



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:09 AM UTC

PDB ID : 5JVG / pdb_00005jvg
Title : The large ribosomal subunit from *Deinococcus radiodurans* in complex with avilamycin
Authors : Krupkin, M.; Wekselman, I.; Matzov, D.; Eyal, Z.; Diskin Posner, Y.; Rozenberg, H.; Zimmerman, E.; Bashan, A.; Yonath, A.
Deposited on : 2016-05-11
Resolution : 3.43 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 Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

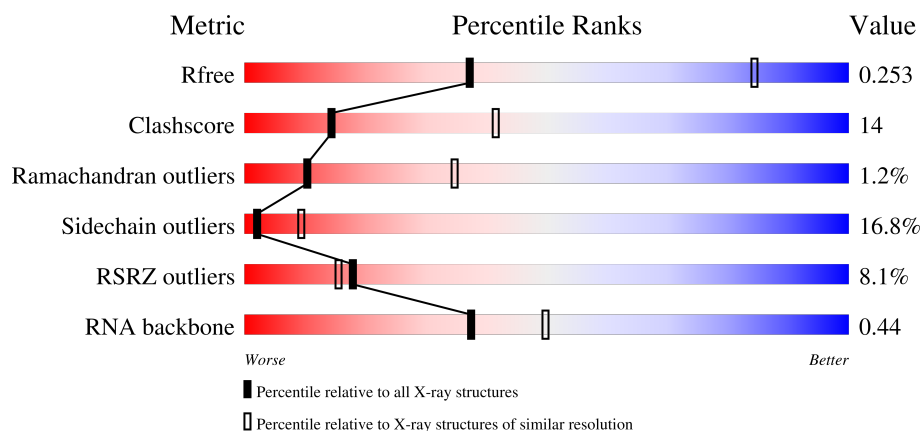
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.43 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}	180053	1210 (3.48-3.36)
Clashscore	190562	1234 (3.48-3.36)
Ramachandran outliers	187476	1222 (3.48-3.36)
Sidechain outliers	187428	1222 (3.48-3.36)
RSRZ outliers	180081	1210 (3.48-3.36)
RNA backbone	3983	1162 (3.84-3.00)

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	2877	21% 46% 37% 11% 6%
2	Y	124	2% 47% 36% 14% .
3	A	275	21% 47% 41% 10% ..

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Mol	Chain	Length	Quality of chain
4	B	211	
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	

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Mol	Chain	Length	Quality of chain
29	3	66	

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	3054	-	-	-	X
31	MG	X	3074	-	-	-	X
31	MG	X	3126	-	-	-	X
31	MG	X	3130	-	-	-	X
31	MG	X	3178	-	-	-	X
31	MG	X	3180	-	-	-	X
31	MG	X	3300	-	-	-	X
31	MG	X	3301	-	-	-	X
31	MG	X	3302	-	-	-	X
32	MPD	X	3316	-	-	X	-

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 85766 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	2710	Total	C	N	O	P	0	1	0
			58191	25957	10742	18782	2710			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1526	U	C	conflict	GB 1026245073
X	1890	A	G	conflict	GB 1026245073

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	120	Total	C	N	O	P	0	0	0
			2561	1143	471	827	120			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	272	Total	C	N	O	S	0	0	0
			2085	1299	416	366	4			

- 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	195	Total	C	N	O	S	0	0	0
			1489	925	285	276	3			

- 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
			1367	869	241	250	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	63	Total	C	N	O	S	0	0	0
			451	280	82	86	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	134	Total	C	N	O	0	0	0
			982	601	195	186			

- 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
			1060	680	192	181	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	115	Total	C	N	O	S	0	0	0
			897	552	183	159	3			

- 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	119	Total	C	N	O		0	0	0
			939	586	185	168				

- 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	97	Total	C	N	O		0	0	0
			759	477	142	140				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	P	128	Total	C	N	O	S	0	0	0
			1015	640	200	173	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
			809	504	153	151	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	S	180	Total	C	N	O	S	0	0	0
			1370	864	241	259	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	T	74	Total	C	N	O	S	0	0	0
			556	351	107	97	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	U	74	Total	C	N	O	S	0	0	0
			549	341	111	97				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	V	65	Total	C	N	O	S	0	0	0
			525	322	106	95	2			

- 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	57	Total	C	N	O	S	0	0	0
			444	273	91	75	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	53	Total	C	N	O	S	0	0	0
			427	271	79	76	1			

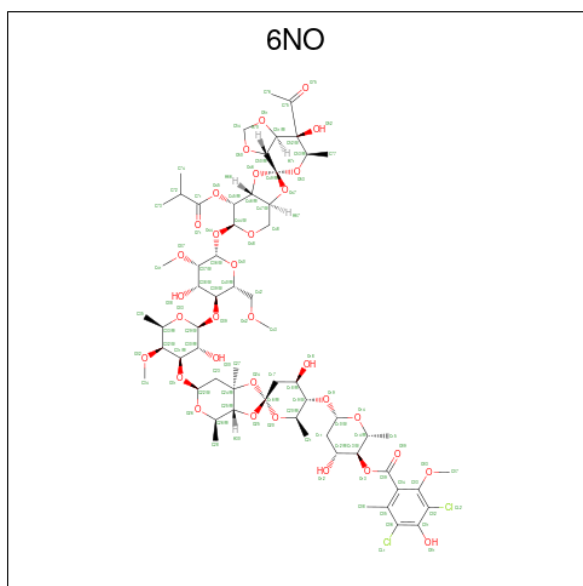
- Molecule 28 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	46	Total	C	N	O	S	0	0	0
			383	230	91	60	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	59	Total	C	N	O	S	0	0	0
			453	285	92	73	3			

- Molecule 30 is Avilamycin (CCD ID: 6NO) (formula: $C_{61}H_{88}Cl_2O_{32}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	X	1	Total	C	Cl	O	0	0
			95	61	2	32		

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

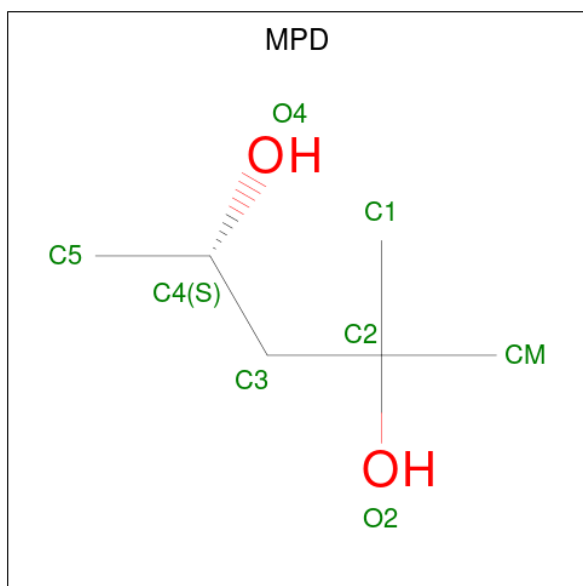
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	X	420	Total	Mg	0	0
			420	420		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	Y	19	Total	Mg	0	0
			19	19		
31	A	1	Total	Mg	0	0
			1	1		
31	J	1	Total	Mg	0	0
			1	1		
31	K	1	Total	Mg	0	0
			1	1		
31	M	1	Total	Mg	0	0
			1	1		
31	N	1	Total	Mg	0	0
			1	1		
31	T	1	Total	Mg	0	0
			1	1		
31	3	1	Total	Mg	0	0
			1	1		

- Molecule 32 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



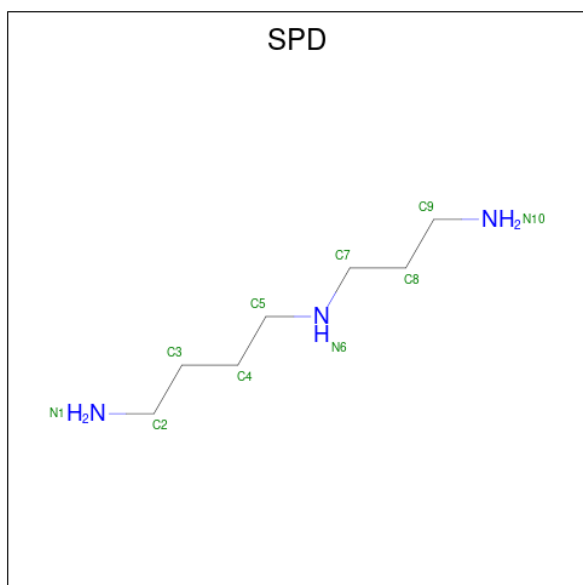
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	X	1	Total	C	O	0	0
			8	6	2		
32	X	1	Total	C	O	0	0
			8	6	2		
32	X	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	X	1	Total	C	O	0	0
			8	6	2		
32	X	1	Total	C	O	0	0
			8	6	2		

- Molecule 33 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).

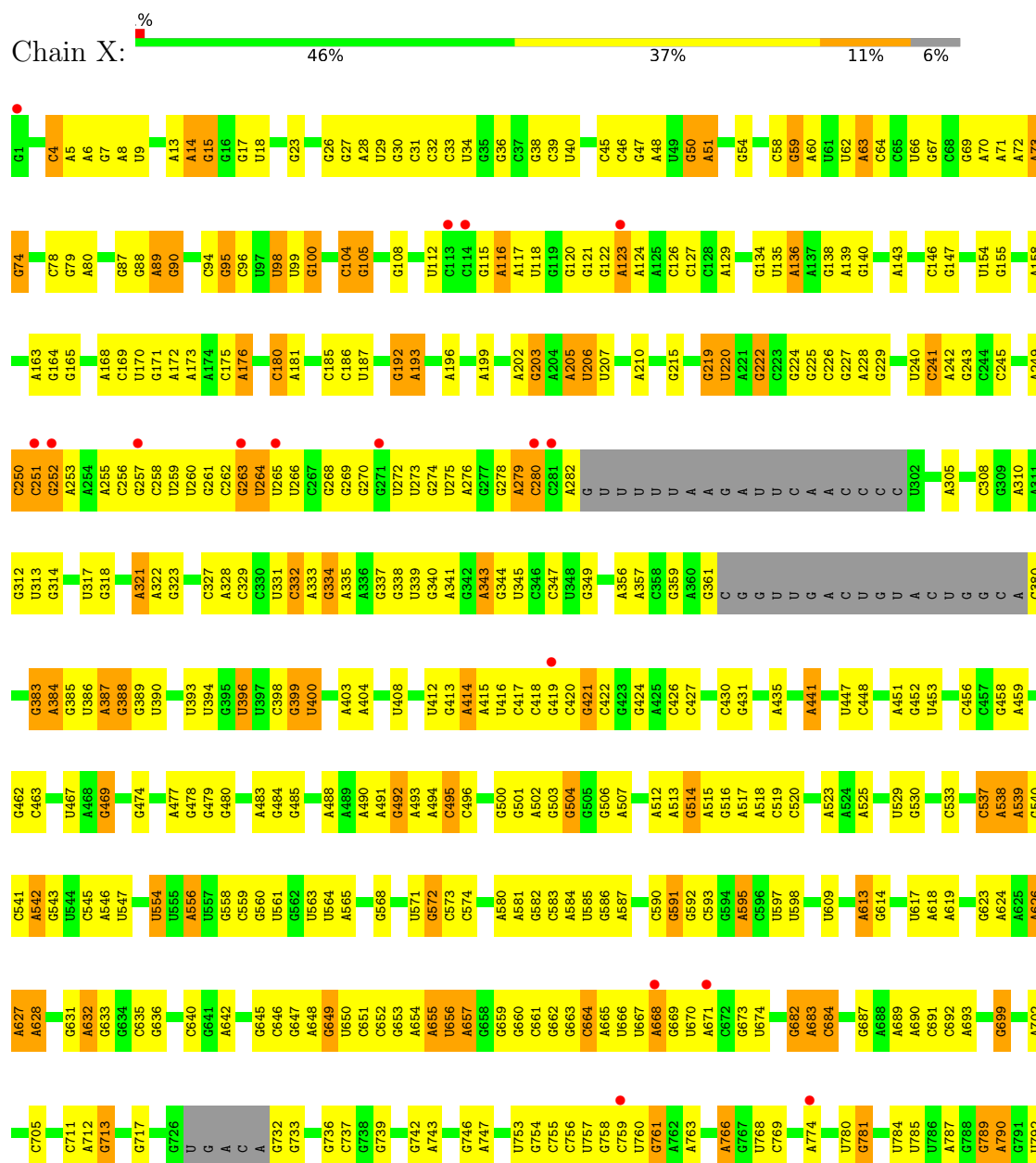


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	X	1	Total	C	N	0	0
			10	7	3		
33	X	1	Total	C	N	0	0
			10	7	3		
33	X	1	Total	C	N	0	0
			10	7	3		

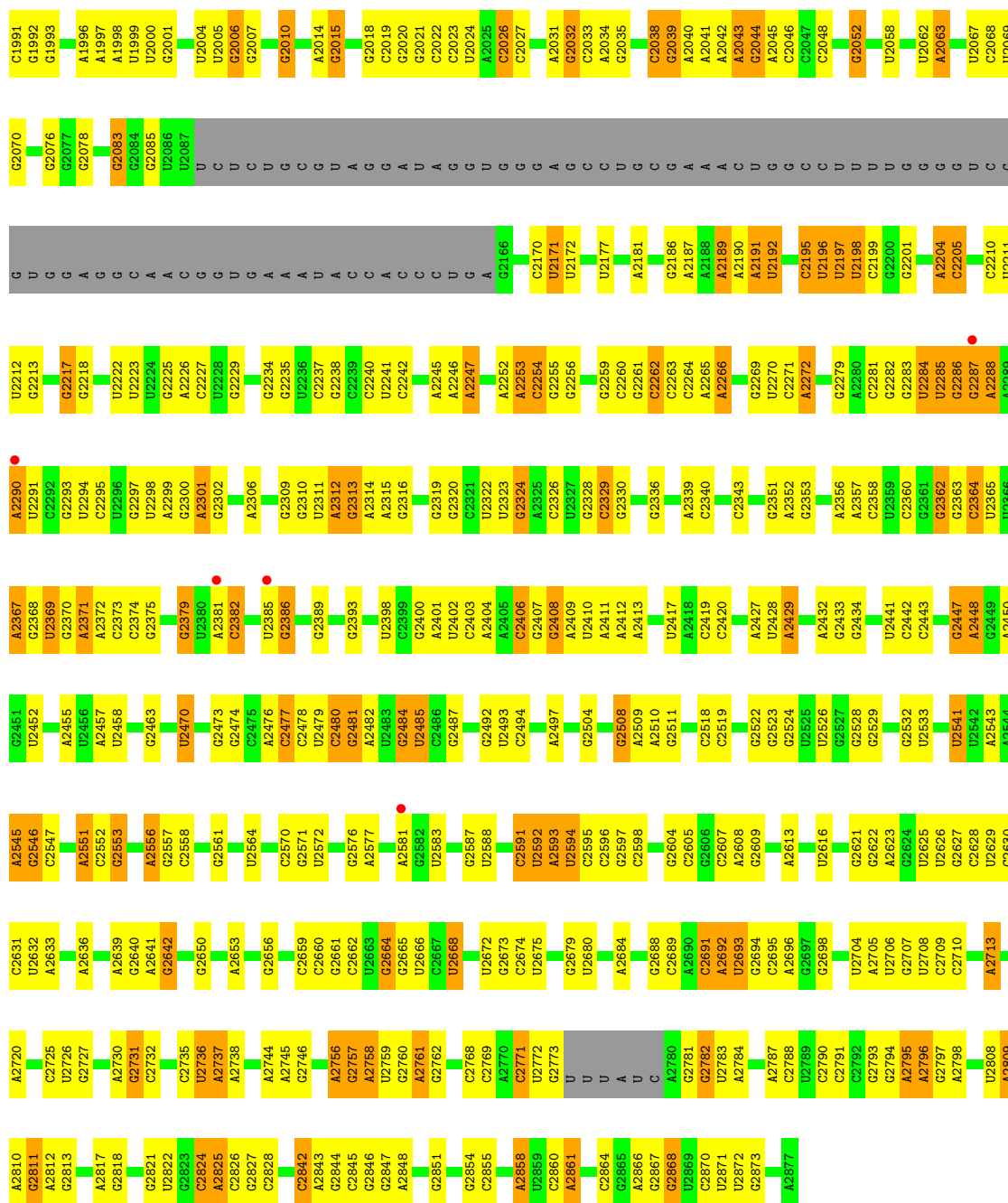
3 Residue-property plots

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.

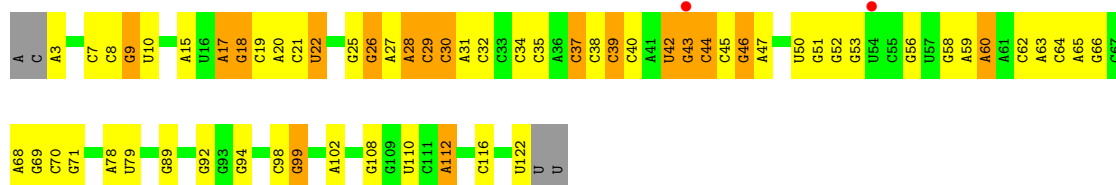
- Molecule 1: 23S ribosomal RNA



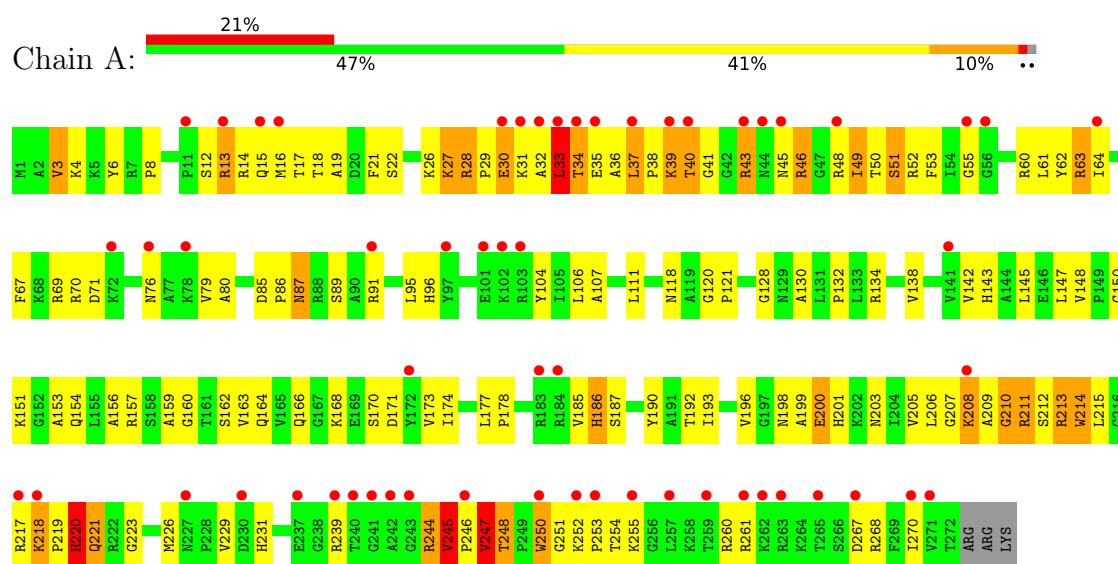
G	G1826	A1751	G1670	A1574	G1479	G1401	C1311	U1213	C1127	G958	G875	G793
U	G1827	U1752	A1671	C1575	G1480	C1404	G1312	U1217	G1128	C959	A876	A794
C	C1830	A1753	A1672	A1582	U1481	A1405	A1314	G1222	A1129	U960	G877	A796
C1908	G1754	G1755	C1673	A1583	U1490	A1406	A1321	G1223	C1134	A964	A879	A797
U1909	C1674	G1760	U1676	A1585	U1499	A1408	G1322	A1224	C1135	G965	C884	G798
A1910	C1675	G1761	U1677	A1586	A1493	U1410	U1325	G1225	G1142	C968	U890	U800
A1911	U1678	A1764	A1680	A1587	G1494	C1411	U1326	U1232	C1145	U969	A	A801
G1912	U1769	G1772	A1681	U1592	G1495	C1412	U1329	U1231	G1146	A970	G	C804
G1913	U1770	C1773	A1682	U1593	G1496	U1413	G1330	U1232	G1147	A971	G	G805
U1914	U1771	A1774	G1683	U1594	C1497	U1414	G1331	G1240	G1148	C972	G	A806
G1918	U1772	A1775	G1684	A1595	A1499	G1417	G1332	U1247	C1150	G985	G	U810
A1919	C1773	C1774	A1685	A1596	U1500	C1418	G1333	U1248	G1151	U986	C	G811
A1920	A1774	A1775	A1686	A1597	G1504	G1419	A1334	G1249	A1152	A986	C	G812
U1921	U1775	A1776	G1687	G1598	U1505	A1420	A1335	G1250	A1153	G987	U	A813
U1922	A1776	A1777	G1688	U1600	A1509	U1421	G1336	G1251	A1154	A	A	G814
U1923	A1777	A1778	G1689	U1601	U1513	C1422	G1337	G1252	G1155	A992	C	G818
C1924	A1778	A1779	A1690	G1602	C1514	A1423	G1338	A1255	U1156	C993	C	G822
C1925	A1779	A1780	A1691	A1603	U1515	G1427	U1341	U1257	U1161	A998	U	C825
U1926	A1781	A1782	A1692	A1604	U1516	A1428	G1342	U1258	A1162	C999	C	U826
C1930	A1783	A1784	A1693	A1605	C1517	G1429	C1343	G1264	C1163	G1000	U	C827
G1937	A1785	A1786	A1694	A1606	G1520	U1430	G1344	G1265	G1164	C1003	A	C830
A1943	U1787	C1788	U1703	C1614	G1521	U1431	G1345	U1266	G1165	A1004	C	G831
A1944	C1788	U1704	U1705	A1619	U1521	A1432	G1346	U1267	G1166	U1005	A	A832
C1945	U1789	U1706	A1707	A1620	C1522	U1433	U1357	U1268	A1167	C1006	C	A833
U1946	G1790	A1708	A1709	A1621	A	U1434	C1358	G1269	U1172	A1007	C	G836
G1947	C1791	A1710	U1710	A1622	C	U1435	G1359	G1270	G1173	C1016	A	U837
A1948	C1792	C1793	C1711	A1623	A1525	G1436	G1360	G1271	A1174	U1019	A	A838
A1949	A1793	A1714	A1715	A1624	A1526	G1437	G1361	U1276	A1175	A1020	C	U839
A1950	A1794	A1716	G1716	A1625	C1528	G1438	G1362	U1277	C1086	A1021	C	U840
A1951	A1795	A1717	A1718	A1626	C1529	G1439	G1363	A1278	C1087	A1022	C	G841
A1953	A1796	A1719	A1720	A1630	C1531	A1441	U1370	U1279	C1090	U1023	C	A842
A1954	A1797	A1721	A1722	A1631	G1539	G1442	G1371	U1280	C1094	U1026	C	G843
G1955	C1801	A1723	A1724	A1632	U1539	G1443	A1372	A1281	A1096	C1027	C	U844
G1963	G1803	U1725	U1726	C1633	C1540	G1444	G1373	U1282	A1097	G1028	C	U845
A1964	U1804	C1725	G1726	G1635	G1541	A1448	G1377	A1283	A1098	C1029	C	U852
U1965	G1805	G1727	U1728	G1636	G1542	A1451	U1378	A1284	A1099	U1030	C	G853
C1967	G1806	A1729	A1730	G1637	U1551	U1452	C1380	A1285	A1099	G1031	C	G854
G1968	A1807	C1730	C1731	G1638	C1552	A1453	G1381	U1286	A1099	U1032	C	U859
U1973	G1808	U1733	U1734	A1643	G1553	U1454	G1382	U1287	A1099	G1033	C	U860
U1974	C1809	A1811	A1812	C1648	A1554	C1455	C1383	A1288	A1099	G1034	C	U865
G1975	U1810	U1735	U1736	C1655	A1555	G1460	G1384	A1289	A1099	U1036	C	U866
A1976	A1811	C1737	C1738	U1656	A1560	A1463	C1385	A1290	A1099	G1037	C	A865
A1977	A1812	A1739	A1740	U1661	A1561	A1464	A1386	G1291	A1099	U1038	C	U866
A1978	G1813	G1741	G1742	C1662	U1562	C1465	A1390	G1296	A1099	A1040	C	C869
C1979	G1814	U1743	U1744	G1663	U1563	C1466	A1391	U1297	A1099	G1041	C	G870
A1980	U1815	C1745	C1746	G1664	U1564	U1467	A1392	G1298	A1099	A1042	C	U871
A1981	G1816	A1747	A1748	C1665	A1569	U1468	G1393	A1300	A1099	U1044	C	U872
C1982	U1817	G1749	G1750	C1668	C1570	U1469	A1394	U1301	A1099	A1045	C	U873
G1983	G1818	A1751	A1752	A1669	C1571	G1470	G1398	C1310	A1099	U1046	C	A874
A1984	A1821	C1825	C1826	A1670	G1572	U1478	G1399		A1126			
U1987	A1822											
A1988	A1823											
C1989	A1824											
U1990	A1825											



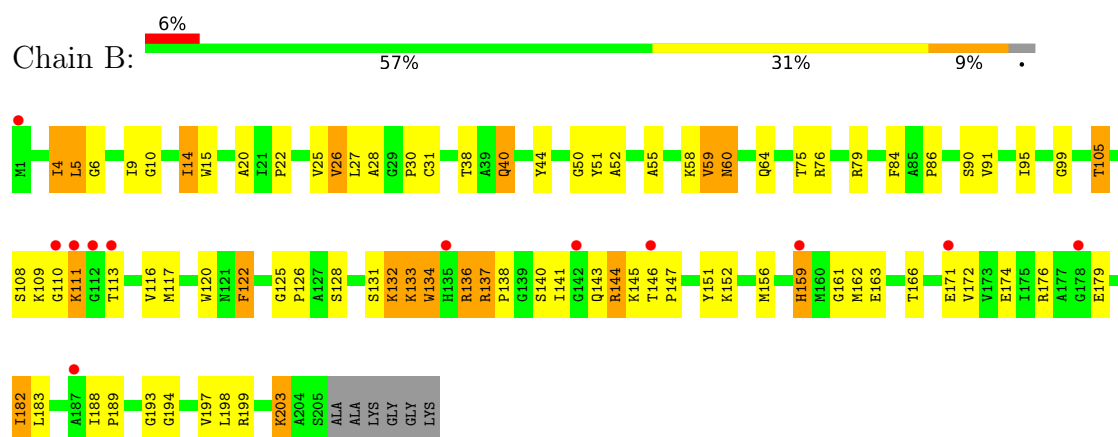
• Molecule 2: 5S ribosomal RNA



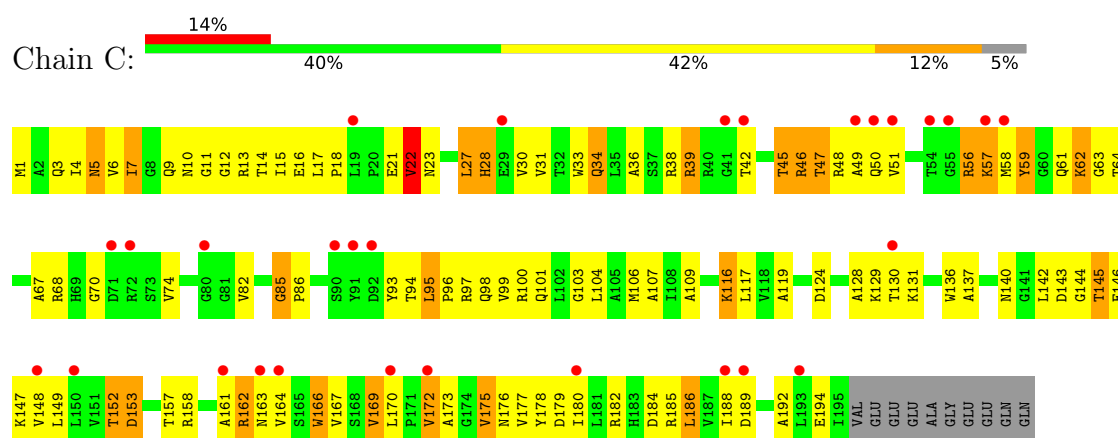
• Molecule 3: 50S ribosomal protein L2



• Molecule 4: 50S ribosomal protein L3

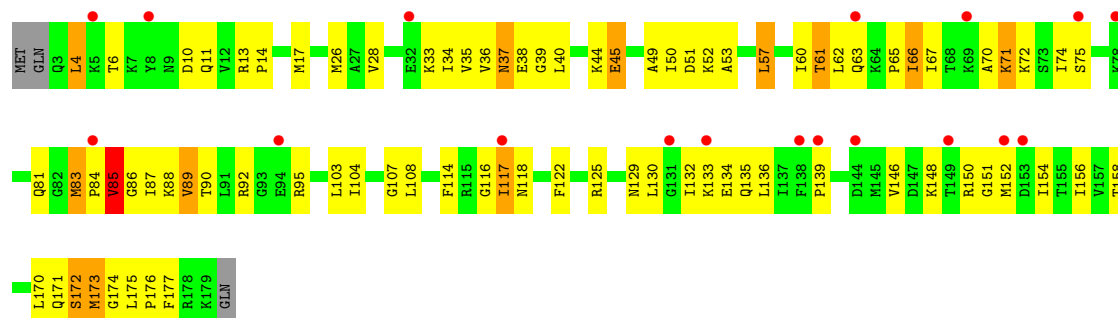


• Molecule 5: 50S ribosomal protein L4

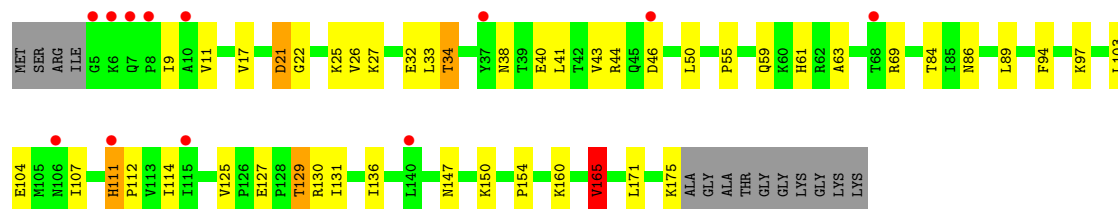


• Molecule 6: 50S ribosomal protein L5

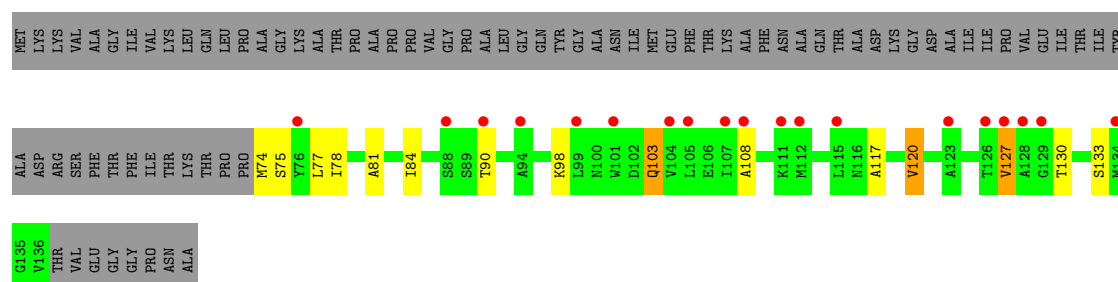
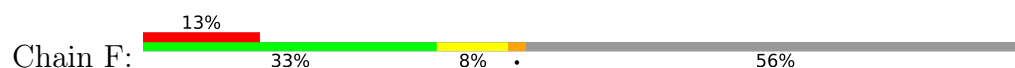




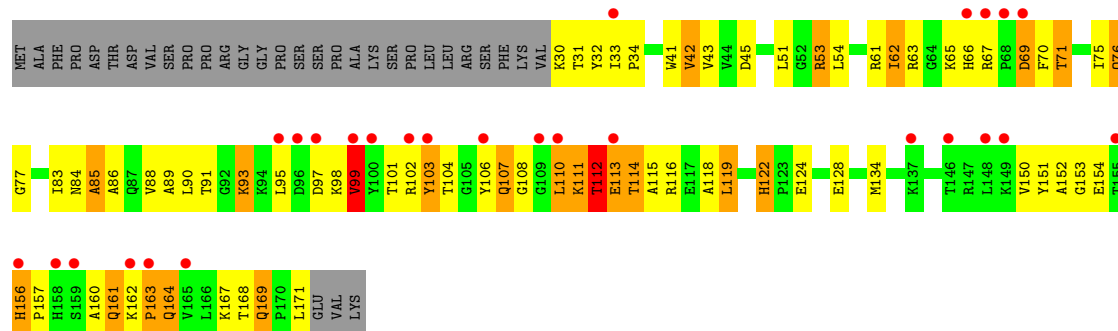
• Molecule 7: 50S ribosomal protein L6



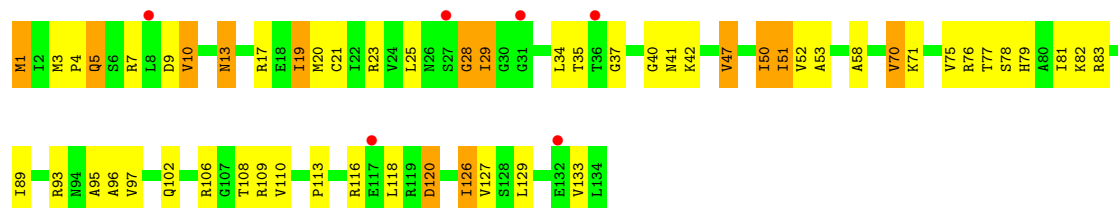
• Molecule 8: 50S ribosomal protein L11



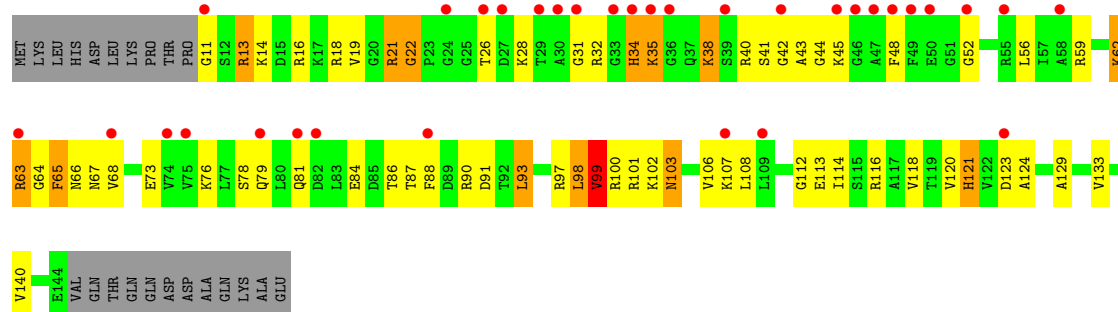
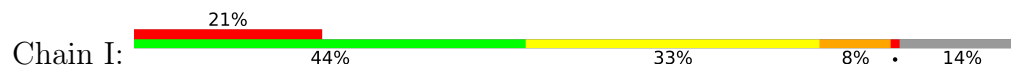
• Molecule 9: 50S ribosomal protein L13



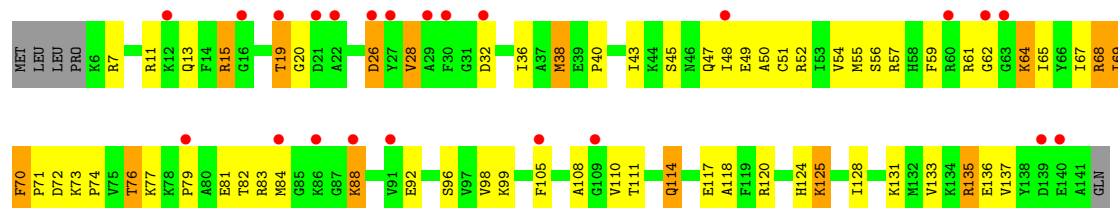
• Molecule 10: 50S ribosomal protein L14



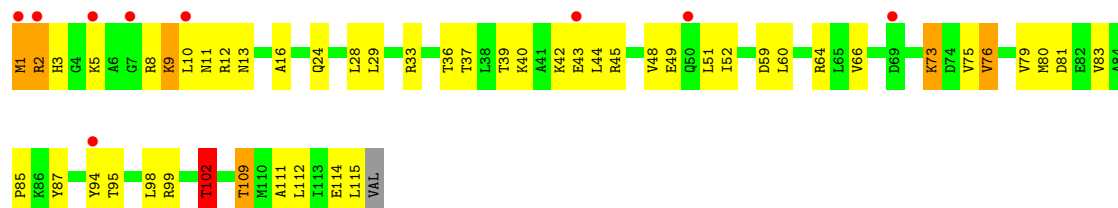
• Molecule 11: 50S ribosomal protein L15



• Molecule 12: 50S ribosomal protein L16

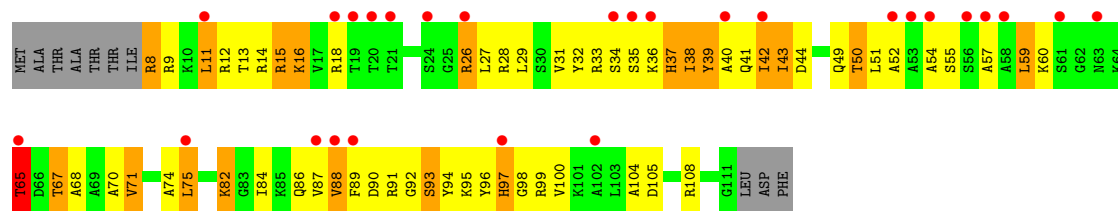


• Molecule 13: 50S ribosomal protein L17

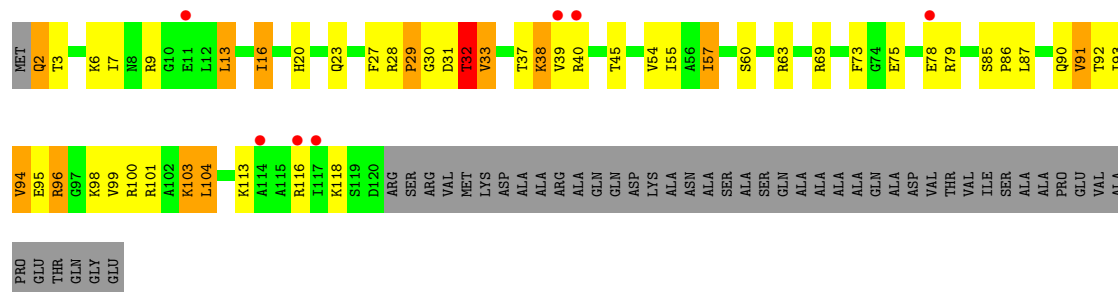
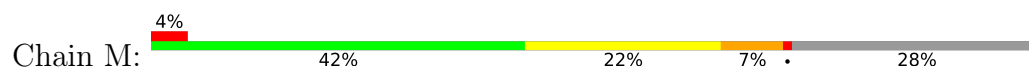


• Molecule 14: 50S ribosomal protein L18

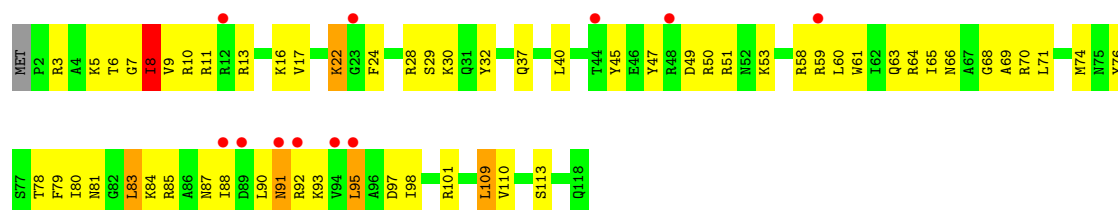




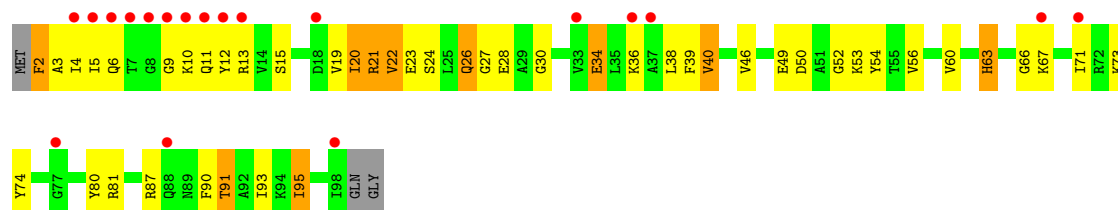
• Molecule 15: 50S ribosomal protein L19



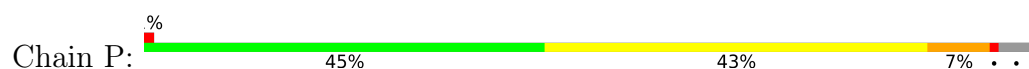
• Molecule 16: 50S ribosomal protein L20



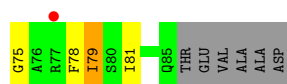
• Molecule 17: 50S ribosomal protein L21



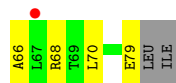
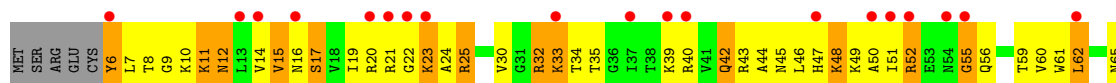
• Molecule 18: 50S ribosomal protein L22



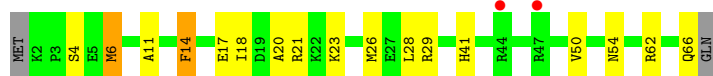
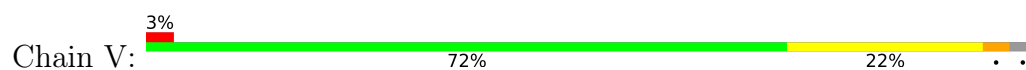




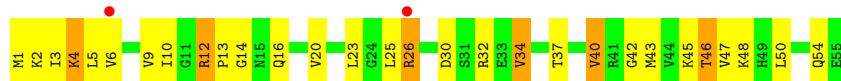
- Molecule 23: 50S ribosomal protein L28



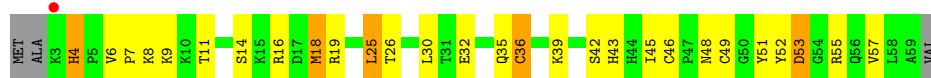
- Molecule 24: 50S ribosomal protein L29



- Molecule 25: 50S ribosomal protein L30



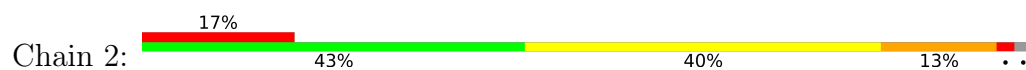
- Molecule 26: 50S ribosomal protein L32



- Molecule 27: 50S ribosomal protein L33

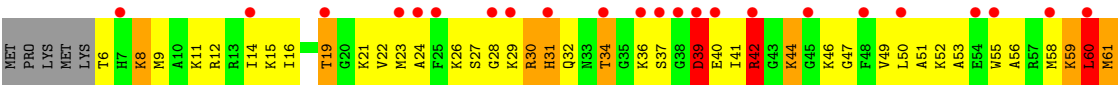
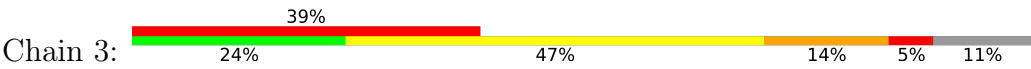


- Molecule 28: 50S ribosomal protein L34





● Molecule 29: 50S ribosomal protein L35



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	170.03Å 412.63Å 698.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.55 – 3.43 49.55 – 3.43	Depositor EDS
% Data completeness (in resolution range)	88.9 (49.55-3.43) 88.9 (49.55-3.43)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 3.40Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.211 , 0.253 0.212 , 0.253	Depositor DCC
R_{free} test set	14626 reflections (4.48%)	wwPDB-VP
Wilson B-factor (Å ²)	99.1	Xtriage
Anisotropy	0.729	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 58.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	85766	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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: SPD, MG, 6NO, MPD

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	0.25	0/65161	0.44	3/101636 (0.0%)
2	Y	0.18	0/2863	0.33	0/4461
3	A	0.48	0/2127	1.06	14/2864 (0.5%)
4	B	0.54	0/1567	1.06	5/2105 (0.2%)
5	C	0.46	0/1512	1.06	10/2046 (0.5%)
6	D	0.37	0/1385	0.94	4/1862 (0.2%)
7	E	0.34	0/1308	0.89	3/1771 (0.2%)
8	F	0.37	0/455	0.94	3/611 (0.5%)
9	G	0.52	0/1138	1.17	13/1539 (0.8%)
10	H	0.55	0/1007	1.09	4/1352 (0.3%)
11	I	0.55	0/991	1.17	9/1328 (0.7%)
12	J	0.57	0/1083	1.09	10/1451 (0.7%)
13	K	0.59	0/905	1.00	4/1212 (0.3%)
14	L	0.50	0/785	0.98	0/1048
15	M	0.60	1/952 (0.1%)	1.11	4/1277 (0.3%)
16	N	0.45	0/994	1.01	2/1323 (0.2%)
17	O	0.48	0/768	0.95	3/1025 (0.3%)
18	P	0.58	0/1028	1.18	10/1375 (0.7%)
19	Q	0.47	0/737	1.04	2/988 (0.2%)
20	R	0.54	0/819	1.17	6/1103 (0.5%)
21	S	0.42	0/1395	1.01	5/1897 (0.3%)
22	T	0.50	0/563	1.10	6/747 (0.8%)
23	U	0.60	0/553	1.15	4/741 (0.5%)
24	V	0.32	0/529	0.87	0/704
25	W	0.45	0/426	0.92	3/568 (0.5%)
26	Z	0.54	0/456	1.01	2/613 (0.3%)
27	1	0.54	0/434	1.29	8/579 (1.4%)
28	2	0.51	0/387	1.17	6/509 (1.2%)
29	3	0.51	0/459	1.19	3/604 (0.5%)
All	All	0.33	1/92787 (0.0%)	0.64	146/139339 (0.1%)

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
6	D	0	2
9	G	0	2
11	I	0	2
14	L	0	2
15	M	0	1
21	S	0	1
22	T	0	1
23	U	0	3
27	1	0	1
28	2	0	1
29	3	0	3
All	All	0	19

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	M	33	VAL	CA-CB	5.21	1.61	1.53

All (146) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	P	60	ILE	CA-C-N	10.60	130.90	119.87
18	P	60	ILE	C-N-CA	10.60	130.90	119.87
3	A	221	GLN	N-CA-C	10.21	125.27	113.01
15	M	31	ASP	N-CA-C	9.94	126.77	111.56
11	I	22	GLY	CA-C-N	9.84	129.96	120.31
11	I	22	GLY	C-N-CA	9.84	129.96	120.31
18	P	22	LYS	CA-C-N	8.60	130.59	119.84
18	P	22	LYS	C-N-CA	8.60	130.59	119.84
19	Q	58	VAL	CA-C-N	8.57	128.22	119.82
19	Q	58	VAL	C-N-CA	8.57	128.22	119.82
15	M	104	LEU	N-CA-C	8.48	123.19	111.74
3	A	211	ARG	N-CA-C	-8.22	101.87	112.23
27	1	41	ASP	CA-C-N	8.12	129.99	119.84
27	1	41	ASP	C-N-CA	8.12	129.99	119.84
3	A	247	VAL	N-CA-C	7.89	118.96	107.75
9	G	71	THR	CA-C-N	7.66	127.20	118.85
9	G	71	THR	C-N-CA	7.66	127.20	118.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	245	VAL	N-CA-C	7.57	125.24	108.88
12	J	19	THR	N-CA-C	7.55	120.79	108.26
21	S	126	GLY	CA-C-N	-7.51	110.45	119.84
21	S	126	GLY	C-N-CA	-7.51	110.45	119.84
11	I	99	VAL	N-CA-C	-7.40	98.58	108.35
11	I	31	GLY	N-CA-C	-7.40	101.20	112.89
11	I	52	GLY	N-CA-C	7.34	119.69	110.29
3	A	33	LEU	N-CA-C	-7.34	95.17	110.80
27	1	18	THR	N-CA-C	7.13	120.99	110.30
22	T	17	ASN	CA-C-N	7.12	126.61	118.85
22	T	17	ASN	C-N-CA	7.12	126.61	118.85
5	C	46	ARG	N-CA-C	7.07	121.61	112.92
5	C	74	VAL	CA-C-N	6.94	127.23	119.32
5	C	74	VAL	C-N-CA	6.94	127.23	119.32
5	C	56	ARG	N-CA-C	6.76	118.00	108.00
9	G	122	HIS	CA-C-N	6.74	126.69	119.28
9	G	122	HIS	C-N-CA	6.74	126.69	119.28
6	D	83	MET	CA-C-N	6.71	128.22	119.84
6	D	83	MET	C-N-CA	6.71	128.22	119.84
15	M	103	LYS	N-CA-C	6.68	121.60	113.38
22	T	16	SER	N-CA-C	6.66	119.32	108.26
9	G	99	VAL	N-CA-C	6.56	117.08	107.37
11	I	84	GLU	CB-CA-C	-6.53	107.20	116.34
3	A	30	GLU	N-CA-C	6.51	117.64	108.00
12	J	92	GLU	N-CA-C	-6.50	103.41	112.12
12	J	81	GLU	N-CA-C	6.40	116.31	107.73
28	2	11	LYS	N-CA-C	-6.40	103.59	111.40
9	G	156	HIS	CA-C-N	-6.30	115.28	121.65
9	G	156	HIS	C-N-CA	-6.30	115.28	121.65
4	B	120	TRP	N-CA-C	6.30	120.67	112.92
20	R	12	ASP	N-CA-C	-6.19	105.68	113.23
29	3	42	ARG	N-CA-C	-6.17	105.51	113.16
23	U	24	ALA	N-CA-C	6.17	116.22	108.45
9	G	111	LYS	N-CA-C	-6.16	101.06	110.30
22	T	20	TYR	N-CA-C	6.14	120.01	111.90
27	1	45	LYS	CB-CA-C	-6.11	107.79	116.34
18	P	9	ARG	CB-CA-C	-6.10	108.94	117.23
20	R	78	ALA	N-CA-C	-6.07	105.93	113.15
12	J	13	GLN	N-CA-C	6.04	122.69	113.51
12	J	11	ARG	N-CA-C	6.03	115.97	108.19
4	B	179	GLU	N-CA-C	-6.01	105.95	113.28
5	C	85	GLY	CA-C-N	5.98	125.74	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	85	GLY	C-N-CA	5.98	125.74	119.76
5	C	152	THR	N-CA-C	5.93	116.24	107.88
15	M	32	THR	N-CA-C	5.93	123.42	110.80
29	3	60	LEU	CA-C-N	-5.92	113.61	123.33
29	3	60	LEU	C-N-CA	-5.92	113.61	123.33
18	P	34	SER	CA-C-N	5.92	126.07	119.32
18	P	34	SER	C-N-CA	5.92	126.07	119.32
22	T	14	ARG	N-CA-C	5.91	120.62	113.17
9	G	110	LEU	N-CA-C	-5.89	105.67	112.92
7	E	111	HIS	CA-C-N	5.88	125.89	119.90
7	E	111	HIS	C-N-CA	5.88	125.89	119.90
21	S	90	GLU	N-CA-C	5.87	122.79	109.81
26	Z	46	CYS	CA-C-N	5.87	125.98	119.87
26	Z	46	CYS	C-N-CA	5.87	125.98	119.87
3	A	120	GLY	CA-C-N	5.78	125.64	119.28
3	A	120	GLY	C-N-CA	5.78	125.64	119.28
9	G	112	THR	N-CA-C	5.77	118.87	109.06
13	K	2	ARG	N-CA-C	5.76	117.64	110.91
13	K	102	THR	N-CA-C	5.73	117.30	110.19
7	E	21	ASP	CB-CA-C	-5.70	109.98	116.54
20	R	22	VAL	N-CA-C	5.70	115.84	107.75
28	2	6	GLN	CA-C-N	5.69	125.16	119.24
28	2	6	GLN	C-N-CA	5.69	125.16	119.24
4	B	125	GLY	CA-C-N	5.69	125.97	119.83
4	B	125	GLY	C-N-CA	5.69	125.97	119.83
18	P	66	GLU	CA-C-N	-5.68	113.76	119.56
18	P	66	GLU	C-N-CA	-5.68	113.76	119.56
4	B	59	VAL	N-CA-C	5.68	117.51	108.87
17	O	9	GLY	N-CA-C	5.66	121.83	112.66
12	J	70	PHE	CA-C-N	5.63	125.81	119.90
12	J	70	PHE	C-N-CA	5.63	125.81	119.90
23	U	25	ARG	N-CA-C	5.56	116.23	108.00
27	1	7	ARG	N-CA-C	5.55	118.09	109.60
10	H	70	VAL	N-CA-C	5.54	115.61	107.75
11	I	32	ARG	N-CA-C	5.49	117.33	110.91
5	C	57	LYS	N-CA-C	-5.48	101.17	108.74
16	N	30	LYS	N-CA-C	5.48	118.43	111.69
6	D	118	ASN	CA-C-N	5.48	125.09	119.56
6	D	118	ASN	C-N-CA	5.48	125.09	119.56
20	R	76	LEU	N-CA-C	5.48	117.51	109.24
18	P	20	LEU	N-CA-C	5.46	117.30	110.91
12	J	76	THR	N-CA-C	5.44	116.91	109.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	11	GLY	N-CA-C	-5.39	107.10	114.64
25	W	14	GLY	N-CA-C	5.35	119.11	112.64
23	U	23	LYS	N-CA-C	5.34	116.81	110.19
21	S	9	THR	CA-C-N	5.34	124.67	118.85
21	S	9	THR	C-N-CA	5.34	124.67	118.85
28	2	39	ARG	CA-C-N	5.34	129.26	121.31
28	2	39	ARG	C-N-CA	5.34	129.26	121.31
25	W	12	ARG	CA-C-N	5.30	125.30	119.89
25	W	12	ARG	C-N-CA	5.30	125.30	119.89
17	O	95	ILE	N-CA-C	5.30	115.53	108.11
1	X	1718[A]	A	OP2-P-O3'	5.29	123.87	108.00
1	X	1718[B]	A	OP2-P-O3'	5.29	123.87	108.00
27	1	5	GLY	CA-C-N	5.27	124.99	119.82
27	1	5	GLY	C-N-CA	5.27	124.99	119.82
8	F	90	THR	CA-C-N	5.27	125.08	119.28
8	F	90	THR	C-N-CA	5.27	125.08	119.28
28	2	18	PHE	N-CA-C	-5.26	105.44	111.07
3	A	201	HIS	N-CA-C	-5.24	105.56	111.28
5	C	59	TYR	N-CA-C	5.23	119.15	112.87
3	A	220	HIS	N-CA-C	5.22	121.93	110.80
10	H	28	GLY	N-CA-C	5.22	125.56	113.18
11	I	34	HIS	N-CA-C	5.22	116.72	109.31
17	O	34	GLU	N-CA-C	5.17	116.82	108.34
10	H	37	GLY	N-CA-C	5.13	117.97	112.33
20	R	85	ASP	N-CA-C	5.12	119.13	112.17
9	G	164	GLN	N-CA-C	5.10	117.74	110.24
13	K	111	ALA	N-CA-C	5.10	116.59	108.79
27	1	32	GLN	N-CA-C	5.10	116.82	109.07
9	G	83	ILE	N-CA-C	5.08	116.18	108.96
11	I	48	PHE	N-CA-C	5.08	121.63	110.80
10	H	53	ALA	N-CA-C	5.07	116.78	108.76
13	K	83	VAL	N-CA-C	5.05	115.20	110.30
3	A	199	ALA	CB-CA-C	-5.05	110.73	116.54
22	T	40	GLN	N-CA-C	5.04	117.31	109.60
1	X	1975	G	C2'-C3'-O3'	5.03	117.05	109.50
8	F	127	VAL	N-CA-C	5.03	115.46	110.23
23	U	9	GLY	N-CA-C	-5.02	105.48	111.36
12	J	81	GLU	CA-C-N	5.02	131.13	121.54
12	J	81	GLU	C-N-CA	5.02	131.13	121.54
9	G	42	VAL	N-CA-C	5.02	114.97	108.35
16	N	95	LEU	N-CA-C	-5.02	106.67	112.89
20	R	112	LYS	CB-CA-C	-5.02	109.31	116.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	210	GLY	N-CA-C	-5.02	108.72	114.69
3	A	244	ARG	CA-C-N	5.00	131.39	122.13
3	A	244	ARG	C-N-CA	5.00	131.39	122.13

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	1	18	THR	Peptide
28	2	37	LYS	Peptide
29	3	39	ASP	Peptide
29	3	60	LEU	Peptide
29	3	61	MET	Peptide
6	D	81	GLN	Peptide
6	D	83	MET	Peptide
9	G	107	GLN	Peptide
9	G	113	GLU	Peptide
11	I	38	LYS	Peptide
11	I	44	GLY	Peptide
14	L	59	LEU	Peptide
14	L	65	THR	Peptide
15	M	30	GLY	Peptide
21	S	90	GLU	Peptide
22	T	71	ASN	Peptide
23	U	32	ARG	Peptide
23	U	33	LYS	Peptide
23	U	55	GLY	Peptide

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	58191	0	29325	966	0
2	Y	2561	0	1306	46	0
3	A	2085	0	2158	111	0
4	B	1539	0	1600	86	0
5	C	1489	0	1516	86	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	1367	0	1408	61	0
7	E	1286	0	1336	24	0
8	F	451	0	474	9	0
9	G	1114	0	1144	72	0
10	H	997	0	1046	36	0
11	I	982	0	1002	54	0
12	J	1060	0	1073	43	0
13	K	897	0	955	50	0
14	L	779	0	820	63	0
15	M	939	0	964	38	0
16	N	978	0	1020	56	0
17	O	759	0	774	37	0
18	P	1015	0	1094	47	0
19	Q	726	0	753	22	0
20	R	809	0	848	45	0
21	S	1370	0	1385	43	0
22	T	556	0	579	18	0
23	U	549	0	584	40	0
24	V	525	0	546	10	0
25	W	424	0	470	17	0
26	Z	444	0	440	28	0
27	1	427	0	445	34	0
28	2	383	0	414	21	0
29	3	453	0	488	37	0
30	X	95	0	0	3	0
31	3	1	0	0	0	0
31	A	1	0	0	0	0
31	J	1	0	0	0	0
31	K	1	0	0	0	0
31	M	1	0	0	0	0
31	N	1	0	0	0	0
31	T	1	0	0	0	0
31	X	420	0	0	0	0
31	Y	19	0	0	0	0
32	X	40	0	70	15	0
33	X	30	0	57	7	0
All	All	85766	0	56094	1918	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 14.

All (1918) 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)
1:X:1277:G:OP1	26:Z:19:ARG:NH2	1.99	0.95
1:X:1669:A:OP2	13:K:9:LYS:NZ	2.00	0.95
1:X:2757:G:H5''	1:X:2758:A:H5'	1.49	0.94
1:X:387:A:HO2'	1:X:388:G:H8	1.09	0.93
1:X:2015:G:N7	32:X:3316:MPD:O4	2.00	0.93
10:H:28:GLY:HA2	10:H:50:ILE:HD11	1.52	0.91
18:P:28:ALA:HB2	18:P:71:VAL:HG21	1.52	0.90
1:X:1976:U:H4'	4:B:128:SER:HB3	1.54	0.89
1:X:1283:C:H5''	1:X:1284:G:H5'	1.57	0.87
3:A:217:ARG:HG2	3:A:219:PRO:HD3	1.56	0.86
1:X:1264:C:H5''	16:N:13:ARG:HH12	1.41	0.85
1:X:278:G:H1	1:X:380:C:H42	1.25	0.84
5:C:116:LYS:HZ2	5:C:117:LEU:H	1.22	0.84
1:X:477:A:H4'	28:2:30:ILE:HD13	1.60	0.83
1:X:699:G:H1	28:2:12:ARG:HD3	1.44	0.83
3:A:53:PHE:HB3	3:A:218:LYS:HA	1.62	0.82
4:B:174:GLU:HB3	4:B:183:LEU:HD12	1.62	0.82
16:N:5:LYS:HG3	16:N:7:GLY:H	1.45	0.82
1:X:1075:C:H42	1:X:1085:G:H1	1.26	0.81
1:X:1373:G:H22	1:X:2192:U:H3	1.28	0.81
1:X:1322:G:H4'	28:2:7:PRO:HB2	1.63	0.81
1:X:2757:G:OP2	1:X:2761:A:O2'	1.98	0.80
3:A:17:THR:HB	3:A:205:VAL:H	1.46	0.80
1:X:251:C:H3'	1:X:252:G:H5''	1.64	0.79
1:X:459:A:H2'	32:X:3315:MPD:H13	1.62	0.79
10:H:17:ARG:H	10:H:58:ALA:HA	1.46	0.79
15:M:57:ILE:HD12	15:M:103:LYS:HE3	1.64	0.79
1:X:2379:G:H4'	27:1:20:PHE:HB2	1.64	0.79
7:E:86:ASN:HB2	7:E:165:VAL:HG22	1.64	0.79
24:V:26:MET:HA	24:V:29:ARG:HE	1.48	0.79
1:X:2659:C:H5'	4:B:189:PRO:HA	1.65	0.78
10:H:75:VAL:HG12	10:H:118:LEU:HD21	1.66	0.78
28:2:38:GLY:C	28:2:40:HIS:H	1.90	0.78
9:G:110:LEU:O	9:G:112:THR:OG1	2.01	0.78
1:X:215:G:H21	1:X:632:A:H8	1.31	0.77
1:X:1429:A:N7	1:X:1600:U:O2'	2.15	0.77
29:3:39:ASP:O	29:3:41:ILE:N	2.11	0.77
1:X:2795:A:H4'	13:K:3:HIS:HD2	1.49	0.77
1:X:220:U:H5'	29:3:62:LEU:HD22	1.67	0.77
6:D:116:GLY:HA3	6:D:176:PRO:HB2	1.65	0.77
23:U:11:LYS:H	23:U:11:LYS:HD3	1.50	0.77
1:X:349:G:OP1	20:R:13:LYS:NZ	2.17	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1668:G:OP2	13:K:40:LYS:NZ	2.18	0.76
25:W:25:LEU:HD22	25:W:30:ASP:HB3	1.66	0.76
1:X:1791:C:OP1	3:A:261:ARG:NH1	2.19	0.76
5:C:124:ASP:HB2	5:C:136:TRP:HD1	1.51	0.76
23:U:47:HIS:O	23:U:48:LYS:NZ	2.15	0.75
9:G:67:ARG:HD3	9:G:70:PHE:HA	1.67	0.75
1:X:2672:U:H2'	1:X:2673:G:H8	1.51	0.75
1:X:1623:C:N4	1:X:1638:G:OP2	2.20	0.75
26:Z:45:ILE:HG22	26:Z:52:TYR:HB2	1.69	0.75
1:X:2795:A:H4'	13:K:3:HIS:CD2	2.21	0.75
1:X:2264:C:OP2	27:1:28:ARG:NH1	2.21	0.74
4:B:132:LYS:HZ3	4:B:132:LYS:HA	1.52	0.74
1:X:640:C:O2	1:X:650:U:O2'	2.03	0.74
1:X:2362:G:N2	1:X:2363:G:N3	2.36	0.74
32:X:3319:MPD:HO2	32:X:3319:MPD:HO4	1.35	0.74
1:X:339:U:H3	1:X:343:A:H2	1.33	0.74
1:X:2795:A:N1	15:M:2:GLN:N	2.36	0.74
9:G:99:VAL:HA	9:G:115:ALA:HB1	1.69	0.74
23:U:19:ILE:HG22	23:U:42:GLN:HG3	1.69	0.74
25:W:45:LYS:HD3	25:W:48:LYS:HD3	1.69	0.74
1:X:833:A:N3	1:X:954:U:O2'	2.20	0.74
1:X:538:A:O2'	1:X:539:A:O5'	2.04	0.73
1:X:2264:C:OP2	27:1:30:ASN:ND2	2.21	0.73
3:A:55:GLY:H	3:A:217:ARG:HB3	1.54	0.73
3:A:28:ARG:HE	3:A:29:PRO:HD2	1.52	0.73
11:I:102:LYS:O	11:I:103:ASN:ND2	2.21	0.73
16:N:88:ILE:HG23	17:O:49:GLU:HB2	1.68	0.73
1:X:1963:G:O2'	1:X:1965:U:OP2	2.05	0.73
14:L:11:LEU:HD23	14:L:14:ARG:HH12	1.53	0.73
27:1:18:THR:HA	27:1:20:PHE:H	1.53	0.73
1:X:2809:A:H8	1:X:2858:A:H62	1.37	0.73
1:X:263:G:N2	1:X:264:U:O4	2.21	0.73
1:X:2450:A:N3	30:X:2901:6NO:O30	2.22	0.73
9:G:32:TYR:HB3	16:N:64:ARG:HH22	1.53	0.72
11:I:66:ASN:HB2	29:3:11:LYS:HE3	1.71	0.72
1:X:1342:U:H5''	1:X:1343:C:H5	1.55	0.72
1:X:2336:G:N2	1:X:2339:A:OP2	2.23	0.72
1:X:1030:U:H3	1:X:1153:A:H62	1.35	0.72
21:S:67:LYS:HD2	21:S:84:TYR:HB2	1.72	0.72
27:1:18:THR:HA	27:1:20:PHE:N	2.04	0.72
1:X:757:U:OP1	4:B:132:LYS:NZ	2.19	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:30:C:OP1	14:L:37:HIS:NE2	2.22	0.71
21:S:104:SER:HA	21:S:139:THR:HA	1.72	0.71
1:X:793:G:H21	1:X:796:A:H62	1.38	0.71
1:X:1202:U:H2'	1:X:1203:A:H8	1.55	0.71
1:X:1811:A:H3'	3:A:178:PRO:HB2	1.72	0.71
1:X:2038:C:N3	32:X:3316:MPD:H13	2.05	0.71
1:X:1562:G:H5'	1:X:1563:U:H5'	1.73	0.71
19:Q:10:PRO:HA	19:Q:27:PHE:HB3	1.73	0.71
15:M:29:PRO:O	15:M:96:ARG:NH2	2.22	0.71
18:P:9:ARG:HG3	18:P:13:GLN:HG3	1.72	0.71
25:W:23:LEU:HD21	25:W:43:MET:HB3	1.71	0.71
13:K:102:THR:HA	13:K:109:THR:HA	1.70	0.71
20:R:63:THR:O	20:R:66:GLN:NE2	2.24	0.71
4:B:183:LEU:HD21	15:M:16:ILE:HG12	1.73	0.71
20:R:55:THR:HG21	20:R:72:ARG:HD3	1.73	0.71
1:X:653:G:H21	1:X:656:U:H5	1.37	0.71
2:Y:51:G:H2'	2:Y:52:G:H8	1.56	0.71
11:I:86:THR:HG21	11:I:116:ARG:HB3	1.72	0.71
26:Z:36:CYS:SG	26:Z:49:CYS:N	2.63	0.71
14:L:16:LYS:NZ	14:L:90:ASP:OD2	2.24	0.70
27:1:14:SER:OG	27:1:23:THR:N	2.24	0.70
1:X:507:A:OP2	18:P:19:LYS:NZ	2.19	0.70
1:X:2417:U:O2'	1:X:2419:C:OP1	2.09	0.70
9:G:84:ASN:O	9:G:86:ALA:N	2.18	0.70
1:X:403:A:H4'	1:X:404:A:H5'	1.73	0.70
1:X:2083:G:H1	1:X:2172:U:H3	1.39	0.70
3:A:41:GLY:O	3:A:43:ARG:NH1	2.25	0.70
1:X:1073:G:H1	1:X:1087:C:H42	1.38	0.70
21:S:25:ASN:ND2	21:S:28:ASN:OD1	2.24	0.70
1:X:1584:G:H5''	3:A:61:LEU:HG	1.72	0.70
2:Y:3:A:H61	2:Y:122:U:H3	1.37	0.70
1:X:2526:U:O2	10:H:23:ARG:NH1	2.25	0.69
14:L:82:LYS:HB3	14:L:84:ILE:HD12	1.72	0.69
10:H:120:ASP:OD1	10:H:120:ASP:N	2.20	0.69
5:C:3:GLN:HB3	5:C:13:ARG:HG3	1.75	0.69
17:O:3:ALA:HB3	17:O:13:ARG:HB2	1.73	0.69
1:X:1882:G:H21	1:X:1885:C:N4	1.91	0.69
4:B:134:TRP:CD1	4:B:134:TRP:H	2.10	0.69
7:E:127:GLU:HB2	7:E:130:ARG:HB3	1.74	0.69
13:K:24:GLN:HB3	13:K:44:LEU:HD22	1.73	0.69
1:X:517:A:H5''	1:X:518:A:H5'	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:172:SER:OG	6:D:173:MET:SD	2.49	0.69
1:X:224:G:OP2	1:X:226:C:N4	2.23	0.69
1:X:1377:G:N7	23:U:6:TYR:N	2.41	0.69
1:X:673:G:N2	11:I:21:ARG:O	2.26	0.69
1:X:1222:G:O2'	1:X:1250:A:N6	2.26	0.69
3:A:34:THR:OG1	3:A:35:GLU:N	2.23	0.69
1:X:1561:A:O2'	1:X:1562:G:O4'	2.11	0.69
1:X:1831:G:H2'	1:X:1832:G:H8	1.58	0.68
4:B:143:GLN:NE2	4:B:151:TYR:OH	2.26	0.68
13:K:1:MET:HE2	13:K:3:HIS:HE1	1.58	0.68
1:X:2622:G:OP2	33:X:3321:SPD:N1	2.25	0.68
3:A:13:ARG:HA	3:A:16:MET:HB3	1.74	0.68
4:B:111:LYS:HD2	13:K:3:HIS:CE1	2.29	0.68
11:I:91:ASP:HA	11:I:121:HIS:HB2	1.75	0.68
18:P:97:VAL:HG22	18:P:124:ILE:HG23	1.74	0.68
1:X:1769:U:H2'	1:X:1775:A:H62	1.57	0.68
1:X:387:A:O2'	1:X:388:G:O5'	2.12	0.68
1:X:1469:U:H1'	13:K:60:LEU:HD13	1.75	0.68
1:X:1582:A:OP1	3:A:211:ARG:NH1	2.25	0.68
6:D:14:PRO:HA	6:D:17:MET:HB3	1.75	0.68
17:O:23:GLU:HG2	17:O:91:THR:HG21	1.75	0.68
1:X:318:G:N2	1:X:321:A:OP2	2.25	0.68
1:X:1673:C:H5''	4:B:136:ARG:HG2	1.76	0.68
9:G:31:THR:HG22	16:N:61:TRP:CH2	2.29	0.68
1:X:168:A:H2'	1:X:169:C:C6	2.29	0.68
1:X:337:G:HO2'	20:R:9:HIS:HD1	1.41	0.68
1:X:1478:U:H2'	1:X:1479:G:C8	2.29	0.68
20:R:96:LYS:HB3	20:R:98:ILE:HG12	1.76	0.68
1:X:1673:C:H2'	1:X:1674:C:H6	1.57	0.68
1:X:1806:G:OP1	3:A:43:ARG:NH1	2.26	0.68
5:C:162:ARG:O	5:C:162:ARG:NE	2.25	0.68
15:M:29:PRO:HA	15:M:54:VAL:HG13	1.76	0.68
1:X:865:A:H5'	25:W:42:GLY:HA3	1.75	0.67
7:E:11:VAL:HG21	7:E:50:LEU:HD13	1.75	0.67
21:S:47:SER:OG	21:S:48:THR:N	2.19	0.67
3:A:244:ARG:O	3:A:252:LYS:NZ	2.21	0.67
4:B:52:ALA:O	4:B:76:ARG:N	2.21	0.67
24:V:50:VAL:O	24:V:54:ASN:ND2	2.28	0.67
1:X:469:G:H2'	28:2:38:GLY:HA2	1.76	0.67
1:X:2551:A:H5''	1:X:2553:G:H4'	1.77	0.67
3:A:210:GLY:HA2	3:A:213:ARG:HB2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:3:16:ILE:N	29:3:64:ARG:O	2.28	0.67
1:X:1004:A:OP1	16:N:50:ARG:NH1	2.28	0.66
1:X:1116:U:H2'	1:X:1117:G:H8	1.60	0.66
1:X:2485:U:OP1	4:B:144:ARG:NH2	2.28	0.66
9:G:41:TRP:HB2	9:G:164:GLN:HB2	1.76	0.66
23:U:70:LEU:HD12	23:U:79:GLU:HA	1.77	0.66
19:Q:14:GLU:O	19:Q:18:SER:OG	2.12	0.66
1:X:1849:G:O6	1:X:1850:G:N2	2.28	0.66
13:K:33:ARG:HG3	13:K:114:GLU:HB3	1.76	0.66
1:X:623:G:O2'	1:X:626:A:N6	2.24	0.66
1:X:2528:G:H2'	1:X:2529:G:H8	1.61	0.66
1:X:1856:U:OP1	1:X:2389:G:O2'	2.13	0.66
29:3:6:THR:HG23	29:3:8:LYS:H	1.61	0.66
1:X:1856:U:H3	1:X:1861:G:H1	1.44	0.66
1:X:2598:C:OP1	4:B:152:LYS:NZ	2.19	0.66
21:S:49:THR:HB	21:S:132:GLN:HA	1.77	0.66
1:X:2237:C:O2'	1:X:2406:C:OP2	2.14	0.66
11:I:133:VAL:HG11	11:I:140:VAL:HG23	1.78	0.66
22:T:64:ASP:OD1	22:T:64:ASP:N	2.28	0.66
1:X:1718[A]:A:H8	1:X:1718[A]:A:OP2	1.78	0.66
20:R:48:VAL:HG13	20:R:50:GLY:H	1.60	0.66
3:A:34:THR:HA	3:A:63:ARG:HA	1.77	0.66
10:H:47:VAL:HG23	10:H:77:THR:HG23	1.78	0.66
1:X:494:A:O2'	20:R:68:GLY:N	2.23	0.66
13:K:9:LYS:HD2	13:K:11:ASN:H	1.60	0.66
1:X:2781:G:O2'	1:X:2782:G:N2	2.28	0.65
3:A:32:ALA:HB1	3:A:35:GLU:HG2	1.79	0.65
1:X:1264:C:OP1	16:N:13:ARG:NH1	2.29	0.65
22:T:42:GLY:O	22:T:57:HIS:ND1	2.29	0.65
29:3:58:MET:SD	29:3:58:MET:N	2.58	0.65
21:S:70:GLN:HB3	21:S:80:HIS:HB3	1.78	0.65
12:J:61:ARG:HD2	21:S:175:ARG:HH21	1.62	0.65
24:V:62:ARG:O	24:V:66:GLN:N	2.30	0.65
25:W:46:THR:HG22	25:W:47:VAL:HG13	1.77	0.65
1:X:2264:C:H41	27:1:26:LYS:HD2	1.61	0.65
1:X:797:A:C5	3:A:229:VAL:HG21	2.32	0.65
5:C:163:ASN:H	5:C:167:VAL:HB	1.62	0.65
9:G:99:VAL:HA	9:G:115:ALA:CB	2.26	0.65
12:J:28:VAL:HG11	12:J:135:ARG:HG2	1.78	0.65
12:J:82:THR:HG23	12:J:84:MET:H	1.62	0.65
21:S:25:ASN:HD22	21:S:27:GLU:HB2	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2225:G:H2'	1:X:2226:A:H8	1.61	0.64
3:A:223:GLY:HA2	3:A:226:MET:HG3	1.79	0.64
1:X:657:A:N3	1:X:2329:C:O2'	2.31	0.64
1:X:833:A:H1'	1:X:954:U:H1'	1.80	0.64
1:X:2034:A:OP1	4:B:137:ARG:HD2	1.96	0.64
7:E:44:ARG:HH22	7:E:46:ASP:HB2	1.62	0.64
1:X:627:A:H2'	1:X:628:A:C8	2.32	0.64
1:X:1276:U:OP1	26:Z:16:ARG:NH1	2.30	0.64
14:L:68:ALA:HA	14:L:71:VAL:HG13	1.80	0.64
27:1:15:SER:HB3	27:1:51:ARG:O	1.97	0.64
3:A:244:ARG:HB2	3:A:246:PRO:HD3	1.80	0.64
20:R:46:VAL:N	20:R:76:LEU:O	2.26	0.64
9:G:114:THR:HA	9:G:116:ARG:HE	1.61	0.64
19:Q:48:VAL:HG21	19:Q:82:LEU:HD13	1.80	0.64
1:X:2369:U:OP2	27:1:2:ALA:N	2.31	0.64
1:X:2371:A:H2	1:X:2403:C:H42	1.46	0.64
1:X:2371:A:OP2	29:3:32:GLN:NE2	2.30	0.64
5:C:136:TRP:O	5:C:140:ASN:ND2	2.28	0.64
11:I:108:LEU:HD22	11:I:120:VAL:HG11	1.80	0.64
4:B:134:TRP:H	4:B:134:TRP:HD1	1.44	0.63
10:H:97:VAL:HG11	10:H:126:ILE:HD11	1.79	0.63
27:1:30:ASN:N	27:1:30:ASN:OD1	2.31	0.63
1:X:2285:U:H5'	1:X:2286:G:C8	2.33	0.63
1:X:2287:G:O2'	1:X:2288:A:O5'	2.15	0.63
29:3:30:ARG:HG3	29:3:31:HIS:H	1.62	0.63
1:X:1093:U:H4'	8:F:117:ALA:HA	1.81	0.63
1:X:2211:U:OP1	23:U:43:ARG:NH1	2.31	0.63
1:X:2283:G:N2	1:X:2284:U:O4	2.32	0.63
20:R:80:LYS:NZ	20:R:81:VAL:O	2.30	0.63
1:X:684:C:H41	11:I:43:ALA:HB1	1.62	0.63
1:X:812:G:H3'	1:X:813:A:H2'	1.79	0.63
9:G:31:THR:HG22	16:N:61:TRP:HH2	1.63	0.63
13:K:9:LYS:HE3	13:K:10:LEU:H	1.64	0.63
1:X:2796:A:H2'	1:X:2797:G:H8	1.63	0.63
9:G:69:ASP:OD1	9:G:69:ASP:N	2.31	0.63
12:J:54:VAL:HG21	12:J:125:LYS:HD3	1.80	0.63
28:2:41:GLN:OE1	28:2:41:GLN:N	2.31	0.63
5:C:5:ASN:N	5:C:5:ASN:OD1	2.31	0.63
1:X:517:A:C5'	1:X:518:A:H5'	2.29	0.63
15:M:39:VAL:HG12	15:M:45:THR:HG23	1.80	0.63
27:1:9:ILE:HA	27:1:28:ARG:HA	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:646:C:O2'	1:X:650:U:OP1	2.16	0.63
1:X:2262:C:OP1	27:1:7:ARG:NH2	2.32	0.63
9:G:31:THR:OG1	9:G:32:TYR:N	2.31	0.63
16:N:66:ASN:HD22	16:N:70:ARG:HH22	1.45	0.63
10:H:10:VAL:HG22	10:H:19:ILE:HG22	1.80	0.62
17:O:36:LYS:HD2	17:O:54:TYR:HB2	1.81	0.62
1:X:837:U:H2'	1:X:838:A:C8	2.35	0.62
1:X:1313:U:H4'	1:X:1314:A:H5'	1.81	0.62
1:X:1382:G:O4'	1:X:1799:A:N6	2.31	0.62
2:Y:21:C:H42	2:Y:66:G:H1	1.47	0.62
3:A:53:PHE:CZ	3:A:220:HIS:HA	2.35	0.62
12:J:15:ARG:HB2	12:J:15:ARG:HH11	1.65	0.62
1:X:1675:C:OP1	4:B:134:TRP:NE1	2.32	0.62
1:X:2281:C:H42	1:X:2293:G:H1	1.46	0.62
1:X:2796:A:OP2	4:B:111:LYS:NZ	2.32	0.62
5:C:45:THR:OG1	5:C:86:PRO:O	2.16	0.62
14:L:12:ARG:NH1	14:L:91:ARG:O	2.33	0.62
23:U:14:VAL:HG23	23:U:15:VAL:HG23	1.81	0.62
6:D:37:ASN:ND2	6:D:87:ILE:O	2.30	0.62
6:D:122:PHE:HD2	6:D:129:ASN:H	1.47	0.62
7:E:41:LEU:HD12	7:E:55:PRO:HD3	1.82	0.62
17:O:27:GLY:HA3	17:O:30:GLY:HA3	1.81	0.62
1:X:746:G:N7	1:X:774:A:C6	2.67	0.62
1:X:2636:A:O3'	7:E:160:LYS:NZ	2.32	0.62
1:X:2713:A:H61	4:B:203:LYS:HE3	1.65	0.62
3:A:213:ARG:HD2	3:A:217:ARG:HG3	1.82	0.62
5:C:56:ARG:HG2	5:C:57:LYS:H	1.65	0.62
1:X:2311:U:O2'	1:X:2315:A:N7	2.33	0.62
1:X:854:G:H1	1:X:948:C:H42	1.47	0.62
8:F:75:SER:HA	8:F:78:ILE:HB	1.81	0.62
12:J:26:ASP:HB2	12:J:68:ARG:HH22	1.65	0.62
1:X:1225:G:H2'	1:X:1249:G:N2	2.14	0.62
1:X:2286:G:H1	6:D:39:GLY:HA3	1.65	0.62
1:X:1787:U:H2'	1:X:1788:C:C6	2.35	0.61
3:A:12:SER:OG	3:A:13:ARG:N	2.32	0.61
6:D:103:LEU:HD12	6:D:107:GLY:HA3	1.81	0.61
21:S:24:TYR:HB3	21:S:29:ASN:HB3	1.80	0.61
26:Z:30:LEU:HD22	26:Z:39:LYS:HB3	1.82	0.61
13:K:60:LEU:HD11	13:K:64:ARG:HE	1.64	0.61
16:N:91:ASN:HB3	16:N:95:LEU:HD13	1.82	0.61
1:X:580:A:H4'	1:X:581:A:OP1	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1919:A:H62	1:X:1946:U:H3	1.48	0.61
4:B:143:GLN:N	4:B:143:GLN:OE1	2.33	0.61
14:L:97:HIS:CG	14:L:98:GLY:N	2.68	0.61
12:J:49:GLU:OE2	12:J:52:ARG:NH2	2.34	0.61
13:K:8:ARG:HD3	13:K:43:GLU:HG2	1.82	0.61
1:X:50:G:H4'	1:X:51:A:O5'	2.00	0.61
4:B:5:LEU:HD13	4:B:51:TYR:HB2	1.81	0.61
1:X:222:G:OP2	11:I:66:ASN:ND2	2.33	0.61
1:X:2085:G:N1	1:X:2171:U:O2	2.34	0.61
1:X:2824:C:P	15:M:100:ARG:HH11	2.24	0.61
1:X:2295:C:O2'	6:D:125:ARG:NH2	2.33	0.61
1:X:661:C:N3	1:X:662:G:N1	2.48	0.61
22:T:51:VAL:HG21	22:T:79:ILE:HG22	1.83	0.61
1:X:1954:A:O2'	1:X:1955:G:OP1	2.16	0.61
1:X:2796:A:H2'	1:X:2797:G:C8	2.35	0.61
1:X:1007:A:H1'	17:O:6:GLN:HG3	1.83	0.61
1:X:1704:G:H21	1:X:1718[B]:A:H2	1.48	0.61
1:X:1975:G:N2	1:X:1979:C:O2'	2.34	0.60
5:C:147:LYS:HA	5:C:166:TRP:HB2	1.81	0.60
3:A:70:ARG:HH21	3:A:150:GLY:H	1.47	0.60
14:L:54:ALA:HB2	14:L:75:LEU:HB2	1.84	0.60
1:X:954:U:OP2	11:I:38:LYS:NZ	2.16	0.60
1:X:1624:A:H1'	1:X:1626:A:OP2	2.01	0.60
4:B:9:ILE:O	15:M:9:ARG:NH1	2.34	0.60
22:T:23:VAL:HG13	22:T:38:VAL:HG23	1.83	0.60
1:X:755:C:H2'	1:X:756:C:H6	1.66	0.60
1:X:2662:C:O2	10:H:82:LYS:NZ	2.34	0.60
20:R:61:SER:OG	20:R:64:ASN:O	2.18	0.60
1:X:135:U:H2'	1:X:136:A:C8	2.37	0.60
1:X:1073:G:H1	1:X:1087:C:N4	1.99	0.60
3:A:134:ARG:HB3	3:A:187:SER:HB2	1.81	0.60
20:R:28:LYS:HG2	20:R:29:HIS:HD2	1.66	0.60
1:X:590:C:H2'	1:X:591:G:H8	1.66	0.60
1:X:2035:G:H4'	4:B:143:GLN:O	2.01	0.60
24:V:4:SER:HA	24:V:6:MET:HE2	1.83	0.60
1:X:478:G:OP1	28:2:33:ARG:HD2	2.01	0.60
1:X:1264:C:H5''	16:N:13:ARG:NH1	2.15	0.60
1:X:2352:A:H2'	1:X:2353:G:C8	2.37	0.60
4:B:14:ILE:HG12	15:M:20:HIS:CD2	2.36	0.60
14:L:8:ARG:HG3	14:L:9:ARG:H	1.66	0.60
1:X:1287:A:N1	1:X:1661:C:O2'	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2001:G:OP1	26:Z:9:LYS:NZ	2.23	0.60
6:D:62:LEU:O	6:D:95:ARG:NH1	2.35	0.60
1:X:4:C:H42	1:X:2873:G:H1	1.48	0.60
1:X:29:U:H5	32:X:3315:MPD:H51	1.67	0.60
1:X:48:A:H61	1:X:154:U:H2'	1.66	0.60
1:X:687:G:H5''	5:C:70:GLY:H	1.67	0.60
1:X:1636:G:O4'	28:2:1:MET:N	2.34	0.59
1:X:1212:U:H2'	1:X:1213:U:C6	2.37	0.59
1:X:1225:G:H2'	1:X:1249:G:H22	1.66	0.59
1:X:1329:U:H2'	1:X:1330:G:H8	1.67	0.59
1:X:1643:A:H61	1:X:1656:U:H3	1.50	0.59
1:X:2265:A:H4'	1:X:2266:A:O4'	2.01	0.59
1:X:1679:U:H1'	1:X:2666:U:H5'	1.84	0.59
1:X:2623:A:H62	33:X:3321:SPD:H22	1.67	0.59
5:C:161:ALA:C	5:C:162:ARG:HG3	2.27	0.59
12:J:19:THR:HG21	12:J:40:PRO:HB3	1.85	0.59
14:L:26:ARG:HE	14:L:86:GLN:HB3	1.67	0.59
1:X:674:U:H1'	11:I:22:GLY:HA3	1.84	0.59
10:H:13:ASN:ND2	10:H:108:THR:OG1	2.35	0.59
16:N:37:GLN:HA	16:N:40:LEU:HD23	1.84	0.59
1:X:1478:U:H2'	1:X:1479:G:H8	1.67	0.59
4:B:38:THR:HG22	4:B:40:GLN:H	1.66	0.59
5:C:45:THR:HG21	5:C:85:GLY:HA3	1.85	0.59
1:X:595:A:N1	1:X:822:G:O2'	2.36	0.59
1:X:1816:G:OP1	3:A:52:ARG:HD3	2.01	0.59
4:B:126:PRO:HG2	4:B:131:SER:HB2	1.83	0.59
9:G:102:ARG:O	9:G:103:TYR:HB2	2.02	0.59
29:3:29:LYS:HD3	29:3:34:THR:HA	1.83	0.59
1:X:1000:G:H5''	25:W:10:ILE:HD11	1.82	0.59
1:X:1675:C:OP1	4:B:134:TRP:CE2	2.56	0.59
1:X:968:C:H5'	12:J:77:LYS:HD2	1.84	0.59
1:X:1288:A:OP2	1:X:1663:C:N4	2.35	0.59
5:C:152:THR:OG1	5:C:153:ASP:N	2.32	0.59
14:L:55:SER:HB3	14:L:57:ALA:H	1.66	0.59
14:L:65:THR:HA	14:L:67:THR:HG23	1.84	0.59
21:S:19:ILE:HD11	21:S:36:ARG:HD3	1.85	0.59
1:X:226:C:OP2	1:X:2373:C:O2'	2.20	0.59
1:X:313:U:H2'	1:X:314:G:H8	1.67	0.59
1:X:2374:C:O2'	23:U:33:LYS:HD3	2.02	0.59
13:K:33:ARG:HH11	13:K:112:LEU:HD13	1.67	0.59
25:W:1:MET:N	25:W:34:VAL:O	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:163:A:H2'	1:X:164:G:C8	2.38	0.59
1:X:2594:U:C2	26:Z:7:PRO:HA	2.36	0.59
2:Y:9:G:H5'	14:L:32:TYR:CZ	2.38	0.59
4:B:108:SER:HB3	4:B:163:GLU:H	1.67	0.59
6:D:13:ARG:HG3	6:D:28:VAL:HG21	1.85	0.59
29:3:30:ARG:HG3	29:3:31:HIS:N	2.18	0.59
1:X:2253:A:H5'	1:X:2254:C:OP2	2.03	0.58
1:X:1291:G:OP1	13:K:36:THR:OG1	2.18	0.58
1:X:1437:A:H2'	1:X:1438:G:H8	1.68	0.58
1:X:1509:A:N3	1:X:2189:A:O2'	2.35	0.58
1:X:655:A:H2'	1:X:656:U:H5'	1.85	0.58
1:X:872:G:O2'	1:X:928:G:O6	2.20	0.58
4:B:50:GLY:HA3	4:B:75:THR:HG21	1.84	0.58
1:X:2311:U:H4'	1:X:2315:A:H62	1.67	0.58
1:X:2674:C:H2'	1:X:2675:U:C6	2.38	0.58
7:E:25:LYS:HG3	7:E:34:THR:HG22	1.86	0.58
1:X:5:A:H2'	1:X:6:A:C8	2.39	0.58
1:X:317:U:O2'	1:X:1224:A:N7	2.37	0.58
1:X:504:G:H4'	18:P:27:VAL:HG13	1.85	0.58
26:Z:53:ASP:OD1	26:Z:53:ASP:N	2.37	0.58
1:X:692:C:H2'	1:X:693:A:H8	1.69	0.58
1:X:841:G:H2'	1:X:842:A:C8	2.39	0.58
1:X:1067:G:H4'	1:X:1097:A:H8	1.69	0.58
1:X:2408:G:O6	11:I:59:ARG:NH2	2.30	0.58
6:D:171:GLN:O	6:D:172:SER:OG	2.22	0.58
14:L:37:HIS:ND1	14:L:37:HIS:O	2.32	0.58
21:S:95:SER:HB3	21:S:119:ASN:HB3	1.86	0.58
6:D:63:GLN:HE21	6:D:89:VAL:HG12	1.68	0.58
11:I:62:LYS:HB3	29:3:12:ARG:HA	1.86	0.58
16:N:66:ASN:HB3	16:N:76:TYR:HB2	1.86	0.58
1:X:1673:C:H2'	1:X:1674:C:C6	2.39	0.58
14:L:28:ARG:HG3	14:L:90:ASP:HB2	1.85	0.58
23:U:47:HIS:CG	23:U:48:LYS:H	2.21	0.58
1:X:7:G:H2'	1:X:8:A:H8	1.68	0.58
1:X:1281:A:H2'	1:X:1282:A:O4'	2.03	0.58
1:X:1296:G:H22	1:X:1299:A:H5'	1.69	0.58
1:X:1919:A:H2	1:X:1926:U:N3	2.01	0.58
1:X:2229:G:C6	12:J:83:ARG:HG2	2.38	0.58
1:X:2522:G:H2'	1:X:2523:G:C8	2.38	0.58
4:B:111:LYS:HD2	13:K:3:HIS:NE2	2.19	0.58
5:C:95:LEU:O	5:C:100:ARG:NH2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:1:32:GLN:HB3	27:1:34:LYS:HG2	1.86	0.58
1:X:73:A:H5''	1:X:74:G:O4'	2.04	0.57
1:X:859:U:HO2'	1:X:860:U:P	2.25	0.57
4:B:55:ALA:H	4:B:58:LYS:HE2	1.69	0.57
1:X:1099:A:N6	8:F:133:SER:OG	2.37	0.57
1:X:1465:G:H2'	1:X:1466:C:C6	2.39	0.57
1:X:1573:G:H3'	1:X:1574:A:H5''	1.86	0.57
1:X:2272:A:OP1	1:X:2356:A:N6	2.35	0.57
1:X:2668:U:OP2	1:X:2847:G:N2	2.36	0.57
3:A:251:GLY:C	3:A:255:LYS:HZ1	2.11	0.57
9:G:90:LEU:HD23	9:G:93:LYS:HZ2	1.68	0.57
1:X:154:U:H3'	1:X:155:G:H8	1.69	0.57
1:X:400:U:OP2	23:U:21:ARG:NH1	2.35	0.57
1:X:1297:A:H62	33:X:3322:SPD:H22	1.68	0.57
1:X:1682:A:O2'	10:H:1:MET:N	2.31	0.57
1:X:2570:C:OP1	3:A:239:ARG:HD2	2.05	0.57
1:X:2596:C:H2'	1:X:2597:G:H8	1.69	0.57
33:X:3320:SPD:H31	33:X:3320:SPD:H71	1.87	0.57
12:J:64:LYS:HB3	12:J:108:ALA:HB3	1.84	0.57
16:N:17:VAL:HG21	16:N:32:TYR:HE1	1.69	0.57
29:3:6:THR:HG23	29:3:8:LYS:N	2.18	0.57
1:X:754:G:H2'	1:X:755:C:C6	2.40	0.57
11:I:81:GLN:HB3	11:I:114:ILE:HG22	1.85	0.57
17:O:22:VAL:HA	17:O:91:THR:HG22	1.87	0.57
23:U:21:ARG:HH21	23:U:23:LYS:HG2	1.68	0.57
29:3:24:ALA:O	29:3:47:GLY:N	2.36	0.57
1:X:2640:G:H2'	1:X:2641:A:C8	2.40	0.57
1:X:2691:C:O2'	1:X:2693:U:H5'	2.05	0.57
23:U:49:LYS:HB2	23:U:61:TRP:CZ3	2.40	0.57
29:3:15:LYS:O	29:3:23:MET:N	2.33	0.57
1:X:859:U:O2'	1:X:860:U:O5'	2.18	0.57
1:X:876:A:H2	1:X:926:C:H41	1.53	0.57
1:X:1046:U:H5'	7:E:59:GLN:HG2	1.85	0.57
3:A:95:LEU:O	3:A:96:HIS:ND1	2.38	0.57
17:O:15:SER:HA	17:O:95:ILE:O	2.05	0.57
25:W:4:LYS:HZ1	25:W:54:GLN:HB2	1.70	0.57
1:X:2639:A:H2'	1:X:2640:G:O4'	2.05	0.57
1:X:837:U:H2'	1:X:838:A:H8	1.69	0.57
10:H:25:LEU:HD11	10:H:52:VAL:HG23	1.87	0.57
1:X:339:U:H4'	20:R:77:HIS:CD2	2.40	0.56
1:X:1339:U:HO2'	1:X:1993:G:HO2'	1.50	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:13:ARG:HH21	11:I:14:LYS:HG3	1.69	0.56
16:N:79:PHE:HE1	16:N:110:VAL:HA	1.69	0.56
21:S:106:GLY:HA3	21:S:142:ASN:HA	1.88	0.56
23:U:11:LYS:HG2	23:U:12:ASN:H	1.70	0.56
1:X:492:G:H1'	1:X:516:G:N2	2.20	0.56
1:X:2319:G:H2'	1:X:2320:G:H8	1.70	0.56
16:N:50:ARG:HH12	17:O:71:ILE:HG13	1.69	0.56
18:P:132:GLY:O	18:P:134:LYS:NZ	2.38	0.56
1:X:1693:A:C2	1:X:1976:U:H5'	2.40	0.56
1:X:2272:A:O3'	14:L:95:LYS:NZ	2.36	0.56
1:X:2594:U:H5'	1:X:2595:C:OP2	2.06	0.56
1:X:2867:G:H4'	1:X:2868:G:O4'	2.06	0.56
7:E:17:VAL:HG22	7:E:26:VAL:HG22	1.87	0.56
14:L:29:LEU:HB3	14:L:89:PHE:HA	1.87	0.56
15:M:29:PRO:HB2	15:M:99:VAL:HG11	1.88	0.56
16:N:66:ASN:HB3	16:N:76:TYR:H	1.71	0.56
1:X:789:G:N2	1:X:806:A:O2'	2.38	0.56
1:X:1342:U:H5''	1:X:1343:C:C5	2.38	0.56
1:X:1542:G:H22	1:X:1562:G:H1	1.53	0.56
1:X:2043:A:O2'	1:X:2044:G:OP2	2.22	0.56
1:X:2736:U:H1'	1:X:2737:A:H5''	1.86	0.56
1:X:568:G:N2	16:N:49:ASP:OD1	2.39	0.56
1:X:1803:G:H21	3:A:46:ARG:HG3	1.70	0.56
1:X:2286:G:O6	6:D:150:ARG:NH2	2.38	0.56
4:B:4:ILE:HD13	4:B:28:ALA:HB1	1.86	0.56
17:O:4:ILE:HG22	17:O:5:ILE:H	1.69	0.56
1:X:1872:A:H2'	1:X:1873:A:C8	2.41	0.56
2:Y:32:C:H1'	2:Y:59:A:H61	1.68	0.56
23:U:21:ARG:HD3	23:U:23:LYS:HG2	1.88	0.56
1:X:495:C:H2'	1:X:496:C:H6	1.70	0.56
1:X:495:C:H2'	1:X:496:C:C6	2.41	0.56
1:X:1850:G:O2'	1:X:1867:A:N6	2.38	0.56
9:G:104:THR:HG22	9:G:106:TYR:H	1.71	0.56
16:N:98:ILE:HD12	16:N:98:ILE:H	1.69	0.56
27:1:18:THR:CA	27:1:20:PHE:H	2.19	0.56
1:X:469:G:H5'	28:2:39:ARG:HB3	1.88	0.56
1:X:2286:G:O2'	1:X:2287:G:N7	2.38	0.56
5:C:146:GLU:OE2	5:C:185:ARG:NH2	2.39	0.56
7:E:104:GLU:HA	7:E:114:ILE:HG22	1.88	0.56
15:M:32:THR:HA	15:M:92:THR:O	2.05	0.56
1:X:493:A:H4'	20:R:56:LYS:HG3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:4:ILE:HG12	4:B:5:LEU:H	1.71	0.56
14:L:27:LEU:HD22	14:L:44:ASP:HA	1.88	0.56
1:X:339:U:N3	1:X:343:A:H2	2.03	0.56
1:X:1223:G:H5'	1:X:1225:G:O4'	2.04	0.56
1:X:1674:C:H2'	1:X:1675:C:C6	2.41	0.56
1:X:2621:G:OP1	9:G:104:THR:HG21	2.05	0.56
3:A:45:ASN:HD21	3:A:50:THR:HG23	1.70	0.56
17:O:66:GLY:O	17:O:87:ARG:NH2	2.28	0.56
9:G:67:ARG:HB2	9:G:70:PHE:HA	1.87	0.55
14:L:27:LEU:C	14:L:88:VAL:HG13	2.31	0.55
1:X:1256:C:O3'	11:I:16:ARG:NH2	2.39	0.55
1:X:1670:G:O6	13:K:9:LYS:HD3	2.06	0.55
1:X:1745:C:P	15:M:101:ARG:HH22	2.29	0.55
1:X:2285:U:H5'	1:X:2286:G:H8	1.69	0.55
2:Y:28:A:H2'	2:Y:28:A:OP2	2.06	0.55
10:H:109:ARG:HA	10:H:129:LEU:HD13	1.87	0.55
21:S:14:LEU:HD22	21:S:36:ARG:HH12	1.71	0.55
1:X:1370:U:H3'	1:X:1371:G:C8	2.40	0.55
3:A:91:ARG:HB2	3:A:107:ALA:HB3	1.88	0.55
9:G:93:LYS:HD3	9:G:93:LYS:H	1.72	0.55
18:P:39:ARG:HD3	18:P:97:VAL:HB	1.89	0.55
1:X:506:G:H4'	18:P:21:ARG:HH12	1.69	0.55
1:X:661:C:OP1	29:3:19:THR:OG1	2.22	0.55
1:X:1337:G:H4'	1:X:1632:A:N7	2.21	0.55
12:J:48:ILE:HA	12:J:51:CYS:HB2	1.88	0.55
12:J:79:PRO:HD3	12:J:88:LYS:HD3	1.89	0.55
18:P:94:GLU:HG3	18:P:127:ILE:HB	1.88	0.55
29:3:36:LYS:HG3	29:3:37:SER:H	1.71	0.55
1:X:99:U:H3'	1:X:100:G:H5'	1.89	0.55
1:X:343:A:O2'	1:X:345:U:OP2	2.24	0.55
1:X:684:C:H41	11:I:43:ALA:CB	2.20	0.55
1:X:1774:A:H5'	1:X:2587:G:H4'	1.87	0.55
1:X:1827:G:H1'	1:X:1914:U:C2	2.41	0.55
1:X:2379:G:H4'	27:1:20:PHE:CB	2.35	0.55
1:X:2508:G:H5''	1:X:2509:A:H5''	1.88	0.55
30:X:2901:6NO:C44	30:X:2901:6NO:O37	2.54	0.55
3:A:252:LYS:HB2	3:A:255:LYS:HZ1	1.72	0.55
12:J:28:VAL:HG21	12:J:135:ARG:HB3	1.89	0.55
1:X:692:C:H2'	1:X:693:A:C8	2.41	0.55
1:X:1718[A]:A:OP2	1:X:1718[A]:A:H2'	2.06	0.55
1:X:2024:U:OP1	9:G:102:ARG:NH2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:63:A:H2'	2:Y:64:C:C6	2.42	0.55
3:A:43:ARG:O	3:A:49:ILE:HA	2.06	0.55
9:G:113:GLU:CD	9:G:113:GLU:H	2.14	0.55
13:K:75:VAL:O	13:K:79:VAL:HG13	2.07	0.55
27:1:33:ALA:C	27:1:35:LEU:H	2.15	0.55
1:X:711:C:O2'	1:X:747:A:N6	2.39	0.55
1:X:2225:G:H2'	1:X:2226:A:C8	2.40	0.55
13:K:12:ARG:HB2	13:K:16:ALA:HB3	1.88	0.55
16:N:83:LEU:HD13	16:N:113:SER:HB2	1.88	0.55
29:3:8:LYS:HA	29:3:8:LYS:NZ	2.22	0.55
5:C:22:VAL:HG12	5:C:23:ASN:H	1.72	0.55
16:N:24:PHE:O	16:N:29:SER:HB3	2.06	0.55
20:R:23:ILE:HG23	20:R:31:GLY:HA2	1.88	0.55
1:X:78:C:H2'	1:X:79:G:H8	1.72	0.55
1:X:1422:C:H2'	1:X:1423:A:C8	2.42	0.55
3:A:69:ARG:CZ	3:A:130:ALA:HB2	2.37	0.55
1:X:1982:C:O2	1:X:2666:U:O2'	2.22	0.54
27:1:9:ILE:HG13	27:1:10:VAL:N	2.21	0.54
1:X:2447:G:HO2'	1:X:2448:A:H8	1.55	0.54
1:X:2621:G:OP2	9:G:110:LEU:HD22	2.07	0.54
2:Y:64:C:H2'	2:Y:65:A:C8	2.42	0.54
5:C:153:ASP:HA	5:C:172:VAL:HG22	1.90	0.54
5:C:173:ALA:HA	5:C:175:VAL:HG12	1.89	0.54
18:P:57:LEU:HD13	18:P:69:ALA:HA	1.88	0.54
20:R:108:VAL:HG13	20:R:109:ALA:H	1.72	0.54
1:X:1098:G:C8	1:X:1100:G:H1'	2.43	0.54
1:X:2629:U:H2'	1:X:2630:C:H6	1.71	0.54
5:C:192:ALA:C	5:C:194:GLU:H	2.15	0.54
6:D:117:ILE:HD12	6:D:117:ILE:H	1.72	0.54
16:N:47:TYR:HE2	17:O:73:LYS:HE2	1.72	0.54
17:O:2:PHE:HE1	17:O:40:VAL:HG11	1.72	0.54
23:U:51:ILE:HG23	23:U:52:ARG:H	1.73	0.54
24:V:20:ALA:HA	24:V:23:LYS:HD3	1.89	0.54
25:W:25:LEU:HD21	25:W:32:ARG:HG2	1.89	0.54
26:Z:36:CYS:SG	26:Z:48:ASN:HB2	2.47	0.54
1:X:413:G:N7	23:U:68:ARG:NH1	2.55	0.54
1:X:673:G:H21	11:I:21:ARG:HG2	1.73	0.54
1:X:1448:A:H61	1:X:1574:A:H61	1.55	0.54
1:X:1451:C:H2'	1:X:1452:U:C6	2.42	0.54
1:X:2492:G:H2'	1:X:2493:U:C6	2.41	0.54
1:X:2812:A:H2'	1:X:2813:G:C8	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:76:LYS:HB3	11:I:79:GLN:HG2	1.90	0.54
13:K:28:LEU:HD23	13:K:48:VAL:HG11	1.90	0.54
1:X:426:C:O2'	1:X:1863:U:O2'	2.23	0.54
1:X:687:G:H21	5:C:68:ARG:HH22	1.56	0.54
1:X:1071:U:P	8:F:74:MET:HB2	2.48	0.54
3:A:121:PRO:HA	3:A:132:PRO:HD2	1.89	0.54
9:G:45:ASP:HB2	9:G:167:LYS:HZ1	1.73	0.54
15:M:69:ARG:HB2	15:M:78:GLU:HG2	1.89	0.54
17:O:10:LYS:HG3	17:O:11:GLN:HG2	1.89	0.54
19:Q:7:LEU:HA	19:Q:29:VAL:HA	1.89	0.54
29:3:21:LYS:HA	29:3:50:LEU:HD21	1.89	0.54
1:X:590:C:H2'	1:X:591:G:C8	2.42	0.54
1:X:1070:G:H5''	1:X:1071:U:H2'	1.89	0.54
1:X:2043:A:H3'	5:C:62:LYS:NZ	2.23	0.54
11:I:79:GLN:HG3	11:I:98:LEU:HD11	1.88	0.54
23:U:11:LYS:HD2	23:U:66:ALA:HB2	1.90	0.54
27:1:13:GLU:HA	27:1:24:THR:HG22	1.89	0.54
1:X:547:U:OP1	1:X:1006:C:N4	2.39	0.54
4:B:144:ARG:CG	4:B:145:LYS:H	2.20	0.54
17:O:22:VAL:HG23	17:O:24:SER:H	1.73	0.54
1:X:1983:G:H5''	13:K:2:ARG:HH21	1.72	0.54
2:Y:46:G:N2	2:Y:50:U:O2	2.41	0.54
6:D:60:ILE:HG13	6:D:61:THR:HG23	1.89	0.54
13:K:49:GLU:O	13:K:52:ILE:HG12	2.07	0.54
18:P:31:VAL:HG21	18:P:124:ILE:HD11	1.90	0.54
20:R:92:THR:O	20:R:92:THR:OG1	2.26	0.54
1:X:78:C:H2'	1:X:79:G:C8	2.43	0.54
1:X:1454:U:H2'	1:X:1455:C:C6	2.43	0.54
1:X:2357:A:H4'	14:L:87:VAL:HG21	1.90	0.54
25:W:2:LYS:HB3	25:W:54:GLN:HB3	1.89	0.54
26:Z:14:SER:O	26:Z:18:MET:HB2	2.07	0.54
1:X:860:U:H3	1:X:945:G:N2	2.06	0.54
1:X:1329:U:H2'	1:X:1330:G:C8	2.43	0.54
1:X:2212:U:H2'	1:X:2213:G:C8	2.43	0.54
1:X:2594:U:H1'	26:Z:7:PRO:HB3	1.90	0.54
8:F:81:ALA:HB3	8:F:103:GLN:HE22	1.72	0.54
15:M:98:LYS:HB3	15:M:118:LYS:HB3	1.90	0.54
1:X:1463:A:H2'	1:X:1464:A:C8	2.43	0.53
14:L:41:GLN:OE1	14:L:50:THR:HG21	2.08	0.53
18:P:59:PHE:CD2	26:Z:30:LEU:HD21	2.43	0.53
1:X:492:G:O2'	1:X:517:A:N6	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:617:U:H5	1:X:632:A:C2	2.27	0.53
1:X:1193:G:H2'	1:X:1194:U:C6	2.43	0.53
3:A:43:ARG:HG2	3:A:51:SER:CB	2.38	0.53
20:R:96:LYS:HG2	20:R:98:ILE:HG23	1.89	0.53
1:X:420:C:H2'	1:X:421:G:C8	2.42	0.53
1:X:2607:C:H1'	1:X:2761:A:H2'	1.90	0.53
1:X:2707:G:H2'	1:X:2708:U:C6	2.43	0.53
23:U:50:ALA:HB3	23:U:62:LEU:HB2	1.91	0.53
1:X:1781:C:H4'	3:A:209:ALA:HB2	1.90	0.53
32:X:3316:MPD:H53	32:X:3316:MPD:H12	1.91	0.53
5:C:45:THR:HG22	5:C:82:VAL:HG11	1.89	0.53
18:P:14:ARG:HA	18:P:17:GLN:HG2	1.91	0.53
1:X:754:G:H2'	1:X:755:C:H6	1.74	0.53
1:X:2062:U:H2'	1:X:2063:A:C8	2.43	0.53
1:X:2170:C:H3'	1:X:2171:U:H5''	1.90	0.53
9:G:119:LEU:HD13	9:G:122:HIS:CE1	2.43	0.53
1:X:1801:C:N4	23:U:49:LYS:HB3	2.24	0.53
2:Y:39:C:H5''	2:Y:40:C:C5	2.44	0.53
4:B:10:GLY:O	4:B:25:VAL:N	2.33	0.53
7:E:154:PRO:HA	7:E:160:LYS:O	2.09	0.53
14:L:90:ASP:OD1	14:L:91:ARG:N	2.38	0.53
22:T:32:LYS:H	22:T:35:ASN:ND2	2.07	0.53
1:X:250:C:H2'	1:X:251:C:H5''	1.91	0.53
1:X:1441:A:H4'	1:X:1442:C:O5'	2.08	0.53
1:X:1451:C:H2'	1:X:1452:U:H6	1.73	0.53
5:C:59:TYR:OH	5:C:67:ALA:O	2.15	0.53
9:G:30:LYS:HE3	17:O:4:ILE:HG23	1.90	0.53
21:S:8:ARG:NE	21:S:8:ARG:O	2.41	0.53
1:X:652:C:H42	1:X:657:A:H61	1.57	0.53
1:X:1134:C:H2'	1:X:1135:C:H6	1.74	0.53
1:X:2005:U:O2'	1:X:2596:C:H5'	2.09	0.53
2:Y:17:A:H1'	2:Y:112:A:C8	2.44	0.53
14:L:43:ILE:HG23	14:L:50:THR:HG23	1.90	0.53
20:R:81:VAL:HG22	20:R:82:ALA:H	1.73	0.53
28:2:38:GLY:O	28:2:40:HIS:N	2.36	0.53
1:X:1668:G:H5'	13:K:39:THR:OG1	2.09	0.53
2:Y:64:C:H2'	2:Y:65:A:H8	1.73	0.53
3:A:43:ARG:HG2	3:A:51:SER:HB3	1.91	0.53
11:I:73:GLU:HB2	11:I:106:VAL:HG22	1.89	0.53
1:X:116:A:N3	1:X:155:G:H1'	2.24	0.53
5:C:128:ALA:C	5:C:130:THR:H	2.17	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:172:SER:O	6:D:174:GLY:N	2.41	0.53
9:G:90:LEU:HD23	9:G:93:LYS:NZ	2.23	0.53
13:K:99:ARG:HG2	13:K:99:ARG:HH11	1.75	0.53
17:O:36:LYS:HZ1	17:O:56:VAL:HG13	1.74	0.53
1:X:1279:G:O5'	18:P:36:ARG:NH2	2.42	0.52
6:D:10:ASP:O	6:D:14:PRO:HD3	2.08	0.52
1:X:642:A:O2'	11:I:65:PHE:HB2	2.10	0.52
1:X:1716:G:O2'	1:X:1718[B]:A:OP1	2.27	0.52
1:X:1865:C:H3'	1:X:1866:G:H8	1.74	0.52
1:X:120:G:H1	1:X:127:C:H42	1.57	0.52
1:X:742:G:OP2	3:A:13:ARG:NH1	2.42	0.52
1:X:1250:A:H2'	1:X:1251:G:O4'	2.09	0.52
1:X:2656:G:H1	1:X:2710:C:H42	1.56	0.52
6:D:134:GLU:HG2	6:D:136:LEU:H	1.74	0.52
9:G:116:ARG:HG3	9:G:118:ALA:HB3	1.90	0.52
1:X:98:U:O2	1:X:100:G:N1	2.42	0.52
1:X:624:A:O2'	1:X:626:A:OP2	2.22	0.52
1:X:1074:G:H1	1:X:1086:C:H42	1.56	0.52
16:N:47:TYR:CE2	17:O:73:LYS:HE2	2.44	0.52
27:1:14:SER:HB3	27:1:23:THR:HB	1.91	0.52
1:X:5:A:H2'	1:X:6:A:H8	1.73	0.52
1:X:1054:C:H42	1:X:1123:G:H1	1.57	0.52
1:X:1443:G:H2'	1:X:1444:C:C6	2.44	0.52
1:X:2339:A:H1'	11:I:59:ARG:HH11	1.75	0.52
12:J:67:ILE:HG12	12:J:105:PHE:HD1	1.74	0.52
1:X:946:U:H2'	1:X:947:C:C6	2.44	0.52
1:X:2282:G:H4'	6:D:122:PHE:HA	1.91	0.52
19:Q:20:MET:HG3	19:Q:25:TYR:CE1	2.45	0.52
1:X:250:C:N3	1:X:270:G:N2	2.58	0.52
1:X:1706:A:H2'	1:X:1707:A:C8	2.45	0.52
3:A:69:ARG:NH2	3:A:192:THR:OG1	2.43	0.52
1:X:559:C:O2	17:O:67:LYS:HB2	2.09	0.52
1:X:830:C:O2'	1:X:852:U:H5''	2.09	0.52
1:X:1685:A:H5''	10:H:5:GLN:HG2	1.90	0.52
1:X:1989:C:O2'	1:X:2798:A:N3	2.43	0.52
6:D:70:ALA:O	6:D:71:LYS:HB3	2.09	0.52
7:E:94:PHE:CG	7:E:107:ILE:HG22	2.45	0.52
18:P:39:ARG:HH11	18:P:39:ARG:HB2	1.74	0.52
1:X:542:A:C5'	16:N:28:ARG:HH21	2.23	0.52
1:X:1817:U:H2'	1:X:1818:G:C8	2.45	0.52
1:X:2324:G:N3	1:X:2360:C:H2'	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:171:GLN:HA	6:D:175:LEU:HD13	1.92	0.52
10:H:9:ASP:O	10:H:96:ALA:N	2.33	0.52
1:X:1417:C:H2'	1:X:1418:C:H6	1.75	0.52
1:X:2479:U:O2	32:X:3316:MPD:O2	2.27	0.52
4:B:26:VAL:HG11	4:B:198:LEU:HD11	1.92	0.52
5:C:5:ASN:ND2	5:C:10:ASN:HB2	2.25	0.52
16:N:59:ARG:O	16:N:63:GLN:HB2	2.10	0.52
28:2:34:ARG:NH1	28:2:42:LEU:HB2	2.25	0.52
1:X:1333:G:N7	1:X:1342:U:H5'	2.25	0.51
1:X:1422:C:H2'	1:X:1423:A:H8	1.76	0.51
1:X:1834:G:H2'	1:X:1835:C:C6	2.45	0.51
1:X:1984:A:P	13:K:2:ARG:HH22	2.33	0.51
9:G:84:ASN:HA	9:G:153:GLY:H	1.74	0.51
13:K:73:LYS:O	13:K:76:VAL:HG12	2.09	0.51
14:L:29:LEU:O	14:L:90:ASP:HB3	2.10	0.51
1:X:946:U:H2'	1:X:947:C:H6	1.76	0.51
1:X:1332:G:C6	1:X:1333:G:N1	2.78	0.51
3:A:246:PRO:O	3:A:247:VAL:HG13	2.10	0.51
11:I:88:PHE:HB2	11:I:90:ARG:NH2	2.25	0.51
12:J:110:VAL:HB	12:J:114:GLN:HB3	1.92	0.51
20:R:58:VAL:HG12	20:R:60:PRO:HD2	1.91	0.51
1:X:1079:G:N2	1:X:1106:A:O2'	2.43	0.51
1:X:1147:G:H2'	1:X:1148:G:H8	1.75	0.51
1:X:1406:A:H62	19:Q:15:LYS:HD3	1.75	0.51
1:X:2713:A:N1	4:B:203:LYS:HG3	2.24	0.51
5:C:23:ASN:O	5:C:27:LEU:HB2	2.11	0.51
5:C:56:ARG:HG2	5:C:57:LYS:N	2.26	0.51
10:H:1:MET:HE3	10:H:79:HIS:NE2	2.24	0.51
12:J:45:SER:O	12:J:49:GLU:HB2	2.10	0.51
21:S:152:ILE:HD11	21:S:168:VAL:HG21	1.92	0.51
1:X:227:G:H2'	1:X:228:A:C8	2.46	0.51
1:X:705:C:C5'	3:A:41:GLY:HA2	2.41	0.51
1:X:2015:G:N2	4:B:146:THR:OG1	2.39	0.51
1:X:2545:A:H61	10:H:40:GLY:HA3	1.76	0.51
16:N:7:GLY:O	16:N:8:ILE:HG12	2.10	0.51
1:X:7:G:H2'	1:X:8:A:C8	2.45	0.51
1:X:826:U:H2'	1:X:827:C:C6	2.46	0.51
1:X:865:A:H2'	1:X:866:U:C6	2.46	0.51
3:A:251:GLY:O	3:A:252:LYS:HB2	2.10	0.51
5:C:28:HIS:HA	5:C:31:VAL:HG22	1.92	0.51
7:E:9:ILE:HG12	7:E:69:ARG:HE	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:38:ILE:HD11	14:L:40:ALA:HB2	1.92	0.51
15:M:27:PHE:HB3	15:M:93:ILE:HD12	1.92	0.51
18:P:32:ARG:NH1	18:P:119:LYS:HE2	2.26	0.51
1:X:69:G:H1'	1:X:72:A:H1'	1.93	0.51
1:X:1128:G:H3'	1:X:1129:A:H5''	1.92	0.51
1:X:2006:G:H5'	1:X:2596:C:H4'	1.92	0.51
1:X:2015:G:OP2	1:X:2433:G:O2'	2.24	0.51
1:X:2312:A:H4'	1:X:2313:G:O5'	2.11	0.51
1:X:2557:G:H2'	1:X:2558:C:C6	2.45	0.51
5:C:129:LYS:C	5:C:131:LYS:H	2.18	0.51
5:C:152:THR:HB	5:C:189:ASP:HB3	1.93	0.51
14:L:27:LEU:O	14:L:88:VAL:HA	2.11	0.51
15:M:32:THR:H	15:M:94:VAL:H	1.57	0.51
18:P:114:ALA:O	18:P:115:ASN:ND2	2.44	0.51
26:Z:35:GLN:HG3	26:Z:51:TYR:CD2	2.45	0.51
1:X:115:G:OP2	1:X:117:A:O2'	2.27	0.51
1:X:421:G:H2'	1:X:422:C:H6	1.76	0.51
1:X:1325:U:H4'	1:X:1326:U:O5'	2.10	0.51
1:X:2432:A:C2	32:X:3316:MPD:HM1	2.46	0.51
1:X:2787:A:H2'	1:X:2788:C:H6	1.75	0.51
1:X:2787:A:H2'	1:X:2788:C:C6	2.46	0.51
14:L:87:VAL:HA	14:L:108:ARG:HH21	1.76	0.51
1:X:163:A:H2'	1:X:164:G:H8	1.75	0.51
1:X:542:A:H5'	16:N:28:ARG:HH21	1.76	0.51
1:X:875:G:H2'	1:X:876:A:O4'	2.11	0.51
1:X:2363:G:OP2	22:T:55:ARG:NH1	2.44	0.51
2:Y:45:C:O2	6:D:92:ARG:NH2	2.44	0.51
7:E:61:HIS:C	7:E:63:ALA:H	2.18	0.51
23:U:17:SER:OG	23:U:45:ASN:N	2.44	0.51
1:X:635:C:O2'	1:X:670:U:OP1	2.26	0.51
1:X:877:G:H1	1:X:924:C:H42	1.59	0.51
1:X:1147:G:H2'	1:X:1148:G:C8	2.46	0.51
1:X:2432:A:H2	32:X:3316:MPD:HM1	1.76	0.51
11:I:62:LYS:CB	29:3:12:ARG:HA	2.41	0.51
29:3:52:LYS:NZ	29:3:56:ALA:HB2	2.26	0.51
1:X:121:G:H2'	1:X:122:G:O4'	2.11	0.51
1:X:1086:C:H3'	1:X:1087:C:H5''	1.93	0.51
1:X:1142:G:H4'	9:G:111:LYS:HE2	1.93	0.51
1:X:2352:A:H2'	1:X:2353:G:H8	1.75	0.51
1:X:2441:U:H1'	1:X:2470:U:O4	2.11	0.51
3:A:268:ARG:NH1	3:A:268:ARG:HA	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:55:ASP:CG	26:Z:39:LYS:HG3	2.36	0.51
1:X:2270:U:O2'	1:X:2353:G:N3	2.43	0.50
1:X:2343:C:H4'	22:T:56:ASP:OD1	2.10	0.50
1:X:2528:G:H2'	1:X:2529:G:C8	2.45	0.50
1:X:2674:C:H2'	1:X:2675:U:H6	1.74	0.50
4:B:143:GLN:HB2	4:B:147:PRO:HG3	1.93	0.50
4:B:152:LYS:HB3	9:G:106:TYR:HA	1.93	0.50
12:J:117:GLU:OE2	12:J:120:ARG:NH2	2.44	0.50
1:X:421:G:H2'	1:X:422:C:C6	2.47	0.50
1:X:1401:G:H1	1:X:1412:C:N4	2.09	0.50
1:X:1952:A:O2'	1:X:1955:G:N3	2.38	0.50
21:S:96:VAL:HG12	21:S:134:LEU:HB2	1.92	0.50
1:X:2845:C:H2'	1:X:2846:G:H5'	1.92	0.50
9:G:61:ARG:NH1	9:G:66:HIS:HB2	2.26	0.50
10:H:4:PRO:O	10:H:5:GLN:HB2	2.10	0.50
11:I:21:ARG:HE	11:I:22:GLY:N	2.08	0.50
11:I:41:SER:O	11:I:41:SER:OG	2.23	0.50
16:N:13:ARG:O	16:N:16:LYS:HB3	2.12	0.50
23:U:11:LYS:HG2	23:U:12:ASN:N	2.26	0.50
1:X:652:C:H42	1:X:657:A:N6	2.09	0.50
1:X:1021:A:O2'	1:X:1163:C:O2	2.29	0.50
1:X:1173:G:H2'	1:X:1174:G:H8	1.76	0.50
1:X:1919:A:H2	1:X:1926:U:H3	1.60	0.50
1:X:2827:G:H2'	1:X:2828:C:O4'	2.11	0.50
19:Q:34:THR:O	19:Q:38:ILE:HG12	2.12	0.50
1:X:705:C:H5'	3:A:41:GLY:HA2	1.94	0.50
1:X:1785:A:H2'	1:X:1786:C:C6	2.47	0.50
1:X:2708:U:H2'	1:X:2709:C:C6	2.47	0.50
7:E:38:ASN:ND2	7:E:40:GLU:OE2	2.37	0.50
13:K:39:THR:O	13:K:42:LYS:N	2.44	0.50
1:X:760:U:HO2'	1:X:761:G:P	2.33	0.50
1:X:1810:U:OP2	3:A:157:ARG:HD2	2.11	0.50
1:X:2314:A:O2'	1:X:2315:A:H2'	2.11	0.50
1:X:2382:C:N4	1:X:2393:G:H1	2.09	0.50
9:G:160:ALA:O	9:G:161:GLN:NE2	2.45	0.50
1:X:1016:C:H1'	1:X:1023:U:N3	2.27	0.50
1:X:2519:C:O2'	1:X:2720:A:N3	2.39	0.50
1:X:2797:G:OP2	4:B:111:LYS:HG3	2.12	0.50
3:A:231:HIS:NE2	3:A:248:THR:HB	2.26	0.50
4:B:99:GLY:N	4:B:172:VAL:O	2.42	0.50
5:C:48:ARG:O	5:C:51:VAL:N	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:113:GLU:O	9:G:114:THR:HB	2.12	0.50
11:I:88:PHE:O	11:I:90:ARG:NH2	2.42	0.50
14:L:15:ARG:HA	14:L:15:ARG:HH11	1.76	0.50
16:N:83:LEU:HD11	16:N:109:LEU:HD13	1.94	0.50
29:3:44:LYS:O	29:3:44:LYS:HE3	2.12	0.50
1:X:2493:U:H2'	1:X:2494:C:C6	2.46	0.50
6:D:4:LEU:C	6:D:6:THR:H	2.20	0.50
9:G:84:ASN:HD21	9:G:154:GLU:HG2	1.76	0.50
10:H:76:ARG:NH1	10:H:113:PRO:O	2.41	0.50
18:P:59:PHE:CE2	26:Z:30:LEU:HD21	2.46	0.50
23:U:51:ILE:HG13	23:U:59:THR:HG23	1.93	0.50
23:U:65:ASN:HA	23:U:68:ARG:HD3	1.93	0.50
26:Z:51:TYR:HE1	26:Z:55:ARG:HD2	1.77	0.50
1:X:586:G:H2'	1:X:587:A:C8	2.47	0.50
1:X:1407:G:H4'	1:X:1619:A:H4'	1.94	0.50
6:D:63:GLN:NE2	6:D:90:THR:O	2.30	0.50
7:E:9:ILE:HA	7:E:69:ARG:HH11	1.76	0.50
14:L:104:ALA:O	14:L:108:ARG:N	2.45	0.50
1:X:691:C:H2'	1:X:692:C:C6	2.47	0.49
1:X:1751:A:H2'	1:X:1752:U:C6	2.47	0.49
1:X:1830:C:N4	1:X:1882:G:OP2	2.43	0.49
1:X:2664:G:O2'	1:X:2665:G:H5'	2.12	0.49
20:R:29:HIS:CG	20:R:51:VAL:HG22	2.47	0.49
1:X:546:A:H2'	1:X:547:U:C6	2.47	0.49
1:X:613:A:N3	1:X:613:A:H2'	2.27	0.49
1:X:1482:U:OP2	1:X:1562:G:O2'	2.29	0.49
1:X:1752:U:H3'	1:X:1753:A:H5''	1.93	0.49
1:X:2432:A:C2	32:X:3316:MPD:H32	2.45	0.49
6:D:132:ILE:HG13	6:D:154:ILE:HD13	1.93	0.49
11:I:78:SER:HB3	11:I:112:GLY:HA3	1.94	0.49
1:X:659:G:H2'	1:X:660:G:C8	2.47	0.49
1:X:757:U:H2'	1:X:758:G:O4'	2.13	0.49
1:X:1504:G:N2	1:X:1517:C:O2	2.45	0.49
1:X:2546:G:H2'	1:X:2547:C:C6	2.47	0.49
3:A:168:LYS:HB3	3:A:173:VAL:HG13	1.94	0.49
14:L:42:ILE:O	14:L:50:THR:HG22	2.12	0.49
1:X:46:C:H2'	1:X:47:G:H8	1.77	0.49
1:X:810:U:OP2	5:C:56:ARG:HG3	2.11	0.49
1:X:1275:A:OP1	18:P:120:ARG:NH1	2.46	0.49
1:X:1584:G:P	3:A:63:ARG:HH22	2.35	0.49
1:X:1679:U:H2'	1:X:1680:U:O4'	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2824:C:OP1	15:M:100:ARG:NH1	2.45	0.49
8:F:108:ALA:HB2	8:F:127:VAL:HG21	1.93	0.49
26:Z:51:TYR:CE1	26:Z:55:ARG:HD2	2.48	0.49
1:X:699:G:N2	28:2:7:PRO:O	2.46	0.49
1:X:1301:U:O2'	1:X:1664:G:N2	2.45	0.49
1:X:2038:C:C2	32:X:3316:MPD:H13	2.47	0.49
1:X:2222:U:H2'	1:X:2223:U:C6	2.48	0.49
2:Y:51:G:H2'	2:Y:52:G:C8	2.42	0.49
26:Z:32:GLU:HA	26:Z:39:LYS:HA	1.95	0.49
1:X:171:G:H2'	1:X:172:A:O4'	2.13	0.49
1:X:387:A:N6	1:X:414:A:O4'	2.46	0.49
1:X:494:A:HO2'	20:R:68:GLY:H	1.53	0.49
1:X:554:U:H5''	1:X:556:A:C2	2.48	0.49
1:X:1005:U:H1'	17:O:21:ARG:HH22	1.78	0.49
1:X:2768:C:O2'	1:X:2784:A:N3	2.41	0.49
1:X:2797:G:N7	4:B:111:LYS:HE3	2.27	0.49
1:X:2860:C:H2'	1:X:2861:A:O4'	2.12	0.49
2:Y:21:C:N4	2:Y:66:G:H1	2.11	0.49
5:C:33:TRP:HD1	5:C:93:TYR:CZ	2.30	0.49
9:G:62:ILE:O	9:G:77:GLY:HA3	2.13	0.49
1:X:812:G:OP1	5:C:50:GLN:NE2	2.43	0.49
1:X:1448:A:N6	1:X:1574:A:H61	2.10	0.49
1:X:2546:G:H2'	1:X:2547:C:H6	1.78	0.49
4:B:144:ARG:HG3	4:B:145:LYS:H	1.78	0.49
14:L:27:LEU:HD13	14:L:42:ILE:HD11	1.95	0.49
21:S:13:LYS:HA	21:S:18:MET:HE3	1.94	0.49
1:X:1406:A:N6	19:Q:15:LYS:HD3	2.27	0.49
1:X:1918:G:H1'	1:X:1947:G:N2	2.27	0.49
1:X:1949:A:H1'	1:X:2572:U:H5'	1.93	0.49
4:B:4:ILE:HG12	4:B:5:LEU:N	2.26	0.49
5:C:36:ALA:O	5:C:39:ARG:HB3	2.12	0.49
12:J:20:GLY:H	12:J:99:LYS:HZ1	1.61	0.49
13:K:9:LYS:HG2	13:K:11:ASN:H	1.78	0.49
16:N:66:ASN:HD22	16:N:70:ARG:NH2	2.09	0.49
25:W:5:LEU:HB2	25:W:25:LEU:HD13	1.94	0.49
1:X:540:G:C6	1:X:2005:U:H5''	2.48	0.49
1:X:971:A:H61	12:J:83:ARG:HH22	1.59	0.49
1:X:1515:U:H2'	1:X:1516:A:H8	1.78	0.49
1:X:2204:A:H4'	1:X:2205:C:O5'	2.13	0.49
4:B:6:GLY:HA3	4:B:27:LEU:O	2.13	0.49
7:E:89:LEU:HB2	7:E:129:THR:HB	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:26:ARG:NE	25:W:26:ARG:HA	2.28	0.49
27:1:12:MET:HE3	27:1:13:GLU:HG2	1.93	0.49
27:1:12:MET:HB3	27:1:27:ASN:ND2	2.28	0.49
29:3:49:VAL:HG22	29:3:51:ALA:H	1.78	0.49
1:X:1164:C:H2'	1:X:1165:G:O4'	2.12	0.49
1:X:1267:A:H5''	1:X:1268:U:H5''	1.94	0.49
1:X:1623:C:H4'	1:X:1624:A:O5'	2.13	0.49
1:X:1727:C:H2'	1:X:1728:A:C8	2.48	0.49
1:X:1949:A:O2'	1:X:2571:G:O3'	2.31	0.49
2:Y:9:G:H5'	14:L:32:TYR:CE1	2.47	0.49
2:Y:39:C:N4	2:Y:51:G:O4'	2.46	0.49
3:A:231:HIS:HE2	3:A:248:THR:HB	1.76	0.49
3:A:252:LYS:HG3	3:A:253:PRO:HD2	1.95	0.49
6:D:70:ALA:O	6:D:71:LYS:NZ	2.39	0.49
12:J:82:THR:OG1	12:J:83:ARG:N	2.44	0.49
1:X:66:U:H2'	1:X:67:G:C8	2.48	0.48
1:X:591:G:H1	1:X:1271:C:H42	1.61	0.48
1:X:732:G:H2'	1:X:733:G:C8	2.48	0.48
1:X:814:G:OP2	5:C:49:ALA:HB3	2.13	0.48
1:X:859:U:H1'	1:X:860:U:C5	2.48	0.48
1:X:2309:G:H2'	1:X:2310:G:O4'	2.13	0.48
1:X:2604:G:H2'	1:X:2605:C:C6	2.48	0.48
6:D:135:GLN:HB3	6:D:151:GLY:HA2	1.95	0.48
7:E:33:LEU:HD22	7:E:136:ILE:HG22	1.94	0.48
9:G:161:GLN:HE21	9:G:161:GLN:HA	1.78	0.48
10:H:116:ARG:HD3	15:M:40:ARG:HE	1.77	0.48
21:S:113:VAL:HA	21:S:171:VAL:HG22	1.95	0.48
23:U:33:LYS:HD2	23:U:34:THR:H	1.77	0.48
1:X:682:G:H3'	1:X:683:A:C8	2.48	0.48
1:X:1204:G:H2'	1:X:1205:G:H8	1.77	0.48
1:X:1805:G:O2'	3:A:43:ARG:HG3	2.13	0.48
1:X:1831:G:H2'	1:X:1832:G:C8	2.43	0.48
1:X:2301:A:H2'	1:X:2302:G:O4'	2.13	0.48
1:X:2691:C:H2'	1:X:2694:G:H5''	1.94	0.48
2:Y:17:A:H5'	2:Y:18:G:C8	2.48	0.48
1:X:1203:A:OP1	11:I:35:LYS:NZ	2.33	0.48
1:X:2197:U:H5'	1:X:2198:U:OP1	2.14	0.48
4:B:132:LYS:N	4:B:132:LYS:HD2	2.28	0.48
21:S:91:PRO:HG3	21:S:127:PRO:HG3	1.95	0.48
1:X:755:C:H2'	1:X:756:C:O4'	2.13	0.48
1:X:795:A:N7	3:A:221:GLN:HG2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1181:C:N4	1:X:1182:U:O4	2.47	0.48
1:X:1810:U:O2'	3:A:154:GLN:O	2.30	0.48
1:X:2281:C:N4	1:X:2293:G:H1	2.11	0.48
4:B:132:LYS:HZ3	4:B:132:LYS:CA	2.23	0.48
5:C:116:LYS:HZ2	5:C:117:LEU:N	2.01	0.48
6:D:114:PHE:CZ	6:D:116:GLY:HA2	2.48	0.48
10:H:1:MET:N	10:H:1:MET:SD	2.83	0.48
16:N:22:LYS:C	16:N:24:PHE:H	2.21	0.48
16:N:50:ARG:HA	16:N:53:LYS:HE3	1.96	0.48
1:X:490:A:HO2'	1:X:492:G:H8	1.62	0.48
1:X:1601:U:O2'	1:X:1602:G:N7	2.42	0.48
1:X:2441:U:H2'	1:X:2442:C:C6	2.47	0.48
2:Y:42:U:H3'	2:Y:43:G:H5'	1.94	0.48
3:A:244:ARG:HH11	3:A:246:PRO:HG2	1.78	0.48
5:C:119:ALA:HB3	5:C:189:ASP:HA	1.96	0.48
12:J:71:PRO:HA	12:J:96:SER:HB2	1.95	0.48
13:K:60:LEU:HD11	13:K:64:ARG:NE	2.27	0.48
13:K:87:TYR:HE1	13:K:94:TYR:HD2	1.59	0.48
17:O:26:GLN:HB2	17:O:63:HIS:CE1	2.48	0.48
23:U:16:ASN:O	23:U:17:SER:OG	2.19	0.48
27:1:9:ILE:HB	27:1:27:ASN:O	2.12	0.48
1:X:334:G:C8	5:C:164:VAL:HA	2.49	0.48
1:X:689:A:H8	1:X:2052:G:H21	1.60	0.48
1:X:736:G:H2'	1:X:737:C:O4'	2.14	0.48
1:X:757:U:H3	1:X:766:A:H61	1.61	0.48
1:X:1296:G:N2	1:X:1299:A:H5'	2.29	0.48
1:X:2441:U:H2'	1:X:2442:C:H6	1.77	0.48
1:X:2679:G:H2'	1:X:2680:U:C6	2.48	0.48
3:A:13:ARG:NH1	3:A:16:MET:SD	2.87	0.48
4:B:176:ARG:HH22	15:M:16:ILE:HA	1.77	0.48
5:C:147:LYS:H	5:C:184:ASP:CG	2.21	0.48
16:N:84:LYS:HA	16:N:92:ARG:HH22	1.79	0.48
20:R:84:VAL:HG12	20:R:90:LYS:O	2.13	0.48
1:X:1151:U:OP1	9:G:53:ARG:NH2	2.47	0.48
1:X:1782:A:O2'	3:A:207:GLY:O	2.27	0.48
1:X:1978:U:H1'	10:H:3:MET:HE1	1.95	0.48
3:A:166:GLN:HB3	3:A:174:ILE:HB	1.94	0.48
1:X:691:C:H2'	1:X:692:C:H6	1.78	0.48
1:X:859:U:O2'	1:X:860:U:H6	1.95	0.48
6:D:133:LYS:O	6:D:151:GLY:HA3	2.12	0.48
1:X:279:A:N6	1:X:280:C:H41	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:545:C:H2'	1:X:546:A:C8	2.49	0.48
1:X:859:U:H1'	1:X:860:U:H5	1.77	0.48
1:X:1412:C:O2'	1:X:1413:U:O5'	2.32	0.48
1:X:1514:C:H4'	1:X:1592:U:O2'	2.13	0.48
1:X:1563:U:H2'	1:X:1564:U:C6	2.49	0.48
1:X:2039:G:C2	1:X:2040:A:C8	3.02	0.48
1:X:2039:G:O2'	26:Z:8:LYS:HE2	2.14	0.48
1:X:2591:C:O2'	1:X:2592:U:OP1	2.30	0.48
1:X:2821:G:H2'	1:X:2822:U:O4'	2.14	0.48
2:Y:19:C:H2'	2:Y:20:A:C8	2.48	0.48
3:A:145:LEU:HD21	3:A:185:VAL:HG21	1.95	0.48
10:H:76:ARG:HB2	10:H:95:ALA:HB3	1.94	0.48
13:K:9:LYS:HD2	13:K:11:ASN:N	2.27	0.48
15:M:113:LYS:HA	15:M:113:LYS:HE2	1.96	0.48
19:Q:89:GLU:HB3	19:Q:90:ALA:H	1.51	0.48
1:X:513:A:H5''	1:X:514:G:H5'	1.96	0.48
1:X:1974:U:H2'	1:X:1975:G:H5''	1.95	0.48
3:A:45:ASN:CG	3:A:46:ARG:H	2.22	0.48
4:B:113:THR:HA	4:B:159:HIS:HA	1.96	0.48
11:I:97:ARG:HD3	11:I:99:VAL:HG22	1.96	0.48
11:I:120:VAL:HB	11:I:140:VAL:HG22	1.96	0.48
12:J:38:MET:SD	12:J:131:LYS:HE3	2.54	0.48
13:K:13:ASN:HB2	13:K:16:ALA:H	1.78	0.48
14:L:29:LEU:HD12	14:L:42:ILE:HB	1.96	0.48
1:X:165:G:H1	1:X:185:C:H42	1.60	0.47
1:X:825:C:O2'	1:X:1239:A:O2'	2.30	0.47
1:X:1500:U:H3	1:X:1520:G:H1	1.62	0.47
5:C:97:ARG:O	5:C:101:GLN:HG2	2.14	0.47
6:D:36:VAL:HG13	6:D:154:ILE:HG13	1.96	0.47
9:G:128:GLU:HG3	9:G:150:VAL:HG21	1.97	0.47
23:U:17:SER:CB	23:U:44:ALA:HA	2.44	0.47
1:X:313:U:H2'	1:X:314:G:C8	2.47	0.47
1:X:529:U:H2'	1:X:530:G:C8	2.49	0.47
1:X:1004:A:H2	17:O:21:ARG:HH21	1.60	0.47
1:X:1026:U:H2'	1:X:1027:C:C6	2.49	0.47
1:X:1427:G:H2'	1:X:1428:G:H4'	1.95	0.47
1:X:2015:G:N7	32:X:3316:MPD:H11	2.30	0.47
1:X:2040:A:H2'	1:X:2041:A:C8	2.50	0.47
1:X:2809:A:H8	1:X:2858:A:N6	2.06	0.47
3:A:163:VAL:HG22	3:A:177:LEU:HA	1.95	0.47
5:C:149:LEU:HD23	5:C:180:ILE:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:63:ARG:O	29:3:11:LYS:HB3	2.14	0.47
13:K:81:ASP:O	13:K:85:PRO:HG2	2.14	0.47
16:N:76:TYR:CZ	16:N:80:ILE:HG13	2.49	0.47
17:O:20:ILE:HD12	17:O:21:ARG:HG2	1.96	0.47
18:P:60:ILE:HA	18:P:61:PRO:HD3	1.47	0.47
1:X:196:A:N6	1:X:441:A:OP1	2.47	0.47
1:X:572:G:H5'	1:X:581:A:H4'	1.96	0.47
1:X:1116:U:H2'	1:X:1117:G:C8	2.46	0.47
1:X:2727:G:O6	1:X:2735:C:H5''	2.14	0.47
5:C:56:ARG:CG	5:C:57:LYS:H	2.23	0.47
18:P:9:ARG:HH11	18:P:10:ASN:HD21	1.61	0.47
1:X:477:A:H5'	28:2:21:ARG:NH2	2.29	0.47
1:X:502:A:H2'	1:X:503:G:O4'	2.15	0.47
1:X:794:A:H2	1:X:1767:G:N3	2.12	0.47
1:X:1909:U:H4'	1:X:1910:A:OP1	2.15	0.47
1:X:1981:A:O2'	1:X:2704:U:O2'	2.22	0.47
3:A:132:PRO:HD3	3:A:190:TYR:CE1	2.49	0.47
13:K:99:ARG:NH1	26:Z:43:HIS:O	2.43	0.47
1:X:240:U:H2'	1:X:241:C:O4'	2.14	0.47
1:X:537:C:H2'	1:X:538:A:C2	2.49	0.47
1:X:2844:G:H2'	1:X:2845:C:O4'	2.15	0.47
4:B:105:THR:HG21	4:B:199:ARG:HH11	1.80	0.47
9:G:61:ARG:HA	9:G:61:ARG:HE	1.79	0.47
12:J:43:ILE:HG21	12:J:48:ILE:HG23	1.96	0.47
20:R:17:LYS:HG2	20:R:18:LYS:H	1.79	0.47
1:X:1729:C:H2'	1:X:1730:G:C8	2.50	0.47
1:X:2367:A:N7	1:X:2368:G:C6	2.83	0.47
1:X:2557:G:N7	4:B:140:SER:HB2	2.29	0.47
3:A:91:ARG:CZ	3:A:198:ASN:H	2.28	0.47
18:P:22:LYS:HA	18:P:23:PRO:HD3	1.59	0.47
1:X:59:G:H1'	1:X:73:A:C2	2.50	0.47
1:X:202:A:C2	1:X:203:G:H1'	2.50	0.47
1:X:512:A:OP1	18:P:16:GLN:HB3	2.15	0.47
1:X:1070:G:N2	8:F:130:THR:OG1	2.47	0.47
1:X:1560:A:C6	1:X:1561:A:C6	3.03	0.47
1:X:2478:C:N3	32:X:3316:MPD:H52	2.29	0.47
1:X:2616:U:H5'	4:B:44:TYR:CE2	2.50	0.47
3:A:8:PRO:HB3	3:A:14:ARG:HB3	1.96	0.47
3:A:160:GLY:H	3:A:196:VAL:HB	1.80	0.47
4:B:14:ILE:HA	15:M:20:HIS:CD2	2.49	0.47
4:B:133:LYS:O	4:B:134:TRP:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:22:VAL:HG13	5:C:106:MET:HB3	1.97	0.47
5:C:148:VAL:HG12	5:C:166:TRP:CD1	2.49	0.47
5:C:158:ARG:HD2	5:C:169:VAL:HG13	1.97	0.47
6:D:74:ILE:HG23	6:D:75:SER:H	1.79	0.47
17:O:50:ASP:O	17:O:53:LYS:HB3	2.14	0.47
21:S:69:VAL:HG13	21:S:81:VAL:HG22	1.97	0.47
29:3:14:ILE:HG21	29:3:56:ALA:HB1	1.96	0.47
1:X:655:A:C2'	1:X:656:U:H5'	2.45	0.47
1:X:790:A:O2'	3:A:48:ARG:NH2	2.47	0.47
1:X:810:U:H2'	1:X:811:G:O4'	2.14	0.47
1:X:825:C:H2'	1:X:826:U:H6	1.80	0.47
1:X:1003:C:H2'	1:X:1004:A:H8	1.78	0.47
1:X:2245:A:H4'	1:X:2246:A:N3	2.29	0.47
14:L:39:TYR:N	14:L:39:TYR:CD1	2.83	0.47
16:N:66:ASN:OD1	16:N:66:ASN:N	2.48	0.47
1:X:597:U:H2'	1:X:598:U:C6	2.49	0.47
1:X:1573:G:O6	1:X:1574:A:N6	2.47	0.47
1:X:2000:U:H4'	26:Z:8:LYS:O	2.15	0.47
1:X:2370:G:O6	1:X:2406:C:H1'	2.15	0.47
1:X:2511:G:N2	1:X:2642:G:O2'	2.48	0.47
2:Y:32:C:H1'	2:Y:59:A:N6	2.29	0.47
3:A:231:HIS:CE1	3:A:247:VAL:HG12	2.50	0.47
4:B:5:LEU:HB3	4:B:197:VAL:HG22	1.97	0.47
4:B:26:VAL:HG12	4:B:182:ILE:HG23	1.96	0.47
5:C:33:TRP:CE3	5:C:95:LEU:HD12	2.49	0.47
5:C:116:LYS:NZ	5:C:186:LEU:O	2.48	0.47
6:D:174:GLY:O	6:D:176:PRO:HD3	2.15	0.47
1:X:1148:G:N3	9:G:134:MET:HE2	2.30	0.47
1:X:1554:G:H2'	1:X:1555:A:H8	1.80	0.47
1:X:2314:A:HO2'	1:X:2315:A:H8	1.61	0.47
1:X:2543:A:C2	1:X:2626:U:H4'	2.50	0.47
27:1:24:THR:O	27:1:24:THR:OG1	2.27	0.47
1:X:1336:G:H2'	1:X:1337:G:H5'	1.97	0.46
1:X:1582:A:O4'	3:A:214:TRP:HB3	2.15	0.46
5:C:179:ASP:HA	5:C:182:ARG:HD3	1.97	0.46
8:F:77:LEU:O	8:F:103:GLN:NE2	2.48	0.46
13:K:66:VAL:HG12	13:K:76:VAL:HG23	1.95	0.46
15:M:104:LEU:HD23	15:M:104:LEU:HA	1.65	0.46
27:1:53:LYS:HG2	27:1:54:LYS:H	1.80	0.46
1:X:387:A:O2'	1:X:388:G:H8	1.83	0.46
1:X:768:U:C4	1:X:769:C:C4	3.03	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:941:U:H2'	1:X:942:U:O4'	2.16	0.46
1:X:2270:U:H2'	1:X:2271:C:C6	2.51	0.46
2:Y:89:G:N2	2:Y:92:G:OP2	2.34	0.46
3:A:18:THR:OG1	3:A:19:ALA:N	2.47	0.46
5:C:149:LEU:HD11	5:C:170:LEU:HB2	1.98	0.46
15:M:60:SER:O	15:M:63:ARG:NH1	2.48	0.46
16:N:79:PHE:CE1	16:N:110:VAL:HA	2.48	0.46
19:Q:7:LEU:HD13	19:Q:7:LEU:H	1.80	0.46
1:X:884:C:H4'	12:J:70:PHE:CE1	2.50	0.46
1:X:1257:U:OP1	11:I:16:ARG:NH1	2.48	0.46
1:X:1710:U:O2'	3:A:14:ARG:NH2	2.49	0.46
1:X:2058:U:C4	1:X:2217:G:C6	3.03	0.46
1:X:2448:A:H4'	12:J:57:ARG:HD2	1.97	0.46
1:X:2557:G:C5	4:B:140:SER:HB2	2.51	0.46
9:G:114:THR:O	9:G:119:LEU:HG	2.16	0.46
9:G:156:HIS:HB2	9:G:157:PRO:HD3	1.97	0.46
11:I:93:LEU:HD12	11:I:97:ARG:HB2	1.97	0.46
14:L:26:ARG:NE	14:L:87:VAL:HG22	2.30	0.46
19:Q:26:SER:HB3	19:Q:79:ILE:HG12	1.97	0.46
22:T:29:GLU:O	22:T:67:VAL:HG12	2.15	0.46
1:X:123:A:C5	28:2:10:ARG:HB2	2.50	0.46
1:X:987:G:O2'	1:X:1166:A:O2'	2.32	0.46
1:X:1812:U:N3	3:A:200:GLU:OE1	2.48	0.46
1:X:2241:U:OP1	22:T:19:LYS:HG3	2.16	0.46
4:B:193:GLY:O	15:M:2:GLN:N	2.49	0.46
16:N:47:TYR:O	16:N:51:ARG:NH1	2.45	0.46
21:S:72:ASP:HB2	21:S:79:ILE:HG23	1.97	0.46
22:T:15:ASP:OD1	22:T:16:SER:N	2.48	0.46
1:X:29:U:C5	32:X:3315:MPD:H51	2.50	0.46
1:X:533:C:O2	1:X:563:U:O2'	2.34	0.46
1:X:663:G:H8	1:X:664:C:H4'	1.79	0.46
1:X:2186:G:H2'	1:X:2187:A:C8	2.50	0.46
1:X:2772:U:H2'	1:X:2773:G:C8	2.50	0.46
2:Y:39:C:H5'	2:Y:40:C:OP2	2.16	0.46
4:B:31:CYS:HB2	4:B:90:SER:HB3	1.98	0.46
14:L:43:ILE:HA	14:L:50:THR:HA	1.98	0.46
1:X:717:G:N3	1:X:739:G:C2	2.84	0.46
1:X:1149:G:O2'	1:X:1154:A:N1	2.44	0.46
1:X:1586:A:H2'	1:X:1587:A:C8	2.50	0.46
1:X:1599:G:H2'	1:X:1600:U:H4'	1.97	0.46
1:X:1670:G:C6	13:K:9:LYS:HG3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1725:C:H42	1:X:1741:G:H1	1.62	0.46
1:X:1781:C:H2'	1:X:1782:A:C5	2.51	0.46
1:X:1845:A:N3	1:X:2212:U:O2'	2.36	0.46
1:X:2210:C:OP1	23:U:45:ASN:HA	2.14	0.46
1:X:2672:U:H2'	1:X:2673:G:C8	2.41	0.46
5:C:104:LEU:HA	5:C:107:ALA:HB3	1.97	0.46
12:J:20:GLY:H	12:J:99:LYS:NZ	2.14	0.46
1:X:646:C:H2'	1:X:647:G:O4'	2.16	0.46
1:X:1361:G:H1	1:X:1614:C:H42	1.63	0.46
1:X:2447:G:O2'	1:X:2448:A:H8	1.97	0.46
3:A:247:VAL:N	3:A:250:TRP:O	2.49	0.46
5:C:163:ASN:OD1	5:C:164:VAL:N	2.41	0.46
6:D:38:GLU:O	6:D:87:ILE:HG12	2.16	0.46
10:H:51:ILE:HG12	10:H:52:VAL:N	2.31	0.46
27:1:13:GLU:HB2	27:1:24:THR:HG22	1.98	0.46
1:X:227:G:H5'	29:3:8:LYS:HD3	1.96	0.46
1:X:308:C:H5''	20:R:95:ARG:HD3	1.98	0.46
1:X:554:U:H5''	1:X:556:A:N3	2.31	0.46
1:X:1991:C:H2'	1:X:1992:G:H8	1.80	0.46
1:X:2226:A:H2'	1:X:2227:C:C6	2.51	0.46
1:X:2428:U:H4'	1:X:2429:A:OP1	2.15	0.46
1:X:2552:C:H5''	1:X:2553:G:H5''	1.98	0.46
1:X:2725:C:H2'	1:X:2726:U:C6	2.51	0.46
1:X:2790:C:H2'	1:X:2791:C:C6	2.51	0.46
4:B:60:ASN:O	4:B:64:GLN:HG3	2.16	0.46
6:D:152:MET:HE3	6:D:154:ILE:HD11	1.98	0.46
16:N:6:THR:HG21	16:N:10:ARG:NH2	2.31	0.46
21:S:25:ASN:HB3	21:S:85:MET:HG3	1.98	0.46
21:S:62:PHE:HD2	21:S:85:MET:HE2	1.81	0.46
21:S:116:VAL:N	21:S:168:VAL:O	2.44	0.46
1:X:104:C:H2'	1:X:105:G:H8	1.80	0.46
1:X:224:G:H4'	1:X:399:G:C4	2.50	0.46
1:X:500:G:H8	1:X:500:G:OP1	1.99	0.46
1:X:540:G:C5	1:X:2005:U:H5''	2.51	0.46
1:X:1437:A:H2'	1:X:1438:G:C8	2.50	0.46
1:X:2842:C:H6	1:X:2842:C:H2'	1.57	0.46
7:E:147:ASN:O	7:E:150:LYS:HB2	2.16	0.46
15:M:13:LEU:HD12	15:M:13:LEU:HA	1.66	0.46
18:P:17:GLN:HG3	18:P:18:VAL:HG23	1.98	0.46
1:X:26:G:C6	1:X:27:G:N1	2.84	0.46
1:X:139:A:H2'	1:X:140:G:H8	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:420:C:H2'	1:X:421:G:H8	1.81	0.46
1:X:1336:G:O6	1:X:1337:G:C6	2.69	0.46
1:X:1623:C:H5''	1:X:1624:A:H5'	1.98	0.46
1:X:2078:G:H1	1:X:2177:U:H3	1.62	0.46
1:X:2171:U:H4'	1:X:2171:U:OP1	2.14	0.46
6:D:40:LEU:HD11	6:D:53:ALA:HB3	1.97	0.46
6:D:104:ILE:HA	6:D:108:LEU:HD12	1.98	0.46
9:G:70:PHE:HB3	16:N:64:ARG:HG2	1.97	0.46
9:G:103:TYR:CG	9:G:104:THR:N	2.83	0.46
16:N:81:ASN:O	16:N:85:ARG:N	2.40	0.46
1:X:172:A:H61	1:X:175:C:H3'	1.81	0.45
1:X:1124:U:H2'	1:X:1125:G:H8	1.81	0.45
1:X:1310:C:H2'	1:X:1311:C:H6	1.80	0.45
1:X:1706:A:H2'	1:X:1707:A:H8	1.80	0.45
1:X:1806:G:O5'	3:A:43:ARG:NE	2.48	0.45
2:Y:28:A:H8	2:Y:29:C:C2	2.34	0.45
3:A:71:ASP:OD1	3:A:71:ASP:N	2.49	0.45
19:Q:25:TYR:OH	19:Q:87:SER:HA	2.16	0.45
1:X:219:G:H4'	1:X:220:U:O5'	2.15	0.45
1:X:1268:U:C5	5:C:67:ALA:HA	2.51	0.45
1:X:2240:C:OP1	22:T:17:ASN:ND2	2.49	0.45
3:A:170:SER:OG	3:A:171:ASP:N	2.48	0.45
6:D:33:LYS:HD3	6:D:92:ARG:NH1	2.30	0.45
7:E:27:LYS:HG2	7:E:32:GLU:HB3	1.98	0.45
11:I:123:ASP:OD1	11:I:123:ASP:N	2.50	0.45
12:J:59:PHE:C	12:J:61:ARG:H	2.24	0.45
16:N:3:ARG:HH21	16:N:5:LYS:HB3	1.81	0.45
18:P:9:ARG:HD2	18:P:10:ASN:ND2	2.31	0.45
23:U:22:GLY:HA3	23:U:39:LYS:CB	2.47	0.45
23:U:47:HIS:CG	23:U:48:LYS:N	2.84	0.45
23:U:55:GLY:O	23:U:56:GLN:HB3	2.16	0.45
1:X:36:G:N3	1:X:462:G:O2'	2.48	0.45
1:X:116:A:OP2	1:X:117:A:H2'	2.17	0.45
1:X:1016:C:C2	1:X:1154:A:C5	3.04	0.45
1:X:2411:A:C6	1:X:2412:A:C6	3.04	0.45
26:Z:25:LEU:HD12	26:Z:25:LEU:HA	1.83	0.45
28:2:34:ARG:HD3	28:2:42:LEU:HD13	1.98	0.45
1:X:32:C:O2'	1:X:33:C:H5'	2.16	0.45
1:X:58:C:H1'	1:X:72:A:H2'	1.98	0.45
1:X:503:G:H2'	1:X:504:G:O4'	2.16	0.45
1:X:1278:A:H2	1:X:1997:A:H62	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1493:A:H2'	1:X:1494:G:O4'	2.15	0.45
1:X:1542:G:H22	1:X:1562:G:N2	2.15	0.45
1:X:1715:A:O4'	1:X:1717:A:H4'	2.16	0.45
1:X:1973:C:H2'	1:X:1974:U:O4'	2.16	0.45
1:X:2328:G:OP2	29:3:42:ARG:HG3	2.16	0.45
6:D:135:GLN:N	6:D:150:ARG:O	2.41	0.45
9:G:70:PHE:O	16:N:64:ARG:NH1	2.48	0.45
12:J:62:GLY:HA3	12:J:64:LYS:HD2	1.98	0.45
1:X:250:C:C2'	1:X:251:C:H5''	2.46	0.45
1:X:396:U:O4	1:X:398:C:H2'	2.16	0.45
1:X:1432:G:H21	1:X:1596:A:H62	1.63	0.45
1:X:1672:A:C2	1:X:1673:C:H1'	2.51	0.45
3:A:33:LEU:O	3:A:64:ILE:HB	2.17	0.45
3:A:36:ALA:HB3	3:A:61:LEU:HD22	1.97	0.45
3:A:86:PRO:O	3:A:87:ASN:ND2	2.50	0.45
4:B:84:PHE:CD1	4:B:86:PRO:HD3	2.51	0.45
4:B:117:MET:HE3	4:B:122:PHE:O	2.16	0.45
14:L:38:ILE:HG22	14:L:99:ARG:HH21	1.80	0.45
18:P:31:VAL:HG22	18:P:122:SER:O	2.17	0.45
18:P:32:ARG:NH1	18:P:119:LYS:HB3	2.32	0.45
28:2:10:ARG:HA	28:2:13:ALA:HB3	1.99	0.45
1:X:784:U:H2'	1:X:785:U:C6	2.52	0.45
1:X:1074:G:H1	1:X:1086:C:N4	2.15	0.45
1:X:1891:C:H2'	1:X:1892:C:O4'	2.17	0.45
1:X:1997:A:H2'	1:X:1998:A:C8	2.51	0.45
1:X:2033:C:N4	1:X:2034:A:N1	2.65	0.45
1:X:2048:C:O2	1:X:2428:U:N3	2.39	0.45
2:Y:7:C:H2'	2:Y:8:C:C6	2.51	0.45
10:H:20:MET:HG2	10:H:21:CYS:N	2.29	0.45
12:J:48:ILE:HG21	12:J:69:ILE:HD12	1.98	0.45
14:L:90:ASP:CG	14:L:91:ARG:N	2.74	0.45
21:S:149:ALA:HB1	21:S:160:LEU:HD11	1.97	0.45
27:1:43:VAL:HG23	27:1:44:ALA:H	1.81	0.45
29:3:51:ALA:O	29:3:55:TRP:HZ3	2.00	0.45
1:X:26:G:H1'	1:X:525:A:H61	1.82	0.45
1:X:79:G:H2'	1:X:80:A:C8	2.52	0.45
1:X:347:C:H4'	20:R:15:HIS:CD2	2.52	0.45
1:X:780:U:O2'	1:X:781:G:OP2	2.32	0.45
1:X:992:A:N1	1:X:2010:G:O2'	2.48	0.45
1:X:1289:A:C2	1:X:1290:A:C8	3.04	0.45
1:X:1811:A:OP2	3:A:156:ALA:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2034:A:H4'	4:B:141:ILE:HG12	1.99	0.45
1:X:2076:G:N3	1:X:2181:A:N6	2.62	0.45
1:X:2660:C:C2	1:X:2704:U:O4	2.70	0.45
3:A:76:ASN:OD1	3:A:118:ASN:ND2	2.46	0.45
9:G:93:LYS:HZ3	9:G:93:LYS:HG2	1.38	0.45
9:G:162:LYS:N	9:G:163:PRO:HD2	2.32	0.45
14:L:42:ILE:HG23	14:L:52:ALA:H	1.82	0.45
21:S:3:LEU:HD11	21:S:6:LYS:HD3	1.99	0.45
1:X:1893:G:H4'	1:X:1908:C:C6	2.52	0.45
1:X:1999:U:O2	26:Z:7:PRO:HG2	2.16	0.45
1:X:2661:G:N3	4:B:22:PRO:HB3	2.31	0.45
5:C:6:VAL:HG21	5:C:136:TRP:CZ2	2.52	0.45
5:C:17:LEU:HG	5:C:109:ALA:HB1	1.99	0.45
6:D:65:PRO:HA	6:D:89:VAL:HG13	1.99	0.45
14:L:51:LEU:HD11	14:L:82:LYS:HG2	1.99	0.45
18:P:37:LYS:O	18:P:40:LEU:HB2	2.17	0.45
27:1:27:ASN:OD1	27:1:27:ASN:N	2.50	0.45
29:3:15:LYS:HB2	29:3:23:MET:HB2	1.98	0.45
1:X:18:U:O2'	1:X:563:U:OP1	2.34	0.45
1:X:1066:G:O2'	1:X:1096:A:N1	2.49	0.45
1:X:1134:C:H2'	1:X:1135:C:C6	2.50	0.45
1:X:1684:G:O2'	1:X:1974:U:O4	2.32	0.45
1:X:1882:G:H21	1:X:1885:C:H41	1.62	0.45
1:X:2543:A:OP1	1:X:2627:G:O2'	2.21	0.45
1:X:2556:A:H5''	1:X:2557:G:H5'	1.99	0.45
7:E:103:LEU:HD21	7:E:131:ILE:HD13	1.98	0.45
9:G:89:ALA:O	9:G:90:LEU:HD12	2.17	0.45
12:J:47:GLN:O	12:J:50:ALA:N	2.50	0.45
18:P:91:PHE:CD1	18:P:131:LYS:HD3	2.52	0.45
22:T:46:LYS:HB3	22:T:78:PHE:CE1	2.52	0.45
1:X:609:U:H4'	11:I:18:ARG:NH2	2.31	0.45
1:X:687:G:O2'	5:C:61:GLN:NE2	2.50	0.45
1:X:836:G:H2'	1:X:837:U:H6	1.81	0.45
1:X:1182:U:O2'	1:X:1183:C:H5''	2.16	0.45
1:X:2523:G:H2'	1:X:2524:G:O4'	2.17	0.45
1:X:2541:U:O2'	10:H:23:ARG:NH2	2.47	0.45
1:X:2596:C:H2'	1:X:2597:G:C8	2.50	0.45
2:Y:94:G:H5''	21:S:74:ARG:HH22	1.82	0.45
3:A:67:PHE:HB3	3:A:153:ALA:H	1.81	0.45
9:G:97:ASP:O	9:G:99:VAL:HG13	2.17	0.45
11:I:42:GLY:HA2	11:I:45:LYS:NZ	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:24:LYS:HB2	22:T:36:ILE:O	2.17	0.45
1:X:94:C:O2'	24:V:41:HIS:ND1	2.41	0.44
1:X:832:A:OP2	1:X:1201:G:N2	2.42	0.44
1:X:1173:G:H2'	1:X:1174:G:C8	2.52	0.44
1:X:1727:C:H2'	1:X:1728:A:H8	1.82	0.44
1:X:2067:U:H2'	1:X:2068:C:C6	2.52	0.44
1:X:2255:G:C2	1:X:2256:G:C8	3.05	0.44
6:D:10:ASP:HB3	6:D:11:GLN:H	1.63	0.44
20:R:23:ILE:HB	20:R:81:VAL:HG11	1.98	0.44
21:S:91:PRO:HG3	21:S:127:PRO:CG	2.47	0.44
29:3:15:LYS:HA	29:3:15:LYS:HD3	1.56	0.44
1:X:79:G:H2'	1:X:80:A:H8	1.81	0.44
1:X:427:C:H1'	1:X:1856:U:H1'	1.99	0.44
1:X:545:C:O3'	16:N:53:LYS:NZ	2.34	0.44
1:X:1212:U:H2'	1:X:1213:U:H6	1.81	0.44
1:X:1419:G:H2'	1:X:1420:A:C8	2.52	0.44
1:X:1469:U:H1'	13:K:60:LEU:CD1	2.44	0.44
1:X:2043:A:O2'	1:X:2481:G:O4'	2.35	0.44
1:X:2484:G:HO2'	1:X:2485:U:H6	1.61	0.44
1:X:2551:A:N7	4:B:145:LYS:HB3	2.32	0.44
2:Y:10:U:OP1	14:L:12:ARG:NH2	2.50	0.44
11:I:11:GLY:HA3	11:I:14:LYS:HD2	2.00	0.44
17:O:19:VAL:HG13	17:O:90:PHE:CD2	2.53	0.44
17:O:38:LEU:HD13	17:O:39:PHE:N	2.32	0.44
20:R:46:VAL:HG21	20:R:80:LYS:HE3	1.98	0.44
21:S:70:GLN:HB3	21:S:80:HIS:CB	2.45	0.44
27:1:12:MET:HE2	27:1:53:LYS:C	2.42	0.44
1:X:742:G:O6	3:A:208:LYS:HB3	2.17	0.44
1:X:787:A:H2	1:X:800:U:O2'	1.99	0.44
1:X:1921:A:O2'	1:X:1922:U:H5''	2.18	0.44
1:X:2241:U:H2'	1:X:2242:C:H6	1.82	0.44
1:X:2684:A:O5'	1:X:2684:A:H8	2.01	0.44
1:X:2825:A:C2	1:X:2826:C:C2	3.06	0.44
1:X:2827:G:C6	1:X:2828:C:N3	2.85	0.44
4:B:105:THR:HG21	4:B:199:ARG:NH1	2.32	0.44
6:D:34:ILE:HD13	6:D:156:ILE:HA	1.99	0.44
6:D:84:PRO:O	6:D:85:VAL:HG22	2.18	0.44
16:N:50:ARG:O	16:N:53:LYS:HG2	2.18	0.44
19:Q:43:GLN:HG2	19:Q:48:VAL:O	2.17	0.44
1:X:123:A:H2'	28:2:13:ALA:HB1	1.99	0.44
1:X:334:G:C6	5:C:164:VAL:HG22	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:699:G:C6	28:2:12:ARG:HA	2.53	0.44
1:X:761:G:C8	1:X:763:A:C8	3.06	0.44
1:X:1433:A:OP2	1:X:1593:C:N4	2.50	0.44
1:X:1919:A:N6	1:X:1946:U:H3	2.14	0.44
1:X:2020:G:H2'	1:X:2021:G:C8	2.52	0.44
1:X:2197:U:H2'	1:X:2198:U:C2	2.52	0.44
1:X:2629:U:H2'	1:X:2630:C:C6	2.52	0.44
33:X:3321:SPD:H31	9:G:110:LEU:HD11	1.98	0.44
3:A:6:TYR:HB2	3:A:13:ARG:O	2.18	0.44
10:H:83:ARG:HH22	15:M:38:LYS:NZ	2.15	0.44
14:L:33:ARG:HG3	14:L:99:ARG:NH2	2.33	0.44
16:N:66:ASN:HA	16:N:69:ALA:HB3	1.99	0.44
16:N:68:GLY:O	16:N:71:LEU:HB3	2.17	0.44
21:S:138:VAL:O	21:S:141:MET:HG2	2.18	0.44
1:X:28:A:H1'	1:X:523:A:C2	2.52	0.44
1:X:192:G:H4'	1:X:193:A:H4'	1.99	0.44
1:X:219:G:H1'	1:X:220:U:OP2	2.17	0.44
1:X:865:A:H2'	1:X:866:U:H6	1.83	0.44
1:X:939:C:OP2	1:X:940:G:H8	2.01	0.44
1:X:1061:A:N1	1:X:2731:G:C6	2.86	0.44
1:X:1599:G:C2	1:X:1600:U:H1'	2.52	0.44
1:X:1662:G:H5''	1:X:1663:C:H5'	1.98	0.44
1:X:2487:G:C2	1:X:2561:G:C6	3.06	0.44
7:E:111:HIS:HA	7:E:112:PRO:HD2	1.76	0.44
14:L:11:LEU:HD22	14:L:93:SER:HA	1.99	0.44
16:N:7:GLY:O	16:N:9:VAL:HG23	2.18	0.44
1:X:38:G:H1	1:X:453:U:H3	1.64	0.44
1:X:252:G:H4'	1:X:252:G:OP1	2.17	0.44
1:X:573:C:H2'	1:X:574:C:O4'	2.18	0.44
1:X:1255:A:H2'	1:X:1256:C:C6	2.52	0.44
1:X:1811:A:O2'	1:X:1812:U:OP2	2.26	0.44
1:X:2195:C:H2'	1:X:2196:U:C5	2.53	0.44
1:X:2811:G:H2'	1:X:2812:A:C8	2.52	0.44
2:Y:39:C:N4	2:Y:50:U:O2'	2.51	0.44
18:P:46:ARG:NE	18:P:95:ALA:O	2.51	0.44
19:Q:71:GLN:HG2	19:Q:72:ARG:HB2	1.99	0.44
1:X:334:G:N7	5:C:164:VAL:HA	2.33	0.44
1:X:636:G:O2'	1:X:669:G:H4'	2.18	0.44
1:X:1201:G:H5''	17:O:80:TYR:CE1	2.52	0.44
1:X:1585:A:H2'	1:X:1586:A:C8	2.53	0.44
1:X:1998:A:N3	26:Z:6:VAL:HG12	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2196:U:H3'	1:X:2197:U:C4'	2.48	0.44
12:J:76:THR:HB	12:J:88:LYS:O	2.18	0.44
18:P:28:ALA:O	18:P:123:HIS:HA	2.17	0.44
20:R:15:HIS:O	20:R:16:PHE:CG	2.71	0.44
25:W:16:GLN:O	25:W:20:VAL:HG23	2.18	0.44
1:X:998:C:H2'	1:X:999:A:O4'	2.18	0.44
1:X:1152:C:O2'	1:X:1153:A:OP1	2.33	0.44
1:X:1313:U:H4'	1:X:1314:A:C5'	2.46	0.44
1:X:1769:U:C4	1:X:1775:A:C8	3.05	0.44
1:X:2297:G:O2'	1:X:2300:G:O6	2.22	0.44
1:X:2362:G:H21	1:X:2363:G:H1'	1.83	0.44
1:X:2796:A:P	4:B:111:LYS:HZ3	2.41	0.44
4:B:203:LYS:HA	4:B:203:LYS:HD2	1.53	0.44
5:C:176:ASN:OD1	5:C:178:TYR:HB3	2.18	0.44
15:M:29:PRO:O	15:M:96:ARG:NH1	2.50	0.44
1:X:79:G:H1	1:X:104:C:H42	1.65	0.44
1:X:356:A:H2'	1:X:357:A:C8	2.53	0.44
1:X:712:A:H2'	1:X:713:G:O4'	2.18	0.44
1:X:939:C:OP2	1:X:940:G:C8	2.71	0.44
1:X:1021:A:H1'	1:X:1164:C:H1'	1.99	0.44
1:X:1094:C:O2	1:X:1096:A:H2'	2.18	0.44
1:X:1987:G:C5	1:X:1988:A:C8	3.06	0.44
1:X:2653:A:O3'	10:H:42:LYS:HA	2.18	0.44
2:Y:25:G:H1	2:Y:62:C:H42	1.66	0.44
3:A:3:VAL:HG13	3:A:17:THR:HG23	1.98	0.44
3:A:200:GLU:HG2	3:A:203:ASN:CG	2.43	0.44
5:C:1:MET:HA	5:C:14:THR:HA	2.00	0.44
6:D:13:ARG:NH1	6:D:14:PRO:HG3	2.33	0.44
19:Q:60:GLY:HA3	19:Q:74:ASP:H	1.83	0.44
1:X:656:U:O2'	1:X:657:A:O5'	2.27	0.43
1:X:945:G:H2'	1:X:946:U:H6	1.82	0.43
1:X:1072:U:O4'	1:X:1081:A:H1'	2.17	0.43
1:X:2364:C:H2'	1:X:2365:U:C6	2.53	0.43
2:Y:28:A:C8	2:Y:29:C:C2	3.06	0.43
4:B:10:GLY:O	4:B:25:VAL:HG23	2.18	0.43
10:H:28:GLY:CA	10:H:50:ILE:HD11	2.37	0.43
14:L:28:ARG:O	14:L:43:ILE:HD12	2.17	0.43
21:S:48:THR:HG22	21:S:66:VAL:O	2.18	0.43
29:3:9:MET:HA	29:3:12:ARG:HB3	1.99	0.43
1:X:1194:U:O2'	1:X:1195:U:O4'	2.37	0.43
1:X:1655:C:H5''	1:X:2689:C:O2'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:61:LEU:HB2	3:A:63:ARG:HH12	1.84	0.43
4:B:14:ILE:HG12	15:M:20:HIS:NE2	2.33	0.43
4:B:55:ALA:HB3	4:B:58:LYS:HE2	2.01	0.43
6:D:135:GLN:HG3	6:D:136:LEU:HD23	2.01	0.43
11:I:107:LYS:HG3	11:I:124:ALA:C	2.43	0.43
12:J:36:ILE:HG22	12:J:38:MET:HE3	2.00	0.43
14:L:37:HIS:ND1	14:L:37:HIS:C	2.76	0.43
14:L:96:TYR:O	14:L:97:HIS:ND1	2.38	0.43
21:S:84:TYR:CG	21:S:85:MET:N	2.86	0.43
1:X:13:A:N3	1:X:15:G:C6	2.86	0.43
1:X:564:U:H2'	1:X:565:A:C8	2.54	0.43
1:X:702:A:N3	1:X:792:U:O2'	2.49	0.43
1:X:1374:G:N2	1:X:1384:G:H1'	2.33	0.43
1:X:2023:C:H2'	1:X:2024:U:C6	2.53	0.43
3:A:128:GLY:HA2	3:A:192:THR:HG23	2.00	0.43
12:J:15:ARG:HD2	12:J:73:LYS:HG3	2.00	0.43
17:O:10:LYS:CG	17:O:11:GLN:HG2	2.48	0.43
18:P:21:ARG:HD3	18:P:83:ASP:OD1	2.18	0.43
18:P:40:LEU:HD12	26:Z:25:LEU:HD13	1.99	0.43
20:R:88:THR:HG22	20:R:89:GLY:H	1.83	0.43
24:V:17:GLU:O	24:V:21:ARG:HD3	2.18	0.43
28:2:38:GLY:C	28:2:40:HIS:N	2.63	0.43
1:X:205:A:H2'	1:X:206:U:H5'	2.00	0.43
1:X:538:A:H2'	1:X:538:A:N3	2.33	0.43
1:X:636:G:N7	11:I:101:ARG:NH1	2.63	0.43
1:X:1173:G:H4'	17:O:22:VAL:HG22	1.99	0.43
1:X:1310:C:C2	1:X:1311:C:C5	3.06	0.43
1:X:1418:C:H2'	1:X:1419:G:C8	2.54	0.43
1:X:2287:G:O2'	1:X:2288:A:P	2.76	0.43
1:X:2621:G:OP1	9:G:110:LEU:HD13	2.18	0.43
1:X:2871:U:H2'	1:X:2872:U:C6	2.54	0.43
2:Y:53:G:C6	14:L:36:LYS:HD2	2.52	0.43
3:A:27:LYS:HE2	3:A:27:LYS:HB2	1.88	0.43
5:C:47:THR:HB	5:C:48:ARG:H	1.46	0.43
17:O:30:GLY:O	17:O:60:VAL:HG23	2.18	0.43
20:R:77:HIS:C	20:R:79:SER:H	2.25	0.43
1:X:70:A:H5''	1:X:71:A:H2'	2.00	0.43
1:X:387:A:H5'	1:X:435:A:H2	1.84	0.43
1:X:415:A:N6	1:X:416:U:O4	2.51	0.43
1:X:1040:A:C8	1:X:1041:G:C8	3.06	0.43
1:X:1670:G:C6	13:K:9:LYS:HD3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2069:U:H2'	1:X:2070:G:C8	2.53	0.43
1:X:2262:C:C2	1:X:2368:G:C2	3.07	0.43
2:Y:34:C:H2'	2:Y:35:C:C6	2.54	0.43
4:B:79:ARG:HA	4:B:79:ARG:HD3	1.87	0.43
5:C:30:VAL:HA	5:C:95:LEU:HD11	2.01	0.43
6:D:148:LYS:HE3	6:D:150:ARG:HG3	1.99	0.43
9:G:63:ARG:HA	9:G:63:ARG:HD2	1.83	0.43
11:I:34:HIS:O	11:I:35:LYS:HE3	2.17	0.43
11:I:129:ALA:O	11:I:133:VAL:HG23	2.19	0.43
20:R:81:VAL:HG13	20:R:82:ALA:N	2.32	0.43
22:T:74:LYS:HB3	22:T:75:GLY:H	1.57	0.43
1:X:618:A:H2'	1:X:619:A:C8	2.53	0.43
1:X:1357:U:H4'	1:X:1397:A:C6	2.53	0.43
1:X:2476:A:N3	1:X:2477:C:N4	2.67	0.43
4:B:122:PHE:HE2	4:B:138:PRO:HA	1.83	0.43
5:C:144:GLY:HA2	5:C:166:TRP:CD2	2.53	0.43
6:D:70:ALA:C	6:D:72:LYS:H	2.25	0.43
16:N:70:ARG:HG2	16:N:74:MET:O	2.18	0.43
20:R:22:VAL:HG23	20:R:83:LEU:H	1.82	0.43
20:R:35:LYS:HE2	20:R:35:LYS:HB3	1.88	0.43
21:S:122:ILE:O	21:S:123:VAL:HB	2.18	0.43
23:U:8:THR:HA	23:U:14:VAL:HG22	1.99	0.43
1:X:389:G:H2'	1:X:390:U:C6	2.54	0.43
1:X:458:G:H4'	1:X:459:A:H5'	2.01	0.43
1:X:755:C:H2'	1:X:756:C:C6	2.49	0.43
1:X:836:G:H2'	1:X:837:U:C6	2.53	0.43
1:X:854:G:N2	1:X:948:C:N3	2.56	0.43
1:X:914:C:H2'	1:X:915:C:C6	2.54	0.43
4:B:6:GLY:HA2	4:B:51:TYR:CZ	2.54	0.43
6:D:66:ILE:N	6:D:88:LYS:O	2.46	0.43
13:K:87:TYR:CE1	13:K:94:TYR:HD2	2.35	0.43
24:V:11:ALA:HA	24:V:14:PHE:HB2	2.01	0.43
1:X:479:G:C6	1:X:480:G:C4	3.07	0.43
1:X:1413:U:H2'	1:X:1414:G:H8	1.84	0.43
1:X:2201:G:H5''	3:A:186:HIS:NE2	2.33	0.43
5:C:144:GLY:HA2	5:C:166:TRP:CE2	2.54	0.43
20:R:77:HIS:HB3	20:R:79:SER:H	1.84	0.43
23:U:34:THR:OG1	23:U:35:THR:N	2.52	0.43
28:2:10:ARG:O	28:2:14:LYS:HB2	2.19	0.43
1:X:8:A:H2'	1:X:9:U:C6	2.53	0.43
1:X:224:G:O2'	1:X:227:G:N7	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:593:C:OP2	16:N:6:THR:OG1	2.36	0.43
1:X:759:C:H1'	18:P:111:ARG:HH22	1.84	0.43
1:X:2263:C:H3'	27:1:28:ARG:HH12	1.82	0.43
1:X:2279:G:H8	1:X:2279:G:O5'	2.02	0.43
1:X:2474:G:H4'	12:J:82:THR:HA	1.99	0.43
29:3:22:VAL:HG21	29:3:53:ALA:HB1	2.01	0.43
1:X:170:U:N3	1:X:180:C:O2	2.51	0.43
1:X:338:G:H5'	20:R:9:HIS:CE1	2.54	0.43
1:X:504:G:H4'	18:P:27:VAL:CG1	2.47	0.43
1:X:1194:U:O2'	1:X:1195:U:H6	2.02	0.43
1:X:1596:A:H2'	1:X:1597:A:O4'	2.18	0.43
1:X:2237:C:H3'	1:X:2238:G:H8	1.83	0.43
1:X:2260:C:O2'	1:X:2261:G:H5'	2.19	0.43
1:X:2314:A:O2'	1:X:2315:A:H8	2.02	0.43
1:X:2628:C:H2'	1:X:2629:U:H6	1.83	0.43
1:X:2845:C:C2'	1:X:2846:G:H5'	2.48	0.43
3:A:33:LEU:HD12	3:A:104:TYR:HD2	1.84	0.43
6:D:40:LEU:H	6:D:86:GLY:HA2	1.83	0.43
9:G:67:ARG:HB2	9:G:70:PHE:H	1.84	0.43
10:H:89:ILE:HG12	15:M:79:ARG:HD3	2.00	0.43
11:I:62:LYS:HD3	11:I:63:ARG:N	2.33	0.43
16:N:109:LEU:HD22	16:N:109:LEU:HA	1.84	0.43
22:T:33:ALA:HB2	22:T:64:ASP:OD1	2.19	0.43
23:U:20:ARG:HD2	23:U:43:ARG:NE	2.34	0.43
23:U:65:ASN:O	23:U:68:ARG:HB2	2.18	0.43
1:X:393:U:H2'	1:X:394:U:C6	2.54	0.42
1:X:1383:C:H3'	1:X:1384:G:H8	1.83	0.42
1:X:2043:A:H1'	1:X:2481:G:C1'	2.49	0.42
1:X:2234:G:H2'	1:X:2235:G:O4'	2.18	0.42
1:X:2310:G:H4'	22:T:43:THR:H	1.84	0.42
1:X:2631:C:H2'	1:X:2632:U:O4'	2.19	0.42
3:A:128:GLY:HA2	3:A:192:THR:CG2	2.49	0.42
5:C:31:VAL:HA	5:C:34:GLN:HB2	2.00	0.42
9:G:116:ARG:HB2	9:G:118:ALA:H	1.84	0.42
10:H:76:ARG:NE	15:M:75:GLU:OE1	2.45	0.42
13:K:2:ARG:O	13:K:5:LYS:NZ	2.47	0.42
15:M:103:LYS:HA	15:M:103:LYS:HD2	1.73	0.42
21:S:72:ASP:OD2	21:S:75:LYS:HD3	2.19	0.42
25:W:40:VAL:HA	25:W:43:MET:HE3	2.00	0.42
1:X:175:C:H2'	1:X:176:A:H5''	2.01	0.42
1:X:430:C:H1'	1:X:2386:G:N2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:761:G:O5'	18:P:110:ALA:HB2	2.19	0.42
1:X:2362:G:N2	1:X:2363:G:H1'	2.34	0.42
4:B:110:GLY:HA3	4:B:161:GLY:HA3	2.00	0.42
4:B:159:HIS:CD2	4:B:159:HIS:C	2.98	0.42
11:I:62:LYS:HE2	11:I:64:GLY:N	2.34	0.42
12:J:15:ARG:HB2	12:J:15:ARG:NH1	2.31	0.42
1:X:95:G:H2'	1:X:96:C:C6	2.54	0.42
1:X:224:G:H4'	1:X:399:G:C5	2.53	0.42
1:X:640:C:H4'	1:X:660:G:H21	1.83	0.42
1:X:705:C:H5''	3:A:40:THR:O	2.19	0.42
1:X:1469:U:O2'	1:X:1470:G:O5'	2.31	0.42
1:X:1515:U:H2'	1:X:1516:A:C8	2.54	0.42
1:X:2026:C:H2'	1:X:2027:C:H6	1.85	0.42
1:X:2269:G:N2	1:X:2322:U:H1'	2.34	0.42
1:X:2442:C:H2'	1:X:2443:C:H6	1.84	0.42
4:B:6:GLY:HA3	4:B:28:ALA:HA	2.01	0.42
5:C:22:VAL:CG1	5:C:106:MET:HB3	2.49	0.42
13:K:29:LEU:HA	13:K:29:LEU:HD23	1.81	0.42
21:S:97:PRO:HA	21:S:119:ASN:H	1.83	0.42
24:V:14:PHE:O	24:V:18:ILE:HG13	2.19	0.42
1:X:591:G:H2'	1:X:592:G:C8	2.54	0.42
1:X:938:G:HO2'	1:X:939:C:P	2.42	0.42
1:X:1278:A:N6	1:X:1996:A:H5''	2.34	0.42
1:X:1699:A:H2'	1:X:1700:C:C6	2.54	0.42
1:X:2532:G:C2	1:X:2533:U:H1'	2.55	0.42
1:X:2695:C:C2	1:X:2696:A:C8	3.08	0.42
2:Y:30:C:OP1	14:L:37:HIS:CE1	2.72	0.42
3:A:37:LEU:H	3:A:37:LEU:HD22	1.85	0.42
5:C:158:ARG:O	5:C:161:ALA:HB2	2.19	0.42
9:G:70:PHE:HB3	16:N:64:ARG:NE	2.34	0.42
10:H:28:GLY:O	10:H:29:ILE:HG13	2.20	0.42
11:I:91:ASP:HB3	11:I:121:HIS:CD2	2.54	0.42
11:I:93:LEU:HD22	11:I:93:LEU:HA	1.71	0.42
14:L:87:VAL:HA	14:L:108:ARG:NH2	2.34	0.42
20:R:92:THR:HA	20:R:108:VAL:HB	2.00	0.42
21:S:46:GLN:O	21:S:49:THR:OG1	2.31	0.42
1:X:383:G:H4'	1:X:384:A:OP2	2.19	0.42
1:X:1361:G:H1	1:X:1614:C:N4	2.17	0.42
1:X:1448:A:H61	1:X:1574:A:N6	2.15	0.42
1:X:1842:G:H1	1:X:1875:C:H42	1.67	0.42
1:X:2044:G:H2'	1:X:2480:C:O2'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2442:C:H2'	1:X:2443:C:C6	2.54	0.42
1:X:2708:U:H2'	1:X:2709:C:H6	1.85	0.42
2:Y:26:G:N7	2:Y:58:G:O2'	2.31	0.42
3:A:21:PHE:O	3:A:22:SER:HB3	2.20	0.42
9:G:30:LYS:NZ	17:O:13:ARG:HH22	2.18	0.42
12:J:55:MET:HG2	12:J:118:ALA:O	2.19	0.42
12:J:135:ARG:H	12:J:135:ARG:HG3	1.66	0.42
14:L:8:ARG:HE	14:L:9:ARG:HG3	1.84	0.42
17:O:27:GLY:H	17:O:60:VAL:HG21	1.84	0.42
20:R:88:THR:HB	20:R:90:LYS:HG3	2.02	0.42
22:T:19:LYS:HD3	22:T:19:LYS:HA	1.84	0.42
29:3:50:LEU:HA	29:3:53:ALA:HB3	2.01	0.42
1:X:1332:G:C2	1:X:1333:G:C2	3.08	0.42
1:X:1479:G:H2'	1:X:1480:G:H8	1.84	0.42
1:X:1908:C:O2'	1:X:1909:U:OP1	2.37	0.42
1:X:2756:A:H3'	1:X:2756:A:OP1	2.19	0.42
33:X:3322:SPD:H51	33:X:3322:SPD:H82	1.85	0.42
5:C:33:TRP:HB2	5:C:93:TYR:OH	2.19	0.42
6:D:107:GLY:HA2	6:D:139:PRO:HD3	2.01	0.42
11:I:13:ARG:HD3	11:I:14:LYS:HG3	2.01	0.42
13:K:80:MET:HE2	13:K:80:MET:HB2	1.84	0.42
16:N:97:ASP:OD1	16:N:101:ARG:NH1	2.53	0.42
18:P:101:PRO:O	18:P:121:THR:OG1	2.27	0.42
19:Q:28:TRP:CZ3	19:Q:75:ARG:HG3	2.54	0.42
21:S:93:GLU:HG2	21:S:123:VAL:HB	2.01	0.42
1:X:39:C:H2'	1:X:40:U:C6	2.54	0.42
1:X:597:U:O4	1:X:683:A:H1'	2.19	0.42
1:X:1386:A:H5''	1:X:2191:A:N6	2.35	0.42
1:X:1815:G:H2'	1:X:1816:G:H8	1.85	0.42
1:X:2226:A:H2'	1:X:2227:C:H6	1.84	0.42
1:X:2329:C:H2'	1:X:2330:G:O4'	2.20	0.42
1:X:2628:C:H2'	1:X:2629:U:C6	2.55	0.42
2:Y:116:C:H4'	14:L:49:GLN:HG2	2.00	0.42
5:C:143:ASP:HB2	5:C:145:THR:H	1.85	0.42
12:J:73:LYS:HA	12:J:74:PRO:HD2	1.96	0.42
15:M:55:ILE:O	15:M:104:LEU:HB2	2.20	0.42
19:Q:17:TYR:O	19:Q:20:MET:HB3	2.20	0.42
19:Q:82:LEU:HD11	19:Q:88:ILE:HG23	2.02	0.42
27:1:51:ARG:HH11	27:1:53:LYS:HG2	1.85	0.42
1:X:64:C:OP1	19:Q:71:GLN:HB2	2.20	0.42
1:X:2007:G:C2	1:X:2023:C:C2	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2398:U:OP1	29:3:41:ILE:HG21	2.20	0.42
1:X:2794:G:O2'	1:X:2795:A:H5''	2.20	0.42
30:X:2901:6NO:CL1	12:J:56:SER:OG	2.71	0.42
4:B:117:MET:HE2	4:B:117:MET:HB3	1.89	0.42
5:C:30:VAL:HG11	5:C:177:VAL:HG21	2.01	0.42
5:C:99:VAL:O	5:C:103:GLY:N	2.52	0.42
9:G:85:ALA:HB3	9:G:152:ALA:HA	2.02	0.42
9:G:124:GLU:OE2	9:G:152:ALA:N	2.52	0.42
14:L:15:ARG:HA	14:L:15:ARG:HD3	1.72	0.42
14:L:26:ARG:CZ	14:L:87:VAL:HG22	2.50	0.42
14:L:42:ILE:HG13	14:L:88:VAL:HG11	2.01	0.42
15:M:85:SER:HA	15:M:86:PRO:HD3	1.83	0.42
18:P:25:PHE:HA	18:P:127:ILE:HG12	2.02	0.42
18:P:46:ARG:HH11	18:P:46:ARG:HG2	1.84	0.42
20:R:38:LEU:HB3	20:R:47:VAL:CG2	2.49	0.42
28:2:15:THR:O	28:2:17:GLY:N	2.53	0.42
1:X:640:C:H1'	1:X:650:U:H1'	2.02	0.42
1:X:1217:U:O2	11:I:13:ARG:HB3	2.19	0.42
1:X:1996:A:H4'	18:P:117:ILE:HD13	2.02	0.42
3:A:89:SER:O	3:A:159:ALA:HB2	2.19	0.42
3:A:142:VAL:HG12	3:A:193:ILE:HA	2.01	0.42
3:A:267:ASP:O	3:A:268:ARG:HD2	2.20	0.42
4:B:15:TRP:NE1	4:B:20:ALA:HB2	2.35	0.42
7:E:21:ASP:HB3	7:E:22:GLY:H	1.63	0.42
14:L:35:SER:OG	14:L:36:LYS:N	2.52	0.42
19:Q:12:ILE:H	19:Q:12:ILE:HG13	1.72	0.42
22:T:45:PHE:CE1	22:T:69:PHE:HE2	2.37	0.42
23:U:61:TRP:O	23:U:62:LEU:HD12	2.20	0.42
26:Z:4:HIS:C	26:Z:4:HIS:ND1	2.77	0.42
29:3:6:THR:CG2	29:3:59:LYS:HG3	2.49	0.42
1:X:88:G:C8	1:X:89:A:H2'	2.55	0.42
1:X:321:A:C6	1:X:323:G:C4	3.07	0.42
1:X:958:G:H2'	1:X:959:C:C6	2.54	0.42
1:X:960:U:H2'	1:X:961:G:C8	2.55	0.42
1:X:1007:A:O3'	16:N:93:LYS:HB3	2.19	0.42
1:X:1377:G:O5'	23:U:7:LEU:HD21	2.20	0.42
1:X:1411:C:N4	1:X:1412:C:H41	2.18	0.42
1:X:1625:A:H4'	1:X:1626:A:OP1	2.18	0.42
13:K:76:VAL:O	13:K:79:VAL:HG22	2.20	0.42
17:O:34:GLU:HB2	17:O:56:VAL:HG23	2.01	0.42
1:X:585:U:H4'	1:X:2481:G:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1330:G:H2'	1:X:1331:G:O4'	2.20	0.41
1:X:1370:U:H3'	1:X:1371:G:H8	1.83	0.41
1:X:1391:A:O2'	1:X:1393:G:N7	2.42	0.41
1:X:1539:U:H2'	1:X:1540:C:C6	2.55	0.41
1:X:1703:C:H2'	1:X:1704:G:O4'	2.19	0.41
1:X:2510:A:C8	7:E:175:LYS:HB2	2.54	0.41
2:Y:31:A:O2'	2:Y:60:A:N1	2.48	0.41
6:D:171:GLN:HA	6:D:175:LEU:HD22	2.01	0.41
16:N:40:LEU:HD12	17:O:74:TYR:CE1	2.55	0.41
16:N:61:TRP:O	16:N:65:ILE:HG13	2.20	0.41
19:Q:11:VAL:HG23	19:Q:27:PHE:HA	2.01	0.41
20:R:44:GLN:HB3	20:R:45:LYS:H	1.65	0.41
1:X:839:U:OP1	1:X:2407:G:H3'	2.21	0.41
1:X:1693:A:H2	1:X:1976:U:H5'	1.84	0.41
1:X:2170:C:H3'	1:X:2171:U:C5'	2.50	0.41
2:Y:70:C:H2'	2:Y:71:G:O4'	2.20	0.41
3:A:80:ALA:N	3:A:95:LEU:HA	2.34	0.41
5:C:46:ARG:HD2	5:C:46:ARG:HA	1.75	0.41
5:C:48:ARG:O	5:C:50:GLN:N	2.53	0.41
5:C:58:MET:HG2	5:C:59:TYR:H	1.85	0.41
6:D:36:VAL:HG11	6:D:57:LEU:HD21	2.02	0.41
9:G:169:GLN:HG3	9:G:171:LEU:N	2.35	0.41
10:H:28:GLY:O	10:H:34:LEU:HA	2.20	0.41
14:L:28:ARG:CG	14:L:90:ASP:HB2	2.50	0.41
25:W:4:LYS:HE2	25:W:4:LYS:HB3	1.88	0.41
25:W:12:ARG:HD2	25:W:13:PRO:HD2	2.02	0.41
1:X:17:G:H2'	1:X:18:U:C6	2.55	0.41
1:X:334:G:OP1	1:X:349:G:N2	2.53	0.41
1:X:812:G:H2'	1:X:813:A:C8	2.56	0.41
1:X:965:G:O2'	1:X:2253:A:N1	2.34	0.41
1:X:1060:C:H1'	1:X:1124:U:O2'	2.19	0.41
1:X:1310:C:H2'	1:X:1311:C:C6	2.55	0.41
1:X:1793:A:H2'	1:X:1794:A:C8	2.55	0.41
1:X:1979:C:H4'	1:X:1980:A:OP1	2.20	0.41
1:X:2042:A:O3'	5:C:63:GLY:HA2	2.20	0.41
1:X:2293:G:H2'	1:X:2294:U:C6	2.55	0.41
1:X:2870:C:H2'	1:X:2871:U:H6	1.84	0.41
2:Y:98:C:H2'	2:Y:99:G:C8	2.55	0.41
20:R:56:LYS:H	20:R:56:LYS:HD3	1.85	0.41
26:Z:35:GLN:HE21	26:Z:51:TYR:HD2	1.67	0.41
1:X:494:A:O4'	20:R:56:LYS:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1745:C:OP1	15:M:101:ARG:NH2	2.49	0.41
1:X:1817:U:H5''	3:A:247:VAL:HG11	2.02	0.41
1:X:2504:G:C2	1:X:2518:C:C2	3.08	0.41
1:X:2771:C:H2'	1:X:2772:U:O4'	2.21	0.41
5:C:137:ALA:HB1	5:C:142:LEU:HB2	2.03	0.41
9:G:51:LEU:HD13	9:G:88:VAL:HG21	2.03	0.41
9:G:67:ARG:CD	9:G:70:PHE:HA	2.45	0.41
9:G:69:ASP:OD2	9:G:76:GLN:HB3	2.21	0.41
10:H:70:VAL:HG22	10:H:71:LYS:N	2.36	0.41
11:I:93:LEU:HB3	11:I:97:ARG:HB2	2.01	0.41
12:J:83:ARG:HD3	12:J:83:ARG:HA	1.89	0.41
21:S:99:HIS:CD2	21:S:133:GLU:HB2	2.55	0.41
21:S:137:ASP:O	21:S:140:LYS:HE2	2.21	0.41
26:Z:49:CYS:SG	26:Z:51:TYR:HB2	2.61	0.41
1:X:186:C:H2'	1:X:187:U:C6	2.56	0.41
1:X:1429:A:H62	1:X:1600:U:H4'	1.85	0.41
1:X:1463:A:H2'	1:X:1464:A:H8	1.83	0.41
1:X:1693:A:H2'	1:X:1694:A:O4'	2.20	0.41
1:X:1718[A]:A:H2'	1:X:1718[A]:A:P	2.61	0.41
1:X:1750:A:H4'	1:X:2695:C:O4'	2.20	0.41
3:A:33:LEU:HD22	3:A:33:LEU:HA	1.86	0.41
3:A:164:GLN:NE2	3:A:166:GLN:OE1	2.35	0.41
5:C:9:GLN:OE1	5:C:12:GLY:HA2	2.21	0.41
5:C:57:LYS:CG	5:C:58:MET:H	2.34	0.41
6:D:45:GLU:HB3	6:D:49:ALA:H	1.84	0.41
17:O:49:GLU:O	17:O:52:GLY:N	2.53	0.41
1:X:451:A:H2'	1:X:452:G:C8	2.55	0.41
1:X:871:U:O2	1:X:2247:A:H2'	2.21	0.41
1:X:1054:C:N4	1:X:1123:G:H1	2.19	0.41
1:X:1676:U:O2'	1:X:2692:A:N1	2.50	0.41
1:X:2195:C:H5'	1:X:2196:U:OP1	2.21	0.41
1:X:2433:G:H1'	32:X:3316:MPD:C4	2.51	0.41
3:A:37:LEU:HB2	3:A:39:LYS:NZ	2.34	0.41
3:A:85:ASP:HA	3:A:86:PRO:HD2	1.82	0.41
4:B:95:ILE:HD13	4:B:95:ILE:HA	1.87	0.41
6:D:170:LEU:O	6:D:175:LEU:HB3	2.20	0.41
9:G:75:ILE:O	9:G:75:ILE:HG13	2.20	0.41
13:K:99:ARG:HG2	13:K:99:ARG:NH1	2.35	0.41
15:M:37:THR:O	15:M:87:LEU:HD13	2.21	0.41
1:X:500:G:C2	1:X:501:G:H1'	2.56	0.41
1:X:854:G:H1	1:X:948:C:N4	2.15	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:874:A:H2'	1:X:875:G:O4'	2.19	0.41
1:X:1161:U:H2'	1:X:1162:A:C8	2.56	0.41
1:X:1301:U:C2	1:X:1340:C:O2	2.74	0.41
1:X:1333:G:N2	1:X:1344:C:H41	2.18	0.41
1:X:1815:G:H2'	1:X:1816:G:C8	2.55	0.41
1:X:1943:A:H5'	1:X:1944:C:OP2	2.21	0.41
1:X:2044:G:N2	1:X:2046:C:C2	2.89	0.41
1:X:2433:G:C4	1:X:2434:G:C8	3.09	0.41
1:X:2705:A:O2'	1:X:2706:U:C6	2.73	0.41
2:Y:42:U:H2'	2:Y:45:C:H5	1.86	0.41
2:Y:44:C:O2	6:D:90:THR:N	2.36	0.41
2:Y:56:G:H21	6:D:26:MET:HG3	1.85	0.41
4:B:99:GLY:O	4:B:171:GLU:HG3	2.21	0.41
4:B:194:GLY:HA2	15:M:2:GLN:HB3	2.03	0.41
5:C:6:VAL:HG21	5:C:136:TRP:HZ2	1.85	0.41
14:L:12:ARG:HD2	14:L:92:GLY:HA2	2.02	0.41
14:L:29:LEU:HB2	14:L:88:VAL:HG12	2.01	0.41
14:L:55:SER:O	14:L:71:VAL:HB	2.21	0.41
23:U:52:ARG:HG2	23:U:79:GLU:OE1	2.21	0.41
27:1:9:ILE:O	27:1:10:VAL:HB	2.21	0.41
1:X:613:A:H5''	1:X:668:A:H61	1.86	0.41
1:X:670:U:H2'	1:X:671:A:C8	2.55	0.41
1:X:1142:G:O4'	9:G:111:LYS:HD3	2.21	0.41
1:X:1631:C:C2	18:P:108:PRO:HG3	2.56	0.41
1:X:2262:C:H2'	1:X:2263:C:O4'	2.20	0.41
6:D:44:LYS:HD2	6:D:44:LYS:HA	1.90	0.41
9:G:107:GLN:O	9:G:108:GLY:C	2.64	0.41
12:J:70:PHE:HA	12:J:71:PRO:HD3	1.81	0.41
29:3:16:ILE:HB	29:3:64:ARG:HA	2.03	0.41
1:X:89:A:H4'	1:X:90:G:H5'	2.03	0.41
1:X:322:A:H3'	1:X:323:G:C8	2.56	0.41
1:X:328:A:H2'	1:X:329:C:C6	2.56	0.41
1:X:953:G:H5''	11:I:38:LYS:HA	2.02	0.41
1:X:1050:G:H1	1:X:1127:C:H42	1.67	0.41
1:X:1172:U:O2'	17:O:21:ARG:HG3	2.20	0.41
1:X:1584:G:OP2	3:A:63:ARG:NH2	2.53	0.41
1:X:2021:G:C6	1:X:2022:C:C4	3.08	0.41
1:X:2262:C:C5	1:X:2368:G:H2'	2.56	0.41
1:X:2290:A:N7	1:X:2291:U:C4	2.89	0.41
1:X:2557:G:OP1	1:X:2593:A:N6	2.53	0.41
1:X:2817:A:H2'	1:X:2818:G:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:37:C:H2'	2:Y:38:C:O4'	2.21	0.41
3:A:79:VAL:HA	3:A:95:LEU:HB3	2.03	0.41
5:C:128:ALA:O	5:C:130:THR:N	2.51	0.41
6:D:66:ILE:HG23	6:D:88:LYS:HB3	2.02	0.41
6:D:175:LEU:H	6:D:175:LEU:HD23	1.86	0.41
9:G:32:TYR:CE2	9:G:34:PRO:HG3	2.56	0.41
10:H:113:PRO:HD3	15:M:73:PHE:HB2	2.03	0.41
13:K:1:MET:HE2	13:K:3:HIS:CE1	2.46	0.41
13:K:59:ASP:OD1	13:K:59:ASP:N	2.54	0.41
14:L:51:LEU:HD22	14:L:84:ILE:HG21	2.02	0.41
20:R:23:ILE:H	20:R:81:VAL:HG12	1.86	0.41
20:R:72:ARG:HB3	20:R:73:GLU:H	1.62	0.41
21:S:62:PHE:HB2	21:S:85:MET:CE	2.51	0.41
1:X:474:G:N2	1:X:477:A:OP2	2.37	0.41
1:X:1020:A:OP1	9:G:65:LYS:NZ	2.45	0.41
1:X:1296:G:H4'	33:X:3322:SPD:HN6	1.86	0.41
1:X:1954:A:HO2'	1:X:1955:G:P	2.40	0.41
1:X:2204:A:H1'	1:X:2205:C:OP2	2.21	0.41
1:X:2271:C:P	14:L:18:ARG:HH22	2.43	0.41
1:X:2812:A:H2'	1:X:2813:G:H8	1.84	0.41
2:Y:78:A:H2'	2:Y:79:U:O4'	2.20	0.41
3:A:69:ARG:NH1	3:A:130:ALA:HB2	2.36	0.41
5:C:95:LEU:HD23	5:C:96:PRO:HD2	2.03	0.41
5:C:148:VAL:N	5:C:166:TRP:O	2.47	0.41
8:F:98:LYS:HE2	8:F:98:LYS:HB3	1.81	0.41
9:G:65:LYS:HD2	9:G:65:LYS:HA	1.82	0.41
12:J:124:HIS:O	12:J:125:LYS:HB2	2.21	0.41
15:M:32:THR:HG23	15:M:91:VAL:HG13	2.02	0.41
17:O:12:TYR:CB	17:O:40:VAL:HG22	2.51	0.41
20:R:15:HIS:ND1	20:R:82:ALA:HB2	2.36	0.41
23:U:15:VAL:HG13	23:U:45:ASN:O	2.21	0.41
27:1:38:LYS:O	27:1:49:VAL:HG23	2.21	0.41
29:3:28:GLY:HA2	29:3:29:LYS:HA	1.62	0.41
1:X:331:U:H4'	1:X:333:A:C8	2.56	0.40
1:X:485:G:C6	1:X:520:C:N4	2.88	0.40
1:X:492:G:O2'	1:X:516:G:N2	2.54	0.40
1:X:652:C:N4	1:X:657:A:H61	2.18	0.40
1:X:1065:A:N6	1:X:1117:G:O6	2.54	0.40
1:X:2576:G:C5	1:X:2577:A:C6	3.08	0.40
3:A:38:PRO:HG3	3:A:60:ARG:O	2.20	0.40
9:G:101:THR:HA	9:G:112:THR:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:102:THR:H	13:K:102:THR:HG23	1.63	0.40
16:N:45:TYR:O	16:N:49:ASP:HB2	2.21	0.40
24:V:62:ARG:C	24:V:66:GLN:HG3	2.46	0.40
1:X:571:U:C2	1:X:581:A:C8	3.09	0.40
1:X:649:G:C6	1:X:662:G:N2	2.89	0.40
1:X:796:A:H8	1:X:797:A:H4'	1.85	0.40
1:X:1006:C:N3	9:G:31:THR:HG23	2.37	0.40
1:X:1156:U:H2'	1:X:1157:G:C8	2.56	0.40
1:X:1753:A:OP1	1:X:1753:A:H4'	2.21	0.40
1:X:2340:C:OP2	29:3:26:LYS:HE2	2.21	0.40
1:X:2481:G:H5''	1:X:2482:A:H5''	2.03	0.40
3:A:36:ALA:HB1	3:A:62:TYR:N	2.35	0.40
9:G:98:LYS:O	9:G:115:ALA:HB1	2.22	0.40
14:L:97:HIS:CG	14:L:98:GLY:H	2.37	0.40
18:P:11:LYS:HG3	18:P:14:ARG:NH2	2.36	0.40
18:P:32:ARG:O	18:P:33:MET:HG2	2.21	0.40
18:P:62:ARG:H	18:P:62:ARG:HG2	1.60	0.40
27:1:48:VAL:HG12	27:1:50:PHE:HE1	1.86	0.40
1:X:104:C:O2'	1:X:105:G:OP1	2.24	0.40
1:X:251:C:N4	1:X:269:G:N3	2.69	0.40
1:X:609:U:O2'	11:I:18:ARG:NH1	2.42	0.40
1:X:1231:A:H2'	1:X:1232:U:C6	2.56	0.40
1:X:1735:G:H2'	1:X:1736:C:C6	2.57	0.40
1:X:1835:C:H2'	1:X:1836:C:C6	2.56	0.40
1:X:2571:G:C6	1:X:2572:U:N3	2.90	0.40
2:Y:22:U:H1'	2:Y:66:G:H22	1.86	0.40
4:B:30:PRO:HB3	4:B:91:VAL:HG22	2.03	0.40
4:B:105:THR:HB	4:B:166:THR:HA	2.04	0.40
6:D:65:PRO:HB3	6:D:89:VAL:HG22	2.02	0.40
9:G:85:ALA:HB3	9:G:152:ALA:CA	2.51	0.40
11:I:93:LEU:HB3	11:I:97:ARG:CB	2.51	0.40
21:S:5:ALA:O	21:S:33:ALA:HB3	2.21	0.40
21:S:168:VAL:HG12	21:S:169:VAL:HG23	2.03	0.40
23:U:10:LYS:HD2	23:U:10:LYS:HA	1.97	0.40
1:X:14:A:H5''	1:X:15:G:OP2	2.21	0.40
1:X:59:G:O6	1:X:62:U:C2	2.75	0.40
1:X:63:A:H1'	19:Q:65:VAL:HB	2.04	0.40
1:X:388:G:H2'	1:X:389:G:O4'	2.21	0.40
1:X:626:A:H5'	5:C:38:ARG:NE	2.37	0.40
1:X:650:U:H2'	1:X:651:C:C6	2.56	0.40
1:X:757:U:P	4:B:132:LYS:HZ2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1175:A:C2	1:X:1176:U:C2	3.10	0.40
1:X:1922:U:OP1	1:X:2583:U:O2'	2.39	0.40
1:X:2031:A:H2'	1:X:2032:G:O4'	2.21	0.40
2:Y:17:A:H1'	2:Y:112:A:C4	2.57	0.40
3:A:268:ARG:HA	3:A:268:ARG:CZ	2.52	0.40
4:B:109:LYS:O	4:B:110:GLY:C	2.64	0.40
5:C:7:ILE:HD12	5:C:7:ILE:HA	1.80	0.40
6:D:172:SER:N	6:D:175:LEU:HD22	2.37	0.40
10:H:97:VAL:HG21	10:H:126:ILE:HD11	2.04	0.40
11:I:93:LEU:H	11:I:97:ARG:NH1	2.19	0.40
13:K:10:LEU:O	13:K:12:ARG:HG2	2.22	0.40
14:L:70:ALA:O	14:L:74:ALA:N	2.50	0.40
20:R:77:HIS:CG	20:R:78:ALA:H	2.39	0.40
25:W:47:VAL:HB	25:W:50:LEU:HD12	2.02	0.40
1:X:30:G:C6	1:X:31:C:C4	3.10	0.40
1:X:332:C:H5''	5:C:130:THR:OG1	2.22	0.40
1:X:387:A:H2	1:X:413:G:H21	1.70	0.40
1:X:661:C:N3	1:X:662:G:C2	2.90	0.40
1:X:844:G:C6	1:X:845:U:C4	3.09	0.40
1:X:1321:A:N6	1:X:1322:G:C2	2.90	0.40
1:X:1704:G:N2	1:X:1718[B]:A:H2	2.18	0.40
1:X:2293:G:H5'	6:D:35:VAL:HG11	2.03	0.40
1:X:2375:G:C2	1:X:2400:G:C2	3.10	0.40
3:A:245:VAL:O	3:A:253:PRO:HD2	2.21	0.40
9:G:61:ARG:HA	9:G:61:ARG:NE	2.36	0.40
13:K:29:LEU:HD13	13:K:79:VAL:CG1	2.51	0.40
18:P:10:ASN:OD1	18:P:12:LYS:HB3	2.22	0.40
18:P:29:LYS:HB3	18:P:30:TYR:CD2	2.56	0.40
21:S:130:ILE:H	21:S:130:ILE:HG13	1.52	0.40
23:U:48:LYS:HD3	23:U:48:LYS:HA	1.72	0.40
27:1:37:LEU:HA	27:1:51:ARG:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	270/275 (98%)	226 (84%)	44 (16%)	0	100	100
4	B	203/211 (96%)	189 (93%)	13 (6%)	1 (0%)	24	54
5	C	193/205 (94%)	163 (84%)	27 (14%)	3 (2%)	7	29
6	D	175/180 (97%)	145 (83%)	27 (15%)	3 (2%)	7	27
7	E	169/185 (91%)	160 (95%)	8 (5%)	1 (1%)	21	49
8	F	61/144 (42%)	54 (88%)	6 (10%)	1 (2%)	7	29
9	G	140/174 (80%)	120 (86%)	16 (11%)	4 (3%)	3	19
10	H	132/134 (98%)	125 (95%)	7 (5%)	0	100	100
11	I	132/156 (85%)	103 (78%)	27 (20%)	2 (2%)	8	30
12	J	134/141 (95%)	111 (83%)	23 (17%)	0	100	100
13	K	113/116 (97%)	103 (91%)	10 (9%)	0	100	100
14	L	102/114 (90%)	79 (78%)	20 (20%)	3 (3%)	3	19
15	M	117/166 (70%)	109 (93%)	6 (5%)	2 (2%)	7	27
16	N	115/118 (98%)	105 (91%)	9 (8%)	1 (1%)	14	41
17	O	95/100 (95%)	83 (87%)	12 (13%)	0	100	100
18	P	126/134 (94%)	120 (95%)	6 (5%)	0	100	100
19	Q	91/95 (96%)	74 (81%)	15 (16%)	2 (2%)	5	23
20	R	108/115 (94%)	87 (81%)	20 (18%)	1 (1%)	14	41
21	S	178/237 (75%)	153 (86%)	21 (12%)	4 (2%)	5	23
22	T	72/91 (79%)	62 (86%)	10 (14%)	0	100	100
23	U	72/81 (89%)	52 (72%)	15 (21%)	5 (7%)	1	6
24	V	63/67 (94%)	59 (94%)	4 (6%)	0	100	100
25	W	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
26	Z	55/60 (92%)	52 (94%)	3 (6%)	0	100	100
27	1	51/55 (93%)	33 (65%)	15 (29%)	3 (6%)	1	9
28	2	44/47 (94%)	36 (82%)	7 (16%)	1 (2%)	5	23
29	3	57/66 (86%)	42 (74%)	13 (23%)	2 (4%)	3	16
All	All	3121/3522 (89%)	2696 (86%)	386 (12%)	39 (1%)	10	35

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	D	85	VAL
6	D	173	MET
9	G	85	ALA
28	2	39	ARG
29	3	40	GLU
5	C	22	VAL
9	G	103	TYR
9	G	114	THR
21	S	123	VAL
27	1	9	ILE
27	1	10	VAL
29	3	39	ASP
14	L	60	LYS
19	Q	6	ILE
19	Q	69	ILE
21	S	122	ILE
23	U	40	ARG
23	U	60	VAL
5	C	15	ILE
7	E	165	VAL
8	F	120	VAL
14	L	88	VAL
20	R	99	VAL
23	U	15	VAL
23	U	17	SER
23	U	32	ARG
4	B	40	GLN
6	D	172	SER
14	L	59	LEU
15	M	28	ARG
15	M	29	PRO
16	N	8	ILE
27	1	49	VAL
9	G	163	PRO
21	S	81	VAL
11	I	68	VAL
5	C	18	PRO
11	I	19	VAL
21	S	125	PRO

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	212/216 (98%)	167 (79%)	45 (21%)	1	4
4	B	155/157 (99%)	133 (86%)	22 (14%)	3	13
5	C	155/163 (95%)	126 (81%)	29 (19%)	1	6
6	D	143/156 (92%)	125 (87%)	18 (13%)	4	17
7	E	136/144 (94%)	128 (94%)	8 (6%)	18	43
8	F	46/107 (43%)	43 (94%)	3 (6%)	15	41
9	G	118/146 (81%)	99 (84%)	19 (16%)	2	10
10	H	103/103 (100%)	81 (79%)	22 (21%)	1	3
11	I	96/121 (79%)	76 (79%)	20 (21%)	1	4
12	J	104/115 (90%)	83 (80%)	21 (20%)	1	4
13	K	92/93 (99%)	80 (87%)	12 (13%)	4	16
14	L	74/82 (90%)	50 (68%)	24 (32%)	0	1
15	M	99/134 (74%)	82 (83%)	17 (17%)	2	9
16	N	96/97 (99%)	85 (88%)	11 (12%)	5	20
17	O	76/79 (96%)	64 (84%)	12 (16%)	2	10
18	P	108/115 (94%)	91 (84%)	17 (16%)	2	10
19	Q	75/76 (99%)	63 (84%)	12 (16%)	2	10
20	R	88/96 (92%)	69 (78%)	19 (22%)	1	3
21	S	149/192 (78%)	133 (89%)	16 (11%)	6	22
22	T	55/67 (82%)	45 (82%)	10 (18%)	2	7
23	U	55/66 (83%)	45 (82%)	10 (18%)	2	7
24	V	53/55 (96%)	50 (94%)	3 (6%)	18	44
25	W	48/48 (100%)	39 (81%)	9 (19%)	1	6
26	Z	49/53 (92%)	40 (82%)	9 (18%)	1	7
27	1	45/48 (94%)	34 (76%)	11 (24%)	1	2
28	2	39/40 (98%)	28 (72%)	11 (28%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	3	44/52 (85%)	31 (70%)	13 (30%)	0	1
All	All	2513/2821 (89%)	2090 (83%)	423 (17%)	2	9

All (423) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	3	VAL
3	A	4	LYS
3	A	13	ARG
3	A	15	GLN
3	A	26	LYS
3	A	27	LYS
3	A	28	ARG
3	A	30	GLU
3	A	31	LYS
3	A	33	LEU
3	A	34	THR
3	A	37	LEU
3	A	39	LYS
3	A	40	THR
3	A	43	ARG
3	A	46	ARG
3	A	49	ILE
3	A	51	SER
3	A	63	ARG
3	A	87	ASN
3	A	106	LEU
3	A	111	LEU
3	A	138	VAL
3	A	143	HIS
3	A	147	LEU
3	A	148	VAL
3	A	151	LYS
3	A	162	SER
3	A	186	HIS
3	A	200	GLU
3	A	206	LEU
3	A	208	LYS
3	A	212	SER
3	A	213	ARG
3	A	214	TRP
3	A	215	LEU

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Mol	Chain	Res	Type
3	A	218	LYS
3	A	220	HIS
3	A	245	VAL
3	A	247	VAL
3	A	248	THR
3	A	250	TRP
3	A	254	THR
3	A	260	ARG
3	A	270	ILE
4	B	4	ILE
4	B	5	LEU
4	B	14	ILE
4	B	26	VAL
4	B	59	VAL
4	B	60	ASN
4	B	105	THR
4	B	111	LYS
4	B	116	VAL
4	B	122	PHE
4	B	132	LYS
4	B	133	LYS
4	B	134	TRP
4	B	136	ARG
4	B	137	ARG
4	B	144	ARG
4	B	156	MET
4	B	159	HIS
4	B	162	MET
4	B	182	ILE
4	B	188	ILE
4	B	203	LYS
5	C	4	ILE
5	C	5	ASN
5	C	7	ILE
5	C	16	GLU
5	C	21	GLU
5	C	22	VAL
5	C	27	LEU
5	C	28	HIS
5	C	34	GLN
5	C	39	ARG
5	C	42	THR

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Mol	Chain	Res	Type
5	C	45	THR
5	C	47	THR
5	C	62	LYS
5	C	64	THR
5	C	94	THR
5	C	95	LEU
5	C	98	GLN
5	C	116	LYS
5	C	145	THR
5	C	153	ASP
5	C	157	THR
5	C	162	ARG
5	C	166	TRP
5	C	169	VAL
5	C	172	VAL
5	C	175	VAL
5	C	186	LEU
5	C	188	ILE
6	D	4	LEU
6	D	37	ASN
6	D	45	GLU
6	D	50	ILE
6	D	51	ASP
6	D	52	LYS
6	D	57	LEU
6	D	61	THR
6	D	66	ILE
6	D	67	ILE
6	D	71	LYS
6	D	85	VAL
6	D	89	VAL
6	D	117	ILE
6	D	130	LEU
6	D	146	VAL
6	D	158	THR
6	D	177	PHE
7	E	34	THR
7	E	43	VAL
7	E	84	THR
7	E	97	LYS
7	E	125	VAL
7	E	129	THR

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Mol	Chain	Res	Type
7	E	165	VAL
7	E	171	LEU
8	F	84	ILE
8	F	103	GLN
8	F	120	VAL
9	G	33	ILE
9	G	42	VAL
9	G	43	VAL
9	G	53	ARG
9	G	54	LEU
9	G	62	ILE
9	G	69	ASP
9	G	71	THR
9	G	76	GLN
9	G	91	THR
9	G	93	LYS
9	G	95	LEU
9	G	99	VAL
9	G	112	THR
9	G	119	LEU
9	G	151	TYR
9	G	161	GLN
9	G	168	THR
9	G	169	GLN
10	H	1	MET
10	H	5	GLN
10	H	7	ARG
10	H	10	VAL
10	H	13	ASN
10	H	19	ILE
10	H	29	ILE
10	H	35	THR
10	H	41	ASN
10	H	47	VAL
10	H	50	ILE
10	H	51	ILE
10	H	78	SER
10	H	81	ILE
10	H	93	ARG
10	H	102	GLN
10	H	106	ARG
10	H	110	VAL

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Mol	Chain	Res	Type
10	H	120	ASP
10	H	126	ILE
10	H	127	VAL
10	H	133	VAL
11	I	13	ARG
11	I	21	ARG
11	I	26	THR
11	I	28	LYS
11	I	35	LYS
11	I	40	ARG
11	I	56	LEU
11	I	62	LYS
11	I	63	ARG
11	I	65	PHE
11	I	67	ASN
11	I	87	THR
11	I	93	LEU
11	I	98	LEU
11	I	99	VAL
11	I	100	ARG
11	I	103	ASN
11	I	113	GLU
11	I	118	VAL
11	I	121	HIS
12	J	7	ARG
12	J	15	ARG
12	J	26	ASP
12	J	28	VAL
12	J	32	ASP
12	J	38	MET
12	J	64	LYS
12	J	65	ILE
12	J	68	ARG
12	J	69	ILE
12	J	72	ASP
12	J	88	LYS
12	J	98	VAL
12	J	111	THR
12	J	114	GLN
12	J	125	LYS
12	J	128	ILE
12	J	133	VAL

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Mol	Chain	Res	Type
12	J	135	ARG
12	J	136	GLU
12	J	137	VAL
13	K	1	MET
13	K	9	LYS
13	K	37	THR
13	K	45	ARG
13	K	51	LEU
13	K	73	LYS
13	K	76	VAL
13	K	95	THR
13	K	98	LEU
13	K	102	THR
13	K	109	THR
13	K	115	LEU
14	L	8	ARG
14	L	11	LEU
14	L	13	THR
14	L	15	ARG
14	L	16	LYS
14	L	26	ARG
14	L	31	VAL
14	L	34	SER
14	L	37	HIS
14	L	38	ILE
14	L	39	TYR
14	L	42	ILE
14	L	43	ILE
14	L	50	THR
14	L	65	THR
14	L	67	THR
14	L	71	VAL
14	L	75	LEU
14	L	82	LYS
14	L	93	SER
14	L	94	TYR
14	L	97	HIS
14	L	100	VAL
14	L	105	ASP
15	M	2	GLN
15	M	3	THR
15	M	6	LYS

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Mol	Chain	Res	Type
15	M	7	ILE
15	M	13	LEU
15	M	16	ILE
15	M	23	GLN
15	M	32	THR
15	M	33	VAL
15	M	38	LYS
15	M	57	ILE
15	M	90	GLN
15	M	91	VAL
15	M	94	VAL
15	M	95	GLU
15	M	96	ARG
15	M	116	ARG
16	N	8	ILE
16	N	11	ARG
16	N	22	LYS
16	N	58	ARG
16	N	60	LEU
16	N	78	THR
16	N	83	LEU
16	N	87	ASN
16	N	90	LEU
16	N	91	ASN
16	N	109	LEU
17	O	2	PHE
17	O	20	ILE
17	O	21	ARG
17	O	22	VAL
17	O	26	GLN
17	O	28	GLU
17	O	40	VAL
17	O	46	VAL
17	O	63	HIS
17	O	81	ARG
17	O	91	THR
17	O	93	ILE
18	P	9	ARG
18	P	20	LEU
18	P	27	VAL
18	P	32	ARG
18	P	39	ARG

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Mol	Chain	Res	Type
18	P	40	LEU
18	P	44	VAL
18	P	45	ILE
18	P	46	ARG
18	P	49	SER
18	P	62	ARG
18	P	89	ARG
18	P	102	THR
18	P	109	ARG
18	P	113	SER
18	P	125	THR
18	P	126	ILE
19	Q	7	LEU
19	Q	12	ILE
19	Q	15	LYS
19	Q	26	SER
19	Q	27	PHE
19	Q	34	THR
19	Q	58	VAL
19	Q	69	ILE
19	Q	74	ASP
19	Q	84	GLU
19	Q	86	GLN
19	Q	91	LEU
20	R	8	SER
20	R	11	ASN
20	R	21	THR
20	R	44	GLN
20	R	48	VAL
20	R	51	VAL
20	R	55	THR
20	R	56	LYS
20	R	58	VAL
20	R	74	LEU
20	R	80	LYS
20	R	81	VAL
20	R	83	LEU
20	R	88	THR
20	R	94	VAL
20	R	95	ARG
20	R	104	VAL
20	R	106	VAL

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Mol	Chain	Res	Type
20	R	113	THR
21	S	8	ARG
21	S	19	ILE
21	S	22	VAL
21	S	25	ASN
21	S	26	LYS
21	S	32	PHE
21	S	34	LEU
21	S	60	GLU
21	S	88	TYR
21	S	118	HIS
21	S	120	LEU
21	S	128	ARG
21	S	130	ILE
21	S	154	LEU
21	S	160	LEU
21	S	175	ARG
22	T	21	LEU
22	T	31	VAL
22	T	37	LEU
22	T	38	VAL
22	T	43	THR
22	T	64	ASP
22	T	68	VAL
22	T	70	ILE
22	T	79	ILE
22	T	81	ILE
23	U	6	TYR
23	U	11	LYS
23	U	12	ASN
23	U	25	ARG
23	U	30	VAL
23	U	42	GLN
23	U	46	LEU
23	U	48	LYS
23	U	52	ARG
23	U	62	LEU
24	V	6	MET
24	V	14	PHE
24	V	28	LEU
25	W	3	ILE
25	W	4	LYS

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Mol	Chain	Res	Type
25	W	6	VAL
25	W	9	VAL
25	W	26	ARG
25	W	34	VAL
25	W	37	THR
25	W	40	VAL
25	W	46	THR
26	Z	4	HIS
26	Z	11	THR
26	Z	18	MET
26	Z	25	LEU
26	Z	26	THR
26	Z	36	CYS
26	Z	42	SER
26	Z	53	ASP
26	Z	57	VAL
27	1	8	ILE
27	1	9	ILE
27	1	27	ASN
27	1	28	ARG
27	1	30	ASN
27	1	35	LEU
27	1	40	TYR
27	1	41	ASP
27	1	43	VAL
27	1	51	ARG
27	1	52	GLU
28	2	10	ARG
28	2	11	LYS
28	2	14	LYS
28	2	24	THR
28	2	25	LYS
28	2	31	LEU
28	2	40	HIS
28	2	41	GLN
28	2	42	LEU
28	2	44	VAL
28	2	45	SER
29	3	8	LYS
29	3	19	THR
29	3	27	SER
29	3	30	ARG

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Mol	Chain	Res	Type
29	3	31	HIS
29	3	34	THR
29	3	42	ARG
29	3	44	LYS
29	3	46	LYS
29	3	59	LYS
29	3	60	LEU
29	3	61	MET
29	3	62	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	154	GLN
4	B	92	ASN
4	B	168	GLN
5	C	66	ASN
5	C	112	GLN
6	D	63	GLN
8	F	103	GLN
9	G	40	ASN
12	J	124	HIS
13	K	3	HIS
13	K	13	ASN
14	L	86	GLN
15	M	20	HIS
17	O	79	GLN
17	O	89	ASN
18	P	10	ASN
18	P	73	ASN
18	P	115	ASN
19	Q	43	GLN
19	Q	57	ASN
19	Q	86	GLN
20	R	44	GLN
20	R	77	HIS
21	S	142	ASN
22	T	17	ASN
24	V	54	ASN
26	Z	35	GLN
26	Z	48	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2700/2877 (93%)	586 (21%)	42 (1%)
2	Y	119/124 (95%)	25 (21%)	1 (0%)
All	All	2819/3001 (93%)	611 (21%)	43 (1%)

All (611) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	4	C
1	X	14	A
1	X	15	G
1	X	23	G
1	X	34	U
1	X	45	C
1	X	50	G
1	X	51	A
1	X	54	G
1	X	59	G
1	X	60	A
1	X	63	A
1	X	73	A
1	X	74	G
1	X	87	G
1	X	89	A
1	X	90	G
1	X	95	G
1	X	98	U
1	X	100	G
1	X	104	C
1	X	105	G
1	X	108	G
1	X	112	U
1	X	116	A
1	X	118	U
1	X	123	A
1	X	124	A
1	X	126	C
1	X	129	A
1	X	134	G
1	X	136	A
1	X	138	G
1	X	143	A

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Mol	Chain	Res	Type
1	X	146	C
1	X	147	G
1	X	158	A
1	X	173	A
1	X	176	A
1	X	180	C
1	X	181	A
1	X	192	G
1	X	193	A
1	X	199	A
1	X	203	G
1	X	205	A
1	X	206	U
1	X	207	U
1	X	210	A
1	X	219	G
1	X	220	U
1	X	222	G
1	X	225	G
1	X	229	G
1	X	241	C
1	X	242	A
1	X	243	G
1	X	245	C
1	X	249	A
1	X	250	C
1	X	251	C
1	X	252	G
1	X	253	A
1	X	255	A
1	X	256	C
1	X	257	G
1	X	258	C
1	X	259	U
1	X	260	U
1	X	261	G
1	X	262	C
1	X	263	G
1	X	264	U
1	X	266	U
1	X	268	G
1	X	272	U

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Mol	Chain	Res	Type
1	X	273	U
1	X	274	G
1	X	275	U
1	X	276	A
1	X	279	A
1	X	280	C
1	X	282	A
1	X	305	A
1	X	310	A
1	X	312	G
1	X	321	A
1	X	327	C
1	X	332	C
1	X	335	A
1	X	340	G
1	X	341	A
1	X	343	A
1	X	344	G
1	X	359	G
1	X	361	G
1	X	384	A
1	X	385	G
1	X	386	U
1	X	387	A
1	X	388	G
1	X	396	U
1	X	399	G
1	X	400	U
1	X	408	U
1	X	412	U
1	X	414	A
1	X	417	C
1	X	418	C
1	X	419	G
1	X	421	G
1	X	424	G
1	X	431	G
1	X	441	A
1	X	447	U
1	X	448	C
1	X	456	C
1	X	463	C

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Mol	Chain	Res	Type
1	X	467	U
1	X	469	G
1	X	483	A
1	X	484	G
1	X	488	A
1	X	491	A
1	X	492	G
1	X	495	C
1	X	504	G
1	X	514	G
1	X	515	A
1	X	519	C
1	X	537	C
1	X	538	A
1	X	539	A
1	X	541	C
1	X	542	A
1	X	543	G
1	X	554	U
1	X	556	A
1	X	558	G
1	X	560	G
1	X	561	U
1	X	572	G
1	X	582	G
1	X	583	C
1	X	584	A
1	X	591	G
1	X	595	A
1	X	613	A
1	X	614	G
1	X	626	A
1	X	627	A
1	X	628	A
1	X	631	G
1	X	632	A
1	X	633	G
1	X	645	G
1	X	648	A
1	X	649	G
1	X	654	A
1	X	655	A

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Mol	Chain	Res	Type
1	X	656	U
1	X	657	A
1	X	664	C
1	X	665	A
1	X	666	U
1	X	667	U
1	X	668	A
1	X	682	G
1	X	683	A
1	X	684	C
1	X	690	A
1	X	699	G
1	X	713	G
1	X	743	A
1	X	753	U
1	X	761	G
1	X	766	A
1	X	781	G
1	X	789	G
1	X	790	A
1	X	795	A
1	X	797	A
1	X	798	G
1	X	801	A
1	X	804	C
1	X	805	G
1	X	806	A
1	X	814	G
1	X	818	G
1	X	825	C
1	X	832	A
1	X	839	U
1	X	840	U
1	X	859	U
1	X	860	U
1	X	869	C
1	X	872	G
1	X	879	A
1	X	922	A
1	X	926	C
1	X	938	G
1	X	939	C

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Mol	Chain	Res	Type
1	X	940	G
1	X	944	A
1	X	952	A
1	X	956	A
1	X	957	G
1	X	964	A
1	X	969	U
1	X	972	C
1	X	973	U
1	X	985	G
1	X	994	A
1	X	998	C
1	X	1000	G
1	X	1006	C
1	X	1007	A
1	X	1016	C
1	X	1019	U
1	X	1022	A
1	X	1023	U
1	X	1028	G
1	X	1032	A
1	X	1033	G
1	X	1034	U
1	X	1036	G
1	X	1037	U
1	X	1044	U
1	X	1049	C
1	X	1052	C
1	X	1053	G
1	X	1055	A
1	X	1056	U
1	X	1058	G
1	X	1061	A
1	X	1072	U
1	X	1077	U
1	X	1079	G
1	X	1081	A
1	X	1082	G
1	X	1086	C
1	X	1087	C
1	X	1090	C
1	X	1096	A

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Mol	Chain	Res	Type
1	X	1097	A
1	X	1099	A
1	X	1100	G
1	X	1101	U
1	X	1121	G
1	X	1123	G
1	X	1128	G
1	X	1129	A
1	X	1145	C
1	X	1146	G
1	X	1149	G
1	X	1152	C
1	X	1153	A
1	X	1154	A
1	X	1166	A
1	X	1167	A
1	X	1176	U
1	X	1183	C
1	X	1185	C
1	X	1192	A
1	X	1194	U
1	X	1195	U
1	X	1223	G
1	X	1225	G
1	X	1240	G
1	X	1247	U
1	X	1250	A
1	X	1266	G
1	X	1269	G
1	X	1284	G
1	X	1285	A
1	X	1289	A
1	X	1301	U
1	X	1313	U
1	X	1314	A
1	X	1325	U
1	X	1334	A
1	X	1337	G
1	X	1342	U
1	X	1345	G
1	X	1359	G
1	X	1370	U

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Mol	Chain	Res	Type
1	X	1372	A
1	X	1378	A
1	X	1379	A
1	X	1381	G
1	X	1391	A
1	X	1392	U
1	X	1398	G
1	X	1404	C
1	X	1409	U
1	X	1413	U
1	X	1428	G
1	X	1430	G
1	X	1432	G
1	X	1433	A
1	X	1434	U
1	X	1440	G
1	X	1442	C
1	X	1443	G
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	1482	U
1	X	1490	U
1	X	1497	C
1	X	1498	G
1	X	1505	U
1	X	1513	U
1	X	1528	C
1	X	1531	C
1	X	1551	U
1	X	1552	C
1	X	1553	G
1	X	1554	G
1	X	1562	G
1	X	1563	U
1	X	1569	A
1	X	1570	C
1	X	1571	G
1	X	1574	A

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Mol	Chain	Res	Type
1	X	1575	C
1	X	1582	A
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	1608	U
1	X	1624	A
1	X	1625	A
1	X	1626	A
1	X	1630	A
1	X	1631	C
1	X	1632	A
1	X	1634	A
1	X	1648	C
1	X	1656	U
1	X	1661	C
1	X	1665	C
1	X	1668	G
1	X	1671	A
1	X	1686	A
1	X	1691	G
1	X	1710	U
1	X	1711	C
1	X	1714	A
1	X	1717	A
1	X	1719	G
1	X	1733	U
1	X	1734	C
1	X	1735	G
1	X	1747	G
1	X	1753	A
1	X	1754	G
1	X	1755	G
1	X	1760	G
1	X	1764	A
1	X	1772	C
1	X	1775	A
1	X	1780	A
1	X	1782	A

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Mol	Chain	Res	Type
1	X	1790	G
1	X	1791	C
1	X	1792	C
1	X	1793	A
1	X	1796	A
1	X	1799	A
1	X	1801	C
1	X	1802	A
1	X	1807	A
1	X	1808	C
1	X	1811	A
1	X	1812	U
1	X	1813	A
1	X	1821	A
1	X	1825	C
1	X	1830	C
1	X	1831	G
1	X	1838	G
1	X	1839	A
1	X	1845	A
1	X	1861	G
1	X	1865	C
1	X	1867	A
1	X	1868	A
1	X	1875	C
1	X	1882	G
1	X	1884	A
1	X	1886	G
1	X	1887	G
1	X	1889	G
1	X	1891	C
1	X	1892	C
1	X	1893	G
1	X	1909	U
1	X	1910	A
1	X	1912	G
1	X	1920	A
1	X	1921	A
1	X	1922	U
1	X	1923	U
1	X	1924	C
1	X	1930	C

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Mol	Chain	Res	Type
1	X	1943	A
1	X	1944	C
1	X	1946	U
1	X	1947	G
1	X	1948	C
1	X	1949	A
1	X	1950	C
1	X	1953	A
1	X	1954	A
1	X	1955	G
1	X	1965	U
1	X	1976	U
1	X	1979	C
1	X	1980	A
1	X	2004	U
1	X	2006	G
1	X	2010	G
1	X	2014	A
1	X	2015	G
1	X	2019	C
1	X	2026	C
1	X	2032	G
1	X	2038	C
1	X	2039	G
1	X	2043	A
1	X	2044	G
1	X	2045	A
1	X	2052	G
1	X	2063	A
1	X	2083	G
1	X	2171	U
1	X	2189	A
1	X	2190	A
1	X	2191	A
1	X	2192	U
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

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Mol	Chain	Res	Type
1	X	2217	G
1	X	2218	G
1	X	2247	A
1	X	2252	A
1	X	2253	A
1	X	2254	C
1	X	2259	G
1	X	2262	C
1	X	2266	A
1	X	2272	A
1	X	2284	U
1	X	2285	U
1	X	2286	G
1	X	2287	G
1	X	2288	A
1	X	2290	A
1	X	2298	U
1	X	2299	A
1	X	2301	A
1	X	2306	A
1	X	2312	A
1	X	2313	G
1	X	2316	G
1	X	2323	U
1	X	2324	G
1	X	2326	C
1	X	2329	C
1	X	2351	G
1	X	2358	C
1	X	2362	G
1	X	2364	C
1	X	2367	A
1	X	2369	U
1	X	2371	A
1	X	2372	A
1	X	2379	G
1	X	2381	A
1	X	2382	C
1	X	2385	U
1	X	2386	G
1	X	2401	A
1	X	2402	U

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Mol	Chain	Res	Type
1	X	2404	A
1	X	2406	C
1	X	2408	G
1	X	2410	U
1	X	2413	A
1	X	2420	C
1	X	2427	A
1	X	2429	A
1	X	2447	G
1	X	2448	A
1	X	2452	U
1	X	2455	A
1	X	2457	A
1	X	2458	U
1	X	2463	G
1	X	2470	U
1	X	2473	G
1	X	2477	C
1	X	2480	C
1	X	2481	G
1	X	2484	G
1	X	2485	U
1	X	2497	A
1	X	2508	G
1	X	2541	U
1	X	2545	A
1	X	2546	G
1	X	2551	A
1	X	2553	G
1	X	2556	A
1	X	2564	U
1	X	2581	A
1	X	2588	U
1	X	2591	C
1	X	2592	U
1	X	2594	U
1	X	2608	A
1	X	2609	G
1	X	2613	A
1	X	2625	U
1	X	2633	A
1	X	2642	G

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Mol	Chain	Res	Type
1	X	2650	G
1	X	2664	G
1	X	2668	U
1	X	2688	G
1	X	2691	C
1	X	2692	A
1	X	2693	U
1	X	2698	G
1	X	2713	A
1	X	2730	A
1	X	2731	G
1	X	2732	C
1	X	2737	A
1	X	2738	A
1	X	2744	A
1	X	2745	A
1	X	2746	G
1	X	2756	A
1	X	2757	G
1	X	2758	A
1	X	2759	U
1	X	2760	G
1	X	2761	A
1	X	2762	G
1	X	2769	C
1	X	2771	C
1	X	2782	G
1	X	2783	U
1	X	2793	G
1	X	2795	A
1	X	2796	A
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	2842	C
1	X	2843	A
1	X	2848	A
1	X	2851	G
1	X	2854	G

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Mol	Chain	Res	Type
1	X	2855	C
1	X	2858	A
1	X	2861	A
1	X	2864	C
1	X	2866	A
1	X	2868	G
2	Y	9	G
2	Y	15	A
2	Y	17	A
2	Y	18	G
2	Y	22	U
2	Y	26	G
2	Y	27	A
2	Y	28	A
2	Y	29	C
2	Y	30	C
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	60	A
2	Y	68	A
2	Y	69	G
2	Y	99	G
2	Y	102	A
2	Y	108	G
2	Y	110	U
2	Y	112	A

All (43) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	50	G
1	X	104	C
1	X	219	G
1	X	265	U
1	X	334	G
1	X	383	G
1	X	483	A

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Mol	Chain	Res	Type
1	X	537	C
1	X	656	U
1	X	838	A
1	X	840	U
1	X	859	U
1	X	938	G
1	X	939	C
1	X	1031	C
1	X	1071	U
1	X	1096	A
1	X	1182	U
1	X	1223	G
1	X	1313	U
1	X	1391	A
1	X	1441	A
1	X	1466	C
1	X	1496	G
1	X	1607	A
1	X	1625	A
1	X	1811	A
1	X	1908	C
1	X	1923	U
1	X	1975	G
1	X	2018	G
1	X	2043	A
1	X	2204	A
1	X	2252	A
1	X	2287	G
1	X	2312	A
1	X	2409	A
1	X	2591	C
1	X	2593	A
1	X	2736	U
1	X	2756	A
1	X	2824	C
2	Y	27	A

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

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 455 ligands modelled in this entry, 446 are monoatomic - leaving 9 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	$\# Z > 2$
33	SPD	X	3322	-	9,9,9	0.32	0	8,8,8	0.62	0
33	SPD	X	3321	-	9,9,9	0.29	0	8,8,8	0.78	0
32	MPD	X	3317	-	7,7,7	0.31	0	9,10,10	0.28	0
30	6NO	X	2901	-	99,105,105	1.54	13 (13%)	129,164,164	1.69	27 (20%)
32	MPD	X	3315	-	7,7,7	0.23	0	9,10,10	0.53	0
33	SPD	X	3320	-	9,9,9	0.30	0	8,8,8	0.91	0
32	MPD	X	3316	-	7,7,7	0.50	0	9,10,10	1.13	1 (11%)
32	MPD	X	3319	-	7,7,7	0.33	0	9,10,10	0.16	0
32	MPD	X	3318	-	7,7,7	0.31	0	9,10,10	0.32	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	SPD	X	3322	-	-	2/7/7/7	-
33	SPD	X	3321	-	-	2/7/7/7	-
32	MPD	X	3317	-	-	1/5/5/5	-
30	6NO	X	2901	-	-	13/47/211/211	0/11/11/11
32	MPD	X	3315	-	-	5/5/5/5	-
33	SPD	X	3320	-	-	1/7/7/7	-
32	MPD	X	3316	-	-	1/5/5/5	-
32	MPD	X	3319	-	-	5/5/5/5	-
32	MPD	X	3318	-	-	4/5/5/5	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	X	2901	6NO	C08-C05	-6.32	1.39	1.51
30	X	2901	6NO	O53-C49	5.70	1.47	1.40
30	X	2901	6NO	C04-C09	-4.28	1.40	1.50
30	X	2901	6NO	O25-C16	4.09	1.48	1.41
30	X	2901	6NO	C51-C50	-3.88	1.47	1.54
30	X	2901	6NO	O50-C54	3.66	1.47	1.41
30	X	2901	6NO	O51-C54	3.56	1.47	1.41
30	X	2901	6NO	O44-C36	2.63	1.49	1.41
30	X	2901	6NO	O48-C44	2.52	1.47	1.41
30	X	2901	6NO	O44-C44	2.21	1.48	1.41
30	X	2901	6NO	O19-C10	2.13	1.47	1.41
30	X	2901	6NO	O26-C22	2.11	1.47	1.42
30	X	2901	6NO	O20-C16	2.04	1.43	1.41

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	X	2901	6NO	C44-O44-C36	-5.69	104.11	114.33
30	X	2901	6NO	O47-C47-C46	-4.31	96.54	103.54
30	X	2901	6NO	C06-C01-C02	3.88	121.94	117.78
30	X	2901	6NO	O44-C36-O40	3.67	120.34	110.69
30	X	2901	6NO	C24-C23-C22	-3.56	108.98	114.99
30	X	2901	6NO	C13-O13-C09	-3.42	111.78	117.24
30	X	2901	6NO	C16-O20-C20	-3.32	109.14	112.16
30	X	2901	6NO	O46-C46-C47	-3.29	98.90	103.48
30	X	2901	6NO	O44-C44-O48	3.26	115.66	108.92
30	X	2901	6NO	C41-O37-C37	-3.20	106.26	114.47
30	X	2901	6NO	C35-C33-C32	-3.04	108.87	113.39
30	X	2901	6NO	O25-C25-C26	3.03	114.18	108.20
30	X	2901	6NO	C48-C47-C46	-3.00	106.91	112.56
30	X	2901	6NO	C01-C06-C05	-2.91	119.54	122.65
30	X	2901	6NO	O44-C44-C45	2.75	114.44	109.09
30	X	2901	6NO	O24-C24-C25	-2.73	98.27	102.03
30	X	2901	6NO	O50-C50-C51	-2.65	98.31	105.36
30	X	2901	6NO	O20-C20-C21	2.56	109.06	105.94
30	X	2901	6NO	O24-C24-C23	2.46	114.51	109.38
30	X	2901	6NO	C01-C02-C03	-2.45	117.44	120.68
30	X	2901	6NO	O51-C51-C50	-2.38	99.02	105.36
30	X	2901	6NO	C30-C31-C32	-2.29	106.56	111.72
30	X	2901	6NO	O24-C24-C27	2.19	112.58	108.61
30	X	2901	6NO	C08-C05-C06	-2.15	117.34	121.23
32	X	3316	MPD	C5-C4-C3	2.14	121.62	111.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	X	2901	6NO	C03-C02-CL2	2.12	122.21	118.95
30	X	2901	6NO	O26-C26-C28	2.08	111.34	106.74
30	X	2901	6NO	C76-C75-C52	-2.04	115.57	118.85

There are no chirality outliers.

All (34) torsion outliers are listed below:

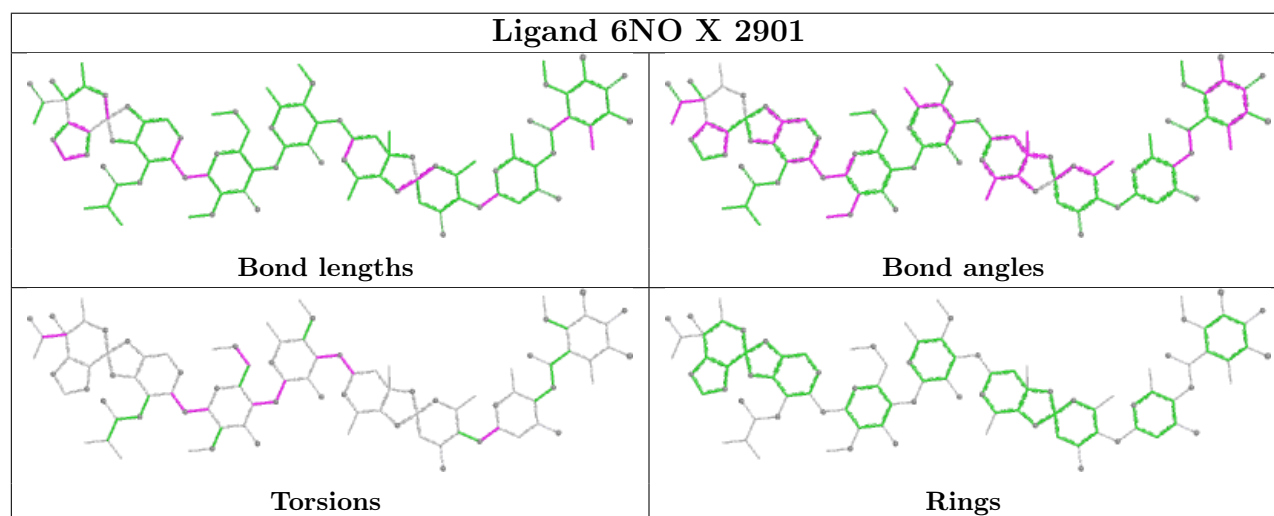
Mol	Chain	Res	Type	Atoms
30	X	2901	6NO	O33-C29-O39-C39
30	X	2901	6NO	C37-C36-O44-C44
30	X	2901	6NO	O40-C36-O44-C44
30	X	2901	6NO	O52-C52-C75-O75
32	X	3315	MPD	C2-C3-C4-C5
32	X	3316	MPD	C2-C3-C4-C5
32	X	3317	MPD	C2-C3-C4-C5
32	X	3319	MPD	C2-C3-C4-O4
33	X	3321	SPD	C3-C4-C5-N6
30	X	2901	6NO	O14-C10-O19-C19
33	X	3322	SPD	C8-C7-N6-C5
30	X	2901	6NO	C40-C42-O42-C43
30	X	2901	6NO	C45-C44-O44-C36
33	X	3321	SPD	N1-C2-C3-C4
30	X	2901	6NO	O48-C44-O44-C36
30	X	2901	6NO	C38-C39-O39-C29
32	X	3315	MPD	CM-C2-C3-C4
32	X	3319	MPD	CM-C2-C3-C4
30	X	2901	6NO	C40-C39-O39-C29
32	X	3318	MPD	C2-C3-C4-C5
32	X	3319	MPD	C2-C3-C4-C5
30	X	2901	6NO	C30-C31-O31-C22
30	X	2901	6NO	O26-C22-O31-C31
33	X	3320	SPD	C7-C8-C9-N10
30	X	2901	6NO	C32-C31-O31-C22
33	X	3322	SPD	C2-C3-C4-C5
32	X	3315	MPD	O2-C2-C3-C4
32	X	3318	MPD	O2-C2-C3-C4
32	X	3319	MPD	O2-C2-C3-C4
32	X	3315	MPD	C2-C3-C4-O4
32	X	3318	MPD	C2-C3-C4-O4
32	X	3315	MPD	C1-C2-C3-C4
32	X	3318	MPD	C1-C2-C3-C4
32	X	3319	MPD	C1-C2-C3-C4

There are no ring outliers.

7 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	X	3322	SPD	3	0
33	X	3321	SPD	3	0
30	X	2901	6NO	3	0
32	X	3315	MPD	3	0
33	X	3320	SPD	1	0
32	X	3316	MPD	11	0
32	X	3319	MPD	1	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	2710/2877 (94%)	-0.23	42 (1%) 72 58	25, 91, 200, 334	1 (0%)
2	Y	120/124 (96%)	-0.01	2 (1%) 69 54	97, 137, 188, 213	0
3	A	272/275 (98%)	1.05	57 (20%) 2 4	53, 112, 177, 240	0
4	B	205/211 (97%)	0.24	12 (5%) 28 21	28, 66, 136, 250	0
5	C	195/205 (95%)	0.76	29 (14%) 5 7	56, 103, 204, 281	0
6	D	177/180 (98%)	0.55	18 (10%) 12 12	120, 178, 253, 296	0
7	E	171/185 (92%)	0.26	12 (7%) 22 18	69, 137, 216, 268	0
8	F	63/144 (43%)	1.46	19 (30%) 1 2	142, 200, 295, 418	0
9	G	142/174 (81%)	0.94	27 (19%) 3 4	48, 89, 188, 342	0
10	H	134/134 (100%)	0.16	6 (4%) 38 28	29, 61, 104, 144	0
11	I	134/156 (85%)	1.27	33 (24%) 2 3	51, 120, 206, 280	0
12	J	136/141 (96%)	0.78	23 (16%) 4 5	58, 99, 176, 252	0
13	K	115/116 (99%)	0.17	9 (7%) 19 16	25, 47, 100, 192	0
14	L	104/114 (91%)	1.16	27 (25%) 1 3	65, 124, 188, 298	0
15	M	119/166 (71%)	0.32	7 (5%) 28 21	40, 62, 136, 200	0
16	N	117/118 (99%)	0.58	11 (9%) 14 13	51, 82, 127, 243	0
17	O	97/100 (97%)	0.95	19 (19%) 3 4	63, 107, 193, 284	0
18	P	128/134 (95%)	-0.06	1 (0%) 82 71	17, 64, 110, 190	0
19	Q	93/95 (97%)	0.51	10 (10%) 11 11	57, 103, 159, 219	0
20	R	110/115 (95%)	1.06	25 (22%) 2 3	65, 110, 221, 253	0
21	S	180/237 (75%)	0.57	19 (10%) 11 11	95, 152, 223, 265	0
22	T	74/91 (81%)	0.47	9 (12%) 8 9	66, 101, 148, 193	0
23	U	74/81 (91%)	1.34	20 (27%) 1 2	62, 127, 214, 239	0
24	V	65/67 (97%)	0.32	2 (3%) 51 38	84, 131, 191, 271	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	55/55 (100%)	-0.02	2 (3%) 46 33	57, 93, 139, 184	0
26	Z	57/60 (95%)	0.06	1 (1%) 67 53	28, 55, 117, 149	0
27	1	53/55 (96%)	1.22	13 (24%) 2 3	82, 147, 236, 292	0
28	2	46/47 (97%)	1.17	8 (17%) 4 5	56, 78, 116, 190	0
29	3	59/66 (89%)	2.13	26 (44%) 0 1	59, 106, 166, 333	0
All	All	6005/6523 (92%)	0.25	489 (8%) 18 15	17, 100, 205, 418	1 (0%)

All (489) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	I	34	HIS	11.5
28	2	46	ASP	10.1
5	C	49	ALA	10.0
9	G	159	SER	9.9
23	U	52	ARG	8.4
9	G	110	LEU	8.3
17	O	7	THR	8.3
3	A	44	ASN	7.6
6	D	94	GLU	7.4
1	X	1718[A]	A	7.1
11	I	35	LYS	7.1
29	3	40	GLU	6.9
5	C	50	GLN	6.8
12	J	27	TYR	6.8
3	A	101	GLU	6.8
11	I	31	GLY	6.7
29	3	42	ARG	6.7
3	A	270	ILE	6.7
9	G	97	ASP	6.6
28	2	39	ARG	6.4
11	I	52	GLY	6.3
9	G	155	THR	6.2
11	I	63	ARG	6.1
16	N	88	ILE	6.1
11	I	36	GLY	6.0
12	J	84	MET	6.0
14	L	87	VAL	5.8
13	K	50	GLN	5.8
15	M	11	GLU	5.8
26	Z	3	LYS	5.7

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Mol	Chain	Res	Type	RSRZ
29	3	37	SER	5.7
8	F	128	ALA	5.6
14	L	36	LYS	5.6
9	G	99	VAL	5.6
17	O	11	GLN	5.5
8	F	127	VAL	5.5
29	3	63	PRO	5.5
20	R	93	ARG	5.4
11	I	49	PHE	5.3
23	U	13	LEU	5.3
3	A	243	GLY	5.3
11	I	42	GLY	5.3
29	3	58	MET	5.3
24	V	44	ARG	5.2
14	L	89	PHE	5.2
16	N	94	VAL	5.1
1	X	1889	G	5.1
28	2	44	VAL	5.1
7	E	5	GLY	5.0
3	A	30	GLU	5.0
13	K	94	TYR	5.0
15	M	116	ARG	4.9
20	R	74	LEU	4.9
3	A	45	ASN	4.9
23	U	67	LEU	4.9
3	A	43	ARG	4.9
5	C	163	ASN	4.8
3	A	37	LEU	4.8
9	G	102	ARG	4.7
3	A	32	ALA	4.7
29	3	62	LEU	4.7
3	A	40	THR	4.7
14	L	19	THR	4.6
29	3	38	GLY	4.6
29	3	54	GLU	4.6
23	U	47	HIS	4.6
11	I	45	LYS	4.6
16	N	23	GLY	4.6
29	3	45	GLY	4.5
23	U	16	ASN	4.5
3	A	97	TYR	4.5
12	J	62	GLY	4.5

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Mol	Chain	Res	Type	RSRZ
13	K	7	GLY	4.5
5	C	29	GLU	4.5
14	L	88	VAL	4.4
8	F	105	LEU	4.4
5	C	90	SER	4.4
5	C	164	VAL	4.3
29	3	34	THR	4.3
2	Y	43	G	4.3
11	I	39	SER	4.3
3	A	237	GLU	4.3
1	X	1098	G	4.2
12	J	91	VAL	4.2
20	R	108	VAL	4.2
3	A	250	TRP	4.2
28	2	37	LYS	4.2
20	R	26	SER	4.1
1	X	1920	A	4.1
27	1	38	LYS	4.1
20	R	106	VAL	4.1
28	2	42	LEU	4.1
23	U	54	ASN	4.1
11	I	55	ARG	4.0
5	C	55	GLY	4.0
17	O	4	ILE	4.0
29	3	14	ILE	4.0
14	L	18	ARG	4.0
8	F	108	ALA	4.0
14	L	57	ALA	4.0
17	O	13	ARG	4.0
5	C	161	ALA	4.0
12	J	12	LYS	4.0
11	I	48	PHE	3.9
20	R	6	ALA	3.9
29	3	29	LYS	3.9
17	O	36	LYS	3.9
16	N	91	ASN	3.9
3	A	263	ARG	3.9
28	2	43	THR	3.8
17	O	10	LYS	3.8
27	1	34	LYS	3.8
16	N	12	ARG	3.8
11	I	74	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
23	U	21	ARG	3.7
3	A	253	PRO	3.7
1	X	1085	G	3.7
1	X	1923	U	3.7
4	B	142	GLY	3.7
21	S	23	ALA	3.6
3	A	262	LYS	3.6
23	U	50	ALA	3.6
4	B	146	THR	3.6
23	U	51	ILE	3.6
9	G	156	HIS	3.6
20	R	79	SER	3.6
10	H	36	THR	3.6
19	Q	52	GLY	3.6
20	R	90	LYS	3.6
10	H	8	LEU	3.6
8	F	90	THR	3.6
15	M	40	ARG	3.5
15	M	114	ALA	3.5
7	E	7	GLN	3.5
14	L	24	SER	3.5
3	A	267	ASP	3.5
1	X	2381	A	3.5
1	X	1734	C	3.5
14	L	65	THR	3.5
17	O	18	ASP	3.5
3	A	35	GLU	3.5
29	3	31	HIS	3.5
4	B	159	HIS	3.4
12	J	29	ALA	3.4
25	W	26	ARG	3.4
10	H	31	GLY	3.4
3	A	242	ALA	3.4
23	U	37	ILE	3.4
3	A	208	LYS	3.4
11	I	47	ALA	3.4
23	U	20	ARG	3.4
3	A	15	GLN	3.4
20	R	88	THR	3.4
15	M	78	GLU	3.4
3	A	241	GLY	3.4
20	R	92	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	X	265	U	3.4
8	F	88	SER	3.4
23	U	23	LYS	3.4
5	C	91	TYR	3.3
5	C	54	THR	3.3
14	L	58	ALA	3.3
12	J	60	ARG	3.3
13	K	2	ARG	3.3
28	2	41	GLN	3.3
5	C	189	ASP	3.3
3	A	240	THR	3.3
14	L	56	SER	3.2
11	I	75	VAL	3.2
20	R	81	VAL	3.2
20	R	94	VAL	3.2
9	G	95	LEU	3.2
19	Q	63	LYS	3.2
6	D	84	PRO	3.2
21	S	29	ASN	3.2
9	G	100	TYR	3.2
17	O	6	GLN	3.2
1	X	1951	G	3.2
27	1	36	GLU	3.2
19	Q	2	SER	3.2
27	1	48	VAL	3.1
29	3	23	MET	3.1
11	I	24	GLY	3.1
29	3	28	GLY	3.1
16	N	48	ARG	3.1
23	U	6	TYR	3.1
5	C	57	LYS	3.1
7	E	115	ILE	3.1
17	O	88	GLN	3.1
20	R	78	ALA	3.1
21	S	116	VAL	3.1
21	S	22	VAL	3.1
22	T	15	ASP	3.1
7	E	6	LYS	3.1
3	A	55	GLY	3.1
5	C	42	THR	3.1
14	L	20	THR	3.1
3	A	184	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
9	G	165	VAL	3.1
9	G	113	GLU	3.1
18	P	19	LYS	3.1
21	S	72	ASP	3.1
9	G	68	PRO	3.1
14	L	40	ALA	3.0
21	S	76	ARG	3.0
1	X	1551	U	3.0
3	A	39	LYS	3.0
22	T	19	LYS	3.0
13	K	1	MET	3.0
9	G	69	ASP	3.0
27	1	27	ASN	3.0
5	C	80	GLY	3.0
7	E	10	ALA	3.0
7	E	37	TYR	3.0
5	C	72	ARG	3.0
16	N	92	ARG	3.0
4	B	135	HIS	3.0
1	X	280	C	3.0
29	3	36	LYS	3.0
14	L	97	HIS	3.0
23	U	22	GLY	3.0
3	A	33	LEU	2.9
12	J	140	GLU	2.9
1	X	2290	A	2.9
12	J	21	ASP	2.9
12	J	32	ASP	2.9
3	A	172	TYR	2.9
11	I	68	VAL	2.9
3	A	103	ARG	2.9
29	3	24	ALA	2.9
23	U	14	VAL	2.9
14	L	34	SER	2.9
19	Q	15	LYS	2.9
1	X	1753	A	2.9
1	X	1890	A	2.9
23	U	40	ARG	2.9
12	J	88	LYS	2.9
8	F	126	THR	2.9
22	T	74	LYS	2.9
1	X	2385	U	2.8

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Mol	Chain	Res	Type	RSRZ
3	A	78	LYS	2.8
22	T	45	PHE	2.8
6	D	152	MET	2.8
7	E	111	HIS	2.8
14	L	61	SER	2.8
20	R	84	VAL	2.8
20	R	83	LEU	2.8
27	1	17	GLY	2.8
8	F	123	ALA	2.8
12	J	86	LYS	2.8
13	K	43	GLU	2.8
3	A	227	ASN	2.8
12	J	105	PHE	2.8
3	A	48	ARG	2.8
29	3	39	ASP	2.8
1	X	251	C	2.8
1	X	281	C	2.8
9	G	163	PRO	2.8
3	A	230	ASP	2.7
5	C	41	GLY	2.7
3	A	76	ASN	2.7
5	C	172	VAL	2.7
12	J	109	GLY	2.7
8	F	111	LYS	2.7
9	G	106	TYR	2.7
5	C	51	VAL	2.7
17	O	33	VAL	2.7
2	Y	54	U	2.7
8	F	107	ILE	2.7
12	J	48	ILE	2.7
17	O	5	ILE	2.7
6	D	133	LYS	2.7
12	J	139	ASP	2.7
3	A	16	MET	2.7
11	I	50	GLU	2.7
3	A	261	ARG	2.7
11	I	27	ASP	2.7
17	O	71	ILE	2.7
6	D	131	GLY	2.7
6	D	75	SER	2.7
5	C	150	LEU	2.7
9	G	137	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
7	E	68	THR	2.6
21	S	20	ALA	2.6
29	3	60	LEU	2.6
20	R	29	HIS	2.6
15	M	117	ILE	2.6
11	I	81	GLN	2.6
27	1	18	THR	2.6
3	A	217	ARG	2.6
16	N	89	ASP	2.6
21	S	151	ASP	2.6
11	I	11	GLY	2.6
20	R	21	THR	2.6
22	T	69	PHE	2.6
3	A	72	LYS	2.6
4	B	111	LYS	2.6
9	G	67	ARG	2.6
24	V	47	ARG	2.6
4	B	112	GLY	2.6
6	D	153	ASP	2.6
27	1	19	GLY	2.6
14	L	63	ASN	2.6
19	Q	14	GLU	2.6
3	A	102	LYS	2.6
3	A	183	ARG	2.6
1	X	1922	U	2.5
3	A	239	ARG	2.5
3	A	252	LYS	2.5
29	3	64	ARG	2.5
21	S	177	THR	2.5
8	F	76	TYR	2.5
12	J	16	GLY	2.5
20	R	91	ALA	2.5
8	F	134	MET	2.5
6	D	78	LYS	2.5
22	T	40	GLN	2.5
21	S	86	VAL	2.5
21	S	171	VAL	2.5
14	L	52	ALA	2.5
21	S	68	ALA	2.5
4	B	113	THR	2.5
3	A	31	LYS	2.5
9	G	158	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
27	1	11	LYS	2.5
3	A	255	LYS	2.5
5	C	71	ASP	2.4
16	N	59	ARG	2.4
22	T	77	ARG	2.4
29	3	55	TRP	2.4
1	X	1390	G	2.4
1	X	1937	G	2.4
1	X	2287	G	2.4
3	A	271	VAL	2.4
8	F	104	VAL	2.4
6	D	32	GLU	2.4
6	D	69	LYS	2.4
19	Q	4	TYR	2.4
1	X	257	G	2.4
1	X	1223	G	2.4
10	H	132	GLU	2.4
14	L	75	LEU	2.4
16	N	44	THR	2.4
20	R	86	PRO	2.4
21	S	82	ASP	2.4
9	G	162	LYS	2.4
19	Q	71	GLN	2.4
1	X	114	C	2.4
3	A	257	LEU	2.4
10	H	117	GLU	2.4
11	I	109	LEU	2.4
9	G	66	HIS	2.4
11	I	123	ASP	2.4
5	C	58	MET	2.4
7	E	140	LEU	2.4
1	X	671	A	2.4
14	L	21	THR	2.3
1	X	252	G	2.3
1	X	1716	G	2.3
9	G	109	GLY	2.3
12	J	63	GLY	2.3
11	I	30	ALA	2.3
9	G	148	LEU	2.3
4	B	171	GLU	2.3
11	I	107	LYS	2.3
20	R	41	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
9	G	146	THR	2.3
12	J	19	THR	2.3
12	J	22	ALA	2.3
14	L	53	ALA	2.3
29	3	19	THR	2.3
14	L	11	LEU	2.3
16	N	95	LEU	2.3
3	A	91	ARG	2.3
5	C	188	ILE	2.3
6	D	139	PRO	2.3
22	T	13	GLY	2.3
20	R	25	LEU	2.3
1	X	263	G	2.3
5	C	92	ASP	2.3
13	K	5	LYS	2.3
27	1	3	LYS	2.3
1	X	774	A	2.3
1	X	2581	A	2.3
17	O	8	GLY	2.3
8	F	101	TRP	2.3
20	R	77	HIS	2.3
6	D	8	TYR	2.3
7	E	46	ASP	2.3
3	A	246	PRO	2.2
11	I	58	ALA	2.2
17	O	77	GLY	2.2
1	X	1792	C	2.2
5	C	180	ILE	2.2
9	G	33	ILE	2.2
17	O	98	ILE	2.2
8	F	94	ALA	2.2
8	F	112	MET	2.2
8	F	129	GLY	2.2
13	K	10	LEU	2.2
1	X	419	G	2.2
20	R	56	LYS	2.2
29	3	7	HIS	2.2
21	S	30	VAL	2.2
21	S	92	VAL	2.2
6	D	117	ILE	2.2
11	I	46	GLY	2.2
9	G	149	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
6	D	138	PHE	2.2
29	3	25	PHE	2.2
3	A	265	THR	2.2
27	1	22	TYR	2.2
3	A	141	VAL	2.2
15	M	39	VAL	2.2
14	L	35	SER	2.2
1	X	271	G	2.2
3	A	56	GLY	2.2
14	L	102	ALA	2.2
17	O	9	GLY	2.2
6	D	5	LYS	2.2
3	A	13	ARG	2.2
21	S	83	PHE	2.2
4	B	1	MET	2.2
14	L	54	ALA	2.2
1	X	1	G	2.2
5	C	148	VAL	2.1
11	I	29	THR	2.1
1	X	1570	C	2.1
5	C	193	LEU	2.1
8	F	115	LEU	2.1
12	J	79	PRO	2.1
14	L	26	ARG	2.1
20	R	11	ASN	2.1
12	J	26	ASP	2.1
13	K	69	ASP	2.1
5	C	130	THR	2.1
19	Q	51	ILE	2.1
21	S	172	LEU	2.1
28	2	31	LEU	2.1
17	O	37	ALA	2.1
22	T	73	GLY	2.1
11	I	88	PHE	2.1
29	3	48	PHE	2.1
21	S	94	VAL	2.1
19	Q	3	HIS	2.1
3	A	64	ILE	2.1
9	G	103	TYR	2.1
17	O	67	LYS	2.1
6	D	63	GLN	2.1
11	I	79	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	X	123	A	2.1
7	E	106	ASN	2.1
20	R	53	VAL	2.1
1	X	113	C	2.1
1	X	759	C	2.1
6	D	144	ASP	2.1
19	Q	61	LYS	2.1
27	1	26	LYS	2.1
8	F	99	LEU	2.1
17	O	12	TYR	2.1
7	E	8	PRO	2.1
1	X	668	A	2.1
23	U	33	LYS	2.1
23	U	39	LYS	2.1
3	A	34	THR	2.1
4	B	110	GLY	2.1
23	U	55	GLY	2.1
1	X	1909	U	2.0
14	L	42	ILE	2.0
23	U	62	LEU	2.0
29	3	50	LEU	2.0
3	A	259	THR	2.0
6	D	149	THR	2.0
9	G	96	ASP	2.0
11	I	26	THR	2.0
12	J	30	PHE	2.0
3	A	218	LYS	2.0
10	H	27	SER	2.0
1	X	1482	U	2.0
4	B	187	ALA	2.0
21	S	148	THR	2.0
27	1	44	ALA	2.0
11	I	82	ASP	2.0
4	B	178	GLY	2.0
11	I	33	GLY	2.0
3	A	11	PRO	2.0
25	W	6	VAL	2.0
5	C	19	LEU	2.0
5	C	170	LEU	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
31	MG	X	3144	1/1	0.34	0.15	76,76,76,76	0
31	MG	X	3273	1/1	0.40	0.15	70,70,70,70	0
31	MG	X	3218	1/1	0.41	0.28	78,78,78,78	0
31	MG	X	3268	1/1	0.43	0.24	115,115,115,115	0
31	MG	X	3313	1/1	0.47	0.28	74,74,74,74	0
31	MG	X	3130	1/1	0.48	0.47	62,62,62,62	0
31	MG	X	3169	1/1	0.51	0.22	77,77,77,77	0
31	MG	X	3262	1/1	0.53	0.15	113,113,113,113	0
31	MG	X	3178	1/1	0.55	0.79	60,60,60,60	0
31	MG	X	2915	1/1	0.55	0.18	39,39,39,39	0
31	MG	X	3142	1/1	0.59	0.25	57,57,57,57	0
31	MG	X	3306	1/1	0.59	0.15	116,116,116,116	0
31	MG	X	3241	1/1	0.59	0.19	85,85,85,85	0
31	MG	X	3309	1/1	0.60	0.23	87,87,87,87	0
31	MG	X	3300	1/1	0.60	0.70	67,67,67,67	0
31	MG	X	3091	1/1	0.64	0.26	49,49,49,49	0
31	MG	X	3229	1/1	0.64	0.40	71,71,71,71	0
31	MG	X	3054	1/1	0.66	0.51	72,72,72,72	0
31	MG	X	3097	1/1	0.66	0.31	63,63,63,63	0
31	MG	X	3126	1/1	0.66	0.45	42,42,42,42	0
31	MG	X	3246	1/1	0.68	0.17	87,87,87,87	0
31	MG	Y	213	1/1	0.68	0.14	83,83,83,83	0
31	MG	X	3314	1/1	0.69	0.29	62,62,62,62	0
31	MG	X	3072	1/1	0.69	0.34	73,73,73,73	0
31	MG	X	3189	1/1	0.70	0.29	61,61,61,61	0
31	MG	X	3102	1/1	0.70	0.36	46,46,46,46	0
31	MG	X	3301	1/1	0.71	0.44	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	MG	X	3059	1/1	0.71	0.19	51,51,51,51	0
31	MG	X	2965	1/1	0.71	0.32	52,52,52,52	0
31	MG	Y	216	1/1	0.71	0.11	70,70,70,70	0
31	MG	X	3145	1/1	0.72	0.30	83,83,83,83	0
31	MG	X	3087	1/1	0.72	0.21	54,54,54,54	0
31	MG	X	3230	1/1	0.72	0.40	99,99,99,99	0
31	MG	X	3202	1/1	0.72	0.15	64,64,64,64	0
31	MG	X	3216	1/1	0.73	0.32	70,70,70,70	0
31	MG	X	3296	1/1	0.73	0.35	56,56,56,56	0
31	MG	X	3192	1/1	0.73	0.21	55,55,55,55	0
31	MG	X	3234	1/1	0.73	0.37	83,83,83,83	0
31	MG	X	3240	1/1	0.73	0.30	82,82,82,82	0
31	MG	X	3177	1/1	0.74	0.16	75,75,75,75	0
33	SPD	X	3320	10/10	0.74	0.30	44,44,44,44	0
31	MG	Y	218	1/1	0.75	0.16	83,83,83,83	0
31	MG	X	3279	1/1	0.75	0.28	50,50,50,50	0
31	MG	X	3180	1/1	0.76	0.57	115,115,115,115	0
31	MG	X	3263	1/1	0.76	0.23	59,59,59,59	0
31	MG	X	2962	1/1	0.77	0.19	84,84,84,84	0
31	MG	X	3190	1/1	0.77	0.26	56,56,56,56	0
31	MG	X	3089	1/1	0.77	0.31	79,79,79,79	0
31	MG	Y	207	1/1	0.77	0.24	93,93,93,93	0
31	MG	X	3073	1/1	0.78	0.26	94,94,94,94	0
31	MG	X	3105	1/1	0.78	0.23	80,80,80,80	0
31	MG	X	2902	1/1	0.78	0.23	27,27,27,27	0
31	MG	X	3277	1/1	0.78	0.27	39,39,39,39	0
31	MG	X	2973	1/1	0.78	0.24	23,23,23,23	0
31	MG	X	3067	1/1	0.78	0.20	60,60,60,60	0
31	MG	X	3261	1/1	0.78	0.15	78,78,78,78	0
31	MG	X	3039	1/1	0.78	0.33	51,51,51,51	0
32	MPD	X	3318	8/8	0.78	0.20	79,79,79,79	0
31	MG	X	3304	1/1	0.78	0.15	88,88,88,88	0
31	MG	Y	215	1/1	0.79	0.15	81,81,81,81	0
31	MG	X	3302	1/1	0.79	0.48	100,100,100,100	0
31	MG	X	3278	1/1	0.79	0.20	50,50,50,50	0
31	MG	X	3074	1/1	0.79	0.51	61,61,61,61	0
31	MG	X	3289	1/1	0.79	0.31	74,74,74,74	0
31	MG	X	3109	1/1	0.80	0.16	74,74,74,74	0
31	MG	X	3070	1/1	0.80	0.18	39,39,39,39	0
31	MG	X	3249	1/1	0.80	0.24	103,103,103,103	0
31	MG	X	3324	1/1	0.80	0.32	26,26,26,26	0
31	MG	X	3250	1/1	0.80	0.39	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	MG	X	3251	1/1	0.80	0.12	85,85,85,85	0
31	MG	X	3051	1/1	0.80	0.16	29,29,29,29	0
31	MG	X	3133	1/1	0.80	0.21	73,73,73,73	0
31	MG	X	3198	1/1	0.80	0.17	66,66,66,66	0
31	MG	X	3235	1/1	0.80	0.32	79,79,79,79	0
31	MG	X	3075	1/1	0.80	0.28	52,52,52,52	0
31	MG	X	3195	1/1	0.81	0.47	90,90,90,90	0
31	MG	X	3255	1/1	0.81	0.16	69,69,69,69	0
31	MG	X	3259	1/1	0.81	0.12	69,69,69,69	0
31	MG	X	3137	1/1	0.81	0.23	57,57,57,57	0
31	MG	X	3084	1/1	0.81	0.19	37,37,37,37	0
31	MG	X	3057	1/1	0.81	0.14	36,36,36,36	0
31	MG	X	3088	1/1	0.81	0.12	51,51,51,51	0
31	MG	X	2958	1/1	0.81	0.25	38,38,38,38	0
31	MG	X	3276	1/1	0.81	0.41	114,114,114,114	0
31	MG	X	3174	1/1	0.81	0.42	52,52,52,52	0
31	MG	X	3185	1/1	0.82	0.08	87,87,87,87	0
31	MG	X	3214	1/1	0.82	0.17	71,71,71,71	0
31	MG	X	3292	1/1	0.82	0.22	28,28,28,28	0
31	MG	X	3001	1/1	0.82	0.41	57,57,57,57	0
31	MG	X	3220	1/1	0.83	0.11	66,66,66,66	0
31	MG	X	3298	1/1	0.83	0.23	20,20,20,20	0
31	MG	Y	206	1/1	0.83	0.26	70,70,70,70	0
31	MG	X	3064	1/1	0.83	0.31	76,76,76,76	0
31	MG	Y	212	1/1	0.83	0.20	78,78,78,78	0
31	MG	X	3210	1/1	0.83	0.09	62,62,62,62	0
31	MG	X	3031	1/1	0.83	0.27	64,64,64,64	0
31	MG	X	3287	1/1	0.83	0.24	65,65,65,65	0
31	MG	X	2931	1/1	0.83	0.25	25,25,25,25	0
31	MG	X	3291	1/1	0.83	0.21	116,116,116,116	0
31	MG	X	3132	1/1	0.83	0.20	70,70,70,70	0
31	MG	X	3168	1/1	0.84	0.24	76,76,76,76	0
31	MG	X	3312	1/1	0.84	0.08	71,71,71,71	0
31	MG	X	3094	1/1	0.84	0.32	76,76,76,76	0
31	MG	X	3063	1/1	0.84	0.27	52,52,52,52	0
31	MG	X	3290	1/1	0.84	0.18	71,71,71,71	0
31	MG	Y	201	1/1	0.84	0.20	57,57,57,57	0
31	MG	X	3176	1/1	0.84	0.09	47,47,47,47	0
31	MG	X	3000	1/1	0.84	0.47	82,82,82,82	0
31	MG	X	3236	1/1	0.84	0.12	56,56,56,56	0
31	MG	X	3239	1/1	0.84	0.20	84,84,84,84	0
31	MG	X	3104	1/1	0.84	0.33	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	MG	X	2919	1/1	0.84	0.27	40,40,40,40	0
31	MG	X	3245	1/1	0.84	0.22	98,98,98,98	0
31	MG	Y	219	1/1	0.84	0.11	81,81,81,81	0
31	MG	X	3003	1/1	0.84	0.39	49,49,49,49	0
31	MG	X	3078	1/1	0.84	0.33	82,82,82,82	0
33	SPD	X	3321	10/10	0.84	0.40	88,88,88,88	0
31	MG	X	3049	1/1	0.85	0.31	70,70,70,70	0
31	MG	X	3173	1/1	0.85	0.28	82,82,82,82	0
31	MG	X	3020	1/1	0.85	0.41	47,47,47,47	0
31	MG	X	3275	1/1	0.85	0.21	70,70,70,70	0
31	MG	X	3069	1/1	0.85	0.23	49,49,49,49	0
31	MG	X	3208	1/1	0.85	0.11	61,61,61,61	0
31	MG	X	2999	1/1	0.85	0.11	29,29,29,29	0
31	MG	X	3033	1/1	0.85	0.21	75,75,75,75	0
31	MG	X	3247	1/1	0.85	0.17	101,101,101,101	0
31	MG	X	3248	1/1	0.85	0.07	87,87,87,87	0
31	MG	X	3215	1/1	0.85	0.40	54,54,54,54	0
31	MG	X	3034	1/1	0.85	0.16	35,35,35,35	0
31	MG	X	3181	1/1	0.85	0.19	51,51,51,51	0
31	MG	X	3293	1/1	0.85	0.21	71,71,71,71	0
31	MG	X	3182	1/1	0.85	0.31	75,75,75,75	0
31	MG	X	3256	1/1	0.85	0.26	48,48,48,48	0
31	MG	T	101	1/1	0.85	0.19	30,30,30,30	0
31	MG	X	3111	1/1	0.85	0.27	49,49,49,49	0
31	MG	X	3161	1/1	0.85	0.23	25,25,25,25	0
31	MG	X	2948	1/1	0.85	0.22	32,32,32,32	0
31	MG	X	3010	1/1	0.86	0.39	72,72,72,72	0
31	MG	X	3266	1/1	0.86	0.28	56,56,56,56	0
31	MG	X	2989	1/1	0.86	0.13	45,45,45,45	0
31	MG	X	3139	1/1	0.86	0.24	29,29,29,29	0
31	MG	X	3283	1/1	0.87	0.14	50,50,50,50	0
31	MG	X	3113	1/1	0.87	0.14	38,38,38,38	0
31	MG	X	3159	1/1	0.87	0.11	31,31,31,31	0
31	MG	X	3329	1/1	0.87	0.14	95,95,95,95	0
31	MG	X	2975	1/1	0.87	0.24	38,38,38,38	0
31	MG	X	3095	1/1	0.87	0.34	65,65,65,65	0
31	MG	X	2981	1/1	0.87	0.19	52,52,52,52	0
31	MG	X	3264	1/1	0.87	0.20	47,47,47,47	0
31	MG	X	2984	1/1	0.87	0.15	22,22,22,22	0
31	MG	X	2905	1/1	0.87	0.24	13,13,13,13	0
31	MG	X	3225	1/1	0.87	0.53	79,79,79,79	0
31	MG	X	3274	1/1	0.87	0.37	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	MG	X	2990	1/1	0.87	0.07	60,60,60,60	0
31	MG	X	2956	1/1	0.87	0.15	31,31,31,31	0
31	MG	X	2941	1/1	0.87	0.20	40,40,40,40	0
32	MPD	X	3319	8/8	0.87	0.45	91,91,91,91	0
31	MG	X	3252	1/1	0.87	0.46	111,111,111,111	0
31	MG	X	3207	1/1	0.87	0.15	75,75,75,75	0
33	SPD	X	3322	10/10	0.87	0.28	90,90,90,90	0
31	MG	X	3328	1/1	0.88	0.25	33,33,33,33	0
31	MG	X	3212	1/1	0.88	0.20	53,53,53,53	0
31	MG	X	3213	1/1	0.88	0.11	34,34,34,34	0
31	MG	Y	205	1/1	0.88	0.10	44,44,44,44	0
31	MG	X	3056	1/1	0.88	0.33	66,66,66,66	0
31	MG	X	3237	1/1	0.88	0.36	88,88,88,88	0
31	MG	Y	210	1/1	0.88	0.32	64,64,64,64	0
31	MG	X	3194	1/1	0.88	0.15	70,70,70,70	0
31	MG	X	2923	1/1	0.88	0.29	13,13,13,13	0
31	MG	X	3258	1/1	0.88	0.30	56,56,56,56	0
31	MG	X	3303	1/1	0.88	0.18	67,67,67,67	0
31	MG	X	2979	1/1	0.88	0.14	37,37,37,37	0
31	MG	X	3281	1/1	0.88	0.22	54,54,54,54	0
31	MG	X	3307	1/1	0.88	0.18	25,25,25,25	0
31	MG	X	3244	1/1	0.88	0.06	61,61,61,61	0
31	MG	X	3060	1/1	0.88	0.15	47,47,47,47	0
31	MG	X	3021	1/1	0.88	0.22	48,48,48,48	0
31	MG	X	3103	1/1	0.88	0.21	84,84,84,84	0
31	MG	X	3037	1/1	0.88	0.38	60,60,60,60	0
31	MG	X	2932	1/1	0.89	0.25	31,31,31,31	0
31	MG	X	3223	1/1	0.89	0.13	34,34,34,34	0
31	MG	X	3149	1/1	0.89	0.06	24,24,24,24	0
31	MG	X	2971	1/1	0.89	0.34	38,38,38,38	0
31	MG	X	3254	1/1	0.89	0.21	19,19,19,19	0
31	MG	X	2925	1/1	0.89	0.20	9,9,9,9	0
31	MG	X	3233	1/1	0.89	0.51	63,63,63,63	0
31	MG	X	3165	1/1	0.89	0.23	8,8,8,8	0
31	MG	X	3119	1/1	0.89	0.26	62,62,62,62	0
31	MG	X	2988	1/1	0.89	0.32	48,48,48,48	0
31	MG	X	3017	1/1	0.89	0.14	30,30,30,30	0
31	MG	X	3294	1/1	0.89	0.28	78,78,78,78	0
31	MG	X	3131	1/1	0.89	0.11	36,36,36,36	0
31	MG	X	2974	1/1	0.89	0.30	45,45,45,45	0
31	MG	X	3055	1/1	0.89	0.19	49,49,49,49	0
31	MG	X	3135	1/1	0.89	0.37	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	MG	X	3271	1/1	0.89	0.18	78,78,78,78	0
31	MG	X	3272	1/1	0.89	0.10	105,105,105,105	0
31	MG	X	2914	1/1	0.89	0.22	4,4,4,4	0
31	MG	X	2997	1/1	0.89	0.34	47,47,47,47	0
31	MG	X	3032	1/1	0.89	0.29	39,39,39,39	0
31	MG	X	2978	1/1	0.89	0.21	42,42,42,42	0
31	MG	X	3311	1/1	0.89	0.36	59,59,59,59	0
31	MG	Y	203	1/1	0.90	0.18	30,30,30,30	0
31	MG	X	3127	1/1	0.90	0.61	52,52,52,52	0
31	MG	X	3100	1/1	0.90	0.23	69,69,69,69	0
31	MG	X	2926	1/1	0.90	0.32	23,23,23,23	0
31	MG	Y	209	1/1	0.90	0.15	81,81,81,81	0
31	MG	X	3086	1/1	0.90	0.11	41,41,41,41	0
31	MG	Y	211	1/1	0.90	0.10	59,59,59,59	0
31	MG	X	3166	1/1	0.90	0.21	18,18,18,18	0
31	MG	X	3004	1/1	0.90	0.14	43,43,43,43	0
31	MG	X	2995	1/1	0.90	0.29	41,41,41,41	0
31	MG	X	3170	1/1	0.90	0.62	105,105,105,105	0
31	MG	X	3036	1/1	0.90	0.18	41,41,41,41	0
31	MG	X	2927	1/1	0.90	0.23	9,9,9,9	0
31	MG	J	201	1/1	0.90	0.24	55,55,55,55	0
31	MG	X	3201	1/1	0.90	0.27	69,69,69,69	0
30	6NO	X	2901	95/95	0.90	0.10	114,114,114,114	0
31	MG	X	3204	1/1	0.90	0.19	51,51,51,51	0
31	MG	X	2955	1/1	0.90	0.13	14,14,14,14	0
31	MG	X	3297	1/1	0.90	0.20	25,25,25,25	0
31	MG	X	2970	1/1	0.90	0.36	30,30,30,30	0
31	MG	X	3077	1/1	0.91	0.19	61,61,61,61	0
31	MG	X	2998	1/1	0.91	0.20	50,50,50,50	0
31	MG	X	3114	1/1	0.91	0.49	70,70,70,70	0
31	MG	X	3082	1/1	0.91	0.25	51,51,51,51	0
31	MG	X	3308	1/1	0.91	0.13	46,46,46,46	0
31	MG	X	3026	1/1	0.91	0.24	35,35,35,35	0
31	MG	X	3265	1/1	0.91	0.14	74,74,74,74	0
31	MG	X	2960	1/1	0.91	0.16	30,30,30,30	0
31	MG	X	3128	1/1	0.91	0.11	73,73,73,73	0
31	MG	X	3179	1/1	0.91	0.18	62,62,62,62	0
31	MG	X	2986	1/1	0.91	0.14	42,42,42,42	0
31	MG	X	3325	1/1	0.91	0.10	104,104,104,104	0
31	MG	X	2906	1/1	0.91	0.18	35,35,35,35	0
31	MG	X	3062	1/1	0.91	0.33	49,49,49,49	0
31	MG	X	3184	1/1	0.91	0.25	131,131,131,131	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	MG	X	3002	1/1	0.91	0.21	34,34,34,34	0
31	MG	Y	204	1/1	0.91	0.27	60,60,60,60	0
31	MG	X	2920	1/1	0.91	0.29	19,19,19,19	0
31	MG	X	3136	1/1	0.91	0.08	43,43,43,43	0
31	MG	X	2966	1/1	0.91	0.29	32,32,32,32	0
31	MG	Y	208	1/1	0.91	0.05	72,72,72,72	0
31	MG	X	3243	1/1	0.91	0.14	83,83,83,83	0
31	MG	X	3038	1/1	0.91	0.36	32,32,32,32	0
31	MG	X	3286	1/1	0.91	0.08	47,47,47,47	0
31	MG	X	2991	1/1	0.91	0.09	22,22,22,22	0
31	MG	X	3046	1/1	0.91	0.07	64,64,64,64	0
31	MG	X	3016	1/1	0.91	0.19	60,60,60,60	0
31	MG	X	2918	1/1	0.91	0.22	6,6,6,6	0
31	MG	X	2942	1/1	0.91	0.11	19,19,19,19	0
31	MG	X	3160	1/1	0.91	0.24	92,92,92,92	0
31	MG	X	3106	1/1	0.91	0.20	57,57,57,57	0
31	MG	X	3209	1/1	0.91	0.15	52,52,52,52	0
31	MG	3	101	1/1	0.91	0.19	31,31,31,31	0
31	MG	X	3162	1/1	0.91	0.20	20,20,20,20	0
31	MG	X	3107	1/1	0.91	0.08	67,67,67,67	0
31	MG	X	3076	1/1	0.91	0.47	90,90,90,90	0
31	MG	X	3257	1/1	0.91	0.30	77,77,77,77	0
31	MG	X	3110	1/1	0.91	0.14	55,55,55,55	0
31	MG	X	3211	1/1	0.92	0.10	32,32,32,32	0
31	MG	X	3152	1/1	0.92	0.36	74,74,74,74	0
31	MG	X	3156	1/1	0.92	0.44	72,72,72,72	0
31	MG	X	2949	1/1	0.92	0.24	16,16,16,16	0
31	MG	X	2936	1/1	0.92	0.27	21,21,21,21	0
31	MG	X	3053	1/1	0.92	0.17	64,64,64,64	0
31	MG	X	2982	1/1	0.92	0.19	40,40,40,40	0
31	MG	X	3219	1/1	0.92	0.11	85,85,85,85	0
31	MG	X	2937	1/1	0.92	0.16	31,31,31,31	0
31	MG	X	2940	1/1	0.92	0.17	32,32,32,32	0
31	MG	X	2928	1/1	0.92	0.20	10,10,10,10	0
31	MG	X	2916	1/1	0.92	0.21	0,0,0,0	0
31	MG	X	3023	1/1	0.92	0.20	50,50,50,50	0
31	MG	X	3172	1/1	0.92	0.31	60,60,60,60	0
31	MG	X	3043	1/1	0.92	0.41	33,33,33,33	0
31	MG	X	3115	1/1	0.92	0.23	75,75,75,75	0
31	MG	X	3143	1/1	0.92	0.30	56,56,56,56	0
31	MG	X	3260	1/1	0.92	0.13	63,63,63,63	0
31	MG	X	2904	1/1	0.92	0.13	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	MG	X	3238	1/1	0.92	0.13	50,50,50,50	0
31	MG	X	3122	1/1	0.92	0.19	52,52,52,52	0
31	MG	X	3080	1/1	0.92	0.11	29,29,29,29	0
31	MG	X	3155	1/1	0.93	0.23	68,68,68,68	0
31	MG	X	3083	1/1	0.93	0.21	50,50,50,50	0
31	MG	X	3158	1/1	0.93	0.31	118,118,118,118	0
31	MG	X	3183	1/1	0.93	0.15	40,40,40,40	0
31	MG	X	3052	1/1	0.93	0.11	21,21,21,21	0
31	MG	X	3068	1/1	0.93	0.52	48,48,48,48	0
31	MG	X	3187	1/1	0.93	0.15	57,57,57,57	0
31	MG	X	2912	1/1	0.93	0.26	3,3,3,3	0
31	MG	X	2994	1/1	0.93	0.37	58,58,58,58	0
31	MG	X	2950	1/1	0.93	0.41	31,31,31,31	0
31	MG	X	3228	1/1	0.93	0.33	85,85,85,85	0
31	MG	X	3193	1/1	0.93	0.09	63,63,63,63	0
31	MG	X	3025	1/1	0.93	0.16	33,33,33,33	0
31	MG	X	3231	1/1	0.93	0.09	96,96,96,96	0
31	MG	X	2947	1/1	0.93	0.14	33,33,33,33	0
31	MG	X	3196	1/1	0.93	0.33	95,95,95,95	0
31	MG	X	3141	1/1	0.93	0.20	62,62,62,62	0
31	MG	Y	214	1/1	0.93	0.07	64,64,64,64	0
31	MG	X	3200	1/1	0.93	0.17	64,64,64,64	0
31	MG	X	3058	1/1	0.93	0.15	35,35,35,35	0
31	MG	X	3040	1/1	0.93	0.70	70,70,70,70	0
31	MG	X	3267	1/1	0.93	0.21	50,50,50,50	0
31	MG	A	301	1/1	0.93	0.19	46,46,46,46	0
31	MG	X	3030	1/1	0.93	0.19	0,0,0,0	0
31	MG	M	201	1/1	0.93	0.28	7,7,7,7	0
31	MG	X	2972	1/1	0.93	0.19	33,33,33,33	0
31	MG	X	2980	1/1	0.93	0.13	23,23,23,23	0
32	MPD	X	3317	8/8	0.93	0.31	73,73,73,73	0
31	MG	X	3242	1/1	0.93	0.17	72,72,72,72	0
31	MG	X	3310	1/1	0.93	0.15	63,63,63,63	0
31	MG	X	3150	1/1	0.93	0.26	65,65,65,65	0
31	MG	X	3151	1/1	0.93	0.29	79,79,79,79	0
31	MG	X	2933	1/1	0.93	0.30	32,32,32,32	0
31	MG	X	2907	1/1	0.94	0.17	18,18,18,18	0
31	MG	X	3138	1/1	0.94	0.12	44,44,44,44	0
31	MG	X	3007	1/1	0.94	0.14	30,30,30,30	0
31	MG	X	2908	1/1	0.94	0.18	15,15,15,15	0
31	MG	X	3171	1/1	0.94	0.26	39,39,39,39	0
31	MG	X	3199	1/1	0.94	0.17	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	MG	X	3012	1/1	0.94	0.31	49,49,49,49	0
31	MG	X	3050	1/1	0.94	0.20	41,41,41,41	0
31	MG	X	3118	1/1	0.94	0.51	113,113,113,113	0
31	MG	X	3099	1/1	0.94	0.20	46,46,46,46	0
31	MG	X	3206	1/1	0.94	0.20	57,57,57,57	0
31	MG	X	3146	1/1	0.94	0.26	46,46,46,46	0
31	MG	X	3121	1/1	0.94	0.22	30,30,30,30	0
31	MG	X	3013	1/1	0.94	0.10	42,42,42,42	0
31	MG	X	3101	1/1	0.94	0.10	52,52,52,52	0
31	MG	X	3014	1/1	0.94	0.36	28,28,28,28	0
31	MG	X	2953	1/1	0.94	0.15	53,53,53,53	0
31	MG	X	3129	1/1	0.94	0.14	21,21,21,21	0
31	MG	X	2961	1/1	0.94	0.25	35,35,35,35	0
31	MG	X	3085	1/1	0.94	0.17	45,45,45,45	0
31	MG	X	2992	1/1	0.94	0.10	25,25,25,25	0
31	MG	X	3188	1/1	0.94	0.11	68,68,68,68	0
32	MPD	X	3316	8/8	0.94	0.17	62,62,62,62	0
31	MG	X	2917	1/1	0.94	0.26	6,6,6,6	0
31	MG	X	3108	1/1	0.94	0.10	74,74,74,74	0
31	MG	X	2987	1/1	0.94	0.65	32,32,32,32	0
31	MG	X	3284	1/1	0.94	0.05	56,56,56,56	0
31	MG	X	3285	1/1	0.94	0.19	84,84,84,84	0
31	MG	X	3224	1/1	0.94	0.07	32,32,32,32	0
31	MG	X	2913	1/1	0.95	0.24	0,0,0,0	0
31	MG	X	3112	1/1	0.95	0.27	42,42,42,42	0
31	MG	X	2929	1/1	0.95	0.20	21,21,21,21	0
31	MG	X	3270	1/1	0.95	0.25	85,85,85,85	0
31	MG	X	3153	1/1	0.95	0.27	58,58,58,58	0
31	MG	X	3065	1/1	0.95	0.34	57,57,57,57	0
31	MG	X	3221	1/1	0.95	0.13	49,49,49,49	0
31	MG	X	3197	1/1	0.95	0.06	49,49,49,49	0
31	MG	X	3019	1/1	0.95	0.14	44,44,44,44	0
31	MG	X	3157	1/1	0.95	0.23	77,77,77,77	0
31	MG	X	3226	1/1	0.95	0.24	145,145,145,145	0
31	MG	X	2935	1/1	0.95	0.18	15,15,15,15	0
31	MG	X	3009	1/1	0.95	0.21	31,31,31,31	0
31	MG	X	3022	1/1	0.95	0.15	53,53,53,53	0
31	MG	X	2954	1/1	0.95	0.16	36,36,36,36	0
31	MG	X	3125	1/1	0.95	0.12	37,37,37,37	0
31	MG	X	3011	1/1	0.95	0.24	33,33,33,33	0
31	MG	X	2930	1/1	0.95	0.14	26,26,26,26	0
31	MG	N	201	1/1	0.95	0.14	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	MG	X	3323	1/1	0.95	0.17	22,22,22,22	0
31	MG	X	3186	1/1	0.95	0.10	45,45,45,45	0
31	MG	X	3167	1/1	0.95	0.14	7,7,7,7	0
31	MG	X	3327	1/1	0.95	0.10	66,66,66,66	0
31	MG	X	3044	1/1	0.95	0.07	10,10,10,10	0
31	MG	X	2921	1/1	0.95	0.16	7,7,7,7	0
31	MG	X	2976	1/1	0.95	0.15	29,29,29,29	0
31	MG	Y	202	1/1	0.95	0.20	52,52,52,52	0
31	MG	X	3191	1/1	0.95	0.14	32,32,32,32	0
31	MG	X	2959	1/1	0.96	0.22	39,39,39,39	0
31	MG	X	3047	1/1	0.96	0.34	23,23,23,23	0
31	MG	X	3253	1/1	0.96	0.11	25,25,25,25	0
31	MG	X	3222	1/1	0.96	0.07	21,21,21,21	0
31	MG	X	3164	1/1	0.96	0.19	16,16,16,16	0
31	MG	X	3048	1/1	0.96	0.22	0,0,0,0	0
31	MG	X	2996	1/1	0.96	0.15	41,41,41,41	0
31	MG	X	3005	1/1	0.96	0.09	45,45,45,45	0
31	MG	X	3018	1/1	0.96	0.32	35,35,35,35	0
31	MG	X	3093	1/1	0.96	0.14	44,44,44,44	0
31	MG	X	3295	1/1	0.96	0.12	59,59,59,59	0
31	MG	X	3006	1/1	0.96	0.17	29,29,29,29	0
31	MG	X	2946	1/1	0.96	0.13	11,11,11,11	0
31	MG	X	3116	1/1	0.96	0.08	61,61,61,61	0
31	MG	X	3117	1/1	0.96	0.43	64,64,64,64	0
31	MG	X	3096	1/1	0.96	0.12	50,50,50,50	0
31	MG	X	2910	1/1	0.96	0.15	25,25,25,25	0
31	MG	X	3147	1/1	0.96	0.11	82,82,82,82	0
31	MG	X	3148	1/1	0.96	0.13	29,29,29,29	0
31	MG	X	3269	1/1	0.96	0.10	62,62,62,62	0
31	MG	X	3098	1/1	0.96	0.11	23,23,23,23	0
31	MG	X	2952	1/1	0.96	0.11	31,31,31,31	0
31	MG	K	201	1/1	0.96	0.11	48,48,48,48	0
31	MG	X	3123	1/1	0.96	0.20	18,18,18,18	0
31	MG	X	3124	1/1	0.96	0.10	47,47,47,47	0
31	MG	X	2964	1/1	0.96	0.20	9,9,9,9	0
31	MG	X	2957	1/1	0.96	0.13	26,26,26,26	0
32	MPD	X	3315	8/8	0.96	0.16	62,62,62,62	0
31	MG	X	3041	1/1	0.96	0.08	30,30,30,30	0
31	MG	X	3042	1/1	0.96	0.06	42,42,42,42	0
31	MG	X	2943	1/1	0.96	0.16	35,35,35,35	0
31	MG	X	3217	1/1	0.96	0.18	48,48,48,48	0
31	MG	X	3029	1/1	0.96	0.09	48,48,48,48	0

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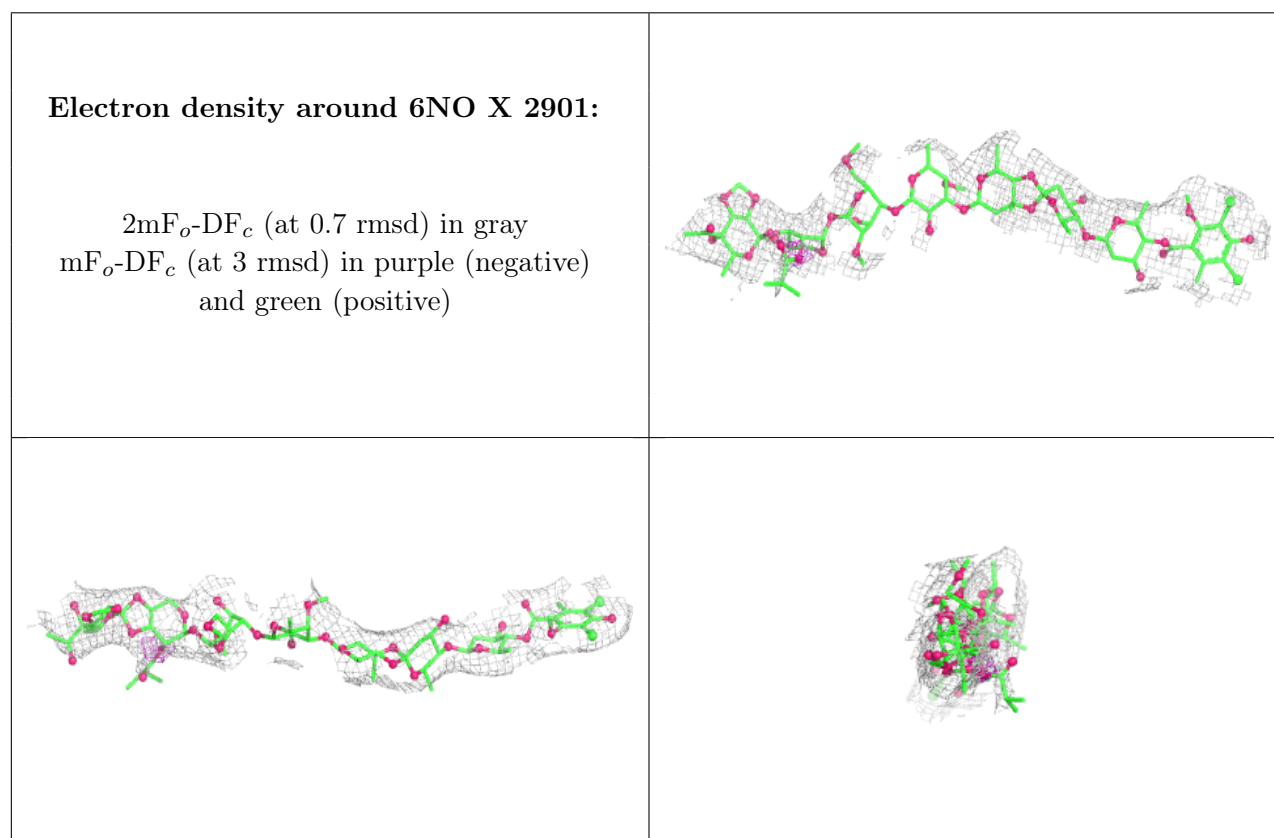
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	MG	X	3326	1/1	0.96	0.19	55,55,55,55	0
31	MG	X	3045	1/1	0.96	0.78	30,30,30,30	0
31	MG	X	2977	1/1	0.97	0.11	33,33,33,33	0
31	MG	X	3175	1/1	0.97	0.33	72,72,72,72	0
31	MG	X	3027	1/1	0.97	0.13	14,14,14,14	0
31	MG	X	3288	1/1	0.97	0.11	54,54,54,54	0
31	MG	X	2968	1/1	0.97	0.40	34,34,34,34	0
31	MG	X	3134	1/1	0.97	0.28	25,25,25,25	0
31	MG	Y	217	1/1	0.97	0.08	65,65,65,65	0
31	MG	X	2922	1/1	0.97	0.15	12,12,12,12	0
31	MG	X	2909	1/1	0.97	0.13	24,24,24,24	0
31	MG	X	3061	1/1	0.97	0.12	38,38,38,38	0
31	MG	X	2924	1/1	0.97	0.16	26,26,26,26	0
31	MG	X	2963	1/1	0.97	0.17	29,29,29,29	0
31	MG	X	3120	1/1	0.97	0.21	56,56,56,56	0
31	MG	X	2983	1/1	0.97	0.10	27,27,27,27	0
31	MG	X	2951	1/1	0.97	0.13	15,15,15,15	0
31	MG	X	3299	1/1	0.97	0.09	89,89,89,89	0
31	MG	X	3066	1/1	0.97	0.43	48,48,48,48	0
31	MG	X	3008	1/1	0.97	0.37	39,39,39,39	0
31	MG	X	2985	1/1	0.97	0.29	29,29,29,29	0
31	MG	X	2939	1/1	0.97	0.15	24,24,24,24	0
31	MG	X	3024	1/1	0.97	0.23	27,27,27,27	0
31	MG	X	3071	1/1	0.97	0.17	46,46,46,46	0
31	MG	X	3092	1/1	0.97	0.20	53,53,53,53	0
31	MG	X	2934	1/1	0.97	0.17	64,64,64,64	0
31	MG	X	2911	1/1	0.98	0.18	11,11,11,11	0
31	MG	X	3154	1/1	0.98	0.17	70,70,70,70	0
31	MG	X	3015	1/1	0.98	0.12	46,46,46,46	0
31	MG	X	3305	1/1	0.98	0.07	125,125,125,125	0
31	MG	X	3081	1/1	0.98	0.06	16,16,16,16	0
31	MG	X	3227	1/1	0.98	0.13	44,44,44,44	0
31	MG	X	2944	1/1	0.98	0.06	1,1,1,1	0
31	MG	X	2938	1/1	0.98	0.16	8,8,8,8	0
31	MG	X	3203	1/1	0.98	0.06	42,42,42,42	0
31	MG	X	2993	1/1	0.98	0.25	26,26,26,26	0
31	MG	X	3232	1/1	0.98	0.21	8,8,8,8	0
31	MG	X	3205	1/1	0.98	0.05	55,55,55,55	0
31	MG	X	2967	1/1	0.98	0.17	14,14,14,14	0
31	MG	X	3280	1/1	0.98	0.04	84,84,84,84	0
31	MG	X	2903	1/1	0.98	0.10	11,11,11,11	0
31	MG	X	3282	1/1	0.98	0.12	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	MG	X	3028	1/1	0.98	0.06	3,3,3,3	0
31	MG	X	3163	1/1	0.98	0.18	0,0,0,0	0
31	MG	X	3079	1/1	0.99	0.07	62,62,62,62	0
31	MG	X	2945	1/1	0.99	0.05	32,32,32,32	0
31	MG	X	3035	1/1	0.99	0.05	31,31,31,31	0
31	MG	X	2969	1/1	0.99	0.11	8,8,8,8	0
31	MG	X	3140	1/1	0.99	0.18	27,27,27,27	0
31	MG	X	3090	1/1	1.00	0.05	11,11,11,11	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.