



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 19, 2020 – 09:50 AM BST

PDB ID : 4WCE  
Title : The crystal structure of the large ribosomal subunit of *Staphylococcus aureus*  
Authors : Eyal, Z.; Matzov, D.; Krupkin, M.; Wekselman, I.; Zimmerman, E.; Rozenberg, H.; Bashan, A.; Yonath, A.  
Deposited on : 2014-09-04  
Resolution : 3.53 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.14.6  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.14.6



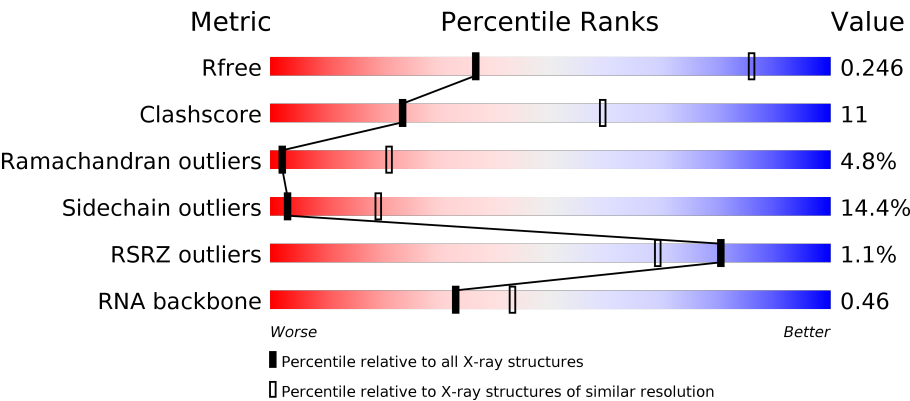
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.53 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	130704	1161 (3.60-3.44)
Clashscore	141614	1244 (3.60-3.44)
Ramachandran outliers	138981	1206 (3.60-3.44)
Sidechain outliers	138945	1207 (3.60-3.44)
RSRZ outliers	127900	1080 (3.60-3.44)
RNA backbone	3102	1003 (4.02-3.00)



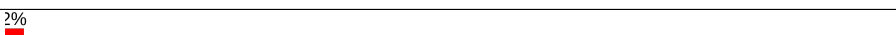



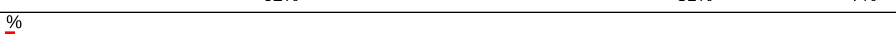







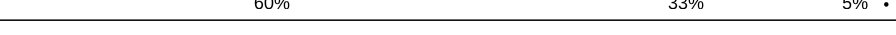






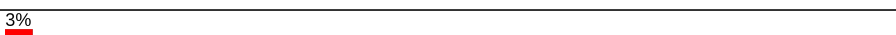

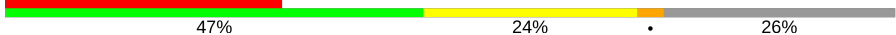
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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	2923	<div><div></div><div><div>44%</div><div>37%</div><div>11%</div><div>7%</div></div></div>
2	Y	114	<div><div></div><div><div>48%</div><div>43%</div><div>6%</div></div></div>
3	A	277	<div><div></div><div><div>%</div><div>66%</div><div>24%</div><div>6%</div></div></div>
4	B	220	<div><div></div><div><div>57%</div><div>35%</div><div>6%</div></div></div>

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Mol	Chain	Length	Quality of chain
5	C	207	
6	D	179	
7	E	178	
8	G	145	
9	H	122	
10	I	146	
11	J	144	
12	K	122	
13	L	119	
14	M	116	
15	N	118	
16	O	102	
17	P	117	
18	Q	91	
19	R	105	
20	S	217	
21	T	94	
22	U	62	
23	V	69	
24	W	59	
25	Z	58	
26	2	45	
27	3	66	
28	4	37	

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



ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	MN	B	303	-	-	-	X
30	MN	X	3050	-	-	-	X
30	MN	X	3053	-	-	-	X
30	MN	X	3308	-	-	-	X
31	MG	X	3013	-	-	-	X
31	MG	X	3113	-	-	-	X
31	MG	X	3173	-	-	-	X
34	EOH	X	3317	-	-	-	X



## 2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 81909 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 rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	2708	Total	C	N	O	P	0	0	0
			58077	25928	10647	18794	2708			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	114	Total	C	N	O	P	0	0	0
			2430	1086	436	794	114			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	269	Total	C	N	O	S	0	0	0
			1686	1024	333	324	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	215	Total	C	N	O	S	0	0	0
			1558	976	291	286	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	199	Total	C	N	O	S	0	0	0
			1320	818	249	251	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	166	Total	C	N	O	S	0	0	0
			866	523	166	175	2			



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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	156	Total	C	N	O	S	0	0	0
			970	596	177	195	2			

- Molecule 8 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	G	145	Total	C	N	O	S	0	0	0
			1106	693	204	206	3			

- Molecule 9 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	122	Total	C	N	O	S	0	0	0
			884	548	167	165	4			

- Molecule 10 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	131	Total	C	N	O	S	0	0	0
			859	527	170	161	1			

- Molecule 11 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	141	Total	C	N	O	S	0	0	0
			1068	684	198	183	3			

- Molecule 12 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	119	Total	C	N	O	S	0	0	0
			908	557	177	173	1			

- Molecule 13 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	L	110	Total	C	N	O	0	0	0
			705	433	137	135			

- Molecule 14 is a protein called 50S ribosomal protein L19.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	M	110	Total	C	N	O			
			826	521	164	141	0	0	0

- Molecule 15 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	N	116	Total	C	N	O	S			
			932	587	187	154	4	0	0	0

- Molecule 16 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	O	102	Total	C	N	O	S			
			751	477	138	135	1	0	0	0

- Molecule 17 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	P	112	Total	C	N	O	S			
			862	537	164	158	3	0	0	0

- Molecule 18 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Q	89	Total	C	N	O	S			
			626	394	113	116	3	0	0	0

- Molecule 19 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	R	100	Total	C	N	O	S			
			683	424	127	131	1	0	0	0

- Molecule 20 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	167	Total	C	N	O	S			
			1097	690	191	214	2	0	0	0

- Molecule 21 is a protein called 50S ribosomal protein L27.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	T	75	Total	C	N	O	0	0	0
			568	352	110	106			

- Molecule 22 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	U	46	Total	C	N	O	0	0	0
			300	182	65	53			

- Molecule 23 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	V	65	Total	C	N	O	0	0	0
			486	299	89	98			

- Molecule 24 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	W	58	Total	C	N	O	S	0	0	0
			449	279	84	85	1			

- Molecule 25 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Z	43	Total	C	N	O	S	0	0	0
			339	208	70	57	4			

- Molecule 26 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	2	44	Total	C	N	O	S	0	0	0
			362	222	86	53	1			

- Molecule 27 is a protein called 50S ribosomal protein L35.

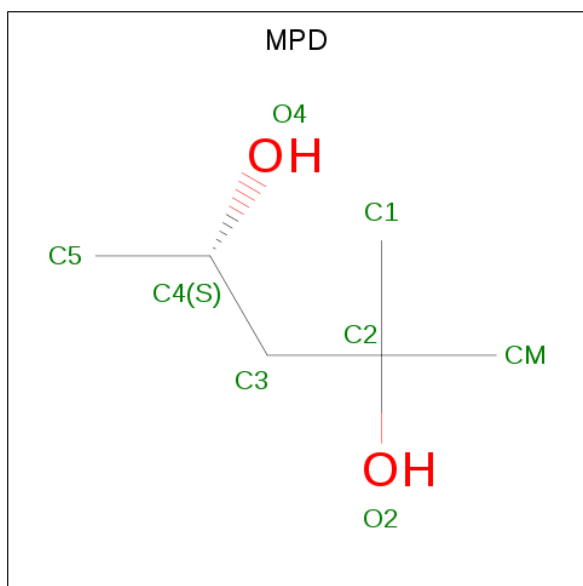
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	3	60	Total	C	N	O	S	0	0	0
			420	260	84	74	2			

- Molecule 28 is a protein called 50S ribosomal protein L36.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	4	37	Total	C	N	O	S	0	0	0
			277	173	58	41	5			

- Molecule 29 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



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

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

- Molecule 30 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

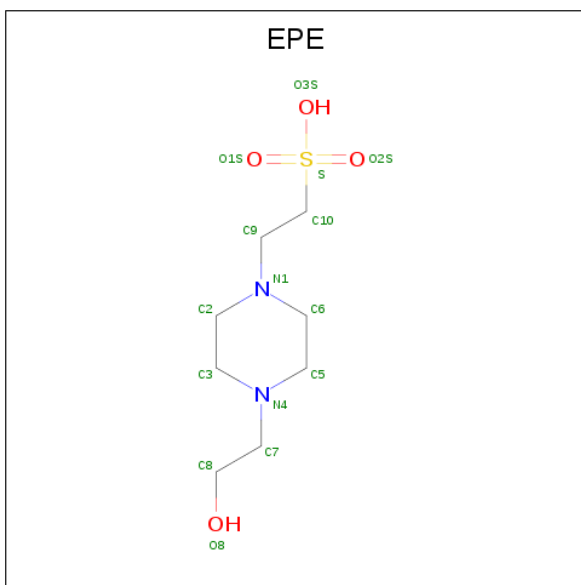
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	J	1	Total	Mn	0	0
			1	1		
30	B	1	Total	Mn	0	0
			1	1		
30	I	2	Total	Mn	0	0
			2	2		
30	X	223	Total	Mn	0	0
			223	223		
30	R	2	Total	Mn	0	0
			2	2		
30	Y	2	Total	Mn	0	0
			2	2		

- Molecule 31 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	G	3	Total	Mg	0	0
			3	3		
31	B	2	Total	Mg	0	0
			2	2		
31	I	1	Total	Mg	0	0
			1	1		
31	C	1	Total	Mg	0	0
			1	1		
31	X	80	Total	Mg	0	0
			80	80		
31	O	1	Total	Mg	0	0
			1	1		
31	Y	3	Total	Mg	0	0
			3	3		

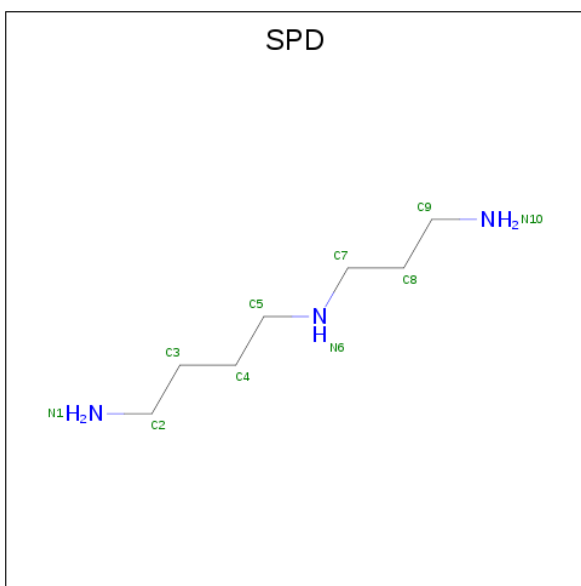
- Molecule 32 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
32	X	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 33 is SPERMIDINE (three-letter code: 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		

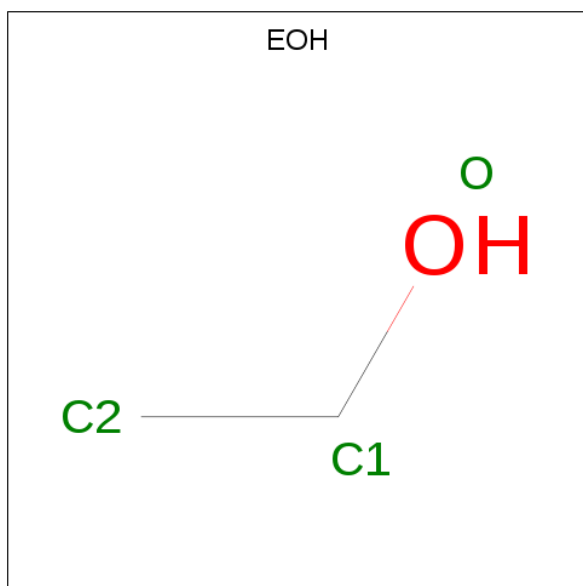
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	X	1	Total	C	N	0	0
			10	7	3		

- Molecule 34 is ETHANOL (three-letter code: EOH) (formula:  $C_2H_6O$ ).



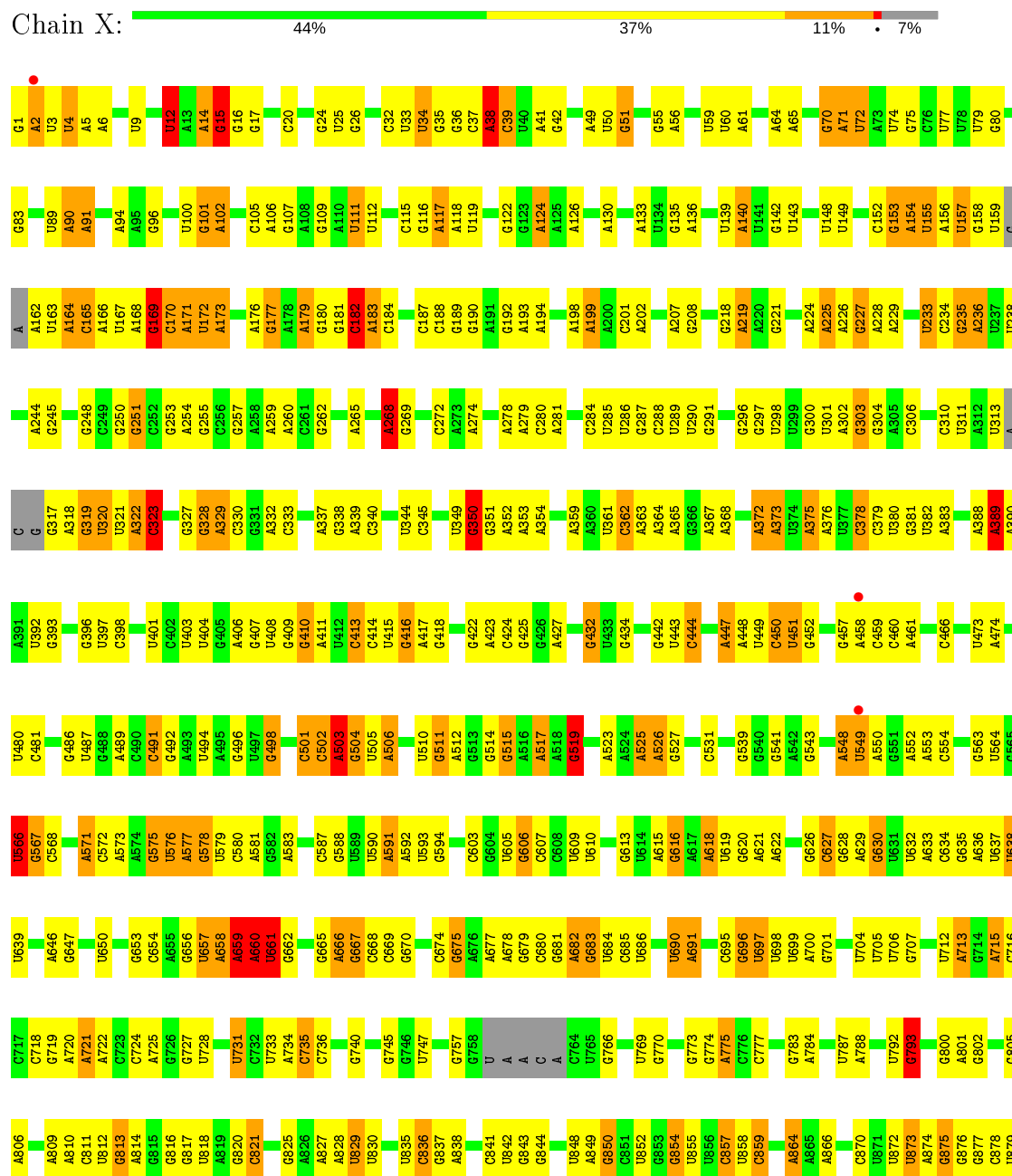
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	X	1	Total	C	O	0	0
			3	2	1		
34	X	1	Total	C	O	0	0
			3	2	1		
34	X	1	Total	C	O	0	0
			3	2	1		
34	X	1	Total	C	O	0	0
			3	2	1		
34	X	1	Total	C	O	0	0
			3	2	1		
34	X	1	Total	C	O	0	0
			3	2	1		



### 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 rRNA



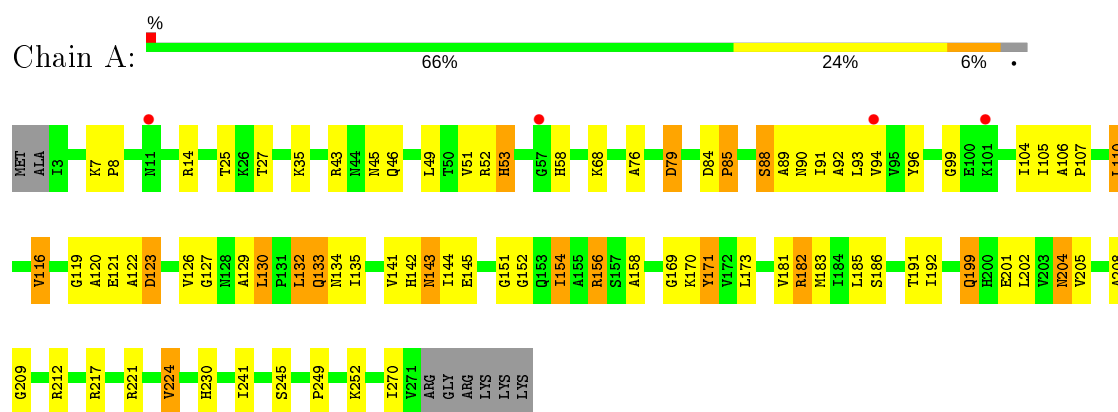


A1997	A1998	A1999	G1922	G1923	G1924	C1833	G1759	A1653	C	G1518	U1451	U1379	U1301	U1209	A	U1059	G966	A880
G2007	G2008	G2009	G1930	G1931	G1932	G1834	G1760	G1653	U	U1519	C1452	A1379	G1302	C1213	A	U1060	G967	A887
G2012	G2013	G2014	G1933	G1934	G1935	G1835	G1761	G1658	U	A1521	U1454	G1380	G1303	C1214	G	U1061	U970	G888
G2018	G2019	G2020	G1936	G1937	G1938	G1836	U1762	U1658	U	G1522	U	G1382	G1305	U1215	A	U1062	U971	G889
G2027	G2028	G2029	G1939	G1940	G1941	G1837	U1763	U1661	U	G1523	U	G1383	G1306	U	G	U1063	U972	G890
G2031	G2032	G2033	G1942	G1943	G1944	G1838	U1764	U1662	A	G1524	U	G1384	G1309	U1217	U	U1064	A977	G891
G2036	G2037	G2038	G1945	G1946	G1947	G1839	U1765	U1663	U	G1525	A	G1385	G1310	G1218	G	U1065	A985	G892
G2040	G2041	G2042	G1948	G1949	G1950	G1840	U1766	U1664	C	G1526	U	U1389	G1311	G1219	C	U1066	U985	G893
G2047	G2048	G2049	G1951	G1952	G1953	G1841	U1767	U1665	U	G1527	U	U1390	G1312	G1220	U	U1067	U986	G894
G2051	G2052	G2053	G1954	G1955	G1956	G1842	U1768	U1666	U	G1528	U	U1391	G1313	A1222	U	U1068	U989	G905
G2056	G2057	G2058	G1957	G1958	G1959	G1843	U1769	U1667	U	G1529	U	U1392	G1314	G1225	A	U1069	U990	G906
G2061	G2062	G2063	G1960	G1961	G1962	G1844	U1770	U1668	U	G1530	U	G1393	G1315	G1226	A	U1070	G990	G907
G2066	G2067	G2068	G1963	G1964	G1965	G1845	U1771	U1669	U	A1531	U	U1394	G1316	U1227	U	U1071	U995	A902
G2071	G2072	G2073	G1966	G1967	G1968	G1846	U1772	U1670	U	U1532	U	U1395	G1317	U1228	G	U1072	G996	A903
G2076	G2077	G2078	G1969	G1970	G1971	G1847	U1773	U1671	U	U1533	U	U1396	G1318	A1229	A	U1073	G997	G904
G2081	G2082	G2083	G1972	G1973	G1974	G1848	U1774	U1672	U	U1534	U	U1397	G1319	G1230	U	U1074	G998	G905
G2086	G2087	G2088	G1975	G1976	G1977	G1849	U1775	U1673	U	U1535	U	U1398	G1320	U1240	U	U1075	G1000	A906
G2091	G2092	G2093	G1978	G1979	G1980	G1850	U1776	U1674	U	U1536	U	U1399	G1321	U1241	U	U1076	G1001	G907
G2096	G2097	G2098	G1981	G1982	G1983	G1851	U1777	U1675	U	U1537	U	U1400	G1322	U1242	U	U1077	U999	A911
G2101	G2102	G2103	G1984	G1985	G1986	G1852	U1778	U1676	U	U1538	U	U1401	G1323	U1243	U	U1078	U1002	U916
G2106	G2107	G2108	G1987	G1988	G1989	G1853	U1779	U1677	U	U1539	U	U1402	G1324	U1244	U	U1079	U1003	G922
G2111	G2112	G2113	G1990	G1991	G1992	G1854	U1780	U1678	U	U1540	U	U1403	G1325	U1245	U	U1080	U1004	A923
G2116	G2117	G2118	G1993	G1994	G1995	G1855	U1781	U1679	U	U1541	U	U1404	G1326	U1246	U	U1081	U1005	G925
G2121	G2122	G2123	G1996	G1997	G1998	G1856	U1782	U1680	U	U1542	U	U1405	G1327	U1247	U	U1082	U1006	G
G2126	G2127	G2128	G1999	G2000	G2001	G1857	U1783	U1681	U	U1543	U	U1406	G1328	U1248	U	U1083	U1007	G
G2131	G2132	G2133	G2002	G2003	G2004	G1858	U1784	U1682	U	U1544	U	U1407	G1329	U1249	U	U1084	U1008	G
G2136	G2137	G2138	G2005	G2006	G2007	G1859	U1785	U1683	U	U1545	U	U1408	G1330	U1250	U	U1085	U1009	G
G2141	G2142	G2143	G2008	G2009	G2010	G1860	U1786	U1684	U	U1546	U	U1409	G1331	U1251	U	U1086	U1010	G
G2146	G2147	G2148	G2011	G2012	G2013	G1861	U1787	U1685	U	U1547	U	U1410	G1332	U1252	U	U1087	U1011	G
G2151	G2152	G2153	G2014	G2015	G2016	G1862	U1788	U1686	U	U1548	U	U1411	G1333	U1253	U	U1088	U1012	G
G2156	G2157	G2158	G2017	G2018	G2019	G1863	U1789	U1687	U	U1549	U	U1412	G1334	U1254	U	U1089	U1013	G
G2161	G2162	G2163	G2020	G2021	G2022	G1864	U1790	U1688	U	U1550	U	U1413	G1335	U1255	U	U1090	U1014	G
G2166	G2167	G2168	G2023	G2024	G2025	G1865	U1791	U1689	U	U1551	U	U1414	G1336	U1256	U	U1091	U1015	G
G2171	G2172	G2173	G2026	G2027	G2028	G1866	U1792	U1690	U	U1552	U	U1415	G1337	U1257	U	U1092	U1016	G
G2176	G2177	G2178	G2029	G2030	G2031	G1867	U1793	U1691	U	U1553	U	U1416	G1338	U1258	U	U1093	U1017	G
G2181	G2182	G2183	G2032	G2033	G2034	G1868	U1794	U1692	U	U1554	U	U1417	G1339	U1259	U	U1094	U1018	G
G2186	G2187	G2188	G2035	G2036	G2037	G1869	U1795	U1693	U	U1555	U	U1418	G1340	U1260	U	U1095	U1019	G
G2191	G2192	G2193	G2038	G2039	G2040	G1870	U1796	U1694	U	U1556	U	U1419	G1341	U1261	U	U1096	U1020	G
G2196	G2197	G2198	G2041	G2042	G2043	G1871	U1797	U1695	U	U1557	U	U1420	G1342	U1262	U	U1097	U1021	G
G2201	G2202	G2203	G2044	G2045	G2046	G1872	U1798	U1696	U	U1558	U	U1421	G1343	U1263	U	U1098	U1022	G
G2206	G2207	G2208	G2047	G2048	G2049	G1873	U1799	U1697	U	U1559	U	U1422	G1344	U1264	U	U1099	U1023	G
G2211	G2212	G2213	G2050	G2051	G2052	G1874	U1800	U1700	U	U1560	U	U1423	G1345	U1265	U	U1100	U1024	G
G2216	G2217	G2218	G2053	G2054	G2055	G1875	U1801	U1701	U	U1561	U	U1424	G1346	U1266	U	U1101	U1025	G
G2221	G2222	G2223	G2056	G2057	G2058	G1876	U1802	U1702	U	U1562	U	U1425	G1347	U1267	U	U1102	U1026	G
G2226	G2227	G2228	G2059	G2060	G2061	G1877	U1803	U1703	U	U1563	U	U1426	G1348	U1268	U	U1103	U1027	G
G2231	G2232	G2233	G2062	G2063	G2064	G1878	U1804	U1704	U	U1564	U	U1427	G1349	U1269	U	U1104	U1028	G
G2236	G2237	G2238	G2065	G2066	G2067	G1879	U1805	U1705	U	U1565	U	U1428	G1350	U1270	U	U1105	U1029	G
G2241	G2242	G2243	G2068	G2069	G2070	G1880	U1806	U1706	U	U1566	U	U1429	G1351	U1271	U	U1106	U1030	G
G2246	G2247	G2248	G2071	G2072	G2073	G1881	U1807	U1707	U	U1567	U	U1430	G1352	U1272	U	U1107	U1031	G
G2251	G2252	G2253	G2074	G2075	G2076	G1882	U1808	U1708	U	U1568	U	U1431	G1353	U1273	U	U1108	U1032	G
G2256	G2257	G2258	G2077	G2078	G2079	G1883	U1809	U1709	U	U1569	U	U1432	G1354	U1274	U	U1109	U1033	G
G2261	G2262	G2263	G2080	G2081	G2082	G1884	U1810	U1710	U	U1570	U	U1433	G1355	U1275	U	U1110	U1034	G
G2266	G2267	G2268	G2083	G2084	G2085	G1885	U1811	U1711	U	U1571	U	U1434	G1356	U1276	U	U1111	U1035	G
G2271	G2272	G2273	G2086	G2087	G2088	G1886	U1812	U1712	U	U1572	U	U1435	G1357	U1277	U	U1112	U1036	G
G2276	G2277	G2278	G2089	G2090	G2091	G1887	U1813	U1713	U	U1573	U	U1436	G1358	U1278	U	U1113	U1037	G
G2281	G2282	G2283	G2092	G2093	G2094	G1888	U1814	U1714	U	U1574	U	U1437	G1359	U1279	U	U1114	U1038	G
G2286	G2287	G2288	G2095	G2096	G2097	G1889	U1815	U1715	U	U1575	U	U1438	G1360	U1280	U	U1115	U1039	G
G2291	G2292	G2293	G2098	G2099	G2100	G1890	U1816	U1716	U	U1576	U	U1439	G1361	U1281	U	U1116	U1040	G
G2296	G2297	G2298	G2101	G2102	G2103	G1891	U1817	U1717	U	U1577	U	U1440	G1362	U1282	U	U1117	U1041	G
G2301	G2302	G2303	G2104	G2105	G2106	G1892	U1818	U1718	U	U1578	U	U1441	G1363	U1283	U	U1118	U1042	G
G2306	G2307	G2308	G2107	G2108	G2109	G1893	U1819	U1719	U	U1579	U	U1442	G1364	U1284	U	U1119	U1043	G
G2311	G2312	G2313	G2110	G2111	G2112	G1894	U1820	U1720	U	U1580	U	U1443	G1365	U1285	U	U1120	U1044	G
G2316	G2317	G2318	G2113	G2114	G2115	G1895	U1821	U1721	U	U1581	U	U1444	G1366	U1286	U	U1121	U1045	G
G2321	G2322	G2323	G2116	G2117	G2118	G1896	U1822	U1722	U	U1582	U	U1445	G1367	U1287	U	U1122	U1046	G
G2326	G2327	G2328	G2119	G2120	G2121	G1897	U1823	U1723	U	U1583	U	U1446	G1368	U1288	U	U1123	U1047	G
G2331	G2332	G2333	G2122	G2123	G2124	G1898	U1824	U1724	U	U1584	U	U1447	G1369	U1289	U	U1124	U1048	G
G2336	G2337	G2338	G2125	G2126	G2127	G1899	U1825	U1725	U	U1585	U	U1448	G1370	U1290	U	U1125	U1049	G
G2341	G2342	G2343	G2128	G2129	G2130	G1900	U1826	U1726	U	U1586	U	U1449	G1371	U1291	U	U1126	U1050	G
G2346	G2347	G2348	G2131	G2132	G2133	G1901	U1827	U1727	U	U1587	U	U1450	G1372	U1292	U	U1127	U1051	G
G2351	G2352	G2353	G2134	G2135	G2136	G1902	U1828	U1728	U	U1588	U	U1451	G1373	U1293	U	U1128	U1052	G
G2356	G2357	G2358	G2137	G2138	G2139	G1903	U1829	U1729	U	U1589	U	U1452	G1374	U1294	U	U1129	U1053	G
G2361	G2362	G2363	G2140	G2141	G2142	G1904	U1830	U1730	U	U1590	U							

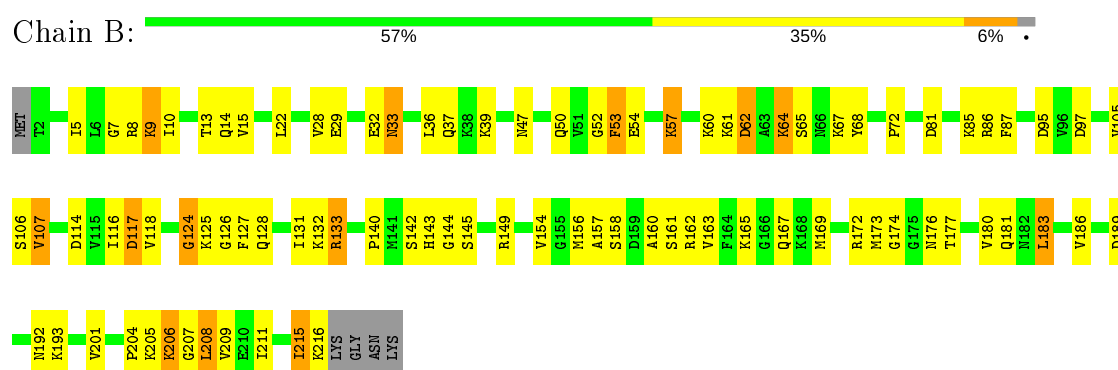




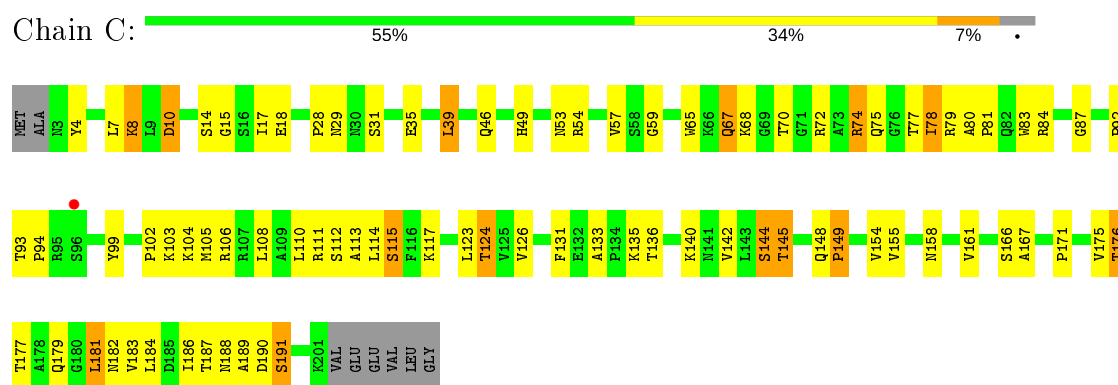




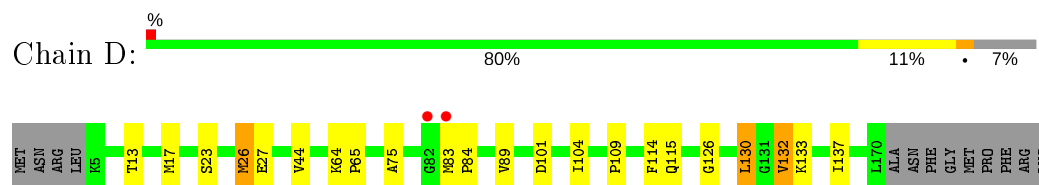
• Molecule 4: 50S ribosomal protein L3



• Molecule 5: 50S ribosomal protein L4



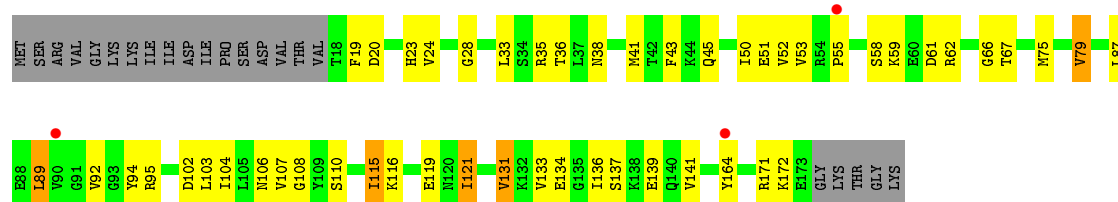
• Molecule 6: 50S ribosomal protein L5



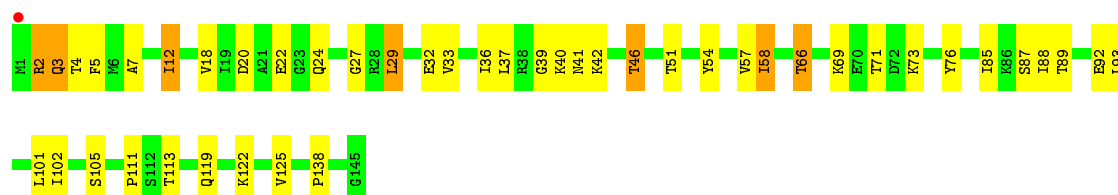
• Molecule 7: 50S ribosomal protein L6







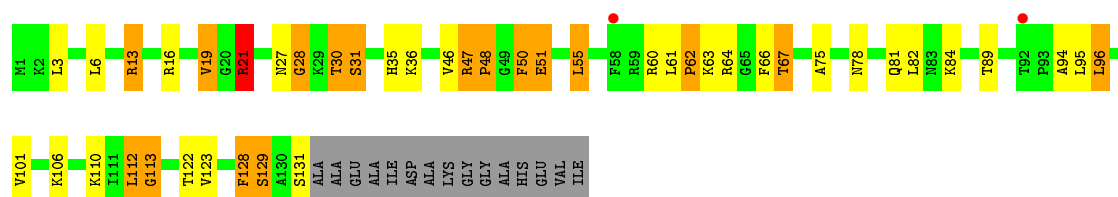
• Molecule 8: 50S ribosomal protein L13



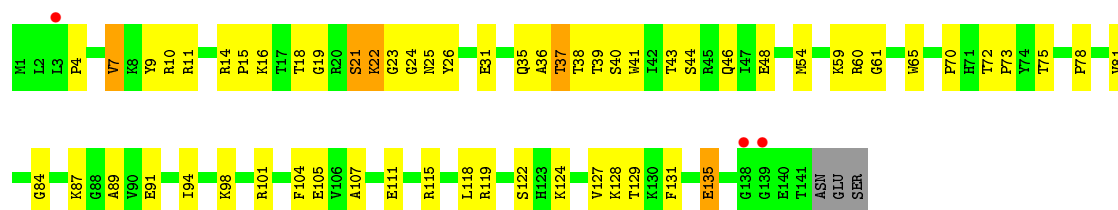
• Molecule 9: 50S ribosomal protein L14



• Molecule 10: 50S ribosomal protein L15



• Molecule 11: 50S ribosomal protein L16



• Molecule 12: 50S ribosomal protein L17



Chain K: 



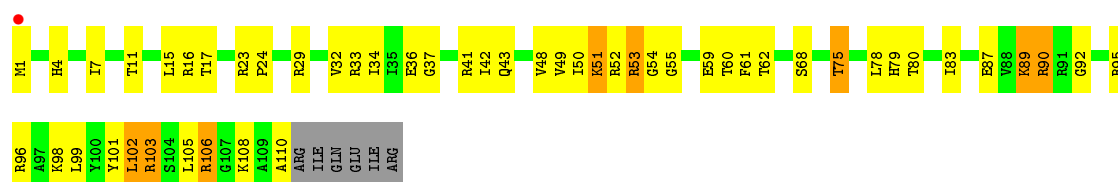
- Molecule 13: 50S ribosomal protein L18

Chain L: 



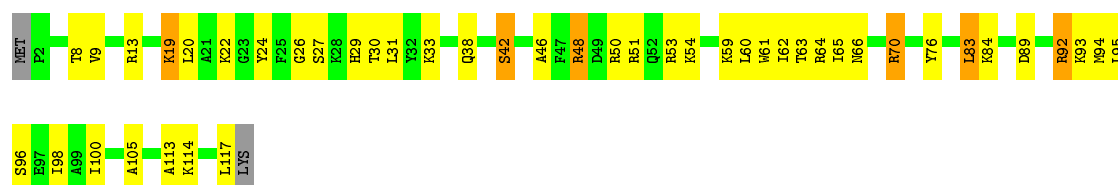
- Molecule 14: 50S ribosomal protein L19

Chain M: 



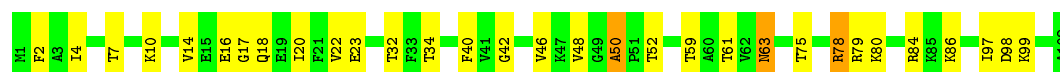
- Molecule 15: 50S ribosomal protein L20

Chain N: 



- Molecule 16: 50S ribosomal protein L21

Chain O: 



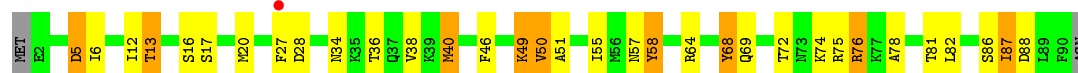
- Molecule 17: 50S ribosomal protein L22

Chain P: 

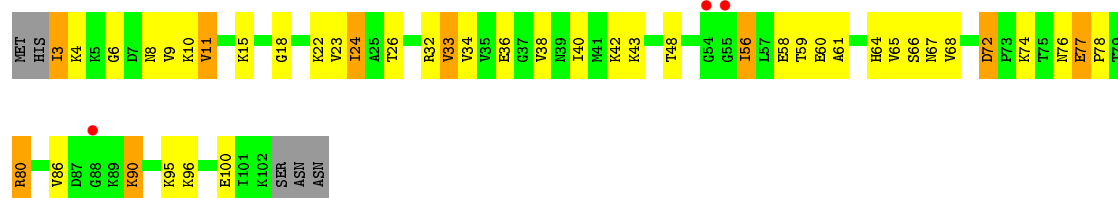




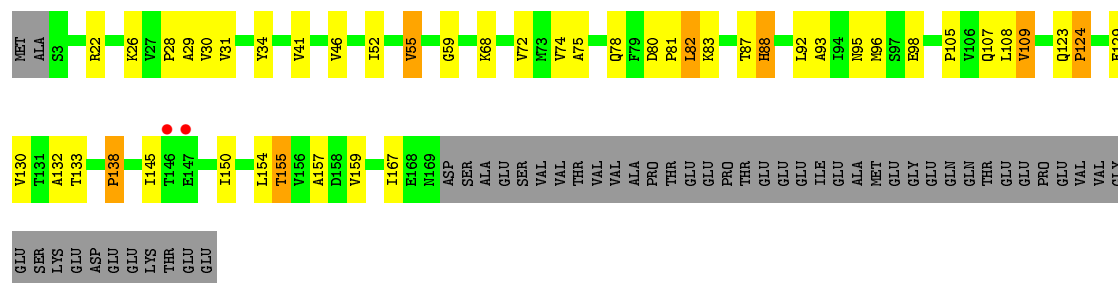
- Molecule 18: 50S ribosomal protein L23



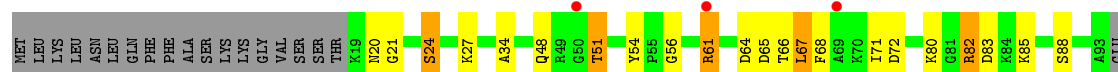
- Molecule 19: 50S ribosomal protein L24



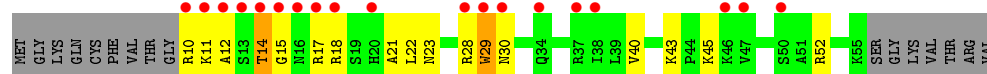
- Molecule 20: 50S ribosomal protein L25



- Molecule 21: 50S ribosomal protein L27



- Molecule 22: 50S ribosomal protein L28



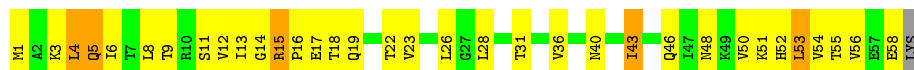
- Molecule 23: 50S ribosomal protein L29



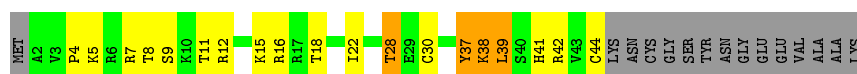




- Molecule 24: 50S ribosomal protein L30



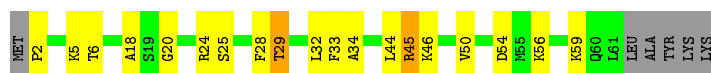
- Molecule 25: 50S ribosomal protein L32



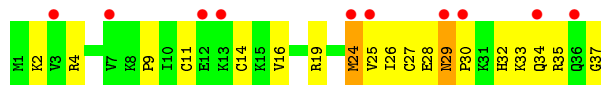
- Molecule 26: 50S ribosomal protein L34



- Molecule 27: 50S ribosomal protein L35



- Molecule 28: 50S ribosomal protein L36





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	279.76Å 279.76Å 872.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.74 – 3.53 49.74 – 3.53	Depositor EDS
% Data completeness (in resolution range)	96.0 (49.74-3.53) 96.0 (49.74-3.53)	Depositor EDS
$R_{merge}$	0.25	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.22 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.202 , 0.246 0.202 , 0.246	Depositor DCC
$R_{free}$ test set	11858 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	108.0	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.21 , 41.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	81909	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.29% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, MN, EOH, MPD, EPE, SPD

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	0.64	12/65032 (0.0%)	1.16	279/101388 (0.3%)
2	Y	0.56	0/2717	1.14	17/4232 (0.4%)
3	A	0.25	0/1717	0.55	0/2361
4	B	0.32	0/1581	0.62	0/2129
5	C	0.48	0/1338	0.72	0/1831
6	D	0.23	0/869	0.48	0/1205
7	E	0.27	0/982	0.51	0/1354
8	G	0.37	0/1128	0.58	0/1525
9	H	0.28	0/891	0.53	0/1203
10	I	0.58	0/868	0.91	1/1172 (0.1%)
11	J	0.30	0/1092	0.54	0/1473
12	K	0.31	0/911	0.59	0/1219
13	L	0.25	0/711	0.54	0/970
14	M	0.51	0/838	0.76	0/1132
15	N	0.38	0/944	0.59	0/1252
16	O	0.30	0/761	0.58	1/1022 (0.1%)
17	P	0.55	0/870	0.78	0/1171
18	Q	0.40	0/633	0.66	0/859
19	R	0.27	0/688	0.59	0/930
20	S	0.28	0/1109	0.58	0/1522
21	T	0.26	0/574	0.48	0/763
22	U	0.28	0/305	0.55	0/419
23	V	0.29	0/487	0.53	0/654
24	W	0.54	0/451	0.69	0/607
25	Z	0.48	0/345	0.67	0/460
26	2	0.47	0/366	0.65	0/480
27	3	0.32	0/424	0.66	0/566
28	4	0.39	0/280	0.63	0/371
All	All	0.59	12/88912 (0.0%)	1.07	298/134270 (0.2%)

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
3	A	0	1
7	E	0	1
27	3	0	1
All	All	0	3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	1289	A	N9-C4	-8.14	1.32	1.37
1	X	1065	A	N9-C4	-6.85	1.33	1.37
1	X	350	G	N9-C4	6.79	1.43	1.38
1	X	2845	G	N9-C4	-6.28	1.32	1.38
1	X	1186	A	N9-C4	-6.07	1.34	1.37
1	X	659	A	N9-C4	6.06	1.41	1.37
1	X	721	A	C5-C6	-5.68	1.35	1.41
1	X	2081	A	N9-C4	-5.66	1.34	1.37
1	X	721	A	N9-C4	-5.65	1.34	1.37
1	X	1027	A	N9-C4	-5.28	1.34	1.37
1	X	1004	A	N9-C4	-5.23	1.34	1.37
1	X	1065	A	C5-C6	-5.11	1.36	1.41

All (298) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2845	G	N3-C4-C5	11.31	134.26	128.60
1	X	955	A	N1-C6-N6	11.28	125.37	118.60
1	X	350	G	N3-C4-C5	-10.89	123.15	128.60
2	Y	86	C	N3-C2-O2	-10.49	114.56	121.90
1	X	1065	A	C2-N3-C4	-9.90	105.65	110.60
1	X	515	G	C4-C5-N7	9.80	114.72	110.80
1	X	2845	G	C2-N3-C4	-9.76	107.02	111.90
1	X	721	A	C2-N3-C4	-9.38	105.91	110.60
1	X	575	G	C2-N3-C4	9.21	116.51	111.90
1	X	2523	C	C6-N1-C2	9.07	123.93	120.30
1	X	1186	A	C2-N3-C4	-9.01	106.09	110.60
2	Y	86	C	N1-C2-O2	9.00	124.30	118.90
2	Y	93	C	N3-C2-O2	-8.86	115.70	121.90
1	X	515	G	C5-N7-C8	-8.72	99.94	104.30
1	X	350	G	C4-N9-C1'	8.55	137.62	126.50

*Continued on next page...*



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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1806	U	C5-C6-N1	-8.50	118.45	122.70
2	Y	86	C	C2-N1-C1'	8.44	128.08	118.80
1	X	515	G	C6-C5-N7	-8.33	125.40	130.40
1	X	1289	A	C2-N3-C4	-8.28	106.46	110.60
1	X	2081	A	C2-N3-C4	-8.26	106.47	110.60
1	X	721	A	C5-N7-C8	-8.25	99.77	103.90
1	X	955	A	C5-C6-N6	-8.22	117.12	123.70
1	X	350	G	N3-C4-N9	8.20	130.92	126.00
1	X	1030	C	C6-N1-C2	8.09	123.53	120.30
1	X	12	U	C2-N1-C1'	7.99	127.29	117.70
1	X	2544	C	C6-N1-C2	7.99	123.50	120.30
1	X	12	U	N3-C2-O2	-7.98	116.62	122.20
1	X	515	G	N7-C8-N9	7.96	117.08	113.10
1	X	496	G	N1-C6-O6	7.90	124.64	119.90
1	X	2845	G	C4-C5-N7	7.81	113.92	110.80
1	X	2845	G	N3-C4-N9	-7.79	121.33	126.00
1	X	1065	A	C5-N7-C8	-7.72	100.04	103.90
1	X	2081	A	N1-C6-N6	7.67	123.20	118.60
1	X	350	G	C8-N9-C4	-7.61	103.36	106.40
1	X	2062	G	C5-C6-O6	-7.56	124.06	128.60
1	X	660	A	P-O3'-C3'	7.54	128.75	119.70
1	X	721	A	C4-C5-N7	7.52	114.46	110.70
2	Y	93	C	N1-C2-O2	7.49	123.39	118.90
1	X	1294	G	C4-N9-C1'	7.47	136.22	126.50
1	X	721	A	N1-C6-N6	7.46	123.08	118.60
1	X	955	A	N9-C4-C5	-7.46	102.82	105.80
1	X	1491	C	C6-N1-C2	-7.44	117.32	120.30
1	X	1395	G	N3-C4-C5	-7.43	124.88	128.60
1	X	2642	U	C2-N1-C1'	7.35	126.52	117.70
1	X	515	G	C5-C6-O6	-7.27	124.24	128.60
1	X	2845	G	N1-C6-O6	7.24	124.25	119.90
1	X	1180	G	N1-C6-O6	7.23	124.24	119.90
1	X	568	C	C6-N1-C2	7.23	123.19	120.30
1	X	2071	C	C6-N1-C2	-7.20	117.42	120.30
2	Y	88	U	N3-C2-O2	-7.13	117.21	122.20
1	X	12	U	N1-C2-O2	7.11	127.78	122.80
1	X	1289	A	C5-N7-C8	-7.07	100.36	103.90
1	X	2483	C	C6-N1-C2	7.07	123.13	120.30
1	X	2479	C	C2-N1-C1'	7.07	126.57	118.80
1	X	1017	A	C8-N9-C4	-7.06	102.98	105.80
1	X	1065	A	N1-C6-N6	7.03	122.82	118.60
2	Y	92	G	N3-C4-C5	7.01	132.11	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	I	21	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	X	1516	C	C6-N1-C2	-6.97	117.51	120.30
1	X	2036	G	O5'-P-OP2	-6.94	99.45	105.70
1	X	2845	G	C5-N7-C8	-6.93	100.83	104.30
1	X	2716	U	C2-N1-C1'	-6.90	109.42	117.70
1	X	591	A	N1-C6-N6	6.89	122.73	118.60
1	X	1289	A	O4'-C1'-N9	-6.89	102.69	108.20
1	X	2062	G	N1-C6-O6	6.88	124.03	119.90
2	Y	93	C	C6-N1-C2	-6.84	117.56	120.30
1	X	1360	G	N1-C6-O6	6.83	124.00	119.90
1	X	503	A	C5-N7-C8	-6.82	100.49	103.90
1	X	515	G	N1-C6-O6	6.81	123.99	119.90
1	X	571	A	N1-C6-N6	-6.77	114.54	118.60
1	X	793	G	O5'-P-OP2	-6.75	99.62	105.70
1	X	504	G	C4-C5-N7	-6.72	108.11	110.80
1	X	2608	G	N1-C6-O6	-6.72	115.87	119.90
1	X	2772	C	C6-N1-C2	6.69	122.98	120.30
1	X	1294	G	C8-N9-C1'	-6.69	118.31	127.00
1	X	1350	U	C2-N1-C1'	6.64	125.66	117.70
1	X	519	G	O5'-P-OP2	-6.62	99.74	105.70
1	X	657	U	C2-N1-C1'	6.61	125.63	117.70
1	X	2566	C	C6-N1-C2	6.59	122.94	120.30
1	X	1395	G	N3-C4-N9	6.59	129.95	126.00
1	X	1395	G	C4-N9-C1'	6.58	135.06	126.50
1	X	1200	A	N1-C6-N6	6.57	122.54	118.60
2	Y	109	C	N3-C2-O2	-6.55	117.32	121.90
1	X	1968	C	C6-N1-C2	-6.54	117.69	120.30
1	X	34	U	N1-C2-O2	6.53	127.37	122.80
1	X	376	A	C8-N9-C4	-6.51	103.19	105.80
1	X	2716	U	C5-C4-O4	6.51	129.81	125.90
1	X	657	U	C6-N1-C1'	-6.49	112.11	121.20
1	X	2881	C	C6-N1-C2	-6.49	117.70	120.30
1	X	2591	A	C8-N9-C4	-6.46	103.22	105.80
1	X	661	U	C5-C6-N1	6.46	125.93	122.70
1	X	2535	G	N1-C6-O6	6.45	123.77	119.90
1	X	2845	G	N3-C2-N2	-6.43	115.40	119.90
1	X	657	U	N1-C2-O2	6.42	127.29	122.80
1	X	1335	C	C6-N1-C2	-6.42	117.73	120.30
1	X	2546	U	C2-N1-C1'	-6.41	110.00	117.70
2	Y	86	C	C6-N1-C1'	-6.41	113.11	120.80
1	X	659	A	O4'-C1'-N9	6.39	113.31	108.20
1	X	1149	U	N1-C2-O2	6.38	127.26	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1304	G	C8-N9-C4	6.36	108.94	106.40
1	X	2716	U	N3-C4-O4	-6.34	114.96	119.40
1	X	1291	A	O5'-P-OP2	-6.34	100.00	105.70
1	X	496	G	C6-C5-N7	-6.33	126.60	130.40
1	X	515	G	O4'-C1'-N9	6.32	113.26	108.20
1	X	656	G	C8-N9-C4	-6.32	103.87	106.40
2	Y	109	C	C6-N1-C2	-6.30	117.78	120.30
1	X	2600	C	N1-C2-O2	6.26	122.66	118.90
1	X	38	A	O5'-P-OP1	-6.25	100.07	105.70
1	X	2058	A	N9-C4-C5	6.25	108.30	105.80
1	X	2805	A	O5'-P-OP2	-6.24	100.08	105.70
1	X	2613	C	C6-N1-C2	-6.23	117.81	120.30
2	Y	99	U	N3-C2-O2	-6.23	117.84	122.20
1	X	854	G	C8-N9-C4	-6.21	103.92	106.40
1	X	498	G	N9-C4-C5	-6.20	102.92	105.40
1	X	350	G	C8-N9-C1'	-6.18	118.97	127.00
1	X	389	A	C8-N9-C4	-6.17	103.33	105.80
1	X	1250	G	O4'-C1'-N9	6.15	113.12	108.20
1	X	1661	C	C6-N1-C2	6.14	122.76	120.30
1	X	2708	C	C6-N1-C2	6.14	122.76	120.30
1	X	955	A	C6-C5-N7	-6.13	128.00	132.30
1	X	1065	A	N7-C8-N9	6.12	116.86	113.80
1	X	2474	G	C6-C5-N7	-6.12	126.73	130.40
1	X	2479	C	N1-C2-O2	6.11	122.57	118.90
1	X	2647	C	C6-N1-C2	-6.11	117.86	120.30
1	X	2048	G	C2-N3-C4	6.10	114.95	111.90
1	X	2474	G	N9-C4-C5	-6.09	102.96	105.40
1	X	1721	A	N1-C6-N6	-6.06	114.97	118.60
1	X	1371	U	N1-C2-O2	-6.03	118.58	122.80
1	X	548	A	O4'-C1'-N9	6.03	113.02	108.20
1	X	721	A	N3-C4-C5	6.02	131.02	126.80
1	X	1149	U	N3-C2-O2	-5.99	118.00	122.20
1	X	591	A	O5'-P-OP1	-5.99	100.31	105.70
1	X	1079	U	C6-N1-C2	-5.97	117.42	121.00
1	X	607	C	C6-N1-C2	-5.94	117.92	120.30
1	X	531	C	C6-N1-C2	-5.94	117.92	120.30
1	X	1499	U	N3-C2-O2	-5.90	118.07	122.20
1	X	1568	U	P-O3'-C3'	5.90	126.78	119.70
1	X	491	C	C6-N1-C2	-5.89	117.94	120.30
1	X	491	C	C5-C6-N1	5.89	123.94	121.00
1	X	1466	G	C4-N9-C1'	5.89	134.15	126.50
1	X	2843	A	O5'-P-OP2	-5.89	100.40	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1065	A	C6-C5-N7	-5.87	128.19	132.30
1	X	1561	G	C8-N9-C4	-5.84	104.06	106.40
1	X	503	A	C4-C5-N7	5.82	113.61	110.70
1	X	511	G	C8-N9-C4	-5.82	104.07	106.40
1	X	350	G	C2-N3-C4	5.82	114.81	111.90
1	X	2058	A	N1-C6-N6	-5.80	115.12	118.60
2	Y	92	G	N3-C4-N9	-5.79	122.53	126.00
1	X	1289	A	N3-C4-C5	5.78	130.85	126.80
1	X	2474	G	N1-C6-O6	5.76	123.36	119.90
1	X	890	G	N3-C4-C5	5.75	131.47	128.60
1	X	2674	U	C6-N1-C2	5.75	124.45	121.00
1	X	2844	U	N1-C2-O2	-5.75	118.78	122.80
1	X	1368	C	C6-N1-C2	5.74	122.60	120.30
1	X	1200	A	C5-C6-N6	-5.73	119.12	123.70
1	X	505	U	C2-N1-C1'	5.73	124.57	117.70
1	X	2280	G	C6-C5-N7	-5.72	126.97	130.40
2	Y	106	U	N3-C2-O2	-5.71	118.20	122.20
1	X	1042	C	C6-N1-C2	5.71	122.58	120.30
1	X	875	G	N1-C6-O6	-5.69	116.49	119.90
1	X	1144	C	C6-N1-C2	-5.69	118.03	120.30
2	Y	114	C	N1-C2-O2	5.64	122.28	118.90
1	X	2909	C	C6-N1-C2	-5.62	118.05	120.30
1	X	1065	A	C4-C5-N7	5.62	113.51	110.70
1	X	2290	C	C6-N1-C2	-5.61	118.06	120.30
1	X	34	U	C2-N1-C1'	5.60	124.42	117.70
1	X	2081	A	N1-C2-N3	5.60	132.10	129.30
1	X	2278	G	C6-C5-N7	-5.59	127.04	130.40
1	X	955	A	C4-C5-N7	5.55	113.47	110.70
1	X	2905	C	C6-N1-C2	-5.55	118.08	120.30
1	X	1360	G	C4-C5-N7	5.54	113.02	110.80
1	X	1068	G	N1-C6-O6	5.54	123.22	119.90
1	X	199	A	O5'-P-OP1	-5.53	100.72	105.70
1	X	1351	C	C5-C6-N1	5.53	123.76	121.00
1	X	1186	A	N1-C6-N6	5.52	121.91	118.60
1	X	721	A	C6-C5-N7	-5.52	128.44	132.30
1	X	2757	U	C6-N1-C2	-5.52	117.69	121.00
1	X	515	G	C8-N9-C4	-5.51	104.20	106.40
1	X	836	C	C6-N1-C2	5.51	122.50	120.30
1	X	661	U	C2-N1-C1'	5.51	124.31	117.70
1	X	1721	A	N9-C4-C5	5.50	108.00	105.80
1	X	34	U	C6-N1-C1'	-5.50	113.50	121.20
1	X	1492	G	C8-N9-C4	-5.50	104.20	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2310	C	C6-N1-C2	-5.49	118.10	120.30
1	X	116	G	N3-C4-C5	-5.49	125.86	128.60
1	X	2012	G	N1-C6-O6	-5.48	116.61	119.90
1	X	1230	G	N7-C8-N9	-5.48	110.36	113.10
1	X	2523	C	C5-C6-N1	-5.48	118.26	121.00
1	X	696	G	O5'-P-OP1	5.47	117.27	110.70
1	X	2036	G	O5'-P-OP1	5.47	117.27	110.70
1	X	1370	C	N3-C4-C5	5.47	124.09	121.90
1	X	2637	C	C6-N1-C2	5.47	122.49	120.30
1	X	268	A	O4'-C1'-N9	5.46	112.57	108.20
1	X	2803	A	OP1-P-O3'	5.46	117.20	105.20
1	X	389	A	N7-C8-N9	5.45	116.53	113.80
1	X	2491	C	C6-N1-C2	5.45	122.48	120.30
1	X	707	G	N3-C4-N9	5.44	129.26	126.00
1	X	1304	G	N7-C8-N9	-5.44	110.38	113.10
1	X	1277	C	C6-N1-C2	-5.43	118.13	120.30
1	X	1721	A	C5-C6-N6	5.43	128.04	123.70
1	X	2052	C	C6-N1-C2	-5.42	118.13	120.30
1	X	323	C	C6-N1-C2	-5.42	118.13	120.30
1	X	1350	U	N3-C2-O2	-5.42	118.41	122.20
1	X	1702	C	C6-N1-C2	5.39	122.46	120.30
2	Y	105	G	C2-N3-C4	-5.38	109.21	111.90
1	X	503	A	N1-C6-N6	5.38	121.83	118.60
1	X	955	A	N3-C4-N9	5.37	131.69	127.40
1	X	2755	U	C6-N1-C2	-5.36	117.78	121.00
1	X	169	G	O4'-C1'-N9	5.36	112.49	108.20
1	X	2027	G	C8-N9-C4	5.36	108.54	106.40
1	X	1042	C	N3-C4-C5	5.35	124.04	121.90
1	X	2599	A	C8-N9-C4	5.35	107.94	105.80
1	X	515	G	C4-N9-C1'	5.34	133.45	126.50
1	X	1506	C	N1-C2-O2	5.34	122.11	118.90
1	X	2642	U	C6-N1-C1'	-5.34	113.73	121.20
1	X	2756	G	N3-C4-C5	-5.33	125.93	128.60
1	X	1524	C	C6-N1-C2	-5.33	118.17	120.30
1	X	496	G	C8-N9-C1'	-5.32	120.08	127.00
1	X	2682	G	O4'-C1'-N9	5.32	112.45	108.20
1	X	2712	G	N3-C2-N2	-5.32	116.18	119.90
1	X	2549	U	N3-C4-O4	5.31	123.12	119.40
1	X	378	C	C6-N1-C2	-5.31	118.18	120.30
1	X	2599	A	N9-C4-C5	-5.30	103.68	105.80
1	X	1360	G	C5-C6-O6	-5.30	125.42	128.60
1	X	1179	C	C6-N1-C2	5.30	122.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	660	A	OP1-P-O3'	5.29	116.84	105.20
1	X	1016	G	N1-C6-O6	-5.29	116.73	119.90
1	X	659	A	C2-N3-C4	5.28	113.24	110.60
1	X	1664	G	N1-C6-O6	5.28	123.07	119.90
1	X	1230	G	C8-N9-C4	5.28	108.51	106.40
1	X	2655	U	N3-C4-O4	5.28	123.09	119.40
2	Y	79	C	C5-C4-N4	-5.28	116.51	120.20
1	X	1395	G	C8-N9-C1'	-5.28	120.14	127.00
1	X	2062	G	C4-C5-N7	5.27	112.91	110.80
1	X	2527	U	OP2-P-O3'	5.27	116.79	105.20
1	X	1229	G	OP2-P-O3'	5.27	116.78	105.20
16	O	50	ALA	C-N-CD	5.25	139.44	128.40
1	X	15	G	C8-N9-C4	5.25	108.50	106.40
1	X	16	G	C4-C5-C6	5.25	121.95	118.80
1	X	1091	G	P-O3'-C3'	5.25	126.00	119.70
1	X	576	U	O5'-P-OP2	-5.24	100.98	105.70
1	X	2479	C	N3-C2-O2	-5.24	118.23	121.90
1	X	372	A	C8-N9-C4	5.23	107.89	105.80
1	X	859	C	C6-N1-C2	-5.23	118.21	120.30
1	X	2535	G	C5-C6-O6	-5.23	125.46	128.60
1	X	1661	C	C2-N1-C1'	-5.22	113.06	118.80
1	X	2599	A	N1-C6-N6	5.22	121.73	118.60
1	X	199	A	C8-N9-C4	-5.21	103.72	105.80
1	X	2661	A	N1-C6-N6	-5.20	115.48	118.60
1	X	504	G	N3-C4-C5	-5.20	126.00	128.60
1	X	728	U	C6-N1-C2	-5.20	117.88	121.00
1	X	2716	U	C6-N1-C1'	5.19	128.47	121.20
1	X	182	C	N1-C2-O2	5.19	122.01	118.90
1	X	1079	U	N3-C2-O2	-5.19	118.57	122.20
1	X	2740	A	N1-C6-N6	5.18	121.71	118.60
1	X	1149	U	C2-N1-C1'	5.18	123.91	117.70
1	X	1186	A	C5-N7-C8	-5.16	101.32	103.90
1	X	2278	G	N1-C6-O6	5.16	123.00	119.90
1	X	875	G	C5-C6-O6	5.16	131.69	128.60
1	X	102	A	N1-C6-N6	5.15	121.69	118.60
1	X	985	A	O5'-P-OP1	-5.15	101.07	105.70
1	X	1708	A	C8-N9-C4	-5.14	103.74	105.80
1	X	2053	U	N3-C4-O4	5.14	123.00	119.40
1	X	20	C	C5-C4-N4	-5.14	116.60	120.20
1	X	1294	G	N3-C4-N9	5.14	129.08	126.00
1	X	2510	C	C6-N1-C2	-5.13	118.25	120.30
1	X	498	G	C4-C5-N7	5.13	112.85	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	880	A	N1-C6-N6	5.13	121.68	118.60
1	X	591	A	C5-C6-N6	-5.12	119.61	123.70
1	X	1968	C	C2-N1-C1'	5.11	124.42	118.80
1	X	1006	G	N3-C2-N2	-5.09	116.34	119.90
1	X	2905	C	C5-C6-N1	5.07	123.54	121.00
1	X	2479	C	C6-N1-C2	-5.07	118.27	120.30
1	X	875	G	C4-C5-N7	-5.07	108.77	110.80
1	X	362	C	C6-N1-C2	-5.07	118.27	120.30
1	X	552	A	N1-C6-N6	5.07	121.64	118.60
1	X	675	G	N1-C6-O6	5.07	122.94	119.90
1	X	2064	A	C8-N9-C4	-5.07	103.77	105.80
1	X	517	A	C8-N9-C4	5.06	107.82	105.80
1	X	1351	C	C2-N1-C1'	5.06	124.36	118.80
1	X	1758	A	C8-N9-C4	-5.05	103.78	105.80
1	X	638	U	N1-C2-O2	5.05	126.33	122.80
1	X	1065	A	C8-N9-C4	-5.05	103.78	105.80
1	X	2546	U	N3-C4-O4	-5.04	115.87	119.40
1	X	36	G	N3-C4-N9	5.04	129.03	126.00
1	X	2014	G	O5'-P-OP2	-5.04	101.16	105.70
1	X	376	A	N7-C8-N9	5.04	116.32	113.80
1	X	2639	C	N3-C4-C5	5.03	123.91	121.90
1	X	2836	C	N3-C4-C5	-5.03	119.89	121.90
1	X	1064	A	C8-N9-C4	5.02	107.81	105.80
1	X	12	U	C6-N1-C1'	-5.02	114.17	121.20
1	X	2298	G	N9-C4-C5	-5.02	103.39	105.40
1	X	350	G	C5-C6-N1	5.02	114.01	111.50
1	X	1312	A	OP1-P-O3'	5.02	116.23	105.20
1	X	656	G	N7-C8-N9	5.01	115.60	113.10
1	X	566	U	O4'-C1'-N1	5.00	112.20	108.20
1	X	2893	A	O4'-C1'-N9	5.00	112.20	108.20
1	X	568	C	C5-C6-N1	-5.00	118.50	121.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	3	24	ARG	Peptide
3	A	52	ARG	Peptide
7	E	119	GLU	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	58077	0	29209	849	0
2	Y	2430	0	1229	48	0
3	A	1686	0	1350	48	0
4	B	1558	0	1545	60	0
5	C	1320	0	1171	54	0
6	D	866	0	470	8	0
7	E	970	0	741	23	0
8	G	1106	0	1072	31	0
9	H	884	0	902	26	0
10	I	859	0	772	37	0
11	J	1068	0	1078	42	0
12	K	908	0	935	28	0
13	L	705	0	589	10	0
14	M	826	0	831	41	0
15	N	932	0	995	37	0
16	O	751	0	743	14	0
17	P	862	0	920	37	0
18	Q	626	0	567	21	0
19	R	683	0	661	21	0
20	S	1097	0	956	18	0
21	T	568	0	575	11	0
22	U	300	0	231	9	0
23	V	486	0	469	6	0
24	W	449	0	490	25	0
25	Z	339	0	350	19	0
26	2	362	0	398	14	0
27	3	420	0	405	7	0
28	4	277	0	301	17	0
29	X	88	0	154	14	0
29	Z	8	0	14	0	0
30	B	1	0	0	0	0
30	I	2	0	0	0	0
30	J	1	0	0	0	0
30	R	2	0	0	0	0
30	X	223	0	0	0	0
30	Y	2	0	0	0	0
31	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	C	1	0	0	0	0
31	G	3	0	0	0	0
31	I	1	0	0	0	0
31	O	1	0	0	0	0
31	X	80	0	0	0	0
31	Y	3	0	0	0	0
32	X	15	0	17	0	0
33	X	40	0	76	0	0
34	X	21	0	42	0	0
All	All	81909	0	50258	1401	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 11.

All (1401) 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:2231:C:HO2'	1:X:2232:A:H8	1.06	0.97
2:Y:80:A:H61	2:Y:91:C:H42	1.05	0.94
2:Y:79:C:H42	2:Y:92:G:H1	1.06	0.94
1:X:1487:G:H1	1:X:1597:U:H3	1.17	0.93
26:2:36:ARG:HG3	26:2:43:LEU:HD21	1.52	0.90
2:Y:15:C:H42	2:Y:105:G:H21	1.19	0.88
8:G:87:SER:O	8:G:89:THR:N	2.09	0.86
1:X:65:A:N1	1:X:90:A:N6	2.26	0.84
28:4:25:VAL:HG22	28:4:34:GLN:HB2	1.59	0.83
1:X:2850:G:H5'	4:B:67:LYS:HE3	1.58	0.83
5:C:7:LEU:HD21	5:C:126:VAL:H	1.42	0.82
1:X:864:A:OP2	1:X:1226:G:N2	2.09	0.82
1:X:1448:U:H3'	1:X:1449:A:H5''	1.62	0.82
19:R:6:GLY:HA2	19:R:23:VAL:HG22	1.61	0.81
1:X:1522:G:H1	1:X:1558:U:H3	1.28	0.81
1:X:1323:A:O2'	1:X:1325:U:OP2	1.98	0.80
1:X:268:A:N6	1:X:473:U:O2'	2.14	0.80
1:X:2432:G:OP1	10:I:63:LYS:NZ	2.14	0.80
1:X:1492:G:N2	1:X:1508:C:N3	2.31	0.78
9:H:63:VAL:HG21	9:H:102:VAL:HG22	1.64	0.78
1:X:627:C:OP2	29:X:3007:MPD:O2	2.01	0.78
1:X:878:C:H1'	10:I:48:PRO:HB3	1.66	0.78
1:X:498:G:H21	1:X:503:A:H8	1.31	0.77
1:X:2314:A:O2'	1:X:2315:A:H2'	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:77:G:H1	2:Y:94:U:H3	1.30	0.77
1:X:1513:A:H3'	1:X:1514:A:H8	1.49	0.77
1:X:1518:G:H1	1:X:1562:C:H42	1.30	0.77
4:B:117:ASP:HB3	4:B:181:GLN:HA	1.66	0.76
1:X:2852:U:OP1	4:B:61:LYS:NZ	2.17	0.76
1:X:1250:G:O2'	1:X:1275:A:N6	2.18	0.76
1:X:1781:C:H5	14:M:96:ARG:HH22	1.31	0.76
2:Y:18:G:H1	2:Y:61:U:H3	1.32	0.76
18:Q:55:ILE:HG13	18:Q:78:ALA:HB2	1.67	0.76
1:X:1851:G:OP2	3:A:53:HIS:NE2	2.18	0.76
1:X:1063:U:H3	1:X:1186:A:H62	1.34	0.76
1:X:1515:G:H1	1:X:1565:U:H3	1.34	0.76
1:X:459:C:O2'	1:X:1907:U:O2'	2.04	0.76
1:X:501:C:H3'	1:X:502:C:H5''	1.67	0.76
2:Y:15:C:H42	2:Y:105:G:N2	1.83	0.75
4:B:67:LYS:HA	4:B:86:ARG:HH22	1.49	0.75
1:X:1894:G:O6	1:X:1902:G:N2	2.19	0.75
1:X:1501:G:H22	1:X:2729:G:H22	1.31	0.75
1:X:304:G:H1	1:X:413:C:H42	1.34	0.75
1:X:2228:C:O2	1:X:2249:G:N2	2.19	0.74
2:Y:78:C:N3	2:Y:93:C:N4	2.34	0.74
3:A:89:ALA:HB2	3:A:158:ALA:HA	1.68	0.74
3:A:68:LYS:HA	3:A:151:GLY:HA2	1.69	0.74
2:Y:81:A:H61	2:Y:90:C:H42	1.31	0.74
1:X:1512:U:H2'	1:X:1513:A:C8	2.23	0.73
1:X:193:A:OP2	22:U:28:ARG:NH2	2.21	0.73
1:X:2649:U:O2'	1:X:2845:G:N2	2.21	0.73
15:N:61:TRP:CE2	15:N:93:LYS:HB2	2.24	0.73
9:H:4:GLN:HG2	9:H:5:GLU:HG2	1.71	0.73
20:S:133:THR:HG21	20:S:159:VAL:HB	1.70	0.73
24:W:26:LEU:HD21	24:W:46:GLN:HB3	1.71	0.72
1:X:1683:U:H2'	1:X:1684:A:H5''	1.70	0.72
4:B:158:SER:O	4:B:161:SER:OG	2.07	0.72
4:B:124:GLY:HA2	4:B:174:GLY:HA3	1.70	0.72
4:B:33:ASN:HB3	4:B:105:VAL:HG22	1.71	0.72
2:Y:31:G:H1	2:Y:47:C:H42	1.37	0.72
2:Y:69:C:H42	2:Y:102:A:H61	1.38	0.72
18:Q:13:THR:HG23	18:Q:16:SER:HB3	1.71	0.72
1:X:1563:U:H2'	1:X:1564:G:H8	1.55	0.72
13:L:36:SER:OG	13:L:37:ASN:N	2.23	0.71
23:V:45:THR:HA	23:V:48:LYS:HD2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1490:G:O2'	1:X:1491:C:O4'	2.09	0.71
1:X:1845:U:H5''	3:A:156:ARG:HB2	1.71	0.71
1:X:657:U:O4	1:X:659:A:N6	2.24	0.71
10:I:112:LEU:HD22	10:I:112:LEU:H	1.56	0.70
1:X:427:A:H5''	22:U:18:ARG:HE	1.56	0.70
2:Y:15:C:N4	2:Y:105:G:H21	1.89	0.70
1:X:2650:G:O5'	1:X:2845:G:N2	2.24	0.70
1:X:2883:U:H2'	1:X:2884:G:H8	1.55	0.70
28:4:27:CYS:HB3	28:4:32:HIS:HB2	1.71	0.70
19:R:80:ARG:NH1	19:R:95:LYS:O	2.24	0.70
28:4:27:CYS:SG	28:4:32:HIS:ND1	2.65	0.70
11:J:40:SER:HB3	11:J:127:VAL:HG22	1.73	0.70
2:Y:79:C:N4	2:Y:92:G:H1	1.87	0.70
19:R:3:ILE:HG13	19:R:4:LYS:HG2	1.74	0.70
14:M:102:LEU:O	14:M:103:ARG:NH2	2.24	0.69
1:X:735:C:O2'	1:X:825:G:OP1	2.08	0.69
1:X:736:C:OP1	3:A:217:ARG:NH1	2.25	0.69
1:X:2711:U:OP2	14:M:53:ARG:NH1	2.25	0.69
1:X:37:C:H2'	1:X:38:A:C8	2.28	0.69
3:A:209:GLY:HA2	3:A:212:ARG:HB2	1.75	0.69
1:X:1563:U:H2'	1:X:1564:G:C8	2.27	0.69
1:X:2051:C:H2'	1:X:2052:C:H6	1.58	0.69
13:L:45:ILE:HG23	13:L:52:THR:HG22	1.74	0.69
16:O:42:GLY:HA2	16:O:46:VAL:HG12	1.75	0.69
5:C:166:SER:OG	5:C:167:ALA:N	2.26	0.69
1:X:503:A:H2	1:X:517:A:H62	1.41	0.69
1:X:2804:G:H5''	1:X:2805:A:H5'	1.74	0.68
1:X:2495:A:OP1	11:J:119:ARG:NH2	2.27	0.68
20:S:22:ARG:HH21	20:S:28:PRO:HG3	1.58	0.68
1:X:1492:G:N7	1:X:1493:U:H5	1.91	0.68
7:E:102:ASP:H	7:E:115:ILE:HD13	1.59	0.68
2:Y:80:A:N6	2:Y:91:C:H42	1.87	0.68
5:C:133:ALA:HB1	5:C:135:LYS:H	1.58	0.68
17:P:2:GLU:HG3	17:P:109:ASP:H	1.57	0.68
1:X:1472:C:N4	1:X:1617:A:OP2	2.27	0.67
1:X:1998:A:O2'	1:X:1999:G:OP1	2.11	0.67
1:X:1250:G:H2'	1:X:1274:G:N2	2.08	0.67
1:X:1521:A:H61	1:X:1560:A:H1'	1.59	0.67
1:X:2817:A:O2'	1:X:2818:A:OP2	2.13	0.67
1:X:922:G:H22	1:X:944:G:H1	1.43	0.67
1:X:83:G:H21	1:X:102:A:H2	1.41	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:351:G:O2'	19:R:15:LYS:NZ	2.28	0.67
1:X:2835:C:H1'	25:Z:39:LEU:HD23	1.75	0.67
5:C:103:LYS:HA	5:C:106:ARG:NE	2.10	0.67
9:H:87:ILE:HD11	9:H:91:LYS:HA	1.77	0.67
12:K:24:LEU:O	12:K:28:GLU:N	2.28	0.67
8:G:2:ARG:HG3	8:G:3:GLN:H	1.59	0.67
14:M:105:LEU:O	14:M:106:ARG:NH1	2.27	0.67
15:N:27:SER:HB2	15:N:31:LEU:HG	1.76	0.67
1:X:2673:C:OP2	1:X:2759:G:O2'	2.12	0.67
1:X:2419:A:H2	1:X:2451:C:H42	1.41	0.66
1:X:1591:G:N2	1:X:1591:G:OP2	2.28	0.66
18:Q:58:TYR:HB2	18:Q:75:ARG:HB2	1.76	0.66
1:X:1931:G:H1	1:X:1957:G:H22	1.43	0.66
1:X:787:U:H2'	1:X:788:A:C8	2.31	0.66
1:X:721:A:H8	1:X:2096:G:H21	1.41	0.66
1:X:1491:C:O2	1:X:1492:G:N2	2.29	0.66
1:X:1575:A:H2'	1:X:1576:A:H5'	1.76	0.66
1:X:2360:A:H5'	1:X:2362:A:H1'	1.77	0.66
1:X:2554:C:H5''	28:4:30:PRO:HB3	1.76	0.66
11:J:22:LYS:HE3	11:J:23:GLY:H	1.61	0.66
1:X:388:A:H1'	1:X:389:A:H2	1.61	0.66
28:4:9:PRO:HB3	28:4:14:CYS:HB2	1.78	0.65
1:X:2313:A:H4'	1:X:2314:A:O4'	1.97	0.65
2:Y:6:U:OP1	13:L:11:ARG:NH2	2.25	0.65
1:X:1490:G:O2'	1:X:1491:C:O5'	2.14	0.65
1:X:2330:G:H4'	6:D:114:PHE:HA	1.78	0.65
1:X:1513:A:H3'	1:X:1514:A:C8	2.31	0.65
1:X:877:G:H2'	1:X:878:C:C6	2.32	0.65
1:X:24:G:O2'	17:P:78:GLU:O	2.14	0.64
1:X:1523:G:N2	1:X:1557:C:N3	2.42	0.64
19:R:10:LYS:HE3	19:R:18:GLY:HA2	1.78	0.64
1:X:665:G:H4'	1:X:666:A:H5''	1.79	0.64
4:B:67:LYS:HA	4:B:86:ARG:NH2	2.11	0.64
1:X:1337:A:H4'	1:X:1338:U:H5''	1.79	0.64
1:X:17:G:OP1	25:Z:11:THR:HG22	1.97	0.64
1:X:700:A:H4'	1:X:701:G:H5'	1.80	0.64
25:Z:38:LYS:HZ2	25:Z:38:LYS:HB2	1.62	0.64
9:H:19:VAL:HG12	9:H:43:VAL:HA	1.80	0.64
10:I:51:GLU:H	10:I:51:GLU:CD	1.97	0.64
1:X:2860:U:H5''	12:K:49:THR:HG21	1.80	0.64
1:X:1395:G:OP2	1:X:1395:G:N2	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1523:G:H1	1:X:1557:C:H42	1.45	0.64
29:X:3003:MPD:HO4	29:X:3003:MPD:HO2	1.43	0.64
5:C:108:LEU:O	5:C:112:SER:OG	2.09	0.63
1:X:1826:G:N2	1:X:1845:U:O2'	2.31	0.63
28:4:27:CYS:O	28:4:29:ASN:N	2.31	0.63
1:X:1467:G:O2'	1:X:1543:G:O2'	2.14	0.63
15:N:92:ARG:O	15:N:93:LYS:HB3	1.97	0.63
21:T:61:ARG:NH1	21:T:65:ASP:OD1	2.32	0.63
1:X:1498:U:HO2'	1:X:1499:U:H5	1.47	0.63
1:X:1065:A:H3'	1:X:1065:A:C8	2.34	0.63
1:X:460:C:O2	1:X:1891:U:O2'	2.17	0.63
1:X:2112:C:H42	1:X:2261:A:H61	1.46	0.63
1:X:637:U:H2'	1:X:638:U:C6	2.33	0.63
1:X:2717:A:H62	12:K:13:ARG:HD2	1.64	0.63
14:M:15:LEU:HD22	14:M:79:HIS:CE1	2.34	0.63
1:X:280:C:H2'	1:X:281:A:H8	1.63	0.63
1:X:444:C:H41	22:U:52:ARG:HH12	1.46	0.63
5:C:14:SER:OG	5:C:15:GLY:N	2.31	0.62
1:X:1769:C:N4	1:X:1770:C:H41	1.98	0.62
1:X:2354:A:H2'	1:X:2355:A:C8	2.34	0.62
3:A:92:ALA:H	3:A:106:ALA:HB2	1.64	0.62
24:W:19:GLN:O	24:W:23:VAL:HG23	1.98	0.62
9:H:15:GLY:HA3	9:H:50:GLY:HA3	1.80	0.62
9:H:76:TYR:HB2	14:M:75:THR:HG23	1.80	0.62
1:X:904:G:O2'	1:X:961:G:O6	2.16	0.62
1:X:79:U:H2'	1:X:389:A:H8	1.65	0.62
9:H:101:PRO:HD3	14:M:68:SER:HB2	1.82	0.62
18:Q:49:LYS:HD3	18:Q:50:VAL:N	2.15	0.62
8:G:89:THR:HG21	8:G:93:LEU:HD12	1.82	0.62
1:X:2018:U:O2'	1:X:2019:G:H5'	2.00	0.62
1:X:2619:G:H2'	1:X:2620:U:O4'	2.00	0.62
1:X:262:G:H21	1:X:666:A:H8	1.48	0.62
1:X:2749:G:H2'	1:X:2750:C:C6	2.35	0.62
3:A:123:ASP:OD1	3:A:123:ASP:N	2.33	0.61
1:X:606:G:OP2	16:O:78:ARG:NH2	2.32	0.61
5:C:140:LYS:HA	5:C:142:VAL:HG12	1.82	0.61
9:H:34:ASN:ND2	9:H:68:GLY:O	2.31	0.61
14:M:23:ARG:HH21	14:M:23:ARG:HG3	1.64	0.61
22:U:21:ALA:O	22:U:23:ASN:N	2.33	0.61
1:X:1737:U:O2'	3:A:14:ARG:NH2	2.33	0.61
1:X:903:G:OP2	21:T:85:LYS:NZ	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:199:GLN:HG3	3:A:202:LEU:HB2	1.83	0.61
1:X:956:A:C6	11:J:11:ARG:HD3	2.35	0.61
1:X:1:G:H3'	1:X:2:A:H4'	1.83	0.61
12:K:105:LYS:HB2	25:Z:41:HIS:HA	1.82	0.61
11:J:31:GLU:H	11:J:107:ALA:HB2	1.64	0.61
3:A:133:GLN:HG3	3:A:186:SER:HB3	1.83	0.61
5:C:77:THR:HG22	5:C:79:ARG:H	1.66	0.61
4:B:116:ILE:HD12	4:B:211:ILE:HG23	1.83	0.61
1:X:1415:A:O2'	1:X:1417:G:N7	2.29	0.61
1:X:1510:U:O4	1:X:1572:G:N2	2.33	0.61
11:J:111:GLU:OE2	11:J:115:ARG:NH1	2.32	0.61
1:X:2120:G:H21	1:X:2225:A:H62	1.48	0.61
4:B:118:VAL:HG12	4:B:211:ILE:HA	1.82	0.61
1:X:2050:A:H5'	1:X:2644:C:H4'	1.82	0.60
1:X:2776:A:H4'	7:E:62:ARG:HG3	1.84	0.60
19:R:40:ILE:HG23	19:R:61:ALA:HB2	1.82	0.60
1:X:1567:A:H5''	1:X:1568:U:H2'	1.82	0.60
1:X:1816:A:OP2	3:A:221:ARG:NH1	2.31	0.60
1:X:2370:U:O2'	1:X:2400:U:O2'	2.14	0.60
1:X:613:G:H2'	1:X:2057:A:N7	2.16	0.60
1:X:1465:G:H2'	1:X:1466:G:C8	2.36	0.60
1:X:2470:C:H2'	1:X:2471:G:H8	1.65	0.60
11:J:36:ALA:HA	11:J:129:THR:HG22	1.84	0.60
1:X:615:A:OP2	16:O:79:ARG:NH2	2.34	0.60
1:X:1289:A:N7	29:X:3007:MPD:H11	2.16	0.60
24:W:50:VAL:HB	24:W:53:LEU:HD11	1.82	0.60
11:J:65:TRP:HB2	11:J:105:GLU:HG3	1.84	0.60
1:X:1512:U:H2'	1:X:1513:A:H8	1.64	0.60
1:X:1514:A:N6	1:X:1566:G:H1	1.99	0.60
4:B:8:ARG:NH1	4:B:206:LYS:O	2.35	0.60
1:X:1250:G:H2'	1:X:1274:G:H22	1.65	0.60
1:X:2682:G:O2'	1:X:2683:U:H5	1.84	0.60
1:X:683:G:C6	1:X:696:G:C6	2.90	0.60
1:X:857:C:HO2'	1:X:1264:A:HO2'	1.50	0.60
1:X:1056:U:OP2	15:N:70:ARG:NH2	2.35	0.60
2:Y:80:A:H61	2:Y:91:C:N4	1.88	0.60
9:H:31:LYS:HG3	9:H:32:THR:HG22	1.83	0.59
24:W:22:THR:HG23	24:W:46:GLN:HG2	1.84	0.59
1:X:2089:A:OP1	29:X:3003:MPD:O2	2.14	0.59
1:X:2355:A:H2'	1:X:2356:A:C8	2.37	0.59
1:X:858:U:H2'	1:X:859:C:C6	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:V:44:ARG:HG2	23:V:48:LYS:HE3	1.84	0.59
1:X:2351:U:H3	1:X:2358:G:H1	1.49	0.59
1:X:2431:C:H42	1:X:2440:G:H1	1.51	0.59
1:X:1527:A:H2'	1:X:1528:G:H5'	1.83	0.59
28:4:35:ARG:HG2	28:4:37:GLY:H	1.67	0.59
5:C:190:ASP:OD1	5:C:191:SER:N	2.31	0.59
7:E:53:VAL:HA	7:E:66:GLY:HA2	1.82	0.59
1:X:1658:A:H61	17:P:88:ARG:H	1.50	0.59
1:X:1765:A:O2'	1:X:1766:C:O4'	2.19	0.59
1:X:2358:G:O2'	1:X:2363:A:N1	2.32	0.59
1:X:2845:G:O6	4:B:172:ARG:NH2	2.35	0.59
1:X:38:A:O2'	1:X:39:C:OP1	2.17	0.59
19:R:11:VAL:HA	19:R:67:ASN:HB3	1.83	0.59
1:X:1487:G:N2	1:X:1597:U:O2	2.36	0.59
1:X:2089:A:OP1	29:X:3003:MPD:O4	2.21	0.59
1:X:683:G:C6	1:X:696:G:N1	2.70	0.59
14:M:55:GLY:H	14:M:59:GLU:HG3	1.67	0.59
1:X:1208:A:H2'	1:X:1209:U:C6	2.38	0.59
1:X:2883:U:H2'	1:X:2884:G:C8	2.37	0.59
7:E:133:VAL:HG11	7:E:141:VAL:HG13	1.85	0.59
1:X:1440:A:HO2'	1:X:1514:A:HO2'	1.47	0.59
5:C:4:TYR:HA	5:C:18:GLU:HA	1.84	0.59
1:X:1072:A:N3	1:X:2513:G:O2'	2.33	0.59
1:X:1568:U:O2'	1:X:1569:G:OP2	2.20	0.59
17:P:73:GLU:HG2	17:P:106:VAL:HB	1.83	0.59
1:X:218:G:H4'	1:X:219:A:H4'	1.85	0.59
4:B:53:PHE:HB3	4:B:87:PHE:HB2	1.85	0.58
12:K:23:SER:HA	12:K:26:ILE:HD12	1.85	0.58
1:X:1300:G:OP2	17:P:99:ARG:NH2	2.35	0.58
1:X:2051:C:H2'	1:X:2052:C:C6	2.36	0.58
26:2:20:ARG:HB2	26:2:20:ARG:NH1	2.18	0.58
3:A:119:GLY:O	3:A:121:GLU:N	2.35	0.58
17:P:61:ASN:HB2	17:P:62:TYR:CE1	2.38	0.58
1:X:666:A:H2'	1:X:667:G:H5'	1.85	0.58
1:X:1465:G:H2'	1:X:1466:G:H8	1.68	0.58
20:S:28:PRO:O	20:S:88:HIS:HA	2.03	0.58
8:G:111:PRO:HB2	8:G:113:THR:HG23	1.84	0.58
1:X:1565:U:H2'	1:X:1566:G:C8	2.39	0.58
17:P:86:ARG:HG3	17:P:87:PRO:HD2	1.86	0.58
1:X:1395:G:O2'	1:X:1410:A:N6	2.37	0.58
22:U:14:THR:OG1	22:U:15:GLY:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:15:G:O2'	25:Z:18:THR:HG21	2.03	0.58
1:X:1197:C:OP1	15:N:92:ARG:NH2	2.37	0.58
1:X:659:A:H1'	1:X:660:A:H5'	1.86	0.58
20:S:107:GLN:HA	20:S:138:PRO:HD2	1.86	0.57
1:X:2856:U:H2'	1:X:2857:A:C8	2.39	0.57
1:X:2905:C:H42	25:Z:39:LEU:HG	1.69	0.57
17:P:4:LYS:HB2	17:P:106:VAL:HG22	1.85	0.57
1:X:1423:C:O2'	1:X:1512:U:O2	2.16	0.57
1:X:460:C:H2'	1:X:461:A:H8	1.67	0.57
28:4:16:VAL:HG22	28:4:25:VAL:HG12	1.85	0.57
2:Y:74:G:H22	2:Y:97:A:H61	1.51	0.57
1:X:1041:G:OP1	15:N:92:ARG:HG2	2.04	0.57
1:X:956:A:C5	11:J:11:ARG:HD3	2.39	0.57
1:X:1491:C:O2	1:X:1509:G:N2	2.37	0.57
1:X:2059:G:H22	1:X:2599:A:H5'	1.69	0.57
24:W:6:ILE:HD12	24:W:56:VAL:HG12	1.85	0.57
1:X:2618:C:H2'	1:X:2619:G:C8	2.40	0.57
2:Y:22:G:N2	2:Y:26:C:N3	2.53	0.57
10:I:3:LEU:HA	10:I:6:LEU:HD21	1.87	0.57
1:X:1424:A:H2'	1:X:1425:G:C8	2.39	0.57
1:X:2470:C:H2'	1:X:2471:G:C8	2.39	0.57
20:S:81:PRO:O	20:S:83:LYS:N	2.36	0.57
1:X:1962:G:H1'	1:X:1991:G:N2	2.20	0.57
1:X:1761:G:O2'	1:X:1762:U:O4'	2.22	0.57
3:A:169:GLY:O	3:A:171:TYR:N	2.37	0.56
13:L:89:ILE:HG23	13:L:90:LYS:H	1.68	0.56
1:X:677:A:H4'	10:I:60:ARG:HH22	1.70	0.56
1:X:1614:A:O4'	1:X:1615:G:N2	2.38	0.56
22:U:43:LYS:O	22:U:45:LYS:N	2.33	0.56
1:X:1257:G:OP2	15:N:19:LYS:NZ	2.32	0.56
1:X:1293:U:H5''	1:X:1294:G:H5''	1.85	0.56
8:G:20:ASP:HA	8:G:58:ILE:HG22	1.87	0.56
11:J:4:PRO:HG2	11:J:48:GLU:HG2	1.87	0.56
1:X:1037:A:OP1	15:N:50:ARG:NH1	2.38	0.56
1:X:1353:A:H2'	1:X:1354:G:C8	2.41	0.56
1:X:1424:A:H2'	1:X:1425:G:H8	1.69	0.56
1:X:327:G:O2'	1:X:328:G:H8	1.89	0.56
1:X:1835:U:H2'	1:X:1836:A:H5''	1.86	0.56
1:X:183:A:H5'	1:X:481:C:H1'	1.86	0.56
5:C:111:ARG:O	5:C:115:SER:OG	2.20	0.56
7:E:23:HIS:HA	7:E:28:GLY:HA3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1281:U:H2'	1:X:1282:A:H8	1.71	0.56
1:X:684:U:H2'	1:X:685:C:C6	2.40	0.56
3:A:116:VAL:HG13	3:A:127:GLY:HA3	1.88	0.56
8:G:18:VAL:HG23	8:G:138:PRO:HB2	1.87	0.56
1:X:1352:C:H2'	1:X:1353:A:C8	2.41	0.56
1:X:1450:A:H5''	1:X:1451:U:H5	1.70	0.56
1:X:1637:A:O2'	1:X:1638:G:O4'	2.23	0.56
1:X:2007:G:O2'	1:X:2009:U:OP2	2.23	0.56
1:X:2060:A:O2'	1:X:2062:G:OP2	2.19	0.56
1:X:622:A:H62	29:X:3011:MPD:H52	1.69	0.56
4:B:95:ASP:O	4:B:97:ASP:N	2.39	0.56
10:I:28:GLY:H	10:I:30:THR:H	1.52	0.56
1:X:501:C:H3'	1:X:502:C:C5'	2.35	0.56
1:X:1016:G:H3'	1:X:1017:A:H5''	1.87	0.56
1:X:38:A:H2'	1:X:39:C:O4'	2.06	0.56
5:C:136:THR:HG22	5:C:140:LYS:NZ	2.20	0.56
12:K:18:ARG:NE	12:K:65:THR:O	2.38	0.56
1:X:2358:G:H4'	21:T:51:THR:H	1.71	0.56
1:X:1065:A:H3'	1:X:1065:A:H8	1.70	0.56
1:X:1813:A:H1'	1:X:1965:A:N6	2.20	0.56
1:X:2887:G:O2'	1:X:2888:A:OP2	2.22	0.56
1:X:501:C:N3	1:X:519:G:H5'	2.21	0.56
1:X:955:A:C4	11:J:15:PRO:HG3	2.41	0.56
24:W:4:LEU:HB3	24:W:58:GLU:HB2	1.87	0.56
1:X:731:U:O5'	26:2:12:LYS:NZ	2.36	0.56
14:M:106:ARG:HA	14:M:106:ARG:CZ	2.36	0.55
1:X:1466:G:H3'	1:X:1467:G:H5''	1.87	0.55
11:J:22:LYS:HD3	11:J:101:ARG:HB2	1.88	0.55
18:Q:64:ARG:HA	18:Q:69:GLN:HA	1.88	0.55
1:X:1359:A:N1	1:X:1370:C:O2'	2.37	0.55
2:Y:36:C:H2'	2:Y:37:A:H8	1.71	0.55
16:O:78:ARG:O	16:O:80:LYS:N	2.39	0.55
14:M:106:ARG:HA	14:M:106:ARG:NE	2.21	0.55
1:X:1515:G:N2	1:X:1565:U:O2	2.35	0.55
6:D:132:VAL:HG22	6:D:133:LYS:H	1.70	0.55
1:X:1281:U:H2'	1:X:1282:A:C8	2.42	0.55
8:G:76:TYR:HB3	8:G:85:ILE:HD11	1.89	0.55
5:C:114:LEU:HG	5:C:181:LEU:HD11	1.89	0.55
11:J:39:THR:HG23	11:J:98:LYS:HA	1.88	0.55
24:W:4:LEU:HA	24:W:58:GLU:HG3	1.89	0.55
1:X:1280:U:H2'	1:X:1281:U:C6	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1825:U:H3	1:X:1848:A:H61	1.55	0.55
1:X:322:A:H2'	1:X:323:C:H5'	1.89	0.55
1:X:422:G:H2'	1:X:423:A:C8	2.42	0.55
1:X:916:U:H5'	11:J:7:VAL:HG12	1.89	0.55
5:C:158:ASN:HA	5:C:161:VAL:HG22	1.89	0.55
1:X:2599:A:N7	4:B:158:SER:HB3	2.22	0.55
15:N:94:MET:O	15:N:98:ILE:HG12	2.07	0.55
1:X:2725:U:H2'	1:X:2726:C:C6	2.42	0.55
1:X:1492:G:N2	1:X:1508:C:C4	2.75	0.55
1:X:153:G:C6	1:X:177:G:C6	2.95	0.55
1:X:658:A:H3'	1:X:659:A:C5'	2.37	0.55
4:B:132:LYS:HG2	4:B:173:MET:HE1	1.88	0.54
1:X:706:U:H1'	10:I:13:ARG:HA	1.89	0.54
11:J:14:ARG:HD2	11:J:73:PRO:HD2	1.89	0.54
12:K:50:LEU:HD22	12:K:58:SER:HB2	1.89	0.54
1:X:1806:U:H5	1:X:1811:A:N7	2.05	0.54
1:X:333:C:H42	1:X:393:G:H1	1.55	0.54
1:X:2446:U:H2'	1:X:2447:C:C6	2.43	0.54
1:X:245:G:O2'	1:X:257:G:O6	2.17	0.54
1:X:680:C:O2'	1:X:684:U:OP1	2.24	0.54
10:I:21:ARG:HG2	10:I:21:ARG:HH11	1.73	0.54
15:N:105:ALA:HB1	16:O:40:PHE:HZ	1.70	0.54
1:X:1340:G:P	29:X:3005:MPD:H32	2.48	0.54
1:X:226:A:O2'	1:X:466:C:O2	2.25	0.54
1:X:1544:G:O2'	3:A:99:GLY:O	2.18	0.54
7:E:95:ARG:HA	7:E:104:ILE:HA	1.88	0.54
14:M:78:LEU:HB3	14:M:79:HIS:HD2	1.72	0.54
16:O:14:VAL:HG12	16:O:20:ILE:HG21	1.90	0.54
17:P:30:ALA:HA	17:P:33:ILE:HD12	1.89	0.54
1:X:2749:G:H2'	1:X:2750:C:H6	1.72	0.54
1:X:2811:U:H2'	1:X:2812:U:H6	1.72	0.54
1:X:690:U:H4'	1:X:691:A:OP2	2.07	0.54
15:N:83:LEU:HD23	15:N:113:ALA:HB2	1.90	0.54
1:X:1523:G:H1	1:X:1557:C:N4	2.05	0.54
5:C:10:ASP:N	5:C:10:ASP:OD1	2.41	0.54
7:E:102:ASP:N	7:E:115:ILE:HD13	2.23	0.54
1:X:1875:A:H2'	1:X:1876:G:O4'	2.08	0.54
11:J:43:THR:HG22	11:J:46:GLN:CD	2.28	0.54
1:X:37:C:H2'	1:X:38:A:H8	1.70	0.54
1:X:718:C:H5''	5:C:81:PRO:HD2	1.89	0.54
1:X:1242:A:H4'	10:I:3:LEU:HD23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:86:VAL:O	19:R:90:LYS:HB2	2.08	0.54
1:X:100:U:H3'	1:X:101:G:H5'	1.90	0.54
1:X:1340:G:OP1	29:X:3005:MPD:O4	2.19	0.54
1:X:1514:A:H2'	1:X:1515:G:H5'	1.90	0.54
1:X:1644:C:P	18:Q:76:ARG:HH22	2.30	0.54
1:X:1410:A:H2'	1:X:1411:G:O4'	2.07	0.54
2:Y:91:C:H2'	2:Y:92:G:H8	1.71	0.54
1:X:1347:G:OP2	26:2:10:LYS:HE2	2.08	0.54
9:H:1:MET:N	9:H:67:SER:OG	2.40	0.54
1:X:1213:C:H42	1:X:1219:G:H1	1.56	0.54
1:X:2507:C:C2'	1:X:2508:G:H5'	2.38	0.54
3:A:88:SER:HB2	3:A:158:ALA:HB2	1.90	0.53
18:Q:5:ASP:OD1	18:Q:5:ASP:N	2.41	0.53
1:X:2081:A:C2	1:X:2643:C:N3	2.76	0.53
1:X:629:A:H62	1:X:1289:A:H2	1.55	0.53
7:E:89:LEU:HD11	7:E:94:TYR:HA	1.90	0.53
1:X:2268:A:H2'	1:X:2269:G:C8	2.43	0.53
1:X:1391:A:H2'	1:X:1392:G:O4'	2.08	0.53
1:X:1514:A:N6	1:X:1566:G:H22	2.06	0.53
1:X:2241:C:H2'	1:X:2242:G:O4'	2.09	0.53
1:X:2784:A:N1	7:E:67:THR:HG21	2.23	0.53
1:X:379:C:C2	1:X:380:U:C5	2.96	0.53
1:X:460:C:H2'	1:X:461:A:C8	2.42	0.53
1:X:1888:U:O4	1:X:1910:G:N2	2.42	0.53
1:X:1097:U:O4	1:X:1098:A:N6	2.42	0.53
1:X:329:A:N6	1:X:398:C:H42	2.06	0.53
1:X:712:U:H2'	1:X:713:A:O4'	2.09	0.53
2:Y:91:C:H2'	2:Y:92:G:C8	2.42	0.53
1:X:257:G:N7	27:3:5:LYS:HE3	2.24	0.53
28:4:24:MET:HG3	28:4:34:GLN:O	2.08	0.53
3:A:142:HIS:N	3:A:191:THR:O	2.40	0.53
1:X:1290:G:OP2	15:N:13:ARG:NH2	2.41	0.53
11:J:59:LYS:O	11:J:61:GLY:N	2.42	0.53
12:K:23:SER:O	12:K:25:ILE:N	2.40	0.53
1:X:1091:G:H2'	1:X:1154:G:H1	1.74	0.53
1:X:1395:G:C6	1:X:1408:G:N7	2.77	0.53
1:X:1540:U:H1'	1:X:1625:U:H4'	1.90	0.53
1:X:1630:A:H2'	1:X:1631:G:H5'	1.91	0.53
1:X:2255:G:H2'	1:X:2256:U:H6	1.72	0.53
4:B:125:LYS:HB2	4:B:173:MET:HB3	1.89	0.53
20:S:75:ALA:HB2	20:S:92:LEU:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2120:G:H21	1:X:2225:A:N6	2.07	0.53
1:X:946:A:H2'	1:X:947:U:H5'	1.91	0.53
1:X:1072:A:N6	1:X:1169:G:H2'	2.24	0.53
1:X:1460:U:H3	1:X:1628:A:N6	2.07	0.53
1:X:2774:G:O2'	7:E:67:THR:HG22	2.09	0.53
1:X:1313:G:OP2	1:X:1689:G:O2'	2.20	0.53
1:X:1501:G:N2	1:X:2729:G:H22	2.03	0.53
1:X:1186:A:C4	1:X:1188:A:C8	2.97	0.52
1:X:55:G:H2'	1:X:56:A:H8	1.72	0.52
1:X:587:C:O2'	1:X:588:G:H5'	2.09	0.52
1:X:774:G:H5'	1:X:775:A:H5''	1.91	0.52
1:X:233:U:O2'	1:X:234:C:H5'	2.10	0.52
1:X:2725:U:H2'	1:X:2726:C:H6	1.74	0.52
1:X:2385:A:N1	10:I:50:PHE:HZ	2.08	0.52
1:X:154:A:O2'	1:X:155:U:H5''	2.09	0.52
1:X:2294:A:H5''	1:X:2295:A:H5'	1.90	0.52
1:X:955:A:C6	11:J:15:PRO:HD3	2.45	0.52
1:X:2047:A:H5'	25:Z:9:SER:HB3	1.91	0.52
24:W:4:LEU:HD13	24:W:6:ILE:HD11	1.92	0.52
1:X:179:A:OP2	1:X:179:A:H8	1.91	0.52
2:Y:65:G:O6	2:Y:105:G:N2	2.33	0.52
9:H:120:GLU:N	9:H:120:GLU:OE1	2.43	0.52
19:R:56:ILE:HB	19:R:58:GLU:HG2	1.91	0.52
1:X:2646:U:OP1	4:B:165:LYS:NZ	2.30	0.52
1:X:339:A:H2'	1:X:340:C:C6	2.45	0.52
1:X:79:U:HO2'	1:X:389:A:H8	1.57	0.52
1:X:1013:U:O3'	24:W:14:GLY:HA2	2.09	0.52
1:X:897:A:H2'	1:X:898:U:H6	1.75	0.52
3:A:142:HIS:CE1	3:A:143:ASN:HB2	2.44	0.52
10:I:78:ASN:ND2	10:I:106:LYS:O	2.43	0.52
15:N:26:GLY:O	15:N:29:HIS:ND1	2.43	0.52
1:X:489:A:N3	1:X:1240:U:H1'	2.23	0.52
1:X:1472:C:O2'	1:X:1616:A:OP2	2.24	0.52
1:X:2314:A:H2	1:X:2373:A:H62	1.58	0.52
3:A:132:LEU:H	3:A:134:ASN:H	1.58	0.52
1:X:142:G:N2	1:X:1640:U:O3'	2.38	0.52
1:X:1864:C:O2'	1:X:1955:A:N3	2.38	0.52
1:X:632:U:H2'	1:X:633:A:C8	2.45	0.52
22:U:10:ARG:NH1	22:U:11:LYS:O	2.43	0.52
1:X:1053:A:N3	1:X:1197:C:O2'	2.41	0.52
7:E:136:ILE:HG13	7:E:137:SER:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:11:ARG:HA	17:P:100:THR:HG22	1.92	0.51
1:X:83:G:N2	1:X:102:A:H2	2.06	0.51
1:X:2694:C:N3	7:E:110:SER:OG	2.43	0.51
11:J:44:SER:HB3	11:J:70:PRO:HG3	1.92	0.51
1:X:2895:G:N2	14:M:1:MET:HA	2.25	0.51
15:N:61:TRP:CD2	15:N:93:LYS:HB2	2.45	0.51
24:W:40:ASN:HB2	24:W:43:ILE:H	1.75	0.51
1:X:1767:G:HO2'	1:X:1768:C:H6	1.57	0.51
24:W:50:VAL:HB	24:W:53:LEU:CD1	2.41	0.51
1:X:1460:U:H3	1:X:1628:A:H61	1.56	0.51
1:X:1651:C:OP1	29:X:3005:MPD:O2	2.22	0.51
1:X:2459:A:H2'	1:X:2460:A:C8	2.46	0.51
1:X:947:U:H2'	1:X:948:U:C6	2.45	0.51
12:K:105:LYS:HA	12:K:117:VAL:HG12	1.92	0.51
1:X:874:A:N7	1:X:2274:A:O2'	2.43	0.51
17:P:20:VAL:HG21	17:P:43:SER:HB2	1.93	0.51
1:X:1039:C:O2'	15:N:93:LYS:NZ	2.44	0.51
1:X:1575:A:H2'	1:X:1576:A:C5'	2.40	0.51
1:X:2759:G:H3'	1:X:2760:A:O4'	2.10	0.51
1:X:2783:U:H3'	28:4:19:ARG:O	2.10	0.51
28:4:19:ARG:HG3	28:4:24:MET:SD	2.51	0.51
8:G:32:GLU:O	8:G:36:ILE:HG12	2.11	0.51
8:G:7:ALA:H	8:G:46:THR:HG21	1.76	0.51
19:R:24:ILE:O	19:R:34:VAL:HB	2.10	0.51
1:X:1185:U:H2'	8:G:66:THR:HG21	1.92	0.51
1:X:1452:C:O2	1:X:1631:G:N2	2.43	0.51
1:X:1599:G:OP1	1:X:1761:G:N2	2.44	0.51
1:X:637:U:H2'	1:X:638:U:H6	1.74	0.51
1:X:1329:G:H2'	1:X:1330:U:C6	2.45	0.51
1:X:1700:C:H2'	1:X:1701:U:C6	2.46	0.51
6:D:23:SER:N	6:D:27:GLU:OE1	2.43	0.51
1:X:1094:A:C2	1:X:2778:G:C5	2.98	0.51
1:X:124:A:C6	26:2:11:ARG:HD3	2.46	0.51
1:X:581:A:H5'	15:N:53:ARG:HD3	1.93	0.51
14:M:51:LYS:HD2	14:M:53:ARG:HG2	1.93	0.51
1:X:1796:A:O2'	1:X:1985:C:OP1	2.24	0.51
1:X:2286:G:C6	1:X:2287:C:C4	2.99	0.51
1:X:2534:C:C2	1:X:2535:G:C8	2.99	0.51
1:X:658:A:H3'	1:X:659:A:H5''	1.92	0.51
5:C:59:GLY:HA3	5:C:79:ARG:HG3	1.94	0.50
1:X:2425:U:H2'	1:X:2426:G:C8	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2732:A:H2'	1:X:2733:A:O4'	2.10	0.50
1:X:2895:G:H21	14:M:1:MET:HA	1.76	0.50
1:X:650:U:H3	1:X:666:A:H2	1.59	0.50
1:X:704:U:H2'	1:X:705:U:O4'	2.11	0.50
2:Y:87:G:N1	11:J:39:THR:O	2.45	0.50
5:C:179:GLN:O	5:C:183:VAL:HG12	2.11	0.50
1:X:2856:U:H2'	1:X:2857:A:H8	1.76	0.50
1:X:1833:C:H2'	1:X:1834:G:H8	1.77	0.50
1:X:793:G:C8	17:P:89:ALA:HB1	2.47	0.50
11:J:10:ARG:O	11:J:11:ARG:HG3	2.10	0.50
1:X:1197:C:H2'	1:X:1198:G:O4'	2.11	0.50
1:X:1867:G:C8	1:X:1954:A:C2	2.99	0.50
1:X:2037:G:OP2	17:P:41:LYS:NZ	2.33	0.50
1:X:1303:A:H8	1:X:1303:A:OP1	1.95	0.50
1:X:1561:G:H8	1:X:1562:C:C6	2.29	0.50
1:X:1846:A:H4'	1:X:1847:U:H5''	1.92	0.50
1:X:2473:G:H2'	1:X:2474:G:H5''	1.92	0.50
1:X:2549:U:O2'	1:X:2674:U:OP1	2.15	0.50
1:X:407:G:H2'	1:X:408:U:C6	2.46	0.50
28:4:2:LYS:HG2	28:4:4:ARG:HD2	1.93	0.50
1:X:2602:C:H5'	4:B:157:ALA:HB2	1.94	0.50
8:G:57:VAL:HB	8:G:125:VAL:HG13	1.94	0.50
14:M:102:LEU:O	14:M:103:ARG:CZ	2.60	0.50
1:X:2869:G:OP1	14:M:95:ARG:NH1	2.45	0.50
12:K:109:ARG:NH1	12:K:112:ASP:OD2	2.45	0.50
1:X:1423:C:H2'	1:X:1424:A:C8	2.47	0.50
1:X:1450:A:N6	1:X:1635:A:H62	2.09	0.50
1:X:157:U:H2'	1:X:158:G:H8	1.77	0.50
1:X:450:C:H4'	1:X:451:U:H5'	1.94	0.50
1:X:679:G:H2'	1:X:680:C:C6	2.46	0.50
1:X:841:C:H2'	1:X:842:U:C6	2.46	0.50
10:I:21:ARG:CG	10:I:21:ARG:HH11	2.24	0.50
18:Q:17:SER:HA	18:Q:20:MET:HE2	1.93	0.50
1:X:168:A:H2	1:X:169:G:C2	2.29	0.50
1:X:2903:A:C5'	1:X:2904:U:H5'	2.42	0.50
7:E:87:LEU:HD23	7:E:164:TYR:HA	1.94	0.50
8:G:5:PHE:O	15:N:64:ARG:NH2	2.45	0.50
1:X:1023:A:H2'	1:X:1026:C:H42	1.75	0.50
1:X:788:A:O2'	1:X:1703:U:OP1	2.26	0.50
1:X:1817:C:H2'	1:X:1818:A:C5	2.47	0.50
1:X:381:G:N2	1:X:382:U:H1'	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:719:G:O2'	5:C:74:ARG:HG3	2.12	0.50
26:2:16:VAL:H	26:2:21:LYS:HG3	1.76	0.49
1:X:1775:G:H2'	1:X:1776:A:C8	2.47	0.49
1:X:1229:G:OP1	10:I:31:SER:HA	2.13	0.49
1:X:1382:C:N4	1:X:1383:G:O6	2.45	0.49
1:X:620:G:H2'	1:X:621:A:C8	2.47	0.49
1:X:665:G:H4'	1:X:666:A:C5'	2.41	0.49
1:X:89:U:H3	1:X:90:A:H62	1.57	0.49
5:C:29:ASN:HB3	5:C:108:LEU:HD11	1.94	0.49
10:I:60:ARG:HB3	10:I:60:ARG:CZ	2.43	0.49
14:M:16:ARG:HH12	14:M:83:ILE:HG22	1.77	0.49
1:X:1091:G:O2'	1:X:1092:A:O5'	2.25	0.49
1:X:1379:A:O2'	1:X:1381:U:OP2	2.19	0.49
1:X:2770:U:OP1	28:4:33:LYS:NZ	2.44	0.49
1:X:319:G:N3	1:X:319:G:H2'	2.27	0.49
1:X:396:G:H2'	1:X:397:U:H5'	1.94	0.49
4:B:133:ARG:NH1	4:B:172:ARG:O	2.45	0.49
1:X:677:A:H2'	1:X:678:A:C8	2.46	0.49
1:X:734:A:H2'	1:X:735:C:C6	2.48	0.49
4:B:142:SER:HG	4:B:143:HIS:HD1	1.60	0.49
7:E:106:ASN:O	7:E:108:GLY:N	2.45	0.49
1:X:850:G:O4'	10:I:36:LYS:HE3	2.12	0.49
12:K:110:ARG:HG3	12:K:111:GLY:N	2.28	0.49
15:N:59:LYS:O	15:N:63:THR:HG23	2.12	0.49
19:R:64:HIS:O	19:R:66:SER:N	2.46	0.49
1:X:1065:A:H62	1:X:1185:U:H3	1.60	0.49
1:X:2255:G:H2'	1:X:2256:U:C6	2.47	0.49
1:X:272:C:H42	1:X:416:G:H1	1.60	0.49
1:X:627:C:OP2	29:X:3007:MPD:H4	2.13	0.49
1:X:1315:C:H2'	1:X:1316:G:H8	1.77	0.49
1:X:1487:G:O6	1:X:1596:G:N1	2.46	0.49
1:X:1700:C:H2'	1:X:1701:U:H6	1.76	0.49
1:X:327:G:O2'	1:X:328:G:O5'	2.31	0.49
4:B:163:VAL:HG13	4:B:167:GLN:HG3	1.94	0.49
5:C:7:LEU:HD21	5:C:126:VAL:N	2.21	0.49
17:P:69:LEU:HD22	17:P:107:VAL:HG12	1.95	0.49
1:X:378:C:H2'	1:X:379:C:H6	1.76	0.49
8:G:5:PHE:HD2	15:N:100:ILE:HD13	1.76	0.49
12:K:28:GLU:HG3	12:K:121:LEU:HD11	1.95	0.49
14:M:24:PRO:HA	14:M:49:VAL:HG12	1.94	0.49
17:P:11:ARG:O	17:P:11:ARG:NE	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2372:G:H1'	1:X:2409:G:H5'	1.94	0.49
25:Z:28:THR:HG23	25:Z:37:TYR:CD1	2.47	0.49
9:H:44:LYS:O	9:H:54:LYS:HE2	2.12	0.49
17:P:13:ALA:HB1	17:P:14:PRO:HD2	1.95	0.49
1:X:1381:U:O2'	1:X:1421:A:H2'	2.11	0.49
1:X:1867:G:C2	1:X:1868:U:C2	3.00	0.49
1:X:2774:G:O6	1:X:2782:C:H5''	2.13	0.49
1:X:379:C:H2'	1:X:380:U:C6	2.48	0.49
2:Y:57:G:H3'	2:Y:58:G:H8	1.78	0.49
1:X:2079:G:O2'	4:B:160:ALA:O	2.29	0.49
1:X:630:G:P	10:I:21:ARG:HH22	2.35	0.49
1:X:1494:G:C8	1:X:1495:C:H5	2.31	0.49
1:X:1806:U:C5	1:X:1811:A:N7	2.80	0.49
1:X:2377:C:H2'	1:X:2378:G:O4'	2.12	0.49
1:X:2543:G:C4	1:X:2596:G:N2	2.81	0.49
1:X:352:A:H5'	19:R:15:LYS:HG3	1.94	0.49
1:X:805:G:H4'	1:X:1803:G:OP1	2.13	0.48
1:X:2332:U:H2'	1:X:2333:U:H5'	1.95	0.48
1:X:274:A:N3	1:X:414:C:O2'	2.45	0.48
1:X:615:A:H5''	1:X:616:G:OP2	2.13	0.48
1:X:828:A:H2'	1:X:828:A:N3	2.27	0.48
12:K:55:ASP:OD1	12:K:55:ASP:N	2.45	0.48
1:X:1331:C:O2'	12:K:67:ARG:HG3	2.13	0.48
15:N:98:ILE:HD11	16:O:4:ILE:HD11	1.93	0.48
1:X:1698:A:H1'	1:X:2843:A:H5'	1.94	0.48
2:Y:86:C:H3'	2:Y:86:C:O2	2.13	0.48
3:A:43:ARG:HD3	3:A:49:LEU:HA	1.96	0.48
4:B:116:ILE:HG12	4:B:183:LEU:O	2.14	0.48
19:R:8:ASN:HA	19:R:22:LYS:HG2	1.96	0.48
1:X:12:U:H2'	1:X:12:U:O2	2.13	0.48
1:X:1818:A:H4'	3:A:205:VAL:HB	1.94	0.48
1:X:1886:A:H3'	1:X:1887:G:H8	1.77	0.48
1:X:460:C:H1'	1:X:1891:U:O2'	2.12	0.48
1:X:2101:U:H2'	1:X:2102:U:C6	2.49	0.48
1:X:2788:A:H2'	1:X:2789:U:C6	2.48	0.48
1:X:379:C:H2'	1:X:380:U:H6	1.79	0.48
1:X:674:C:N4	1:X:675:G:O6	2.46	0.48
1:X:79:U:C2'	1:X:389:A:H8	2.25	0.48
1:X:810:A:H2'	1:X:811:C:C6	2.48	0.48
11:J:22:LYS:HD2	11:J:98:LYS:HB2	1.95	0.48
16:O:18:GLN:O	16:O:97:ILE:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1400:C:O2'	1:X:1836:A:H1'	2.14	0.48
1:X:1491:C:C2	1:X:1492:G:C2	3.01	0.48
1:X:548:A:H4'	1:X:549:U:H5''	1.94	0.48
5:C:123:LEU:O	5:C:188:ASN:HA	2.13	0.48
17:P:40:ASN:O	17:P:41:LYS:HD2	2.12	0.48
1:X:1091:G:H2'	1:X:1154:G:N1	2.28	0.48
1:X:1492:G:N3	1:X:1593:G:N2	2.62	0.48
1:X:1521:A:O2'	1:X:1522:G:OP1	2.30	0.48
1:X:2717:A:H5''	12:K:4:ARG:HH21	1.79	0.48
1:X:424:C:N4	1:X:425:G:O6	2.46	0.48
1:X:685:C:H2'	1:X:686:U:C6	2.48	0.48
1:X:897:A:H2'	1:X:898:U:C6	2.47	0.48
13:L:30:ARG:N	13:L:45:ILE:O	2.46	0.48
17:P:36:LEU:HD13	17:P:48:GLU:HA	1.95	0.48
22:U:29:TRP:CG	22:U:30:ASN:N	2.76	0.48
1:X:2494:C:H2'	1:X:2495:A:O4'	2.14	0.48
1:X:32:C:O2'	1:X:33:U:H5'	2.13	0.48
4:B:189:ASP:OD1	4:B:192:ASN:N	2.38	0.48
8:G:12:ILE:HD11	8:G:51:THR:HA	1.96	0.48
12:K:32:THR:HG22	12:K:33:THR:N	2.29	0.48
1:X:526:A:H4'	19:R:42:LYS:HB2	1.96	0.48
1:X:1295:C:H4'	5:C:83:TRP:CE3	2.48	0.48
1:X:1510:U:H2'	1:X:1511:C:C6	2.48	0.48
1:X:1833:C:H2'	1:X:1834:G:C8	2.49	0.48
1:X:2382:C:C4	1:X:2383:C:C4	3.01	0.48
2:Y:90:C:H2'	2:Y:91:C:C6	2.49	0.48
10:I:19:VAL:HG22	10:I:27:ASN:HB3	1.96	0.48
10:I:95:LEU:HD12	10:I:96:LEU:N	2.29	0.48
1:X:1059:A:H2'	1:X:1060:U:C6	2.49	0.48
1:X:1218:G:H2'	1:X:1219:G:C8	2.49	0.48
1:X:1922:C:H2'	1:X:1923:A:H8	1.77	0.48
20:S:155:THR:HG22	20:S:159:VAL:HG13	1.95	0.48
23:V:63:GLU:HA	23:V:66:LYS:HG3	1.94	0.48
24:W:6:ILE:CD1	24:W:56:VAL:HG12	2.44	0.48
1:X:1819:G:O2'	1:X:1857:C:OP1	2.24	0.48
4:B:154:VAL:HG21	4:B:169:MET:HE3	1.96	0.48
4:B:205:LYS:O	4:B:207:GLY:N	2.46	0.48
8:G:69:LYS:HG2	8:G:73:LYS:HB2	1.96	0.48
1:X:1494:G:HO2'	1:X:1495:C:C5'	2.26	0.48
1:X:1574:G:H2'	1:X:1575:A:O4'	2.14	0.48
1:X:1710:G:O3'	9:H:6:THR:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:280:C:H2'	1:X:281:A:C8	2.44	0.48
2:Y:6:U:H3	2:Y:109:C:H42	1.61	0.48
2:Y:49:G:C6	2:Y:50:A:C6	3.02	0.48
25:Z:15:LYS:O	25:Z:18:THR:HG23	2.14	0.48
5:C:8:LYS:HA	5:C:14:SER:H	1.79	0.47
11:J:22:LYS:HE2	11:J:101:ARG:CZ	2.44	0.47
1:X:626:G:N2	1:X:1296:C:C2	2.82	0.47
1:X:1302:G:OP1	25:Z:16:ARG:NH2	2.37	0.47
1:X:1609:U:H2'	1:X:1610:G:C8	2.49	0.47
1:X:302:A:HO2'	1:X:303:G:H8	1.62	0.47
1:X:575:G:N3	1:X:575:G:H2'	2.29	0.47
1:X:680:C:H2'	1:X:681:G:O4'	2.14	0.47
11:J:22:LYS:HG2	11:J:101:ARG:HB2	1.96	0.47
20:S:55:VAL:HB	20:S:59:GLY:HA3	1.96	0.47
1:X:1013:U:H2'	1:X:1014:U:C6	2.49	0.47
1:X:1521:A:HO2'	1:X:1522:G:P	2.36	0.47
1:X:1694:A:O3'	12:K:33:THR:HG21	2.14	0.47
1:X:2311:U:H1'	1:X:2352:G:N2	2.28	0.47
1:X:2632:U:H2'	1:X:2633:C:C6	2.49	0.47
1:X:2811:U:H2'	1:X:2812:U:C6	2.49	0.47
4:B:53:PHE:CG	4:B:54:GLU:N	2.81	0.47
7:E:75:MET:O	7:E:79:VAL:HB	2.15	0.47
13:L:95:ASP:O	13:L:97:GLY:N	2.47	0.47
14:M:54:GLY:HA3	14:M:59:GLU:HA	1.96	0.47
21:T:20:ASN:OD1	21:T:21:GLY:N	2.47	0.47
1:X:1346:G:H4'	26:2:8:PRO:HG2	1.97	0.47
1:X:1869:G:H2'	1:X:1870:C:C6	2.50	0.47
1:X:1985:C:H2'	1:X:1986:G:H8	1.78	0.47
4:B:14:GLN:NE2	4:B:22:LEU:HD21	2.30	0.47
7:E:103:LEU:H	7:E:115:ILE:HD11	1.79	0.47
1:X:1183:G:H5'	8:G:105:SER:OG	2.15	0.47
17:P:6:VAL:HG22	17:P:104:THR:HG23	1.95	0.47
1:X:1151:G:H2'	1:X:1152:U:C6	2.49	0.47
1:X:24:G:H2'	1:X:25:U:H6	1.80	0.47
1:X:250:G:H4'	1:X:432:G:C4	2.49	0.47
1:X:2903:A:H5''	1:X:2904:U:H5'	1.96	0.47
17:P:9:THR:HG22	17:P:80:PRO:HD2	1.95	0.47
20:S:105:PRO:HD2	20:S:123:GLN:O	2.15	0.47
1:X:51:G:H1'	1:X:117:A:H61	1.78	0.47
1:X:1182:G:H2'	1:X:1183:G:O4'	2.14	0.47
1:X:136:A:H61	1:X:143:U:H3	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:187:C:H2'	1:X:188:C:C6	2.50	0.47
1:X:1973:U:H2'	1:X:1974:C:C6	2.49	0.47
1:X:2111:C:H2'	1:X:2112:C:H6	1.78	0.47
1:X:870:C:H4'	1:X:2455:G:N7	2.28	0.47
1:X:719:G:O2'	5:C:67:GLN:OE1	2.29	0.47
7:E:45:GLN:OE1	7:E:45:GLN:N	2.48	0.47
17:P:24:ILE:HD11	17:P:36:LEU:HG	1.96	0.47
1:X:1818:A:N6	1:X:1855:G:O2'	2.47	0.47
1:X:2122:A:H2'	1:X:2123:A:C8	2.50	0.47
1:X:605:U:O2	1:X:615:A:H1'	2.15	0.47
1:X:638:U:H2'	1:X:639:U:C6	2.48	0.47
1:X:813:G:H2'	1:X:814:A:C8	2.50	0.47
14:M:78:LEU:HB3	14:M:79:HIS:CD2	2.50	0.47
1:X:1651:C:H5''	1:X:1652:A:H5'	1.96	0.47
1:X:2334:G:O2'	1:X:2337:A:N6	2.30	0.47
1:X:70:G:N2	1:X:71:A:N1	2.63	0.47
1:X:71:A:H4'	1:X:72:U:H5''	1.95	0.47
1:X:769:U:H2'	1:X:770:G:O4'	2.14	0.47
2:Y:21:G:N1	2:Y:22:G:O6	2.48	0.47
12:K:51:GLY:HA2	12:K:86:PHE:CZ	2.49	0.47
1:X:1353:A:H2'	1:X:1354:G:H8	1.79	0.47
1:X:1376:G:OP1	18:Q:13:THR:HG21	2.14	0.47
1:X:2905:C:N4	25:Z:39:LEU:HG	2.29	0.47
1:X:1815:C:H5''	3:A:224:VAL:HG11	1.97	0.47
14:M:102:LEU:HA	14:M:102:LEU:HD13	1.54	0.47
14:M:29:ARG:HH11	14:M:89:LYS:NZ	2.13	0.47
1:X:1373:U:H2'	1:X:1374:G:C8	2.50	0.47
1:X:183:A:OP2	1:X:183:A:H3'	2.15	0.47
1:X:1931:G:H1	1:X:1957:G:N2	2.12	0.47
1:X:2425:U:H2'	1:X:2426:G:H8	1.80	0.47
1:X:510:U:H5'	26:2:6:TYR:CD1	2.49	0.47
1:X:5:A:H2'	1:X:6:A:C8	2.50	0.47
6:D:13:THR:O	6:D:17:MET:HB2	2.15	0.47
10:I:60:ARG:HB3	10:I:60:ARG:NH1	2.30	0.47
1:X:1279:C:H2'	1:X:1280:U:H6	1.79	0.47
1:X:2438:A:H2'	1:X:2439:A:C8	2.50	0.47
10:I:96:LEU:HB2	10:I:113:GLY:O	2.15	0.47
1:X:1448:U:H3'	1:X:1449:A:C5'	2.41	0.47
1:X:1487:G:C6	1:X:1596:G:N1	2.83	0.47
1:X:1793:C:H2'	1:X:1794:C:H6	1.80	0.47
1:X:1854:U:H2'	1:X:1855:G:O4'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1893:A:N6	1:X:1902:G:O2'	2.48	0.47
1:X:353:A:O2'	1:X:354:A:H2'	2.15	0.47
1:X:811:C:N4	1:X:812:U:O4	2.48	0.47
17:P:14:PRO:O	17:P:18:ARG:HG3	2.15	0.46
19:R:26:THR:HA	19:R:33:VAL:HA	1.97	0.46
1:X:2817:A:HO2'	1:X:2818:A:P	2.36	0.46
1:X:682:A:H4'	1:X:683:G:H5'	1.96	0.46
1:X:2782:C:H3'	28:4:19:ARG:NH2	2.30	0.46
24:W:51:LYS:NZ	24:W:56:VAL:H	2.13	0.46
1:X:1437:U:H2'	1:X:1438:G:O4'	2.16	0.46
1:X:1468:G:H2'	1:X:1469:G:O4'	2.16	0.46
1:X:2093:C:C2'	1:X:2094:G:H5'	2.46	0.46
1:X:24:G:H2'	1:X:25:U:C6	2.51	0.46
1:X:2881:C:H2'	1:X:2882:A:H8	1.80	0.46
1:X:494:U:H1'	5:C:84:ARG:HG3	1.97	0.46
4:B:9:LYS:O	4:B:28:VAL:HA	2.15	0.46
5:C:104:LYS:HE2	5:C:104:LYS:HB3	1.61	0.46
17:P:5:ALA:HB3	17:P:54:ALA:HB2	1.97	0.46
24:W:15:ARG:HD2	24:W:53:LEU:HD23	1.96	0.46
1:X:1053:A:H5''	15:N:63:THR:HG22	1.97	0.46
1:X:1352:C:H42	1:X:1374:G:H1	1.62	0.46
1:X:140:A:O2'	1:X:1446:U:H5'	2.15	0.46
4:B:7:GLY:HA2	4:B:53:PHE:CZ	2.50	0.46
5:C:113:ALA:HB3	5:C:181:LEU:HD13	1.97	0.46
6:D:101:ASP:HA	6:D:130:LEU:HD11	1.98	0.46
16:O:2:PHE:CE1	16:O:42:GLY:HA3	2.51	0.46
11:J:37:THR:HG22	20:S:82:LEU:HD23	1.98	0.46
1:X:1268:C:H2'	1:X:1269:A:C8	2.51	0.46
1:X:1611:C:H2'	1:X:1612:C:C6	2.51	0.46
1:X:2419:A:H2	1:X:2451:C:N4	2.12	0.46
1:X:566:U:H2'	1:X:567:G:N7	2.31	0.46
1:X:747:U:H3	1:X:775:A:H61	1.62	0.46
3:A:91:ILE:HB	3:A:104:ILE:O	2.16	0.46
1:X:1295:C:H5'	5:C:75:GLN:NE2	2.29	0.46
10:I:21:ARG:HG2	10:I:21:ARG:NH1	2.30	0.46
1:X:2111:C:H2'	1:X:2112:C:C6	2.50	0.46
1:X:234:C:O2'	1:X:235:G:O4'	2.26	0.46
1:X:1038:C:OP2	15:N:54:LYS:NZ	2.49	0.46
17:P:86:ARG:HG3	17:P:87:PRO:CD	2.45	0.46
1:X:2349:A:H2'	1:X:2350:G:O4'	2.15	0.46
1:X:2740:A:H3'	1:X:2741:G:H5''	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:145:THR:HG21	5:C:186:ILE:HG13	1.97	0.46
17:P:7:ALA:HB1	17:P:10:ILE:HD11	1.98	0.46
1:X:1438:G:H2'	1:X:1439:U:C6	2.50	0.46
1:X:1441:C:H2'	1:X:1442:C:H6	1.80	0.46
1:X:1451:U:H2'	1:X:1452:C:C6	2.51	0.46
1:X:198:A:N6	1:X:201:C:OP2	2.46	0.46
1:X:788:A:OP1	4:B:144:GLY:HA2	2.16	0.46
1:X:906:A:H2'	1:X:907:G:O4'	2.15	0.46
1:X:2642:U:N1	25:Z:4:PRO:HA	2.30	0.46
14:M:92:GLY:HA2	14:M:110:ALA:HA	1.97	0.46
17:P:50:VAL:HG12	17:P:105:ILE:HD12	1.97	0.46
24:W:26:LEU:HB2	24:W:28:LEU:HD12	1.97	0.46
1:X:1053:A:OP2	8:G:40:LYS:NZ	2.46	0.46
1:X:1065:A:C3'	1:X:1065:A:C8	2.96	0.46
1:X:1241:A:H2'	1:X:1242:A:C8	2.49	0.46
1:X:1450:A:H5''	1:X:1451:U:C5	2.48	0.46
1:X:409:G:N2	1:X:411:A:H61	2.14	0.46
1:X:506:A:N1	1:X:515:G:H8	2.14	0.46
2:Y:94:U:H2'	2:Y:95:A:O4'	2.16	0.46
25:Z:38:LYS:H	25:Z:38:LYS:NZ	2.14	0.46
26:2:13:HIS:O	26:2:17:HIS:HB2	2.16	0.46
1:X:2077:C:H1'	4:B:169:MET:HE1	1.98	0.46
1:X:2860:U:C5'	12:K:49:THR:HG21	2.45	0.46
1:X:1003:A:N3	1:X:2484:U:O2'	2.43	0.46
1:X:2507:C:H2'	1:X:2508:G:H5'	1.98	0.46
1:X:720:A:C8	1:X:849:A:C6	3.04	0.46
28:4:27:CYS:O	28:4:29:ASN:ND2	2.47	0.46
7:E:87:LEU:HB2	7:E:131:VAL:HG23	1.98	0.46
8:G:20:ASP:OD2	8:G:22:GLU:HG2	2.15	0.46
12:K:55:ASP:O	12:K:58:SER:OG	2.26	0.46
14:M:99:LEU:HA	14:M:101:TYR:CE1	2.50	0.46
18:Q:74:LYS:HG3	18:Q:74:LYS:H	1.48	0.46
21:T:82:ARG:NH2	21:T:83:ASP:HB3	2.31	0.46
24:W:51:LYS:HZ1	24:W:55:THR:HA	1.81	0.46
1:X:997:G:N2	1:X:1008:C:O2	2.32	0.46
1:X:1034:A:N6	1:X:1225:G:H1'	2.31	0.46
1:X:2833:U:H2'	1:X:2834:C:H6	1.81	0.46
5:C:149:PRO:HD2	5:C:187:THR:HA	1.98	0.45
1:X:1289:A:H5''	15:N:13:ARG:HH12	1.80	0.45
1:X:1390:A:OP2	1:X:1414:G:N1	2.38	0.45
1:X:1476:G:H2'	1:X:1477:U:C6	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1916:A:H1'	1:X:2114:G:H5'	1.98	0.45
1:X:318:A:C6	1:X:319:G:H1'	2.51	0.45
1:X:1699:A:H1'	4:B:127:PHE:CD1	2.51	0.45
11:J:14:ARG:HD3	11:J:72:THR:HG22	1.98	0.45
14:M:4:HIS:HB2	14:M:7:ILE:HB	1.98	0.45
17:P:33:ILE:O	17:P:37:LYS:HB2	2.15	0.45
18:Q:75:ARG:HA	18:Q:75:ARG:HD3	1.71	0.45
1:X:1422:A:O2'	1:X:1423:C:O4'	2.21	0.45
1:X:1385:G:C2	1:X:1643:C:N3	2.84	0.45
1:X:181:G:H2'	1:X:182:C:O4'	2.16	0.45
1:X:628:G:N7	29:X:3007:MPD:H13	2.32	0.45
1:X:668:C:H2'	1:X:669:C:C6	2.52	0.45
25:Z:28:THR:CG2	25:Z:39:LEU:HD12	2.46	0.45
4:B:107:VAL:HG21	4:B:193:LYS:HA	1.97	0.45
10:I:128:PHE:HD2	10:I:129:SER:H	1.63	0.45
19:R:77:GLU:HA	19:R:78:PRO:HD3	1.78	0.45
1:X:170:C:H2'	1:X:171:A:C8	2.51	0.45
1:X:189:G:H2'	1:X:190:G:H8	1.80	0.45
1:X:416:G:OP2	1:X:416:G:H8	1.98	0.45
1:X:603:C:O2	15:N:48:ARG:NH1	2.49	0.45
18:Q:34:ASN:O	18:Q:38:VAL:HG23	2.17	0.45
1:X:2392:G:H4'	21:T:68:PHE:CZ	2.51	0.45
1:X:718:C:OP1	5:C:54:ARG:NH1	2.47	0.45
1:X:61:A:C5	1:X:94:A:C2	3.04	0.45
4:B:53:PHE:O	4:B:85:LYS:HD2	2.16	0.45
2:Y:87:G:H22	11:J:38:THR:HB	1.81	0.45
1:X:579:U:H5'	15:N:42:SER:OG	2.17	0.45
1:X:169:G:O2'	1:X:170:C:O5'	2.34	0.45
1:X:2457:A:H2'	1:X:2457:A:N3	2.32	0.45
1:X:2581:U:H2'	1:X:2582:U:C6	2.52	0.45
1:X:695:C:N4	1:X:696:G:C6	2.85	0.45
4:B:61:LYS:HD2	4:B:68:TYR:CZ	2.52	0.45
1:X:677:A:H4'	10:I:60:ARG:NH2	2.30	0.45
17:P:24:ILE:HD13	17:P:24:ILE:HA	1.74	0.45
1:X:1644:C:OP1	18:Q:76:ARG:NH2	2.49	0.45
20:S:29:ALA:HB3	20:S:41:VAL:HG23	1.99	0.45
1:X:1092:A:N6	1:X:1155:A:C4	2.84	0.45
1:X:1628:A:OP1	1:X:1628:A:H4'	2.16	0.45
1:X:2284:U:O2'	1:X:2285:C:H5'	2.16	0.45
1:X:806:A:OP2	1:X:806:A:H8	1.99	0.45
1:X:879:U:H2'	1:X:880:A:H8	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:52:LYS:HD2	12:K:94:THR:HA	1.99	0.45
1:X:2435:U:H2'	1:X:2436:G:C8	2.51	0.45
1:X:2833:U:H2'	1:X:2834:C:C6	2.51	0.45
1:X:725:A:OP1	1:X:821:C:N4	2.50	0.45
2:Y:64:A:N6	2:Y:104:C:H2'	2.31	0.45
15:N:65:ILE:HD11	15:N:95:LEU:HB3	1.98	0.45
1:X:1461:C:H2'	1:X:1462:G:O4'	2.17	0.45
1:X:1867:G:C8	1:X:1954:A:H2	2.34	0.45
1:X:2494:C:O2	11:J:124:LYS:NZ	2.41	0.45
1:X:388:A:H1'	1:X:389:A:C2	2.46	0.45
1:X:410:G:H21	1:X:411:A:H62	1.65	0.45
1:X:685:C:H2'	1:X:686:U:H6	1.82	0.45
28:4:11:CYS:HB2	28:4:32:HIS:CE1	2.51	0.45
4:B:126:GLY:O	4:B:128:GLN:HG2	2.17	0.45
8:G:102:ILE:HB	8:G:125:VAL:HG11	1.99	0.45
11:J:118:LEU:HD12	11:J:131:PHE:HD1	1.82	0.45
21:T:54:TYR:HD2	21:T:80:LYS:HE3	1.82	0.45
1:X:1089:C:H4'	1:X:1090:A:H5''	1.99	0.45
1:X:1092:A:HO2'	1:X:1093:C:H6	1.63	0.45
1:X:1290:G:C2	1:X:1291:A:C2	3.04	0.45
1:X:1352:C:H2'	1:X:1353:A:H8	1.82	0.45
1:X:2418:G:C6	1:X:2454:C:H1'	2.52	0.45
1:X:2623:U:H2'	1:X:2624:G:O4'	2.16	0.45
1:X:630:G:C6	10:I:30:THR:HG21	2.52	0.45
1:X:684:U:C2	1:X:696:G:N2	2.85	0.45
2:Y:21:G:H22	2:Y:58:G:H1	1.65	0.45
5:C:39:LEU:HD12	5:C:39:LEU:O	2.17	0.45
8:G:5:PHE:CD2	15:N:100:ILE:HD13	2.51	0.45
24:W:11:SER:OG	24:W:13:ILE:HG13	2.17	0.45
1:X:111:U:H5'	1:X:112:U:OP2	2.17	0.45
1:X:1315:C:OP1	12:K:32:THR:HG23	2.17	0.45
1:X:1422:A:O2'	1:X:1423:C:O5'	2.34	0.45
1:X:2031:G:C6	1:X:2032:A:C4	3.05	0.45
1:X:2851:G:C8	4:B:64:LYS:HG3	2.52	0.45
1:X:674:C:H2'	1:X:675:G:C8	2.51	0.45
4:B:14:GLN:HB3	4:B:22:LEU:HD11	1.98	0.44
9:H:107:ARG:HB2	9:H:107:ARG:HH11	1.81	0.44
9:H:64:ARG:HA	9:H:79:PHE:CD2	2.52	0.44
10:I:55:LEU:HA	10:I:55:LEU:HD23	1.79	0.44
1:X:2887:G:C4	14:M:23:ARG:NH1	2.85	0.44
1:X:1185:U:H4'	1:X:1186:A:O4'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:86:C:N4	2:Y:88:U:C2	2.85	0.44
5:C:57:VAL:O	5:C:59:GLY:N	2.50	0.44
14:M:29:ARG:HB2	14:M:87:GLU:HB2	1.99	0.44
24:W:5:GLN:HG3	24:W:36:VAL:HG22	2.00	0.44
1:X:1357:G:C2	1:X:1366:U:H5'	2.52	0.44
1:X:1492:G:N7	1:X:1493:U:C5	2.79	0.44
1:X:1845:U:OP2	3:A:156:ARG:HD2	2.17	0.44
1:X:2599:A:O2'	1:X:2602:C:OP1	2.35	0.44
1:X:1340:G:OP2	29:X:3005:MPD:H32	2.17	0.44
1:X:344:U:H1'	1:X:345:C:C6	2.52	0.44
2:Y:102:A:H2'	2:Y:103:A:H8	1.82	0.44
15:N:19:LYS:HA	15:N:19:LYS:HD2	1.68	0.44
18:Q:50:VAL:HG13	18:Q:51:ALA:H	1.82	0.44
18:Q:46:PHE:CD1	18:Q:87:ILE:HD13	2.52	0.44
1:X:1687:G:C6	1:X:1688:U:C4	3.05	0.44
1:X:1886:A:N6	1:X:1910:G:O2'	2.49	0.44
1:X:2577:G:C6	1:X:2578:C:C4	3.06	0.44
2:Y:3:U:H3	2:Y:112:G:H1	1.65	0.44
3:A:76:ALA:HB2	3:A:96:TYR:HD1	1.83	0.44
1:X:1494:G:O2'	1:X:1495:C:H6	2.01	0.44
1:X:1506:C:H2'	1:X:1507:A:C8	2.52	0.44
1:X:1306:A:C2	1:X:2040:A:C4	3.06	0.44
1:X:854:G:C6	1:X:855:U:C4	3.05	0.44
1:X:1184:C:H5'	8:G:27:GLY:HA3	1.99	0.44
17:P:41:LYS:HE3	17:P:41:LYS:HB3	1.78	0.44
1:X:55:G:O2'	1:X:126:A:N1	2.43	0.44
1:X:2079:G:H4'	4:B:156:MET:O	2.17	0.44
1:X:2088:G:H2'	1:X:2528:C:O2'	2.17	0.44
1:X:2634:G:H2'	1:X:2635:G:O4'	2.18	0.44
1:X:970:U:OP1	1:X:970:U:H3'	2.17	0.44
5:C:80:ALA:HB3	5:C:83:TRP:CD1	2.53	0.44
13:L:31:LEU:HD12	13:L:44:ILE:HG12	2.00	0.44
1:X:1167:C:H2'	1:X:1168:C:H6	1.83	0.44
1:X:1471:A:H1'	1:X:1472:C:C5	2.53	0.44
1:X:1477:U:H2'	1:X:1478:A:C8	2.53	0.44
1:X:228:A:N6	1:X:234:C:H42	2.15	0.44
5:C:70:THR:HG22	5:C:72:ARG:HG3	1.99	0.44
1:X:2575:G:N3	9:H:23:LYS:HE2	2.32	0.44
10:I:112:LEU:HD13	10:I:131:SER:HA	2.00	0.44
11:J:72:THR:O	11:J:94:ILE:N	2.47	0.44
16:O:20:ILE:HD13	16:O:97:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Q:51:ALA:HB3	18:Q:81:THR:O	2.18	0.44
1:X:1292:A:H5''	1:X:1293:U:H5'	2.00	0.44
1:X:1542:C:H3'	1:X:1543:G:H5''	1.98	0.44
1:X:2668:A:H2'	1:X:2669:G:H8	1.82	0.44
1:X:2757:U:H2'	1:X:2758:G:H8	1.83	0.44
1:X:304:G:N2	1:X:413:C:N3	2.47	0.44
26:2:31:VAL:O	26:2:35:ARG:HG3	2.18	0.44
4:B:57:LYS:HD2	4:B:68:TYR:CE1	2.52	0.44
14:M:34:ILE:HB	14:M:41:ARG:O	2.18	0.44
18:Q:49:LYS:HD3	18:Q:50:VAL:H	1.83	0.44
1:X:895:U:O2	24:W:46:GLN:NE2	2.50	0.44
1:X:1429:G:C6	1:X:1430:A:N6	2.86	0.44
1:X:2279:G:H2'	1:X:2280:G:C8	2.53	0.44
1:X:3:U:H2'	1:X:4:U:C6	2.53	0.44
1:X:661:U:O2'	1:X:662:G:OP2	2.34	0.44
2:Y:4:G:H1	2:Y:111:A:H62	1.64	0.44
2:Y:90:C:H2'	2:Y:91:C:H6	1.83	0.44
1:X:1346:G:OP1	26:2:10:LYS:HG3	2.18	0.44
3:A:143:ASN:ND2	3:A:143:ASN:O	2.47	0.44
3:A:182:ARG:HB2	3:A:270:ILE:HA	2.00	0.44
4:B:9:LYS:HD3	4:B:205:LYS:H	1.82	0.44
7:E:121:ILE:HD11	7:E:136:ILE:HG12	1.99	0.44
1:X:677:A:C4'	10:I:60:ARG:HH22	2.31	0.44
14:M:96:ARG:HA	14:M:96:ARG:HD3	1.58	0.44
1:X:1446:U:O2	1:X:1638:G:N2	2.51	0.44
1:X:172:U:H2'	1:X:173:A:H8	1.82	0.44
1:X:2348:G:H5''	1:X:2349:A:OP2	2.17	0.44
1:X:319:G:N2	1:X:320:U:O3'	2.50	0.44
1:X:713:A:H2'	1:X:715:A:H62	1.83	0.44
2:Y:114:C:H6	2:Y:114:C:H2'	1.57	0.44
2:Y:21:G:H1	2:Y:58:G:H1	1.66	0.44
4:B:5:ILE:HG13	4:B:211:ILE:HB	2.00	0.43
9:H:24:VAL:HB	9:H:30:ARG:HD2	2.00	0.43
9:H:35:ILE:HD13	9:H:62:ILE:HG22	1.99	0.43
15:N:46:ALA:O	15:N:50:ARG:HG3	2.17	0.43
19:R:38:VAL:O	19:R:61:ALA:N	2.35	0.43
19:R:72:ASP:OD1	19:R:72:ASP:N	2.51	0.43
20:S:78:GLN:HB2	20:S:87:THR:O	2.18	0.43
1:X:1504:U:H6	1:X:1504:U:H2'	1.63	0.43
1:X:2571:G:H2'	1:X:2572:G:H8	1.81	0.43
1:X:339:A:H2'	1:X:340:C:H6	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:351:G:H2'	1:X:352:A:O4'	2.18	0.43
1:X:578:G:C5	1:X:579:U:C4	3.05	0.43
4:B:131:ILE:HD11	4:B:149:ARG:NH2	2.34	0.43
1:X:1371:U:H2'	1:X:1372:C:C6	2.53	0.43
1:X:1518:G:N2	1:X:1562:C:N3	2.49	0.43
1:X:1746:G:C2	1:X:1747:G:N7	2.86	0.43
1:X:1781:C:H2'	1:X:1782:A:O4'	2.18	0.43
1:X:1931:G:O2'	1:X:1955:A:N6	2.51	0.43
1:X:306:C:H42	1:X:409:G:H1	1.67	0.43
1:X:660:A:N3	1:X:660:A:O4'	2.49	0.43
1:X:59:U:C2	1:X:74:U:H5	2.36	0.43
2:Y:87:G:N3	2:Y:87:G:H2'	2.32	0.43
12:K:105:LYS:O	25:Z:42:ARG:N	2.39	0.43
1:X:1441:C:H2'	1:X:1442:C:C6	2.52	0.43
1:X:2448:G:H5''	1:X:2449:C:OP2	2.17	0.43
1:X:843:G:H2'	1:X:844:G:C8	2.53	0.43
4:B:140:PRO:HG2	4:B:145:SER:HB2	2.01	0.43
4:B:37:GLN:HE21	4:B:39:LYS:HG3	1.84	0.43
5:C:110:LEU:HD23	5:C:110:LEU:HA	1.74	0.43
11:J:22:LYS:HA	11:J:98:LYS:HB2	2.00	0.43
21:T:71:ILE:HG12	21:T:72:ASP:N	2.34	0.43
1:X:158:G:H2'	1:X:158:G:N3	2.32	0.43
1:X:487:U:O2'	5:C:46:GLN:NE2	2.50	0.43
2:Y:74:G:H1	2:Y:97:A:H62	1.66	0.43
3:A:201:GLU:HG3	3:A:202:LEU:HD12	1.98	0.43
9:H:113:LYS:O	9:H:117:LEU:HB2	2.18	0.43
13:L:2:ILE:HG12	13:L:3:SER:H	1.84	0.43
14:M:89:LYS:HB2	14:M:90:ARG:H	1.63	0.43
1:X:1494:G:C8	1:X:1495:C:C5	3.07	0.43
1:X:2489:U:H2'	1:X:2490:C:O4'	2.19	0.43
1:X:259:A:H2'	1:X:260:A:C8	2.53	0.43
1:X:2567:C:O2	1:X:2767:A:H2	2.02	0.43
1:X:800:G:H2'	1:X:801:A:H8	1.84	0.43
4:B:37:GLN:NE2	4:B:39:LYS:HE3	2.34	0.43
1:X:1092:A:O2'	1:X:1093:C:H6	2.02	0.43
1:X:1518:G:H1	1:X:1562:C:N4	2.07	0.43
1:X:1521:A:N7	1:X:1561:G:N1	2.67	0.43
1:X:1700:C:C2	1:X:1701:U:C5	3.06	0.43
1:X:1930:G:C5	1:X:1931:G:N7	2.87	0.43
1:X:2106:U:H2'	1:X:2107:G:O4'	2.18	0.43
1:X:2289:U:OP1	1:X:2414:U:O2'	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:251:G:N7	1:X:253:G:H1'	2.34	0.43
1:X:2646:U:H2'	1:X:2647:C:H6	1.83	0.43
1:X:2712:G:P	14:M:51:LYS:HZ1	2.41	0.43
1:X:2760:A:N1	4:B:216:LYS:HB2	2.34	0.43
1:X:354:A:C8	1:X:375:A:C5	3.07	0.43
1:X:817:G:H2'	1:X:818:U:H6	1.84	0.43
5:C:177:THR:HB	5:C:179:GLN:OE1	2.18	0.43
9:H:88:ARG:O	9:H:90:ASP:N	2.46	0.43
11:J:38:THR:HG23	11:J:128:LYS:HB3	1.99	0.43
11:J:59:LYS:HD3	11:J:59:LYS:HA	1.74	0.43
20:S:95:ASN:OD1	20:S:96:MET:N	2.52	0.43
1:X:1039:C:O2	8:G:4:THR:OG1	2.31	0.43
1:X:1092:A:N6	1:X:1155:A:C2	2.86	0.43
1:X:1510:U:O2'	1:X:1511:C:O5'	2.36	0.43
1:X:1576:A:N3	1:X:1577:G:C8	2.86	0.43
1:X:1383:G:N2	1:X:1644:C:O2	2.49	0.43
1:X:618:A:O2'	1:X:619:U:H5'	2.19	0.43
25:Z:8:THR:HG22	25:Z:12:ARG:HB3	2.01	0.43
4:B:160:ALA:C	4:B:162:ARG:H	2.22	0.43
5:C:182:ASN:OD1	5:C:182:ASN:N	2.49	0.43
9:H:102:VAL:O	9:H:122:LEU:N	2.51	0.43
1:X:999:U:H5''	11:J:87:LYS:HD3	2.00	0.43
13:L:73:ALA:HB1	13:L:107:ALA:HB2	2.01	0.43
14:M:62:THR:OG1	14:M:75:THR:HB	2.19	0.43
1:X:1286:G:H5'	5:C:92:PRO:HD3	2.01	0.43
1:X:1514:A:C2'	1:X:1515:G:H5'	2.49	0.43
1:X:828:A:H2'	1:X:829:U:H4'	2.00	0.43
3:A:145:GLU:HA	3:A:152:GLY:HA2	2.01	0.43
4:B:37:GLN:HB3	4:B:50:GLN:HB3	2.01	0.43
6:D:64:LYS:HA	6:D:65:PRO:HD2	1.79	0.43
8:G:2:ARG:HG3	8:G:3:GLN:N	2.31	0.43
8:G:42:LYS:HE2	8:G:51:THR:O	2.18	0.43
11:J:54:MET:HE1	11:J:104:PHE:CD1	2.54	0.43
19:R:80:ARG:NH2	19:R:96:LYS:HA	2.33	0.43
1:X:106:A:H2'	1:X:107:G:H8	1.83	0.43
1:X:296:G:C6	1:X:297:G:C2	3.07	0.43
1:X:49:A:H4'	1:X:50:U:H5''	2.01	0.43
1:X:995:U:H2'	1:X:996:G:C8	2.54	0.43
10:I:62:PRO:O	10:I:63:LYS:HG3	2.19	0.43
1:X:1498:U:O2'	1:X:1499:U:H5	2.01	0.43
1:X:164:A:O2'	1:X:165:C:H5'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1880:A:H1'	1:X:2261:A:H5'	2.01	0.43
1:X:2318:U:O2'	1:X:2401:C:O2	2.31	0.43
1:X:2507:C:O2'	1:X:2508:G:H5'	2.19	0.43
1:X:2652:G:H2'	1:X:2653:C:C6	2.54	0.43
1:X:2805:A:H8	1:X:2805:A:H5''	1.84	0.43
1:X:2839:A:O2'	1:X:2840:A:H5''	2.18	0.43
1:X:2907:A:H2'	1:X:2908:U:C6	2.54	0.43
1:X:349:U:H2'	1:X:350:G:O4'	2.19	0.43
1:X:265:A:H5'	1:X:653:G:O2'	2.19	0.43
1:X:902:A:H61	1:X:965:G:H1	1.67	0.43
5:C:65:TRP:CZ2	5:C:75:GLN:HG3	2.54	0.42
5:C:78:ILE:HD13	5:C:78:ILE:H	1.83	0.42
8:G:29:LEU:O	8:G:33:VAL:HG23	2.19	0.42
17:P:24:ILE:HD12	17:P:32:ALA:HB1	2.00	0.42
20:S:80:ASP:OD2	20:S:83:LYS:HB2	2.19	0.42
21:T:56:GLY:HA3	21:T:88:SER:HB3	2.01	0.42
1:X:192:G:H2'	1:X:208:G:N2	2.34	0.42
1:X:317:G:H2'	1:X:318:A:O4'	2.19	0.42
1:X:539:G:OP1	17:P:8:ARG:NH1	2.50	0.42
3:A:76:ALA:HB2	3:A:96:TYR:CD1	2.53	0.42
8:G:12:ILE:CD1	8:G:51:THR:HA	2.50	0.42
9:H:106:LEU:HD22	9:H:111:PHE:HB2	2.01	0.42
9:H:24:VAL:HA	9:H:39:ILE:HG22	2.01	0.42
10:I:81:GLN:CB	10:I:110:LYS:H	2.32	0.42
10:I:61:LEU:HA	10:I:62:PRO:HD3	1.85	0.42
17:P:95:ALA:O	17:P:96:ILE:HG13	2.18	0.42
24:W:52:HIS:CD2	24:W:53:LEU:HG	2.53	0.42
1:X:1314:A:H2'	1:X:1315:C:C6	2.54	0.42
1:X:889:U:H3'	1:X:890:G:C8	2.54	0.42
1:X:889:U:H3'	1:X:890:G:H8	1.85	0.42
1:X:90:A:O2'	1:X:91:A:O4'	2.37	0.42
26:2:20:ARG:HB2	26:2:20:ARG:HH11	1.82	0.42
4:B:62:ASP:OD1	4:B:62:ASP:N	2.52	0.42
15:N:61:TRP:CZ2	15:N:93:LYS:HD2	2.54	0.42
1:X:1490:G:H1'	1:X:1491:C:OP1	2.19	0.42
1:X:1526:G:N2	1:X:1549:C:N3	2.66	0.42
1:X:1819:G:H5''	3:A:204:ASN:HB2	2.01	0.42
1:X:189:G:H2'	1:X:190:G:C8	2.54	0.42
1:X:1923:A:H2'	1:X:1924:G:C8	2.54	0.42
1:X:2823:G:H2'	1:X:2824:G:O4'	2.20	0.42
1:X:250:G:H4'	1:X:432:G:C5	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:84:ASP:OD1	3:A:85:PRO:HD2	2.20	0.42
4:B:39:LYS:O	4:B:47:ASN:HA	2.19	0.42
8:G:54:TYR:CE1	8:G:122:LYS:HG2	2.54	0.42
14:M:78:LEU:CB	14:M:79:HIS:HD2	2.31	0.42
20:S:108:LEU:HB3	20:S:109:VAL:H	1.74	0.42
21:T:48:GLN:HE22	21:T:67:LEU:HD22	1.84	0.42
1:X:1208:A:H2'	1:X:1209:U:H6	1.84	0.42
1:X:1279:C:H2'	1:X:1280:U:C6	2.54	0.42
1:X:1326:C:H2'	1:X:1327:C:C6	2.54	0.42
1:X:158:G:H2'	1:X:159:U:H5'	2.01	0.42
1:X:1631:G:O2'	1:X:1632:A:OP2	2.32	0.42
1:X:1762:U:H5'	1:X:1763:U:OP2	2.19	0.42
1:X:1711:G:N2	1:X:2018:U:H2'	2.34	0.42
1:X:2289:U:H4'	1:X:2355:A:C2	2.53	0.42
1:X:2900:C:O2	12:K:99:GLY:HA3	2.19	0.42
1:X:695:C:N4	1:X:696:G:O6	2.49	0.42
7:E:121:ILE:HD11	7:E:136:ILE:CG1	2.50	0.42
15:N:66:ASN:HA	15:N:76:TYR:HB2	2.01	0.42
15:N:62:ILE:HG23	15:N:76:TYR:CZ	2.55	0.42
1:X:1024:A:C6	1:X:1025:A:N1	2.87	0.42
1:X:1765:A:H2'	1:X:1765:A:N3	2.34	0.42
1:X:2360:A:C5'	1:X:2362:A:H1'	2.47	0.42
1:X:2668:A:H2'	1:X:2669:G:C8	2.54	0.42
1:X:502:C:H5	18:Q:68:TYR:CD1	2.37	0.42
1:X:14:A:C6	1:X:571:A:C2	3.08	0.42
1:X:854:G:C4	1:X:855:U:C5	3.07	0.42
27:3:32:LEU:HB3	27:3:33:PHE:CE1	2.55	0.42
3:A:133:GLN:CD	3:A:133:GLN:H	2.23	0.42
3:A:142:HIS:NE2	3:A:191:THR:HB	2.35	0.42
9:H:88:ARG:C	9:H:90:ASP:H	2.22	0.42
10:I:19:VAL:HG21	10:I:30:THR:HG23	2.02	0.42
14:M:98:LYS:HD3	14:M:98:LYS:HA	1.83	0.42
1:X:1149:U:H2'	1:X:1149:U:O2	2.18	0.42
1:X:148:U:H2'	1:X:149:U:C6	2.54	0.42
1:X:2058:A:C6	1:X:2525:C:H1'	2.54	0.42
1:X:2615:G:H2'	1:X:2616:A:O4'	2.19	0.42
1:X:41:A:H2'	1:X:42:G:C8	2.55	0.42
3:A:122:ALA:HA	3:A:130:LEU:HD12	2.00	0.42
3:A:144:ILE:HB	3:A:154:ILE:HD12	2.02	0.42
1:X:1929:C:H5''	3:A:241:ILE:HG13	2.02	0.42
3:A:7:LYS:HA	3:A:8:PRO:HD3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:93:THR:HB	5:C:94:PRO:HD2	2.01	0.42
12:K:22:THR:OG1	12:K:67:ARG:HB2	2.19	0.42
1:X:1352:C:N3	1:X:1374:G:N2	2.56	0.42
1:X:1356:G:C5	1:X:1357:G:C6	3.08	0.42
1:X:1567:A:OP2	1:X:1568:U:O2'	2.37	0.42
1:X:162:A:H5''	1:X:163:U:H2'	2.00	0.42
1:X:2372:G:H4'	1:X:2373:A:H5''	2.01	0.42
1:X:619:U:H4'	1:X:2529:G:C8	2.54	0.42
1:X:874:A:H5'	1:X:876:G:N7	2.35	0.42
2:Y:57:G:H3'	2:Y:58:G:C8	2.53	0.42
3:A:173:LEU:HA	3:A:183:MET:HA	2.02	0.42
15:N:51:ARG:O	15:N:54:LYS:HB2	2.20	0.42
16:O:22:VAL:HG22	16:O:23:GLU:H	1.85	0.42
18:Q:50:VAL:O	18:Q:82:LEU:HA	2.19	0.42
20:S:123:GLN:HB2	20:S:124:PRO:HD3	2.01	0.42
24:W:51:LYS:NZ	24:W:55:THR:HA	2.35	0.42
1:X:1000:G:N2	1:X:1004:A:OP2	2.45	0.42
1:X:1070:A:H1'	1:X:1178:C:H41	1.85	0.42
1:X:1312:A:N3	1:X:1313:G:H1'	2.35	0.42
1:X:1432:A:C6	1:X:1435:C:C2	3.07	0.42
1:X:1834:G:N1	1:X:1835:U:H1'	2.34	0.42
1:X:1889:G:C6	1:X:1908:A:C6	3.08	0.42
1:X:2287:C:H2'	1:X:2288:C:H6	1.84	0.42
1:X:272:C:N3	1:X:416:G:N2	2.63	0.42
2:Y:55:A:C4	6:D:26:MET:HB3	2.54	0.42
1:X:995:U:P	2:Y:85:A:H61	2.43	0.42
3:A:171:TYR:HB3	3:A:185:LEU:HA	2.01	0.42
3:A:79:ASP:OD2	3:A:93:LEU:HD23	2.20	0.42
4:B:36:LEU:N	4:B:50:GLN:O	2.52	0.42
10:I:95:LEU:HD12	10:I:96:LEU:H	1.85	0.42
11:J:22:LYS:HG3	11:J:24:GLY:H	1.85	0.42
11:J:78:PRO:HB2	11:J:81:VAL:HG21	2.01	0.42
20:S:108:LEU:HD23	20:S:108:LEU:HA	1.94	0.42
1:X:864:A:C4	1:X:1228:A:C2	3.07	0.42
1:X:1901:C:O2'	1:X:1902:G:O5'	2.25	0.42
1:X:2571:G:H2'	1:X:2572:G:C8	2.55	0.42
1:X:2719:C:H2'	1:X:2720:A:O4'	2.19	0.42
1:X:407:G:H2'	1:X:408:U:H6	1.83	0.42
1:X:514:G:C2'	1:X:515:G:H5'	2.49	0.42
11:J:18:THR:OG1	11:J:19:GLY:N	2.53	0.42
19:R:4:LYS:NZ	19:R:4:LYS:HB3	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:16:PRO:HD2	24:W:19:GLN:CD	2.39	0.42
1:X:1680:U:H2'	1:X:1681:U:C6	2.55	0.42
1:X:1830:A:C8	1:X:1831:A:C8	3.07	0.42
1:X:1886:A:H3'	1:X:1887:G:C8	2.53	0.42
1:X:2322:C:H2'	1:X:2323:U:H6	1.85	0.42
1:X:615:A:N6	1:X:616:G:C6	2.87	0.42
5:C:124:THR:HA	5:C:189:ALA:O	2.20	0.41
17:P:86:ARG:NH1	17:P:86:ARG:HB2	2.35	0.41
18:Q:57:ASN:OD1	18:Q:76:ARG:HG2	2.20	0.41
1:X:1357:G:N2	1:X:1366:U:H5'	2.35	0.41
1:X:1760:G:C2	1:X:1761:G:N7	2.88	0.41
1:X:2051:C:C2	1:X:2052:C:C5	3.08	0.41
1:X:616:G:N2	1:X:2058:A:OP1	2.45	0.41
1:X:235:G:HO2'	1:X:236:A:C5'	2.34	0.41
1:X:2456:G:H5''	1:X:2457:A:OP2	2.20	0.41
1:X:367:A:H2'	1:X:368:A:O4'	2.20	0.41
1:X:373:A:H2	1:X:1248:U:H2'	1.85	0.41
3:A:105:ILE:O	3:A:107:PRO:HD3	2.20	0.41
8:G:40:LYS:O	8:G:41:ASN:HB2	2.20	0.41
9:H:91:LYS:HD2	9:H:111:PHE:CZ	2.55	0.41
15:N:114:LYS:O	15:N:117:LEU:HB2	2.20	0.41
1:X:2279:G:H2'	1:X:2280:G:H8	1.85	0.41
1:X:2379:A:C4	1:X:2393:A:C2	3.08	0.41
1:X:253:G:C6	1:X:254:A:C6	3.08	0.41
1:X:2585:C:H2'	1:X:2586:C:O4'	2.20	0.41
1:X:2814:C:H1'	4:B:72:PRO:HG3	2.02	0.41
1:X:873:U:H4'	1:X:876:G:N1	2.36	0.41
1:X:1817:C:O2'	3:A:208:ALA:HB2	2.21	0.41
4:B:52:GLY:HA3	4:B:85:LYS:HG3	2.02	0.41
5:C:117:LYS:NZ	5:C:182:ASN:HA	2.35	0.41
8:G:119:GLN:HA	8:G:122:LYS:HD3	2.00	0.41
11:J:118:LEU:HD12	11:J:131:PHE:CD1	2.55	0.41
12:K:109:ARG:HD2	12:K:112:ASP:OD1	2.21	0.41
14:M:50:ILE:HD13	14:M:50:ILE:HA	1.82	0.41
1:X:1650:G:H5''	1:X:1651:C:OP1	2.19	0.41
1:X:1963:A:OP2	1:X:1988:C:N4	2.54	0.41
1:X:2089:A:OP2	29:X:3003:MPD:HM1	2.20	0.41
1:X:2288:C:C2'	1:X:2289:U:H5'	2.50	0.41
1:X:2660:A:H2'	1:X:2661:A:O4'	2.20	0.41
1:X:609:U:H2'	1:X:610:U:O4'	2.20	0.41
10:I:16:ARG:HG2	10:I:16:ARG:H	1.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1013:U:OP1	24:W:17:GLU:HG2	2.19	0.41
1:X:361:U:H2'	1:X:362:C:H6	1.85	0.41
1:X:733:U:O2'	1:X:734:A:H5'	2.20	0.41
27:3:20:GLY:O	27:3:45:ARG:HA	2.21	0.41
4:B:208:LEU:HA	4:B:208:LEU:HD12	1.76	0.41
5:C:142:VAL:HG13	5:C:144:SER:HB2	2.02	0.41
5:C:28:PRO:HB3	5:C:112:SER:O	2.20	0.41
5:C:39:LEU:HD11	5:C:99:TYR:O	2.21	0.41
7:E:41:MET:O	7:E:43:PHE:N	2.42	0.41
20:S:72:VAL:HG12	20:S:93:ALA:HA	2.02	0.41
1:X:2418:G:O6	1:X:2452:A:H5''	2.20	0.41
1:X:278:A:N1	1:X:279:A:N6	2.68	0.41
1:X:2793:G:C2	1:X:2794:C:C6	3.09	0.41
1:X:302:A:N6	1:X:450:C:C2	2.89	0.41
2:Y:81:A:N1	2:Y:90:C:N3	2.69	0.41
27:3:59:LYS:HA	27:3:59:LYS:HD3	1.90	0.41
5:C:53:ASN:O	5:C:57:VAL:HG23	2.21	0.41
8:G:39:GLY:HA3	8:G:51:THR:HG23	2.01	0.41
14:M:33:ARG:HA	14:M:42:ILE:HG12	2.01	0.41
14:M:50:ILE:HG23	14:M:50:ILE:HD12	1.86	0.41
1:X:1086:G:C6	1:X:1158:G:C6	3.09	0.41
1:X:1906:C:H2'	1:X:1907:U:O4'	2.21	0.41
1:X:2342:U:H2'	1:X:2343:U:C6	2.54	0.41
1:X:2725:U:C2	1:X:2726:C:C5	3.09	0.41
1:X:619:U:H2'	1:X:620:G:C8	2.55	0.41
1:X:745:G:H1	1:X:777:C:H42	1.68	0.41
3:A:8:PRO:HB3	3:A:14:ARG:HB2	2.02	0.41
10:I:66:PHE:HB3	10:I:67:THR:H	1.68	0.41
1:X:1515:G:N2	1:X:1516:C:C2	2.89	0.41
1:X:2311:U:H1'	1:X:2352:G:C2	2.56	0.41
1:X:442:G:O2'	1:X:443:U:H5'	2.19	0.41
1:X:696:G:H2'	1:X:697:U:C6	2.55	0.41
1:X:696:G:H2'	1:X:697:U:H6	1.86	0.41
1:X:800:G:H2'	1:X:801:A:C8	2.56	0.41
5:C:184:LEU:O	5:C:186:ILE:N	2.51	0.41
14:M:51:LYS:O	14:M:61:PHE:HA	2.21	0.41
1:X:1290:G:N3	15:N:33:LYS:HE2	2.36	0.41
1:X:1272:U:H2'	1:X:1273:G:O4'	2.21	0.41
1:X:1438:G:H2'	1:X:1439:U:H6	1.86	0.41
1:X:1823:U:H2'	1:X:1824:C:C6	2.56	0.41
1:X:1959:A:H2'	1:X:1960:G:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2256:U:H2'	1:X:2257:G:C8	2.55	0.41
1:X:2594:G:H2'	1:X:2595:C:C6	2.55	0.41
1:X:2665:G:C4	1:X:2802:A:C2	3.08	0.41
1:X:268:A:O2'	1:X:269:G:H4'	2.21	0.41
1:X:2757:U:H2'	1:X:2758:G:C8	2.56	0.41
1:X:344:U:C2	1:X:345:C:C5	3.09	0.41
1:X:306:C:O2	1:X:411:A:N6	2.54	0.41
1:X:511:G:C6	1:X:512:A:N6	2.89	0.41
5:C:102:PRO:HB2	5:C:105:MET:HG3	2.03	0.41
12:K:22:THR:O	12:K:26:ILE:HG13	2.21	0.41
18:Q:36:THR:O	18:Q:40:MET:HG2	2.20	0.41
1:X:105:C:O2	1:X:337:A:O2'	2.38	0.41
1:X:2120:G:N2	1:X:2225:A:H62	2.17	0.41
1:X:225:A:N6	1:X:227:G:C2	2.89	0.41
1:X:25:U:H2'	1:X:26:G:O4'	2.21	0.41
1:X:365:A:C5	1:X:383:A:C2	3.09	0.41
1:X:447:A:H2'	1:X:448:A:O4'	2.21	0.41
1:X:514:G:H2'	1:X:515:G:H5'	2.02	0.41
2:Y:68:A:N1	2:Y:103:A:N1	2.68	0.41
26:2:3:LYS:HE3	26:2:3:LYS:HB2	1.81	0.41
4:B:118:VAL:HG21	4:B:201:VAL:HG12	2.02	0.41
6:D:65:PRO:HD2	6:D:83:MET:HA	2.03	0.41
11:J:75:THR:HG21	11:J:87:LYS:HE2	2.03	0.41
13:L:30:ARG:HD3	13:L:91:GLU:HG3	2.02	0.41
23:V:25:LEU:HA	23:V:28:LEU:HD12	2.02	0.41
23:V:25:LEU:HB2	23:V:46:VAL:HG11	2.03	0.41
1:X:1356:G:O2'	1:X:1357:G:H5'	2.21	0.41
1:X:1491:C:H4'	1:X:1593:G:H5''	2.02	0.41
1:X:1445:C:C2	1:X:1639:G:N2	2.89	0.41
1:X:1658:A:H8	1:X:1658:A:P	2.44	0.41
1:X:1410:A:H4'	1:X:2239:A:H1'	2.02	0.41
1:X:363:A:H4'	1:X:365:A:C8	2.56	0.41
1:X:577:A:N3	1:X:577:A:H2'	2.34	0.41
1:X:77:U:OP1	23:V:52:ARG:HD2	2.21	0.41
3:A:230:HIS:CD2	3:A:249:PRO:HG3	2.56	0.41
4:B:8:ARG:NH2	4:B:54:GLU:OE2	2.53	0.41
7:E:103:LEU:H	7:E:115:ILE:CD1	2.34	0.41
10:I:47:ARG:HA	10:I:48:PRO:HD3	1.85	0.41
22:U:17:ARG:O	22:U:29:TRP:HD1	2.04	0.41
1:X:1983:U:H1'	1:X:2579:U:OP1	2.21	0.41
1:X:563:G:H2'	1:X:564:U:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:946:A:C2'	1:X:947:U:H5'	2.51	0.41
27:3:56:LYS:HE3	27:3:56:LYS:HB2	1.87	0.40
28:4:14:CYS:SG	28:4:32:HIS:ND1	2.74	0.40
15:N:60:LEU:O	15:N:64:ARG:HD2	2.21	0.40
1:X:1241:A:C6	1:X:1242:A:C6	3.09	0.40
1:X:135:G:C2	1:X:136:A:C8	3.09	0.40
1:X:1681:U:H5'	1:X:1787:A:O2'	2.21	0.40
1:X:852:U:O2'	1:X:2087:A:N1	2.53	0.40
1:X:713:A:OP2	29:X:3008:MPD:HM3	2.20	0.40
1:X:579:U:H2'	1:X:580:C:C6	2.55	0.40
1:X:634:C:HO2'	27:3:2:PRO:N	2.18	0.40
1:X:635:G:C2	1:X:636:A:C8	3.09	0.40
1:X:724:C:H2'	1:X:725:A:C8	2.56	0.40
2:Y:1:U:O2'	2:Y:2:C:OP2	2.33	0.40
25:Z:39:LEU:O	25:Z:41:HIS:ND1	2.46	0.40
3:A:142:HIS:CD2	3:A:191:THR:HB	2.55	0.40
4:B:215:ILE:O	4:B:216:LYS:HG2	2.21	0.40
7:E:19:PHE:HB3	7:E:20:ASP:H	1.58	0.40
12:K:106:GLN:H	12:K:117:VAL:HA	1.84	0.40
14:M:34:ILE:CD1	14:M:43:GLN:HB2	2.52	0.40
16:O:32:THR:HG22	16:O:61:THR:HA	2.03	0.40
17:P:1:MET:HG2	17:P:2:GLU:OE2	2.20	0.40
19:R:11:VAL:HA	19:R:67:ASN:CB	2.48	0.40
1:X:1168:C:H2'	1:X:1169:G:O4'	2.21	0.40
1:X:1313:G:N7	1:X:1689:G:C2	2.89	0.40
1:X:221:G:N2	1:X:238:U:H4'	2.36	0.40
1:X:2584:G:H2'	1:X:2585:C:C6	2.57	0.40
1:X:2848:G:O2'	1:X:2849:A:H5'	2.22	0.40
1:X:525:A:H4'	1:X:526:A:OP1	2.20	0.40
1:X:810:A:H2'	1:X:811:C:H6	1.86	0.40
17:P:19:LEU:HD22	25:Z:22:ILE:HG23	2.04	0.40
27:3:32:LEU:HD22	27:3:33:PHE:CE1	2.56	0.40
3:A:129:ALA:HA	3:A:191:THR:HA	2.02	0.40
5:C:57:VAL:HG21	5:C:87:GLY:HA2	2.04	0.40
8:G:33:VAL:O	8:G:37:LEU:HG	2.22	0.40
15:N:24:TYR:CE2	15:N:38:GLN:HG3	2.56	0.40
17:P:72:LYS:N	17:P:106:VAL:O	2.54	0.40
24:W:51:LYS:HZ2	24:W:56:VAL:H	1.69	0.40
1:X:1326:C:H2'	1:X:1327:C:H6	1.86	0.40
1:X:1460:U:C2'	1:X:1461:C:H5'	2.51	0.40
1:X:2686:G:O5'	1:X:2686:G:H8	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:616:G:O6	1:X:2056:G:O2'	2.25	0.40
10:I:66:PHE:CD1	10:I:94:ALA:HB3	2.56	0.40
1:X:793:G:H5''	17:P:89:ALA:HB2	2.03	0.40
1:X:1730:C:H2'	1:X:1731:G:O4'	2.21	0.40
1:X:1825:U:C4	1:X:1846:A:C2	3.09	0.40
1:X:2329:U:H2'	1:X:2330:G:C8	2.56	0.40
1:X:854:G:C5	1:X:855:U:C5	3.09	0.40
2:Y:87:G:N2	11:J:38:THR:HB	2.36	0.40
25:Z:28:THR:HG21	25:Z:39:LEU:HD12	2.02	0.40
1:X:1663:G:HO2'	26:2:2:VAL:N	2.20	0.40
5:C:177:THR:O	5:C:181:LEU:HB2	2.22	0.40
9:H:64:ARG:HD3	9:H:101:PRO:HG2	2.03	0.40
11:J:75:THR:HG21	11:J:87:LYS:HB3	2.02	0.40
14:M:23:ARG:NH2	14:M:23:ARG:HG3	2.32	0.40
16:O:17:GLY:H	16:O:97:ILE:HB	1.86	0.40
16:O:63:ASN:OD1	16:O:63:ASN:N	2.55	0.40
1:X:967:C:O2'	21:T:34:ALA:HB2	2.21	0.40
24:W:8:LEU:HD23	24:W:31:THR:HA	2.03	0.40
1:X:1016:G:C3'	1:X:1017:A:H5''	2.49	0.40
1:X:122:G:O3'	1:X:1413:C:H4'	2.22	0.40
1:X:2269:G:H2'	1:X:2270:U:O4'	2.21	0.40
1:X:2720:A:H2'	1:X:2721:G:H8	1.86	0.40
1:X:2757:U:O2'	1:X:2758:G:H5'	2.21	0.40
1:X:491:C:N4	1:X:492:G:O6	2.55	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	A	267/277 (96%)	222 (83%)	27 (10%)	18 (7%)	<b>1</b> <b>15</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	B	213/220 (97%)	182 (85%)	18 (8%)	13 (6%)	1	16
5	C	197/207 (95%)	169 (86%)	20 (10%)	8 (4%)	3	25
6	D	164/179 (92%)	134 (82%)	19 (12%)	11 (7%)	1	15
7	E	154/178 (86%)	112 (73%)	27 (18%)	15 (10%)	0	8
8	G	143/145 (99%)	129 (90%)	12 (8%)	2 (1%)	11	47
9	H	120/122 (98%)	109 (91%)	8 (7%)	3 (2%)	5	35
10	I	129/146 (88%)	91 (70%)	25 (19%)	13 (10%)	0	7
11	J	139/144 (96%)	124 (89%)	9 (6%)	6 (4%)	2	23
12	K	117/122 (96%)	101 (86%)	15 (13%)	1 (1%)	17	57
13	L	108/119 (91%)	88 (82%)	15 (14%)	5 (5%)	2	22
14	M	108/116 (93%)	93 (86%)	11 (10%)	4 (4%)	3	28
15	N	114/118 (97%)	108 (95%)	6 (5%)	0	100	100
16	O	100/102 (98%)	85 (85%)	11 (11%)	4 (4%)	3	25
17	P	110/117 (94%)	107 (97%)	3 (3%)	0	100	100
18	Q	87/91 (96%)	78 (90%)	7 (8%)	2 (2%)	6	37
19	R	98/105 (93%)	76 (78%)	18 (18%)	4 (4%)	3	25
20	S	165/217 (76%)	130 (79%)	19 (12%)	16 (10%)	0	8
21	T	73/94 (78%)	65 (89%)	7 (10%)	1 (1%)	11	47
22	U	44/62 (71%)	31 (70%)	9 (20%)	4 (9%)	1	9
23	V	63/69 (91%)	58 (92%)	4 (6%)	1 (2%)	9	45
24	W	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
25	Z	41/58 (71%)	38 (93%)	3 (7%)	0	100	100
26	2	42/45 (93%)	38 (90%)	2 (5%)	2 (5%)	2	21
27	3	58/66 (88%)	46 (79%)	4 (7%)	8 (14%)	0	4
28	4	35/37 (95%)	32 (91%)	2 (6%)	1 (3%)	4	33
All	All	2945/3215 (92%)	2499 (85%)	304 (10%)	142 (5%)	2	21

All (142) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	27	THR
3	A	51	VAL
3	A	120	ALA

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Mol	Chain	Res	Type
3	A	126	VAL
3	A	141	VAL
3	A	154	ILE
4	B	9	LYS
4	B	10	ILE
4	B	208	LEU
5	C	154	VAL
6	D	84	PRO
6	D	104	ILE
6	D	109	PRO
6	D	137	ILE
7	E	55	PRO
7	E	107	VAL
7	E	171	ARG
8	G	88	ILE
10	I	13	ARG
10	I	46	VAL
10	I	48	PRO
10	I	62	PRO
10	I	75	ALA
10	I	101	VAL
12	K	81	ALA
13	L	90	LYS
13	L	100	LEU
16	O	50	ALA
19	R	76	ASN
20	S	34	TYR
20	S	130	VAL
20	S	145	ILE
22	U	22	LEU
27	3	54	ASP
3	A	170	LYS
3	A	192	ILE
3	A	224	VAL
4	B	32	GLU
4	B	53	PHE
4	B	60	LYS
5	C	131	PHE
5	C	145	THR
6	D	44	VAL
6	D	115	GLN
6	D	126	GLY

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Mol	Chain	Res	Type
7	E	50	ILE
7	E	52	VAL
7	E	59	LYS
9	H	25	LEU
10	I	64	ARG
10	I	113	GLY
11	J	21	SER
11	J	84	GLY
11	J	135	GLU
13	L	89	ILE
14	M	89	LYS
16	O	52	THR
16	O	99	LYS
18	Q	50	VAL
20	S	109	VAL
20	S	129	GLU
20	S	132	ALA
22	U	14	THR
22	U	40	VAL
26	2	16	VAL
27	3	25	SER
28	4	28	GLU
3	A	110	LEU
3	A	132	LEU
4	B	106	SER
4	B	186	VAL
4	B	206	LYS
6	D	75	ALA
6	D	130	LEU
7	E	24	VAL
7	E	35	ARG
7	E	51	GLU
7	E	134	GLU
8	G	2	ARG
9	H	119	PRO
10	I	129	SER
11	J	60	ARG
13	L	96	ARG
14	M	36	GLU
18	Q	86	SER
19	R	65	VAL
19	R	74	LYS

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Mol	Chain	Res	Type
20	S	82	LEU
20	S	88	HIS
20	S	98	GLU
20	S	138	PRO
20	S	150	ILE
21	T	24	SER
27	3	29	THR
3	A	25	THR
3	A	245	SER
3	A	252	LYS
4	B	176	ASN
5	C	171	PRO
5	C	191	SER
6	D	89	VAL
7	E	33	LEU
7	E	36	THR
7	E	116	LYS
7	E	121	ILE
7	E	172	LYS
9	H	64	ARG
10	I	30	THR
10	I	128	PHE
11	J	89	ALA
14	M	108	LYS
16	O	16	GLU
19	R	77	GLU
20	S	68	LYS
20	S	157	ALA
20	S	167	ILE
22	U	12	ALA
23	V	12	SER
26	2	6	TYR
27	3	18	ALA
27	3	46	LYS
3	A	35	LYS
3	A	135	ILE
3	A	156	ARG
4	B	204	PRO
4	B	209	VAL
5	C	175	VAL
10	I	28	GLY
10	I	35	HIS

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Mol	Chain	Res	Type
13	L	65	THR
27	3	28	PHE
27	3	34	ALA
4	B	124	GLY
5	C	176	THR
6	D	132	VAL
11	J	25	ASN
27	3	45	ARG
14	M	37	GLY
20	S	124	PRO
3	A	85	PRO
20	S	74	VAL
5	C	149	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	120/224 (54%)	101 (84%)	19 (16%)	2	16
4	B	153/177 (86%)	136 (89%)	17 (11%)	6	29
5	C	106/169 (63%)	88 (83%)	18 (17%)	2	12
6	D	18/158 (11%)	17 (94%)	1 (6%)	21	55
7	E	67/155 (43%)	58 (87%)	9 (13%)	4	22
8	G	111/123 (90%)	101 (91%)	10 (9%)	9	38
9	H	91/100 (91%)	78 (86%)	13 (14%)	3	20
10	I	67/112 (60%)	52 (78%)	15 (22%)	1	5
11	J	103/119 (87%)	91 (88%)	12 (12%)	5	27
12	K	91/102 (89%)	81 (89%)	10 (11%)	6	30
13	L	47/95 (50%)	39 (83%)	8 (17%)	2	12
14	M	80/102 (78%)	66 (82%)	14 (18%)	2	11
15	N	93/98 (95%)	79 (85%)	14 (15%)	3	18
16	O	71/86 (83%)	60 (84%)	11 (16%)	2	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	P	91/94 (97%)	84 (92%)	7 (8%)	13	43
18	Q	53/82 (65%)	39 (74%)	14 (26%)	0	3
19	R	63/90 (70%)	46 (73%)	17 (27%)	0	3
20	S	91/190 (48%)	83 (91%)	8 (9%)	10	39
21	T	56/75 (75%)	48 (86%)	8 (14%)	3	20
22	U	18/52 (35%)	17 (94%)	1 (6%)	21	55
23	V	47/62 (76%)	42 (89%)	5 (11%)	6	31
24	W	52/53 (98%)	40 (77%)	12 (23%)	1	5
25	Z	38/51 (74%)	30 (79%)	8 (21%)	1	6
26	2	37/40 (92%)	32 (86%)	5 (14%)	4	21
27	3	37/57 (65%)	33 (89%)	4 (11%)	6	30
28	4	30/35 (86%)	27 (90%)	3 (10%)	7	33
All	All	1831/2701 (68%)	1568 (86%)	263 (14%)	3	19

All (263) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	45	ASN
3	A	46	GLN
3	A	53	HIS
3	A	58	HIS
3	A	79	ASP
3	A	88	SER
3	A	90	ASN
3	A	94	VAL
3	A	110	LEU
3	A	116	VAL
3	A	123	ASP
3	A	130	LEU
3	A	133	GLN
3	A	143	ASN
3	A	171	TYR
3	A	181	VAL
3	A	182	ARG
3	A	199	GLN
3	A	204	ASN
4	B	13	THR
4	B	15	VAL

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Mol	Chain	Res	Type
4	B	29	GLU
4	B	33	ASN
4	B	57	LYS
4	B	62	ASP
4	B	64	LYS
4	B	65	SER
4	B	81	ASP
4	B	107	VAL
4	B	114	ASP
4	B	117	ASP
4	B	133	ARG
4	B	177	THR
4	B	180	VAL
4	B	183	LEU
4	B	215	ILE
5	C	8	LYS
5	C	10	ASP
5	C	17	ILE
5	C	31	SER
5	C	35	GLU
5	C	39	LEU
5	C	49	HIS
5	C	67	GLN
5	C	68	LYS
5	C	74	ARG
5	C	78	ILE
5	C	115	SER
5	C	124	THR
5	C	144	SER
5	C	148	GLN
5	C	155	VAL
5	C	176	THR
5	C	181	LEU
6	D	26	MET
7	E	38	ASN
7	E	58	SER
7	E	61	ASP
7	E	79	VAL
7	E	89	LEU
7	E	92	VAL
7	E	115	ILE
7	E	131	VAL

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Mol	Chain	Res	Type
7	E	139	GLU
8	G	3	GLN
8	G	12	ILE
8	G	24	GLN
8	G	29	LEU
8	G	46	THR
8	G	58	ILE
8	G	66	THR
8	G	71	THR
8	G	92	GLU
8	G	101	LEU
9	H	8	LEU
9	H	23	LYS
9	H	24	VAL
9	H	32	THR
9	H	37	ASP
9	H	42	THR
9	H	52	VAL
9	H	58	VAL
9	H	63	VAL
9	H	88	ARG
9	H	107	ARG
9	H	112	MET
9	H	117	LEU
10	I	19	VAL
10	I	21	ARG
10	I	31	SER
10	I	47	ARG
10	I	50	PHE
10	I	51	GLU
10	I	55	LEU
10	I	67	THR
10	I	82	LEU
10	I	84	LYS
10	I	89	THR
10	I	96	LEU
10	I	112	LEU
10	I	122	THR
10	I	123	VAL
11	J	7	VAL
11	J	9	TYR
11	J	16	LYS

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Mol	Chain	Res	Type
11	J	21	SER
11	J	22	LYS
11	J	26	TYR
11	J	35	GLN
11	J	37	THR
11	J	41	TRP
11	J	91	GLU
11	J	122	SER
11	J	135	GLU
12	K	4	ARG
12	K	8	ARG
12	K	9	THR
12	K	28	GLU
12	K	33	THR
12	K	50	LEU
12	K	55	ASP
12	K	67	ARG
12	K	76	GLU
12	K	110	ARG
13	L	36	SER
13	L	41	TYR
13	L	45	ILE
13	L	46	ASP
13	L	53	LEU
13	L	91	GLU
13	L	92	ILE
13	L	99	TYR
14	M	11	THR
14	M	17	THR
14	M	32	VAL
14	M	48	VAL
14	M	51	LYS
14	M	52	ARG
14	M	53	ARG
14	M	60	THR
14	M	75	THR
14	M	80	THR
14	M	90	ARG
14	M	102	LEU
14	M	103	ARG
14	M	106	ARG
15	N	8	THR

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Mol	Chain	Res	Type
15	N	9	VAL
15	N	19	LYS
15	N	20	LEU
15	N	22	LYS
15	N	30	THR
15	N	42	SER
15	N	48	ARG
15	N	70	ARG
15	N	83	LEU
15	N	84	LYS
15	N	89	ASP
15	N	92	ARG
15	N	96	SER
16	O	7	THR
16	O	10	LYS
16	O	34	THR
16	O	48	VAL
16	O	59	THR
16	O	63	ASN
16	O	75	THR
16	O	78	ARG
16	O	84	ARG
16	O	86	LYS
16	O	98	ASP
17	P	2	GLU
17	P	11	ARG
17	P	19	LEU
17	P	38	LEU
17	P	62	TYR
17	P	81	THR
17	P	109	ASP
18	Q	5	ASP
18	Q	6	ILE
18	Q	12	ILE
18	Q	13	THR
18	Q	27	PHE
18	Q	28	ASP
18	Q	40	MET
18	Q	49	LYS
18	Q	58	TYR
18	Q	68	TYR
18	Q	72	THR

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Mol	Chain	Res	Type
18	Q	76	ARG
18	Q	87	ILE
18	Q	88	ASP
19	R	3	ILE
19	R	9	VAL
19	R	11	VAL
19	R	24	ILE
19	R	32	ARG
19	R	33	VAL
19	R	36	GLU
19	R	43	LYS
19	R	48	THR
19	R	56	ILE
19	R	59	THR
19	R	60	GLU
19	R	68	VAL
19	R	72	ASP
19	R	80	ARG
19	R	90	LYS
19	R	100	GLU
20	S	26	LYS
20	S	30	VAL
20	S	31	VAL
20	S	46	VAL
20	S	52	ILE
20	S	55	VAL
20	S	154	LEU
20	S	155	THR
21	T	24	SER
21	T	27	LYS
21	T	51	THR
21	T	61	ARG
21	T	64	ASP
21	T	66	THR
21	T	67	LEU
21	T	82	ARG
22	U	29	TRP
23	V	30	PHE
23	V	32	LEU
23	V	37	LEU
23	V	38	GLU
23	V	52	ARG

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Mol	Chain	Res	Type
24	W	1	MET
24	W	3	LYS
24	W	4	LEU
24	W	5	GLN
24	W	9	THR
24	W	12	VAL
24	W	15	ARG
24	W	18	THR
24	W	43	ILE
24	W	48	ASN
24	W	53	LEU
24	W	54	VAL
25	Z	5	LYS
25	Z	7	ARG
25	Z	28	THR
25	Z	30	CYS
25	Z	37	TYR
25	Z	38	LYS
25	Z	39	LEU
25	Z	44	CYS
26	2	2	VAL
26	2	5	THR
26	2	23	MET
26	2	42	VAL
26	2	44	SER
27	3	6	THR
27	3	29	THR
27	3	44	LEU
27	3	50	VAL
28	4	24	MET
28	4	26	ILE
28	4	29	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2691/2923 (92%)	627 (23%)	18 (0%)
2	Y	113/114 (99%)	13 (11%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	2804/3037 (92%)	640 (22%)	18 (0%)

All (640) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	2	A
1	X	4	U
1	X	9	U
1	X	12	U
1	X	14	A
1	X	15	G
1	X	34	U
1	X	35	G
1	X	39	C
1	X	51	G
1	X	60	U
1	X	64	A
1	X	70	G
1	X	71	A
1	X	72	U
1	X	75	G
1	X	80	G
1	X	90	A
1	X	91	A
1	X	96	G
1	X	101	G
1	X	109	G
1	X	111	U
1	X	115	C
1	X	117	A
1	X	118	A
1	X	119	U
1	X	124	A
1	X	130	A
1	X	133	A
1	X	139	U
1	X	140	A
1	X	152	C
1	X	153	G
1	X	154	A
1	X	155	U
1	X	156	A

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Mol	Chain	Res	Type
1	X	157	U
1	X	164	A
1	X	165	C
1	X	166	A
1	X	167	U
1	X	169	G
1	X	170	C
1	X	171	A
1	X	172	U
1	X	173	A
1	X	176	A
1	X	177	G
1	X	179	A
1	X	180	G
1	X	182	C
1	X	183	A
1	X	184	C
1	X	194	A
1	X	199	A
1	X	202	A
1	X	207	A
1	X	219	A
1	X	224	A
1	X	225	A
1	X	227	G
1	X	229	A
1	X	233	U
1	X	235	G
1	X	236	A
1	X	244	A
1	X	248	G
1	X	251	G
1	X	255	G
1	X	268	A
1	X	284	C
1	X	285	U
1	X	286	U
1	X	287	G
1	X	288	C
1	X	289	U
1	X	290	U
1	X	291	G

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Mol	Chain	Res	Type
1	X	298	U
1	X	300	G
1	X	301	U
1	X	303	G
1	X	310	C
1	X	311	U
1	X	313	U
1	X	319	G
1	X	320	U
1	X	321	U
1	X	322	A
1	X	323	C
1	X	328	G
1	X	329	A
1	X	330	C
1	X	332	A
1	X	338	G
1	X	350	G
1	X	359	A
1	X	364	A
1	X	372	A
1	X	373	A
1	X	375	A
1	X	389	A
1	X	390	A
1	X	392	U
1	X	401	U
1	X	403	U
1	X	404	U
1	X	406	A
1	X	410	G
1	X	413	C
1	X	415	U
1	X	416	G
1	X	417	A
1	X	418	G
1	X	432	G
1	X	434	G
1	X	444	C
1	X	447	A
1	X	449	U
1	X	450	C

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Mol	Chain	Res	Type
1	X	451	U
1	X	452	G
1	X	457	G
1	X	458	A
1	X	474	A
1	X	480	U
1	X	486	G
1	X	501	C
1	X	502	C
1	X	503	A
1	X	504	G
1	X	506	A
1	X	519	G
1	X	523	A
1	X	526	A
1	X	527	G
1	X	541	G
1	X	543	G
1	X	549	U
1	X	550	A
1	X	553	A
1	X	554	C
1	X	566	U
1	X	567	G
1	X	572	C
1	X	573	A
1	X	576	U
1	X	577	A
1	X	578	G
1	X	583	A
1	X	590	U
1	X	591	A
1	X	592	A
1	X	593	U
1	X	594	G
1	X	606	G
1	X	616	G
1	X	618	A
1	X	627	C
1	X	630	G
1	X	646	A
1	X	647	G

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Mol	Chain	Res	Type
1	X	654	C
1	X	658	A
1	X	659	A
1	X	660	A
1	X	661	U
1	X	666	A
1	X	667	G
1	X	670	G
1	X	682	A
1	X	683	G
1	X	690	U
1	X	691	A
1	X	697	U
1	X	698	U
1	X	699	U
1	X	713	A
1	X	715	A
1	X	716	C
1	X	722	A
1	X	727	G
1	X	731	U
1	X	735	C
1	X	740	G
1	X	757	G
1	X	766	G
1	X	773	G
1	X	775	A
1	X	783	G
1	X	784	A
1	X	792	U
1	X	793	G
1	X	802	G
1	X	809	A
1	X	813	G
1	X	816	G
1	X	820	G
1	X	821	C
1	X	827	A
1	X	829	U
1	X	830	U
1	X	835	U
1	X	836	C

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Mol	Chain	Res	Type
1	X	837	G
1	X	838	A
1	X	848	U
1	X	850	G
1	X	857	C
1	X	864	A
1	X	866	A
1	X	872	U
1	X	873	U
1	X	875	G
1	X	887	A
1	X	892	U
1	X	904	G
1	X	911	A
1	X	922	G
1	X	923	A
1	X	924	G
1	X	943	C
1	X	944	G
1	X	947	U
1	X	955	A
1	X	959	C
1	X	964	U
1	X	970	U
1	X	971	U
1	X	977	A
1	X	985	A
1	X	989	A
1	X	990	G
1	X	1001	A
1	X	1005	G
1	X	1017	A
1	X	1018	A
1	X	1027	A
1	X	1029	C
1	X	1033	G
1	X	1034	A
1	X	1040	A
1	X	1043	U
1	X	1056	U
1	X	1057	A
1	X	1061	G

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Mol	Chain	Res	Type
1	X	1064	A
1	X	1066	G
1	X	1067	U
1	X	1069	G
1	X	1070	A
1	X	1077	U
1	X	1078	G
1	X	1086	G
1	X	1087	C
1	X	1089	C
1	X	1091	G
1	X	1092	A
1	X	1093	C
1	X	1145	U
1	X	1146	C
1	X	1147	A
1	X	1148	C
1	X	1150	A
1	X	1151	G
1	X	1154	G
1	X	1155	A
1	X	1156	G
1	X	1172	A
1	X	1176	U
1	X	1178	C
1	X	1179	C
1	X	1180	G
1	X	1186	A
1	X	1195	A
1	X	1200	A
1	X	1213	C
1	X	1215	U
1	X	1218	G
1	X	1222	A
1	X	1250	G
1	X	1276	G
1	X	1278	G
1	X	1284	A
1	X	1285	A
1	X	1286	G
1	X	1291	A
1	X	1293	U

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Mol	Chain	Res	Type
1	X	1294	G
1	X	1309	G
1	X	1310	A
1	X	1311	A
1	X	1313	G
1	X	1324	A
1	X	1337	A
1	X	1338	U
1	X	1339	U
1	X	1349	U
1	X	1366	U
1	X	1382	C
1	X	1389	U
1	X	1401	G
1	X	1402	A
1	X	1405	G
1	X	1415	A
1	X	1416	U
1	X	1421	A
1	X	1422	A
1	X	1432	A
1	X	1433	U
1	X	1437	U
1	X	1448	U
1	X	1449	A
1	X	1450	A
1	X	1451	U
1	X	1452	C
1	X	1453	G
1	X	1454	U
1	X	1461	C
1	X	1462	G
1	X	1463	A
1	X	1464	U
1	X	1465	G
1	X	1466	G
1	X	1467	G
1	X	1471	A
1	X	1472	C
1	X	1481	A
1	X	1489	A
1	X	1490	G

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Mol	Chain	Res	Type
1	X	1491	C
1	X	1492	G
1	X	1493	U
1	X	1494	G
1	X	1495	C
1	X	1496	G
1	X	1497	A
1	X	1498	U
1	X	1503	U
1	X	1504	U
1	X	1505	G
1	X	1508	C
1	X	1509	G
1	X	1510	U
1	X	1511	C
1	X	1512	U
1	X	1513	A
1	X	1514	A
1	X	1515	G
1	X	1516	C
1	X	1519	U
1	X	1522	G
1	X	1524	C
1	X	1527	A
1	X	1528	G
1	X	1529	U
1	X	1541	C
1	X	1542	C
1	X	1543	G
1	X	1544	G
1	X	1546	A
1	X	1547	C
1	X	1548	U
1	X	1550	G
1	X	1556	G
1	X	1557	C
1	X	1561	G
1	X	1568	U
1	X	1569	G
1	X	1573	A
1	X	1575	A
1	X	1576	A

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Mol	Chain	Res	Type
1	X	1577	G
1	X	1592	A
1	X	1593	G
1	X	1594	U
1	X	1599	G
1	X	1603	U
1	X	1605	A
1	X	1613	G
1	X	1616	A
1	X	1623	U
1	X	1625	U
1	X	1628	A
1	X	1629	U
1	X	1630	A
1	X	1631	G
1	X	1632	A
1	X	1636	U
1	X	1637	A
1	X	1638	G
1	X	1650	G
1	X	1652	A
1	X	1653	A
1	X	1657	G
1	X	1662	A
1	X	1683	U
1	X	1684	A
1	X	1690	A
1	X	1691	G
1	X	1692	C
1	X	1695	G
1	X	1718	G
1	X	1732	U
1	X	1738	C
1	X	1739	G
1	X	1740	G
1	X	1744	A
1	X	1745	A
1	X	1746	G
1	X	1755	U
1	X	1756	U
1	X	1757	U
1	X	1760	G

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Mol	Chain	Res	Type
1	X	1761	G
1	X	1762	U
1	X	1763	U
1	X	1765	A
1	X	1766	C
1	X	1768	C
1	X	1770	C
1	X	1771	A
1	X	1772	G
1	X	1789	A
1	X	1790	G
1	X	1791	G
1	X	1800	A
1	X	1808	U
1	X	1818	A
1	X	1826	G
1	X	1827	C
1	X	1828	U
1	X	1829	A
1	X	1835	U
1	X	1836	A
1	X	1837	A
1	X	1843	U
1	X	1847	U
1	X	1848	A
1	X	1856	A
1	X	1865	C
1	X	1875	A
1	X	1885	G
1	X	1902	G
1	X	1908	A
1	X	1909	C
1	X	1911	A
1	X	1912	A
1	X	1930	G
1	X	1932	C
1	X	1933	G
1	X	1953	U
1	X	1954	A
1	X	1955	A
1	X	1963	A
1	X	1964	A

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Mol	Chain	Res	Type
1	X	1965	A
1	X	1982	U
1	X	1987	A
1	X	1994	C
1	X	1997	A
1	X	1998	A
1	X	1999	G
1	X	2009	U
1	X	2018	U
1	X	2019	G
1	X	2020	U
1	X	2024	A
1	X	2050	A
1	X	2058	A
1	X	2059	G
1	X	2060	A
1	X	2070	C
1	X	2078	A
1	X	2079	G
1	X	2082	C
1	X	2083	G
1	X	2084	G
1	X	2087	A
1	X	2088	G
1	X	2089	A
1	X	2094	G
1	X	2096	G
1	X	2107	G
1	X	2119	U
1	X	2225	A
1	X	2226	A
1	X	2230	G
1	X	2231	C
1	X	2232	A
1	X	2233	C
1	X	2234	C
1	X	2237	U
1	X	2238	U
1	X	2239	A
1	X	2240	U
1	X	2241	C
1	X	2246	U

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Mol	Chain	Res	Type
1	X	2248	G
1	X	2252	A
1	X	2253	C
1	X	2266	G
1	X	2270	U
1	X	2289	U
1	X	2295	A
1	X	2298	G
1	X	2306	G
1	X	2310	C
1	X	2314	A
1	X	2332	U
1	X	2333	U
1	X	2334	G
1	X	2339	U
1	X	2345	A
1	X	2347	A
1	X	2352	G
1	X	2354	A
1	X	2361	U
1	X	2362	A
1	X	2363	A
1	X	2374	C
1	X	2377	C
1	X	2398	G
1	X	2399	G
1	X	2406	G
1	X	2410	G
1	X	2412	C
1	X	2417	U
1	X	2429	U
1	X	2433	C
1	X	2434	A
1	X	2440	G
1	X	2441	G
1	X	2449	C
1	X	2450	U
1	X	2452	A
1	X	2456	G
1	X	2457	A
1	X	2458	U
1	X	2461	A

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Mol	Chain	Res	Type
1	X	2468	C
1	X	2472	G
1	X	2475	A
1	X	2497	G
1	X	2500	U
1	X	2501	U
1	X	2503	A
1	X	2505	A
1	X	2514	G
1	X	2519	U
1	X	2525	C
1	X	2529	G
1	X	2532	G
1	X	2533	U
1	X	2534	C
1	X	2545	A
1	X	2546	U
1	X	2547	C
1	X	2556	G
1	X	2561	C
1	X	2576	G
1	X	2581	U
1	X	2591	A
1	X	2593	A
1	X	2594	G
1	X	2600	C
1	X	2609	G
1	X	2612	U
1	X	2613	C
1	X	2629	A
1	X	2630	G
1	X	2631	U
1	X	2636	U
1	X	2640	U
1	X	2641	A
1	X	2642	U
1	X	2648	G
1	X	2656	A
1	X	2661	A
1	X	2663	U
1	X	2666	A
1	X	2681	A

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Mol	Chain	Res	Type
1	X	2682	G
1	X	2690	G
1	X	2698	A
1	X	2712	G
1	X	2715	G
1	X	2716	U
1	X	2717	A
1	X	2737	C
1	X	2741	G
1	X	2745	G
1	X	2753	U
1	X	2760	A
1	X	2766	U
1	X	2771	G
1	X	2775	A
1	X	2778	G
1	X	2784	A
1	X	2787	C
1	X	2792	A
1	X	2805	A
1	X	2806	U
1	X	2807	G
1	X	2817	A
1	X	2818	A
1	X	2819	C
1	X	2820	U
1	X	2821	U
1	X	2824	G
1	X	2827	A
1	X	2832	A
1	X	2838	C
1	X	2840	A
1	X	2843	A
1	X	2850	G
1	X	2854	A
1	X	2856	U
1	X	2877	G
1	X	2887	G
1	X	2892	G
1	X	2896	A
1	X	2899	A
1	X	2900	C

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Mol	Chain	Res	Type
1	X	2913	G
1	X	2920	U
2	Y	10	U
2	Y	23	U
2	Y	24	C
2	Y	38	U
2	Y	39	G
2	Y	42	G
2	Y	43	A
2	Y	54	U
2	Y	86	C
2	Y	87	G
2	Y	88	U
2	Y	106	U
2	Y	114	C

All (18) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	38	A
1	X	90	A
1	X	165	C
1	X	373	A
1	X	525	A
1	X	660	A
1	X	1091	G
1	X	1490	G
1	X	1503	U
1	X	1510	U
1	X	1521	A
1	X	1526	G
1	X	1568	U
1	X	1575	A
1	X	1576	A
1	X	1901	C
1	X	2457	A
1	X	2823	G

## 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 346 ligands modelled in this entry, 322 are monoatomic - leaving 24 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	$\# Z  > 2$
29	MPD	X	3011	-	7,7,7	0.88	0	9,10,10	0.45	0
29	MPD	X	3003	-	7,7,7	0.30	0	9,10,10	0.37	0
34	EOH	X	3317	-	2,2,2	0.53	0	1,1,1	0.66	0
32	EPE	X	3311	-	15,15,15	1.27	1 (6%)	18,20,20	0.45	0
29	MPD	X	3010	-	7,7,7	0.63	0	9,10,10	0.35	0
29	MPD	X	3001	-	7,7,7	0.33	0	9,10,10	0.45	0
29	MPD	X	3009	-	7,7,7	0.66	0	9,10,10	0.25	0
34	EOH	X	3320	-	2,2,2	0.58	0	1,1,1	0.63	0
29	MPD	X	3002	-	7,7,7	0.96	1 (14%)	9,10,10	0.53	0
34	EOH	X	3321	-	2,2,2	0.58	0	1,1,1	0.62	0
29	MPD	X	3008	-	7,7,7	0.69	0	9,10,10	0.32	0
33	SPD	X	3313	-	9,9,9	0.19	0	8,8,8	0.27	0
34	EOH	X	3322	-	2,2,2	0.54	0	1,1,1	0.66	0
29	MPD	X	3004	-	7,7,7	0.58	0	9,10,10	0.19	0
33	SPD	X	3314	-	9,9,9	0.14	0	8,8,8	0.22	0
29	MPD	X	3007	-	7,7,7	0.79	0	9,10,10	0.41	0
34	EOH	X	3316	-	2,2,2	0.67	0	1,1,1	0.41	0
34	EOH	X	3319	-	2,2,2	0.50	0	1,1,1	0.76	0
29	MPD	X	3006	-	7,7,7	0.46	0	9,10,10	0.10	0
33	SPD	X	3315	-	9,9,9	0.23	0	8,8,8	0.23	0
33	SPD	X	3312	-	9,9,9	0.28	0	8,8,8	0.34	0
29	MPD	Z	101	-	7,7,7	0.30	0	9,10,10	0.36	0
29	MPD	X	3005	-	7,7,7	0.67	0	9,10,10	0.23	0
34	EOH	X	3318	-	2,2,2	0.56	0	1,1,1	0.64	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
29	MPD	X	3009	-	-	1/5/5/5	-
29	MPD	X	3011	-	-	2/5/5/5	-
29	MPD	X	3003	-	-	3/5/5/5	-
29	MPD	X	3008	-	-	1/5/5/5	-
33	SPD	X	3313	-	-	2/7/7/7	-
29	MPD	X	3006	-	-	1/5/5/5	-
33	SPD	X	3315	-	-	2/7/7/7	-
33	SPD	X	3312	-	-	1/7/7/7	-
32	EPE	X	3311	-	-	6/9/19/19	0/1/1/1
29	MPD	Z	101	-	-	3/5/5/5	-
29	MPD	X	3005	-	-	3/5/5/5	-
29	MPD	X	3010	-	-	3/5/5/5	-
29	MPD	X	3004	-	-	0/5/5/5	-
29	MPD	X	3001	-	-	0/5/5/5	-
33	SPD	X	3314	-	-	2/7/7/7	-
29	MPD	X	3007	-	-	5/5/5/5	-
29	MPD	X	3002	-	-	2/5/5/5	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	X	3311	EPE	C10-S	-4.67	1.70	1.77
29	X	3002	MPD	C3-C2	2.32	1.60	1.53

There are no bond angle outliers.

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	X	3009	MPD	C2-C3-C4-C5
29	X	3011	MPD	C2-C3-C4-O4
29	X	3011	MPD	C2-C3-C4-C5
29	X	3007	MPD	C2-C3-C4-O4
29	X	3003	MPD	C2-C3-C4-C5
32	X	3311	EPE	C8-C7-N4-C3
32	X	3311	EPE	C9-C10-S-O1S
32	X	3311	EPE	C9-C10-S-O3S

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Mol	Chain	Res	Type	Atoms
29	X	3006	MPD	C2-C3-C4-C5
29	X	3010	MPD	C2-C3-C4-O4
29	X	3002	MPD	C2-C3-C4-O4
32	X	3311	EPE	C10-C9-N1-C2
32	X	3311	EPE	C10-C9-N1-C6
33	X	3313	SPD	C8-C7-N6-C5
29	X	3007	MPD	O2-C2-C3-C4
29	X	3002	MPD	O2-C2-C3-C4
33	X	3312	SPD	C8-C7-N6-C5
29	X	3007	MPD	C2-C3-C4-C5
32	X	3311	EPE	C9-C10-S-O2S
29	X	3008	MPD	CM-C2-C3-C4
29	Z	101	MPD	C1-C2-C3-C4
29	X	3007	MPD	C1-C2-C3-C4
29	X	3007	MPD	CM-C2-C3-C4
29	X	3010	MPD	C1-C2-C3-C4
29	X	3005	MPD	C1-C2-C3-C4
33	X	3314	SPD	C2-C3-C4-C5
33	X	3315	SPD	C8-C7-N6-C5
29	Z	101	MPD	O2-C2-C3-C4
29	X	3003	MPD	O2-C2-C3-C4
29	X	3010	MPD	O2-C2-C3-C4
33	X	3314	SPD	C4-C5-N6-C7
33	X	3313	SPD	C7-C8-C9-N10
29	Z	101	MPD	C2-C3-C4-C5
29	X	3005	MPD	C2-C3-C4-C5
33	X	3315	SPD	N1-C2-C3-C4
29	X	3003	MPD	C2-C3-C4-O4
29	X	3005	MPD	C2-C3-C4-O4

There are no ring outliers.

5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	X	3011	MPD	1	0
29	X	3003	MPD	4	0
29	X	3008	MPD	1	0
29	X	3007	MPD	4	0
29	X	3005	MPD	4	0



## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	X	2708/2923 (92%)	-0.47	9 (0%) 94 89	11, 51, 139, 230	0
2	Y	114/114 (100%)	-0.66	0 100 100	22, 67, 115, 151	0
3	A	269/277 (97%)	-0.24	4 (1%) 73 61	43, 74, 106, 136	0
4	B	215/220 (97%)	-0.32	0 100 100	12, 28, 66, 97	0
5	C	199/207 (96%)	-0.53	1 (0%) 91 84	12, 35, 71, 107	0
6	D	166/179 (92%)	-0.41	2 (1%) 79 67	80, 102, 132, 150	0
7	E	156/178 (87%)	-0.26	3 (1%) 66 53	61, 86, 120, 131	0
8	G	145/145 (100%)	-0.28	1 (0%) 87 79	9, 26, 58, 114	0
9	H	122/122 (100%)	-0.39	0 100 100	17, 41, 74, 102	0
10	I	131/146 (89%)	-0.11	2 (1%) 73 61	14, 47, 91, 108	0
11	J	141/144 (97%)	-0.04	3 (2%) 63 50	25, 43, 97, 121	0
12	K	119/122 (97%)	-0.44	0 100 100	14, 37, 86, 97	0
13	L	110/119 (92%)	-0.50	0 100 100	39, 62, 92, 111	0
14	M	110/116 (94%)	-0.48	1 (0%) 84 73	23, 43, 89, 115	0
15	N	116/118 (98%)	-0.54	0 100 100	6, 21, 59, 69	0
16	O	102/102 (100%)	-0.57	0 100 100	7, 35, 75, 92	0
17	P	112/117 (95%)	-0.35	0 100 100	7, 21, 86, 125	0
18	Q	89/91 (97%)	-0.22	1 (1%) 80 69	39, 60, 93, 108	0
19	R	100/105 (95%)	0.18	3 (3%) 50 37	43, 66, 122, 142	0
20	S	167/217 (76%)	-0.19	2 (1%) 79 67	42, 61, 120, 130	0
21	T	75/94 (79%)	0.20	3 (4%) 38 28	21, 39, 81, 102	0
22	U	46/62 (74%)	1.90	19 (41%) 0 0	60, 91, 122, 130	0
23	V	65/69 (94%)	-0.29	0 100 100	48, 71, 105, 119	0
24	W	58/59 (98%)	-0.11	0 100 100	12, 24, 72, 108	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	Z	43/58 (74%)	-0.39	0 100 100	11, 20, 99, 127	0
26	2	44/45 (97%)	0.01	1 (2%) 60 46	19, 41, 73, 93	0
27	3	60/66 (90%)	-0.43	0 100 100	10, 32, 69, 83	0
28	4	37/37 (100%)	1.54	10 (27%) 0 0	39, 60, 89, 103	0
All	All	5819/6252 (93%)	-0.35	65 (1%) 80 69	6, 51, 123, 230	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	U	13	SER	6.3
22	U	12	ALA	6.1
22	U	14	THR	5.3
22	U	11	LYS	5.1
20	S	146	THR	4.1
22	U	17	ARG	4.1
22	U	38	ILE	4.0
22	U	30	ASN	3.9
28	4	12	GLU	3.7
1	X	1148	C	3.7
6	D	82	GLY	3.5
22	U	28	ARG	3.4
22	U	15	GLY	3.4
11	J	3	LEU	3.3
28	4	36	GLN	3.2
22	U	47	VAL	3.1
18	Q	27	PHE	3.0
1	X	2	A	3.0
22	U	16	ASN	3.0
26	2	2	VAL	2.8
14	M	1	MET	2.8
28	4	30	PRO	2.7
19	R	88	GLY	2.7
11	J	138	GLY	2.6
3	A	11	ASN	2.6
1	X	942	C	2.6
22	U	37	ARG	2.6
22	U	10	ARG	2.5
20	S	147	GLU	2.4
28	4	34	GLN	2.4
21	T	50	GLY	2.4
28	4	24	MET	2.4

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Mol	Chain	Res	Type	RSRZ
22	U	50	SER	2.4
3	A	57	GLY	2.4
1	X	2439	A	2.3
28	4	29	ASN	2.3
1	X	458	A	2.3
8	G	1	MET	2.3
22	U	20	HIS	2.3
1	X	1147	A	2.3
1	X	2629	A	2.3
22	U	18	ARG	2.3
22	U	46	LYS	2.3
11	J	139	GLY	2.2
22	U	29	TRP	2.2
7	E	55	PRO	2.2
7	E	90	VAL	2.2
1	X	549	U	2.2
3	A	101	LYS	2.2
5	C	96	SER	2.2
28	4	7	VAL	2.1
19	R	54	GLY	2.1
3	A	94	VAL	2.1
28	4	3	VAL	2.1
7	E	164	TYR	2.1
28	4	13	LYS	2.1
21	T	69	ALA	2.1
6	D	83	MET	2.1
19	R	55	GLY	2.1
10	I	58	PHE	2.0
1	X	2760	A	2.0
28	4	25	VAL	2.0
21	T	61	ARG	2.0
22	U	34	GLN	2.0
10	I	92	THR	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.



## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
30	MN	X	3308	1/1	0.39	0.74	92,92,92,92	0
31	MG	G	203	1/1	0.47	0.33	17,17,17,17	0
30	MN	X	3055	1/1	0.62	0.21	94,94,94,94	0
30	MN	X	3053	1/1	0.63	0.54	89,89,89,89	0
31	MG	X	3113	1/1	0.66	1.07	45,45,45,45	0
30	MN	X	3132	1/1	0.67	0.16	97,97,97,97	0
30	MN	X	3044	1/1	0.70	0.24	94,94,94,94	0
30	MN	B	303	1/1	0.70	0.74	102,102,102,102	0
31	MG	X	3083	1/1	0.70	0.34	37,37,37,37	0
34	EOH	X	3317	3/3	0.71	0.51	46,46,46,46	0
31	MG	X	3173	1/1	0.71	1.13	26,26,26,26	0
30	MN	X	3213	1/1	0.71	0.23	95,95,95,95	0
30	MN	X	3057	1/1	0.71	0.20	71,71,71,71	0
30	MN	X	3133	1/1	0.72	0.31	98,98,98,98	0
30	MN	X	3222	1/1	0.73	0.35	71,71,71,71	0
30	MN	X	3168	1/1	0.73	0.21	74,74,74,74	0
31	MG	X	3034	1/1	0.73	0.39	18,18,18,18	0
30	MN	X	3015	1/1	0.74	0.38	75,75,75,75	0
30	MN	X	3050	1/1	0.74	0.47	99,99,99,99	0
31	MG	X	3016	1/1	0.74	0.39	23,23,23,23	0
30	MN	X	3148	1/1	0.75	0.25	79,79,79,79	0
31	MG	X	3084	1/1	0.76	0.14	14,14,14,14	0
31	MG	X	3013	1/1	0.76	0.83	30,30,30,30	0
33	SPD	X	3312	10/10	0.77	0.29	47,47,47,47	0
30	MN	X	3182	1/1	0.77	0.38	107,107,107,107	0
31	MG	X	3023	1/1	0.78	0.29	37,37,37,37	0
30	MN	X	3121	1/1	0.78	0.31	88,88,88,88	0
29	MPD	X	3008	8/8	0.79	0.35	70,70,70,70	0
30	MN	X	3128	1/1	0.79	0.16	84,84,84,84	0
30	MN	X	3066	1/1	0.79	0.12	56,56,56,56	0
30	MN	X	3143	1/1	0.79	0.18	94,94,94,94	0
30	MN	J	201	1/1	0.80	0.20	78,78,78,78	0
30	MN	X	3111	1/1	0.80	0.13	99,99,99,99	0
31	MG	X	3175	1/1	0.80	0.30	0,0,0,0	0
31	MG	X	3137	1/1	0.80	0.92	17,17,17,17	0
29	MPD	X	3010	8/8	0.81	0.33	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
30	MN	X	3293	1/1	0.81	0.19	70,70,70,70	0
30	MN	X	3220	1/1	0.81	0.43	68,68,68,68	0
30	MN	X	3124	1/1	0.81	0.11	77,77,77,77	0
30	MN	X	3126	1/1	0.81	0.24	77,77,77,77	0
31	MG	X	3298	1/1	0.82	1.02	23,23,23,23	0
31	MG	X	3114	1/1	0.82	0.57	36,36,36,36	0
30	MN	X	3130	1/1	0.82	0.13	102,102,102,102	0
30	MN	X	3140	1/1	0.82	0.17	71,71,71,71	0
30	MN	X	3076	1/1	0.83	0.09	74,74,74,74	0
30	MN	X	3135	1/1	0.83	0.14	94,94,94,94	0
34	EOH	X	3318	3/3	0.83	0.27	47,47,47,47	0
30	MN	X	3052	1/1	0.83	0.21	71,71,71,71	0
30	MN	X	3123	1/1	0.83	0.42	97,97,97,97	0
30	MN	X	3138	1/1	0.83	0.10	112,112,112,112	0
31	MG	X	3109	1/1	0.83	0.70	24,24,24,24	0
29	MPD	X	3002	8/8	0.83	0.32	45,45,45,45	0
30	MN	X	3254	1/1	0.83	0.23	48,48,48,48	0
31	MG	X	3093	1/1	0.84	0.27	21,21,21,21	0
30	MN	X	3059	1/1	0.84	0.10	61,61,61,61	0
30	MN	X	3122	1/1	0.84	0.50	89,89,89,89	0
30	MN	X	3090	1/1	0.84	0.35	96,96,96,96	0
31	MG	X	3095	1/1	0.84	0.34	26,26,26,26	0
31	MG	X	3079	1/1	0.84	0.74	27,27,27,27	0
30	MN	X	3042	1/1	0.84	0.11	104,104,104,104	0
33	SPD	X	3315	10/10	0.84	0.31	46,46,46,46	0
30	MN	X	3131	1/1	0.85	0.48	89,89,89,89	0
29	MPD	X	3011	8/8	0.85	0.24	39,39,39,39	0
30	MN	I	202	1/1	0.85	0.25	64,64,64,64	0
29	MPD	X	3006	8/8	0.85	0.18	88,88,88,88	0
34	EOH	X	3316	3/3	0.85	0.40	10,10,10,10	0
31	MG	X	3106	1/1	0.85	0.22	37,37,37,37	0
30	MN	X	3158	1/1	0.85	0.22	62,62,62,62	0
30	MN	X	3125	1/1	0.85	0.32	79,79,79,79	0
31	MG	X	3294	1/1	0.86	0.34	37,37,37,37	0
31	MG	G	201	1/1	0.86	0.20	19,19,19,19	0
30	MN	X	3268	1/1	0.86	0.29	27,27,27,27	0
33	SPD	X	3313	10/10	0.86	0.29	30,30,30,30	0
30	MN	X	3068	1/1	0.87	0.21	70,70,70,70	0
31	MG	X	3172	1/1	0.87	0.79	27,27,27,27	0
31	MG	Y	203	1/1	0.87	0.76	21,21,21,21	0
33	SPD	X	3314	10/10	0.87	0.48	26,26,26,26	0
30	MN	X	3118	1/1	0.87	0.31	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	X	3302	1/1	0.87	0.30	20,20,20,20	0
30	MN	X	3183	1/1	0.88	0.15	41,41,41,41	0
34	EOH	X	3321	3/3	0.88	0.30	18,18,18,18	0
30	MN	X	3073	1/1	0.88	0.14	86,86,86,86	0
31	MG	Y	201	1/1	0.88	0.11	34,34,34,34	0
31	MG	X	3039	1/1	0.88	0.30	7,7,7,7	0
31	MG	Y	205	1/1	0.88	0.14	12,12,12,12	0
30	MN	Y	202	1/1	0.88	0.14	57,57,57,57	0
31	MG	X	3174	1/1	0.88	0.31	5,5,5,5	0
31	MG	X	3082	1/1	0.88	0.17	31,31,31,31	0
30	MN	X	3276	1/1	0.88	0.17	42,42,42,42	0
34	EOH	X	3320	3/3	0.88	0.28	28,28,28,28	0
30	MN	X	3216	1/1	0.89	0.19	54,54,54,54	0
31	MG	X	3035	1/1	0.89	0.34	23,23,23,23	0
31	MG	X	3031	1/1	0.89	0.33	11,11,11,11	0
30	MN	X	3074	1/1	0.89	0.06	78,78,78,78	0
30	MN	X	3223	1/1	0.89	0.24	60,60,60,60	0
30	MN	X	3273	1/1	0.89	0.27	41,41,41,41	0
31	MG	B	301	1/1	0.89	0.14	0,0,0,0	0
30	MN	X	3169	1/1	0.89	0.67	78,78,78,78	0
34	EOH	X	3319	3/3	0.90	0.19	47,47,47,47	0
30	MN	X	3290	1/1	0.90	0.18	89,89,89,89	0
31	MG	C	301	1/1	0.90	0.25	2,2,2,2	0
31	MG	X	3305	1/1	0.90	0.91	15,15,15,15	0
31	MG	X	3028	1/1	0.90	0.30	34,34,34,34	0
30	MN	X	3127	1/1	0.90	0.13	44,44,44,44	0
30	MN	X	3155	1/1	0.90	0.38	87,87,87,87	0
29	MPD	Z	101	8/8	0.90	0.35	48,48,48,48	0
30	MN	X	3146	1/1	0.90	0.23	101,101,101,101	0
30	MN	X	3244	1/1	0.90	0.18	57,57,57,57	0
31	MG	X	3097	1/1	0.90	0.23	14,14,14,14	0
30	MN	X	3192	1/1	0.90	0.32	84,84,84,84	0
30	MN	X	3134	1/1	0.91	0.18	58,58,58,58	0
31	MG	X	3085	1/1	0.91	0.21	9,9,9,9	0
30	MN	X	3250	1/1	0.91	0.27	80,80,80,80	0
31	MG	X	3115	1/1	0.91	0.72	1,1,1,1	1
31	MG	X	3300	1/1	0.91	0.16	11,11,11,11	0
31	MG	X	3022	1/1	0.91	0.60	25,25,25,25	0
30	MN	X	3058	1/1	0.91	0.14	64,64,64,64	0
31	MG	X	3098	1/1	0.91	0.33	14,14,14,14	0
31	MG	X	3038	1/1	0.91	0.29	23,23,23,23	0
30	MN	X	3288	1/1	0.91	0.11	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
30	MN	X	3178	1/1	0.91	0.46	78,78,78,78	0
30	MN	X	3067	1/1	0.91	0.19	51,51,51,51	0
34	EOH	X	3322	3/3	0.91	0.47	34,34,34,34	0
30	MN	X	3041	1/1	0.91	0.22	84,84,84,84	0
31	MG	X	3026	1/1	0.91	0.61	18,18,18,18	0
29	MPD	X	3004	8/8	0.92	0.34	73,73,73,73	0
30	MN	X	3230	1/1	0.92	0.28	65,65,65,65	0
30	MN	X	3255	1/1	0.92	0.56	35,35,35,35	0
30	MN	X	3233	1/1	0.92	0.26	63,63,63,63	0
30	MN	X	3065	1/1	0.92	0.10	60,60,60,60	0
31	MG	O	201	1/1	0.92	0.28	7,7,7,7	0
31	MG	X	3297	1/1	0.92	0.31	5,5,5,5	0
30	MN	X	3186	1/1	0.92	0.29	51,51,51,51	0
29	MPD	X	3009	8/8	0.92	0.15	76,76,76,76	0
30	MN	X	3063	1/1	0.92	0.13	60,60,60,60	0
31	MG	X	3107	1/1	0.92	0.59	18,18,18,18	0
30	MN	X	3117	1/1	0.92	0.25	80,80,80,80	0
31	MG	I	201	1/1	0.92	0.26	0,0,0,0	0
30	MN	X	3226	1/1	0.92	0.33	89,89,89,89	0
30	MN	X	3227	1/1	0.92	0.17	57,57,57,57	0
31	MG	X	3103	1/1	0.92	0.45	3,3,3,3	0
30	MN	X	3207	1/1	0.92	0.44	62,62,62,62	0
30	MN	X	3199	1/1	0.92	0.36	51,51,51,51	0
31	MG	X	3299	1/1	0.93	0.26	5,5,5,5	0
30	MN	X	3072	1/1	0.93	0.17	80,80,80,80	0
30	MN	X	3269	1/1	0.93	0.24	36,36,36,36	0
31	MG	X	3018	1/1	0.93	0.47	15,15,15,15	0
30	MN	X	3061	1/1	0.93	0.12	63,63,63,63	0
31	MG	X	3019	1/1	0.93	0.25	15,15,15,15	0
30	MN	X	3202	1/1	0.93	0.23	54,54,54,54	0
31	MG	X	3309	1/1	0.93	0.24	20,20,20,20	0
31	MG	X	3100	1/1	0.93	0.21	17,17,17,17	0
31	MG	X	3136	1/1	0.93	0.34	27,27,27,27	0
30	MN	X	3119	1/1	0.93	0.15	63,63,63,63	0
30	MN	X	3231	1/1	0.93	0.24	74,74,74,74	0
30	MN	X	3149	1/1	0.93	0.27	94,94,94,94	0
31	MG	X	3304	1/1	0.93	0.78	15,15,15,15	0
30	MN	X	3291	1/1	0.93	0.52	94,94,94,94	0
30	MN	X	3229	1/1	0.93	0.13	79,79,79,79	0
30	MN	X	3211	1/1	0.93	0.20	60,60,60,60	0
30	MN	X	3046	1/1	0.93	0.30	94,94,94,94	0
31	MG	X	3099	1/1	0.94	0.14	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
30	MN	X	3218	1/1	0.94	0.31	65,65,65,65	0
31	MG	X	3108	1/1	0.94	0.10	12,12,12,12	0
30	MN	X	3187	1/1	0.94	0.28	74,74,74,74	0
30	MN	X	3160	1/1	0.94	0.18	45,45,45,45	0
29	MPD	X	3001	8/8	0.94	0.14	33,33,33,33	0
31	MG	X	3089	1/1	0.94	0.15	13,13,13,13	0
30	MN	X	3054	1/1	0.94	0.28	86,86,86,86	0
30	MN	X	3069	1/1	0.94	0.14	68,68,68,68	0
30	MN	X	3157	1/1	0.94	0.22	68,68,68,68	0
30	MN	X	3261	1/1	0.94	0.16	30,30,30,30	0
30	MN	X	3162	1/1	0.94	0.31	43,43,43,43	0
30	MN	X	3263	1/1	0.94	0.33	52,52,52,52	0
31	MG	X	3310	1/1	0.94	0.13	15,15,15,15	0
30	MN	X	3188	1/1	0.94	0.45	87,87,87,87	0
30	MN	X	3184	1/1	0.94	0.36	88,88,88,88	0
30	MN	X	3209	1/1	0.94	0.20	24,24,24,24	0
31	MG	X	3303	1/1	0.94	0.25	4,4,4,4	0
30	MN	X	3191	1/1	0.94	0.15	51,51,51,51	0
30	MN	X	3224	1/1	0.94	0.25	53,53,53,53	0
31	MG	G	202	1/1	0.94	0.37	12,12,12,12	0
31	MG	X	3295	1/1	0.94	0.68	18,18,18,18	0
31	MG	X	3021	1/1	0.94	0.18	21,21,21,21	0
30	MN	X	3208	1/1	0.94	0.25	37,37,37,37	0
30	MN	X	3267	1/1	0.94	0.31	48,48,48,48	0
30	MN	X	3221	1/1	0.94	0.12	46,46,46,46	0
31	MG	X	3027	1/1	0.94	0.19	29,29,29,29	0
31	MG	X	3032	1/1	0.94	0.25	21,21,21,21	0
30	MN	X	3177	1/1	0.95	0.21	82,82,82,82	0
30	MN	X	3040	1/1	0.95	0.19	74,74,74,74	0
31	MG	X	3036	1/1	0.95	0.14	8,8,8,8	0
30	MN	X	3049	1/1	0.95	0.39	82,82,82,82	0
30	MN	X	3265	1/1	0.95	0.24	43,43,43,43	0
29	MPD	X	3005	8/8	0.95	0.17	65,65,65,65	0
31	MG	X	3105	1/1	0.95	0.24	35,35,35,35	0
30	MN	X	3153	1/1	0.95	0.29	95,95,95,95	0
32	EPE	X	3311	15/15	0.95	0.18	57,57,57,57	0
30	MN	X	3156	1/1	0.95	0.22	53,53,53,53	0
30	MN	X	3179	1/1	0.95	0.21	83,83,83,83	0
30	MN	X	3129	1/1	0.95	0.07	73,73,73,73	0
31	MG	X	3176	1/1	0.95	0.16	14,14,14,14	0
30	MN	X	3070	1/1	0.95	0.10	78,78,78,78	0
31	MG	X	3087	1/1	0.95	0.32	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
30	MN	X	3048	1/1	0.95	0.10	59,59,59,59	0
30	MN	X	3142	1/1	0.95	0.39	72,72,72,72	0
30	MN	X	3110	1/1	0.95	0.13	96,96,96,96	0
30	MN	X	3171	1/1	0.95	0.15	86,86,86,86	0
31	MG	X	3104	1/1	0.96	0.32	28,28,28,28	0
30	MN	X	3112	1/1	0.96	0.06	54,54,54,54	0
31	MG	X	3102	1/1	0.96	0.34	6,6,6,6	0
30	MN	X	3120	1/1	0.96	0.17	55,55,55,55	0
30	MN	X	3225	1/1	0.96	0.41	41,41,41,41	0
30	MN	R	201	1/1	0.96	0.10	63,63,63,63	0
30	MN	X	3325	1/1	0.96	0.22	59,59,59,59	0
30	MN	X	3324	1/1	0.96	0.18	12,12,12,12	0
30	MN	X	3206	1/1	0.96	0.45	57,57,57,57	0
30	MN	R	202	1/1	0.96	0.23	58,58,58,58	0
30	MN	X	3260	1/1	0.96	0.30	40,40,40,40	0
30	MN	X	3071	1/1	0.96	0.08	69,69,69,69	0
30	MN	X	3196	1/1	0.96	0.33	51,51,51,51	0
31	MG	X	3296	1/1	0.96	0.47	9,9,9,9	0
31	MG	X	3091	1/1	0.96	0.43	30,30,30,30	0
30	MN	X	3228	1/1	0.96	0.34	85,85,85,85	0
31	MG	X	3092	1/1	0.96	0.15	20,20,20,20	0
31	MG	X	3037	1/1	0.96	0.12	11,11,11,11	0
30	MN	X	3262	1/1	0.96	0.22	50,50,50,50	0
30	MN	X	3281	1/1	0.96	0.17	40,40,40,40	0
30	MN	X	3252	1/1	0.96	0.30	17,17,17,17	0
30	MN	X	3180	1/1	0.96	0.54	76,76,76,76	0
30	MN	X	3259	1/1	0.96	0.15	13,13,13,13	0
30	MN	X	3258	1/1	0.96	0.22	35,35,35,35	0
30	MN	X	3240	1/1	0.96	0.19	28,28,28,28	0
30	MN	X	3194	1/1	0.96	0.17	31,31,31,31	0
31	MG	X	3086	1/1	0.96	0.10	26,26,26,26	0
30	MN	X	3025	1/1	0.96	0.21	52,52,52,52	0
29	MPD	X	3007	8/8	0.96	0.28	9,9,9,9	0
31	MG	X	3307	1/1	0.96	0.04	21,21,21,21	0
30	MN	X	3014	1/1	0.97	0.20	12,12,12,12	0
31	MG	X	3029	1/1	0.97	0.39	19,19,19,19	0
30	MN	X	3075	1/1	0.97	0.11	76,76,76,76	0
31	MG	X	3088	1/1	0.97	0.13	36,36,36,36	0
30	MN	X	3282	1/1	0.97	0.21	49,49,49,49	0
30	MN	X	3152	1/1	0.97	0.29	68,68,68,68	0
31	MG	X	3306	1/1	0.97	0.06	29,29,29,29	0
30	MN	X	3323	1/1	0.97	0.15	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
30	MN	X	3212	1/1	0.97	0.27	56,56,56,56	0
30	MN	X	3278	1/1	0.97	0.30	35,35,35,35	0
31	MG	X	3080	1/1	0.97	0.19	33,33,33,33	0
30	MN	X	3287	1/1	0.97	0.31	78,78,78,78	0
30	MN	X	3166	1/1	0.97	0.23	62,62,62,62	0
31	MG	X	3020	1/1	0.97	0.25	20,20,20,20	0
30	MN	X	3165	1/1	0.97	0.16	63,63,63,63	0
30	MN	X	3024	1/1	0.97	0.43	107,107,107,107	0
30	MN	X	3151	1/1	0.97	0.17	44,44,44,44	0
30	MN	X	3219	1/1	0.97	0.31	53,53,53,53	0
30	MN	X	3289	1/1	0.97	0.28	57,57,57,57	0
30	MN	Y	204	1/1	0.97	0.11	63,63,63,63	0
30	MN	X	3239	1/1	0.97	0.36	15,15,15,15	0
30	MN	X	3078	1/1	0.97	0.19	78,78,78,78	0
30	MN	X	3141	1/1	0.97	0.35	69,69,69,69	0
30	MN	I	203	1/1	0.97	0.22	33,33,33,33	0
30	MN	X	3181	1/1	0.97	0.19	39,39,39,39	0
30	MN	X	3047	1/1	0.97	0.20	69,69,69,69	0
30	MN	X	3147	1/1	0.97	0.12	82,82,82,82	0
31	MG	X	3144	1/1	0.97	0.18	8,8,8,8	0
30	MN	X	3266	1/1	0.97	0.18	22,22,22,22	0
30	MN	X	3193	1/1	0.97	0.18	33,33,33,33	0
30	MN	X	3241	1/1	0.97	0.28	20,20,20,20	0
30	MN	X	3242	1/1	0.97	0.30	22,22,22,22	0
30	MN	X	3236	1/1	0.97	0.15	36,36,36,36	0
30	MN	X	3292	1/1	0.97	0.28	99,99,99,99	0
31	MG	X	3030	1/1	0.97	0.21	15,15,15,15	0
30	MN	X	3204	1/1	0.97	0.16	21,21,21,21	0
30	MN	X	3170	1/1	0.97	0.10	54,54,54,54	0
29	MPD	X	3003	8/8	0.97	0.19	21,21,21,21	0
30	MN	X	3159	1/1	0.97	0.15	42,42,42,42	0
30	MN	X	3012	1/1	0.97	0.31	19,19,19,19	0
30	MN	X	3253	1/1	0.97	0.34	26,26,26,26	0
30	MN	X	3256	1/1	0.98	0.22	13,13,13,13	0
30	MN	X	3251	1/1	0.98	0.19	8,8,8,8	0
31	MG	X	3096	1/1	0.98	0.24	9,9,9,9	0
30	MN	X	3214	1/1	0.98	0.11	81,81,81,81	0
30	MN	X	3203	1/1	0.98	0.37	27,27,27,27	0
30	MN	X	3077	1/1	0.98	0.20	78,78,78,78	0
30	MN	X	3280	1/1	0.98	0.27	39,39,39,39	0
31	MG	X	3033	1/1	0.98	0.19	19,19,19,19	0
30	MN	X	3277	1/1	0.98	0.17	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
30	MN	X	3238	1/1	0.98	0.22	34,34,34,34	0
30	MN	X	3195	1/1	0.98	0.21	30,30,30,30	0
30	MN	X	3043	1/1	0.98	0.11	61,61,61,61	0
30	MN	X	3274	1/1	0.98	0.10	36,36,36,36	0
30	MN	X	3285	1/1	0.98	0.21	85,85,85,85	0
31	MG	X	3101	1/1	0.98	0.35	9,9,9,9	0
31	MG	B	302	1/1	0.98	0.11	4,4,4,4	0
31	MG	X	3081	1/1	0.98	0.07	36,36,36,36	0
30	MN	X	3232	1/1	0.98	0.30	55,55,55,55	0
30	MN	X	3161	1/1	0.98	0.23	46,46,46,46	0
30	MN	X	3197	1/1	0.98	0.24	34,34,34,34	0
30	MN	X	3235	1/1	0.98	0.39	40,40,40,40	0
30	MN	X	3210	1/1	0.98	0.20	57,57,57,57	0
30	MN	X	3060	1/1	0.98	0.15	51,51,51,51	0
30	MN	X	3205	1/1	0.98	0.27	61,61,61,61	0
30	MN	X	3283	1/1	0.98	0.34	14,14,14,14	0
30	MN	X	3163	1/1	0.98	0.16	61,61,61,61	0
30	MN	X	3217	1/1	0.98	0.27	38,38,38,38	0
30	MN	X	3272	1/1	0.98	0.36	44,44,44,44	0
30	MN	X	3051	1/1	0.98	0.18	67,67,67,67	0
30	MN	X	3164	1/1	0.98	0.23	48,48,48,48	0
30	MN	X	3017	1/1	0.98	0.36	103,103,103,103	0
30	MN	X	3245	1/1	0.99	0.21	28,28,28,28	0
30	MN	X	3257	1/1	0.99	0.23	25,25,25,25	0
30	MN	X	3139	1/1	0.99	0.29	97,97,97,97	0
30	MN	X	3264	1/1	0.99	0.33	52,52,52,52	0
30	MN	X	3247	1/1	0.99	0.25	25,25,25,25	0
30	MN	X	3243	1/1	0.99	0.42	28,28,28,28	0
30	MN	X	3326	1/1	0.99	0.17	57,57,57,57	0
30	MN	X	3056	1/1	0.99	0.19	61,61,61,61	0
30	MN	X	3286	1/1	0.99	0.31	57,57,57,57	0
30	MN	X	3279	1/1	0.99	0.25	25,25,25,25	0
30	MN	X	3237	1/1	0.99	0.23	47,47,47,47	0
30	MN	X	3064	1/1	0.99	0.14	68,68,68,68	0
30	MN	X	3185	1/1	0.99	0.21	28,28,28,28	0
30	MN	X	3275	1/1	0.99	0.18	30,30,30,30	0
30	MN	X	3167	1/1	0.99	0.20	57,57,57,57	0
31	MG	X	3094	1/1	0.99	0.16	5,5,5,5	0
30	MN	X	3249	1/1	0.99	0.21	51,51,51,51	0
30	MN	X	3200	1/1	0.99	0.26	37,37,37,37	0
31	MG	X	3116	1/1	0.99	0.13	20,20,20,20	0
30	MN	X	3190	1/1	0.99	0.41	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
30	MN	X	3270	1/1	0.99	0.16	30,30,30,30	0
30	MN	X	3198	1/1	0.99	0.20	64,64,64,64	0
30	MN	X	3201	1/1	0.99	0.20	40,40,40,40	0
30	MN	X	3150	1/1	0.99	0.13	50,50,50,50	0
30	MN	X	3284	1/1	0.99	0.15	21,21,21,21	0
31	MG	X	3301	1/1	0.99	0.13	8,8,8,8	0
30	MN	X	3154	1/1	0.99	0.22	40,40,40,40	0
30	MN	X	3145	1/1	0.99	0.16	51,51,51,51	0
30	MN	X	3246	1/1	0.99	0.19	13,13,13,13	0
30	MN	X	3062	1/1	0.99	0.16	42,42,42,42	0
30	MN	X	3234	1/1	0.99	0.18	17,17,17,17	0
30	MN	X	3045	1/1	0.99	0.28	3,3,3,3	0
30	MN	X	3215	1/1	0.99	0.28	26,26,26,26	0
30	MN	X	3271	1/1	0.99	0.25	17,17,17,17	0
30	MN	X	3248	1/1	0.99	0.28	37,37,37,37	0
30	MN	X	3189	1/1	0.99	0.30	64,64,64,64	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.