	X	554	U
1	X	557	U
1	X	558	G
1	X	559	C
1	X	580	A
1	X	583	C
1	X	648	A
1	X	655	A
1	X	664	C
1	X	668	A
1	X	672	C
1	X	682	G
1	X	683	A
1	X	698	A
1	X	751	G
1	X	758	G
1	X	759	C
1	X	761	G
1	X	777	A
1	X	780	U
1	X	788	G
1	X	789	G
1	X	796	A

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Mol	Chain	Res	Type
1	X	802	A
1	X	803	C
1	X	806	A
1	X	813	A
1	X	814	G
1	X	824	U
1	X	841	G
1	X	842	A
1	X	858	G
1	X	859	U
1	X	872	G
1	X	878	C
1	X	879	A
1	X	939	C
1	X	940	G
1	X	955	G
1	X	969	U
1	X	972	C
1	X	994	A
1	X	1000	G
1	X	1031	C
1	X	1033	G
1	X	1037	U
1	X	1053	G
1	X	1055	A
1	X	1056	U
1	X	1072	U
1	X	1081	A
1	X	1086	C
1	X	1096	A
1	X	1099	A
1	X	1120	C
1	X	1121	G
1	X	1139	A
1	X	1141	U
1	X	1152	C
1	X	1154	A
1	X	1182	U
1	X	1186	G
1	X	1191	G
1	X	1194	U
1	X	1223	G

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Mol	Chain	Res	Type
1	X	1233	A
1	X	1249	G
1	X	1288	A
1	X	1299	A
1	X	1313	U
1	X	1314	A
1	X	1353	A
1	X	1357	U
1	X	1378	A
1	X	1409	U
1	X	1410	U
1	X	1412	C
1	X	1432	G
1	X	1433	A
1	X	1441	A
1	X	1442	C
1	X	1459	U
1	X	1473	U
1	X	1475	U
1	X	1496	G
1	X	1505	U
1	X	1513	U
1	X	1531	C
1	X	1541	G
1	X	1552	C
1	X	1561	A
1	X	1562	G
1	X	1574	A
1	X	1575	C
1	X	1581	C
1	X	1583	A
1	X	1601	U
1	X	1607	A
1	X	1618	U
1	X	1624	A
1	X	1625	A
1	X	1631	C
1	X	1680	U
1	X	1710	U
1	X	1711	C
1	X	1716	G
1	X	1732	U

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Mol	Chain	Res	Type
1	X	1775	A
1	X	1777	A
1	X	1790	G
1	X	1791	C
1	X	1799	A
1	X	1800	A
1	X	1807	A
1	X	1810	U
1	X	1811	A
1	X	1812	U
1	X	1820	G
1	X	1865	C
1	X	1872	A
1	X	1882	G
1	X	1883	A
1	X	1909	U
1	X	1920	A
1	X	1921	A
1	X	1938	U
1	X	1953	A
1	X	1963	G
1	X	1975	G
1	X	1980	A
1	X	2014	A
1	X	2018	G
1	X	2075	U
1	X	2083	G
1	X	2088	U
1	X	2180	U
1	X	2181	A
1	X	2189	A
1	X	2198	U
1	X	2204	A
1	X	2217	G
1	X	2228	U
1	X	2254	C
1	X	2258	G
1	X	2261	G
1	X	2298	U
1	X	2299	A
1	X	2305	C
1	X	2312	A

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Mol	Chain	Res	Type
1	X	2314	A
1	X	2324	G
1	X	2354	G
1	X	2361	G
1	X	2370	G
1	X	2381	A
1	X	2401	A
1	X	2404	A
1	X	2409	A
1	X	2447	G
1	X	2477	C
1	X	2482	A
1	X	2497	A
1	X	2498	U
1	X	2560	G
1	X	2564	U
1	X	2580	C
1	X	2608	A
1	X	2615	U
1	X	2624	G
1	X	2660	C
1	X	2669	C
1	X	2691	C
1	X	2705	A
1	X	2706	U
1	X	2731	G
1	X	2736	U
1	X	2744	A
1	X	2758	A
1	X	2769	C
1	X	2770	A
1	X	2778	U
1	X	2807	U
1	X	2808	U
1	X	2810	A
1	X	2824	C
1	X	2846	G
1	X	2848	A
1	X	2854	G
1	X	2867	G
2	Y	26	G
2	Y	46	G

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Mol	Chain	Res	Type
2	Y	54	U
2	Y	58	G
2	Y	86	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 35 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
32	1F3	X	2931	-	63,64,64	1.32	7 (11%)	83,96,96	1.87	19 (22%)

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
32	1F3	X	2931	-	-	9/78/119/119	0/5/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	X	2931	1F3	C50-C49	4.20	1.50	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	X	2931	1F3	C48-C47	-4.14	1.51	1.54
32	X	2931	1F3	C50-N45	3.34	1.44	1.38
32	X	2931	1F3	O17-C5	-3.08	1.43	1.47
32	X	2931	1F3	C47-N45	-2.63	1.43	1.47
32	X	2931	1F3	C41-N40	2.53	1.37	1.33
32	X	2931	1F3	C51-C47	-2.02	1.48	1.51

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	X	2931	1F3	C59-C58-N57	-5.48	106.72	114.95
32	X	2931	1F3	C28-O20-C8	-4.96	107.83	116.26
32	X	2931	1F3	C23-C6-C5	-4.94	108.42	115.23
32	X	2931	1F3	O60-C58-N57	3.83	128.31	123.06
32	X	2931	1F3	C47-N45-C50	3.52	113.23	109.61
32	X	2931	1F3	O29-C30-C38	-3.41	100.49	106.88
32	X	2931	1F3	C48-C47-N45	3.02	105.56	103.17
32	X	2931	1F3	C27-C12-C13	-3.00	106.28	113.00
32	X	2931	1F3	C48-C47-C51	-2.89	108.03	113.91
32	X	2931	1F3	C4-N40-C41	-2.66	108.91	112.39
32	X	2931	1F3	C30-C31-C32	-2.62	105.99	110.46
32	X	2931	1F3	C47-C48-C49	2.36	107.55	103.04
32	X	2931	1F3	O43-C13-C12	-2.35	103.66	107.84
32	X	2931	1F3	C9-C7-C2	2.30	119.85	116.10
32	X	2931	1F3	O10-C6-C23	2.30	111.63	107.36
32	X	2931	1F3	C52-C51-C47	-2.27	116.42	120.76
32	X	2931	1F3	O10-C11-O26	2.25	128.02	123.95
32	X	2931	1F3	C48-C49-C50	-2.17	106.31	111.47
32	X	2931	1F3	C16-C1-C3	-2.10	104.41	108.09

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	X	2931	1F3	C59-C58-N57-C54
32	X	2931	1F3	O60-C58-N57-C54
32	X	2931	1F3	C16-C1-C4-N40
32	X	2931	1F3	O20-C8-C9-C7
32	X	2931	1F3	C3-C2-C7-C9
32	X	2931	1F3	C14-C8-C9-C7
32	X	2931	1F3	O20-C8-C9-C22
32	X	2931	1F3	C3-C1-C4-N40

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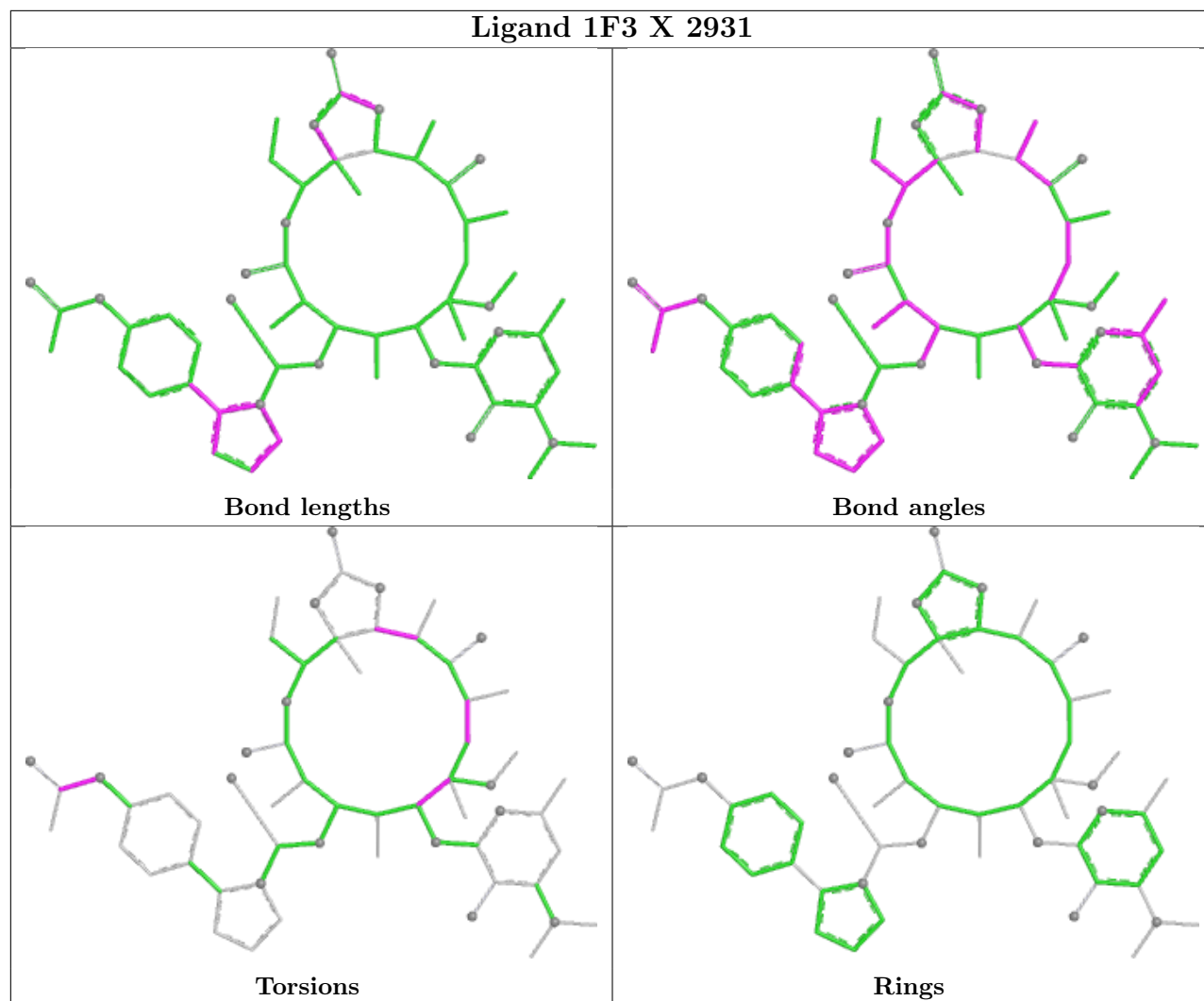
Mol	Chain	Res	Type	Atoms
32	X	2931	1F3	C16-C1-C4-C5

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	X	2931	1F3	2	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	X	2686/2880 (93%)	0.16	128 (4%) 36 25	43, 87, 194, 279	0
2	Y	122/123 (99%)	0.62	8 (6%) 26 17	82, 129, 165, 187	0
3	A	240/274 (87%)	1.19	48 (20%) 3 3	63, 107, 137, 156	0
4	B	205/211 (97%)	0.15	10 (4%) 36 25	38, 68, 99, 145	0
5	C	197/205 (96%)	1.26	47 (23%) 2 2	55, 107, 150, 178	0
6	D	177/180 (98%)	1.17	39 (22%) 3 2	148, 178, 210, 216	0
7	E	171/185 (92%)	0.82	22 (12%) 9 6	98, 139, 178, 188	0
8	F	71/144 (49%)	2.39	35 (49%) 0 1	221, 234, 251, 259	0
9	G	142/174 (81%)	1.18	36 (25%) 2 2	65, 89, 137, 149	0
10	H	134/134 (100%)	-0.10	2 (1%) 71 56	49, 62, 88, 110	0
11	I	141/156 (90%)	2.11	54 (38%) 1 1	54, 120, 171, 195	0
12	J	136/141 (96%)	0.91	25 (18%) 4 3	83, 106, 147, 172	0
13	K	113/116 (97%)	0.01	7 (6%) 28 18	37, 53, 71, 99	0
14	L	104/114 (91%)	1.41	30 (28%) 1 1	91, 122, 149, 166	0
15	M	108/166 (65%)	0.13	6 (5%) 31 20	44, 64, 106, 128	0
16	N	117/118 (99%)	0.54	11 (9%) 15 11	54, 86, 124, 152	0
17	O	94/100 (94%)	0.80	13 (13%) 8 5	67, 106, 146, 160	0
18	P	127/134 (94%)	-0.15	1 (0%) 82 70	48, 64, 103, 143	0
19	Q	93/95 (97%)	1.00	18 (19%) 4 3	69, 101, 156, 193	0
20	R	110/115 (95%)	1.46	31 (28%) 1 1	84, 113, 170, 173	0
21	S	175/237 (73%)	0.93	25 (14%) 7 5	119, 154, 178, 190	0
22	T	84/91 (92%)	1.06	16 (19%) 4 3	72, 103, 176, 195	0
23	U	72/81 (88%)	1.97	29 (40%) 1 1	86, 122, 146, 182	0
24	V	66/67 (98%)	0.71	8 (12%) 10 7	88, 128, 213, 230	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9	
25	W	55/55 (100%)	0.14	0	100	100	76, 96, 123, 161	0
26	Z	58/60 (96%)	0.46	4 (6%)	24	17	47, 64, 96, 108	0
27	1	53/55 (96%)	5.65	34 (64%)	0	1	6, 28, 62, 73	0
28	2	46/47 (97%)	5.10	37 (80%)	0	0	3, 10, 27, 42	0
29	3	63/66 (95%)	5.52	41 (65%)	0	1	3, 18, 41, 84	0
30	4	37/37 (100%)	5.54	31 (83%)	0	0	191, 239, 247, 252	0
All	All	5997/6561 (91%)	0.71	796 (13%)	8	6	3, 96, 193, 279	0

All (796) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
27	1	7	ARG	50.7
27	1	4	ASP	44.3
29	3	60	LEU	38.8
28	2	46	ASP	21.7
27	1	3	LYS	19.3
29	3	41	ILE	19.2
29	3	20	GLY	18.8
29	3	28	GLY	16.6
27	1	44	ALA	15.2
29	3	33	ASN	14.6
9	G	97	ASP	13.7
30	4	20	HIS	13.4
30	4	24	LEU	12.1
28	2	7	PRO	11.8
11	I	52	GLY	11.6
27	1	2	ALA	11.5
27	1	21	TYR	11.4
28	2	34	ARG	11.2
29	3	38	GLY	11.1
29	3	2	PRO	11.1
29	3	56	ALA	11.1
23	U	16	ASN	10.9
29	3	11	LYS	10.8
27	1	40	TYR	10.7
29	3	43	GLY	10.4
28	2	35	ARG	10.1
29	3	19	THR	10.0
29	3	14	ILE	9.9
29	3	62	LEU	9.8

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Mol	Chain	Res	Type	RSRZ
11	I	29	THR	9.8
26	Z	2	ALA	9.7
29	3	51	ALA	9.7
12	J	84	MET	9.6
27	1	41	ASP	9.5
11	I	9	THR	9.5
30	4	17	VAL	9.5
27	1	24	THR	9.4
11	I	48	PHE	9.2
27	1	43	VAL	9.2
3	A	203	ASN	9.1
8	F	127	VAL	9.0
30	4	19	ARG	8.9
29	3	30	ARG	8.9
29	3	39	ASP	8.8
30	4	21	GLY	8.7
30	4	36	GLN	8.7
1	X	248	A	8.6
30	4	31	LYS	8.5
30	4	23	VAL	8.5
27	1	19	GLY	8.5
29	3	17	THR	8.4
28	2	36	ALA	8.4
24	V	2	LYS	8.3
19	Q	64	ARG	8.3
28	2	38	GLY	8.1
11	I	63	ARG	8.0
8	F	115	LEU	7.8
28	2	31	LEU	7.7
28	2	27	GLY	7.6
8	F	126	THR	7.5
30	4	5	SER	7.5
30	4	30	VAL	7.4
28	2	21	ARG	7.4
29	3	37	SER	7.3
27	1	5	GLY	7.3
30	4	35	ARG	7.3
14	L	34	SER	7.3
19	Q	69	ILE	7.2
3	A	220	HIS	7.0
28	2	37	LYS	6.9
28	2	3	ARG	6.9

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Mol	Chain	Res	Type	RSRZ
28	2	11	LYS	6.9
29	3	35	GLY	6.8
8	F	123	ALA	6.7
30	4	37	GLY	6.7
30	4	4	ARG	6.7
11	I	8	PRO	6.7
3	A	85	ASP	6.6
20	R	82	ALA	6.5
28	2	1	MET	6.5
20	R	77	HIS	6.5
28	2	20	ALA	6.4
30	4	16	VAL	6.4
17	O	5	ILE	6.4
3	A	219	PRO	6.3
23	U	27	ASP	6.3
30	4	22	ARG	6.2
29	3	4	MET	6.2
5	C	189	ASP	6.2
1	X	731	A	6.2
4	B	135	HIS	6.2
22	T	9	SER	6.2
28	2	15	THR	6.2
11	I	36	GLY	6.2
30	4	26	ILE	6.1
1	X	1069	G	6.1
28	2	6	GLN	6.1
7	E	5	GLY	6.0
5	C	165	SER	6.0
20	R	78	ALA	6.0
30	4	33	LYS	6.0
11	I	31	GLY	5.9
5	C	47	THR	5.9
28	2	41	GLN	5.9
28	2	23	LYS	5.8
11	I	53	ARG	5.8
28	2	4	THR	5.8
29	3	34	THR	5.8
9	G	129	HIS	5.8
8	F	136	VAL	5.8
30	4	3	VAL	5.8
8	F	129	GLY	5.8
9	G	103	TYR	5.7

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Mol	Chain	Res	Type	RSRZ
5	C	193	LEU	5.7
30	4	1	MET	5.7
20	R	58	VAL	5.7
30	4	18	ARG	5.6
5	C	91	TYR	5.6
29	3	63	PRO	5.6
28	2	8	ASN	5.6
1	X	1082	G	5.5
27	1	29	ARG	5.4
28	2	28	ARG	5.4
11	I	50	GLU	5.4
28	2	9	ASN	5.4
1	X	1091	C	5.4
3	A	260	ARG	5.3
29	3	55	TRP	5.3
30	4	29	ASN	5.3
5	C	190	ALA	5.3
22	T	10	SER	5.3
3	A	46	ARG	5.3
27	1	36	GLU	5.3
3	A	250	TRP	5.3
14	L	33	ARG	5.3
9	G	110	LEU	5.3
9	G	106	TYR	5.3
22	T	15	ASP	5.2
8	F	99	LEU	5.2
14	L	40	ALA	5.2
5	C	174	GLY	5.2
1	X	2327	U	5.2
7	E	37	TYR	5.2
16	N	48	ARG	5.2
22	T	11	LYS	5.2
8	F	137	THR	5.1
14	L	36	LYS	5.1
5	C	44	SER	5.1
6	D	42	SER	5.1
11	I	33	GLY	5.0
5	C	48	ARG	5.0
23	U	47	HIS	5.0
27	1	34	LYS	5.0
29	3	18	GLY	5.0
17	O	39	PHE	4.9

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Mol	Chain	Res	Type	RSRZ
29	3	8	LYS	4.9
1	X	413	G	4.9
17	O	23	GLU	4.9
30	4	2	LYS	4.9
1	X	483	A	4.9
27	1	30	ASN	4.8
12	J	14	PHE	4.8
5	C	49	ALA	4.8
1	X	225	G	4.8
8	F	114	ASP	4.8
2	Y	123	U	4.8
7	E	6	LYS	4.8
29	3	9	MET	4.8
14	L	57	ALA	4.8
20	R	81	VAL	4.8
23	U	52	ARG	4.8
29	3	32	GLN	4.8
21	S	24	TYR	4.8
11	I	10	PRO	4.7
30	4	32	HIS	4.7
5	C	57	LYS	4.7
11	I	30	ALA	4.7
16	N	94	VAL	4.7
22	T	7	VAL	4.7
14	L	39	TYR	4.7
11	I	32	ARG	4.6
1	X	1083	C	4.6
12	J	18	MET	4.6
8	F	125	ASN	4.6
29	3	42	ARG	4.6
1	X	2326	C	4.6
29	3	40	GLU	4.6
6	D	43	SER	4.5
21	S	67	LYS	4.5
20	R	91	ALA	4.5
9	G	171	LEU	4.5
16	N	91	ASN	4.4
21	S	114	ASP	4.4
11	I	64	GLY	4.4
23	U	21	ARG	4.4
5	C	66	ASN	4.4
19	Q	65	VAL	4.4

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Mol	Chain	Res	Type	RSRZ
5	C	55	GLY	4.4
11	I	54	SER	4.4
3	A	43	ARG	4.3
23	U	39	LYS	4.3
20	R	92	THR	4.3
27	1	18	THR	4.3
7	E	143	GLN	4.3
8	F	130	THR	4.3
8	F	124	ALA	4.3
20	R	100	ASP	4.3
20	R	7	GLY	4.3
27	1	27	ASN	4.3
3	A	239	ARG	4.2
1	X	1086	C	4.2
23	U	34	THR	4.2
20	R	79	SER	4.2
1	X	1913	G	4.2
3	A	102	LYS	4.2
28	2	14	LYS	4.2
12	J	141	ALA	4.2
28	2	32	ALA	4.2
30	4	28	SER	4.2
21	S	1	MET	4.2
29	3	58	MET	4.2
14	L	21	THR	4.2
28	2	39	ARG	4.2
30	4	8	LYS	4.2
27	1	17	GLY	4.2
1	X	774	A	4.2
5	C	161	ALA	4.2
1	X	2328	G	4.1
6	D	153	ASP	4.1
12	J	140	GLU	4.1
14	L	20	THR	4.1
24	V	6	MET	4.1
22	T	12	ASN	4.1
28	2	24	THR	4.1
1	X	356	A	4.1
20	R	102	LYS	4.1
21	S	91	PRO	4.0
9	G	156	HIS	4.0
28	2	40	HIS	4.0

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Mol	Chain	Res	Type	RSRZ
3	A	249	PRO	4.0
19	Q	56	MET	4.0
1	X	434	C	4.0
12	J	86	LYS	4.0
23	U	46	LEU	4.0
12	J	27	TYR	4.0
20	R	43	ASP	4.0
30	4	25	VAL	4.0
13	K	17	ARG	3.9
14	L	111	GLY	3.9
12	J	82	THR	3.9
11	I	28	LYS	3.9
12	J	17	ARG	3.9
24	V	1	MET	3.9
19	Q	42	ILE	3.9
1	X	1068	A	3.9
19	Q	62	ARG	3.9
28	2	44	VAL	3.9
13	K	3	HIS	3.9
11	I	60	LEU	3.9
1	X	1429	A	3.9
9	G	65	LYS	3.9
12	J	88	LYS	3.9
1	X	1428	G	3.8
28	2	12	ARG	3.8
11	I	103	ASN	3.8
11	I	97	ARG	3.8
29	3	7	HIS	3.8
11	I	37	GLN	3.8
29	3	29	LYS	3.8
8	F	128	ALA	3.8
11	I	58	ALA	3.8
22	T	13	GLY	3.8
1	X	1085	G	3.7
3	A	186	HIS	3.7
6	D	8	TYR	3.7
1	X	435	A	3.7
1	X	1070	G	3.7
14	L	53	ALA	3.7
19	Q	55	THR	3.7
17	O	34	GLU	3.7
21	S	92	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
23	U	65	ASN	3.7
3	A	101	GLU	3.7
6	D	130	LEU	3.7
1	X	1037	U	3.6
8	F	131	ALA	3.6
1	X	358	C	3.6
3	A	242	ALA	3.6
27	1	31	THR	3.6
11	I	56	LEU	3.6
17	O	36	LYS	3.6
7	E	52	VAL	3.6
1	X	123	A	3.6
1	X	2280	A	3.6
11	I	15	ASP	3.6
21	S	14	LEU	3.6
9	G	163	PRO	3.6
19	Q	72	ARG	3.5
22	T	8	GLY	3.5
11	I	88	PHE	3.5
3	A	259	THR	3.5
1	X	1117	G	3.5
11	I	6	LEU	3.5
20	R	94	VAL	3.5
3	A	248	THR	3.5
24	V	48	ARG	3.5
26	Z	56	GLN	3.5
12	J	90	ALA	3.5
1	X	1089	C	3.5
1	X	1100	G	3.5
14	L	58	ALA	3.5
1	X	1524	C	3.4
27	1	52	GLU	3.4
11	I	86	THR	3.4
1	X	1092	U	3.4
23	U	49	LYS	3.4
8	F	111	LYS	3.4
6	D	154	ILE	3.4
17	O	37	ALA	3.4
29	3	31	HIS	3.4
3	A	39	LYS	3.4
12	J	16	GLY	3.4
28	2	45	SER	3.4

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Mol	Chain	Res	Type	RSRZ
5	C	194	GLU	3.4
21	S	7	PRO	3.4
4	B	94	ASP	3.4
9	G	37	ASP	3.4
11	I	5	ASP	3.4
15	M	34	ARG	3.4
27	1	28	ARG	3.4
11	I	41	SER	3.4
30	4	6	SER	3.4
11	I	95	ALA	3.4
15	M	40	ARG	3.4
20	R	26	SER	3.4
23	U	63	SER	3.4
11	I	45	LYS	3.3
6	D	85	VAL	3.3
8	F	120	VAL	3.3
9	G	160	ALA	3.3
27	1	51	ARG	3.3
9	G	119	LEU	3.3
3	A	224	SER	3.3
1	X	1084	A	3.3
29	3	24	ALA	3.3
3	A	272	THR	3.3
21	S	15	ASP	3.3
17	O	8	GLY	3.3
22	T	19	LYS	3.3
12	J	21	ASP	3.3
11	I	59	ARG	3.3
27	1	49	VAL	3.3
18	P	19	LYS	3.3
29	3	3	LYS	3.3
3	A	254	THR	3.3
12	J	28	VAL	3.3
20	R	83	LEU	3.3
23	U	62	LEU	3.3
1	X	304	A	3.2
21	S	87	THR	3.2
11	I	74	VAL	3.2
1	X	1067	G	3.2
6	D	149	THR	3.2
24	V	19	ASP	3.2
5	C	19	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
20	R	90	LYS	3.2
11	I	55	ARG	3.2
16	N	92	ARG	3.2
20	R	93	ARG	3.2
1	X	2323	U	3.2
1	X	1090	C	3.2
17	O	11	GLN	3.2
20	R	27	GLY	3.2
22	T	6	GLY	3.2
14	L	18	ARG	3.2
3	A	237	GLU	3.2
9	G	162	LYS	3.2
1	X	2776	U	3.2
23	U	28	GLY	3.2
3	A	261	ARG	3.2
1	X	2329	C	3.2
23	U	45	ASN	3.2
1	X	2330	G	3.2
27	1	45	LYS	3.2
27	1	8	ILE	3.2
11	I	27	ASP	3.1
4	B	205	SER	3.1
3	A	188	GLU	3.1
9	G	36	ASN	3.1
27	1	53	LYS	3.1
1	X	2288	A	3.1
22	T	14	ARG	3.1
23	U	31	GLY	3.1
8	F	86	LYS	3.1
23	U	44	ALA	3.1
1	X	346	C	3.1
1	X	1888	C	3.1
6	D	131	GLY	3.1
6	D	12	VAL	3.1
5	C	160	ALA	3.1
19	Q	14	GLU	3.1
2	Y	28	A	3.1
6	D	138	PHE	3.1
16	N	56	ASP	3.1
17	O	98	ILE	3.1
1	X	361	G	3.1
9	G	155	THR	3.1

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Mol	Chain	Res	Type	RSRZ
23	U	55	GLY	3.1
27	1	25	THR	3.1
11	I	62	LYS	3.1
3	A	252	LYS	3.0
23	U	8	THR	3.0
1	X	1951	G	3.0
13	K	94	TYR	3.0
3	A	243	GLY	3.0
1	X	1523	A	3.0
1	X	1093	U	3.0
23	U	51	ILE	3.0
10	H	117	GLU	3.0
3	A	50	THR	3.0
7	E	69	ARG	3.0
1	X	1095	A	3.0
20	R	96	LYS	3.0
8	F	121	GLU	3.0
19	Q	54	SER	3.0
28	2	19	ARG	3.0
3	A	34	THR	3.0
1	X	1432	G	3.0
8	F	107	ILE	3.0
19	Q	71	GLN	3.0
27	1	26	LYS	3.0
3	A	244	ARG	3.0
7	E	10	ALA	3.0
20	R	57	ASN	3.0
7	E	59	GLN	2.9
4	B	136	ARG	2.9
1	X	357	A	2.9
6	D	156	ILE	2.9
3	A	218	LYS	2.9
29	3	5	LYS	2.9
29	3	27	SER	2.9
6	D	118	ASN	2.9
11	I	21	ARG	2.9
6	D	44	LYS	2.9
19	Q	63	LYS	2.9
6	D	121	ALA	2.9
1	X	2385	U	2.9
3	A	44	ASN	2.9
14	L	38	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
21	S	124	ALA	2.9
8	F	92	ASN	2.9
1	X	540	G	2.9
6	D	4	LEU	2.9
6	D	152	MET	2.9
13	K	10	LEU	2.9
20	R	89	GLY	2.9
29	3	21	LYS	2.9
13	K	43	GLU	2.9
11	I	43	ALA	2.9
3	A	40	THR	2.9
5	C	124	ASP	2.9
12	J	87	GLY	2.9
1	X	1522	C	2.9
1	X	1734	C	2.9
8	F	78	ILE	2.9
16	N	88	ILE	2.9
4	B	202	ALA	2.8
30	4	34	GLN	2.8
5	C	90	SER	2.8
11	I	11	GLY	2.8
1	X	655	A	2.8
3	A	91	ARG	2.8
2	Y	2	C	2.8
7	E	17	VAL	2.8
3	A	201	HIS	2.8
9	G	69	ASP	2.8
5	C	188	ILE	2.8
8	F	84	ILE	2.8
19	Q	27	PHE	2.8
28	2	33	ARG	2.8
3	A	33	LEU	2.8
1	X	1872	A	2.8
5	C	112	GLN	2.8
7	E	12	PRO	2.8
30	4	15	LYS	2.8
1	X	1467	U	2.8
9	G	76	GLN	2.8
9	G	107	GLN	2.8
11	I	79	GLN	2.8
4	B	86	PRO	2.8
1	X	247	A	2.8

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Mol	Chain	Res	Type	RSRZ
1	X	1753	A	2.8
1	X	2290	A	2.8
1	X	537	C	2.8
28	2	26	SER	2.8
19	Q	53	ILE	2.8
21	S	54	ILE	2.8
7	E	80	SER	2.7
26	Z	3	LYS	2.7
3	A	223	GLY	2.7
7	E	150	LYS	2.7
1	X	1071	U	2.7
1	X	1112	U	2.7
24	V	3	PRO	2.7
7	E	46	ASP	2.7
14	L	55	SER	2.7
1	X	1121	G	2.7
1	X	1887	G	2.7
21	S	93	GLU	2.7
1	X	1078	A	2.7
1	X	1468	A	2.7
7	E	8	PRO	2.7
9	G	122	HIS	2.7
6	D	169	LEU	2.7
27	1	37	LEU	2.7
6	D	26	MET	2.7
9	G	100	TYR	2.7
16	N	58	ARG	2.7
11	I	89	ASP	2.7
12	J	139	ASP	2.7
30	4	9	LYS	2.7
7	E	111	HIS	2.7
1	X	559	C	2.7
11	I	101	ARG	2.7
12	J	25	GLY	2.6
4	B	204	ALA	2.6
6	D	139	PRO	2.6
5	C	94	THR	2.6
5	C	191	ALA	2.6
14	L	37	HIS	2.6
5	C	39	ARG	2.6
5	C	159	ARG	2.6
20	R	106	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
22	T	20	TYR	2.6
1	X	1393	G	2.6
1	X	2283	G	2.6
1	X	436	A	2.6
23	U	48	LYS	2.6
3	A	100	GLY	2.6
12	J	85	GLY	2.6
1	X	1120	C	2.6
9	G	159	SER	2.6
15	M	29	PRO	2.6
5	C	166	TRP	2.6
9	G	66	HIS	2.6
8	F	117	ALA	2.6
8	F	122	ALA	2.6
1	X	730	C	2.6
1	X	1104	G	2.6
1	X	1912	G	2.6
8	F	76	TYR	2.6
3	A	251	GLY	2.6
14	L	99	ARG	2.6
6	D	172	SER	2.6
24	V	36	GLN	2.5
1	X	2265	A	2.5
1	X	2581	A	2.5
2	Y	41	A	2.5
14	L	59	LEU	2.5
9	G	94	LYS	2.5
20	R	51	VAL	2.5
28	2	25	LYS	2.5
6	D	23	SER	2.5
20	R	98	ILE	2.5
11	I	72	TYR	2.5
9	G	108	GLY	2.5
8	F	132	ARG	2.5
6	D	5	LYS	2.5
11	I	68	VAL	2.5
21	S	86	VAL	2.5
3	A	174	ILE	2.5
1	X	1553	G	2.5
11	I	12	SER	2.5
3	A	99	ASP	2.5
11	I	49	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
12	J	26	ASP	2.5
21	S	62	PHE	2.5
16	N	12	ARG	2.5
5	C	29	GLU	2.5
1	X	1059	A	2.5
1	X	519	C	2.5
2	Y	111	C	2.5
1	X	1881	U	2.5
12	J	134	LYS	2.5
26	Z	8	LYS	2.5
27	1	6	PRO	2.5
6	D	132	ILE	2.5
14	L	19	THR	2.5
21	S	68	ALA	2.5
15	M	39	VAL	2.5
21	S	168	VAL	2.5
19	Q	12	ILE	2.4
1	X	641	G	2.4
5	C	162	ARG	2.4
8	F	94	ALA	2.4
8	F	133	SER	2.4
14	L	56	SER	2.4
21	S	170	SER	2.4
8	F	116	ASN	2.4
1	X	1188	A	2.4
6	D	117	ILE	2.4
5	C	56	ARG	2.4
6	D	41	GLY	2.4
9	G	90	LEU	2.4
22	T	36	ILE	2.4
23	U	40	ARG	2.4
1	X	343	A	2.4
1	X	1954	A	2.4
2	Y	42	U	2.4
3	A	262	LYS	2.4
1	X	583	C	2.4
1	X	2195	C	2.4
4	B	134	TRP	2.4
4	B	146	THR	2.4
8	F	113	PRO	2.4
7	E	71	LEU	2.4
27	1	35	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
28	2	29	ASN	2.4
12	J	77	LYS	2.4
1	X	1189	G	2.4
14	L	68	ALA	2.4
5	C	51	VAL	2.4
6	D	35	VAL	2.4
1	X	2281	C	2.4
2	Y	14	C	2.4
8	F	91	PRO	2.4
20	R	65	PRO	2.4
11	I	17	LYS	2.4
14	L	100	VAL	2.4
1	X	843	G	2.4
1	X	1355	A	2.4
14	L	9	ARG	2.4
5	C	20	PRO	2.3
17	O	25	LEU	2.3
5	C	24	SER	2.3
4	B	34	VAL	2.3
5	C	22	VAL	2.3
11	I	40	ARG	2.3
12	J	83	ARG	2.3
5	C	7	ILE	2.3
16	N	2	PRO	2.3
1	X	360	A	2.3
1	X	625	A	2.3
5	C	123	PHE	2.3
1	X	1223	G	2.3
20	R	12	ASP	2.3
7	E	152	ARG	2.3
8	F	138	VAL	2.3
11	I	118	VAL	2.3
16	N	110	VAL	2.3
21	S	171	VAL	2.3
29	3	36	LYS	2.3
8	F	90	THR	2.3
15	M	2	GLN	2.3
14	L	24	SER	2.3
1	X	305	A	2.3
9	G	131	VAL	2.3
23	U	26	ALA	2.3
1	X	2084	G	2.3

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Mol	Chain	Res	Type	RSRZ
3	A	233	HIS	2.3
17	O	10	LYS	2.3
27	1	42	PRO	2.3
9	G	53	ARG	2.3
3	A	247	VAL	2.3
6	D	38	GLU	2.3
12	J	137	VAL	2.3
20	R	59	LYS	2.3
27	1	38	LYS	2.3
24	V	53	LEU	2.3
9	G	41	TRP	2.3
20	R	86	PRO	2.3
21	S	4	THR	2.3
9	G	93	LYS	2.3
5	C	128	ALA	2.3
28	2	13	ALA	2.3
6	D	136	LEU	2.3
20	R	54	ILE	2.2
9	G	34	PRO	2.2
23	U	75	TYR	2.2
23	U	33	LYS	2.2
20	R	108	VAL	2.2
14	L	52	ALA	2.2
6	D	66	ILE	2.2
5	C	23	ASN	2.2
19	Q	46	PHE	2.2
11	I	92	THR	2.2
14	L	65	THR	2.2
6	D	13	ARG	2.2
9	G	116	ARG	2.2
5	C	164	VAL	2.2
1	X	1525	A	2.2
21	S	79	ILE	2.2
5	C	163	ASN	2.2
6	D	144	ASP	2.2
21	S	32	PHE	2.2
22	T	17	ASN	2.2
14	L	108	ARG	2.2
1	X	1562	G	2.2
1	X	2731	G	2.2
23	U	14	VAL	2.2
1	X	2284	U	2.2

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Mol	Chain	Res	Type	RSRZ
6	D	27	ALA	2.2
1	X	2777	A	2.2
7	E	175	LYS	2.2
6	D	113	ASP	2.2
8	F	74	MET	2.2
29	3	6	THR	2.2
1	X	1094	C	2.2
14	L	54	ALA	2.2
1	X	192	G	2.2
1	X	200	A	2.2
1	X	1516	A	2.2
1	X	2189	A	2.2
30	4	10	MET	2.2
7	E	11	VAL	2.2
17	O	78	VAL	2.2
8	F	97	GLY	2.1
13	K	52	ILE	2.1
3	A	222	ARG	2.1
3	A	255	LYS	2.1
1	X	2198	U	2.1
1	X	2286	G	2.1
9	G	95	LEU	2.1
21	S	169	VAL	2.1
11	I	123	ASP	2.1
1	X	1099	A	2.1
11	I	42	GLY	2.1
2	Y	29	C	2.1
5	C	173	ALA	2.1
21	S	5	ALA	2.1
3	A	45	ASN	2.1
7	E	7	GLN	2.1
3	A	217	ARG	2.1
6	D	125	ARG	2.1
9	G	35	LYS	2.1
19	Q	32	LYS	2.1
20	R	13	LYS	2.1
1	X	1109	A	2.1
9	G	68	PRO	2.1
23	U	30	VAL	2.1
10	H	27	SER	2.1
3	A	207	GLY	2.1
12	J	15	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
14	L	41	GLN	2.1
1	X	653	G	2.1
1	X	1588	A	2.1
6	D	155	THR	2.1
9	G	64	GLY	2.1
7	E	13	SER	2.1
6	D	11	GLN	2.1
1	X	1812	U	2.1
5	C	172	VAL	2.1
5	C	187	VAL	2.1
7	E	149	ARG	2.0
11	I	7	LYS	2.0
22	T	24	LYS	2.0
22	T	74	LYS	2.0
23	U	20	ARG	2.0
29	3	53	ALA	2.0
1	X	341	A	2.0
1	X	2427	A	2.0
1	X	732	G	2.0
1	X	1073	G	2.0
1	X	2076	G	2.0
3	A	236	GLY	2.0
15	M	30	GLY	2.0
23	U	29	GLY	2.0
5	C	157	THR	2.0
6	D	143	TYR	2.0
5	C	50	GLN	2.0
14	L	89	PHE	2.0
11	I	108	LEU	2.0
28	2	22	MET	2.0
14	L	17	VAL	2.0
1	X	429	C	2.0
1	X	1183	C	2.0
1	X	1552	C	2.0
21	S	118	HIS	2.0
5	C	53	LYS	2.0
6	D	71	LYS	2.0
23	U	79	GLU	2.0
5	C	114	GLY	2.0
9	G	112	THR	2.0
1	X	632	A	2.0
1	X	388	G	2.0

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Mol	Chain	Res	Type	RSRZ
1	X	2324	G	2.0
12	J	78	LYS	2.0
13	K	114	GLU	2.0
1	X	1365	U	2.0
1	X	75	C	2.0
1	X	226	C	2.0
1	X	1190	C	2.0
5	C	11	GLY	2.0
16	N	23	GLY	2.0
17	O	27	GLY	2.0
19	Q	66	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	MG	X	2922	1/1	0.53	0.83	81,81,81,81	0
31	MG	X	2904	1/1	0.58	0.92	90,90,90,90	0
31	MG	X	2930	1/1	0.80	1.20	71,71,71,71	0
31	MG	X	2910	1/1	0.82	0.42	85,85,85,85	0
31	MG	Y	205	1/1	0.84	0.12	77,77,77,77	0
31	MG	X	2912	1/1	0.85	0.31	60,60,60,60	0
31	MG	X	2906	1/1	0.86	0.85	79,79,79,79	0
31	MG	X	2901	1/1	0.86	0.62	110,110,110,110	0
31	MG	X	2911	1/1	0.87	0.34	35,35,35,35	0
31	MG	X	2929	1/1	0.87	0.35	77,77,77,77	0
31	MG	X	2926	1/1	0.88	0.51	56,56,56,56	0
31	MG	X	2907	1/1	0.88	0.38	53,53,53,53	0

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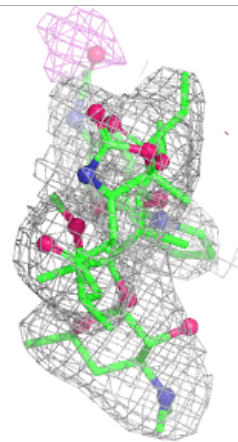
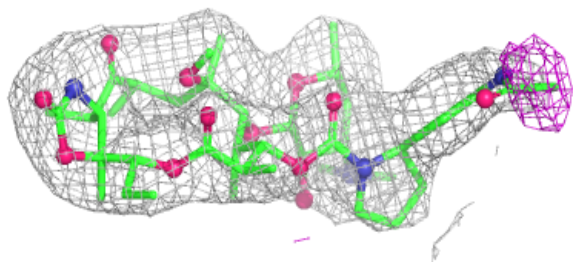
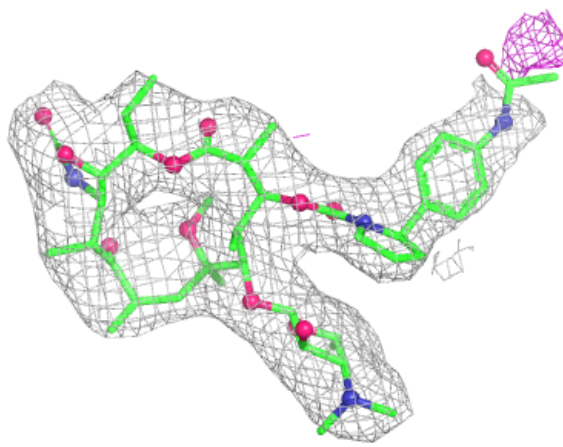
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	MG	Y	201	1/1	0.89	0.63	82,82,82,82	0
31	MG	X	2908	1/1	0.89	0.39	49,49,49,49	0
31	MG	X	2925	1/1	0.90	0.50	39,39,39,39	0
31	MG	X	2913	1/1	0.91	0.45	66,66,66,66	0
31	MG	X	2905	1/1	0.92	0.22	104,104,104,104	0
31	MG	Y	203	1/1	0.92	0.47	87,87,87,87	0
31	MG	Y	204	1/1	0.92	0.16	67,67,67,67	0
31	MG	X	2923	1/1	0.92	0.63	74,74,74,74	0
31	MG	X	2916	1/1	0.93	0.50	53,53,53,53	0
31	MG	X	2903	1/1	0.93	0.17	82,82,82,82	0
31	MG	Y	202	1/1	0.93	0.34	54,54,54,54	0
31	MG	X	2920	1/1	0.94	0.56	38,38,38,38	0
31	MG	X	2927	1/1	0.94	0.20	106,106,106,106	0
31	MG	X	2919	1/1	0.94	0.60	56,56,56,56	0
31	MG	X	2924	1/1	0.95	0.42	39,39,39,39	0
32	1F3	X	2931	60/60	0.95	0.10	38,60,90,99	0
31	MG	X	2917	1/1	0.96	0.47	37,37,37,37	0
31	MG	X	2902	1/1	0.97	0.63	45,45,45,45	0
31	MG	X	2915	1/1	0.97	0.26	24,24,24,24	0
31	MG	X	2914	1/1	0.98	0.54	51,51,51,51	0
31	MG	X	2918	1/1	0.98	0.48	32,32,32,32	0
31	MG	X	2921	1/1	0.98	0.38	18,18,18,18	0
31	MG	X	2928	1/1	0.98	0.58	42,42,42,42	0
31	MG	X	2909	1/1	0.99	0.45	37,37,37,37	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 1F3 X 2931:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.