



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 10:43 pm BST

PDB ID : 1Q82  
Title : Crystal Structure of CC-Puromycin bound to the A-site of the 50S ribosomal subunit  
Authors : Hansen, J.L.; Schmeing, T.M.; Moore, P.B.; Steitz, T.A.  
Deposited on : 2003-08-20  
Resolution : 2.98 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 : 2.11  
buster-report : 1.1.7 (2018)  
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) : 2.11

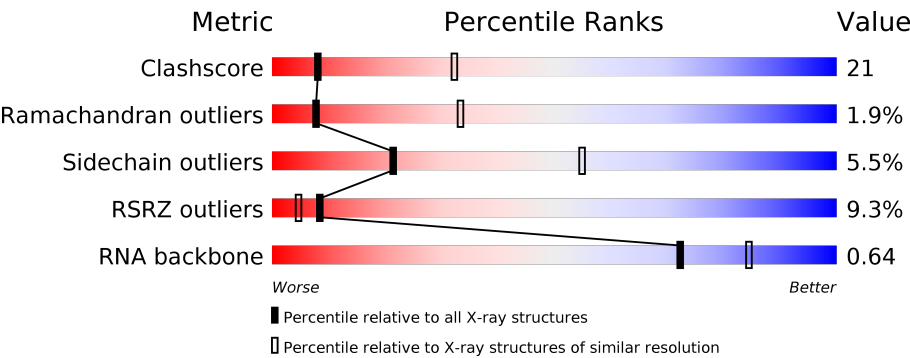
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.98 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.



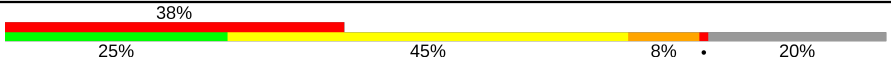


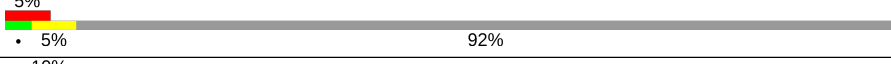
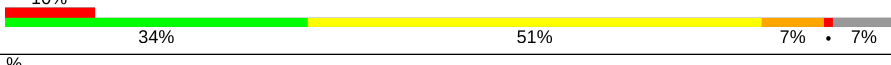
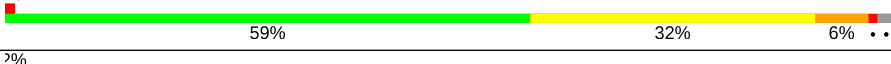
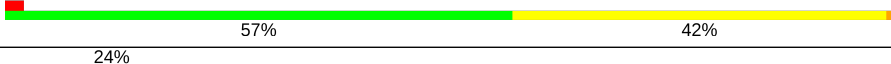
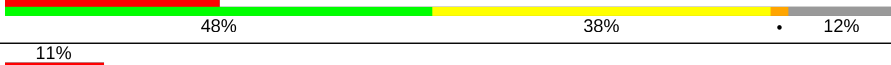
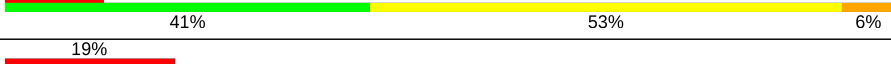
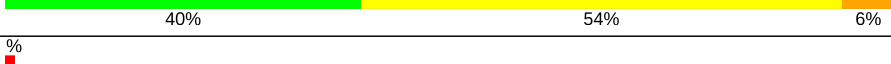

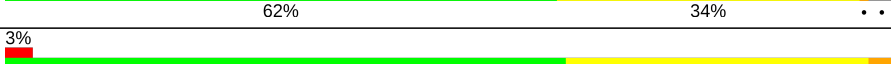

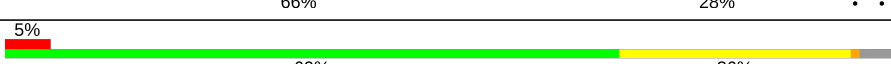

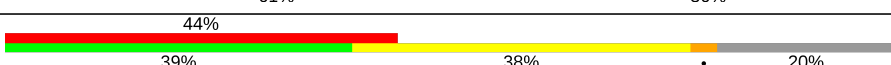


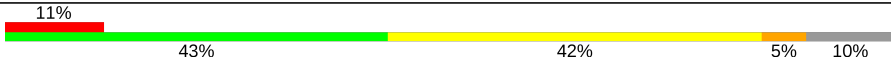
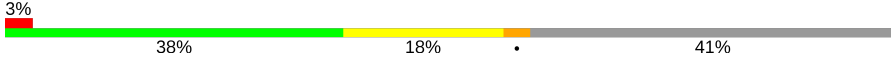

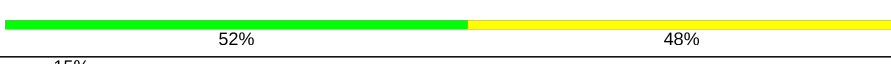
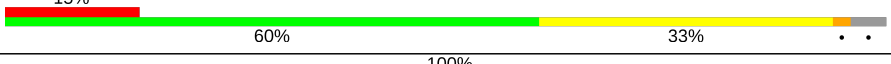
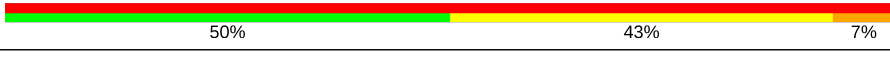

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)
RNA backbone	3102	1088 (3.26-2.70)

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	A	2922	<div><div>3%</div><div><div></div><div>50%</div><div>36%</div><div>7%</div><div>6%</div></div></div>
2	B	122	<div><div>5%</div><div><div></div><div>51%</div><div>35%</div><div>10%</div><div></div></div></div>
3	5	2	<div><div></div><div><div>50%</div><div>50%</div></div></div>
4	C	239	<div><div>11%</div><div><div></div><div>54%</div><div>40%</div><div>5%</div><div></div></div></div>
5	D	337	<div><div>2%</div><div><div></div><div>48%</div><div>46%</div><div>6%</div></div></div>
6	E	246	<div><div>2%</div><div><div></div><div>54%</div><div>40%</div><div>5%</div></div></div>

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Mol	Chain	Length	Quality of chain
7	F	176	
8	G	177	
9	H	119	
10	I	348	
11	J	167	
12	K	145	
13	L	132	
14	M	164	
15	N	194	
16	O	186	
17	P	115	
18	Q	148	
19	R	95	
20	S	154	
21	T	84	
22	U	119	
23	V	66	
24	W	70	
25	X	154	
26	Y	91	
27	Z	240	
28	1	73	
29	2	56	
30	3	48	
31	4	92	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	MG	1	8105	-	-	-	X
32	MG	A	8011	-	-	X	-
32	MG	A	8024	-	-	-	X
32	MG	A	8049	-	-	-	X
32	MG	A	8092	-	-	-	X
32	MG	A	8102	-	-	-	X
32	MG	A	8114	-	-	-	X
34	NA	A	8307	-	-	-	X
34	NA	A	8310	-	-	-	X
34	NA	A	8326	-	-	-	X
34	NA	A	8328	-	-	-	X
34	NA	A	8332	-	-	-	X
34	NA	A	8340	-	-	-	X
34	NA	A	8363	-	-	-	X
34	NA	A	8365	-	-	-	X
34	NA	A	8371	-	-	-	X
34	NA	A	8372	-	-	-	X
34	NA	A	8382	-	-	-	X
34	NA	A	8384	-	-	-	X
34	NA	B	8383	-	-	-	X
34	NA	S	8386	-	-	-	X
34	NA	T	8312	-	-	-	X
35	CL	A	8522	-	-	-	X
35	CL	M	8510	-	-	-	X
35	CL	N	8518	-	-	X	-
37	CD	4	8404	-	-	-	X

## 2 Entry composition [i](#)

There are 38 unique types of molecules in this entry. The entry contains 98593 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2754	Total	C	N	O	P	0	0	0
			59017	26346	10878	19048	2745			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	122	Total	C	N	O	P	0	0	0
			2600	1160	472	847	121			

- Molecule 3 is a RNA chain called CC-puromycin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	5	2	Total	C	N	O	P	0	0	0
			40	18	6	14	2			

- Molecule 4 is a protein called 50S ribosomal protein L2P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	237	Total	C	N	O	S	0	0	0
			1754	1072	352	325	5			

- Molecule 5 is a protein called 50S ribosomal protein L3P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	337	Total	C	N	O	S	0	0	0
			2624	1616	493	510	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	PRO	DELETION	UNP P20279
D	310	ARG	PHE	CONFLICT	UNP P20279

- Molecule 6 is a protein called 50S ribosomal protein L4E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	246	Total	C	N	O	S	0	0	0
			1858	1131	344	382	1			

- Molecule 7 is a protein called 50S ribosomal protein L5P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	F	140	Total	C	N	O	S	0	0	0
			1094	685	195	210	4			

- Molecule 8 is a protein called 50S ribosomal protein L6P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	G	172	Total	C	N	O	S	0	0	0
			1357	840	224	289	4			

- Molecule 9 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	119	Total	C	N	O	S	0	0	0
			885	552	141	191	1			

- Molecule 10 is a protein called Acidic ribosomal protein P0 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	29	Total	C	N	O	S	0	0	0
			240	149	39	51	1			

- Molecule 11 is a protein called L10 Ribosomal Protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	156	Total	C	N	O	S	0	0	0
			1215	766	233	212	4			

- Molecule 12 is a protein called 50S ribosomal protein L13P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	142	Total	C	N	O	S	0	0	0
			1119	696	199	221	3			

- Molecule 13 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	132	Total	C	N	O	S	0	0	0
			993	609	189	191	4			

- Molecule 14 is a protein called 50S ribosomal protein L15P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	M	145	Total	C	N	O	S	0	0	0
			1114	668	222	224				

- Molecule 15 is a protein called L15 Ribosomal Protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	N	194	Total	C	N	O	S	0	0	0
			1605	988	346	266	5			

- Molecule 16 is a protein called 50S ribosomal protein L18P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	O	186	Total	C	N	O	S	0	0	0
			1444	895	262	285	2			

- Molecule 17 is a protein called 50S ribosomal protein L18e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	P	115	Total	C	N	O	S	0	0	0
			864	529	161	174				

- Molecule 18 is a protein called 50S ribosomal protein L19E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Q	143	Total	C	N	O	S	0	0	0
			1133	680	230	223				

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	71	LYS	TYR	CONFLICT	UNP P14119

- Molecule 19 is a protein called 50S ribosomal protein L21e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	R	95	Total	C	N	O			
			734	450	141	143	0	0	0

- Molecule 20 is a protein called 50S ribosomal protein L22P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	S	150	Total	C	N	O	S		
			1149	713	209	223	4	0	0

- Molecule 21 is a protein called 50S ribosomal protein L23P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	T	81	Total	C	N	O	S		
			641	389	111	138	3	0	0

- Molecule 22 is a protein called 50S ribosomal protein L24P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	U	119	Total	C	N	O			
			949	568	180	201		0	0

- Molecule 23 is a protein called 50S ribosomal protein L24E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	V	53	Total	C	N	O	S		
			410	244	75	86	5	0	0

- Molecule 24 is a protein called 50S ribosomal protein L29P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	W	65	Total	C	N	O	S		
			499	304	94	100	1	0	0

- Molecule 25 is a protein called 50S ribosomal protein L30P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	X	154	Total	C	N	O	S		
			1195	737	209	243	6	0	0

- Molecule 26 is a protein called 50S ribosomal protein L31e.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Y	82	Total	C	N	O	S	0	0	0
			654	402	129	122	1			

- Molecule 27 is a protein called 50S ribosomal protein L32E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	Z	142	Total	C	N	O	S	0	0	0
			1130	686	228	216				

- Molecule 28 is a protein called L37Ae 50S ribosomal protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	1	73	Total	C	N	O	S	0	0	0
			563	359	111	86	7			

- Molecule 29 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	2	56	Total	C	N	O	S	0	0	0
			430	258	86	82	4			

- Molecule 30 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	3	46	Total	C	N	O	S	0	0	0
			393	238	86	68	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	?	-	ARG	DELETION	UNP P22452

- Molecule 31 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	4	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	1	1	Total Mg 1 1	0	0
32	D	1	Total Mg 1 1	0	0
32	B	1	Total Mg 1 1	0	0
32	C	1	Total Mg 1 1	0	0
32	Z	1	Total Mg 1 1	0	0
32	A	109	Total Mg 109 109	0	0
32	4	1	Total Mg 1 1	0	0
32	U	1	Total Mg 1 1	0	0
32	L	1	Total Mg 1 1	0	0

- Molecule 33 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	A	2	Total K 2 2	0	0

- Molecule 34 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	J	2	Total Na 2 2	0	0
34	K	1	Total Na 1 1	0	0
34	E	1	Total Na 1 1	0	0
34	B	2	Total Na 2 2	0	0
34	C	1	Total Na 1 1	0	0
34	A	71	Total Na 71 71	0	0
34	T	1	Total Na 1 1	0	0
34	N	1	Total Na 1 1	0	0

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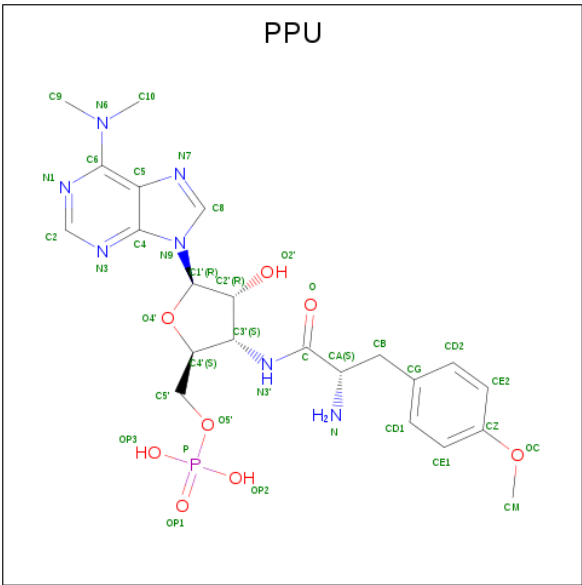
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	U	1	Total 1	Na 1	0	0
34	4	1	Total 1	Na 1	0	0
34	R	1	Total 1	Na 1	0	0
34	S	2	Total 2	Na 2	0	0
34	M	1	Total 1	Na 1	0	0

- Molecule 35 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	P	1	Total 1	Cl 1	0	0
35	D	1	Total 1	Cl 1	0	0
35	K	4	Total 4	Cl 4	0	0
35	C	1	Total 1	Cl 1	0	0
35	Z	2	Total 2	Cl 2	0	0
35	A	7	Total 7	Cl 7	0	0
35	4	1	Total 1	Cl 1	0	0
35	N	1	Total 1	Cl 1	0	0
35	O	1	Total 1	Cl 1	0	0
35	R	1	Total 1	Cl 1	0	0
35	S	1	Total 1	Cl 1	0	0
35	M	1	Total 1	Cl 1	0	0

- Molecule 36 is PUROMYCIN-5'-MONOPHOSPHATE (three-letter code: PPU) (formula: C<sub>22</sub>H<sub>30</sub>N<sub>7</sub>O<sub>8</sub>P).



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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	C	140	Total 140	O 140	0	0
38	D	146	Total 146	O 146	0	0
38	E	176	Total 176	O 176	0	0
38	F	52	Total 52	O 52	0	0
38	G	45	Total 45	O 45	0	0
38	H	32	Total 32	O 32	0	0
38	I	22	Total 22	O 22	0	0
38	J	78	Total 78	O 78	0	0
38	K	54	Total 54	O 54	0	0
38	L	64	Total 64	O 64	0	0
38	M	86	Total 86	O 86	0	0
38	N	138	Total 138	O 138	0	0
38	O	64	Total 64	O 64	0	0
38	P	44	Total 44	O 44	0	0
38	Q	70	Total 70	O 70	0	0
38	R	57	Total 57	O 57	0	0
38	S	83	Total 83	O 83	0	0
38	T	36	Total 36	O 36	0	0
38	U	38	Total 38	O 38	0	0
38	V	22	Total 22	O 22	0	0
38	W	16	Total 16	O 16	0	0

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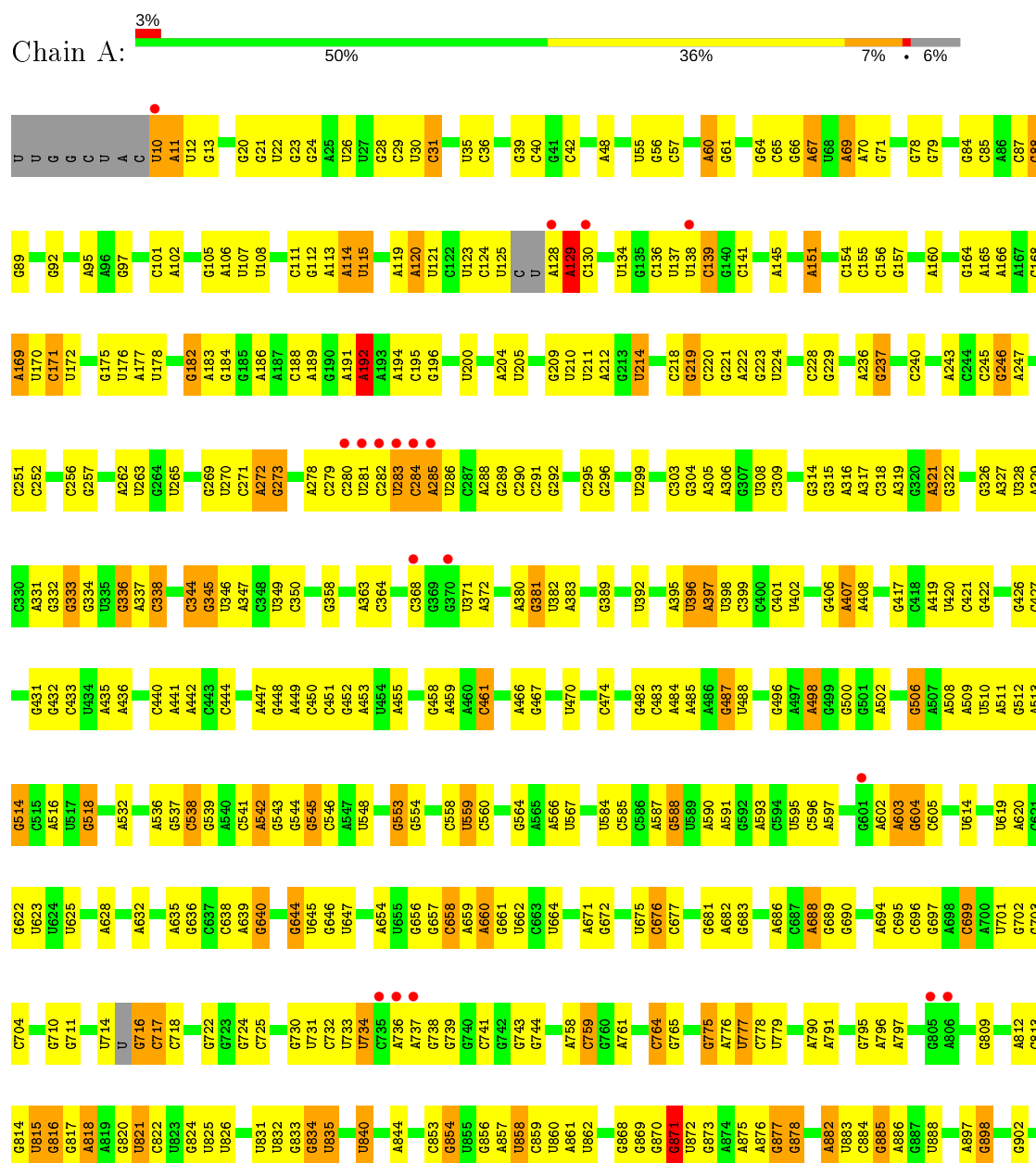
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	X	67	Total 67	O 67	0	0
38	Y	28	Total 28	O 28	0	0
38	Z	100	Total 100	O 100	0	0
38	1	36	Total 36	O 36	0	0
38	2	58	Total 58	O 58	0	0
38	3	37	Total 37	O 37	0	0
38	4	70	Total 70	O 70	0	0

### 3 Residue-property plots

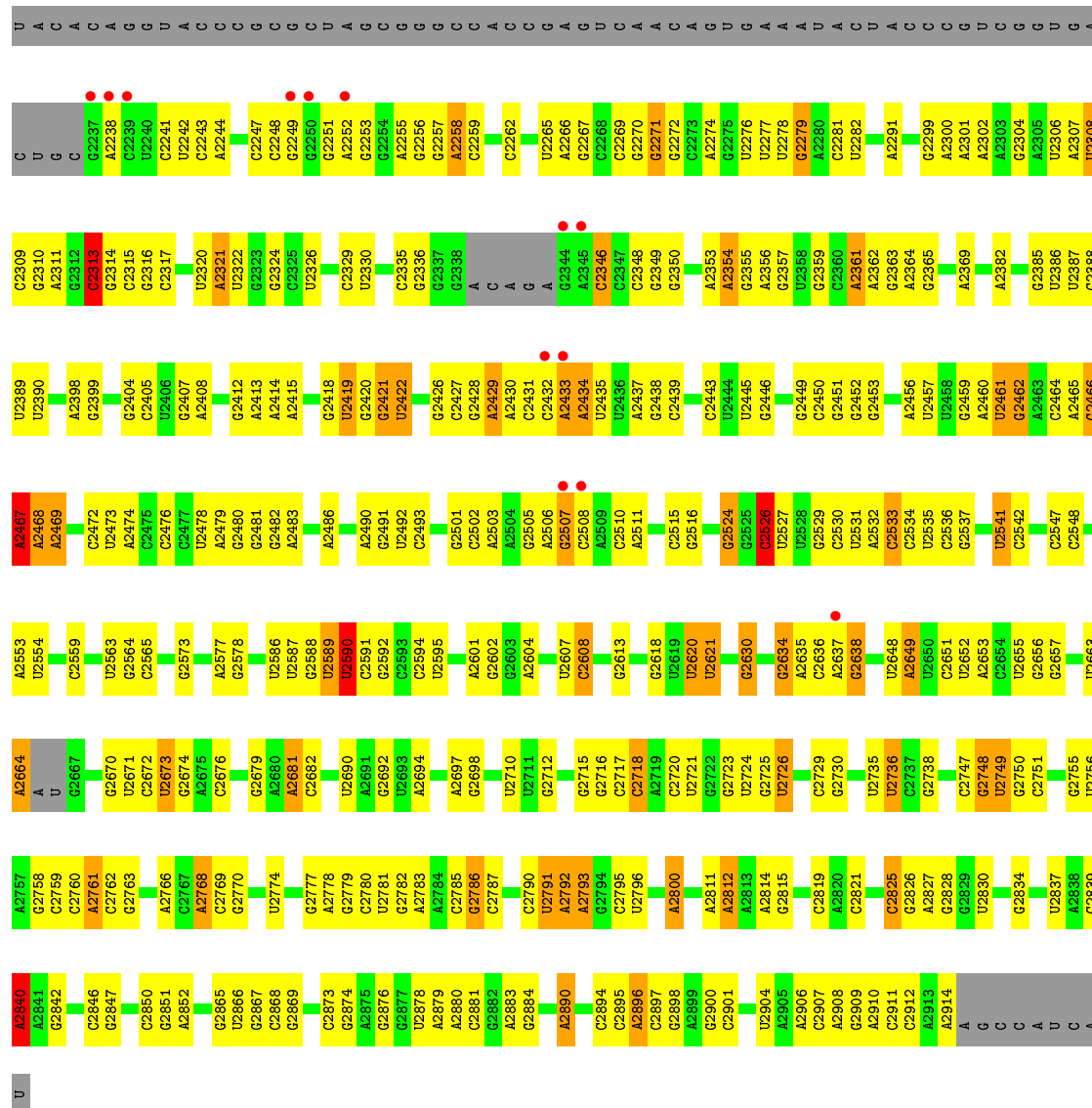
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 23S ribosomal rna

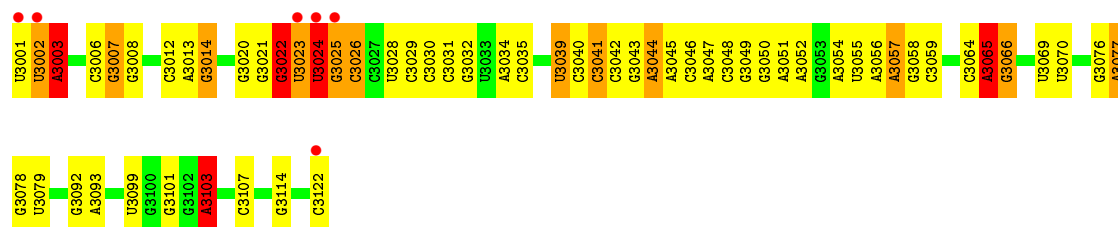


C2106	A2007	G1827	A1733	G1563	A1471	U1362	A1261	G1087	C905
U2107	U2008	G1828	C1734	C1564	C1472	U1368	G1265	A1088	C906
A2108	G2009	A1829	C1735	C1565	C1473	U1368	G1265	A1088	G911
A2010	A2010	A1830	A1736	C1566	C1474	A1372	U1266	A1097	A912
G2110	U2011	U1834	C1737	A1567	C1477	G1376	C1267	U1109	A913
G2111	U2012	U1835	C1738	U1568	U1478	G1377	G1268	G1110	U917
A2112	A1921	A1839	U1741	A1572	C1483	U1380	G1269	U1116	G918
G2013	A1922	A1840	A1742	A1573	A1484	U1380	G1270	A1117	U919
G2014	G1923	A1841	G1743	A1485	A1485	U1380	U1279	A1118	C920
A2015	G1925	A1842	U1749	A1580	U1488	U1383	G1289	G1119	G921
U2016	G1926	A1843	C1750	A1580	U1488	U1384	G1289	U1120	A922
A2019	G1929	A1844	G1751	A1589	A1494	G1385	U1297	G1121	A923
A2022	A1930	G1847	C1752	G1589	C1495	G1386	U1298	U1122	G924
G2026	G1931	G1848	C1753	A1669	A1496	G1387	G1299	A1123	G925
A2027	G1932	U1850	A1754	G1670	G1496	U1388	U1304	U1124	A926
A2123	G1933	G1851	A1755	U1677	G1497	G1389	U1305	U1125	A929
G2124	A1852	A1852	A1755	C1677	G1498	U1390	C1306	C1126	U932
G2128	G1855	C1856	A1759	U1678	U1499	G1391	U1307	U1127	G941
G2134	G2033	A1859	C1762	C1679	U1500	A1392	A1308	C1129	U942
A2135	U2034	A1860	U1766	G1680	A1501	C1393	U1309	G1130	G948
G2136	A2039	U1861	A1767	A1587	A1502	C1394	A1311	G1131	U949
A	G2044	C1862	C1768	G1601	U1503	A1407	G1312	G1132	G950
C	G	G1868	C1769	C1602	U1505	U1408	A1313	A1133	A951
U	C2047	U1871	U1770	G1603	C1512	U1412	A1314	G1134	G952
G	G2050	C1870	U1771	G1604	C1513	G1417	G1315	U1136	G953
G	G2051	U1872	G1772	G1605	C1514	U1417	G1316	G1137	U954
C	G2053	C1873	G1773	C1609	C1515	U1422	G1324	G1151	A955
A	A2054	U1874	A1776	G1610	C1516	A1423	G1325	G1159	G958
C	A2055	U1874	G1777	G1611	U1517	A1424	A1328	G1160	C959
G	U2063	U1879	A1779	C1613	C1523	A1427	A1329	A1161	G960
A	U2064	C1880	C1787	A1614	U1524	G1430	A1330	G1162	A961
U	C2071	C1881	U1788	A1615	A1525	G1430	A1331	G1163	C962
G	G2072	C1882	C1795	A1616	A1527	A1434	C1332	U1164	G968
C	G2073	U1883	G1796	C1617	A1528	U1435	U1333	G1165	G969
G	A2074	G1884	A1796	A1624	U1529	C1436	C1334	A1166	U970
A	A2081	A1885	A1797	U1625	U1530	U1440	C1335	G1167	G
C	G	U1886	C1798	A1626	U1531	U1441	U1336	U1168	G
C	A2089	U1887	A1804	G1627	C1534	U1442	A1337	U1169	C
A	G2090	G1896	G1805	C1633	G1535	G1442	G1340	U1170	U
A	G2091	U1897	G1806	U1634	C1536	A1442	A1341	A1171	G
G	G2092	G1902	U1813	U1635	G1543	A1448	C1342	A1172	C
G	G2093	U1903	G1814	U1636	U1544	G1449	U1343	A1173	G
U	G2094	A1904	G1815	A1637	U1545	C1450	G1344	A1174	C
A	A2096	U1981	C1816	U1638	G1546	U1451	A1345	G1175	G
G	A2100	C1982	U1817	U1641	G1546	U1461	U1346	C1176	C
A	A2101	U1907	G1723	A1642	U1547	A1462	U1347	A1177	U
G	G2102	A1909	U1724	C1643	G1557	C1463	A1351	U1180	C
A	A2103	A1910	C1725	C1644	C1558	U1464	A1352	A1181	G
C	C2104	U2004	G1730	U1645	U1559	U1467	C1353	C1182	A
C	C2105	G2005	C1731	G1646	U	C1467	C1360	C1183	G
C		C2006	A1732	G1647	U1561		C1361	U1185	A
					C1562			C1186	G





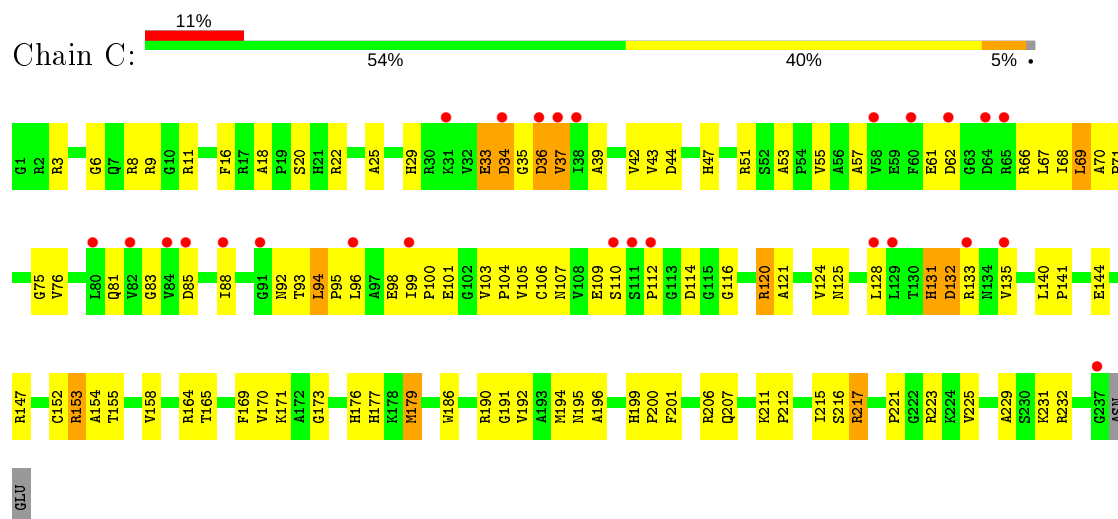
• Molecule 2: 5S ribosomal RNA



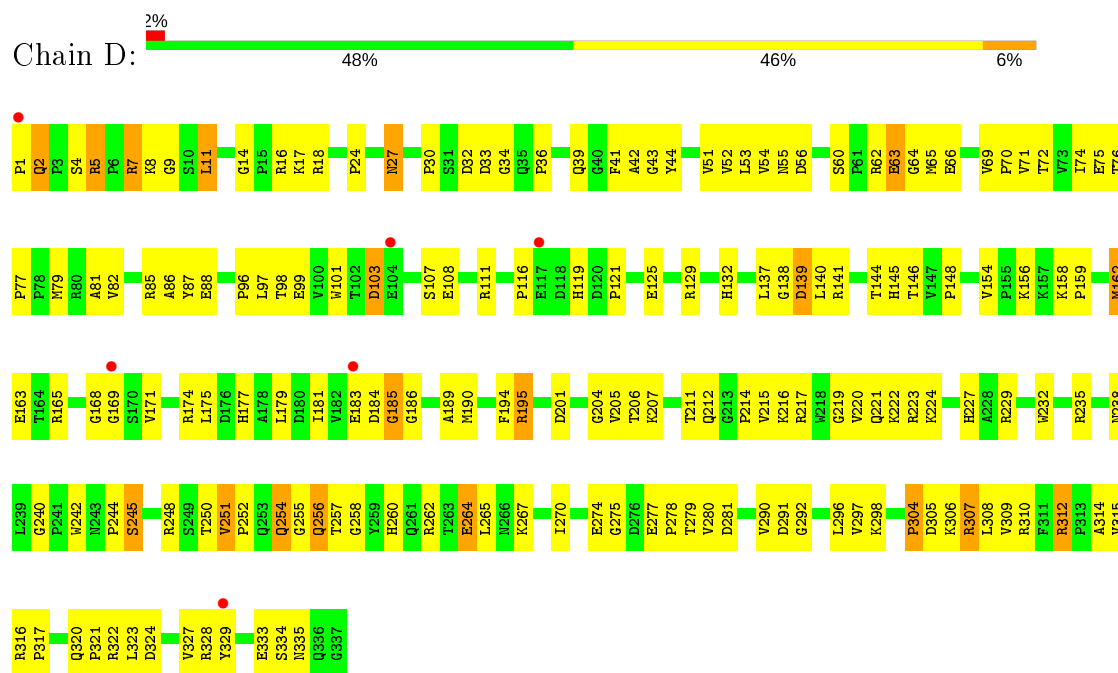
• Molecule 3: CC-puromycin



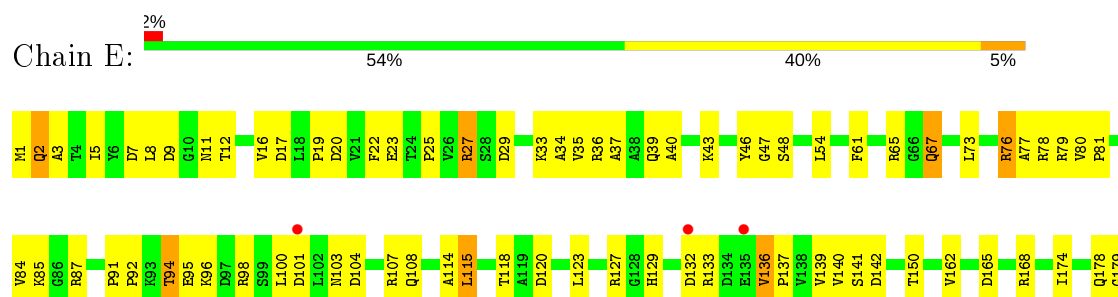
• Molecule 4: 50S ribosomal protein L2P



• Molecule 5: 50S ribosomal protein L3P

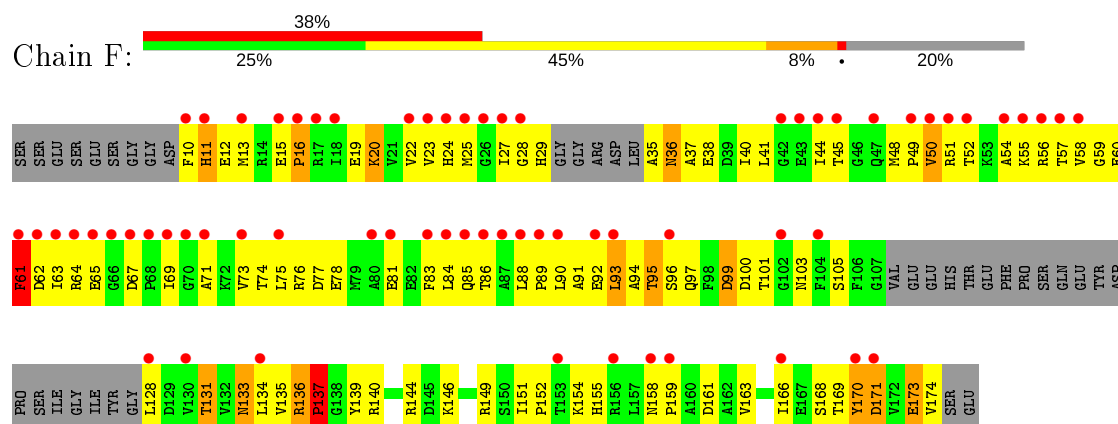


• Molecule 6: 50S ribosomal protein L4E

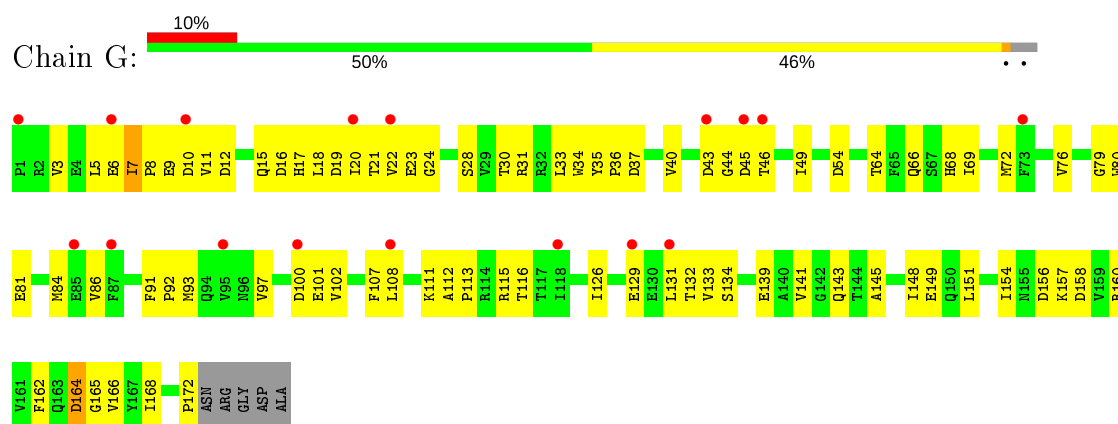




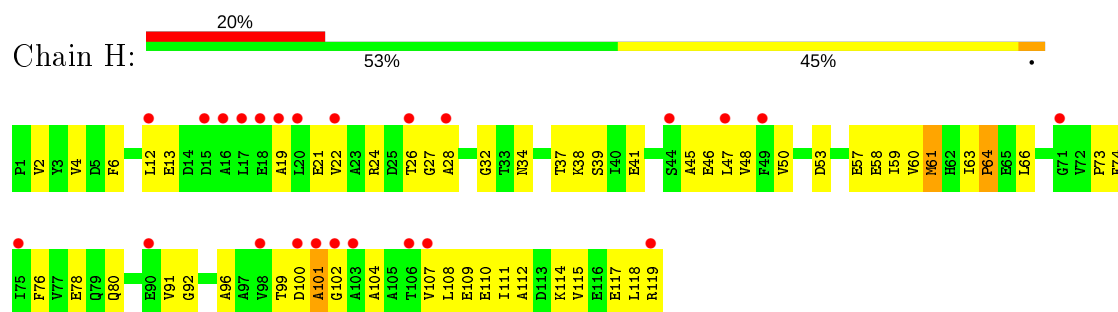
- Molecule 7: 50S ribosomal protein L5P



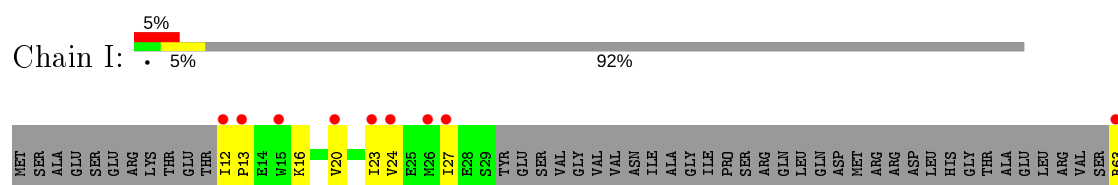
- Molecule 8: 50S ribosomal protein L6P

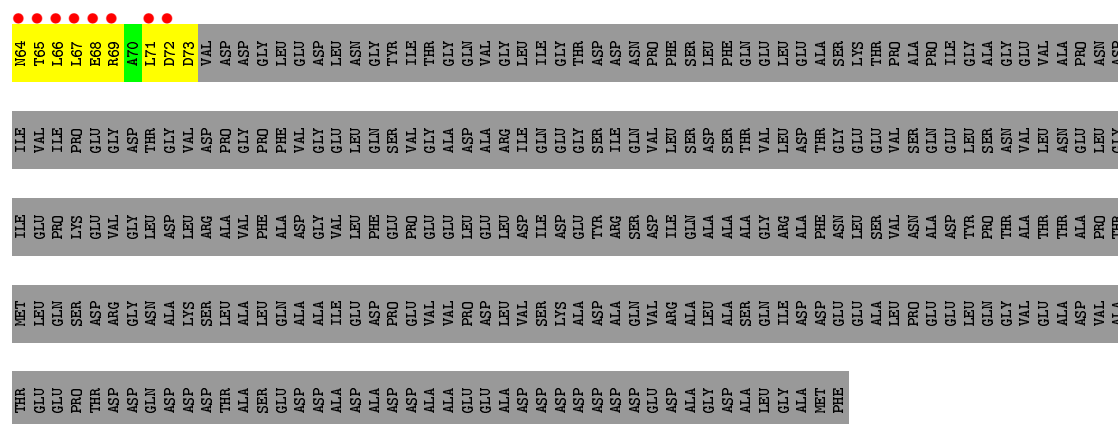


- Molecule 9: 50S ribosomal protein L7Ae

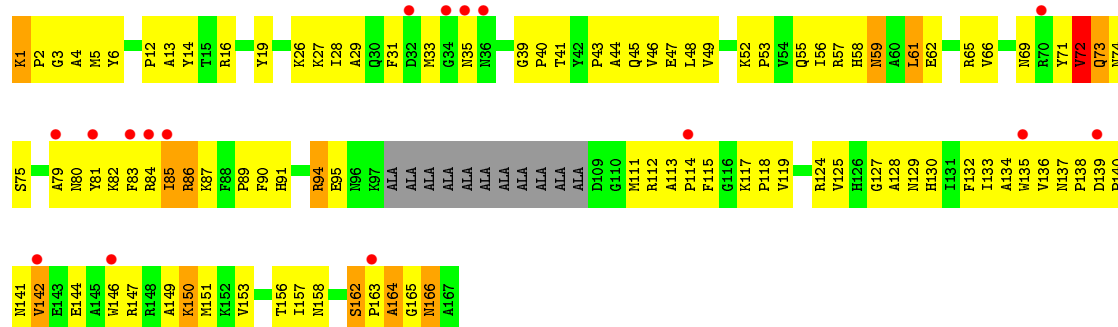


- Molecule 10: Acidic ribosomal protein P0 homolog

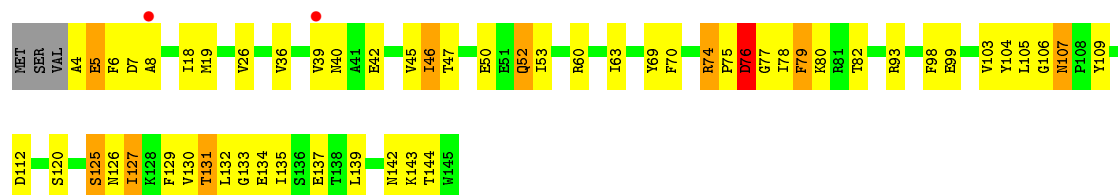




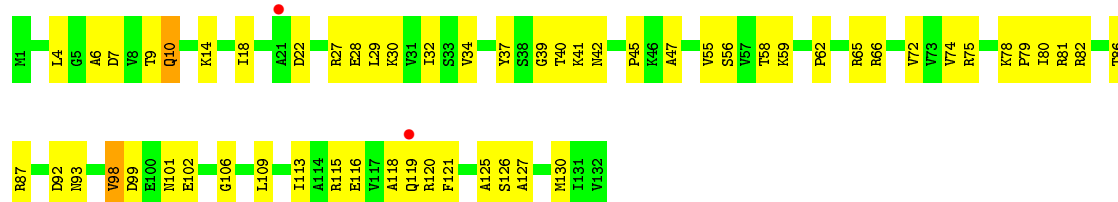
### • Molecule 11: L10 Ribosomal Protein



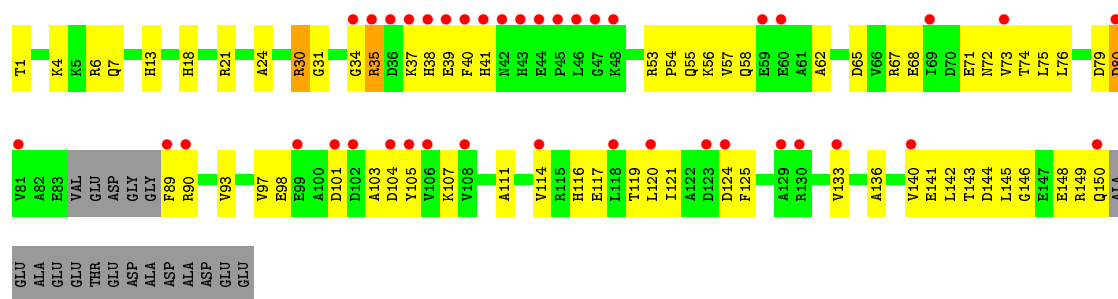
### • Molecule 12: 50S ribosomal protein L13P



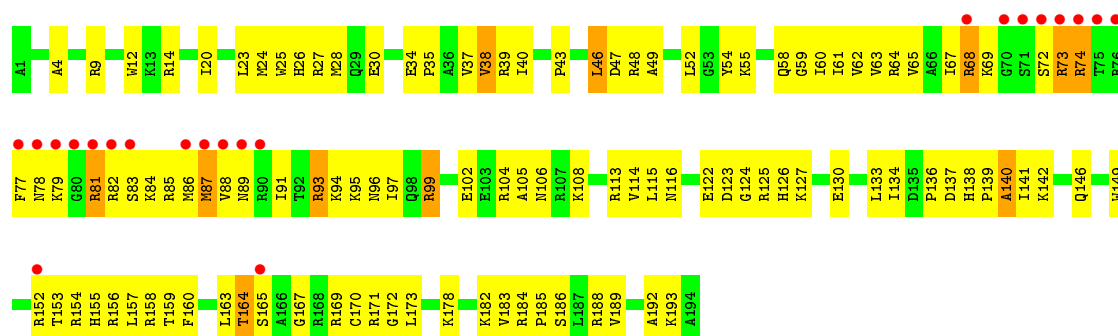
### • Molecule 13: 50S ribosomal protein L14P



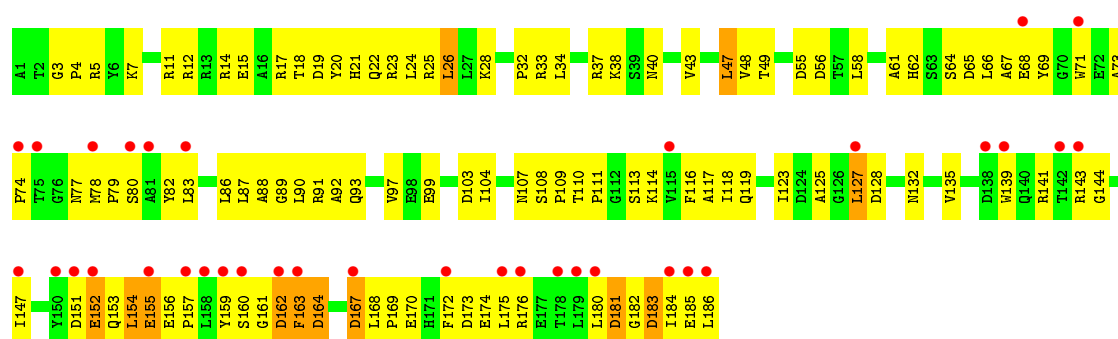
### • Molecule 14: 50S ribosomal protein L15P



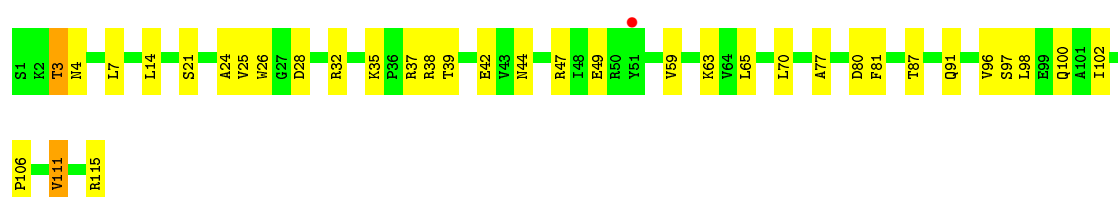
• Molecule 15: L15 Ribosomal Protein



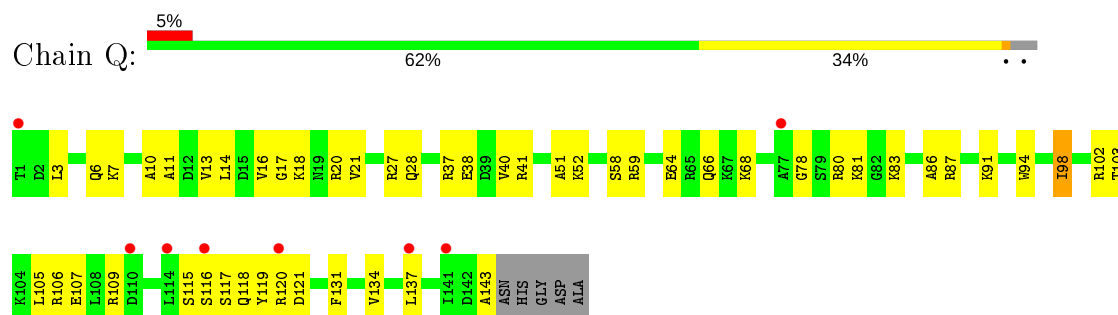
• Molecule 16: 50S ribosomal protein L18P



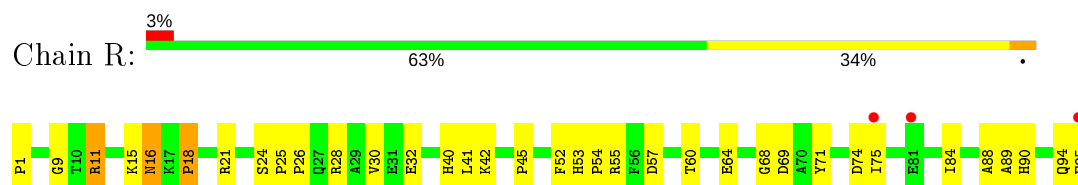
• Molecule 17: 50S ribosomal protein L18e



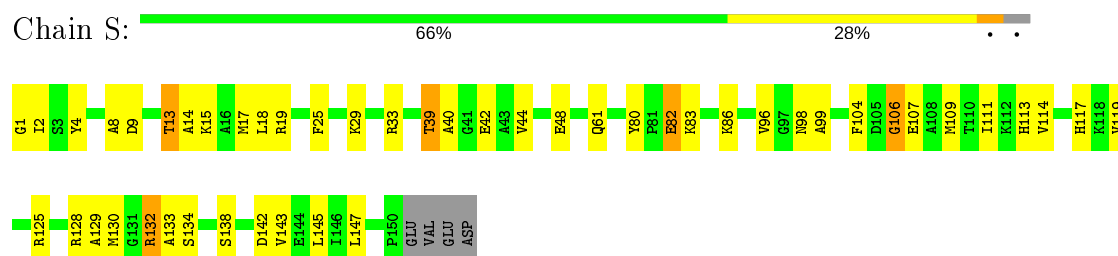
- Molecule 18: 50S ribosomal protein L19E



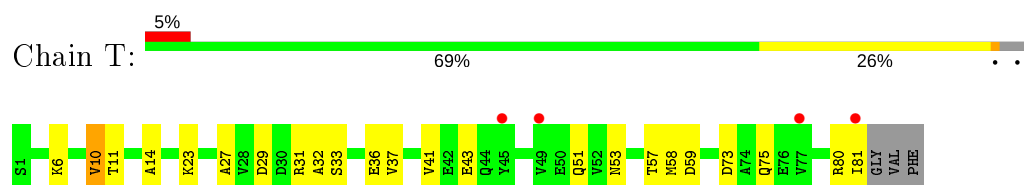
- Molecule 19: 50S ribosomal protein L21e



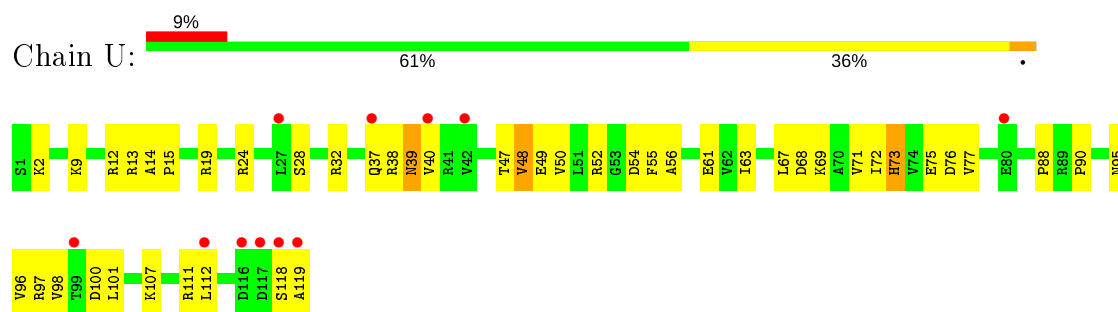
- Molecule 20: 50S ribosomal protein L22P



- Molecule 21: 50S ribosomal protein L23P

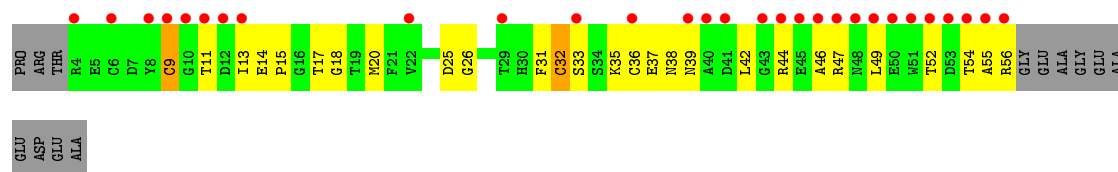


- Molecule 22: 50S ribosomal protein L24P

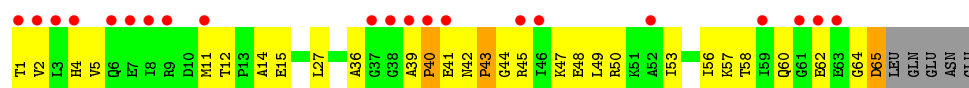


- Molecule 23: 50S ribosomal protein L24E





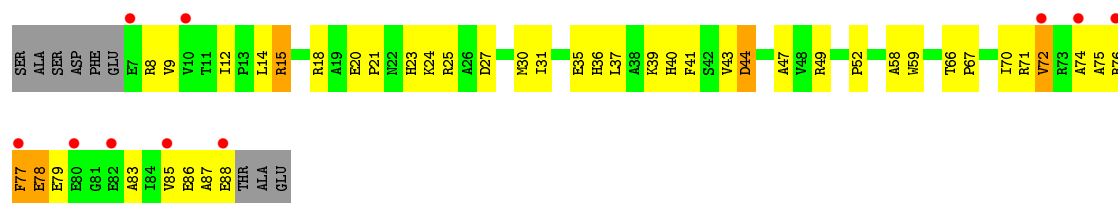
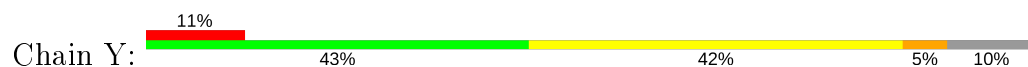
- Molecule 24: 50S ribosomal protein L29P



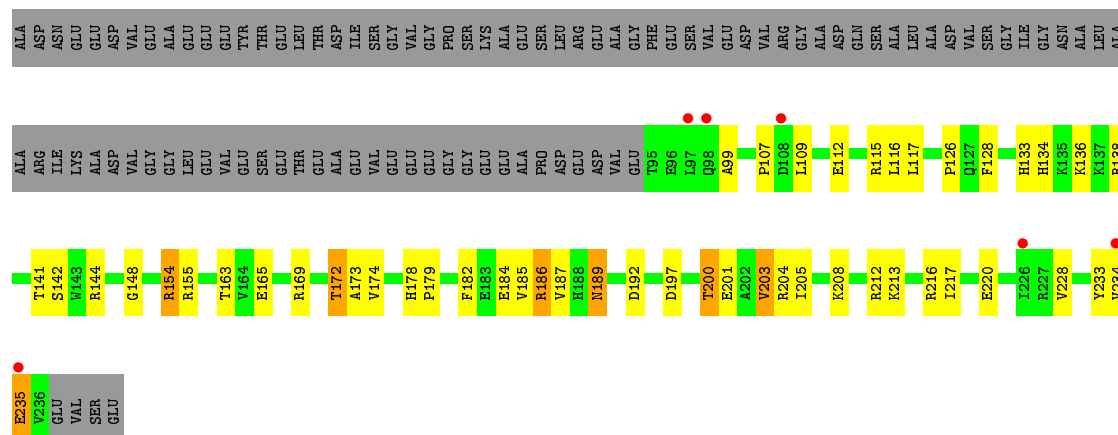
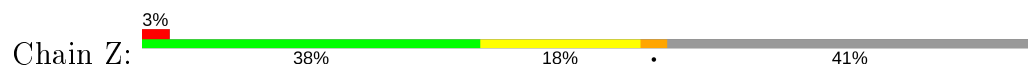
- Molecule 25: 50S ribosomal protein L30P



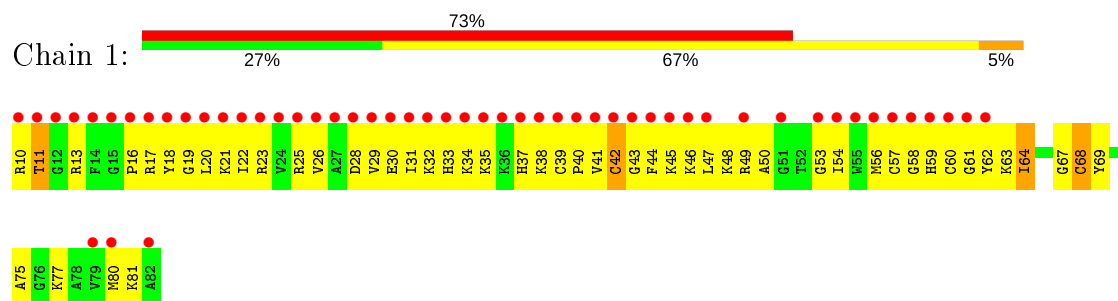
- Molecule 26: 50S ribosomal protein L31e



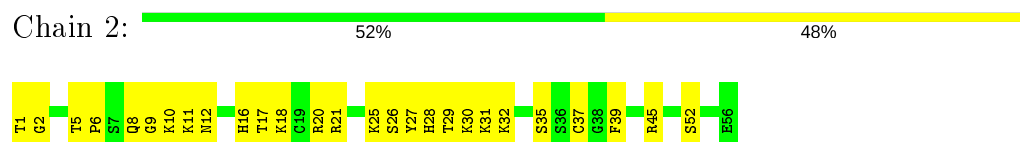
- Molecule 27: 50S ribosomal protein L32E



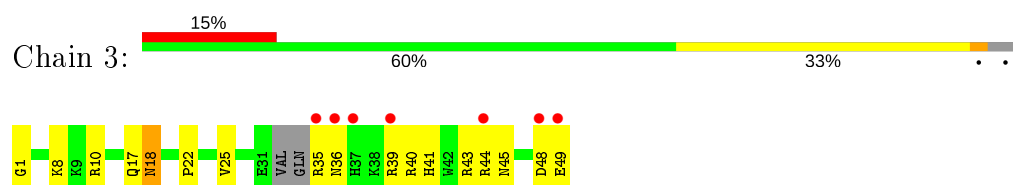
- Molecule 28: L37Ae 50S ribosomal protein



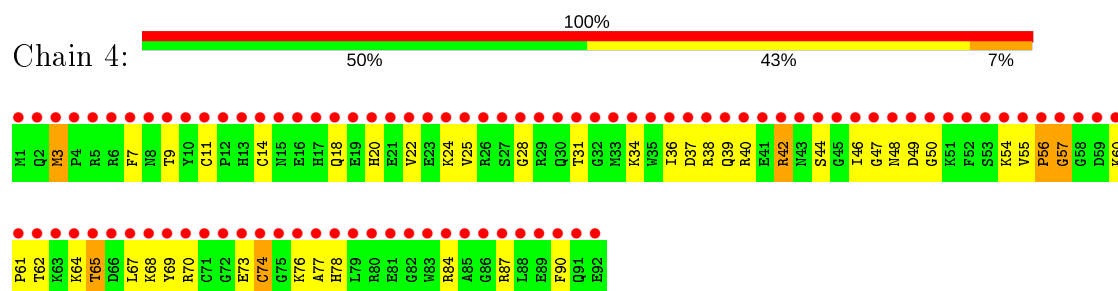
- Molecule 29: 50S ribosomal protein L37e



- Molecule 30: 50S ribosomal protein L39e



- Molecule 31: 50S ribosomal protein L44E





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	213.16 Å   301.29 Å   575.40 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	20.00 – 2.98 49.62 – 2.98	Depositor EDS
% Data completeness (in resolution range)	91.7 (20.00-2.98) 91.8 (49.62-2.98)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.50 (at 2.96 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.207   ,   0.251 0.211   ,   (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.6	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 63.9	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	0.91	EDS
Total number of atoms	98593	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% 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, CL, NA, K, CD, PPU

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	A	0.58	2/66076 (0.0%)	0.76	28/103052 (0.0%)
2	B	0.54	0/2905	0.82	4/4528 (0.1%)
3	5	2.09	1/43 (2.3%)	1.94	0/64
4	C	0.45	0/1787	0.75	0/2409
5	D	0.44	0/2689	0.70	0/3652
6	E	0.48	0/1883	0.72	0/2551
7	F	0.40	0/1111	0.63	0/1498
8	G	0.45	0/1382	0.65	0/1880
9	H	0.39	0/896	0.62	0/1219
10	I	0.38	0/241	0.56	0/324
11	J	0.48	0/1246	0.81	2/1686 (0.1%)
12	K	0.49	0/1135	0.70	0/1530
13	L	0.46	0/1003	0.76	0/1351
14	M	0.49	0/1126	0.76	0/1504
15	N	0.61	0/1633	0.83	2/2180 (0.1%)
16	O	0.40	0/1473	0.71	0/1999
17	P	0.47	0/873	0.70	0/1181
18	Q	0.44	0/1143	0.62	0/1521
19	R	0.44	0/748	0.75	1/1005 (0.1%)
20	S	0.49	0/1172	0.73	0/1578
21	T	0.41	0/648	0.65	0/875
22	U	0.39	0/957	0.70	0/1289
23	V	0.58	0/417	0.74	1/562 (0.2%)
24	W	0.38	0/502	0.60	0/675
25	X	0.50	0/1218	0.72	0/1655
26	Y	0.46	0/664	0.71	0/895
27	Z	0.48	0/1146	0.71	0/1536
28	1	0.77	0/575	0.84	0/763
29	2	0.55	0/437	0.77	0/578
30	3	0.44	0/398	0.61	0/527
31	4	0.93	0/771	0.80	0/1024
All	All	0.56	3/98298 (0.0%)	0.75	38/147091 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	143
2	B	1	4
All	All	2	147

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1206	U	N1-C2	5.33	1.43	1.38
1	A	1206	U	C3'-O3'	-5.24	1.34	1.42
3	5	75	C	C4'-C3'	-5.04	1.47	1.52

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1164	U	OP1-P-O3'	-18.53	64.43	105.20
1	A	1164	U	OP2-P-O3'	-18.53	64.44	105.20
1	A	1165	G	O5'-P-OP1	-11.90	94.99	105.70
2	B	3024	U	C2'-C3'-O3'	9.55	130.52	109.50
1	A	1563	G	C2'-C3'-O3'	9.10	129.51	109.50
1	A	1979	G	C2'-C3'-O3'	8.54	128.28	109.50
1	A	1206	U	O5'-P-OP1	-8.21	98.31	105.70
1	A	1942	A	C5'-C4'-C3'	7.54	128.07	116.00
2	B	3003	A	O5'-P-OP1	7.40	119.58	110.70
1	A	1942	A	C5'-C4'-O4'	7.19	117.73	109.10
2	B	3103	A	C5'-C4'-O4'	7.07	117.59	109.10
1	A	871	G	C5'-C4'-O4'	-6.56	101.23	109.10
1	A	1504	A	C1'-O4'-C4'	-6.30	104.86	109.90
2	B	3039	U	N1-C1'-C2'	6.18	122.03	114.00
1	A	1165	G	OP1-P-OP2	6.10	128.75	119.60
1	A	1120	U	C5'-C4'-C3'	-6.07	106.29	116.00
1	A	1165	G	O5'-P-OP2	-6.02	100.28	105.70
1	A	389	G	C5'-C4'-C3'	-6.02	106.38	116.00
23	V	36	CYS	CA-CB-SG	-6.00	103.21	114.00
1	A	2419	U	N1-C1'-C2'	5.98	121.77	114.00
1	A	2313	C	C5'-C4'-O4'	5.89	116.17	109.10
1	A	2012	U	N1-C1'-C2'	5.88	121.65	114.00
1	A	2467	A	O5'-P-OP1	-5.79	100.49	105.70
1	A	2726	U	N1-C1'-C2'	5.66	121.35	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1738	C	O4'-C4'-C3'	-5.61	98.39	104.00
11	J	74	ASN	N-CA-C	-5.56	95.98	111.00
1	A	129	A	C2'-C3'-O3'	5.54	122.56	113.70
1	A	2096	A	N9-C1'-C2'	5.42	121.05	114.00
11	J	156	THR	N-CA-C	-5.38	96.49	111.00
15	N	73	ARG	N-CA-C	-5.35	96.55	111.00
19	R	68	GLY	N-CA-C	-5.28	99.90	113.10
1	A	921	G	N9-C1'-C2'	5.12	120.65	114.00
1	A	192	A	N9-C1'-C2'	5.09	120.62	114.00
1	A	658	C	N1-C1'-C2'	-5.08	106.41	112.00
1	A	2468	A	N9-C1'-C2'	5.04	120.56	114.00
15	N	74	ARG	N-CA-C	5.04	124.60	111.00
1	A	917	U	C5'-C4'-C3'	5.01	124.01	116.00
1	A	1819	G	C5'-C4'-C3'	5.01	124.01	116.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1563	G	C3'
2	B	3024	U	C3'

All (147) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1007	A	Sidechain
1	A	1027	G	Sidechain
1	A	1030	U	Sidechain
1	A	1038	G	Sidechain
1	A	1125	U	Sidechain
1	A	115	U	Sidechain
1	A	1191	A	Sidechain
1	A	1206	U	Sidechain
1	A	1226	G	Sidechain
1	A	1236	A	Sidechain
1	A	1244	U	Sidechain
1	A	1260	G	Sidechain
1	A	1261	A	Sidechain
1	A	1266	U	Sidechain
1	A	1297	U	Sidechain
1	A	1298	U	Sidechain
1	A	1309	U	Sidechain
1	A	1332	C	Sidechain

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Mol	Chain	Res	Type	Group
1	A	1347	U	Sidechain
1	A	1368	U	Sidechain
1	A	1376	G	Sidechain
1	A	1387	G	Sidechain
1	A	1412	U	Sidechain
1	A	1417	G	Sidechain
1	A	1430	G	Sidechain
1	A	1467	C	Sidechain
1	A	1478	U	Sidechain
1	A	1503	U	Sidechain
1	A	1531	U	Sidechain
1	A	1635	U	Sidechain
1	A	1645	U	Sidechain
1	A	1647	G	Sidechain
1	A	1681	G	Sidechain
1	A	1684	A	Sidechain
1	A	1688	G	Sidechain
1	A	1696	U	Sidechain
1	A	1701	A	Sidechain
1	A	1706	G	Sidechain
1	A	171	C	Sidechain
1	A	1736	A	Sidechain
1	A	1750	C	Sidechain
1	A	176	U	Sidechain
1	A	1777	G	Sidechain
1	A	1818	C	Sidechain
1	A	182	G	Sidechain
1	A	1826	C	Sidechain
1	A	1828	G	Sidechain
1	A	1835	U	Sidechain
1	A	1839	A	Sidechain
1	A	1846	U	Sidechain
1	A	1848	G	Sidechain
1	A	1878	G	Sidechain
1	A	1933	G	Sidechain
1	A	1972	U	Sidechain
1	A	1978	A	Sidechain
1	A	2022	A	Sidechain
1	A	2026	C	Sidechain
1	A	2063	U	Sidechain
1	A	2102	G	Sidechain
1	A	211	U	Sidechain

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Mol	Chain	Res	Type	Group
1	A	2110	G	Sidechain
1	A	2119	C	Sidechain
1	A	2124	G	Sidechain
1	A	214	U	Sidechain
1	A	22	U	Sidechain
1	A	224	U	Sidechain
1	A	2279	G	Sidechain
1	A	2306	U	Sidechain
1	A	2308	U	Sidechain
1	A	2313	C	Sidechain
1	A	2336	G	Sidechain
1	A	2390	U	Sidechain
1	A	2421	G	Sidechain
1	A	2429	A	Sidechain
1	A	2433	A	Sidechain
1	A	2434	A	Sidechain
1	A	246	G	Sidechain
1	A	2461	U	Sidechain
1	A	2492	U	Sidechain
1	A	2493	C	Sidechain
1	A	2524	G	Sidechain
1	A	2526	C	Sidechain
1	A	2535	U	Sidechain
1	A	2590	U	Sidechain
1	A	26	U	Sidechain
1	A	2620	U	Sidechain
1	A	2621	U	Sidechain
1	A	2630	G	Sidechain
1	A	2634	G	Sidechain
1	A	265	U	Sidechain
1	A	2663	U	Sidechain
1	A	2673	U	Sidechain
1	A	2692	G	Sidechain
1	A	2736	U	Sidechain
1	A	2774	U	Sidechain
1	A	2790	C	Sidechain
1	A	2793	A	Sidechain
1	A	28	G	Sidechain
1	A	2800	A	Sidechain
1	A	2840	A	Sidechain
1	A	2842	G	Sidechain
1	A	315	G	Sidechain

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Mol	Chain	Res	Type	Group
1	A	321	A	Sidechain
1	A	333	G	Sidechain
1	A	344	C	Sidechain
1	A	395	A	Sidechain
1	A	396	U	Sidechain
1	A	407	A	Sidechain
1	A	435	A	Sidechain
1	A	436	A	Sidechain
1	A	458	G	Sidechain
1	A	459	A	Sidechain
1	A	48	A	Sidechain
1	A	483	C	Sidechain
1	A	502	A	Sidechain
1	A	506	G	Sidechain
1	A	518	G	Sidechain
1	A	548	U	Sidechain
1	A	55	U	Sidechain
1	A	614	U	Sidechain
1	A	619	U	Sidechain
1	A	640	G	Sidechain
1	A	664	U	Sidechain
1	A	676	C	Sidechain
1	A	722	G	Sidechain
1	A	734	U	Sidechain
1	A	743	G	Sidechain
1	A	761	A	Sidechain
1	A	764	C	Sidechain
1	A	775	G	Sidechain
1	A	815	U	Sidechain
1	A	816	G	Sidechain
1	A	818	A	Sidechain
1	A	854	G	Sidechain
1	A	873	G	Sidechain
1	A	888	U	Sidechain
1	A	897	A	Sidechain
1	A	898	G	Sidechain
1	A	906	C	Sidechain
1	A	919	U	Sidechain
1	A	932	U	Sidechain
1	A	950	G	Sidechain
1	A	954	U	Sidechain
2	B	3022	G	Sidechain

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Mol	Chain	Res	Type	Group
2	B	3024	U	Sidechain
2	B	3065	A	Sidechain
2	B	3099	U	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	59017	0	29798	1217	0
2	B	2600	0	1326	82	0
3	5	40	0	22	5	0
4	C	1754	0	1763	125	0
5	D	2624	0	2533	189	0
6	E	1858	0	1816	137	0
7	F	1094	0	1085	137	0
8	G	1357	0	1266	83	0
9	H	885	0	854	57	0
10	I	240	0	231	25	0
11	J	1215	0	1215	155	0
12	K	1119	0	1098	70	0
13	L	993	0	1027	67	0
14	M	1114	0	1072	67	0
15	N	1605	0	1676	179	0
16	O	1444	0	1401	142	0
17	P	864	0	873	40	0
18	Q	1133	0	1127	60	0
19	R	734	0	728	28	0
20	S	1149	0	1122	56	0
21	T	641	0	605	28	0
22	U	949	0	923	49	0
23	V	410	0	368	36	0
24	W	499	0	511	27	0
25	X	1195	0	1137	99	0
26	Y	654	0	653	51	0
27	Z	1130	0	1133	63	0
28	1	563	0	601	80	0
29	2	430	0	426	39	0
30	3	393	0	406	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	4	755	0	732	62	0
32	1	1	0	0	0	0
32	4	1	0	0	0	0
32	A	109	0	0	2	0
32	B	1	0	0	0	0
32	C	1	0	0	0	0
32	D	1	0	0	0	0
32	L	1	0	0	0	0
32	U	1	0	0	0	0
32	Z	1	0	0	0	0
33	A	2	0	0	0	0
34	4	1	0	0	0	0
34	A	71	0	0	0	0
34	B	2	0	0	0	0
34	C	1	0	0	0	0
34	E	1	0	0	0	0
34	J	2	0	0	0	0
34	K	1	0	0	0	0
34	M	1	0	0	0	0
34	N	1	0	0	0	0
34	R	1	0	0	0	0
34	S	2	0	0	0	0
34	T	1	0	0	0	0
34	U	1	0	0	0	0
35	4	1	0	0	1	0
35	A	7	0	0	0	0
35	C	1	0	0	0	0
35	D	1	0	0	0	0
35	K	4	0	0	0	0
35	M	1	0	0	0	0
35	N	1	0	0	2	0
35	O	1	0	0	1	0
35	P	1	0	0	0	0
35	R	1	0	0	0	0
35	S	1	0	0	0	0
35	Z	2	0	0	1	0
36	5	37	0	28	4	0
37	1	1	0	0	0	0
37	2	1	0	0	0	0
37	4	1	0	0	0	0
37	P	1	0	0	0	0
37	V	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	1	36	0	0	13	0
38	2	58	0	0	4	0
38	3	37	0	0	4	0
38	4	70	0	0	11	0
38	5	1	0	0	0	0
38	A	5860	0	0	268	0
38	B	146	0	0	15	0
38	C	140	0	0	15	0
38	D	146	0	0	32	0
38	E	176	0	0	34	0
38	F	52	0	0	20	0
38	G	45	0	0	11	0
38	H	32	0	0	9	0
38	I	22	0	0	8	0
38	J	78	0	0	20	0
38	K	54	0	0	4	0
38	L	64	0	0	16	0
38	M	86	0	0	15	0
38	N	138	0	0	27	0
38	O	64	0	0	19	0
38	P	44	0	0	12	0
38	Q	70	0	0	11	0
38	R	57	0	0	4	0
38	S	83	0	0	10	0
38	T	36	0	0	5	0
38	U	38	0	0	2	0
38	V	22	0	0	6	0
38	W	16	0	0	3	0
38	X	67	0	0	10	0
38	Y	28	0	0	6	0
38	Z	100	0	0	16	0
All	All	98593	0	59556	3185	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 21.

All (3185) 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)
11:J:165:GLY:HA3	38:J:8398:HOH:O	1.43	1.15
11:J:86:ARG:NH1	11:J:133:ILE:HG13	1.63	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:164:THR:HG22	15:N:167:GLY:H	1.10	1.12
28:1:46:LYS:HD3	28:1:59:HIS:HB2	1.30	1.10
1:A:1751:G:H2'	1:A:1752:G:H5''	1.30	1.10
6:E:236:THR:HG22	6:E:239:ALA:H	1.01	1.09
6:E:5:ILE:HD11	6:E:16:VAL:HG23	1.34	1.08
7:F:134:LEU:HD11	7:F:166:ILE:HD11	1.34	1.08
28:1:39:CYS:SG	28:1:47:LEU:HD21	1.93	1.08
22:U:71:VAL:HG11	22:U:90:PRO:HB3	1.34	1.08
1:A:2121:G:OP2	38:A:3007:HOH:O	1.69	1.06
24:W:12:THR:HG22	24:W:15:GLU:HG3	1.38	1.06
1:A:1160:G:H5'	1:A:1161:A:H5'	1.36	1.04
27:Z:200:THR:HG22	27:Z:201:GLU:HG3	1.39	1.04
1:A:1134:G:H4'	11:J:151:MET:HE1	1.41	1.03
28:1:40:PRO:HD3	28:1:47:LEU:HD11	1.39	1.03
1:A:156:C:H5''	15:N:171:ARG:HD3	1.39	1.03
1:A:870:G:H2'	1:A:871:G:H5''	1.40	1.02
11:J:45:GLN:HB3	11:J:163:PRO:HD2	1.40	1.02
1:A:2426:G:H1'	38:A:5552:HOH:O	1.57	1.02
15:N:74:ARG:O	15:N:88:VAL:HG13	1.56	1.02
25:X:88:THR:HB	38:X:6679:HOH:O	1.60	1.01
15:N:87:MET:HG2	31:4:46:ILE:HG21	1.39	1.00
1:A:1835:U:H5	1:A:1840:A:N7	1.58	1.00
7:F:105:SER:HB2	7:F:131:THR:HG23	1.43	1.00
6:E:127:ARG:NH2	6:E:225:PRO:HG2	1.77	0.99
1:A:2466:G:H5''	38:A:3142:HOH:O	1.61	0.99
6:E:115:LEU:HD13	6:E:223:LEU:HD21	1.42	0.98
5:D:86:ALA:HA	38:D:8583:HOH:O	1.64	0.98
15:N:35:PRO:HG2	15:N:38:VAL:HG23	1.42	0.98
1:A:1886:A:N3	38:A:4297:HOH:O	1.95	0.97
11:J:86:ARG:HH11	11:J:133:ILE:CG1	1.77	0.97
11:J:86:ARG:HH11	11:J:133:ILE:HG13	0.82	0.97
14:M:68:GLU:HA	38:M:8548:HOH:O	1.62	0.97
1:A:1474:C:H6	1:A:1474:C:H5'	1.30	0.97
2:B:3056:A:H2'	2:B:3057:A:H5''	1.45	0.96
21:T:57:THR:HG22	21:T:59:ASP:H	1.24	0.96
13:L:10:GLN:NE2	13:L:10:GLN:H	1.62	0.96
1:A:2717:C:H2'	1:A:2718:C:H5''	1.47	0.96
18:Q:115:SER:H	18:Q:118:GLN:HE21	0.99	0.96
1:A:2467:A:H2'	38:A:4927:HOH:O	1.64	0.95
5:D:321:PRO:HA	38:D:8657:HOH:O	1.66	0.95
1:A:962:C:H1'	16:O:5:ARG:NH1	1.82	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:871:G:H5'	1:A:871:G:H8	1.31	0.94
16:O:47:LEU:HD11	16:O:127:LEU:HD21	1.50	0.94
38:A:4337:HOH:O	15:N:14:ARG:HG2	1.65	0.93
21:T:57:THR:HG22	21:T:59:ASP:N	1.82	0.93
11:J:142:VAL:HG13	38:J:8381:HOH:O	1.68	0.93
26:Y:37:LEU:HD13	26:Y:85:VAL:HG21	1.47	0.93
7:F:25:MET:HE2	7:F:41:LEU:HG	1.50	0.93
2:B:3006:C:H5''	16:O:37:ARG:NH1	1.83	0.93
1:A:2533:C:H5'	1:A:2533:C:H6	1.32	0.93
2:B:3023:U:H4'	2:B:3024:U:OP2	1.69	0.93
6:E:104:ASP:HA	6:E:107:ARG:HH12	1.33	0.93
13:L:29:LEU:HB3	13:L:55:VAL:HG11	1.49	0.92
1:A:856:G:H2'	38:A:4898:HOH:O	1.68	0.92
1:A:1116:U:HO2'	1:A:1118:A:H2	0.92	0.91
4:C:211:LYS:HB3	4:C:212:PRO:HD2	1.52	0.91
11:J:150:LYS:HB2	11:J:157:ILE:HD12	1.52	0.91
11:J:162:SER:HB2	11:J:163:PRO:HD3	1.53	0.91
20:S:99:ALA:HB1	20:S:109:MET:HE1	1.50	0.91
13:L:10:GLN:HE21	13:L:10:GLN:H	1.10	0.91
6:E:2:GLN:HB3	38:E:8338:HOH:O	1.70	0.91
6:E:236:THR:HG22	6:E:239:ALA:N	1.85	0.90
15:N:35:PRO:CG	15:N:38:VAL:HG23	2.01	0.90
27:Z:212:ARG:HD2	38:Z:8605:HOH:O	1.70	0.90
12:K:19:MET:HE3	12:K:132:LEU:HD11	1.53	0.90
1:A:1372:A:H3'	38:A:6651:HOH:O	1.68	0.90
13:L:14:LYS:HB2	13:L:45:PRO:HG2	1.54	0.90
26:Y:78:GLU:HG2	26:Y:79:GLU:H	1.36	0.90
15:N:69:LYS:O	15:N:73:ARG:NH2	2.04	0.90
15:N:87:MET:CG	31:4:46:ILE:HG21	2.02	0.90
1:A:2122:C:OP2	38:A:6038:HOH:O	1.88	0.90
1:A:871:G:H5'	1:A:871:G:C8	2.06	0.90
2:B:3076:G:H3'	2:B:3077:A:H5''	1.54	0.89
1:A:506:G:H22	1:A:509:A:H5'	1.35	0.89
11:J:27:LYS:H	11:J:58:HIS:HD2	1.14	0.89
5:D:264:GLU:HG2	5:D:267:LYS:HE2	1.51	0.89
16:O:49:THR:HG22	16:O:56:ASP:HB2	1.55	0.89
1:A:2780:C:H1'	8:G:143:GLN:HE21	1.38	0.89
11:J:29:ALA:HB3	11:J:65:ARG:HH12	1.38	0.89
26:Y:25:ARG:HD2	38:Y:3861:HOH:O	1.73	0.88
1:A:1679:C:H5'	38:A:8834:HOH:O	1.74	0.88
30:3:41:HIS:H	30:3:45:ASN:HD22	1.20	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:26:LYS:HD2	11:J:28:ILE:HD12	1.54	0.88
25:X:122:ARG:HH21	25:X:154:ARG:HD2	1.37	0.88
1:A:2717:C:C2'	1:A:2718:C:H5''	2.04	0.88
6:E:132:ASP:HB3	38:E:8364:HOH:O	1.74	0.88
10:I:23:ILE:HD13	10:I:67:LEU:HD23	1.56	0.88
15:N:164:THR:HG22	15:N:167:GLY:N	1.88	0.87
5:D:212:GLN:HB2	5:D:257:THR:HG21	1.56	0.87
16:O:144:GLY:O	16:O:147:ILE:HG22	1.73	0.87
5:D:62:ARG:HA	5:D:65:MET:HE3	1.56	0.87
1:A:1242:A:H5'	12:K:82:THR:HG23	1.53	0.87
4:C:223:ARG:HG3	38:C:8616:HOH:O	1.73	0.87
11:J:13:ALA:HA	11:J:91:HIS:HE1	1.38	0.87
25:X:88:THR:HG22	25:X:89:ASP:H	1.39	0.87
1:A:2123:A:OP2	38:A:4762:HOH:O	1.91	0.86
6:E:236:THR:HG21	38:E:8375:HOH:O	1.74	0.86
26:Y:15:ARG:HH11	26:Y:15:ARG:HB3	1.40	0.86
12:K:19:MET:CE	12:K:132:LEU:HD11	2.05	0.86
18:Q:115:SER:OG	18:Q:118:GLN:HG3	1.75	0.86
2:B:3025:G:H3'	2:B:3026:C:H5'	1.55	0.86
1:A:1166:A:H1'	1:A:1192:A:C2	2.10	0.86
1:A:21:G:H5'	20:S:2:ILE:HA	1.56	0.86
1:A:542:A:H8	1:A:542:A:H5'	1.38	0.86
28:1:39:CYS:HA	28:1:47:LEU:HD11	1.57	0.86
1:A:1116:U:H3	1:A:1246:A:H62	1.23	0.86
1:A:545:G:H5'	1:A:545:G:H8	1.40	0.86
1:A:870:G:C2'	1:A:871:G:H5''	2.06	0.86
20:S:9:ASP:O	20:S:13:THR:HB	1.76	0.86
6:E:5:ILE:HD11	6:E:16:VAL:CG2	2.06	0.85
1:A:1244:U:OP1	12:K:18:ILE:HD13	1.76	0.85
5:D:140:LEU:HA	38:D:8583:HOH:O	1.75	0.85
1:A:2420:G:O2'	1:A:2421:G:H5'	1.75	0.85
15:N:74:ARG:HH11	15:N:74:ARG:HG3	1.41	0.85
18:Q:115:SER:H	18:Q:118:GLN:NE2	1.74	0.85
31:4:25:VAL:HG22	31:4:68:LYS:HG3	1.58	0.85
1:A:1474:C:C6	1:A:1474:C:H5'	2.12	0.85
15:N:164:THR:HG23	15:N:165:SER:N	1.90	0.85
16:O:87:LEU:HD12	16:O:186:LEU:HD21	1.57	0.85
6:E:246:ARG:NH1	6:E:246:ARG:HB3	1.91	0.85
11:J:162:SER:HB2	11:J:163:PRO:CD	2.07	0.85
1:A:506:G:H22	1:A:509:A:C5'	1.88	0.84
15:N:102:GLU:OE1	15:N:164:THR:HG21	1.77	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1450:C:H4'	1:A:1451:C:OP2	1.76	0.84
6:E:140:VAL:HB	38:E:8457:HOH:O	1.77	0.84
1:A:645:U:OP2	14:M:4:LYS:HE2	1.77	0.84
2:B:3025:G:H3'	2:B:3026:C:C5'	2.07	0.84
15:N:52:LEU:HD11	38:N:8616:HOH:O	1.76	0.84
16:O:83:LEU:HD13	16:O:175:LEU:HD23	1.60	0.84
25:X:122:ARG:NH2	25:X:154:ARG:HD2	1.92	0.84
29:2:8:GLN:HE22	29:2:11:LYS:NZ	1.74	0.84
38:B:8459:HOH:O	19:R:25:PRO:HB2	1.78	0.84
11:J:59:ASN:HD22	11:J:59:ASN:H	1.21	0.84
13:L:81:ARG:HB2	13:L:87:ARG:HH11	1.40	0.84
29:2:8:GLN:HE22	29:2:11:LYS:HZ2	1.23	0.83
25:X:88:THR:HG23	25:X:110:GLN:NE2	1.93	0.83
28:1:42:CYS:SG	28:1:44:PHE:HB2	2.17	0.83
1:A:2459:G:P	31:4:64:LYS:HB2	2.18	0.83
11:J:13:ALA:HA	11:J:91:HIS:CE1	2.13	0.83
38:A:3219:HOH:O	15:N:157:LEU:HD11	1.77	0.83
14:M:79:ASP:HB3	38:M:8564:HOH:O	1.78	0.83
1:A:960:G:H4'	38:A:6886:HOH:O	1.76	0.83
27:Z:187:VAL:HG23	27:Z:192:ASP:HB2	1.61	0.83
31:4:70:ARG:HG2	31:4:77:ALA:HB2	1.60	0.83
5:D:201:ASP:HB2	5:D:312:ARG:HD2	1.59	0.83
25:X:6:GLN:HB2	25:X:26:ILE:HD12	1.59	0.83
7:F:27:ILE:HG22	7:F:28:GLY:H	1.43	0.83
13:L:10:GLN:HE21	13:L:10:GLN:N	1.77	0.83
1:A:1603:A:H5'	1:A:1605:G:O4'	1.78	0.82
15:N:74:ARG:NH2	38:N:8632:HOH:O	2.11	0.82
16:O:7:LYS:HE3	19:R:21:ARG:O	1.79	0.82
4:C:121:ALA:O	4:C:124:VAL:HG22	1.79	0.82
12:K:76:ASP:HA	38:K:5907:HOH:O	1.79	0.82
28:1:46:LYS:HB2	28:1:57:CYS:SG	2.19	0.82
16:O:113:SER:HB2	38:O:8556:HOH:O	1.77	0.82
7:F:154:LYS:H	7:F:154:LYS:HD2	1.44	0.82
16:O:86:LEU:HD12	16:O:125:ALA:HB2	1.60	0.82
38:A:7015:HOH:O	31:4:60:LYS:HG3	1.79	0.81
29:2:25:LYS:HE2	38:3:7213:HOH:O	1.79	0.81
38:A:8631:HOH:O	15:N:82:ARG:HD2	1.80	0.81
5:D:18:ARG:HG3	5:D:256:GLN:HG3	1.61	0.81
8:G:100:ASP:HB2	38:G:2789:HOH:O	1.79	0.81
11:J:26:LYS:HG2	11:J:28:ILE:H	1.44	0.81
1:A:2506:A:HO2'	1:A:2507:G:H8	0.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1184:C:H1'	38:A:6922:HOH:O	1.81	0.81
1:A:1835:U:C5	1:A:1840:A:N7	2.48	0.81
38:A:4426:HOH:O	2:B:3103:A:H4'	1.81	0.81
11:J:55:GLN:HE21	11:J:124:ARG:HE	1.28	0.81
11:J:2:PRO:HB2	38:J:8365:HOH:O	1.81	0.80
4:C:192:VAL:HB	38:C:8606:HOH:O	1.81	0.80
28:1:38:LYS:HG2	28:1:45:LYS:HG2	1.62	0.80
7:F:20:LYS:HA	7:F:75:LEU:O	1.82	0.80
27:Z:187:VAL:HG23	27:Z:192:ASP:CB	2.12	0.80
1:A:1974:G:OP1	38:A:6321:HOH:O	1.99	0.80
28:1:47:LEU:HD23	28:1:57:CYS:HB2	1.63	0.80
1:A:2506:A:O2'	1:A:2507:G:H8	1.62	0.80
11:J:5:MET:HG3	38:J:8365:HOH:O	1.80	0.80
1:A:1205:U:H2'	1:A:1206:U:H5'	1.62	0.80
1:A:560:C:H42	1:A:597:A:H61	1.29	0.80
4:C:69:LEU:HD21	4:C:120:ARG:HB3	1.62	0.80
9:H:91:VAL:HG12	9:H:92:GLY:H	1.47	0.80
23:V:9:CYS:SG	23:V:11:THR:HG23	2.21	0.79
1:A:289:G:H22	1:A:363:A:H2	1.30	0.79
1:A:1684:A:H1'	30:3:43:ARG:HH22	1.47	0.79
1:A:1118:A:C8	1:A:1118:A:H3'	2.18	0.79
1:A:2586:U:H3	1:A:2592:G:H22	1.30	0.79
1:A:1165:G:H4'	1:A:1174:A:O2'	1.81	0.79
1:A:2466:G:OP1	38:A:3142:HOH:O	2.00	0.79
14:M:133:VAL:HA	38:M:8577:HOH:O	1.80	0.79
1:A:346:U:H4'	38:A:6302:HOH:O	1.83	0.79
12:K:26:VAL:HG13	12:K:36:VAL:HG11	1.65	0.79
38:A:3278:HOH:O	15:N:189:VAL:HG21	1.83	0.78
1:A:31:C:H4'	38:A:6880:HOH:O	1.83	0.78
13:L:30:LYS:O	13:L:55:VAL:HG13	1.82	0.78
38:A:6460:HOH:O	19:R:9:GLY:HA2	1.82	0.78
6:E:246:ARG:HH11	6:E:246:ARG:HB3	1.45	0.78
12:K:99:GLU:HA	38:K:7377:HOH:O	1.84	0.78
26:Y:76:ARG:HH11	26:Y:76:ARG:HG3	1.49	0.78
1:A:381:G:H5"	38:A:3807:HOH:O	1.84	0.78
7:F:19:GLU:O	7:F:20:LYS:HG2	1.84	0.78
6:E:47:GLY:HA2	6:E:92:PRO:HB2	1.65	0.78
13:L:74:VAL:HG13	13:L:113:ILE:HG23	1.65	0.78
27:Z:185:VAL:HA	38:Z:8566:HOH:O	1.84	0.78
5:D:145:HIS:HD2	5:D:146:THR:O	1.67	0.78
11:J:139:ASP:N	11:J:140:PRO:HD3	1.98	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:3:GLY:HA2	11:J:57:ARG:HH12	1.48	0.78
15:N:87:MET:HG2	31:4:46:ILE:CG2	2.14	0.78
27:Z:216:ARG:HD3	38:Z:8574:HOH:O	1.83	0.78
6:E:107:ARG:NH1	6:E:107:ARG:HB3	1.99	0.77
1:A:2468:A:H61	31:4:48:ASN:HD21	1.27	0.77
1:A:2812:A:H2	1:A:2814:A:H62	1.32	0.77
11:J:150:LYS:HE2	38:J:8383:HOH:O	1.84	0.77
12:K:74:ARG:HB3	12:K:74:ARG:HH11	1.48	0.77
25:X:4:LEU:HD22	25:X:52:VAL:HG21	1.66	0.77
1:A:1160:G:C5'	1:A:1161:A:H5'	2.14	0.77
1:A:288:A:H61	1:A:364:C:H42	1.32	0.77
9:H:91:VAL:HG12	9:H:92:GLY:N	2.00	0.77
38:A:5753:HOH:O	7:F:99:ASP:HA	1.84	0.77
9:H:96:ALA:HA	38:H:3111:HOH:O	1.84	0.77
12:K:103:VAL:HG12	38:K:5907:HOH:O	1.84	0.77
15:N:157:LEU:HA	35:N:8518:CL:CL	2.22	0.77
1:A:1118:A:H3'	1:A:1118:A:H8	1.48	0.77
11:J:130:HIS:CD2	11:J:133:ILE:HD11	2.20	0.77
27:Z:220:GLU:HG2	38:Z:8553:HOH:O	1.85	0.77
1:A:338:C:H4'	6:E:174:ILE:CD1	2.15	0.76
12:K:133:GLY:O	12:K:137:GLU:HG3	1.85	0.76
8:G:97:VAL:HG12	38:G:4191:HOH:O	1.84	0.76
26:Y:71:ARG:HB3	26:Y:88:GLU:OE1	1.85	0.76
2:B:3014:G:H8	2:B:3014:G:H5'	1.50	0.76
2:B:3023:U:H6	2:B:3023:U:H5''	1.50	0.76
18:Q:59:ARG:NH2	18:Q:66:GLN:HE22	1.82	0.76
1:A:1058:A:H2'	1:A:1060:C:H5''	1.68	0.76
18:Q:115:SER:N	18:Q:118:GLN:HE21	1.80	0.76
28:1:29:VAL:O	28:1:33:HIS:HB2	1.86	0.76
1:A:2466:G:C5'	38:A:3142:HOH:O	2.23	0.76
1:A:450:C:OP1	6:E:184:ARG:NH2	2.17	0.76
1:A:559:U:H6	1:A:559:U:H5'	1.51	0.76
1:A:871:G:C5'	1:A:871:G:H8	1.98	0.76
1:A:962:C:H1'	16:O:5:ARG:HH12	1.50	0.76
2:B:3023:U:H3'	38:B:8482:HOH:O	1.85	0.76
11:J:59:ASN:HD22	11:J:59:ASN:N	1.83	0.76
1:A:2578:G:H5'	1:A:2578:G:H8	1.49	0.76
5:D:258:GLY:H	5:D:260:HIS:CE1	2.03	0.76
11:J:141:ASN:HA	38:J:8366:HOH:O	1.84	0.76
1:A:31:C:H2'	38:A:7147:HOH:O	1.86	0.76
25:X:68:THR:HG23	25:X:69:ARG:HG2	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:21:LEU:HD22	25:X:26:ILE:CD1	2.16	0.76
1:A:2271:G:OP2	38:A:8940:HOH:O	2.05	0.75
1:A:2467:A:H3'	38:A:4927:HOH:O	1.85	0.75
9:H:50:VAL:HG21	9:H:63:ILE:HG21	1.65	0.75
8:G:6:GLU:HA	8:G:46:THR:HG22	1.69	0.75
14:M:120:LEU:HD12	14:M:133:VAL:HG21	1.69	0.75
1:A:1741:U:O2'	1:A:2723:G:H4'	1.87	0.75
1:A:282:C:H1'	1:A:368:C:N4	2.00	0.75
4:C:88:ILE:HD13	4:C:100:PRO:HD3	1.68	0.75
11:J:27:LYS:N	11:J:58:HIS:HD2	1.84	0.75
20:S:99:ALA:HB1	20:S:109:MET:CE	2.15	0.75
1:A:711:G:H1'	38:A:6554:HOH:O	1.87	0.75
4:C:35:GLY:O	4:C:36:ASP:HB3	1.86	0.75
13:L:39:GLY:HA2	38:L:4183:HOH:O	1.86	0.75
7:F:146:LYS:NZ	16:O:107:ASN:HD21	1.85	0.75
25:X:72:PRO:HG2	25:X:77:ALA:HB3	1.67	0.75
1:A:1771:U:H4'	28:1:20:LEU:HD21	1.67	0.75
24:W:1:THR:HG23	24:W:2:VAL:H	1.51	0.75
1:A:2094:G:H4'	5:D:245:SER:HB3	1.66	0.75
28:1:46:LYS:HB2	28:1:57:CYS:HG	1.52	0.75
1:A:1191:A:H3'	1:A:1192:A:H5''	1.68	0.75
1:A:2508:C:H2'	38:A:6213:HOH:O	1.86	0.75
1:A:2433:A:H2'	1:A:2434:A:C8	2.22	0.75
6:E:76:ARG:HD2	38:E:8439:HOH:O	1.85	0.75
8:G:107:PHE:CE2	8:G:108:LEU:HD13	2.22	0.75
11:J:28:ILE:HA	11:J:62:GLU:OE1	1.87	0.75
2:B:3069:U:OP1	16:O:4:PRO:HG3	1.86	0.75
28:1:18:TYR:HB3	28:1:22:ILE:HG21	1.68	0.74
14:M:67:ARG:O	14:M:71:GLU:HG3	1.87	0.74
1:A:1751:G:C2'	1:A:1752:G:H5''	2.11	0.74
20:S:8:ALA:HB1	20:S:13:THR:HG21	1.69	0.74
15:N:87:MET:CB	31:4:46:ILE:HG21	2.17	0.74
28:1:38:LYS:HE2	28:1:45:LYS:HE2	1.68	0.74
31:4:65:THR:HG23	31:4:67:LEU:HG	1.69	0.74
8:G:166:VAL:HG12	38:G:3134:HOH:O	1.87	0.74
1:A:2812:A:N7	38:A:6974:HOH:O	2.20	0.74
15:N:152:ARG:HG3	38:N:8559:HOH:O	1.87	0.74
23:V:13:ILE:HG12	23:V:32:CYS:CB	2.17	0.74
6:E:162:VAL:HG12	6:E:192:ILE:HD11	1.69	0.74
7:F:95:THR:O	7:F:97:GLN:N	2.18	0.74
38:B:8467:HOH:O	16:O:147:ILE:HD12	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:1:49:ARG:HD2	38:1:8426:HOH:O	1.87	0.73
2:B:3056:A:C2'	2:B:3057:A:H5''	2.18	0.73
4:C:36:ASP:OD2	4:C:85:ASP:HB2	1.87	0.73
1:A:2755:G:H1'	38:A:4164:HOH:O	1.88	0.73
15:N:173:LEU:HD23	15:N:183:VAL:HG12	1.70	0.73
16:O:61:ALA:HB3	16:O:88:ALA:HB2	1.71	0.73
23:V:47:ARG:HG3	38:V:4381:HOH:O	1.88	0.73
1:A:2748:G:H2'	38:A:6999:HOH:O	1.88	0.73
25:X:137:GLN:HE21	25:X:141:HIS:HE1	1.36	0.73
1:A:820:G:OP1	28:1:17:ARG:NH2	2.20	0.73
1:A:1209:C:H4'	38:A:4753:HOH:O	1.88	0.73
1:A:1701:A:H5'	38:A:5741:HOH:O	1.87	0.73
15:N:79:LYS:HD3	38:N:8563:HOH:O	1.88	0.73
1:A:1130:U:H2'	1:A:1131:G:O4'	1.89	0.73
1:A:1829:A:H61	28:1:18:TYR:HA	1.54	0.73
5:D:71:VAL:HG11	5:D:296:LEU:HB3	1.70	0.73
25:X:122:ARG:HG2	25:X:122:ARG:HH11	1.52	0.73
13:L:62:PRO:HG3	13:L:65:ARG:HH21	1.54	0.73
2:B:3024:U:O2'	2:B:3025:G:H4'	1.88	0.73
1:A:1160:G:H5'	1:A:1161:A:C5'	2.15	0.72
7:F:35:ALA:N	38:F:5576:HOH:O	2.22	0.72
38:A:3951:HOH:O	15:N:146:GLN:HG2	1.89	0.72
1:A:2404:G:O3'	38:A:6058:HOH:O	2.06	0.72
4:C:135:VAL:HG21	4:C:147:ARG:NH1	2.04	0.72
11:J:56:ILE:HG22	11:J:61:LEU:HD22	1.71	0.72
16:O:11:ARG:HG3	16:O:14:ARG:NH1	2.03	0.72
20:S:39:THR:HG23	20:S:107:GLU:O	1.89	0.72
31:4:74:CYS:SG	31:4:76:LYS:HB2	2.28	0.72
15:N:87:MET:CB	31:4:46:ILE:HD13	2.20	0.72
10:I:12:ILE:N	10:I:13:PRO:HD3	2.04	0.72
1:A:182:G:H5'	38:A:4632:HOH:O	1.87	0.72
8:G:101:GLU:HB2	8:G:116:THR:O	1.90	0.72
38:A:4311:HOH:O	12:K:47:THR:HB	1.89	0.72
5:D:179:LEU:O	5:D:183:GLU:HG2	1.90	0.72
15:N:72:SER:O	38:N:8655:HOH:O	2.06	0.72
1:A:1666:C:H2'	1:A:1667:A:H5'	1.70	0.72
1:A:2620:U:O2'	38:A:6629:HOH:O	2.06	0.72
11:J:137:ASN:O	11:J:139:ASP:N	2.22	0.72
20:S:39:THR:HG22	20:S:42:GLU:H	1.53	0.72
1:A:113:A:OP2	1:A:114:A:H2'	1.89	0.72
1:A:172:U:OP2	38:A:5669:HOH:O	2.07	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:141:ARG:HG2	5:D:165:ARG:HA	1.70	0.72
12:K:75:PRO:HG2	12:K:105:LEU:HD21	1.71	0.72
15:N:139:PRO:O	15:N:140:ALA:HB3	1.89	0.72
14:M:114:VAL:HG11	38:M:8577:HOH:O	1.89	0.72
15:N:59:GLY:HA3	15:N:141:ILE:CD1	2.19	0.72
19:R:64:GLU:HG3	19:R:74:ASP:OD2	1.89	0.72
38:A:6880:HOH:O	22:U:9:LYS:HB2	1.89	0.72
1:A:2346:C:H6	1:A:2346:C:O5'	1.73	0.71
1:A:272:A:H3'	38:A:6987:HOH:O	1.88	0.71
8:G:11:VAL:HG12	8:G:12:ASP:N	2.05	0.71
10:I:12:ILE:HA	38:I:4499:HOH:O	1.89	0.71
13:L:106:GLY:HA3	38:L:5264:HOH:O	1.89	0.71
15:N:68:ARG:HD3	15:N:68:ARG:O	1.89	0.71
17:P:32:ARG:HD3	17:P:32:ARG:O	1.87	0.71
17:P:47:ARG:HH11	17:P:47:ARG:HG3	1.55	0.71
1:A:2467:A:C2'	38:A:4927:HOH:O	2.31	0.71
1:A:284:C:H4'	1:A:285:A:O5'	1.88	0.71
15:N:106:ASN:HD22	15:N:114:VAL:HG23	1.56	0.71
24:W:12:THR:HG22	24:W:15:GLU:CG	2.19	0.71
28:1:30:GLU:HA	28:1:33:HIS:HB3	1.73	0.71
4:C:179:MET:HG2	4:C:186:TRP:CB	2.20	0.71
11:J:162:SER:CB	11:J:163:PRO:HD3	2.20	0.71
4:C:76:VAL:HG23	28:1:63:LYS:HB3	1.73	0.71
11:J:139:ASP:HA	38:J:8370:HOH:O	1.88	0.71
1:A:2291:A:C8	1:A:2309:C:H5'	2.25	0.71
1:A:2310:G:OP2	11:J:114:PRO:HD2	1.89	0.71
1:A:2638:G:H1'	38:A:7218:HOH:O	1.90	0.71
5:D:190:MET:HE2	5:D:194:PHE:CD1	2.25	0.71
11:J:33:MET:HB2	11:J:83:PHE:HB3	1.72	0.71
2:B:3006:C:OP1	16:O:37:ARG:NH1	2.22	0.71
1:A:1701:A:H4'	1:A:1702:U:H5''	1.72	0.71
6:E:12:THR:HB	38:E:8447:HOH:O	1.89	0.71
38:A:3555:HOH:O	5:D:27:ASN:HB2	1.90	0.71
23:V:13:ILE:HG12	23:V:32:CYS:HB3	1.70	0.71
1:A:1118:A:H62	1:A:1244:U:H3	1.39	0.71
1:A:877:G:H5'	1:A:878:G:OP1	1.91	0.71
14:M:143:THR:HG22	14:M:144:ASP:N	2.05	0.71
14:M:34:GLY:HA3	14:M:38:HIS:CE1	2.25	0.71
25:X:81:ASP:OD1	25:X:92:ASP:HB2	1.91	0.71
1:A:113:A:H3'	1:A:114:A:H5''	1.71	0.71
13:L:81:ARG:HB2	13:L:87:ARG:NH1	2.04	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1741:U:H5'	1:A:1742:A:OP1	1.90	0.70
1:A:2502:C:C2'	1:A:2503:A:H5'	2.21	0.70
6:E:46:TYR:CE2	6:E:98:ARG:NH1	2.59	0.70
1:A:2346:C:O2'	7:F:52:THR:HG21	1.91	0.70
16:O:48:VAL:CG1	16:O:55:ASP:HB3	2.20	0.70
1:A:1666:C:O2'	1:A:1667:A:H5''	1.91	0.70
1:A:2421:G:H4'	38:A:4257:HOH:O	1.91	0.70
5:D:162:MET:HE3	5:D:308:LEU:HD21	1.72	0.70
15:N:122:GLU:OE2	15:N:127:LYS:HE2	1.91	0.70
38:A:5258:HOH:O	15:N:170:CYS:SG	2.48	0.70
6:E:104:ASP:HA	6:E:107:ARG:NH1	2.06	0.70
6:E:236:THR:H	6:E:239:ALA:HB3	1.55	0.70
7:F:91:ALA:HB1	38:F:5198:HOH:O	1.91	0.70
15:N:164:THR:CG2	15:N:167:GLY:H	1.95	0.70
18:Q:10:ALA:HA	18:Q:13:VAL:HG12	1.73	0.70
20:S:18:LEU:HB2	20:S:143:VAL:HG12	1.72	0.70
1:A:1164:U:H3	1:A:1192:A:H2	1.38	0.70
1:A:1119:G:N2	1:A:1246:A:C2	2.59	0.70
1:A:2467:A:OP1	38:A:8560:HOH:O	2.09	0.70
11:J:14:TYR:H	11:J:91:HIS:CE1	2.09	0.70
23:V:9:CYS:HA	23:V:52:THR:HG23	1.72	0.70
25:X:4:LEU:HD22	25:X:52:VAL:CG2	2.21	0.70
1:A:2281:C:C2'	1:A:2282:U:H5'	2.20	0.70
2:B:3006:C:H5''	16:O:37:ARG:HH12	1.55	0.70
9:H:53:ASP:OD1	9:H:80:GLN:HB2	1.91	0.70
11:J:75:SER:O	11:J:79:ALA:HB2	1.92	0.70
38:A:9293:HOH:O	13:L:39:GLY:HA3	1.90	0.70
6:E:25:PRO:HG2	38:E:8325:HOH:O	1.92	0.70
6:E:78:ARG:HG3	6:E:78:ARG:HH11	1.56	0.70
2:B:3023:U:C6	2:B:3023:U:H5''	2.27	0.70
11:J:26:LYS:HD3	11:J:89:PRO:HG3	1.73	0.70
26:Y:18:ARG:NH1	38:Y:4132:HOH:O	2.16	0.70
11:J:140:PRO:HB3	38:J:8381:HOH:O	1.92	0.70
11:J:27:LYS:H	11:J:58:HIS:CD2	2.04	0.70
12:K:107:ASN:ND2	12:K:109:TYR:H	1.90	0.70
15:N:12:TRP:CE2	15:N:20:ILE:HD11	2.27	0.70
15:N:74:ARG:HG3	15:N:74:ARG:NH1	2.02	0.70
1:A:2837:U:H2'	38:A:6298:HOH:O	1.92	0.69
1:A:299:U:H5'	38:A:6794:HOH:O	1.92	0.69
38:A:6913:HOH:O	6:E:188:ARG:HD3	1.92	0.69
9:H:63:ILE:HB	9:H:64:PRO:HD3	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2526:C:O2'	1:A:2527:U:H5'	1.92	0.69
5:D:148:PRO:HD2	38:D:8584:HOH:O	1.91	0.69
20:S:39:THR:HB	20:S:42:GLU:HG3	1.73	0.69
1:A:1080:C:H4'	1:A:1081:A:OP1	1.90	0.69
1:A:1377:C:H5'	1:A:1377:C:H6	1.57	0.69
1:A:2249:G:OP2	38:A:4912:HOH:O	2.10	0.69
1:A:461:C:H2'	38:A:3491:HOH:O	1.92	0.69
1:A:541:C:C2'	1:A:542:A:H5''	2.22	0.69
1:A:1625:U:H4'	38:A:4149:HOH:O	1.92	0.69
6:E:139:VAL:HG13	38:E:8454:HOH:O	1.90	0.69
1:A:182:G:H4'	15:N:157:LEU:HD13	1.75	0.69
4:C:199:HIS:CD2	4:C:201:PHE:H	2.10	0.69
11:J:55:GLN:HE22	11:J:91:HIS:CD2	2.10	0.69
1:A:1380:U:OP1	38:A:7331:HOH:O	2.09	0.69
1:A:2433:A:H2'	1:A:2434:A:H8	1.56	0.69
16:O:164:ASP:CG	16:O:167:ASP:HA	2.13	0.69
25:X:88:THR:HG22	25:X:89:ASP:N	2.08	0.69
1:A:541:C:H2'	1:A:542:A:C5'	2.22	0.69
4:C:33:GLU:O	4:C:34:ASP:HB2	1.92	0.69
15:N:139:PRO:O	15:N:140:ALA:CB	2.41	0.69
16:O:159:TYR:HB3	16:O:162:ASP:HB2	1.74	0.69
1:A:2100:A:H5'	38:A:6844:HOH:O	1.92	0.69
2:B:3048:C:H4'	16:O:141:ARG:HH21	1.57	0.69
7:F:88:LEU:HB2	7:F:89:PRO:HD3	1.75	0.69
24:W:39:ALA:N	24:W:40:PRO:HD2	2.08	0.69
30:3:39:ARG:HG2	38:3:3143:HOH:O	1.93	0.69
1:A:214:U:H5'	38:A:5600:HOH:O	1.91	0.69
1:A:69:A:C8	1:A:69:A:H5'	2.28	0.69
2:B:3025:G:C3'	2:B:3026:C:H5'	2.22	0.69
17:P:47:ARG:NH1	38:P:4564:HOH:O	2.24	0.69
22:U:9:LYS:HE3	22:U:13:ARG:NH1	2.08	0.69
26:Y:72:VAL:HG22	26:Y:85:VAL:HG12	1.75	0.69
9:H:110:GLU:HG2	38:H:6926:HOH:O	1.92	0.69
11:J:69:ASN:O	11:J:72:VAL:HG12	1.92	0.69
1:A:447:A:OP1	22:U:2:LYS:HG2	1.92	0.69
38:A:6913:HOH:O	6:E:188:ARG:CD	2.41	0.68
11:J:41:THR:HA	38:J:8396:HOH:O	1.91	0.68
28:1:47:LEU:CD2	28:1:57:CYS:HB2	2.23	0.68
30:3:41:HIS:N	30:3:45:ASN:HD22	1.89	0.68
1:A:1160:G:N3	38:A:5102:HOH:O	2.26	0.68
1:A:1743:G:N7	38:A:8768:HOH:O	2.25	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:254:GLN:HG3	38:D:8530:HOH:O	1.92	0.68
1:A:2467:A:C3'	38:A:4927:HOH:O	2.42	0.68
1:A:371:U:H2'	1:A:372:A:H8	1.58	0.68
1:A:542:A:H5'	1:A:542:A:C8	2.27	0.68
2:B:3039:U:H1'	2:B:3044:A:H61	1.57	0.68
16:O:151:ASP:O	16:O:154:LEU:HB2	1.94	0.68
21:T:51:GLN:HE21	21:T:53:ASN:HD21	1.41	0.68
1:A:1909:A:N1	1:A:2128:G:H1'	2.08	0.68
15:N:37:VAL:HG21	15:N:108:LYS:HG3	1.74	0.68
26:Y:78:GLU:CG	26:Y:79:GLU:H	2.06	0.68
1:A:2316:G:H8	38:A:5124:HOH:O	1.76	0.68
6:E:242:GLU:HG3	38:E:8383:HOH:O	1.92	0.68
1:A:516:A:OP2	38:A:5115:HOH:O	2.10	0.68
22:U:61:GLU:HG3	38:U:3851:HOH:O	1.93	0.68
25:X:13:MET:HE1	25:X:18:GLN:HA	1.75	0.68
25:X:21:LEU:HD22	25:X:26:ILE:HD11	1.76	0.68
25:X:6:GLN:HB2	25:X:26:ILE:CD1	2.23	0.68
28:1:62:TYR:CE2	28:1:64:ILE:HG23	2.29	0.68
1:A:541:C:H2'	1:A:542:A:H5''	1.75	0.68
16:O:164:ASP:OD2	16:O:167:ASP:HA	1.94	0.68
21:T:37:VAL:O	21:T:41:VAL:HG23	1.93	0.68
1:A:21:G:C5'	20:S:2:ILE:HA	2.23	0.68
1:A:2301:A:H5''	1:A:2302:A:H5'	1.75	0.68
1:A:2716:G:H5''	5:D:206:THR:HG21	1.76	0.68
1:A:2830:U:H3'	38:A:4703:HOH:O	1.92	0.68
1:A:485:A:N3	1:A:487:G:H5''	2.09	0.68
2:B:3013:A:O2'	2:B:3014:G:H5''	1.94	0.68
9:H:99:THR:HA	38:H:3461:HOH:O	1.94	0.68
25:X:22:GLU:HG2	25:X:27:HIS:CD2	2.28	0.68
1:A:739:G:C5	38:A:7001:HOH:O	2.47	0.67
12:K:107:ASN:HD21	12:K:109:TYR:HB2	1.59	0.67
1:A:545:G:C8	1:A:545:G:H5'	2.28	0.67
1:A:918:G:N7	38:A:9993:HOH:O	2.27	0.67
2:B:3092:G:H2'	2:B:3093:A:C8	2.29	0.67
15:N:78:ASN:ND2	38:N:8651:HOH:O	2.26	0.67
27:Z:155:ARG:NH1	38:Z:8562:HOH:O	2.26	0.67
1:A:2748:G:H5'	38:A:6999:HOH:O	1.94	0.67
1:A:689:G:N3	38:A:8933:HOH:O	2.26	0.67
1:A:69:A:H8	1:A:69:A:H5'	1.59	0.67
5:D:7:ARG:HG2	5:D:7:ARG:HH11	1.58	0.67
7:F:22:VAL:HG22	7:F:74:THR:HG22	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1172:G:H1'	38:A:4448:HOH:O	1.93	0.67
1:A:2464:C:H5''	1:A:2465:A:OP1	1.93	0.67
1:A:281:U:H2'	1:A:282:C:O4'	1.95	0.67
16:O:119:GLN:O	16:O:123:ILE:HG13	1.94	0.67
16:O:73:ALA:N	38:O:8563:HOH:O	2.28	0.67
26:Y:41:PHE:O	26:Y:43:VAL:HG23	1.94	0.67
7:F:105:SER:CB	7:F:131:THR:HG23	2.21	0.67
15:N:89:ASN:HA	38:N:8557:HOH:O	1.94	0.67
17:P:42:GLU:HB2	38:P:2176:HOH:O	1.92	0.67
1:A:544:G:H2'	1:A:545:G:H5''	1.77	0.67
4:C:8:ARG:HG2	38:C:8558:HOH:O	1.94	0.67
12:K:19:MET:HE2	12:K:79:PHE:HA	1.76	0.67
17:P:38:ARG:NH1	38:P:7674:HOH:O	2.27	0.67
22:U:63:ILE:HD11	22:U:75:GLU:HB2	1.77	0.67
1:A:236:A:H4'	1:A:237:G:H5'	1.77	0.67
5:D:314:ALA:HB3	5:D:317:PRO:HG3	1.77	0.67
1:A:1209:C:H2'	1:A:1210:G:H8	1.58	0.67
1:A:1874:U:H2'	4:C:120:ARG:HG3	1.75	0.67
7:F:97:GLN:O	7:F:97:GLN:HG2	1.95	0.67
1:A:902:G:N7	14:M:18:HIS:HD2	1.92	0.67
23:V:14:GLU:O	23:V:17:THR:HB	1.95	0.67
13:L:55:VAL:HG12	13:L:56:SER:N	2.09	0.67
1:A:2851:G:O2'	1:A:2852:A:H5'	1.94	0.67
5:D:297:VAL:HB	38:D:8606:HOH:O	1.95	0.67
15:N:169:ARG:HD2	38:N:8591:HOH:O	1.95	0.67
1:A:2502:C:H2'	1:A:2503:A:H5'	1.77	0.66
1:A:2635:A:O2'	1:A:2636:C:H5'	1.94	0.66
11:J:127:GLY:O	11:J:128:ALA:HB3	1.95	0.66
25:X:88:THR:HG23	25:X:110:GLN:HE21	1.58	0.66
1:A:111:C:O2'	29:2:20:ARG:HG2	1.95	0.66
5:D:51:VAL:HG23	5:D:329:TYR:O	1.95	0.66
7:F:55:LYS:HA	38:F:6752:HOH:O	1.95	0.66
16:O:71:TRP:CE3	16:O:175:LEU:HD22	2.30	0.66
1:A:1667:A:H5'	1:A:1667:A:H8	1.60	0.66
1:A:2533:C:H5'	1:A:2533:C:C6	2.23	0.66
5:D:41:PHE:HA	5:D:79:MET:HE2	1.76	0.66
13:L:115:ARG:HG3	13:L:116:GLU:N	2.08	0.66
15:N:164:THR:CG2	15:N:165:SER:N	2.58	0.66
1:A:2459:G:OP2	31:4:64:LYS:HD2	1.94	0.66
1:A:2780:C:H1'	8:G:143:GLN:NE2	2.09	0.66
13:L:34:VAL:HG22	13:L:47:ALA:HB2	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:329:TYR:CE2	23:V:15:PRO:HG2	2.30	0.66
1:A:1829:A:N6	28:1:18:TYR:HA	2.10	0.66
4:C:94:LEU:N	4:C:94:LEU:HD23	2.10	0.66
9:H:2:VAL:HG22	9:H:57:GLU:OE1	1.94	0.66
25:X:149:LEU:HG	25:X:153:MET:HE2	1.78	0.66
13:L:74:VAL:HG11	13:L:113:ILE:HG12	1.76	0.66
15:N:172:GLY:O	15:N:183:VAL:HG11	1.96	0.66
7:F:64:ARG:HG2	7:F:67:ASP:HB3	1.77	0.66
5:D:141:ARG:HD2	5:D:163:GLU:OE2	1.95	0.66
7:F:51:ARG:HD3	38:F:7636:HOH:O	1.96	0.66
18:Q:38:GLU:HA	18:Q:41:ARG:HH11	1.60	0.66
28:1:53:GLY:HA2	28:1:67:GLY:O	1.96	0.66
1:A:1119:G:H22	1:A:1246:A:H2	1.42	0.66
1:A:1874:U:OP1	38:A:3810:HOH:O	2.14	0.66
1:A:2505:G:O2'	1:A:2506:A:H5'	1.95	0.66
1:A:2768:A:H2'	1:A:2769:C:O4'	1.94	0.66
1:A:2502:C:H4'	11:J:151:MET:HG2	1.78	0.66
20:S:44:VAL:O	20:S:48:GLU:HG3	1.96	0.66
1:A:2271:G:P	38:A:8940:HOH:O	2.54	0.65
1:A:282:C:O2'	1:A:283:U:H5'	1.96	0.65
13:L:28:GLU:OE2	13:L:58:THR:HG21	1.96	0.65
28:1:30:GLU:HA	28:1:33:HIS:CB	2.26	0.65
1:A:814:G:H4'	38:A:9628:HOH:O	1.96	0.65
2:B:3001:U:O3'	2:B:3003:A:H5''	1.96	0.65
4:C:153:ARG:HB2	4:C:153:ARG:HH11	1.61	0.65
6:E:1:MET:HG2	6:E:2:GLN:H	1.61	0.65
11:J:47:GLU:HB3	11:J:133:ILE:HD13	1.78	0.65
11:J:3:GLY:HA2	11:J:57:ARG:NH1	2.10	0.65
1:A:1130:U:H5'	38:A:7130:HOH:O	1.95	0.65
1:A:1681:G:H5''	1:A:1682:A:H5'	1.79	0.65
2:B:3014:G:H5'	2:B:3014:G:C8	2.31	0.65
5:D:238:ASN:HD22	5:D:240:GLY:H	1.44	0.65
15:N:30:GLU:O	15:N:34:GLU:HG3	1.97	0.65
18:Q:98:ILE:HD12	18:Q:102:ARG:NE	2.12	0.65
27:Z:142:SER:OG	38:Z:8616:HOH:O	2.15	0.65
4:C:191:GLY:HA2	4:C:194:MET:CE	2.27	0.65
7:F:136:ARG:HD2	7:F:155:HIS:O	1.95	0.65
1:A:1477:C:O2'	1:A:1478:U:H5'	1.96	0.65
1:A:2363:G:O3'	19:R:11:ARG:NH1	2.28	0.65
13:L:27:ARG:HD2	38:L:4747:HOH:O	1.97	0.65
15:N:37:VAL:HG21	15:N:108:LYS:CG	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:91:ARG:HG3	16:O:186:LEU:HD23	1.79	0.65
18:Q:87:ARG:HG2	38:Q:190:HOH:O	1.96	0.65
22:U:50:VAL:HG12	22:U:56:ALA:HA	1.78	0.65
25:X:149:LEU:HG	25:X:153:MET:CE	2.27	0.65
1:A:2414:A:H2'	1:A:2415:A:C8	2.31	0.65
4:C:94:LEU:HG	4:C:99:ILE:HD11	1.77	0.65
5:D:140:LEU:HD23	38:D:8583:HOH:O	1.96	0.65
6:E:127:ARG:HG2	6:E:127:ARG:HH11	1.61	0.65
13:L:62:PRO:HG3	13:L:65:ARG:NH2	2.11	0.65
15:N:87:MET:HB2	15:N:91:ILE:HD11	1.78	0.65
31:4:11:CYS:SG	38:4:8534:HOH:O	2.54	0.65
1:A:1886:A:H4'	38:1:8405:HOH:O	1.97	0.65
1:A:2618:G:N7	38:A:3140:HOH:O	2.30	0.65
7:F:41:LEU:HA	7:F:44:ILE:HG22	1.78	0.65
1:A:2432:C:O2'	1:A:2433:A:H5'	1.96	0.65
11:J:118:PRO:HD2	38:J:8340:HOH:O	1.97	0.65
15:N:84:LYS:HA	31:4:46:ILE:O	1.96	0.65
20:S:106:GLY:HA2	20:S:109:MET:HE3	1.77	0.65
27:Z:189:ASN:HD22	27:Z:189:ASN:C	2.00	0.65
1:A:2064:U:H5'	1:A:2652:U:O3'	1.97	0.65
1:A:733:U:OP2	38:A:5671:HOH:O	2.14	0.64
2:B:3029:C:H2'	2:B:3030:C:H5'	1.77	0.64
20:S:18:LEU:HB2	20:S:143:VAL:CG1	2.27	0.64
25:X:4:LEU:HD23	25:X:54:PHE:HB3	1.79	0.64
26:Y:78:GLU:HG2	26:Y:79:GLU:N	2.11	0.64
1:A:2054:A:N3	20:S:128:ARG:NH2	2.45	0.64
1:A:2276:U:H2'	1:A:2277:U:C6	2.33	0.64
8:G:11:VAL:HG13	8:G:23:GLU:O	1.97	0.64
18:Q:38:GLU:HA	18:Q:41:ARG:NH1	2.12	0.64
27:Z:141:THR:HG23	38:Z:8594:HOH:O	1.96	0.64
1:A:2064:U:H4'	1:A:2653:A:OP1	1.97	0.64
28:1:42:CYS:SG	28:1:43:GLY:N	2.70	0.64
28:1:30:GLU:HB2	38:1:8413:HOH:O	1.98	0.64
1:A:2428:G:C5	38:A:3276:HOH:O	2.50	0.64
4:C:88:ILE:O	4:C:88:ILE:HG22	1.97	0.64
12:K:74:ARG:CB	12:K:74:ARG:HH11	2.10	0.64
28:1:31:ILE:O	28:1:35:LYS:HG3	1.98	0.64
15:N:87:MET:HB3	31:4:46:ILE:HG21	1.80	0.64
1:A:1187:U:H2'	38:A:6356:HOH:O	1.98	0.64
1:A:1773:G:C8	28:1:16:PRO:HA	2.32	0.64
1:A:777:U:OP1	38:A:6954:HOH:O	2.14	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:65:VAL:HA	25:X:68:THR:HG22	1.80	0.64
1:A:558:C:O2'	1:A:559:U:H5''	1.97	0.64
1:A:2769:C:H2'	1:A:2770:G:O4'	1.98	0.64
2:B:3023:U:H3'	2:B:3024:U:H5''	1.78	0.64
5:D:248:ARG:NH2	38:D:8524:HOH:O	2.31	0.64
13:L:22:ASP:HB2	38:L:5264:HOH:O	1.96	0.64
13:L:34:VAL:CG2	13:L:47:ALA:HB2	2.27	0.64
29:2:21:ARG:HD2	29:2:37:CYS:SG	2.38	0.64
1:A:1441:G:O2'	1:A:1442:A:H5'	1.98	0.64
1:A:2119:C:O2'	1:A:2120:U:H5'	1.97	0.64
1:A:1942:A:H3'	38:A:6804:HOH:O	1.98	0.64
1:A:2314:G:C2'	1:A:2315:C:H5'	2.28	0.64
4:C:93:THR:C	4:C:94:LEU:HD23	2.18	0.64
6:E:115:LEU:O	6:E:118:THR:HB	1.97	0.64
11:J:71:TYR:C	11:J:73:GLN:H	2.01	0.64
15:N:59:GLY:HA3	15:N:141:ILE:HD11	1.78	0.64
4:C:131:HIS:O	4:C:132:ASP:HB2	1.96	0.63
5:D:36:PRO:HA	5:D:168:GLY:HA3	1.80	0.63
7:F:101:THR:HG22	38:F:7400:HOH:O	1.97	0.63
13:L:58:THR:HG22	13:L:59:LYS:HG3	1.80	0.63
14:M:89:PHE:N	38:M:8575:HOH:O	2.32	0.63
15:N:84:LYS:HE2	38:N:8580:HOH:O	1.97	0.63
20:S:18:LEU:HD12	20:S:143:VAL:HG11	1.79	0.63
25:X:38:THR:HG22	38:X:3580:HOH:O	1.97	0.63
2:B:3049:G:H5''	38:B:8467:HOH:O	1.99	0.63
7:F:23:VAL:HG22	7:F:73:VAL:HB	1.78	0.63
11:J:58:HIS:HA	11:J:61:LEU:HD23	1.80	0.63
13:L:92:ASP:OD1	38:L:5638:HOH:O	2.15	0.63
27:Z:200:THR:HG22	27:Z:201:GLU:CG	2.20	0.63
30:3:22:PRO:HG2	30:3:25:VAL:HG23	1.80	0.63
31:4:55:VAL:HG22	38:4:8510:HOH:O	1.99	0.63
1:A:1923:G:H4'	31:4:31:THR:O	1.98	0.63
1:A:2465:A:H3'	38:A:3142:HOH:O	1.97	0.63
1:A:544:G:C2'	1:A:545:G:H5''	2.28	0.63
8:G:79:GLY:HA3	38:G:7046:HOH:O	1.98	0.63
15:N:60:ILE:C	15:N:61:ILE:HD12	2.17	0.63
24:W:64:GLY:O	24:W:65:ASP:HB2	1.99	0.63
26:Y:31:ILE:O	26:Y:35:GLU:HG3	1.98	0.63
28:1:37:HIS:HB2	28:1:47:LEU:HB2	1.79	0.63
1:A:1329:A:H2	38:A:4165:HOH:O	1.80	0.63
1:A:157:G:H4'	15:N:95:LYS:HE3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:A:8011:MG:MG	38:A:3800:HOH:O	1.40	0.63
4:C:101:GLU:OE2	4:C:131:HIS:HB2	1.99	0.63
6:E:168:ARG:NH2	6:E:190:ALA:O	2.31	0.63
7:F:69:ILE:O	7:F:69:ILE:HG22	1.97	0.63
12:K:45:VAL:HG21	12:K:129:PHE:CD1	2.34	0.63
15:N:37:VAL:HG13	15:N:63:VAL:HG11	1.79	0.63
1:A:2467:A:P	38:A:8560:HOH:O	2.57	0.63
5:D:280:VAL:CG1	5:D:334:SER:HA	2.29	0.63
8:G:7:ILE:HG22	8:G:45:ASP:O	1.98	0.63
9:H:107:VAL:O	9:H:111:ILE:HG13	1.98	0.63
11:J:53:PRO:HG3	11:J:127:GLY:H	1.63	0.63
17:P:87:THR:O	17:P:91:GLN:HG3	1.99	0.63
1:A:1595:G:O2'	1:A:1596:U:H5'	1.98	0.63
7:F:25:MET:HE1	7:F:37:ALA:HB1	1.80	0.63
15:N:34:GLU:HB3	15:N:35:PRO:HD2	1.80	0.63
2:B:3028:U:H5''	16:O:40:ASN:ND2	2.14	0.63
1:A:396:U:OP2	31:4:38:ARG:NH1	2.32	0.63
8:G:20:ILE:CD1	8:G:33:LEU:HD12	2.29	0.63
14:M:143:THR:HG22	14:M:145:LEU:H	1.63	0.63
1:A:2890:A:H1'	23:V:56:ARG:NH2	2.14	0.63
8:G:23:GLU:HG2	8:G:28:SER:HB3	1.81	0.63
11:J:47:GLU:HB3	11:J:133:ILE:CD1	2.28	0.63
15:N:185:PRO:HG2	15:N:189:VAL:HG11	1.81	0.63
21:T:23:LYS:HE2	38:T:8330:HOH:O	1.99	0.63
30:3:35:ARG:HB2	38:3:2691:HOH:O	1.98	0.63
1:A:2105:C:H2'	1:A:2106:C:C6	2.33	0.63
5:D:138:GLY:O	5:D:139:ASP:O	2.16	0.63
5:D:175:LEU:C	5:D:175:LEU:HD23	2.19	0.63
18:Q:103:THR:HA	18:Q:106:ARG:NH1	2.14	0.63
22:U:71:VAL:HG11	22:U:90:PRO:CB	2.22	0.63
12:K:131:THR:HG22	12:K:134:GLU:H	1.63	0.62
1:A:2548:C:OP2	5:D:5:ARG:NH2	2.32	0.62
6:E:233:THR:HG22	6:E:234:VAL:N	2.13	0.62
11:J:166:ASN:N	11:J:166:ASN:HD22	1.96	0.62
12:K:45:VAL:HG23	12:K:130:VAL:O	1.98	0.62
15:N:114:VAL:HG21	15:N:159:THR:HG21	1.80	0.62
27:Z:187:VAL:CG2	27:Z:192:ASP:HB2	2.29	0.62
1:A:1116:U:O2'	1:A:1118:A:H2	1.72	0.62
1:A:2004:U:H4'	38:A:4780:HOH:O	1.98	0.62
7:F:25:MET:HE1	7:F:37:ALA:O	1.99	0.62
10:I:12:ILE:N	10:I:13:PRO:CD	2.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:C:H4'	15:N:146:GLN:NE2	2.15	0.62
27:Z:235:GLU:CD	27:Z:235:GLU:H	2.03	0.62
38:C:8627:HOH:O	28:1:75:ALA:HB3	1.98	0.62
6:E:78:ARG:HG3	6:E:78:ARG:NH1	2.13	0.62
7:F:23:VAL:HG23	7:F:23:VAL:O	1.99	0.62
9:H:46:GLU:N	38:H:3461:HOH:O	2.32	0.62
38:A:4556:HOH:O	5:D:216:LYS:HA	2.00	0.62
6:E:107:ARG:HH11	6:E:107:ARG:HB3	1.64	0.62
15:N:91:ILE:HG23	38:N:8649:HOH:O	1.99	0.62
20:S:104:PHE:HB2	20:S:109:MET:HE1	1.81	0.62
1:A:189:A:OP1	15:N:171:ARG:NH2	2.32	0.62
1:A:56:G:H5''	24:W:50:ARG:NH1	2.13	0.62
1:A:714:U:H3'	38:A:6403:HOH:O	2.00	0.62
7:F:37:ALA:O	7:F:40:ILE:HG12	1.99	0.62
15:N:64:ARG:HD2	38:N:8587:HOH:O	1.98	0.62
20:S:17:MET:HE1	20:S:19:ARG:NH2	2.15	0.62
1:A:1594:C:OP2	18:Q:120:ARG:HD2	2.00	0.62
5:D:41:PHE:HB3	5:D:190:MET:HE1	1.82	0.62
15:N:104:ARG:O	15:N:108:LYS:HE2	2.00	0.62
16:O:183:ASP:OD2	16:O:186:LEU:HD12	1.99	0.62
26:Y:37:LEU:CD1	26:Y:85:VAL:HG21	2.28	0.62
29:2:28:HIS:HD2	29:2:30:LYS:H	1.48	0.62
1:A:280:C:H2'	1:A:281:U:O4'	2.00	0.62
1:A:488:U:H2'	38:A:3497:HOH:O	1.99	0.62
22:U:48:VAL:HG22	22:U:97:ARG:O	2.00	0.62
32:A:8011:MG:MG	38:A:3470:HOH:O	1.42	0.62
5:D:145:HIS:CD2	5:D:146:THR:O	2.52	0.62
15:N:52:LEU:HD13	15:N:116:ASN:HB3	1.82	0.62
16:O:61:ALA:CB	16:O:88:ALA:HB2	2.30	0.62
25:X:26:ILE:O	25:X:26:ILE:HG13	1.97	0.62
28:1:23:ARG:NH1	38:1:8404:HOH:O	2.32	0.62
1:A:1213:C:O2'	1:A:1214:G:H5'	2.00	0.62
1:A:1713:G:H1'	38:A:4547:HOH:O	2.00	0.62
1:A:558:C:H5'	38:A:4732:HOH:O	1.99	0.62
1:A:1534:C:N3	38:A:8988:HOH:O	2.31	0.61
1:A:2421:G:H3'	1:A:2422:U:H5''	1.82	0.61
1:A:2506:A:O2'	1:A:2507:G:O5'	2.18	0.61
1:A:603:A:H5''	1:A:604:G:OP1	1.99	0.61
23:V:44:ARG:HB3	38:V:3805:HOH:O	1.99	0.61
1:A:1669:A:H2'	1:A:1670:G:C8	2.35	0.61
1:A:2281:C:H2'	1:A:2282:U:H5'	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:671:A:O2'	1:A:672:G:H2'	2.00	0.61
9:H:50:VAL:CG2	9:H:63:ILE:HG21	2.30	0.61
24:W:42:ASN:HB3	38:W:7247:HOH:O	2.00	0.61
1:A:56:G:H5''	24:W:50:ARG:HH12	1.63	0.61
28:1:30:GLU:HB3	28:1:34:LYS:HE3	1.81	0.61
1:A:1120:U:C6	1:A:1120:U:H5''	2.36	0.61
5:D:36:PRO:HA	5:D:168:GLY:CA	2.31	0.61
1:A:1886:A:O2'	28:1:20:LEU:HB2	1.99	0.61
1:A:183:A:H5'	15:N:157:LEU:HD12	1.82	0.61
1:A:948:G:N7	38:A:5313:HOH:O	2.30	0.61
8:G:20:ILE:HD11	8:G:40:VAL:HG11	1.81	0.61
11:J:84:ARG:NH2	11:J:135:TRP:HH2	1.98	0.61
18:Q:94:TRP:CZ2	18:Q:98:ILE:HG13	2.35	0.61
27:Z:117:LEU:HD12	27:Z:174:VAL:HG11	1.83	0.61
1:A:1086:A:C6	25:X:11:VAL:HG11	2.34	0.61
1:A:1884:G:O6	4:C:190:ARG:HD2	2.00	0.61
1:A:1234:U:N3	5:D:244:PRO:HB3	2.16	0.61
7:F:25:MET:CE	7:F:37:ALA:HB1	2.31	0.61
11:J:62:GLU:O	11:J:66:VAL:HG23	2.00	0.61
14:M:21:ARG:N	38:M:8534:HOH:O	2.34	0.61
15:N:155:HIS:CE1	15:N:158:ARG:HE	2.18	0.61
5:D:217:ARG:HG3	5:D:257:THR:HG22	1.81	0.61
10:I:12:ILE:HD12	38:I:692:HOH:O	2.00	0.61
11:J:141:ASN:CA	38:J:8366:HOH:O	2.46	0.61
16:O:80:SER:HB2	38:O:8536:HOH:O	2.01	0.61
18:Q:143:ALA:HA	38:Q:170:HOH:O	2.00	0.61
21:T:80:ARG:HG2	38:T:8337:HOH:O	2.01	0.61
28:1:39:CYS:CB	28:1:47:LEU:HD21	2.30	0.61
9:H:50:VAL:HG13	9:H:60:VAL:HG11	1.82	0.61
16:O:89:GLY:O	16:O:92:ALA:HB3	2.00	0.61
26:Y:15:ARG:NH1	26:Y:15:ARG:HB3	2.15	0.61
28:1:19:GLY:O	28:1:23:ARG:HG2	2.01	0.61
1:A:1862:C:H1'	38:A:6681:HOH:O	2.00	0.61
1:A:1878:G:H1'	38:A:5581:HOH:O	2.01	0.61
2:B:3039:U:H1'	2:B:3044:A:N6	2.15	0.61
4:C:191:GLY:HA2	4:C:194:MET:HE3	1.83	0.61
5:D:204:GLY:HA3	38:D:8653:HOH:O	2.00	0.61
5:D:305:ASP:O	5:D:306:LYS:HB2	2.01	0.61
6:E:118:THR:O	6:E:136:VAL:HG13	2.01	0.61
1:A:338:C:H4'	6:E:174:ILE:HD11	1.83	0.61
11:J:55:GLN:NE2	11:J:124:ARG:HE	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1972:U:H2'	1:A:1973:A:H5'	1.82	0.61
5:D:154:VAL:HG12	5:D:156:LYS:HG2	1.83	0.61
5:D:312:ARG:HD3	5:D:315:VAL:HG13	1.83	0.61
6:E:219:ASN:O	6:E:222:ASP:OD1	2.18	0.61
8:G:15:GLN:HG3	8:G:20:ILE:HG12	1.83	0.61
8:G:7:ILE:HD11	8:G:11:VAL:C	2.21	0.61
8:G:7:ILE:HD11	8:G:11:VAL:O	2.01	0.61
13:L:32:ILE:HD11	13:L:56:SER:HB3	1.83	0.61
22:U:55:PHE:CD2	22:U:77:VAL:HG13	2.36	0.61
1:A:1919:A:H4'	38:A:4324:HOH:O	1.99	0.61
2:B:3002:U:H4'	2:B:3002:U:OP2	2.01	0.61
12:K:74:ARG:O	12:K:78:ILE:HG12	2.00	0.61
20:S:132:ARG:HG2	20:S:133:ALA:N	2.16	0.61
11:J:136:VAL:HG22	11:J:137:ASN:O	2.00	0.60
11:J:150:LYS:CB	11:J:157:ILE:HD12	2.27	0.60
15:N:149:TRP:O	15:N:152:ARG:HG2	1.99	0.60
25:X:84:VAL:HG12	38:X:6679:HOH:O	2.01	0.60
1:A:2717:C:H2'	1:A:2718:C:C5'	2.27	0.60
1:A:2827:A:H2'	1:A:2828:G:O4'	2.00	0.60
11:J:26:LYS:HD2	11:J:28:ILE:CD1	2.30	0.60
22:U:49:GLU:OE2	22:U:97:ARG:HD2	2.01	0.60
31:4:48:ASN:ND2	31:4:50:GLY:H	1.99	0.60
1:A:2405:C:P	38:A:6058:HOH:O	2.58	0.60
1:A:871:G:C5'	1:A:871:G:C8	2.77	0.60
2:B:3007:G:H4'	16:O:55:ASP:OD2	2.00	0.60
15:N:55:LYS:HB2	15:N:60:ILE:CD1	2.31	0.60
1:A:2710:U:H1'	38:A:7082:HOH:O	2.01	0.60
1:A:558:C:C2'	1:A:559:U:H5''	2.31	0.60
4:C:105:VAL:HG13	4:C:155:THR:O	2.02	0.60
5:D:81:ALA:O	5:D:186:GLY:HA3	2.01	0.60
5:D:221:GLN:HE22	13:L:42:ASN:HD22	1.49	0.60
12:K:75:PRO:HG2	12:K:105:LEU:CD2	2.31	0.60
28:1:39:CYS:HA	28:1:47:LEU:CD1	2.29	0.60
1:A:553:G:P	27:Z:204:ARG:HH22	2.24	0.60
5:D:85:ARG:NH1	38:D:8634:HOH:O	2.34	0.60
7:F:38:GLU:HB3	7:F:49:PRO:HG2	1.83	0.60
38:B:8477:HOH:O	16:O:23:ARG:HD3	2.00	0.60
22:U:69:LYS:O	22:U:71:VAL:HG23	2.02	0.60
25:X:26:ILE:O	25:X:26:ILE:CG1	2.49	0.60
1:A:659:A:H5''	38:A:6557:HOH:O	2.00	0.60
18:Q:78:GLY:O	38:Q:157:HOH:O	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2089:A:O2'	1:A:2090:G:H5'	2.01	0.60
1:A:2419:U:H5''	1:A:2420:G:H5'	1.84	0.60
1:A:285:A:H2'	1:A:286:U:O4'	2.01	0.60
1:A:2908:A:H2'	1:A:2909:G:O4'	2.01	0.60
7:F:23:VAL:HG21	7:F:45:THR:HG21	1.81	0.60
8:G:23:GLU:HG2	8:G:28:SER:CB	2.32	0.60
1:A:1185:U:H2'	1:A:1186:C:C6	2.36	0.60
1:A:1182:C:H1'	1:A:1192:A:H8	1.67	0.60
1:A:1730:G:H5'	1:A:1731:C:C5	2.36	0.60
15:N:138:HIS:ND1	15:N:139:PRO:O	2.32	0.60
25:X:21:LEU:HD21	25:X:48:VAL:HG11	1.84	0.60
1:A:134:U:C2	1:A:145:A:C2	2.90	0.60
1:A:2019:A:H5'	38:A:4024:HOH:O	2.01	0.60
1:A:282:C:H1'	1:A:368:C:H42	1.65	0.60
6:E:104:ASP:O	6:E:108:GLN:HG3	2.02	0.60
7:F:50:VAL:O	7:F:71:ALA:HA	2.02	0.60
1:A:2690:U:O2'	8:G:111:LYS:HE3	2.00	0.60
9:H:58:GLU:HA	9:H:61:MET:HG3	1.82	0.60
15:N:52:LEU:HD21	38:N:8616:HOH:O	2.01	0.60
15:N:74:ARG:O	15:N:88:VAL:CG1	2.43	0.60
1:A:281:U:H3'	38:A:6668:HOH:O	2.02	0.60
1:A:821:U:H2'	1:A:822:C:H6	1.67	0.60
7:F:57:THR:HG23	7:F:63:ILE:HG22	1.83	0.60
12:K:39:VAL:HG13	12:K:106:GLY:O	2.01	0.60
22:U:48:VAL:HG23	22:U:98:VAL:HA	1.84	0.60
24:W:4:HIS:HB3	38:W:6622:HOH:O	2.02	0.60
1:A:349:U:O2'	1:A:350:C:H5'	2.02	0.59
7:F:25:MET:CE	7:F:41:LEU:HG	2.29	0.59
13:L:109:LEU:HD13	13:L:113:ILE:HD11	1.84	0.59
38:A:9444:HOH:O	26:Y:23:HIS:HD2	1.84	0.59
1:A:263:U:O4'	9:H:59:ILE:HD13	2.03	0.59
1:A:639:A:H2'	1:A:640:G:C8	2.37	0.59
16:O:12:ARG:HD3	16:O:18:THR:OG1	2.01	0.59
23:V:9:CYS:CA	23:V:52:THR:HG23	2.32	0.59
25:X:4:LEU:O	25:X:32:CYS:HA	2.02	0.59
15:N:87:MET:HB3	31:4:46:ILE:HD13	1.83	0.59
1:A:2408:A:H2	38:A:9595:HOH:O	1.84	0.59
5:D:1:PRO:O	5:D:2:GLN:HB2	2.01	0.59
6:E:115:LEU:HD21	6:E:243:VAL:HG13	1.83	0.59
6:E:180:SER:HB2	38:E:8451:HOH:O	2.02	0.59
8:G:81:GLU:HG2	8:G:134:SER:HB3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:28:GLU:HG2	13:L:58:THR:HB	1.84	0.59
1:A:824:G:C8	38:A:3800:HOH:O	2.51	0.59
5:D:2:GLN:HA	38:D:8622:HOH:O	2.02	0.59
5:D:43:GLY:O	5:D:308:LEU:HD12	2.02	0.59
9:H:46:GLU:O	9:H:73:PRO:HD2	2.02	0.59
16:O:48:VAL:HG11	16:O:55:ASP:HB3	1.84	0.59
22:U:47:THR:HB	22:U:100:ASP:HB3	1.83	0.59
1:A:2428:G:O6	1:A:2464:C:H1'	2.03	0.59
1:A:289:G:N2	1:A:363:A:H2	1.98	0.59
4:C:109:GLU:HG2	4:C:116:GLY:N	2.17	0.59
7:F:135:VAL:HG22	7:F:136:ARG:H	1.66	0.59
12:K:80:LYS:HE2	12:K:98:PHE:CZ	2.38	0.59
16:O:37:ARG:NE	38:O:8534:HOH:O	2.34	0.59
24:W:39:ALA:C	24:W:41:GLU:H	2.06	0.59
25:X:141:HIS:HB2	25:X:146:ILE:HG12	1.84	0.59
26:Y:66:THR:HG23	26:Y:67:PRO:HD2	1.84	0.59
1:A:182:G:O3'	15:N:157:LEU:CD1	2.51	0.59
1:A:738:G:H3'	38:A:6507:HOH:O	2.03	0.59
11:J:35:ASN:ND2	11:J:80:ASN:HA	2.18	0.59
16:O:182:GLY:N	38:O:8567:HOH:O	2.32	0.59
25:X:106:THR:OG1	25:X:109:GLU:HG3	2.02	0.59
28:1:28:ASP:O	28:1:31:ILE:HG22	2.02	0.59
1:A:1170:U:O2'	1:A:1172:G:N7	2.27	0.59
14:M:37:LYS:O	38:M:8525:HOH:O	2.17	0.59
14:M:54:PRO:HG2	14:M:57:VAL:CG2	2.33	0.59
1:A:20:G:H21	20:S:117:HIS:HD2	1.51	0.59
1:A:2429:A:O2'	1:A:2430:A:H5'	2.03	0.59
38:A:4990:HOH:O	5:D:298:LYS:HD3	2.02	0.59
7:F:11:HIS:O	7:F:12:GLU:HB3	2.02	0.59
14:M:136:ALA:HB3	38:M:8577:HOH:O	2.03	0.59
16:O:154:LEU:O	16:O:155:GLU:HB3	2.03	0.59
22:U:24:ARG:HH21	22:U:39:ASN:HD22	1.50	0.59
1:A:775:G:OP1	29:2:16:HIS:HE1	1.85	0.59
1:A:449:A:N7	6:E:43:LYS:HG2	2.18	0.59
7:F:170:TYR:O	7:F:171:ASP:HB3	2.01	0.59
2:B:3040:C:N4	7:F:51:ARG:HB2	2.18	0.59
22:U:52:ARG:HB2	22:U:95:ASN:HB3	1.85	0.59
1:A:1666:C:C2'	1:A:1667:A:H5'	2.32	0.59
1:A:1918:U:OP2	38:A:3513:HOH:O	2.17	0.59
1:A:2896:A:H5''	38:A:5559:HOH:O	2.02	0.59
4:C:100:PRO:HG2	4:C:103:VAL:HG21	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:64:ASN:N	10:I:64:ASN:HD22	2.00	0.59
15:N:59:GLY:HA3	15:N:141:ILE:HD12	1.85	0.59
38:A:6333:HOH:O	15:N:178:LYS:HB2	2.02	0.59
16:O:152:GLU:C	16:O:154:LEU:H	2.05	0.59
27:Z:144:ARG:CZ	38:Z:8616:HOH:O	2.51	0.59
1:A:157:G:H4'	15:N:95:LYS:CE	2.33	0.58
1:A:2413:A:N7	16:O:109:PRO:HB3	2.18	0.58
5:D:195:ARG:HG2	5:D:323:LEU:HD22	1.85	0.58
29:2:10:LYS:HG3	38:2:2979:HOH:O	2.02	0.58
1:A:1183:C:N4	38:A:3888:HOH:O	2.32	0.58
7:F:64:ARG:CG	7:F:67:ASP:HB3	2.33	0.58
11:J:56:ILE:HG22	11:J:61:LEU:CD2	2.32	0.58
14:M:125:PHE:CZ	14:M:140:VAL:HG13	2.37	0.58
16:O:163:PHE:HA	38:O:8520:HOH:O	2.02	0.58
20:S:132:ARG:NH2	38:S:8582:HOH:O	2.35	0.58
24:W:49:LEU:O	24:W:53:ILE:HG13	2.03	0.58
1:A:120:A:H2'	1:A:120:A:N3	2.18	0.58
1:A:371:U:H2'	1:A:372:A:C8	2.37	0.58
15:N:72:SER:OG	15:N:74:ARG:HB2	2.02	0.58
1:A:1759:A:N3	1:A:1818:C:H2'	2.17	0.58
2:B:3057:A:N6	38:B:8444:HOH:O	2.36	0.58
5:D:264:GLU:HG2	5:D:267:LYS:CE	2.28	0.58
6:E:107:ARG:CB	6:E:107:ARG:HH11	2.16	0.58
2:B:3044:A:O4'	7:F:76:ARG:NE	2.36	0.58
13:L:37:TYR:CD2	38:L:7169:HOH:O	2.52	0.58
15:N:48:ARG:NH2	38:N:8567:HOH:O	2.35	0.58
38:A:3680:HOH:O	27:Z:186:ARG:HD2	2.03	0.58
27:Z:187:VAL:HB	38:Z:8575:HOH:O	2.03	0.58
1:A:567:U:H5''	38:A:5862:HOH:O	2.03	0.58
4:C:25:ALA:HA	38:C:8573:HOH:O	2.03	0.58
6:E:237:GLU:HB2	38:E:8436:HOH:O	2.01	0.58
27:Z:187:VAL:HG23	27:Z:192:ASP:HB3	1.85	0.58
1:A:1168:C:H2'	1:A:1169:U:O4'	2.03	0.58
1:A:184:G:H5''	15:N:153:THR:HG22	1.86	0.58
1:A:739:G:N7	38:A:7001:HOH:O	2.36	0.58
2:B:3047:A:C2	2:B:3048:C:C2	2.91	0.58
5:D:62:ARG:HA	5:D:65:MET:CE	2.33	0.58
6:E:103:ASN:HB3	38:E:8308:HOH:O	2.02	0.58
7:F:38:GLU:OE2	7:F:51:ARG:CZ	2.52	0.58
20:S:14:ALA:HB3	20:S:147:LEU:HB2	1.86	0.58
1:A:2462:G:N7	31:4:60:LYS:NZ	2.45	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2578:G:H5'	1:A:2578:G:C8	2.36	0.58
1:A:29:C:O2'	1:A:30:U:H5'	2.04	0.58
1:A:661:G:C5	1:A:686:A:C2	2.91	0.58
7:F:99:ASP:HB2	7:F:103:ASN:HB2	1.84	0.58
16:O:169:PRO:O	16:O:172:PHE:HB3	2.04	0.58
1:A:646:G:H2'	1:A:647:U:C6	2.38	0.58
2:B:3006:C:C5'	16:O:37:ARG:NH1	2.61	0.58
2:B:3051:A:H5'	16:O:160:SER:HB3	1.86	0.58
5:D:307:ARG:HH11	5:D:307:ARG:HB2	1.68	0.58
11:J:75:SER:C	11:J:79:ALA:HB2	2.24	0.58
12:K:130:VAL:HG12	12:K:131:THR:N	2.18	0.58
18:Q:10:ALA:HA	18:Q:13:VAL:CG1	2.32	0.58
1:A:1123:A:C6	1:A:1238:C:H5'	2.39	0.58
1:A:1351:G:O2'	38:A:4032:HOH:O	2.17	0.58
1:A:2274:A:H1'	15:N:86:MET:SD	2.43	0.58
1:A:2316:G:H2'	38:A:4385:HOH:O	2.02	0.58
1:A:2073:G:OP2	1:A:2490:A:H5'	2.02	0.58
1:A:820:G:C6	4:C:171:LYS:HB2	2.39	0.58
8:G:3:VAL:HG22	8:G:49:ILE:HB	1.86	0.58
1:A:1053:G:OP1	11:J:12:PRO:HG3	2.02	0.58
18:Q:64:GLU:HG2	38:Q:171:HOH:O	2.04	0.58
27:Z:184:GLU:OE1	27:Z:204:ARG:NH1	2.36	0.58
1:A:2427:C:OP2	31:4:84:ARG:HD2	2.03	0.58
1:A:2878:U:H2'	1:A:2879:A:O4'	2.04	0.58
1:A:542:A:H1'	38:A:4158:HOH:O	2.04	0.58
11:J:44:ALA:HA	11:J:163:PRO:O	2.03	0.58
1:A:2676:C:H4'	12:K:70:PHE:CE1	2.39	0.58
16:O:184:ILE:HG22	16:O:185:GLU:HG3	1.84	0.58
18:Q:59:ARG:HH22	18:Q:66:GLN:HE22	1.51	0.58
1:A:1942:A:O2'	1:A:1943:C:H5'	2.04	0.57
5:D:205:VAL:O	5:D:307:ARG:NE	2.37	0.57
9:H:47:LEU:HB2	9:H:108:LEU:HD11	1.86	0.57
11:J:26:LYS:HD3	11:J:89:PRO:CG	2.33	0.57
15:N:35:PRO:O	38:N:8539:HOH:O	2.17	0.57
1:A:1819:G:H2'	1:A:1820:G:H4'	1.85	0.57
4:C:109:GLU:HG2	4:C:116:GLY:H	1.69	0.57
5:D:82:VAL:HG12	5:D:82:VAL:O	2.04	0.57
6:E:162:VAL:HG13	6:E:232:LEU:HD21	1.85	0.57
15:N:61:ILE:HG13	38:N:8624:HOH:O	2.03	0.57
38:B:8477:HOH:O	16:O:20:TYR:CE2	2.53	0.57
7:F:166:ILE:HD12	38:F:6326:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1162:G:H2'	38:A:6045:HOH:O	2.04	0.57
1:A:2763:G:OP1	13:L:9:THR:OG1	2.20	0.57
4:C:192:VAL:HG12	4:C:207:GLN:HB3	1.86	0.57
14:M:104:ASP:O	14:M:105:TYR:HB3	2.04	0.57
15:N:186:SER:O	15:N:189:VAL:HG12	2.03	0.57
16:O:141:ARG:HB3	38:O:8566:HOH:O	2.05	0.57
1:A:128:A:H3'	1:A:128:A:C8	2.38	0.57
1:A:2324:G:H4'	1:A:2418:G:O2'	2.04	0.57
1:A:2421:G:H3'	1:A:2422:U:C5'	2.35	0.57
1:A:2866:U:C2	38:A:6955:HOH:O	2.53	0.57
1:A:820:G:C5	4:C:171:LYS:HB2	2.40	0.57
4:C:179:MET:HG2	4:C:186:TRP:HB2	1.86	0.57
14:M:143:THR:CG2	14:M:144:ASP:N	2.67	0.57
21:T:43:GLU:HB3	38:T:8345:HOH:O	2.04	0.57
1:A:1528:A:H2'	1:A:1529:G:O4'	2.04	0.57
1:A:1753:C:O2	5:D:229:ARG:NH2	2.38	0.57
1:A:2011:A:P	38:A:5418:HOH:O	2.63	0.57
1:A:2783:A:H3'	38:A:4707:HOH:O	2.02	0.57
9:H:57:GLU:O	9:H:61:MET:HG3	2.05	0.57
25:X:137:GLN:HE21	25:X:141:HIS:CE1	2.21	0.57
25:X:21:LEU:HD22	25:X:26:ILE:HD13	1.86	0.57
1:A:1474:C:H6	1:A:1474:C:C5'	2.11	0.57
1:A:1497:G:H4'	1:A:1627:G:O2'	2.04	0.57
4:C:211:LYS:NZ	38:C:8635:HOH:O	2.38	0.57
4:C:29:HIS:CE1	4:C:107:ASN:ND2	2.73	0.57
5:D:320:GLN:HG3	5:D:321:PRO:HD2	1.87	0.57
1:A:1119:G:H2'	12:K:52:GLN:NE2	2.19	0.57
38:A:9660:HOH:O	15:N:87:MET:HE3	2.03	0.57
17:P:59:VAL:HG23	17:P:111:VAL:HG23	1.86	0.57
1:A:1500:U:P	18:Q:41:ARG:HH22	2.27	0.57
1:A:2365:G:H4'	19:R:45:PRO:O	2.04	0.57
28:1:47:LEU:HD23	28:1:57:CYS:CB	2.34	0.57
1:A:1299:G:O6	14:M:6:ARG:HD3	2.05	0.57
1:A:1669:A:H2'	1:A:1670:G:H8	1.69	0.57
10:I:12:ILE:HG13	38:I:6833:HOH:O	2.04	0.57
15:N:106:ASN:ND2	35:N:8518:CL:CL	2.74	0.57
16:O:49:THR:CG2	16:O:56:ASP:HB2	2.33	0.57
16:O:90:LEU:HB2	16:O:186:LEU:HD22	1.86	0.57
1:A:138:U:H5"	1:A:139:C:OP2	2.05	0.57
11:J:85:ILE:HB	11:J:132:PHE:CE2	2.40	0.57
29:2:52:SER:HA	38:2:4248:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:G:O2'	1:A:106:A:H5'	2.04	0.57
1:A:638:C:H2'	1:A:639:A:C8	2.40	0.57
38:A:4879:HOH:O	4:C:164:ARG:NE	2.36	0.57
25:X:4:LEU:HD21	25:X:52:VAL:HG11	1.87	0.57
27:Z:115:ARG:NE	38:Z:8560:HOH:O	2.37	0.57
30:3:18:ASN:HD21	30:3:40:ARG:H	1.52	0.56
1:A:1086:A:N6	25:X:11:VAL:HG11	2.20	0.56
1:A:1118:A:C8	1:A:1118:A:C3'	2.85	0.56
1:A:1766:U:O2	1:A:1778:A:H5'	2.05	0.56
1:A:2359:G:N7	38:A:3196:HOH:O	2.32	0.56
1:A:2793:A:N3	38:A:3982:HOH:O	2.33	0.56
1:A:396:U:H1'	38:A:7089:HOH:O	2.03	0.56
1:A:825:U:H5''	1:A:826:U:OP1	2.05	0.56
9:H:110:GLU:O	9:H:114:LYS:HG3	2.04	0.56
9:H:21:GLU:O	9:H:24:ARG:HG3	2.05	0.56
15:N:186:SER:OG	15:N:189:VAL:HG12	2.05	0.56
16:O:33:ARG:NH1	16:O:103:ASP:OD2	2.30	0.56
28:1:11:THR:CG2	28:1:23:ARG:HB2	2.35	0.56
4:C:211:LYS:HB3	4:C:212:PRO:CD	2.30	0.56
5:D:30:PRO:HB2	5:D:39:GLN:NE2	2.18	0.56
6:E:27:ARG:HG3	6:E:29:ASP:OD1	2.05	0.56
8:G:69:ILE:HA	8:G:72:MET:CE	2.35	0.56
12:K:39:VAL:HG11	12:K:107:ASN:HB2	1.85	0.56
16:O:139:TRP:HA	16:O:139:TRP:CE3	2.39	0.56
24:W:12:THR:CG2	24:W:15:GLU:HG3	2.25	0.56
30:3:41:HIS:H	30:3:45:ASN:ND2	1.96	0.56
1:A:2314:G:H2'	1:A:2315:C:H5'	1.87	0.56
1:A:2694:A:H4'	8:G:91:PHE:CE1	2.40	0.56
1:A:595:U:O2'	1:A:596:C:H5'	2.05	0.56
5:D:55:ASN:HB3	5:D:64:GLY:H	1.70	0.56
11:J:130:HIS:CG	11:J:133:ILE:HD11	2.40	0.56
14:M:104:ASP:HB3	38:M:8570:HOH:O	2.05	0.56
25:X:60:GLU:O	25:X:63:GLU:HB2	2.05	0.56
4:C:88:ILE:HD13	4:C:100:PRO:CD	2.35	0.56
11:J:13:ALA:CA	11:J:91:HIS:HE1	2.15	0.56
21:T:51:GLN:NE2	21:T:53:ASN:HD21	2.03	0.56
24:W:39:ALA:N	24:W:40:PRO:CD	2.69	0.56
25:X:38:THR:HB	38:X:5390:HOH:O	2.06	0.56
31:4:38:ARG:O	31:4:42:ARG:HB2	2.06	0.56
1:A:383:A:H4'	38:A:4801:HOH:O	2.06	0.56
21:T:51:GLN:HE21	21:T:53:ASN:ND2	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Z:186:ARG:HH11	27:Z:186:ARG:HG2	1.71	0.56
1:A:2620:U:O4	36:5:76:PPU:C	2.54	0.56
1:A:1181:A:H2'	1:A:1182:C:O4'	2.05	0.56
1:A:2241:C:O2'	1:A:2242:U:H5'	2.05	0.56
1:A:2529:G:O2'	1:A:2530:C:H5'	2.05	0.56
1:A:2718:C:H6	1:A:2718:C:H5'	1.70	0.56
1:A:272:A:H5'	1:A:273:G:OP2	2.05	0.56
1:A:2814:A:OP2	38:A:4548:HOH:O	2.17	0.56
6:E:133:ARG:HD2	38:E:8414:HOH:O	2.05	0.56
6:E:162:VAL:HG12	6:E:162:VAL:O	2.04	0.56
16:O:154:LEU:HG	16:O:155:GLU:H	1.70	0.56
18:Q:103:THR:O	18:Q:107:GLU:HG3	2.06	0.56
20:S:29:LYS:HB3	38:S:8531:HOH:O	2.05	0.56
24:W:58:THR:O	24:W:62:GLU:HG3	2.05	0.56
1:A:168:C:O2'	1:A:169:A:H5'	2.06	0.56
1:A:283:U:H5''	1:A:284:C:P	2.45	0.56
1:A:316:A:H5'	22:U:54:ASP:OD2	2.05	0.56
6:E:214:THR:HG21	38:E:8407:HOH:O	2.05	0.56
7:F:44:ILE:HG12	7:F:83:PHE:HE1	1.69	0.56
9:H:19:ALA:O	9:H:22:VAL:HG22	2.06	0.56
14:M:148:GLU:HA	38:M:8576:HOH:O	2.05	0.56
18:Q:105:LEU:CD2	18:Q:137:LEU:HD21	2.36	0.56
18:Q:58:SER:HB3	38:Q:186:HOH:O	2.04	0.56
31:4:74:CYS:SG	31:4:76:LYS:CB	2.94	0.56
2:B:3049:G:O2'	2:B:3050:G:H5'	2.06	0.56
5:D:207:LYS:HG2	5:D:304:PRO:HB3	1.88	0.56
16:O:58:LEU:HD12	16:O:58:LEU:N	2.21	0.56
16:O:80:SER:CB	38:O:8536:HOH:O	2.53	0.56
1:A:2502:C:C4'	11:J:151:MET:HG2	2.35	0.56
5:D:280:VAL:HG13	5:D:334:SER:HA	1.88	0.56
7:F:44:ILE:HG23	7:F:45:THR:HG23	1.88	0.56
12:K:19:MET:HE1	12:K:132:LEU:HD11	1.85	0.56
29:2:8:GLN:NE2	29:2:11:LYS:NZ	2.52	0.56
15:N:87:MET:CG	31:4:46:ILE:HD13	2.36	0.56
1:A:154:C:H2'	1:A:155:C:H6	1.70	0.56
1:A:2093:G:H5''	38:D:8526:HOH:O	2.06	0.56
1:A:2664:A:OP1	1:A:2664:A:H8	1.89	0.56
8:G:31:ARG:NH1	38:G:5919:HOH:O	2.38	0.56
22:U:48:VAL:HG22	22:U:97:ARG:C	2.27	0.56
1:A:2507:G:H2'	1:A:2510:C:H42	1.71	0.56
7:F:144:ARG:NH2	38:F:3839:HOH:O	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:39:GLY:O	11:J:41:THR:N	2.39	0.56
11:J:59:ASN:ND2	11:J:59:ASN:H	1.97	0.56
12:K:126:ASN:O	12:K:129:PHE:HE2	1.89	0.56
1:A:2721:U:H4'	13:L:87:ARG:HG3	1.88	0.56
16:O:34:LEU:HA	16:O:47:LEU:HD23	1.87	0.56
17:P:7:LEU:HD22	38:P:5650:HOH:O	2.05	0.56
22:U:9:LYS:HE3	22:U:13:ARG:HH11	1.71	0.56
1:A:121:U:OP2	30:3:10:ARG:NH2	2.39	0.55
1:A:2672:C:H1'	38:D:8634:HOH:O	2.06	0.55
9:H:107:VAL:HG23	38:H:6617:HOH:O	2.05	0.55
21:T:32:ALA:HA	21:T:36:GLU:OE1	2.06	0.55
1:A:113:A:H3'	1:A:114:A:C5'	2.36	0.55
8:G:133:VAL:HG12	8:G:141:VAL:HG13	1.88	0.55
8:G:21:THR:HG23	8:G:30:THR:OG1	2.06	0.55
15:N:104:ARG:O	15:N:108:LYS:HG2	2.06	0.55
18:Q:109:ARG:NH1	18:Q:119:TYR:CE2	2.74	0.55
26:Y:43:VAL:HG12	26:Y:44:ASP:N	2.21	0.55
31:4:44:SER:HA	31:4:49:ASP:OD1	2.06	0.55
1:A:1682:A:H5''	38:A:8961:HOH:O	2.06	0.55
1:A:558:C:H2'	1:A:559:U:C5'	2.36	0.55
2:B:3028:U:H2'	2:B:3029:C:C6	2.42	0.55
4:C:215:ILE:HG13	4:C:216:SER:N	2.22	0.55
6:E:236:THR:CG2	6:E:239:ALA:H	1.95	0.55
14:M:1:THR:HA	38:M:8526:HOH:O	2.06	0.55
16:O:143:ARG:HA	16:O:172:PHE:CD2	2.41	0.55
16:O:71:TRP:HE3	16:O:175:LEU:HD22	1.72	0.55
1:A:1209:C:H2'	1:A:1210:G:C8	2.41	0.55
1:A:1393:A:H2'	1:A:1394:C:C6	2.41	0.55
14:M:90:ARG:NH2	14:M:121:ILE:HD11	2.20	0.55
25:X:108:ARG:HE	25:X:114:PRO:HG3	1.71	0.55
1:A:338:C:H5''	38:E:8426:HOH:O	2.06	0.55
4:C:95:PRO:HG2	4:C:98:GLU:HG2	1.88	0.55
7:F:27:ILE:HG22	7:F:28:GLY:N	2.15	0.55
23:V:33:SER:O	23:V:37:GLU:HG3	2.07	0.55
1:A:2904:U:H4'	26:Y:8:ARG:NH1	2.20	0.55
27:Z:133:HIS:HD2	38:Z:8588:HOH:O	1.88	0.55
27:Z:216:ARG:CD	38:Z:8574:HOH:O	2.47	0.55
29:2:2:GLY:O	29:2:6:PRO:HG2	2.07	0.55
1:A:506:G:N2	1:A:509:A:H5'	2.16	0.55
1:A:635:A:H2'	1:A:636:G:H5''	1.87	0.55
5:D:195:ARG:HD2	5:D:324:ASP:OD1	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:114:VAL:HB	15:N:159:THR:HG23	1.87	0.55
24:W:64:GLY:O	24:W:65:ASP:CB	2.55	0.55
30:3:22:PRO:HG2	30:3:25:VAL:CG2	2.35	0.55
31:4:34:LYS:HB2	31:4:37:ASP:OD2	2.06	0.55
1:A:1659:A:H2'	1:A:1660:G:O4'	2.07	0.55
1:A:2361:A:H5''	38:A:8523:HOH:O	2.06	0.55
1:A:57:C:H5''	38:A:6218:HOH:O	2.06	0.55
5:D:119:HIS:O	5:D:121:PRO:HD3	2.06	0.55
9:H:100:ASP:HB3	38:H:5691:HOH:O	2.07	0.55
14:M:145:LEU:O	14:M:148:GLU:HG3	2.07	0.55
1:A:182:G:O3'	15:N:157:LEU:HD13	2.07	0.55
19:R:11:ARG:HD3	38:R:5620:HOH:O	2.07	0.55
1:A:1191:A:C3'	1:A:1192:A:H5''	2.37	0.55
1:A:1166:A:H1'	1:A:1192:A:N1	2.21	0.55
1:A:2326:U:H4'	1:A:2412:G:C4'	2.37	0.55
4:C:140:LEU:HB3	4:C:141:PRO:HD2	1.88	0.55
6:E:236:THR:O	6:E:237:GLU:C	2.45	0.55
7:F:140:ARG:O	7:F:144:ARG:HG2	2.06	0.55
1:A:777:U:O2'	29:2:11:LYS:HG2	2.06	0.55
2:B:3029:C:C2'	2:B:3030:C:H5'	2.36	0.55
4:C:211:LYS:NZ	38:C:8582:HOH:O	2.39	0.55
7:F:23:VAL:CG2	7:F:73:VAL:HB	2.36	0.55
8:G:34:TRP:O	12:K:127:ILE:HD11	2.06	0.55
16:O:73:ALA:HB2	16:O:163:PHE:CZ	2.42	0.55
20:S:82:GLU:O	20:S:86:LYS:HG3	2.07	0.55
1:A:2478:U:H2'	1:A:2479:A:C8	2.41	0.55
1:A:970:U:H2'	38:A:5786:HOH:O	2.06	0.55
11:J:48:LEU:HG	11:J:157:ILE:HG21	1.89	0.55
16:O:62:HIS:HB3	16:O:65:ASP:OD1	2.07	0.55
21:T:6:LYS:HB2	21:T:27:ALA:O	2.06	0.55
22:U:37:GLN:OE1	22:U:118:SER:HA	2.06	0.55
26:Y:21:PRO:HG2	26:Y:24:LYS:HD3	1.88	0.55
31:4:3:MET:O	31:4:90:PHE:HA	2.07	0.54
1:A:1159:G:P	38:A:3782:HOH:O	2.65	0.54
1:A:1165:G:H3'	1:A:1165:G:OP1	2.08	0.54
1:A:125:U:H2'	38:A:3261:HOH:O	2.07	0.54
2:B:3023:U:H6	2:B:3023:U:C5'	2.20	0.54
8:G:11:VAL:CG1	8:G:12:ASP:N	2.70	0.54
18:Q:105:LEU:HD21	18:Q:137:LEU:HD21	1.88	0.54
1:A:1187:U:O2'	1:A:1189:A:H2	1.91	0.54
1:A:1512:G:O2'	1:A:1513:C:H5'	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2415:A:N3	16:O:26:LEU:HD13	2.22	0.54
1:A:514:G:O5'	1:A:514:G:H8	1.90	0.54
4:C:192:VAL:CG1	4:C:207:GLN:HB3	2.38	0.54
4:C:192:VAL:O	4:C:192:VAL:HG12	2.07	0.54
11:J:147:ARG:HA	11:J:150:LYS:NZ	2.23	0.54
11:J:46:VAL:HG12	11:J:146:TRP:HZ3	1.72	0.54
13:L:4:LEU:HD22	13:L:116:GLU:HB3	1.89	0.54
16:O:132:ASN:O	16:O:135:VAL:HG12	2.06	0.54
1:A:962:C:C1'	16:O:5:ARG:NH1	2.64	0.54
20:S:132:ARG:CZ	38:S:8582:HOH:O	2.55	0.54
26:Y:15:ARG:HH11	26:Y:15:ARG:CB	2.15	0.54
5:D:314:ALA:CB	5:D:317:PRO:HG3	2.37	0.54
5:D:51:VAL:CG2	5:D:327:VAL:HG13	2.36	0.54
12:K:42:GLU:O	12:K:131:THR:HG23	2.07	0.54
15:N:46:LEU:HG	38:N:8622:HOH:O	2.07	0.54
15:N:61:ILE:N	15:N:61:ILE:HD12	2.21	0.54
22:U:32:ARG:NH1	22:U:38:ARG:HH12	2.05	0.54
1:A:1422:U:H2'	1:A:1423:C:C6	2.42	0.54
1:A:1500:U:OP2	18:Q:41:ARG:NH2	2.40	0.54
1:A:204:A:H2'	1:A:205:U:H5'	1.88	0.54
1:A:2320:U:H4'	1:A:2321:A:O4'	2.08	0.54
1:A:711:G:C2	1:A:718:C:C2	2.96	0.54
2:B:3023:U:C3'	2:B:3024:U:H5''	2.38	0.54
2:B:3042:C:H2'	38:B:8505:HOH:O	2.07	0.54
4:C:199:HIS:HD2	4:C:201:PHE:H	1.52	0.54
5:D:75:GLU:C	5:D:77:PRO:HD3	2.28	0.54
7:F:41:LEU:HA	7:F:44:ILE:CG2	2.36	0.54
9:H:101:ALA:HA	38:H:5413:HOH:O	2.07	0.54
19:R:40:HIS:HD2	19:R:60:THR:OG1	1.90	0.54
1:A:21:G:H4'	20:S:2:ILE:HG22	1.88	0.54
1:A:1120:U:H6	1:A:1120:U:H5''	1.70	0.54
2:B:3020:G:O2'	2:B:3021:G:H5'	2.07	0.54
1:A:2547:C:OP2	5:D:5:ARG:NH1	2.40	0.54
8:G:126:ILE:HB	8:G:131:LEU:CD2	2.37	0.54
11:J:136:VAL:HG23	38:J:8344:HOH:O	2.07	0.54
14:M:149:ARG:O	14:M:150:GLN:HB2	2.07	0.54
17:P:14:LEU:HD23	17:P:102:ILE:HD11	1.88	0.54
28:1:42:CYS:SG	28:1:44:PHE:N	2.61	0.54
1:A:1951:G:N2	38:A:5718:HOH:O	2.40	0.54
1:A:2429:A:H2'	1:A:2430:A:C8	2.42	0.54
1:A:541:C:H2'	1:A:542:A:H5'	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:824:G:N7	38:A:3800:HOH:O	2.39	0.54
4:C:164:ARG:HA	28:1:69:TYR:CE1	2.43	0.54
38:A:6231:HOH:O	16:O:4:PRO:HD2	2.07	0.54
22:U:9:LYS:CE	22:U:13:ARG:NH1	2.71	0.54
25:X:35:VAL:HG23	25:X:41:TYR:CD2	2.42	0.54
31:4:87:ARG:HG3	38:4:8570:HOH:O	2.06	0.54
1:A:2349:G:OP1	7:F:20:LYS:NZ	2.36	0.54
1:A:2761:A:C4	1:A:2763:G:C8	2.95	0.54
1:A:951:A:C2'	1:A:952:G:H5'	2.38	0.54
4:C:173:GLY:O	4:C:176:HIS:HB3	2.07	0.54
6:E:16:VAL:HG12	6:E:17:ASP:N	2.22	0.54
10:I:64:ASN:O	10:I:68:GLU:HG3	2.08	0.54
1:A:2437:A:H2'	1:A:2438:G:C8	2.43	0.54
1:A:2758:G:H2'	1:A:2759:C:C6	2.43	0.54
5:D:66:GLU:OE1	5:D:328:ARG:HD2	2.08	0.54
8:G:126:ILE:HB	8:G:131:LEU:HD23	1.89	0.54
1:A:2015:A:H2'	1:A:2016:U:O4'	2.07	0.54
1:A:2329:C:O2'	1:A:2330:U:H5'	2.08	0.54
1:A:2717:C:O2'	1:A:2718:C:H5''	2.06	0.54
5:D:168:GLY:N	5:D:174:ARG:HD3	2.22	0.54
5:D:55:ASN:HB3	5:D:63:GLU:HA	1.89	0.54
11:J:166:ASN:N	11:J:166:ASN:ND2	2.56	0.54
12:K:131:THR:HG22	12:K:133:GLY:N	2.23	0.54
15:N:164:THR:HB	38:N:8520:HOH:O	2.08	0.54
23:V:44:ARG:CB	38:V:3805:HOH:O	2.54	0.54
1:A:1887:U:OP1	28:1:21:LYS:HG3	2.08	0.54
38:A:5970:HOH:O	30:3:1:GLY:HA3	2.07	0.54
1:A:1527:A:H1'	1:A:1528:A:C8	2.43	0.54
1:A:1713:G:C2'	38:A:4547:HOH:O	2.56	0.54
1:A:1829:A:H5''	38:A:9578:HOH:O	2.07	0.54
1:A:506:G:H22	1:A:509:A:H5''	1.70	0.54
2:B:3035:C:H5''	38:B:8456:HOH:O	2.08	0.54
6:E:236:THR:HA	38:E:8457:HOH:O	2.08	0.54
7:F:65:GLU:HG3	38:F:6752:HOH:O	2.06	0.54
11:J:45:GLN:HE21	11:J:135:TRP:HE1	1.56	0.54
13:L:34:VAL:HB	38:L:7169:HOH:O	2.08	0.54
38:A:7138:HOH:O	15:N:154:ARG:HB2	2.07	0.54
25:X:5:VAL:HG22	25:X:32:CYS:HB2	1.90	0.54
26:Y:76:ARG:HG3	26:Y:76:ARG:NH1	2.21	0.54
1:A:1174:A:C5	1:A:1201:C:H4'	2.43	0.53
1:A:1641:A:H2'	1:A:1642:A:H5'	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2265:U:H2'	1:A:2266:A:C8	2.43	0.53
1:A:329:A:OP2	6:E:206:ASN:HB2	2.08	0.53
1:A:447:A:O2'	1:A:448:G:H5'	2.08	0.53
1:A:778:C:C4	1:A:779:U:C4	2.96	0.53
6:E:43:LYS:NZ	38:E:8392:HOH:O	2.41	0.53
7:F:64:ARG:CD	7:F:67:ASP:HB3	2.38	0.53
13:L:75:ARG:CZ	38:L:4172:HOH:O	2.56	0.53
15:N:87:MET:SD	31:4:46:ILE:HD13	2.48	0.53
17:P:39:THR:O	17:P:115:ARG:NH2	2.41	0.53
25:X:110:GLN:HA	25:X:110:GLN:NE2	2.24	0.53
1:A:1250:C:O2'	1:A:1251:C:H5'	2.08	0.53
1:A:558:C:H2'	1:A:559:U:H5'	1.91	0.53
1:A:816:G:H5'	1:A:1598:A:H4'	1.90	0.53
4:C:164:ARG:HB2	28:1:68:CYS:SG	2.48	0.53
6:E:200:PRO:HB3	6:E:212:VAL:HG23	1.90	0.53
10:I:12:ILE:HG22	10:I:12:ILE:O	2.08	0.53
10:I:12:ILE:N	38:I:4714:HOH:O	2.41	0.53
15:N:172:GLY:C	15:N:183:VAL:HG11	2.29	0.53
17:P:4:ASN:HB3	17:P:7:LEU:HB3	1.90	0.53
21:T:57:THR:CG2	21:T:58:MET:N	2.71	0.53
23:V:9:CYS:HA	23:V:52:THR:CG2	2.38	0.53
29:2:25:LYS:HD2	30:3:49:GLU:H	1.72	0.53
1:A:113:A:OP1	38:A:9242:HOH:O	2.19	0.53
1:A:1909:A:H2'	1:A:1910:A:C8	2.42	0.53
1:A:644:G:H5'	1:A:644:G:N3	2.24	0.53
5:D:248:ARG:O	5:D:251:VAL:CG1	2.56	0.53
5:D:72:THR:HB	38:D:8606:HOH:O	2.09	0.53
8:G:69:ILE:HA	8:G:72:MET:HE3	1.90	0.53
22:U:24:ARG:HH21	22:U:39:ASN:ND2	2.06	0.53
25:X:1:MET:HB2	25:X:103:GLU:HG2	1.90	0.53
1:A:1097:A:H5''	25:X:125:HIS:NE2	2.24	0.53
27:Z:126:PRO:HG2	27:Z:128:PHE:CE1	2.43	0.53
1:A:1666:C:O2'	1:A:1667:A:C5'	2.56	0.53
1:A:1730:G:H5'	1:A:1731:C:C6	2.44	0.53
1:A:2028:U:H2'	1:A:2029:C:C6	2.43	0.53
1:A:2791:U:H1'	1:A:2792:A:H5''	1.90	0.53
4:C:105:VAL:HG11	4:C:154:ALA:HB1	1.89	0.53
7:F:99:ASP:CB	7:F:103:ASN:H	2.22	0.53
8:G:86:VAL:CG1	8:G:129:GLU:HA	2.38	0.53
9:H:28:ALA:HB3	9:H:99:THR:O	2.08	0.53
14:M:54:PRO:HG2	14:M:57:VAL:HG21	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:43:VAL:HG13	16:O:118:ILE:HD11	1.89	0.53
20:S:18:LEU:HD12	20:S:143:VAL:CG1	2.39	0.53
38:L:408:HOH:O	23:V:37:GLU:HB3	2.08	0.53
1:A:1617:C:C4	1:A:1643:C:H4'	2.43	0.53
1:A:42:C:H1'	38:A:4157:HOH:O	2.08	0.53
1:A:681:G:N3	1:A:681:G:H5'	2.24	0.53
4:C:105:VAL:CG1	4:C:154:ALA:HB1	2.39	0.53
4:C:95:PRO:HA	4:C:153:ARG:HA	1.91	0.53
9:H:91:VAL:CG1	9:H:92:GLY:H	2.18	0.53
23:V:46:ALA:HB1	23:V:52:THR:HG21	1.90	0.53
1:A:1192:A:H3'	1:A:1193:A:H5'	1.90	0.53
1:A:1268:C:O2'	1:A:1269:G:H5'	2.09	0.53
1:A:1362:U:H5'	38:A:9762:HOH:O	2.09	0.53
1:A:2326:U:H4'	1:A:2412:G:H4'	1.90	0.53
1:A:344:C:H2'	1:A:345:G:O4'	2.08	0.53
4:C:37:VAL:HG22	38:C:8610:HOH:O	2.08	0.53
7:F:54:ALA:HB2	7:F:69:ILE:HD12	1.90	0.53
9:H:91:VAL:CG1	9:H:92:GLY:N	2.70	0.53
11:J:147:ARG:HA	11:J:150:LYS:HZ2	1.73	0.53
15:N:108:LYS:HE3	38:N:8614:HOH:O	2.08	0.53
15:N:61:ILE:HA	38:N:8624:HOH:O	2.09	0.53
24:W:44:GLY:O	24:W:48:GLU:HG2	2.08	0.53
1:A:1200:A:H4'	38:A:6798:HOH:O	2.09	0.53
4:C:217:ARG:HG2	4:C:229:ALA:HB2	1.91	0.53
5:D:74:ILE:HD13	5:D:309:VAL:HG21	1.91	0.53
9:H:99:THR:O	9:H:100:ASP:HB2	2.08	0.53
10:I:12:ILE:HB	38:I:4714:HOH:O	2.07	0.53
1:A:1242:A:OP2	12:K:60:ARG:NH2	2.38	0.53
1:A:902:G:N7	14:M:18:HIS:CD2	2.75	0.53
1:A:538:C:OP2	27:Z:134:HIS:HE1	1.92	0.53
1:A:1185:U:H5'	38:A:6922:HOH:O	2.09	0.53
38:A:5778:HOH:O	7:F:55:LYS:HB2	2.07	0.53
13:L:55:VAL:HG12	13:L:56:SER:H	1.73	0.53
18:Q:10:ALA:CA	18:Q:13:VAL:HG12	2.39	0.53
24:W:39:ALA:O	24:W:41:GLU:N	2.41	0.53
1:A:1180:U:H2'	1:A:1181:A:O4'	2.09	0.53
1:A:212:A:O4'	1:A:214:U:C6	2.62	0.53
1:A:2256:G:H2'	1:A:2257:G:H5'	1.91	0.53
1:A:2459:G:OP1	31:4:64:LYS:N	2.21	0.53
1:A:703:G:O2'	1:A:704:C:H5'	2.09	0.53
6:E:77:ALA:O	6:E:78:ARG:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A:4311:HOH:O	12:K:47:THR:CB	2.51	0.53
15:N:87:MET:HB2	15:N:91:ILE:CD1	2.39	0.53
18:Q:16:VAL:HG12	18:Q:17:GLY:N	2.24	0.53
1:A:1328:A:OP1	27:Z:169:ARG:HD2	2.08	0.53
1:A:2594:C:O2'	1:A:2595:U:H5'	2.09	0.53
1:A:776:A:OP1	29:2:28:HIS:HE1	1.92	0.53
38:A:9733:HOH:O	4:C:221:PRO:HA	2.07	0.53
5:D:315:VAL:HG23	5:D:316:ARG:HG2	1.91	0.53
7:F:11:HIS:C	7:F:13:MET:H	2.12	0.53
9:H:100:ASP:O	9:H:101:ALA:O	2.27	0.53
12:K:131:THR:HB	12:K:134:GLU:HG3	1.91	0.53
16:O:157:PRO:HA	38:O:8526:HOH:O	2.09	0.53
18:Q:115:SER:O	18:Q:117:SER:N	2.42	0.53
38:A:9566:HOH:O	20:S:83:LYS:HB3	2.08	0.53
25:X:90:TYR:CE2	25:X:99:ALA:HB2	2.44	0.53
27:Z:178:HIS:CG	27:Z:179:PRO:HD2	2.44	0.53
28:1:10:ARG:HG3	28:1:11:THR:N	2.25	0.52
31:4:40:ARG:HD2	38:4:8547:HOH:O	2.07	0.52
1:A:1014:A:H5''	2:B:3101:G:O2'	2.09	0.52
1:A:1060:C:H6	1:A:1060:C:H5'	1.73	0.52
1:A:2107:U:O2'	1:A:2108:A:H5'	2.09	0.52
5:D:27:ASN:HD22	5:D:27:ASN:H	1.57	0.52
5:D:42:ALA:HB1	5:D:308:LEU:HD11	1.90	0.52
6:E:95:GLU:N	6:E:95:GLU:OE1	2.39	0.52
7:F:174:VAL:HG13	38:F:6555:HOH:O	2.08	0.52
8:G:31:ARG:NH1	8:G:68:HIS:CG	2.77	0.52
15:N:65:VAL:HG21	15:N:105:ALA:HB2	1.91	0.52
1:A:1701:A:H4'	1:A:1702:U:C5'	2.39	0.52
1:A:1819:G:H2'	1:A:1820:G:C5'	2.39	0.52
1:A:2478:U:H2'	1:A:2479:A:H8	1.74	0.52
8:G:20:ILE:HD12	8:G:33:LEU:CD1	2.40	0.52
11:J:4:ALA:HB3	38:J:8365:HOH:O	2.08	0.52
20:S:82:GLU:HG3	20:S:83:LYS:N	2.24	0.52
25:X:125:HIS:HE1	38:X:3071:HOH:O	1.92	0.52
28:1:26:VAL:O	28:1:30:GLU:HG3	2.09	0.52
28:1:46:LYS:NZ	38:1:8439:HOH:O	2.43	0.52
1:A:1333:U:H2'	1:A:1334:C:C6	2.44	0.52
1:A:1505:U:H6	1:A:1505:U:H5'	1.73	0.52
1:A:1834:C:H2'	1:A:1840:A:N6	2.24	0.52
1:A:2435:U:H1'	38:A:4900:HOH:O	2.08	0.52
1:A:256:C:H2'	1:A:257:G:O4'	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:U:H2'	1:A:560:C:O4'	2.10	0.52
1:A:88:G:H8	1:A:88:G:H5'	1.75	0.52
2:B:3041:C:H4'	7:F:48:MET:HB2	1.90	0.52
4:C:18:ALA:O	4:C:20:SER:N	2.39	0.52
5:D:62:ARG:CA	5:D:65:MET:HE3	2.33	0.52
7:F:58:VAL:HG12	7:F:59:GLY:N	2.24	0.52
11:J:117:LYS:O	11:J:119:VAL:HG13	2.09	0.52
1:A:2123:A:H5'	15:N:89:ASN:HD21	1.74	0.52
28:1:50:ALA:HB3	28:1:54:ILE:HG22	1.91	0.52
1:A:1015:C:H2'	1:A:1016:U:C6	2.44	0.52
1:A:1159:G:H21	1:A:1189:A:H8	1.56	0.52
1:A:1205:U:H2'	1:A:1206:U:C5'	2.38	0.52
2:B:3025:G:H5''	2:B:3026:C:C6	2.45	0.52
10:I:69:ARG:NH1	38:I:3513:HOH:O	2.42	0.52
11:J:150:LYS:NZ	38:J:8379:HOH:O	2.40	0.52
15:N:184:ARG:HG3	15:N:185:PRO:HA	1.92	0.52
16:O:159:TYR:HE2	16:O:163:PHE:HE2	1.57	0.52
17:P:96:VAL:HA	38:P:4258:HOH:O	2.08	0.52
20:S:61:GLN:NE2	38:S:8539:HOH:O	2.42	0.52
1:A:1008:C:O2'	1:A:1009:U:H5'	2.09	0.52
1:A:1189:A:O2'	1:A:1208:C:H2'	2.09	0.52
1:A:2276:U:H2'	1:A:2277:U:H6	1.74	0.52
1:A:2467:A:O2'	1:A:2468:A:H2'	2.08	0.52
1:A:2587:U:H2'	1:A:2589:U:H5''	1.91	0.52
1:A:401:C:H2'	1:A:402:U:C6	2.45	0.52
1:A:622:G:O2'	1:A:623:U:H5'	2.09	0.52
1:A:657:G:OP1	6:E:27:ARG:NH2	2.40	0.52
6:E:127:ARG:HG2	6:E:127:ARG:NH1	2.24	0.52
6:E:150:THR:HA	6:E:203:ALA:O	2.09	0.52
7:F:146:LYS:NZ	16:O:107:ASN:ND2	2.57	0.52
1:A:380:A:OP2	15:N:9:ARG:HD2	2.09	0.52
27:Z:172:THR:HG22	27:Z:173:ALA:N	2.24	0.52
27:Z:99:ALA:HB2	27:Z:233:TYR:CZ	2.44	0.52
28:1:38:LYS:HE2	28:1:45:LYS:CE	2.38	0.52
1:A:1176:C:H1'	38:A:3422:HOH:O	2.10	0.52
1:A:2064:U:H5'	1:A:2652:U:H4'	1.90	0.52
1:A:2694:A:H4'	8:G:91:PHE:HE1	1.74	0.52
1:A:2769:C:C2'	1:A:2770:G:H5'	2.40	0.52
1:A:566:A:H2'	1:A:567:U:O4'	2.09	0.52
5:D:305:ASP:O	5:D:306:LYS:CB	2.56	0.52
5:D:307:ARG:HH11	5:D:307:ARG:CG	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:11:VAL:HG12	8:G:12:ASP:H	1.74	0.52
13:L:74:VAL:CG1	13:L:113:ILE:HG12	2.40	0.52
1:A:513:A:N3	38:A:3157:HOH:O	2.33	0.52
1:A:797:A:O4'	28:1:10:ARG:N	2.42	0.52
5:D:217:ARG:HG3	5:D:257:THR:CG2	2.39	0.52
5:D:162:MET:CE	5:D:308:LEU:HD21	2.40	0.52
6:E:142:ASP:OD1	6:E:236:THR:HG23	2.09	0.52
6:E:37:ALA:HB2	38:E:8382:HOH:O	2.09	0.52
9:H:58:GLU:OE1	15:N:27:ARG:NH2	2.39	0.52
12:K:93:ARG:HH11	12:K:93:ARG:HB3	1.74	0.52
14:M:73:VAL:HG23	14:M:74:THR:H	1.73	0.52
16:O:64:SER:C	16:O:66:LEU:H	2.12	0.52
1:A:1450:C:C4'	1:A:1451:C:OP2	2.54	0.52
1:A:2505:G:H8	38:A:5108:HOH:O	1.93	0.52
1:A:401:C:P	38:A:5258:HOH:O	2.68	0.52
4:C:199:HIS:HD2	4:C:201:PHE:HB2	1.75	0.52
1:A:2630:G:O6	4:C:206:ARG:NH2	2.43	0.52
5:D:144:THR:HG22	5:D:145:HIS:N	2.25	0.52
7:F:54:ALA:CB	7:F:69:ILE:HD12	2.40	0.52
11:J:46:VAL:O	11:J:146:TRP:HH2	1.93	0.52
11:J:86:ARG:HD3	11:J:130:HIS:HD2	1.74	0.52
1:A:1718:G:OP2	18:Q:20:ARG:HD2	2.09	0.52
28:1:37:HIS:O	28:1:45:LYS:HA	2.10	0.52
30:3:40:ARG:HG2	30:3:40:ARG:HH11	1.74	0.52
1:A:625:U:H5''	1:A:1044:C:N4	2.25	0.52
1:A:1188:A:C5	1:A:1189:A:C2	2.98	0.52
1:A:1654:U:H2'	4:C:47:HIS:CD2	2.45	0.52
1:A:2715:G:N2	5:D:264:GLU:OE1	2.43	0.52
4:C:81:GLN:HB2	4:C:92:ASN:ND2	2.24	0.52
4:C:99:ILE:O	4:C:131:HIS:CE1	2.63	0.52
11:J:144:GLU:HA	11:J:144:GLU:OE1	2.10	0.52
1:A:431:G:P	15:N:48:ARG:HH12	2.33	0.52
17:P:25:VAL:HG23	17:P:26:TRP:N	2.25	0.52
25:X:88:THR:CG2	25:X:89:ASP:H	2.19	0.52
1:A:218:C:OP2	1:A:220:C:N4	2.42	0.52
1:A:832:U:H2'	1:A:833:G:C8	2.45	0.52
5:D:162:MET:CE	5:D:310:ARG:HD3	2.40	0.52
11:J:139:ASP:N	11:J:140:PRO:CD	2.72	0.52
11:J:48:LEU:CD1	11:J:157:ILE:HG21	2.39	0.52
14:M:35:ARG:O	14:M:40:PHE:HA	2.10	0.52
14:M:53:ARG:NH2	14:M:57:VAL:HG12	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:154:LEU:HG	16:O:155:GLU:N	2.24	0.52
1:A:1654:U:H2'	4:C:47:HIS:HD2	1.74	0.51
1:A:2724:U:H2'	1:A:2725:G:O4'	2.10	0.51
1:A:2781:U:H2'	1:A:2782:G:H5'	1.91	0.51
1:A:2896:A:H2'	1:A:2896:A:N3	2.25	0.51
7:F:92:GLU:O	7:F:93:LEU:O	2.28	0.51
10:I:23:ILE:O	10:I:27:ILE:HG13	2.10	0.51
1:A:1055:G:OP2	11:J:94:ARG:NH1	2.43	0.51
13:L:125:ALA:C	13:L:127:ALA:H	2.12	0.51
1:A:2115:U:H2'	1:A:2116:U:C6	2.45	0.51
1:A:2307:A:C2	1:A:2308:U:N3	2.78	0.51
1:A:2524:G:H21	1:A:2526:C:N4	2.08	0.51
1:A:2756:U:H3	1:A:2896:A:H2	1.56	0.51
1:A:920:C:H5''	1:A:921:G:O5'	2.10	0.51
6:E:178:GLN:O	6:E:179:GLY:C	2.48	0.51
11:J:127:GLY:O	11:J:128:ALA:CB	2.58	0.51
14:M:57:VAL:HG12	14:M:57:VAL:O	2.10	0.51
23:V:14:GLU:OE1	23:V:15:PRO:HD2	2.10	0.51
25:X:122:ARG:HG2	25:X:152:ALA:O	2.09	0.51
25:X:90:TYR:CD1	25:X:90:TYR:N	2.78	0.51
1:A:2533:C:H6	1:A:2533:C:C5'	2.15	0.51
1:A:542:A:H2'	1:A:543:G:O4'	2.10	0.51
4:C:125:ASN:ND2	38:C:8542:HOH:O	2.39	0.51
9:H:48:VAL:HG23	9:H:74:PHE:CB	2.41	0.51
22:U:111:ARG:HB3	22:U:119:ALA:HB2	1.93	0.51
25:X:21:LEU:HD21	25:X:48:VAL:CG1	2.40	0.51
31:4:39:GLN:HA	31:4:42:ARG:NH2	2.26	0.51
1:A:1056:U:H2'	1:A:1057:A:O4'	2.11	0.51
1:A:136:C:H2'	1:A:137:U:O4'	2.10	0.51
1:A:2121:G:O2'	31:4:47:GLY:HA2	2.11	0.51
1:A:2432:C:H2'	1:A:2433:A:H8	1.75	0.51
1:A:2749:U:O2'	1:A:2751:C:OP2	2.17	0.51
1:A:911:G:H5'	1:A:932:U:OP1	2.10	0.51
1:A:926:A:O2'	14:M:41:HIS:CD2	2.63	0.51
1:A:1874:U:P	4:C:51:ARG:HD2	2.50	0.51
7:F:169:THR:O	7:F:170:TYR:HB2	2.11	0.51
25:X:154:ARG:C	38:X:4276:HOH:O	2.47	0.51
1:A:797:A:C4'	28:1:10:ARG:N	2.73	0.51
1:A:1568:G:O2'	1:A:1569:U:H5'	2.09	0.51
1:A:2039:A:H4'	1:A:2760:C:O2'	2.11	0.51
1:A:2270:G:H4'	4:C:223:ARG:HH12	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3030:C:OP1	7:F:137:PRO:O	2.28	0.51
4:C:192:VAL:O	4:C:207:GLN:HG2	2.10	0.51
11:J:150:LYS:HA	11:J:153:VAL:HG22	1.92	0.51
16:O:162:ASP:O	38:O:8520:HOH:O	2.18	0.51
16:O:180:LEU:O	16:O:181:ASP:HB3	2.10	0.51
20:S:25:PHE:CE2	20:S:29:LYS:HE2	2.46	0.51
23:V:52:THR:HG22	23:V:54:THR:N	2.26	0.51
26:Y:43:VAL:CG1	26:Y:47:ALA:HB3	2.41	0.51
38:A:6167:HOH:O	27:Z:165:GLU:HB3	2.10	0.51
28:1:25:ARG:O	28:1:29:VAL:HG23	2.10	0.51
1:A:111:C:H2'	1:A:112:G:O4'	2.11	0.51
1:A:2081:A:H4'	12:K:69:TYR:CE1	2.46	0.51
1:A:2256:G:C2'	1:A:2257:G:H5'	2.41	0.51
1:A:245:C:H2'	1:A:246:G:H5'	1.92	0.51
1:A:2787:C:H5	38:A:4115:HOH:O	1.93	0.51
1:A:289:G:O2'	1:A:290:C:H5'	2.11	0.51
1:A:711:G:N2	1:A:718:C:C2	2.79	0.51
6:E:39:GLN:O	6:E:43:LYS:HD3	2.11	0.51
7:F:135:VAL:HG22	7:F:136:ARG:N	2.25	0.51
8:G:5:LEU:HD21	8:G:66:GLN:HG3	1.91	0.51
8:G:7:ILE:CG2	8:G:45:ASP:O	2.58	0.51
10:I:66:LEU:O	10:I:69:ARG:HB3	2.10	0.51
15:N:59:GLY:CA	15:N:141:ILE:HD11	2.41	0.51
23:V:52:THR:HG22	23:V:54:THR:H	1.76	0.51
25:X:14:HIS:HB2	25:X:17:ILE:HG13	1.93	0.51
26:Y:72:VAL:HG22	26:Y:85:VAL:CG1	2.38	0.51
28:1:57:CYS:O	28:1:61:GLY:N	2.41	0.51
1:A:470:U:O2'	29:2:16:HIS:HD2	1.93	0.51
29:2:25:LYS:HG3	30:3:49:GLU:H	1.76	0.51
29:2:25:LYS:HD2	30:3:49:GLU:N	2.25	0.51
1:A:1052:G:H2'	1:A:1052:G:N3	2.24	0.51
1:A:1589:G:N2	1:A:1605:G:H1'	2.26	0.51
1:A:1882:C:O2'	1:A:2012:U:OP2	2.26	0.51
1:A:306:A:P	22:U:38:ARG:HH21	2.33	0.51
5:D:204:GLY:C	38:D:8653:HOH:O	2.49	0.51
7:F:10:PHE:CG	7:F:11:HIS:N	2.79	0.51
8:G:92:PRO:HB2	38:G:4917:HOH:O	2.11	0.51
9:H:99:THR:HG23	9:H:99:THR:O	2.10	0.51
15:N:113:ARG:NH2	15:N:156:ARG:HG2	2.26	0.51
1:A:2363:G:O2'	19:R:11:ARG:HG3	2.11	0.51
1:A:2055:A:H4'	20:S:132:ARG:NH2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1787:C:H4'	1:A:2883:A:O4'	2.10	0.51
1:A:2897:C:H2'	1:A:2898:G:H8	1.75	0.51
5:D:211:THR:HA	5:D:255:GLY:O	2.11	0.51
7:F:86:THR:O	7:F:90:LEU:HG	2.11	0.51
11:J:56:ILE:HG21	11:J:61:LEU:HD13	1.93	0.51
25:X:31:HIS:HB3	38:X:5420:HOH:O	2.11	0.51
1:A:1008:C:OP1	11:J:16:ARG:NH2	2.40	0.51
1:A:305:A:C5	1:A:329:A:C2	2.99	0.51
1:A:960:G:N3	1:A:960:G:H2'	2.26	0.51
38:A:4879:HOH:O	4:C:164:ARG:CZ	2.59	0.51
5:D:125:GLU:O	5:D:129:ARG:HG3	2.10	0.51
5:D:329:TYR:HE2	23:V:15:PRO:HG2	1.74	0.51
6:E:140:VAL:HG12	6:E:141:SER:N	2.26	0.51
9:H:101:ALA:HB2	9:H:108:LEU:HD22	1.93	0.51
16:O:82:TYR:OH	16:O:176:ARG:NH1	2.44	0.51
19:R:30:VAL:O	19:R:30:VAL:HG12	2.11	0.51
20:S:29:LYS:HD3	38:S:8531:HOH:O	2.11	0.51
21:T:58:MET:SD	30:3:8:LYS:HE3	2.50	0.51
31:4:24:LYS:HG2	35:4:8504:CL:CL	2.48	0.51
1:A:737:A:H2'	1:A:738:G:O4'	2.11	0.51
5:D:32:ASP:HA	38:D:8575:HOH:O	2.10	0.51
1:A:2779:G:H21	8:G:143:GLN:NE2	2.09	0.51
11:J:83:PHE:HZ	11:J:146:TRP:HE1	1.55	0.51
16:O:139:TRP:HA	16:O:139:TRP:HE3	1.76	0.51
16:O:3:GLY:HA3	38:O:8512:HOH:O	2.10	0.51
28:1:58:GLY:HA3	38:1:8437:HOH:O	2.10	0.50
1:A:1197:G:N2	38:A:5692:HOH:O	2.43	0.50
1:A:1699:C:H4'	38:A:5901:HOH:O	2.10	0.50
1:A:204:A:C2'	1:A:205:U:H5'	2.40	0.50
1:A:2112:A:H2'	1:A:2113:G:C8	2.46	0.50
1:A:2795:C:O2'	1:A:2796:U:H5'	2.11	0.50
5:D:235:ARG:HA	38:D:8596:HOH:O	2.10	0.50
1:A:2094:G:C4'	5:D:245:SER:HB3	2.39	0.50
6:E:33:LYS:HE2	38:E:8361:HOH:O	2.10	0.50
11:J:71:TYR:C	11:J:73:GLN:N	2.63	0.50
21:T:57:THR:CG2	21:T:59:ASP:HB2	2.40	0.50
31:4:69:TYR:HB2	31:4:78:HIS:CE1	2.46	0.50
1:A:2897:C:O2'	1:A:2898:G:H5'	2.11	0.50
5:D:189:ALA:HB1	38:D:8566:HOH:O	2.10	0.50
26:Y:20:GLU:CD	26:Y:21:PRO:HD2	2.31	0.50
38:A:5651:HOH:O	30:3:44:ARG:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1119:G:H8	12:K:52:GLN:HE22	1.59	0.50
1:A:1559:A:H1'	38:A:5328:HOH:O	2.11	0.50
1:A:192:A:N6	1:A:194:A:C2	2.80	0.50
1:A:2004:U:H1'	38:A:9690:HOH:O	2.10	0.50
1:A:2266:A:H2'	1:A:2267:G:H8	1.76	0.50
1:A:821:U:O2'	1:A:822:C:H5'	2.12	0.50
6:E:5:ILE:CD1	6:E:16:VAL:HG23	2.24	0.50
6:E:127:ARG:HD2	6:E:229:PRO:O	2.11	0.50
8:G:15:GLN:HG2	8:G:19:ASP:O	2.11	0.50
15:N:24:MET:HE2	15:N:28:MET:HE3	1.94	0.50
38:A:4057:HOH:O	15:N:83:SER:HA	2.10	0.50
26:Y:8:ARG:NH1	38:Y:2479:HOH:O	2.23	0.50
1:A:1015:C:O5'	1:A:1015:C:H6	1.93	0.50
1:A:1205:U:C2'	1:A:1206:U:H5'	2.36	0.50
1:A:2266:A:H2'	1:A:2267:G:C8	2.46	0.50
1:A:220:C:OP2	1:A:2431:C:H1'	2.12	0.50
1:A:564:G:H1'	38:A:5768:HOH:O	2.12	0.50
7:F:49:PRO:HG3	38:F:5828:HOH:O	2.10	0.50
7:F:64:ARG:O	7:F:67:ASP:OD2	2.29	0.50
7:F:95:THR:C	7:F:97:GLN:H	2.07	0.50
8:G:20:ILE:CD1	8:G:40:VAL:HG11	2.41	0.50
11:J:47:GLU:CB	11:J:133:ILE:HD13	2.41	0.50
14:M:72:ASN:O	14:M:76:LEU:HG	2.11	0.50
15:N:173:LEU:HD23	15:N:183:VAL:CG1	2.41	0.50
15:N:52:LEU:HD13	15:N:116:ASN:CG	2.31	0.50
23:V:52:THR:CG2	23:V:54:THR:HB	2.42	0.50
25:X:11:VAL:O	25:X:12:ASN:HB2	2.11	0.50
31:4:18:GLN:OE1	31:4:73:GLU:HB3	2.12	0.50
1:A:1768:C:H2'	1:A:1769:C:O4'	2.10	0.50
1:A:1829:A:C8	1:A:1885:A:C8	2.99	0.50
1:A:858:U:H2'	1:A:859:C:C6	2.47	0.50
4:C:191:GLY:HA2	4:C:194:MET:HE2	1.94	0.50
4:C:94:LEU:HG	4:C:99:ILE:CD1	2.42	0.50
6:E:79:ARG:O	6:E:87:ARG:HG2	2.11	0.50
7:F:41:LEU:CA	7:F:44:ILE:HG22	2.40	0.50
14:M:73:VAL:HG23	14:M:74:THR:N	2.26	0.50
20:S:119:VAL:O	20:S:119:VAL:HG12	2.11	0.50
1:A:1523:G:H2'	1:A:1524:U:C6	2.47	0.50
1:A:1787:C:OP1	18:Q:68:LYS:HE2	2.11	0.50
1:A:646:G:H2'	1:A:647:U:H6	1.77	0.50
2:B:3076:G:C3'	2:B:3077:A:H5"	2.35	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:37:ASP:OD1	12:K:125:SER:HB3	2.11	0.50
9:H:48:VAL:CG2	9:H:74:PHE:HB3	2.40	0.50
29:2:25:LYS:O	29:2:25:LYS:HG2	2.12	0.50
1:A:128:A:H3'	1:A:128:A:H8	1.77	0.50
1:A:1804:A:H2'	1:A:1805:G:C8	2.46	0.50
1:A:419:A:C2	1:A:2449:G:C2	3.00	0.50
4:C:51:ARG:HB2	38:C:8620:HOH:O	2.11	0.50
5:D:103:ASP:HB2	38:D:8594:HOH:O	2.11	0.50
9:H:32:GLY:N	38:H:3111:HOH:O	2.44	0.50
18:Q:80:ARG:HG2	18:Q:87:ARG:CZ	2.41	0.50
20:S:96:VAL:HG13	20:S:106:GLY:HA3	1.93	0.50
4:C:75:GLY:HA2	28:1:63:LYS:O	2.12	0.50
31:4:7:PHE:HE2	31:4:22:VAL:HG21	1.76	0.50
1:A:1557:G:O2'	1:A:1558:C:H5'	2.12	0.50
1:A:1636:G:O2'	1:A:1637:A:H5'	2.11	0.50
1:A:2256:G:H2'	1:A:2257:G:C5'	2.42	0.50
1:A:2382:A:H5'	38:4:8531:HOH:O	2.11	0.50
1:A:2404:G:OP1	19:R:69:ASP:N	2.38	0.50
1:A:2531:U:O2'	1:A:2532:A:H5'	2.12	0.50
1:A:702:G:O2'	1:A:703:G:H5'	2.12	0.50
1:A:858:U:H2'	1:A:859:C:H6	1.77	0.50
5:D:4:SER:O	5:D:5:ARG:HB2	2.12	0.50
7:F:65:GLU:HA	38:F:6752:HOH:O	2.12	0.50
8:G:93:MET:HE1	8:G:165:GLY:N	2.27	0.50
11:J:65:ARG:NH1	38:J:8385:HOH:O	2.44	0.50
15:N:85:ARG:NE	38:N:8519:HOH:O	2.34	0.50
22:U:19:ARG:HD3	22:U:67:LEU:O	2.11	0.50
1:A:2304:G:H5'	38:R:1719:HOH:O	2.10	0.50
1:A:2911:C:H2'	1:A:2912:C:C6	2.47	0.50
1:A:303:C:O2'	1:A:304:G:H5'	2.12	0.50
1:A:832:U:H2'	1:A:833:G:H8	1.76	0.50
7:F:23:VAL:HG21	7:F:45:THR:CG2	2.42	0.50
9:H:117:GLU:C	9:H:119:ARG:H	2.15	0.50
9:H:27:GLY:HA3	38:H:5413:HOH:O	2.12	0.50
21:T:53:ASN:ND2	38:T:8321:HOH:O	2.44	0.50
21:T:81:ILE:HG23	38:T:8337:HOH:O	2.11	0.50
24:W:11:MET:HB3	24:W:15:GLU:HB2	1.93	0.50
25:X:122:ARG:CG	25:X:152:ALA:O	2.60	0.50
1:A:119:A:H2'	1:A:120:A:H5''	1.94	0.49
1:A:2278:U:H2'	38:A:7060:HOH:O	2.11	0.49
1:A:2361:A:H2'	1:A:2362:A:C8	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:105:VAL:HG12	4:C:106:CYS:N	2.27	0.49
4:C:53:ALA:HB3	38:C:8620:HOH:O	2.11	0.49
5:D:132:HIS:CE1	5:D:171:VAL:HG21	2.46	0.49
5:D:223:ARG:HG3	5:D:232:TRP:O	2.12	0.49
5:D:56:ASP:OD1	5:D:322:ARG:HB3	2.10	0.49
8:G:18:LEU:HD13	8:G:34:TRP:CD1	2.47	0.49
9:H:34:ASN:HA	15:N:4:ALA:HB2	1.94	0.49
13:L:72:VAL:HG11	13:L:121:PHE:CD1	2.47	0.49
14:M:140:VAL:HG23	38:M:8562:HOH:O	2.11	0.49
1:A:656:G:OP2	17:P:37:ARG:HD2	2.11	0.49
18:Q:7:LYS:HD3	18:Q:21:VAL:HG21	1.94	0.49
20:S:39:THR:HB	20:S:42:GLU:CG	2.41	0.49
1:A:1887:U:OP1	28:1:21:LYS:HE3	2.12	0.49
1:A:1127:C:H2'	1:A:1128:U:H5'	1.93	0.49
1:A:734:U:O2'	1:A:737:A:N6	2.45	0.49
1:A:820:G:O2'	1:A:856:G:H4'	2.12	0.49
1:A:821:U:H2'	1:A:822:C:C6	2.47	0.49
1:A:883:U:O2	1:A:883:U:C2'	2.60	0.49
1:A:922:A:N7	1:A:2281:C:H5'	2.27	0.49
6:E:246:ARG:CB	6:E:246:ARG:HH11	2.18	0.49
19:R:24:SER:O	38:R:2847:HOH:O	2.19	0.49
23:V:39:ASN:ND2	23:V:44:ARG:HH11	2.10	0.49
1:A:1495:C:H1'	1:A:1573:A:H1'	1.94	0.49
1:A:2453:G:H5'	38:A:4173:HOH:O	2.11	0.49
2:B:3031:C:H1'	38:B:8392:HOH:O	2.11	0.49
8:G:116:THR:HG22	8:G:151:LEU:HD22	1.93	0.49
10:I:63:ARG:N	38:I:2569:HOH:O	2.45	0.49
11:J:59:ASN:ND2	11:J:59:ASN:N	2.56	0.49
15:N:122:GLU:HB2	15:N:126:HIS:O	2.12	0.49
1:A:1015:C:H2'	1:A:1016:U:H6	1.75	0.49
1:A:484:A:N1	1:A:506:G:H4'	2.28	0.49
1:A:61:G:OP1	30:3:17:GLN:HG2	2.12	0.49
1:A:920:C:H4'	1:A:921:G:C2	2.47	0.49
6:E:162:VAL:CG1	6:E:192:ILE:HD11	2.42	0.49
12:K:39:VAL:HG12	12:K:40:ASN:ND2	2.26	0.49
12:K:52:GLN:HG3	12:K:53:ILE:N	2.28	0.49
14:M:143:THR:HG22	14:M:144:ASP:H	1.77	0.49
20:S:119:VAL:HG21	20:S:142:ASP:CG	2.32	0.49
26:Y:36:HIS:CE1	26:Y:40:HIS:CD2	3.01	0.49
1:A:1116:U:H3	1:A:1246:A:N6	2.00	0.49
1:A:1160:G:HO2'	1:A:1190:G:H8	1.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1762:C:H4'	38:A:4138:HOH:O	2.11	0.49
1:A:1778:A:H2'	1:A:1779:A:H5'	1.94	0.49
1:A:1819:G:H5'	38:A:5281:HOH:O	2.12	0.49
1:A:2004:U:H2'	1:A:2004:U:O2	2.11	0.49
1:A:2123:A:H3'	1:A:2124:G:H8	1.77	0.49
1:A:2419:U:H5''	1:A:2420:G:C5'	2.41	0.49
1:A:2505:G:C2'	1:A:2506:A:H5'	2.42	0.49
1:A:921:G:H4'	1:A:924:G:C6	2.47	0.49
4:C:57:ALA:HA	4:C:67:LEU:HD23	1.94	0.49
15:N:52:LEU:HD13	15:N:116:ASN:CB	2.42	0.49
1:A:251:C:H1'	15:N:58:GLN:HE22	1.76	0.49
21:T:29:ASP:OD2	21:T:31:ARG:NH1	2.46	0.49
29:2:21:ARG:HD2	29:2:39:PHE:HB2	1.94	0.49
31:4:62:THR:HB	38:4:8549:HOH:O	2.11	0.49
31:4:84:ARG:HB3	38:4:8549:HOH:O	2.11	0.49
1:A:1132:A:N6	1:A:1229:C:H2'	2.28	0.49
1:A:283:U:H5''	1:A:284:C:OP2	2.13	0.49
5:D:2:GLN:CD	38:D:8622:HOH:O	2.50	0.49
6:E:118:THR:HG23	38:E:8305:HOH:O	2.12	0.49
9:H:6:PHE:CD1	9:H:6:PHE:O	2.66	0.49
9:H:13:GLU:OE2	9:H:78:GLU:HG2	2.12	0.49
12:K:142:ASN:O	12:K:144:THR:N	2.45	0.49
12:K:74:ARG:NH1	12:K:76:ASP:HB2	2.27	0.49
38:A:9103:HOH:O	15:N:165:SER:HB3	2.12	0.49
15:N:95:LYS:HG2	15:N:99:ARG:HB3	1.94	0.49
17:P:77:ALA:HA	17:P:96:VAL:O	2.13	0.49
21:T:57:THR:C	21:T:59:ASP:H	2.15	0.49
1:A:1125:U:H2'	1:A:1126:C:H5'	1.95	0.49
1:A:1189:A:H1'	1:A:1209:C:C1'	2.43	0.49
1:A:1883:U:O2'	1:A:1884:G:H5'	2.13	0.49
1:A:219:G:O5'	1:A:220:C:H5''	2.13	0.49
1:A:228:C:H2'	1:A:229:G:H5'	1.95	0.49
1:A:2712:G:H5'	38:L:4183:HOH:O	2.13	0.49
1:A:500:G:H21	20:S:98:ASN:HD21	1.60	0.49
6:E:141:SER:HB3	38:E:8421:HOH:O	2.13	0.49
8:G:43:ASP:HA	38:G:5864:HOH:O	2.12	0.49
12:K:79:PHE:HB3	12:K:103:VAL:HG11	1.94	0.49
16:O:34:LEU:HD13	16:O:47:LEU:HD21	1.94	0.49
23:V:52:THR:HG22	23:V:54:THR:HB	1.95	0.49
25:X:6:GLN:CB	25:X:26:ILE:HD12	2.38	0.49
29:2:17:THR:N	29:2:27:TYR:O	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:C:C2'	1:A:542:A:C5'	2.88	0.49
1:A:553:G:O4'	1:A:1325:G:H5'	2.13	0.49
5:D:304:PRO:HD2	5:D:307:ARG:HD2	1.95	0.49
7:F:35:ALA:HB1	38:F:3279:HOH:O	2.12	0.49
16:O:170:GLU:O	16:O:174:GLU:HG3	2.13	0.49
20:S:111:ILE:HG23	20:S:145:LEU:HD11	1.95	0.49
23:V:35:LYS:NZ	38:V:6621:HOH:O	2.39	0.49
25:X:139:GLY:O	25:X:141:HIS:HD2	1.95	0.49
25:X:3:ALA:O	25:X:54:PHE:HA	2.12	0.49
28:1:11:THR:OG1	28:1:23:ARG:HB2	2.13	0.49
1:A:1164:U:C4'	1:A:1165:G:OP1	2.54	0.49
1:A:1535:G:H2'	1:A:1536:C:C6	2.48	0.49
1:A:1651:C:OP1	38:A:4986:HOH:O	2.20	0.49
1:A:2262:C:O5'	1:A:2262:C:H6	1.95	0.49
1:A:2815:G:N7	12:K:80:LYS:NZ	2.61	0.49
1:A:834:G:H4'	1:A:835:U:OP2	2.13	0.49
6:E:129:HIS:CE1	6:E:231:ARG:HA	2.48	0.49
14:M:65:ASP:CG	14:M:111:ALA:HB3	2.33	0.49
15:N:157:LEU:HB3	15:N:160:PHE:HD1	1.76	0.49
1:A:1813:U:O2'	18:Q:81:LYS:HE3	2.13	0.49
29:2:26:SER:HB3	29:2:35:SER:OG	2.11	0.49
30:3:48:ASP:O	30:3:49:GLU:HB2	2.13	0.49
31:4:73:GLU:HB3	38:4:8559:HOH:O	2.12	0.49
1:A:1218:U:H2'	1:A:1219:U:C6	2.48	0.49
1:A:1299:G:N2	38:A:4165:HOH:O	2.46	0.49
1:A:314:G:N2	1:A:316:A:H3'	2.27	0.49
1:A:558:C:C2'	1:A:559:U:C5'	2.91	0.49
4:C:36:ASP:HA	4:C:83:GLY:HA3	1.95	0.49
38:A:6913:HOH:O	6:E:188:ARG:HD2	2.11	0.49
8:G:80:TRP:O	8:G:134:SER:HA	2.12	0.49
10:I:20:VAL:O	10:I:24:VAL:HG23	2.13	0.49
11:J:81:TYR:CD1	11:J:81:TYR:C	2.86	0.49
20:S:114:VAL:HG13	20:S:114:VAL:O	2.13	0.49
27:Z:144:ARG:NH2	38:Z:8616:HOH:O	2.45	0.49
1:A:1735:C:O2'	1:A:1736:A:H5'	2.13	0.48
1:A:401:C:C5'	38:A:5258:HOH:O	2.61	0.48
1:A:65:C:O2'	1:A:66:G:H5'	2.13	0.48
5:D:108:GLU:HB3	5:D:111:ARG:HD2	1.94	0.48
5:D:44:TYR:OH	5:D:148:PRO:HG3	2.13	0.48
8:G:20:ILE:HD11	8:G:33:LEU:HD12	1.93	0.48
15:N:77:PHE:HD2	38:N:8526:HOH:O	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:154:LEU:O	16:O:155:GLU:CB	2.61	0.48
16:O:18:THR:HA	38:O:8525:HOH:O	2.12	0.48
23:V:31:PHE:CG	23:V:37:GLU:HG2	2.48	0.48
25:X:6:GLN:HA	25:X:52:VAL:HG23	1.93	0.48
31:4:42:ARG:HH11	31:4:42:ARG:HG3	1.78	0.48
1:A:1733:A:H4'	5:D:212:GLN:HA	1.94	0.48
1:A:2010:A:H2'	38:A:5418:HOH:O	2.12	0.48
1:A:2053:G:OP1	20:S:138:SER:OG	2.27	0.48
1:A:2251:G:H2'	1:A:2252:A:C8	2.49	0.48
1:A:2559:C:H4'	38:A:6714:HOH:O	2.13	0.48
1:A:278:A:H2'	1:A:279:C:O4'	2.14	0.48
1:A:926:A:O2'	14:M:41:HIS:HD2	1.96	0.48
2:B:3025:G:N2	38:B:8512:HOH:O	2.45	0.48
5:D:177:HIS:O	5:D:181:ILE:HG13	2.13	0.48
8:G:132:THR:HG23	8:G:132:THR:O	2.12	0.48
9:H:47:LEU:HD22	9:H:108:LEU:CD1	2.44	0.48
13:L:86:THR:HG22	13:L:87:ARG:N	2.29	0.48
14:M:101:ASP:C	14:M:103:ALA:H	2.15	0.48
14:M:143:THR:CG2	14:M:144:ASP:H	2.26	0.48
25:X:122:ARG:HH22	25:X:154:ARG:C	2.17	0.48
28:1:77:LYS:HA	28:1:80:MET:CE	2.43	0.48
1:A:1164:U:O4'	1:A:1165:G:OP1	2.31	0.48
1:A:1166:A:H61	1:A:1180:U:H3	1.60	0.48
1:A:1494:A:H1'	1:A:1495:C:C6	2.48	0.48
1:A:2542:C:H5''	1:A:2608:C:N4	2.27	0.48
5:D:148:PRO:HB2	5:D:156:LYS:O	2.13	0.48
7:F:154:LYS:H	7:F:154:LYS:CD	2.19	0.48
7:F:35:ALA:O	7:F:37:ALA:N	2.46	0.48
7:F:62:ASP:HA	38:F:4233:HOH:O	2.13	0.48
7:F:49:PRO:HA	7:F:73:VAL:HG22	1.95	0.48
11:J:48:LEU:HD13	11:J:146:TRP:HB3	1.95	0.48
11:J:75:SER:HB3	11:J:79:ALA:HB1	1.95	0.48
28:1:56:MET:HA	28:1:62:TYR:O	2.14	0.48
31:4:11:CYS:HB2	31:4:20:HIS:CE1	2.48	0.48
1:A:1119:G:H2'	12:K:52:GLN:HE22	1.77	0.48
1:A:1706:G:C5	1:A:1707:G:C6	3.02	0.48
1:A:2620:U:H1'	38:A:6629:HOH:O	2.13	0.48
1:A:2906:A:H5'	1:A:2907:C:O4'	2.13	0.48
1:A:338:C:H4'	6:E:174:ILE:HD12	1.95	0.48
5:D:251:VAL:HG23	5:D:252:PRO:HD2	1.95	0.48
7:F:36:ASN:HA	38:F:7500:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:154:ARG:HD3	38:N:8646:HOH:O	2.12	0.48
7:F:146:LYS:HZ3	16:O:107:ASN:HD21	1.58	0.48
16:O:155:GLU:O	16:O:156:GLU:HG3	2.14	0.48
16:O:32:PRO:HD2	16:O:99:GLU:O	2.14	0.48
19:R:32:GLU:HA	19:R:71:TYR:OH	2.13	0.48
27:Z:189:ASN:HA	27:Z:217:ILE:HD11	1.95	0.48
1:A:107:U:H2'	1:A:108:U:H5'	1.96	0.48
1:A:870:G:C3'	1:A:871:G:H5''	2.43	0.48
2:B:3054:A:O2'	2:B:3055:U:H5'	2.13	0.48
7:F:86:THR:C	7:F:89:PRO:HD2	2.33	0.48
12:K:107:ASN:C	12:K:107:ASN:HD22	2.17	0.48
38:A:9264:HOH:O	14:M:41:HIS:HE1	1.96	0.48
7:F:146:LYS:HZ1	16:O:107:ASN:HD21	1.59	0.48
22:U:24:ARG:NH2	22:U:39:ASN:HD22	2.10	0.48
23:V:13:ILE:HG12	23:V:32:CYS:HB2	1.95	0.48
26:Y:76:ARG:O	26:Y:77:PHE:HB3	2.12	0.48
30:3:40:ARG:HG3	30:3:45:ASN:CB	2.44	0.48
1:A:1116:U:O2'	1:A:1118:A:C2	2.57	0.48
1:A:1120:U:H5'	1:A:1121:G:OP2	2.13	0.48
1:A:1503:U:H2'	1:A:1504:A:O4'	2.14	0.48
1:A:1574:C:H6	1:A:1574:C:O5'	1.96	0.48
1:A:2679:G:H2'	1:A:2681:A:OP2	2.13	0.48
1:A:488:U:C2'	38:A:3497:HOH:O	2.57	0.48
6:E:54:LEU:HD21	6:E:87:ARG:HD2	1.95	0.48
38:A:7167:HOH:O	6:E:94:THR:HG21	2.14	0.48
13:L:55:VAL:CG1	13:L:56:SER:N	2.77	0.48
16:O:182:GLY:O	16:O:183:ASP:O	2.31	0.48
18:Q:3:LEU:HA	18:Q:6:GLN:OE1	2.13	0.48
22:U:75:GLU:O	22:U:76:ASP:HB2	2.13	0.48
38:A:6603:HOH:O	29:2:1:THR:HB	2.12	0.48
1:A:1687:C:O2	29:2:9:GLY:HA2	2.14	0.48
1:A:221:G:H2'	1:A:222:A:C8	2.48	0.48
1:A:2720:C:O2	13:L:87:ARG:NH2	2.46	0.48
5:D:156:LYS:HE3	38:D:8630:HOH:O	2.13	0.48
5:D:320:GLN:HG3	5:D:321:PRO:CD	2.43	0.48
6:E:19:PRO:HG2	6:E:22:PHE:CD1	2.49	0.48
12:K:39:VAL:CG1	12:K:107:ASN:HB2	2.42	0.48
13:L:82:ARG:NH2	13:L:115:ARG:HG2	2.29	0.48
15:N:115:LEU:HD13	15:N:116:ASN:HB2	1.96	0.48
15:N:38:VAL:C	15:N:63:VAL:HG13	2.34	0.48
20:S:39:THR:O	20:S:40:ALA:C	2.50	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A:6862:HOH:O	22:U:2:LYS:HE2	2.13	0.48
25:X:126:ASP:HB3	25:X:135:GLY:O	2.14	0.48
27:Z:107:PRO:HB3	27:Z:182:PHE:CE2	2.49	0.48
3:5:75:C:N4	36:5:76:PPU:H102	2.28	0.48
1:A:1211:G:O2'	1:A:1212:C:H5'	2.13	0.48
1:A:1269:G:H2'	1:A:1270:U:C6	2.49	0.48
1:A:1434:A:H2'	1:A:1436:C:C5	2.49	0.48
1:A:1562:C:H2'	1:A:1562:C:O2	2.14	0.48
1:A:1788:U:C2	1:A:1805:G:N2	2.81	0.48
1:A:2256:G:O2'	1:A:2257:G:H5'	2.13	0.48
1:A:2428:G:C6	1:A:2464:C:H1'	2.48	0.48
1:A:2472:C:O2'	1:A:2634:G:H4'	2.12	0.48
1:A:420:U:H2'	1:A:421:C:C6	2.48	0.48
5:D:24:PRO:CG	5:D:204:GLY:HA2	2.44	0.48
5:D:27:ASN:HB3	38:D:8628:HOH:O	2.12	0.48
11:J:139:ASP:H	11:J:140:PRO:HD3	1.73	0.48
12:K:107:ASN:HD22	12:K:109:TYR:H	1.59	0.48
16:O:67:ALA:HA	16:O:71:TRP:HB3	1.96	0.48
18:Q:7:LYS:CD	18:Q:21:VAL:CG2	2.92	0.48
24:W:56:ILE:O	24:W:60:GLN:HG3	2.12	0.48
1:A:1543:G:N1	1:A:1641:A:OP2	2.36	0.48
1:A:1819:G:H2'	1:A:1820:G:C4'	2.44	0.48
1:A:2089:A:C2'	1:A:2090:G:H5'	2.44	0.48
1:A:1006:A:N1	1:A:2311:A:H1'	2.29	0.48
1:A:283:U:H5	1:A:284:C:N4	2.11	0.48
1:A:60:A:C2	1:A:61:G:C8	3.02	0.48
5:D:307:ARG:HH11	5:D:307:ARG:CB	2.26	0.48
5:D:55:ASN:HB3	5:D:64:GLY:N	2.28	0.48
7:F:159:PRO:O	7:F:163:VAL:HG23	2.14	0.48
8:G:11:VAL:CG1	8:G:12:ASP:H	2.27	0.48
13:L:18:ILE:HG22	13:L:93:ASN:HB2	1.96	0.48
15:N:67:ILE:HG21	15:N:97:ILE:HG23	1.96	0.48
16:O:22:GLN:HG2	16:O:26:LEU:HD22	1.94	0.48
25:X:13:MET:HE3	25:X:17:ILE:HG22	1.95	0.48
1:A:128:A:C3'	1:A:128:A:C8	2.97	0.48
1:A:1525:G:H5'	1:A:1526:A:OP2	2.14	0.48
1:A:422:G:C6	1:A:2446:G:C6	3.02	0.48
1:A:2729:C:O2'	1:A:2730:G:H5'	2.14	0.48
1:A:2768:A:O2'	1:A:2769:C:H5'	2.14	0.48
4:C:88:ILE:CD1	4:C:100:PRO:HD3	2.43	0.48
4:C:69:LEU:CD2	4:C:120:ARG:HB3	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:76:THR:N	5:D:77:PRO:HD3	2.28	0.48
1:A:1308:A:O4'	6:E:226:GLY:HA3	2.14	0.48
15:N:81:ARG:HB3	15:N:86:MET:HG2	1.96	0.48
17:P:25:VAL:HG23	17:P:26:TRP:H	1.79	0.48
25:X:21:LEU:HB3	25:X:26:ILE:HG12	1.95	0.48
29:2:25:LYS:HD2	30:3:48:ASP:HA	1.95	0.47
1:A:1878:G:O2'	1:A:1879:U:C6	2.66	0.47
1:A:2281:C:O2'	1:A:2282:U:H5'	2.14	0.47
1:A:2456:A:H5'	38:A:5164:HOH:O	2.13	0.47
1:A:282:C:H2'	1:A:283:U:O4'	2.13	0.47
38:A:8728:HOH:O	4:C:11:ARG:HD3	2.13	0.47
6:E:133:ARG:NH2	38:E:8431:HOH:O	2.46	0.47
8:G:18:LEU:HD13	8:G:34:TRP:CG	2.48	0.47
18:Q:18:LYS:O	18:Q:21:VAL:HG22	2.13	0.47
18:Q:27:ARG:HA	38:Q:177:HOH:O	2.13	0.47
26:Y:25:ARG:HG2	38:Y:5356:HOH:O	2.12	0.47
1:A:1666:C:C2'	1:A:1667:A:C5'	2.92	0.47
1:A:195:C:H2'	1:A:196:G:H5'	1.96	0.47
1:A:2120:U:H2'	1:A:2121:G:O4'	2.14	0.47
1:A:2900:G:H2'	1:A:2901:C:O4'	2.14	0.47
1:A:639:A:H2'	1:A:640:G:H8	1.77	0.47
5:D:221:GLN:HE22	13:L:42:ASN:ND2	2.11	0.47
5:D:54:VAL:HB	38:D:8613:HOH:O	2.14	0.47
6:E:61:PHE:HB3	38:E:8450:HOH:O	2.13	0.47
13:L:9:THR:O	13:L:10:GLN:C	2.52	0.47
38:A:9041:HOH:O	18:Q:81:LYS:HG2	2.13	0.47
20:S:113:HIS:O	20:S:145:LEU:HD12	2.13	0.47
23:V:17:THR:HG22	23:V:18:GLY:N	2.28	0.47
25:X:64:THR:O	25:X:68:THR:HG22	2.14	0.47
1:A:1205:U:C2'	1:A:1206:U:C5'	2.92	0.47
1:A:1377:C:C6	1:A:1377:C:H5'	2.44	0.47
1:A:2300:A:H4'	1:A:2301:A:O5'	2.14	0.47
1:A:2445:U:H2'	1:A:2446:G:C8	2.49	0.47
4:C:192:VAL:O	4:C:192:VAL:CG1	2.62	0.47
5:D:85:ARG:NH2	5:D:99:GLU:OE2	2.40	0.47
6:E:162:VAL:CG1	6:E:162:VAL:O	2.61	0.47
38:A:4446:HOH:O	11:J:57:ARG:HG3	2.14	0.47
16:O:24:LEU:O	16:O:28:LYS:HG2	2.14	0.47
1:A:2243:C:HO2'	1:A:2244:A:H8	1.61	0.47
1:A:240:C:O2	1:A:240:C:H2'	2.15	0.47
1:A:694:A:H2'	1:A:695:C:H5'	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:132:ASP:OD1	4:C:133:ARG:N	2.47	0.47
5:D:16:ARG:NE	38:D:8553:HOH:O	2.25	0.47
8:G:107:PHE:CZ	8:G:108:LEU:HD13	2.49	0.47
1:A:1515:A:H2'	1:A:1516:C:C6	2.49	0.47
1:A:2676:C:H4'	12:K:70:PHE:HE1	1.76	0.47
1:A:2715:G:O2'	5:D:262:ARG:HD2	2.14	0.47
1:A:2748:G:C5'	38:A:6999:HOH:O	2.58	0.47
1:A:432:G:O2'	1:A:433:C:H5'	2.13	0.47
1:A:39:G:N2	1:A:444:C:C2	2.83	0.47
4:C:165:THR:O	4:C:165:THR:HG22	2.13	0.47
38:A:9067:HOH:O	5:D:267:LYS:HD3	2.14	0.47
6:E:20:ASP:O	6:E:23:GLU:HB2	2.15	0.47
18:Q:10:ALA:O	18:Q:13:VAL:HG12	2.14	0.47
26:Y:74:ALA:CB	26:Y:85:VAL:HG22	2.45	0.47
27:Z:203:VAL:HG12	27:Z:228:VAL:HG22	1.96	0.47
1:A:1494:A:C4	1:A:1495:C:C5	3.03	0.47
1:A:169:A:HO2'	1:A:170:U:H6	1.62	0.47
1:A:2010:A:C2'	38:A:5418:HOH:O	2.63	0.47
1:A:2781:U:H2'	1:A:2782:G:C5'	2.45	0.47
1:A:2894:C:O2'	1:A:2895:C:H5'	2.14	0.47
1:A:398:U:H2'	1:A:399:C:C6	2.50	0.47
1:A:816:G:C6	1:A:817:G:N1	2.82	0.47
2:B:3042:C:O2	7:F:76:ARG:NH1	2.47	0.47
4:C:96:LEU:HD22	4:C:128:LEU:HD13	1.95	0.47
23:V:38:ASN:O	23:V:42:LEU:HG	2.15	0.47
27:Z:154:ARG:NH1	27:Z:155:ARG:HG3	2.30	0.47
28:1:47:LEU:HD13	28:1:64:ILE:HD11	1.97	0.47
1:A:1072:G:OP2	27:Z:154:ARG:NH2	2.41	0.47
1:A:1268:C:H2'	1:A:1269:G:H8	1.79	0.47
1:A:2697:A:H2'	1:A:2698:G:O4'	2.14	0.47
6:E:233:THR:CG2	6:E:234:VAL:N	2.78	0.47
6:E:25:PRO:HD2	38:E:8434:HOH:O	2.14	0.47
14:M:97:VAL:HG12	14:M:98:GLU:O	2.14	0.47
15:N:69:LYS:O	15:N:73:ARG:CZ	2.62	0.47
18:Q:11:ALA:HB2	18:Q:18:LYS:HA	1.97	0.47
25:X:88:THR:HG23	25:X:110:GLN:HB3	1.97	0.47
26:Y:85:VAL:HG12	26:Y:86:GLU:N	2.29	0.47
1:A:154:C:H2'	1:A:155:C:C6	2.49	0.47
1:A:2407:G:O2'	1:A:2408:A:H5'	2.14	0.47
1:A:1565:C:O4'	1:A:2738:G:H1'	2.15	0.47
1:A:654:A:OP2	17:P:38:ARG:HD3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:39:ALA:HB3	4:C:61:GLU:OE2	2.15	0.47
5:D:41:PHE:CZ	5:D:79:MET:HG3	2.49	0.47
6:E:1:MET:HG2	6:E:2:GLN:NE2	2.30	0.47
9:H:60:VAL:O	9:H:61:MET:C	2.52	0.47
13:L:118:ALA:C	13:L:120:ARG:H	2.18	0.47
29:2:18:LYS:HB2	30:3:49:GLU:HG2	1.97	0.47
1:A:1189:A:H1'	1:A:1209:C:H1'	1.97	0.47
1:A:12:U:H2'	1:A:13:G:H5'	1.97	0.47
1:A:2271:G:H2'	1:A:2271:G:N3	2.29	0.47
1:A:2866:U:H4'	1:A:2867:G:H5'	1.97	0.47
1:A:474:C:O3'	6:E:73:LEU:HD21	2.14	0.47
5:D:322:ARG:HB2	38:D:8608:HOH:O	2.14	0.47
5:D:63:GLU:HG3	5:D:63:GLU:O	2.14	0.47
6:E:236:THR:C	38:E:8454:HOH:O	2.52	0.47
9:H:21:GLU:HA	9:H:24:ARG:HE	1.79	0.47
12:K:45:VAL:HG22	12:K:46:ILE:N	2.29	0.47
1:A:926:A:H1'	14:M:38:HIS:O	2.14	0.47
15:N:184:ARG:HB2	15:N:184:ARG:CZ	2.45	0.47
15:N:46:LEU:HB2	38:N:8607:HOH:O	2.15	0.47
16:O:73:ALA:HB1	16:O:74:PRO:HD2	1.96	0.47
21:T:29:ASP:OD1	21:T:31:ARG:NH1	2.47	0.47
23:V:47:ARG:CG	38:V:4381:HOH:O	2.56	0.47
25:X:122:ARG:HH11	25:X:122:ARG:CG	2.24	0.47
25:X:21:LEU:HD13	25:X:26:ILE:HD11	1.97	0.47
29:2:21:ARG:HD3	29:2:45:ARG:NE	2.30	0.47
1:A:1189:A:H1'	1:A:1209:C:O4'	2.15	0.47
1:A:1342:C:O2'	1:A:1343:C:H5'	2.15	0.47
1:A:2016:U:H6	1:A:2016:U:O5'	1.97	0.47
1:A:331:A:C6	1:A:332:G:C4	3.02	0.47
1:A:383:A:C6	1:A:407:A:C8	3.03	0.47
1:A:929:A:O5'	1:A:929:A:H8	1.98	0.47
7:F:29:HIS:C	38:F:5858:HOH:O	2.53	0.47
16:O:184:ILE:HG22	16:O:185:GLU:N	2.30	0.47
18:Q:115:SER:C	18:Q:117:SER:H	2.18	0.47
20:S:119:VAL:CG2	20:S:142:ASP:HB2	2.44	0.47
26:Y:75:ALA:O	26:Y:83:ALA:HA	2.15	0.47
1:A:1119:G:N2	1:A:1246:A:H2	2.08	0.47
1:A:2104:C:O2	1:A:2486:A:C2	2.68	0.47
1:A:2346:C:H4'	7:F:52:THR:HG22	1.97	0.47
1:A:2781:U:C2'	1:A:2782:G:H5'	2.45	0.47
1:A:392:U:O2'	15:N:182:LYS:HE2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:731:U:H2'	1:A:732:C:C6	2.50	0.47
1:A:84:G:O2'	1:A:85:C:H5'	2.15	0.47
4:C:135:VAL:HG21	4:C:147:ARG:CZ	2.45	0.47
6:E:35:VAL:HG21	6:E:227:GLY:HA2	1.95	0.47
6:E:7:ASP:OD1	6:E:11:ASN:O	2.33	0.47
11:J:162:SER:CB	11:J:163:PRO:CD	2.80	0.47
1:A:2834:G:OP1	26:Y:39:LYS:HE2	2.15	0.47
27:Z:235:GLU:CD	27:Z:235:GLU:N	2.68	0.47
1:A:797:A:H4'	28:I:10:ARG:N	2.30	0.46
1:A:1845:A:OP2	4:C:190:ARG:NH1	2.45	0.46
1:A:544:G:H2'	1:A:545:G:C5'	2.45	0.46
4:C:9:ARG:HG2	4:C:16:PHE:CD2	2.50	0.46
5:D:7:ARG:HH11	5:D:7:ARG:CG	2.25	0.46
5:D:87:TYR:O	5:D:138:GLY:N	2.42	0.46
6:E:65:ARG:HG3	6:E:67:GLN:HB2	1.98	0.46
9:H:37:THR:O	9:H:41:GLU:HG3	2.15	0.46
10:I:16:LYS:O	10:I:20:VAL:HG23	2.15	0.46
15:N:47:ASP:CG	15:N:48:ARG:N	2.68	0.46
17:P:96:VAL:HG13	17:P:100:GLN:HB2	1.97	0.46
18:Q:143:ALA:HA	38:Q:197:HOH:O	2.15	0.46
18:Q:37:ARG:O	18:Q:40:VAL:HB	2.15	0.46
25:X:88:THR:CG2	25:X:110:GLN:NE2	2.72	0.46
31:4:74:CYS:SG	31:4:76:LYS:CG	3.03	0.46
1:A:1007:A:H2'	11:J:19:TYR:CZ	2.50	0.46
1:A:1249:U:H2'	1:A:1250:C:C6	2.51	0.46
1:A:1331:A:OP2	27:Z:142:SER:OG	2.25	0.46
1:A:171:C:C2'	1:A:172:U:H5'	2.45	0.46
1:A:1730:G:H4'	1:A:1731:C:O5'	2.15	0.46
1:A:175:G:H2'	15:N:192:ALA:HB3	1.96	0.46
1:A:2247:C:H5''	38:A:6802:HOH:O	2.15	0.46
1:A:2279:G:OP1	38:A:4571:HOH:O	2.21	0.46
1:A:288:A:H2'	1:A:289:G:C8	2.50	0.46
1:A:383:A:C2	1:A:407:A:C4	3.03	0.46
2:B:3041:C:O4'	7:F:50:VAL:HG23	2.16	0.46
2:B:3049:G:H2'	2:B:3050:G:O4'	2.15	0.46
4:C:211:LYS:HD3	38:C:8625:HOH:O	2.14	0.46
7:F:103:ASN:ND2	7:F:134:LEU:H	2.12	0.46
8:G:22:VAL:O	8:G:28:SER:HA	2.15	0.46
9:H:50:VAL:CG1	9:H:60:VAL:HG11	2.45	0.46
12:K:19:MET:HE1	12:K:132:LEU:CD1	2.45	0.46
1:A:188:C:H5''	15:N:163:LEU:HD21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:5:ARG:HG3	19:R:18:PRO:CB	2.45	0.46
22:U:71:VAL:HG12	22:U:72:ILE:N	2.30	0.46
1:A:1304:U:H2'	1:A:1305:C:C6	2.51	0.46
1:A:1684:A:O2'	1:A:1685:A:H5''	2.15	0.46
1:A:177:A:H2'	1:A:178:U:O4'	2.16	0.46
1:A:2451:G:O6	38:A:9891:HOH:O	2.19	0.46
1:A:407:A:H2'	1:A:408:A:C8	2.51	0.46
2:B:3092:G:C6	2:B:3093:A:C6	3.04	0.46
11:J:95:GLU:HB3	11:J:119:VAL:HG11	1.96	0.46
11:J:140:PRO:HA	11:J:142:VAL:HG12	1.98	0.46
16:O:93:GLN:HG2	38:O:8554:HOH:O	2.13	0.46
31:4:11:CYS:HB2	31:4:20:HIS:HE1	1.80	0.46
1:A:2428:G:N7	38:A:3276:HOH:O	2.46	0.46
1:A:281:U:O2'	1:A:282:C:H5'	2.16	0.46
2:B:3064:C:H2'	2:B:3065:A:H5'	1.98	0.46
5:D:24:PRO:HG2	5:D:204:GLY:HA2	1.96	0.46
8:G:10:ASP:HA	38:G:3707:HOH:O	2.15	0.46
11:J:14:TYR:N	11:J:91:HIS:CE1	2.81	0.46
17:P:47:ARG:NH1	17:P:47:ARG:HG3	2.27	0.46
29:2:29:THR:O	29:2:32:LYS:CE	2.64	0.46
1:A:1342:C:C2'	1:A:1343:C:H5'	2.46	0.46
1:A:1504:A:O2'	1:A:1506:U:OP2	2.31	0.46
1:A:1713:G:C1'	38:A:4547:HOH:O	2.60	0.46
1:A:1776:A:C8	1:A:1778:A:O4'	2.68	0.46
1:A:2265:U:H2'	1:A:2266:A:H8	1.81	0.46
5:D:310:ARG:HD2	38:D:8648:HOH:O	2.15	0.46
11:J:113:ALA:N	11:J:114:PRO:HD3	2.31	0.46
11:J:157:ILE:CG2	11:J:158:ASN:N	2.78	0.46
1:A:952:G:OP1	19:R:42:LYS:HE2	2.15	0.46
1:A:317:A:H5''	22:U:52:ARG:HD2	1.97	0.46
25:X:35:VAL:HA	25:X:36:PRO:HD3	1.78	0.46
1:A:1161:A:O5'	1:A:1161:A:H8	1.99	0.46
1:A:1850:U:H2'	1:A:1851:G:H8	1.80	0.46
1:A:2121:G:C2'	1:A:2122:C:H5'	2.44	0.46
1:A:2840:A:OP1	5:D:211:THR:HG23	2.16	0.46
7:F:99:ASP:HB3	7:F:103:ASN:H	1.80	0.46
7:F:169:THR:C	7:F:170:TYR:HD1	2.18	0.46
16:O:58:LEU:CD1	16:O:58:LEU:N	2.78	0.46
17:P:32:ARG:NE	38:P:3360:HOH:O	2.48	0.46
30:3:18:ASN:ND2	30:3:40:ARG:H	2.14	0.46
1:A:1930:A:H2'	1:A:1931:A:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2769:C:O2'	1:A:2770:G:H5'	2.16	0.46
1:A:95:A:H5''	1:A:97:G:O4'	2.16	0.46
7:F:57:THR:HG23	7:F:63:ILE:CB	2.45	0.46
15:N:153:THR:O	15:N:156:ARG:HG3	2.15	0.46
20:S:39:THR:CB	20:S:42:GLU:HG3	2.42	0.46
23:V:9:CYS:HG	23:V:11:THR:HG23	1.80	0.46
1:A:1754:A:H2'	1:A:1755:A:O4'	2.15	0.46
1:A:2028:U:H2'	1:A:2029:C:H6	1.79	0.46
1:A:2432:C:H4'	31:4:36:ILE:HG12	1.97	0.46
1:A:2443:C:H3'	38:A:9970:HOH:O	2.16	0.46
1:A:169:A:C6	1:A:2469:A:C6	3.04	0.46
1:A:660:A:H4'	1:A:661:G:O5'	2.16	0.46
1:A:815:U:C4	1:A:816:G:C6	3.03	0.46
7:F:23:VAL:CG2	7:F:23:VAL:O	2.63	0.46
11:J:157:ILE:HG22	11:J:158:ASN:N	2.30	0.46
11:J:43:PRO:HD2	11:J:137:ASN:HA	1.97	0.46
11:J:72:VAL:HG11	11:J:81:TYR:CZ	2.51	0.46
15:N:114:VAL:HG21	15:N:159:THR:CG2	2.46	0.46
38:A:5155:HOH:O	16:O:21:HIS:HE1	1.99	0.46
28:1:10:ARG:HA	38:1:8413:HOH:O	2.16	0.46
30:3:40:ARG:HA	30:3:45:ASN:ND2	2.30	0.46
3:5:74:C:H2'	3:5:75:C:C5'	2.46	0.46
1:A:1306:U:OP1	6:E:184:ARG:HD2	2.16	0.46
1:A:2362:A:H2'	1:A:2363:G:C8	2.51	0.46
1:A:2672:C:O2'	1:A:2673:U:H5'	2.16	0.46
1:A:2777:G:O2'	1:A:2778:A:H5'	2.15	0.46
5:D:185:GLY:HA2	38:D:8633:HOH:O	2.16	0.46
5:D:42:ALA:HB3	5:D:79:MET:SD	2.56	0.46
6:E:34:ALA:HB3	6:E:220:THR:HG21	1.98	0.46
7:F:86:THR:HG23	38:F:7477:HOH:O	2.15	0.46
1:A:2781:U:H1'	8:G:139:GLU:OE2	2.15	0.46
15:N:49:ALA:C	15:N:54:TYR:HB3	2.36	0.46
22:U:12:ARG:O	22:U:19:ARG:NH2	2.48	0.46
27:Z:117:LEU:HD12	27:Z:174:VAL:CG1	2.45	0.46
1:A:392:U:H4'	15:N:193:LYS:HB3	1.98	0.46
1:A:941:G:O2'	1:A:942:U:H5'	2.16	0.46
38:A:5700:HOH:O	4:C:22:ARG:HG2	2.16	0.46
7:F:95:THR:C	7:F:97:GLN:N	2.67	0.46
9:H:39:SER:HB3	9:H:45:ALA:HB2	1.97	0.46
10:I:12:ILE:O	10:I:13:PRO:C	2.53	0.46
17:P:32:ARG:HE	17:P:35:LYS:HD2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Z:112:GLU:HA	27:Z:112:GLU:OE1	2.16	0.46
27:Z:189:ASN:ND2	27:Z:192:ASP:H	2.13	0.46
30:3:40:ARG:NH1	30:3:40:ARG:HG2	2.30	0.45
1:A:1151:G:OP1	10:I:16:LYS:NZ	2.40	0.45
1:A:1592:G:O2'	1:A:1593:C:O5'	2.34	0.45
1:A:1634:G:H3'	38:A:3386:HOH:O	2.14	0.45
1:A:1644:C:H2'	1:A:1645:U:H6	1.81	0.45
1:A:407:A:H5'	38:A:5485:HOH:O	2.16	0.45
1:A:419:A:C2	1:A:2449:G:N3	2.84	0.45
2:B:3041:C:C6	7:F:50:VAL:HG21	2.51	0.45
6:E:118:THR:CG2	6:E:137:PRO:HB3	2.45	0.45
6:E:218:VAL:HG12	38:E:8429:HOH:O	2.16	0.45
7:F:135:VAL:HG21	7:F:139:TYR:CD1	2.51	0.45
8:G:20:ILE:HD12	8:G:33:LEU:HD12	1.95	0.45
13:L:6:ALA:HB3	13:L:116:GLU:HG2	1.98	0.45
13:L:130:MET:SD	23:V:25:ASP:O	2.73	0.45
15:N:68:ARG:CD	15:N:68:ARG:O	2.63	0.45
21:T:73:ASP:OD1	21:T:75:GLN:HB2	2.16	0.45
22:U:96:VAL:CG1	22:U:97:ARG:N	2.79	0.45
25:X:121:PRO:HA	25:X:153:MET:HG2	1.98	0.45
1:A:1200:A:C4'	38:A:6798:HOH:O	2.64	0.45
1:A:1246:A:O2'	1:A:1247:A:H3'	2.16	0.45
1:A:1667:A:H5'	1:A:1667:A:C8	2.48	0.45
1:A:1902:G:H2'	1:A:1903:U:O4'	2.16	0.45
1:A:2266:A:P	38:A:5323:HOH:O	2.73	0.45
1:A:2785:C:H4'	1:A:2786:G:OP2	2.17	0.45
1:A:541:C:O2'	1:A:542:A:H5''	2.16	0.45
1:A:677:C:H4'	6:E:246:ARG:NH2	2.32	0.45
4:C:101:GLU:HG2	4:C:131:HIS:ND1	2.31	0.45
4:C:112:PRO:HD3	4:C:152:CYS:SG	2.56	0.45
4:C:217:ARG:CG	4:C:217:ARG:HH11	2.29	0.45
5:D:254:GLN:HG2	5:D:255:GLY:N	2.31	0.45
13:L:74:VAL:HG12	13:L:75:ARG:HG3	1.97	0.45
13:L:99:ASP:OD1	13:L:101:ASN:N	2.49	0.45
14:M:104:ASP:HB2	38:M:8580:HOH:O	2.16	0.45
19:R:28:ARG:NH1	38:R:6206:HOH:O	2.43	0.45
25:X:75:GLY:HA3	38:X:5763:HOH:O	2.17	0.45
26:Y:25:ARG:NH1	38:Y:3861:HOH:O	2.49	0.45
27:Z:115:ARG:HG3	35:Z:8517:CL:CL	2.53	0.45
5:D:7:ARG:CD	5:D:9:GLY:O	2.65	0.45
6:E:178:GLN:C	6:E:180:SER:N	2.67	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:70:PHE:O	12:K:70:PHE:CD2	2.69	0.45
38:A:4393:HOH:O	15:N:14:ARG:HB3	2.16	0.45
18:Q:28:GLN:N	38:Q:203:HOH:O	2.50	0.45
27:Z:136:LYS:HE2	27:Z:138:ARG:NH1	2.31	0.45
1:A:1336:U:C2	1:A:1337:A:C8	3.04	0.45
1:A:1351:G:OP1	6:E:96:LYS:NZ	2.39	0.45
1:A:1384:C:H5'	26:Y:30:MET:HG2	1.99	0.45
1:A:1440:U:P	38:A:3954:HOH:O	2.73	0.45
1:A:1609:C:H2'	1:A:1610:G:H8	1.81	0.45
1:A:380:A:H5''	15:N:48:ARG:NH2	2.31	0.45
1:A:451:C:O2'	1:A:452:G:H5'	2.16	0.45
1:A:466:A:H2'	1:A:467:G:O4'	2.16	0.45
1:A:590:A:H2'	1:A:591:A:H5'	1.99	0.45
1:A:603:A:H4'	1:A:604:G:O5'	2.16	0.45
1:A:790:A:H2'	1:A:791:A:O4'	2.16	0.45
7:F:173:GLU:O	7:F:174:VAL:C	2.54	0.45
7:F:58:VAL:CG1	7:F:59:GLY:N	2.78	0.45
7:F:84:LEU:C	7:F:86:THR:H	2.19	0.45
15:N:37:VAL:CG2	15:N:108:LYS:HG3	2.45	0.45
15:N:59:GLY:C	15:N:141:ILE:HD11	2.37	0.45
23:V:9:CYS:SG	23:V:11:THR:N	2.83	0.45
28:1:59:HIS:HA	38:1:8439:HOH:O	2.15	0.45
1:A:1057:A:C6	1:A:1058:A:C6	3.05	0.45
1:A:1279:U:H5''	38:A:9093:HOH:O	2.16	0.45
1:A:2044:G:OP1	26:Y:23:HIS:HE1	2.00	0.45
1:A:628:A:C8	1:A:2071:C:N4	2.85	0.45
1:A:2314:G:O2'	1:A:2315:C:H5'	2.16	0.45
1:A:2353:A:H4'	1:A:2354:A:O5'	2.16	0.45
1:A:291:C:H2'	1:A:292:G:O4'	2.16	0.45
1:A:382:U:C5	1:A:406:G:N2	2.84	0.45
1:A:818:A:O2'	28:1:13:ARG:HD3	2.16	0.45
4:C:153:ARG:CB	4:C:153:ARG:HH11	2.29	0.45
5:D:162:MET:HE2	5:D:310:ARG:HD3	1.98	0.45
1:A:2819:C:O4'	5:D:96:PRO:HB2	2.16	0.45
6:E:235:PHE:HE2	6:E:243:VAL:HG21	1.80	0.45
7:F:25:MET:SD	7:F:40:ILE:HD11	2.56	0.45
7:F:67:ASP:O	7:F:69:ILE:HG13	2.16	0.45
8:G:157:LYS:NZ	38:G:2401:HOH:O	2.49	0.45
10:I:73:ASP:C	38:I:2994:HOH:O	2.54	0.45
15:N:184:ARG:HB2	15:N:184:ARG:NH1	2.32	0.45
25:X:146:ILE:HG23	25:X:150:LEU:CD1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Z:186:ARG:NH1	27:Z:186:ARG:HG2	2.31	0.45
1:A:1225:C:H4'	38:A:8903:HOH:O	2.16	0.45
1:A:1805:G:H2'	1:A:1806:G:H8	1.81	0.45
4:C:8:ARG:NH1	38:C:8558:HOH:O	2.42	0.45
5:D:248:ARG:O	5:D:251:VAL:HG13	2.17	0.45
10:I:64:ASN:N	10:I:64:ASN:ND2	2.64	0.45
12:K:130:VAL:CG1	12:K:131:THR:N	2.79	0.45
13:L:27:ARG:CD	38:L:4747:HOH:O	2.61	0.45
14:M:121:ILE:HG12	14:M:141:GLU:HB2	1.97	0.45
29:2:25:LYS:CG	30:3:49:GLU:H	2.29	0.45
1:A:2050:G:H5''	20:S:80:TYR:O	2.17	0.45
1:A:2385:G:H2'	1:A:2386:U:C6	2.51	0.45
1:A:247:A:C8	1:A:262:A:N6	2.85	0.45
1:A:2670:G:O2'	1:A:2671:U:H5'	2.16	0.45
16:O:25:ARG:HA	16:O:28:LYS:HG3	1.97	0.45
1:A:1677:U:OP2	30:3:8:LYS:NZ	2.50	0.45
1:A:1878:G:C1'	38:A:5581:HOH:O	2.63	0.45
1:A:2116:U:C4	1:A:2271:G:C6	3.05	0.45
1:A:222:A:H2'	1:A:223:G:O4'	2.16	0.45
1:A:2434:A:O3'	31:4:28:GLY:HA3	2.16	0.45
2:B:3055:U:H4'	2:B:3056:A:C8	2.52	0.45
9:H:28:ALA:CB	9:H:99:THR:HG23	2.46	0.45
11:J:86:ARG:NH1	11:J:130:HIS:CD2	2.85	0.45
11:J:6:TYR:HE2	11:J:94:ARG:O	2.00	0.45
14:M:38:HIS:CD2	14:M:39:GLU:HG3	2.51	0.45
16:O:19:ASP:N	38:O:8525:HOH:O	2.15	0.45
17:P:26:TRP:HA	17:P:26:TRP:CE3	2.52	0.45
38:E:8358:HOH:O	17:P:3:THR:HG21	2.17	0.45
1:A:2299:G:O6	19:R:1:PRO:HA	2.16	0.45
25:X:38:THR:HG22	25:X:39:ASP:N	2.32	0.45
28:1:22:ILE:HG22	28:1:23:ARG:N	2.32	0.45
1:A:2432:C:H2'	1:A:2433:A:C8	2.51	0.45
1:A:2468:A:C8	31:4:54:LYS:HE2	2.51	0.45
1:A:2591:C:H2'	1:A:2592:G:O4'	2.17	0.45
1:A:2656:G:O2'	1:A:2657:G:H5'	2.17	0.45
1:A:758:A:H2'	1:A:759:C:O4'	2.17	0.45
2:B:3034:A:H1'	16:O:153:GLN:HE22	1.82	0.45
8:G:16:ASP:O	8:G:17:HIS:HB2	2.17	0.45
11:J:163:PRO:HG2	38:J:8339:HOH:O	2.16	0.45
12:K:6:PHE:HB3	12:K:109:TYR:OH	2.17	0.45
13:L:87:ARG:CZ	38:L:4854:HOH:O	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:140:VAL:CG2	38:M:8562:HOH:O	2.64	0.45
15:N:49:ALA:HB1	15:N:54:TYR:CB	2.47	0.45
2:B:3008:G:O6	16:O:11:ARG:NH1	2.48	0.45
16:O:73:ALA:HB1	16:O:74:PRO:CD	2.47	0.45
17:P:39:THR:HB	38:P:3360:HOH:O	2.16	0.45
1:A:1014:A:H2'	1:A:1015:C:H5'	1.99	0.45
1:A:101:C:H2'	1:A:102:A:H8	1.82	0.45
1:A:1427:A:N6	38:A:6184:HOH:O	2.40	0.45
1:A:1613:C:H2'	1:A:1614:G:O4'	2.17	0.45
1:A:496:G:C6	1:A:498:A:C6	3.05	0.45
1:A:553:G:H5'	38:A:9994:HOH:O	2.15	0.45
1:A:831:U:O2	38:A:3936:HOH:O	2.21	0.45
1:A:92:G:H4'	24:W:44:GLY:HA3	1.98	0.45
4:C:199:HIS:CE1	4:C:225:VAL:HG11	2.52	0.45
5:D:101:TRP:HB2	5:D:119:HIS:CD2	2.52	0.45
5:D:8:LYS:HG3	5:D:220:VAL:HG12	1.98	0.45
5:D:41:PHE:CD1	5:D:79:MET:HE2	2.51	0.45
6:E:192:ILE:CG2	6:E:234:VAL:HG12	2.48	0.45
8:G:116:THR:CG2	8:G:151:LEU:HD22	2.47	0.45
13:L:29:LEU:HB3	13:L:55:VAL:CG1	2.35	0.45
14:M:7:GLN:HB3	14:M:13:HIS:CE1	2.52	0.45
1:A:392:U:C5'	15:N:193:LYS:HB3	2.47	0.45
15:N:69:LYS:HD3	15:N:125:ARG:HA	1.98	0.45
16:O:141:ARG:N	38:O:8566:HOH:O	2.50	0.45
16:O:15:GLU:HB2	16:O:17:ARG:HG3	1.99	0.45
17:P:21:SER:OG	17:P:106:PRO:HB2	2.17	0.45
18:Q:14:LEU:HD13	18:Q:51:ALA:HB2	1.98	0.45
19:R:41:LEU:HB3	19:R:52:PHE:CZ	2.51	0.45
21:T:11:THR:H	21:T:14:ALA:HB3	1.81	0.45
25:X:139:GLY:O	25:X:141:HIS:CD2	2.70	0.45
27:Z:154:ARG:HH12	27:Z:155:ARG:HG3	1.82	0.45
28:1:57:CYS:O	28:1:61:GLY:HA2	2.17	0.44
1:A:1886:A:C2'	38:A:4297:HOH:O	2.65	0.44
1:A:2356:A:H2'	1:A:2357:G:O4'	2.16	0.44
1:A:2435:U:OP1	31:4:28:GLY:HA3	2.16	0.44
1:A:696:C:C2'	1:A:697:G:H5'	2.48	0.44
1:A:821:U:H5''	38:A:9546:HOH:O	2.16	0.44
5:D:238:ASN:ND2	5:D:240:GLY:H	2.14	0.44
5:D:52:VAL:O	5:D:53:LEU:HD12	2.16	0.44
7:F:173:GLU:HG3	7:F:174:VAL:N	2.32	0.44
15:N:35:PRO:CG	15:N:38:VAL:CG2	2.87	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:163:PHE:O	16:O:164:ASP:O	2.34	0.44
38:A:6880:HOH:O	22:U:9:LYS:HD2	2.17	0.44
1:A:2122:C:H3'	38:A:4762:HOH:O	2.17	0.44
1:A:2547:C:H2'	1:A:2548:C:H6	1.81	0.44
1:A:553:G:H2'	1:A:554:G:H5'	1.98	0.44
1:A:876:A:H2'	1:A:876:A:N3	2.32	0.44
4:C:66:ARG:HH11	4:C:66:ARG:HB2	1.80	0.44
6:E:237:GLU:N	38:E:8454:HOH:O	2.50	0.44
11:J:149:ALA:C	11:J:151:MET:H	2.20	0.44
11:J:150:LYS:HE2	38:J:8379:HOH:O	2.16	0.44
16:O:38:LYS:HB2	16:O:38:LYS:HE3	1.76	0.44
16:O:67:ALA:C	16:O:69:TYR:N	2.70	0.44
17:P:14:LEU:CD2	17:P:102:ILE:HD11	2.46	0.44
20:S:39:THR:CG2	20:S:42:GLU:HG3	2.48	0.44
27:Z:144:ARG:NE	38:Z:8616:HOH:O	2.49	0.44
28:1:77:LYS:HA	28:1:80:MET:HE2	1.98	0.44
29:2:29:THR:O	29:2:32:LYS:HE2	2.18	0.44
31:4:7:PHE:HE2	31:4:22:VAL:CG2	2.30	0.44
31:4:7:PHE:CE1	31:4:9:THR:HB	2.52	0.44
1:A:1461:U:H2'	1:A:1462:C:C6	2.51	0.44
1:A:1523:G:C6	1:A:1524:U:O4	2.70	0.44
1:A:1827:G:H2'	1:A:1828:G:C8	2.52	0.44
1:A:1921:A:C6	1:A:1922:A:C2	3.06	0.44
1:A:1970:G:C5'	38:A:6529:HOH:O	2.65	0.44
1:A:584:U:H3'	38:A:5555:HOH:O	2.17	0.44
5:D:258:GLY:N	5:D:260:HIS:CE1	2.78	0.44
5:D:280:VAL:CG1	5:D:281:ASP:N	2.80	0.44
11:J:45:GLN:NE2	11:J:135:TRP:HE1	2.16	0.44
16:O:108:SER:HA	16:O:109:PRO:HD3	1.81	0.44
20:S:125:ARG:HG2	38:S:8541:HOH:O	2.16	0.44
22:U:73:HIS:CD2	22:U:88:PRO:HG3	2.52	0.44
23:V:49:LEU:O	23:V:55:ALA:CB	2.65	0.44
25:X:121:PRO:CA	25:X:153:MET:HG2	2.48	0.44
1:A:1189:A:N3	38:A:7139:HOH:O	2.50	0.44
1:A:2503:A:OP1	11:J:147:ARG:NH2	2.38	0.44
1:A:407:A:C2	1:A:408:A:C4	3.05	0.44
1:A:602:A:O2'	1:A:605:C:H4'	2.17	0.44
1:A:661:G:C4	1:A:686:A:C2	3.06	0.44
5:D:154:VAL:CG1	5:D:156:LYS:HG2	2.47	0.44
1:A:2766:A:O2'	5:D:265:LEU:O	2.30	0.44
7:F:27:ILE:HD11	7:F:37:ALA:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:81:GLU:O	7:F:85:GLN:HG3	2.17	0.44
8:G:9:GLU:HG3	8:G:10:ASP:N	2.33	0.44
16:O:143:ARG:HH12	16:O:173:ASP:CG	2.21	0.44
20:S:129:ALA:O	20:S:130:MET:HB2	2.17	0.44
1:A:2055:A:H5'	20:S:134:SER:HB2	2.00	0.44
22:U:38:ARG:HG3	22:U:38:ARG:HH11	1.81	0.44
25:X:149:LEU:HG	25:X:153:MET:HE1	1.99	0.44
1:A:1423:C:O2'	1:A:1424:A:H5'	2.18	0.44
1:A:696:C:HO2'	1:A:697:G:H5'	1.82	0.44
5:D:17:LYS:O	5:D:260:HIS:HD2	2.01	0.44
7:F:57:THR:HG23	7:F:63:ILE:CG2	2.46	0.44
10:I:71:LEU:C	10:I:73:ASP:H	2.21	0.44
1:A:1134:G:C4'	11:J:151:MET:HE1	2.28	0.44
14:M:142:LEU:HG	14:M:146:GLY:HA3	2.00	0.44
16:O:104:ILE:O	16:O:107:ASN:HB2	2.17	0.44
16:O:67:ALA:HA	16:O:71:TRP:H	1.81	0.44
19:R:75:ILE:CD1	19:R:84:ILE:HD11	2.48	0.44
25:X:4:LEU:HA	25:X:4:LEU:HD23	1.82	0.44
38:A:3472:HOH:O	31:4:57:GLY:HA2	2.17	0.44
1:A:1041:U:H2'	1:A:1042:U:H5'	2.00	0.44
1:A:1313:A:H5'	27:Z:208:LYS:O	2.17	0.44
1:A:1462:C:H2'	1:A:1463:A:C8	2.53	0.44
1:A:1829:A:H61	28:1:18:TYR:CA	2.26	0.44
1:A:1859:A:H8	1:A:1859:A:O5'	2.01	0.44
1:A:2466:G:P	38:A:3142:HOH:O	2.73	0.44
1:A:2635:A:C2'	1:A:2636:C:H5'	2.46	0.44
1:A:716:G:H2'	1:A:717:C:O5'	2.18	0.44
1:A:764:C:H2'	1:A:765:G:O4'	2.18	0.44
2:B:3092:G:H22	11:J:52:LYS:NZ	2.15	0.44
4:C:199:HIS:CD2	4:C:201:PHE:HB2	2.52	0.44
15:N:123:ASP:C	15:N:123:ASP:OD1	2.55	0.44
38:A:4009:HOH:O	15:N:94:LYS:HE3	2.18	0.44
16:O:161:GLY:O	16:O:162:ASP:C	2.55	0.44
26:Y:9:VAL:HG13	26:Y:88:GLU:OE2	2.18	0.44
27:Z:213:LYS:O	27:Z:217:ILE:HG13	2.18	0.44
28:1:48:LYS:HG2	38:1:8429:HOH:O	2.18	0.44
1:A:1189:A:C4	38:A:7139:HOH:O	2.56	0.44
1:A:1644:C:O2'	1:A:1645:U:H5'	2.17	0.44
1:A:2387:U:H2'	1:A:2388:C:C6	2.53	0.44
1:A:2873:C:N4	1:A:2874:G:C6	2.86	0.44
1:A:40:C:H4'	38:A:6462:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:94:LEU:N	4:C:94:LEU:CD2	2.81	0.44
8:G:84:MET:HE1	8:G:148:ILE:HD12	1.99	0.44
11:J:165:GLY:C	11:J:166:ASN:HD22	2.21	0.44
12:K:39:VAL:HG11	12:K:107:ASN:CB	2.48	0.44
12:K:46:ILE:HG12	12:K:53:ILE:HD13	1.99	0.44
1:A:1299:G:N7	14:M:6:ARG:NH1	2.65	0.44
16:O:152:GLU:C	16:O:154:LEU:N	2.71	0.44
16:O:71:TRP:N	38:O:8539:HOH:O	2.50	0.44
19:R:88:ALA:O	19:R:90:HIS:N	2.51	0.44
31:4:60:LYS:HD2	31:4:61:PRO:HD2	1.99	0.44
1:A:1008:C:H2'	1:A:1009:U:C6	2.53	0.44
1:A:1135:G:H5'	38:A:5388:HOH:O	2.17	0.44
1:A:2620:U:O4	36:5:76:PPU:O	2.36	0.44
1:A:2909:G:H2'	1:A:2910:A:H8	1.83	0.44
6:E:7:ASP:OD2	6:E:9:ASP:HB2	2.18	0.44
8:G:162:PHE:CD1	8:G:162:PHE:N	2.85	0.44
12:K:39:VAL:CG1	12:K:40:ASN:N	2.81	0.44
13:L:80:ILE:HG13	13:L:80:ILE:O	2.17	0.44
17:P:44:ASN:HA	17:P:65:LEU:O	2.18	0.44
28:1:40:PRO:CD	28:1:47:LEU:HD11	2.29	0.44
28:1:33:HIS:HE1	28:1:49:ARG:NE	2.16	0.44
29:2:8:GLN:NE2	29:2:11:LYS:HZ2	2.02	0.44
1:A:1637:A:H2'	1:A:1638:U:C6	2.53	0.44
1:A:1874:U:OP1	4:C:51:ARG:HD2	2.18	0.44
1:A:716:G:C2'	1:A:717:C:O5'	2.66	0.44
11:J:47:GLU:HG2	11:J:133:ILE:HD12	1.99	0.44
11:J:26:LYS:HG3	11:J:58:HIS:HB2	2.00	0.44
13:L:45:PRO:HB2	38:L:7169:HOH:O	2.17	0.44
1:A:2123:A:OP1	15:N:89:ASN:ND2	2.51	0.44
21:T:29:ASP:OD1	21:T:31:ARG:HG3	2.17	0.44
27:Z:126:PRO:HG2	27:Z:128:PHE:CZ	2.53	0.44
27:Z:197:ASP:C	27:Z:197:ASP:OD1	2.55	0.44
28:1:10:ARG:CG	28:1:11:THR:N	2.81	0.43
28:1:38:LYS:HD3	38:1:8423:HOH:O	2.17	0.43
28:1:57:CYS:O	28:1:61:GLY:CA	2.65	0.43
1:A:1391:G:H2'	1:A:1392:A:H5'	2.00	0.43
1:A:1711:A:O2'	1:A:1712:A:H5'	2.18	0.43
1:A:1825:U:O2'	1:A:1826:C:H5'	2.18	0.43
1:A:656:G:H2'	1:A:657:G:H8	1.83	0.43
1:A:883:U:O2	1:A:883:U:H2'	2.17	0.43
2:B:3057:A:H2'	2:B:3058:G:H5'	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:248:ARG:O	5:D:251:VAL:HG12	2.18	0.43
5:D:274:GLU:HA	5:D:292:GLY:O	2.18	0.43
6:E:218:VAL:CG1	38:E:8429:HOH:O	2.66	0.43
11:J:151:MET:HA	11:J:151:MET:CE	2.48	0.43
8:G:36:PRO:HD3	12:K:127:ILE:HD12	2.00	0.43
13:L:98:VAL:HG22	13:L:102:GLU:C	2.38	0.43
16:O:78:MET:HB2	16:O:79:PRO:HD3	1.99	0.43
16:O:86:LEU:HD12	16:O:125:ALA:CB	2.40	0.43
17:P:26:TRP:HA	17:P:26:TRP:HE3	1.82	0.43
17:P:26:TRP:N	38:P:3062:HOH:O	2.49	0.43
22:U:96:VAL:HG13	22:U:97:ARG:N	2.32	0.43
3:5:74:C:H2'	3:5:75:C:H5'	2.01	0.43
1:A:1265:G:H1'	38:A:4475:HOH:O	2.17	0.43
1:A:1385:G:O3'	26:Y:49:ARG:NH1	2.52	0.43
1:A:1471:A:H2'	1:A:1472:C:C6	2.53	0.43
1:A:1730:G:C5'	1:A:1731:C:H6	2.31	0.43
1:A:2255:A:C6	1:A:2256:G:C5	3.06	0.43
1:A:2438:G:H2'	1:A:2439:C:O4'	2.18	0.43
1:A:2779:G:O2'	1:A:2780:C:H5'	2.18	0.43
1:A:24:G:N2	1:A:518:G:H1'	2.33	0.43
1:A:860:U:H2'	1:A:861:A:C8	2.53	0.43
2:B:3107:C:H5	38:B:8437:HOH:O	2.00	0.43
38:A:6486:HOH:O	4:C:211:LYS:HG2	2.17	0.43
5:D:88:GLU:HG3	5:D:88:GLU:O	2.18	0.43
6:E:84:VAL:O	6:E:85:LYS:HB2	2.18	0.43
6:E:7:ASP:C	6:E:9:ASP:H	2.22	0.43
7:F:19:GLU:HG3	38:F:6165:HOH:O	2.18	0.43
9:H:26:THR:HB	9:H:102:GLY:HA3	1.99	0.43
12:K:77:GLY:O	12:K:78:ILE:C	2.57	0.43
14:M:62:ALA:HB2	14:M:103:ALA:CB	2.48	0.43
16:O:116:PHE:CB	38:O:8556:HOH:O	2.66	0.43
16:O:34:LEU:HA	16:O:47:LEU:CD2	2.48	0.43
24:W:5:VAL:HG23	38:W:2271:HOH:O	2.18	0.43
26:Y:76:ARG:NH1	26:Y:76:ARG:CG	2.80	0.43
31:4:73:GLU:HB2	38:4:8525:HOH:O	2.18	0.43
1:A:1329:A:C2	38:A:4165:HOH:O	2.57	0.43
1:A:1624:A:H4'	1:A:1626:A:H5'	2.01	0.43
1:A:1925:G:O2'	1:A:1926:G:H5'	2.19	0.43
1:A:2123:A:H5'	15:N:89:ASN:ND2	2.34	0.43
1:A:2621:U:H5	38:A:9479:HOH:O	2.01	0.43
1:A:295:C:H2'	1:A:296:G:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:U:C5'	38:A:5862:HOH:O	2.65	0.43
1:A:886:A:OP2	1:A:2113:G:H5'	2.19	0.43
4:C:223:ARG:CG	38:C:8616:HOH:O	2.48	0.43
7:F:170:TYR:N	7:F:170:TYR:CD1	2.87	0.43
8:G:112:ALA:HA	8:G:113:PRO:HD3	1.88	0.43
1:A:1119:G:H8	12:K:52:GLN:NE2	2.15	0.43
18:Q:83:LYS:O	18:Q:86:ALA:HB3	2.18	0.43
20:S:33:ARG:NH1	38:S:8542:HOH:O	2.51	0.43
21:T:10:VAL:O	21:T:10:VAL:HG22	2.19	0.43
25:X:122:ARG:NH1	25:X:152:ALA:O	2.51	0.43
25:X:85:ALA:HB2	25:X:91:ASP:O	2.18	0.43
26:Y:9:VAL:HG22	26:Y:88:GLU:OE2	2.18	0.43
27:Z:234:VAL:HG12	27:Z:235:GLU:N	2.33	0.43
28:1:46:LYS:CB	28:1:57:CYS:HG	2.24	0.43
31:4:22:VAL:HG12	31:4:90:PHE:HE2	1.83	0.43
1:A:2461:U:O2	1:A:2466:G:H1'	2.18	0.43
1:A:401:C:H2'	1:A:402:U:H6	1.81	0.43
4:C:195:ASN:O	4:C:196:ALA:C	2.56	0.43
7:F:151:ILE:HA	7:F:152:PRO:HD3	1.80	0.43
7:F:99:ASP:O	7:F:159:PRO:HG3	2.18	0.43
11:J:112:ARG:O	11:J:113:ALA:C	2.57	0.43
13:L:37:TYR:HD2	38:L:7169:HOH:O	1.92	0.43
9:H:61:MET:SD	15:N:23:LEU:HD11	2.58	0.43
1:A:171:C:OP2	15:N:84:LYS:HG3	2.18	0.43
16:O:82:TYR:C	16:O:82:TYR:CD2	2.91	0.43
18:Q:115:SER:C	18:Q:117:SER:N	2.71	0.43
18:Q:16:VAL:HG13	18:Q:20:ARG:NH1	2.33	0.43
22:U:48:VAL:CG2	22:U:98:VAL:HA	2.48	0.43
26:Y:70:ILE:HG23	26:Y:70:ILE:O	2.17	0.43
28:1:13:ARG:NH1	38:1:8419:HOH:O	2.50	0.43
28:1:40:PRO:HG2	28:1:64:ILE:HD13	2.01	0.43
29:2:45:ARG:HB3	38:2:988:HOH:O	2.18	0.43
3:5:74:C:H2'	3:5:75:C:O4'	2.17	0.43
1:A:101:C:H2'	1:A:102:A:C8	2.53	0.43
1:A:160:A:C4	1:A:177:A:C2	3.06	0.43
1:A:1624:A:H5'	1:A:1626:A:O4'	2.19	0.43
1:A:2321:A:O2'	1:A:2322:U:H3'	2.18	0.43
1:A:482:G:H4'	1:A:508:A:N1	2.34	0.43
1:A:536:A:H3'	38:A:4525:HOH:O	2.17	0.43
2:B:3045:A:C8	2:B:3046:C:C5	3.07	0.43
6:E:5:ILE:HG12	38:E:8436:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:15:GLU:HA	7:F:16:PRO:HD3	1.85	0.43
1:A:2780:C:C1'	8:G:143:GLN:NE2	2.81	0.43
11:J:163:PRO:O	11:J:164:ALA:HB2	2.18	0.43
38:A:9957:HOH:O	12:K:46:ILE:HD12	2.18	0.43
16:O:77:ASN:OD1	16:O:80:SER:HB2	2.18	0.43
38:A:3911:HOH:O	31:4:34:LYS:HD3	2.18	0.43
1:A:1058:A:H2'	1:A:1060:C:C5'	2.42	0.43
1:A:1159:G:H1	1:A:1208:C:H42	1.67	0.43
1:A:1311:G:C2	1:A:1312:G:C8	3.07	0.43
1:A:1572:A:H2'	1:A:1573:A:C8	2.53	0.43
1:A:2450:C:O5'	1:A:2450:C:H6	2.02	0.43
1:A:812:A:H2'	1:A:813:C:O4'	2.19	0.43
1:A:844:A:C6	1:A:882:A:C5	3.06	0.43
1:A:913:A:N3	1:A:1042:U:O2'	2.44	0.43
1:A:962:C:H5'	38:A:6424:HOH:O	2.19	0.43
13:L:40:THR:O	13:L:41:LYS:C	2.57	0.43
15:N:37:VAL:CG1	15:N:63:VAL:HG11	2.47	0.43
15:N:96:ASN:ND2	38:N:8541:HOH:O	2.49	0.43
16:O:90:LEU:CB	16:O:186:LEU:HD22	2.49	0.43
20:S:15:LYS:HE3	38:S:8577:HOH:O	2.18	0.43
21:T:57:THR:HG21	21:T:59:ASP:HB2	2.01	0.43
1:A:97:G:C2	22:U:107:LYS:HD2	2.53	0.43
27:Z:187:VAL:HG12	27:Z:205:ILE:HA	2.00	0.43
1:A:1164:U:C1'	1:A:1165:G:OP1	2.67	0.43
1:A:1592:G:H2'	1:A:1593:C:C6	2.54	0.43
1:A:1644:C:C2	1:A:1645:U:C6	3.07	0.43
1:A:2106:C:H2'	1:A:2107:U:C6	2.53	0.43
1:A:2247:C:C5'	38:A:6802:HOH:O	2.67	0.43
1:A:2851:G:C2'	1:A:2852:A:H5'	2.49	0.43
1:A:559:U:C6	1:A:559:U:H5'	2.42	0.43
1:A:675:U:H2'	1:A:676:C:H5'	2.00	0.43
1:A:860:U:H2'	38:A:5151:HOH:O	2.19	0.43
2:B:3003:A:N6	2:B:3022:G:H1'	2.33	0.43
2:B:3065:A:O2'	2:B:3066:G:P	2.75	0.43
8:G:7:ILE:HA	8:G:8:PRO:HD3	1.92	0.43
15:N:39:ARG:NH2	38:N:8624:HOH:O	2.51	0.43
16:O:47:LEU:HD13	16:O:97:VAL:HG11	2.01	0.43
17:P:39:THR:CB	38:P:3360:HOH:O	2.66	0.43
20:S:40:ALA:O	20:S:44:VAL:HG23	2.18	0.43
22:U:38:ARG:HG3	22:U:38:ARG:NH1	2.33	0.43
27:Z:187:VAL:O	27:Z:187:VAL:HG13	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1167:G:O2'	1:A:1168:C:H5'	2.19	0.43
1:A:1422:U:H2'	1:A:1423:C:H6	1.80	0.43
1:A:2563:U:H2'	1:A:2565:C:O5'	2.19	0.43
1:A:290:C:O2'	1:A:291:C:H5'	2.18	0.43
1:A:326:G:O2'	1:A:327:A:H5'	2.18	0.43
1:A:661:G:C6	1:A:686:A:C2	3.06	0.43
1:A:731:U:O2'	1:A:732:C:H5'	2.18	0.43
1:A:885:G:H5''	1:A:886:A:H5'	1.99	0.43
1:A:955:A:C2	1:A:1013:A:C4	3.06	0.43
2:B:3039:U:H3'	2:B:3040:C:H5''	1.99	0.43
4:C:36:ASP:O	4:C:37:VAL:C	2.56	0.43
5:D:204:GLY:CA	38:D:8653:HOH:O	2.61	0.43
5:D:71:VAL:CG1	5:D:296:LEU:HB3	2.46	0.43
7:F:19:GLU:O	7:F:133:ASN:HB3	2.19	0.43
11:J:83:PHE:CD1	11:J:134:ALA:HB2	2.54	0.43
13:L:10:GLN:NE2	13:L:10:GLN:N	2.43	0.43
16:O:47:LEU:HD12	16:O:92:ALA:HB1	2.00	0.43
25:X:26:ILE:HB	38:X:5420:HOH:O	2.17	0.43
25:X:38:THR:CB	38:X:5390:HOH:O	2.66	0.43
25:X:41:TYR:CD2	25:X:44:MET:HE3	2.54	0.43
1:A:1269:G:H2'	1:A:1270:U:H6	1.84	0.43
1:A:1714:C:O2'	1:A:1715:C:H5'	2.18	0.43
1:A:2113:G:C6	1:A:2114:C:C4	3.06	0.43
1:A:2577:A:H5'	38:A:7211:HOH:O	2.19	0.43
1:A:696:C:O2'	1:A:697:G:H5'	2.19	0.43
7:F:60:GLU:C	7:F:62:ASP:N	2.72	0.43
11:J:31:PHE:HA	11:J:85:ILE:CG2	2.49	0.43
11:J:62:GLU:HA	38:J:8385:HOH:O	2.18	0.43
21:T:33:SER:O	21:T:37:VAL:HG23	2.18	0.43
21:T:57:THR:HG22	21:T:59:ASP:HB2	2.01	0.43
1:A:1051:C:H2'	1:A:1052:G:O4'	2.19	0.43
1:A:2515:C:H2'	1:A:2516:G:O4'	2.18	0.43
1:A:2604:A:H5'	38:A:5256:HOH:O	2.18	0.43
1:A:319:A:H4'	1:A:338:C:C5	2.53	0.43
1:A:440:C:H2'	1:A:441:A:C8	2.54	0.43
1:A:818:A:H5''	38:A:6050:HOH:O	2.19	0.43
1:A:952:G:N3	1:A:2302:A:H2'	2.33	0.43
2:B:3003:A:H2'	38:B:8421:HOH:O	2.19	0.43
2:B:3031:C:H2'	2:B:3032:G:O4'	2.19	0.43
4:C:135:VAL:HG11	4:C:147:ARG:NH2	2.34	0.43
6:E:1:MET:HG2	6:E:2:GLN:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:200:PRO:HB3	6:E:212:VAL:CG2	2.49	0.43
7:F:76:ARG:O	7:F:77:ASP:HB2	2.19	0.43
38:A:6363:HOH:O	8:G:157:LYS:HD3	2.18	0.43
16:O:67:ALA:C	16:O:69:TYR:H	2.22	0.43
17:P:96:VAL:CG1	17:P:100:GLN:HB2	2.48	0.43
18:Q:59:ARG:HH22	18:Q:66:GLN:NE2	2.17	0.43
1:A:588:G:O6	25:X:154:ARG:NH1	2.52	0.43
25:X:65:VAL:HA	25:X:68:THR:CG2	2.49	0.43
1:A:1236:A:H2'	1:A:1237:U:O4'	2.19	0.42
1:A:2359:G:H3'	38:A:5160:HOH:O	2.19	0.42
1:A:2502:C:H2'	1:A:2503:A:C5'	2.46	0.42
1:A:854:G:N7	38:A:3800:HOH:O	2.36	0.42
1:A:968:G:O2'	1:A:969:G:H5'	2.19	0.42
4:C:70:ALA:HA	4:C:71:PRO:HD3	1.91	0.42
5:D:11:LEU:C	38:D:8617:HOH:O	2.57	0.42
5:D:215:VAL:O	5:D:219:GLY:HA2	2.18	0.42
6:E:246:ARG:NE	38:E:8429:HOH:O	2.51	0.42
12:K:104:TYR:HA	38:K:2238:HOH:O	2.19	0.42
14:M:146:GLY:C	14:M:148:GLU:H	2.22	0.42
17:P:24:ALA:N	38:P:3062:HOH:O	2.52	0.42
18:Q:13:VAL:HG21	18:Q:41:ARG:HG2	2.01	0.42
25:X:110:GLN:HA	25:X:110:GLN:HE21	1.83	0.42
1:A:622:G:P	27:Z:148:GLY:HA3	2.59	0.42
29:2:28:HIS:CE1	29:2:31:LYS:HE2	2.54	0.42
1:A:1182:C:H1'	1:A:1192:A:C8	2.51	0.42
1:A:128:A:O2'	1:A:129:A:H5'	2.18	0.42
1:A:1667:A:H2'	1:A:1668:U:C6	2.54	0.42
1:A:1771:U:O2'	28:1:23:ARG:NH2	2.50	0.42
1:A:2673:U:C2'	1:A:2674:G:H5'	2.49	0.42
1:A:2735:U:H2'	1:A:2736:U:C6	2.54	0.42
1:A:426:G:H2'	1:A:427:C:O4'	2.18	0.42
5:D:132:HIS:CE1	5:D:171:VAL:CG2	3.02	0.42
5:D:212:GLN:HB2	5:D:257:THR:CG2	2.38	0.42
6:E:107:ARG:CB	6:E:107:ARG:NH1	2.73	0.42
6:E:129:HIS:HD2	6:E:165:ASP:OD2	2.01	0.42
7:F:99:ASP:CB	7:F:103:ASN:HB2	2.49	0.42
7:F:77:ASP:HB3	7:F:78:GLU:H	1.57	0.42
14:M:24:ALA:HB2	14:M:30:ARG:HD2	2.00	0.42
15:N:133:LEU:N	15:N:133:LEU:HD12	2.33	0.42
15:N:38:VAL:HG12	15:N:38:VAL:O	2.17	0.42
38:A:3159:HOH:O	15:N:79:LYS:HD2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:110:THR:HA	16:O:111:PRO:HD3	1.90	0.42
18:Q:134:VAL:O	18:Q:137:LEU:HB3	2.19	0.42
18:Q:58:SER:CB	38:Q:186:HOH:O	2.66	0.42
26:Y:74:ALA:HB2	26:Y:85:VAL:HG13	2.00	0.42
1:A:1298:U:H2'	1:A:1299:G:C8	2.54	0.42
1:A:1389:G:H1'	1:A:1435:U:O2	2.19	0.42
1:A:1681:G:H5''	1:A:1682:A:OP1	2.19	0.42
1:A:1730:G:C5'	1:A:1731:C:C6	3.03	0.42
1:A:1907:U:C4	1:A:1908:G:C5	3.07	0.42
1:A:2247:C:O2'	1:A:2248:C:H5'	2.20	0.42
1:A:2453:G:H3'	38:A:5380:HOH:O	2.18	0.42
2:B:3025:G:C8	2:B:3026:C:H5'	2.55	0.42
4:C:36:ASP:HB2	4:C:85:ASP:H	1.84	0.42
5:D:53:LEU:HD21	5:D:270:ILE:HD12	2.00	0.42
5:D:7:ARG:NH1	5:D:11:LEU:HD22	2.34	0.42
17:P:96:VAL:HG12	17:P:97:SER:O	2.18	0.42
13:L:130:MET:SD	23:V:26:GLY:HA3	2.59	0.42
25:X:119:HIS:HD2	25:X:120:PRO:O	2.02	0.42
26:Y:43:VAL:CG1	26:Y:44:ASP:N	2.81	0.42
1:A:1494:A:C2	1:A:1495:C:C4	3.07	0.42
1:A:1657:A:H2'	1:A:1658:A:C8	2.54	0.42
1:A:1871:U:O4'	1:A:1873:G:C8	2.73	0.42
1:A:1896:G:C6	1:A:1897:U:C4	3.07	0.42
1:A:2122:C:P	38:A:6038:HOH:O	2.67	0.42
1:A:2573:G:N3	38:A:6756:HOH:O	2.36	0.42
1:A:2911:C:H2'	1:A:2912:C:H6	1.84	0.42
1:A:321:A:O2'	1:A:322:G:H5'	2.19	0.42
1:A:332:G:H4'	22:U:2:LYS:O	2.19	0.42
1:A:35:U:O2'	1:A:36:C:H5'	2.20	0.42
1:A:553:G:C2'	1:A:554:G:H5'	2.49	0.42
1:A:951:A:H2'	1:A:952:G:H5'	2.01	0.42
2:B:3045:A:C5	2:B:3046:C:C4	3.07	0.42
2:B:3045:A:C5	2:B:3046:C:C5	3.07	0.42
5:D:277:GLU:N	5:D:278:PRO:CD	2.82	0.42
7:F:94:ALA:HB3	7:F:174:VAL:HA	2.01	0.42
8:G:31:ARG:HH12	8:G:68:HIS:CG	2.37	0.42
9:H:34:ASN:O	9:H:38:LYS:HG3	2.19	0.42
13:L:28:GLU:HB3	13:L:59:LYS:HB2	2.01	0.42
15:N:25:TRP:HE3	15:N:26:HIS:HD2	1.66	0.42
15:N:38:VAL:O	15:N:63:VAL:HG13	2.20	0.42
21:T:29:ASP:CG	21:T:31:ARG:NH1	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:U:19:ARG:NH1	22:U:68:ASP:O	2.52	0.42
25:X:80:ASP:O	25:X:84:VAL:HG23	2.18	0.42
26:Y:71:ARG:HD3	38:Y:2171:HOH:O	2.18	0.42
1:A:1134:G:H4'	11:J:151:MET:CE	2.29	0.42
1:A:1314:U:H5''	1:A:1316:G:O4'	2.18	0.42
1:A:1324:G:C2	1:A:1334:C:O2	2.73	0.42
1:A:1566:C:H2'	1:A:1567:A:H8	1.85	0.42
1:A:1701:A:H5''	1:A:1702:U:H3'	2.02	0.42
1:A:1869:A:H2'	1:A:1870:C:O4'	2.20	0.42
1:A:2112:A:H2'	1:A:2113:G:H8	1.84	0.42
1:A:2530:C:O2'	1:A:2531:U:H5'	2.20	0.42
1:A:2634:G:O2'	1:A:2635:A:H5'	2.19	0.42
1:A:2637:A:H5'	38:A:8784:HOH:O	2.20	0.42
1:A:2883:A:H2'	1:A:2884:G:O4'	2.20	0.42
2:B:3003:A:H2	2:B:3021:G:N3	2.17	0.42
4:C:200:PRO:HG2	4:C:225:VAL:HG21	2.01	0.42
5:D:275:GLY:O	5:D:291:ASP:HA	2.19	0.42
5:D:7:ARG:NH2	5:D:250:THR:O	2.53	0.42
6:E:212:VAL:HG23	6:E:212:VAL:O	2.20	0.42
6:E:76:ARG:HG2	6:E:78:ARG:NH1	2.34	0.42
9:H:22:VAL:HG21	9:H:104:ALA:HB2	2.01	0.42
11:J:84:ARG:CZ	11:J:135:TRP:HH2	2.32	0.42
11:J:49:VAL:O	11:J:157:ILE:HG23	2.20	0.42
11:J:57:ARG:C	11:J:59:ASN:N	2.70	0.42
15:N:84:LYS:O	15:N:87:MET:HG2	2.20	0.42
16:O:86:LEU:O	16:O:90:LEU:HG	2.19	0.42
18:Q:16:VAL:HG12	18:Q:20:ARG:HB2	2.00	0.42
18:Q:7:LYS:HD3	18:Q:21:VAL:CG2	2.49	0.42
22:U:55:PHE:HB2	38:U:6384:HOH:O	2.20	0.42
28:1:38:LYS:HG2	38:1:8408:HOH:O	2.20	0.42
1:A:1044:C:H5''	38:A:8542:HOH:O	2.19	0.42
1:A:1943:C:O4'	4:C:212:PRO:HA	2.19	0.42
1:A:2252:A:C5	1:A:2253:G:H1'	2.54	0.42
1:A:23:G:O2'	1:A:24:G:H5'	2.19	0.42
1:A:2443:C:O3'	14:M:56:LYS:HE3	2.19	0.42
1:A:877:G:C5'	1:A:878:G:OP1	2.64	0.42
1:A:950:G:O2'	1:A:951:A:H5'	2.18	0.42
1:A:960:G:N3	1:A:960:G:C2'	2.82	0.42
4:C:110:SER:N	4:C:114:ASP:OD2	2.52	0.42
4:C:173:GLY:O	4:C:177:HIS:CD2	2.72	0.42
5:D:7:ARG:HD3	5:D:9:GLY:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:184:ARG:NE	38:E:8415:HOH:O	2.43	0.42
6:E:236:THR:O	6:E:239:ALA:N	2.53	0.42
8:G:15:GLN:NE2	8:G:40:VAL:O	2.53	0.42
11:J:53:PRO:HA	11:J:125:VAL:O	2.20	0.42
11:J:84:ARG:CZ	11:J:135:TRP:CH2	3.02	0.42
12:K:79:PHE:O	12:K:79:PHE:HD2	2.01	0.42
14:M:55:GLN:HA	14:M:58:GLN:NE2	2.33	0.42
14:M:53:ARG:HH22	14:M:57:VAL:HG12	1.83	0.42
15:N:63:VAL:O	15:N:130:GLU:HA	2.19	0.42
16:O:47:LEU:HA	16:O:47:LEU:HD23	1.72	0.42
1:A:1010:C:H4'	16:O:4:PRO:HB2	2.02	0.42
19:R:53:HIS:O	19:R:55:ARG:N	2.53	0.42
25:X:65:VAL:HG12	25:X:116:LEU:HD13	2.01	0.42
1:A:171:C:O2'	1:A:172:U:H5'	2.20	0.42
1:A:2004:U:H5''	1:A:2005:G:C8	2.54	0.42
1:A:2335:C:C2	1:A:2350:G:C2	3.07	0.42
2:B:3055:U:H4'	2:B:3056:A:H8	1.83	0.42
2:B:3078:G:O2'	2:B:3079:U:P	2.78	0.42
4:C:125:ASN:HB3	4:C:158:VAL:HG12	2.02	0.42
4:C:169:PHE:O	4:C:170:VAL:HB	2.20	0.42
5:D:82:VAL:HG12	5:D:101:TRP:CE3	2.54	0.42
7:F:59:GLY:C	7:F:61:PHE:H	2.23	0.42
8:G:101:GLU:OE2	8:G:115:ARG:HD3	2.19	0.42
15:N:185:PRO:CG	15:N:189:VAL:HG11	2.48	0.42
16:O:107:ASN:OD1	35:O:8507:CL:CL	2.75	0.42
20:S:4:TYR:N	38:S:8546:HOH:O	2.52	0.42
22:U:28:SER:O	22:U:32:ARG:HG3	2.18	0.42
23:V:9:CYS:SG	38:V:6796:HOH:O	2.62	0.42
25:X:73:LEU:HD12	25:X:73:LEU:HA	1.88	0.42
29:2:12:ASN:HB3	38:2:5389:HOH:O	2.19	0.42
31:4:54:LYS:NZ	38:4:8526:HOH:O	2.52	0.42
1:A:1268:C:H2'	1:A:1269:G:C8	2.54	0.42
1:A:1483:C:O2'	1:A:1484:G:H5'	2.20	0.42
1:A:1603:A:H4'	1:A:1605:G:C8	2.55	0.42
1:A:1743:G:H1'	38:A:4365:HOH:O	2.19	0.42
1:A:1855:G:H8	4:C:144:GLU:OE2	2.03	0.42
1:A:419:A:H1'	1:A:1921:A:C2	2.55	0.42
1:A:2346:C:H4'	7:F:52:THR:CG2	2.48	0.42
1:A:251:C:O2'	1:A:252:C:H5'	2.19	0.42
1:A:553:G:P	27:Z:204:ARG:NH2	2.92	0.42
1:A:67:A:H5''	1:A:69:A:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:949:U:O2'	19:R:40:HIS:HE1	2.03	0.42
2:B:3048:C:H4'	16:O:141:ARG:NH2	2.27	0.42
9:H:4:VAL:HG13	9:H:76:PHE:CE1	2.54	0.42
38:A:5000:HOH:O	15:N:58:GLN:HG3	2.19	0.42
17:P:26:TRP:HB2	38:P:3062:HOH:O	2.20	0.42
38:A:3626:HOH:O	26:Y:59:TRP:HB2	2.19	0.42
26:Y:85:VAL:HG12	26:Y:86:GLU:H	1.85	0.42
1:A:10:U:HO2'	1:A:11:A:P	2.43	0.42
1:A:1501:A:C6	1:A:1502:A:C6	3.07	0.42
1:A:2452:G:OP2	38:A:6202:HOH:O	2.21	0.42
1:A:2456:A:H2'	1:A:2457:U:C6	2.55	0.42
1:A:2607:U:C4	5:D:242:TRP:CZ2	3.07	0.42
1:A:2909:G:O2'	1:A:2910:A:H5'	2.20	0.42
1:A:303:C:H2'	1:A:304:G:O4'	2.20	0.42
4:C:128:LEU:HG	38:C:8583:HOH:O	2.19	0.42
5:D:132:HIS:HB2	5:D:137:LEU:HD22	2.02	0.42
5:D:277:GLU:N	5:D:278:PRO:HD2	2.34	0.42
8:G:145:ALA:HB1	8:G:168:ILE:CD1	2.50	0.42
8:G:24:GLY:HA3	8:G:76:VAL:HB	2.02	0.42
8:G:64:THR:HG22	8:G:68:HIS:CD2	2.55	0.42
1:A:2311:A:H5''	11:J:115:PHE:CD2	2.54	0.42
12:K:4:ALA:O	12:K:5:GLU:O	2.38	0.42
13:L:121:PHE:HB3	38:L:2659:HOH:O	2.19	0.42
15:N:40:ILE:HG13	15:N:40:ILE:O	2.20	0.42
16:O:116:PHE:HB2	38:O:8556:HOH:O	2.18	0.42
16:O:162:ASP:HB3	16:O:163:PHE:H	1.61	0.42
19:R:16:ASN:HA	19:R:16:ASN:HD22	1.59	0.42
24:W:45:ARG:C	24:W:47:LYS:N	2.73	0.42
25:X:28:HIS:HD2	25:X:31:HIS:CE1	2.38	0.42
25:X:76:ASP:O	25:X:77:ALA:C	2.59	0.42
1:A:2896:A:OP1	26:Y:15:ARG:NH1	2.52	0.42
1:A:111:C:O2'	1:A:112:G:H5'	2.20	0.42
1:A:1242:A:H5'	12:K:82:THR:CG2	2.39	0.42
1:A:221:G:C6	1:A:222:A:C6	3.08	0.42
1:A:2655:U:C4	1:A:2656:G:N7	2.88	0.42
1:A:319:A:H4'	1:A:338:C:C4	2.55	0.42
2:B:3012:C:H5'	2:B:3070:U:O4'	2.20	0.42
38:A:8592:HOH:O	5:D:214:PRO:HD2	2.20	0.42
6:E:115:LEU:HD12	6:E:115:LEU:HA	1.90	0.42
1:A:449:A:C8	6:E:43:LYS:HG2	2.54	0.42
7:F:55:LYS:O	7:F:56:ARG:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:69:ILE:HA	8:G:72:MET:HE2	2.01	0.42
11:J:71:TYR:O	11:J:73:GLN:N	2.53	0.42
14:M:90:ARG:NH1	14:M:119:THR:HG21	2.35	0.42
30:3:49:GLU:CD	38:3:719:HOH:O	2.58	0.41
1:A:1384:C:O5'	1:A:1384:C:H6	2.03	0.41
1:A:155:C:OP2	15:N:188:ARG:HD3	2.20	0.41
1:A:2430:A:H2'	1:A:2431:C:C6	2.54	0.41
1:A:512:G:O3'	1:A:513:A:H8	2.03	0.41
1:A:758:A:OP1	14:M:31:GLY:N	2.50	0.41
1:A:795:G:HO2'	1:A:796:A:P	2.43	0.41
1:A:876:A:C2'	1:A:876:A:N3	2.83	0.41
4:C:103:VAL:HA	4:C:104:PRO:HD3	1.80	0.41
4:C:43:VAL:O	4:C:44:ASP:HB2	2.20	0.41
5:D:146:THR:O	5:D:159:PRO:HB3	2.19	0.41
5:D:190:MET:HE2	5:D:194:PHE:HD1	1.83	0.41
5:D:224:LYS:HD3	5:D:224:LYS:HA	1.75	0.41
9:H:109:GLU:O	9:H:112:ALA:HB3	2.21	0.41
11:J:45:GLN:HG3	11:J:135:TRP:NE1	2.35	0.41
8:G:35:TYR:HA	12:K:127:ILE:HD12	2.02	0.41
13:L:115:ARG:CG	13:L:116:GLU:N	2.79	0.41
14:M:73:VAL:HG21	14:M:116:HIS:CD2	2.55	0.41
16:O:91:ARG:HG3	16:O:186:LEU:CD2	2.48	0.41
18:Q:121:ASP:HB2	38:Q:201:HOH:O	2.19	0.41
18:Q:11:ALA:HB1	18:Q:16:VAL:O	2.20	0.41
20:S:25:PHE:N	38:S:8508:HOH:O	2.51	0.41
3:5:74:C:C4	3:5:75:C:C2	3.08	0.41
1:A:1192:A:O2'	1:A:1193:A:OP1	2.29	0.41
1:A:1930:A:H1'	1:A:2128:G:H5'	2.02	0.41
1:A:1973:A:H5'	1:A:1973:A:H8	1.84	0.41
1:A:2385:G:H2'	1:A:2386:U:H6	1.85	0.41
1:A:2506:A:O2'	1:A:2507:G:P	2.78	0.41
1:A:1562:C:H42	1:A:2738:G:H1	1.67	0.41
1:A:2865:G:HO2'	1:A:2866:U:H5	1.67	0.41
1:A:699:C:C2	1:A:744:G:C2	3.08	0.41
5:D:205:VAL:O	5:D:307:ARG:CD	2.68	0.41
6:E:36:ARG:NH1	38:E:8400:HOH:O	2.53	0.41
7:F:158:ASN:HB2	7:F:161:ASP:OD2	2.20	0.41
9:H:26:THR:HB	9:H:102:GLY:C	2.41	0.41
12:K:135:ILE:O	12:K:139:LEU:HG	2.20	0.41
15:N:133:LEU:O	15:N:134:ILE:HD13	2.21	0.41
16:O:69:TYR:HE2	16:O:183:ASP:OD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:146:ILE:HG23	25:X:150:LEU:HD12	2.02	0.41
26:Y:43:VAL:HG12	26:Y:47:ALA:HB3	2.01	0.41
1:A:1448:A:C6	1:A:1451:C:C2	3.09	0.41
1:A:1545:C:H2'	1:A:1546:G:O4'	2.20	0.41
1:A:1851:G:O2'	1:A:1852:A:H5'	2.20	0.41
1:A:209:G:C6	1:A:210:U:N3	2.89	0.41
1:A:2108:A:C2	1:A:2110:G:C8	3.08	0.41
1:A:2388:C:O2'	1:A:2389:U:H5'	2.20	0.41
1:A:245:C:C2'	1:A:246:G:H5'	2.50	0.41
1:A:2769:C:H2'	1:A:2770:G:C5'	2.50	0.41
5:D:279:THR:HG22	5:D:280:VAL:O	2.21	0.41
5:D:69:VAL:HA	5:D:70:PRO:HD3	1.95	0.41
6:E:191:SER:OG	6:E:192:ILE:N	2.53	0.41
8:G:172:PRO:HB3	38:G:6931:HOH:O	2.20	0.41
11:J:111:MET:O	11:J:114:PRO:HD3	2.20	0.41
11:J:65:ARG:CZ	38:J:8385:HOH:O	2.68	0.41
15:N:155:HIS:ND1	15:N:158:ARG:NE	2.55	0.41
1:A:183:A:C5'	15:N:157:LEU:HD12	2.50	0.41
1:A:182:G:C4'	15:N:157:LEU:HD13	2.47	0.41
15:N:93:ARG:H	15:N:93:ARG:HG2	1.54	0.41
16:O:67:ALA:O	16:O:69:TYR:N	2.54	0.41
24:W:39:ALA:C	24:W:41:GLU:N	2.73	0.41
1:A:1217:G:H2'	1:A:1218:U:C6	2.55	0.41
1:A:1506:U:H6	1:A:1506:U:H5'	1.86	0.41
1:A:1513:C:O2'	1:A:1514:C:H5'	2.19	0.41
1:A:590:A:C2'	1:A:591:A:H5'	2.51	0.41
1:A:596:C:H2'	1:A:597:A:C8	2.55	0.41
1:A:638:C:H2'	1:A:639:A:H8	1.85	0.41
4:C:42:VAL:HG11	4:C:75:GLY:O	2.21	0.41
4:C:36:ASP:CB	4:C:85:ASP:H	2.32	0.41
5:D:238:ASN:HD22	5:D:240:GLY:N	2.14	0.41
13:L:118:ALA:O	13:L:120:ARG:N	2.54	0.41
13:L:78:LYS:HA	13:L:79:PRO:HD3	1.88	0.41
14:M:93:VAL:HG12	14:M:97:VAL:HG23	2.03	0.41
16:O:37:ARG:HD3	16:O:37:ARG:HA	1.84	0.41
1:A:710:G:OP1	17:P:24:ALA:HB3	2.20	0.41
17:P:80:ASP:OD1	17:P:81:PHE:N	2.53	0.41
38:A:3268:HOH:O	23:V:17:THR:CG2	2.69	0.41
26:Y:12:ILE:HG23	26:Y:36:HIS:CG	2.55	0.41
1:A:1524:U:O2'	1:A:1525:G:P	2.78	0.41
1:A:1600:G:H8	1:A:1600:G:OP2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2346:C:O3'	7:F:52:THR:HG23	2.20	0.41
1:A:2547:C:H2'	1:A:2548:C:C6	2.56	0.41
1:A:292:G:N2	38:A:5231:HOH:O	2.30	0.41
1:A:736:A:H2'	1:A:737:A:O4'	2.20	0.41
1:A:920:C:H5'	1:A:921:G:C4	2.55	0.41
5:D:280:VAL:HG11	5:D:335:ASN:H	1.86	0.41
5:D:280:VAL:HG13	5:D:333:GLU:O	2.20	0.41
7:F:101:THR:HG22	7:F:101:THR:O	2.20	0.41
12:K:6:PHE:O	12:K:8:ALA:N	2.53	0.41
15:N:74:ARG:HD3	15:N:88:VAL:HA	2.03	0.41
15:N:87:MET:HE1	38:N:8531:HOH:O	2.21	0.41
16:O:164:ASP:OD1	16:O:164:ASP:C	2.58	0.41
22:U:71:VAL:CG1	22:U:72:ILE:N	2.83	0.41
25:X:29:VAL:O	25:X:30:ASN:HB2	2.21	0.41
27:Z:107:PRO:HB3	27:Z:182:PHE:CD2	2.56	0.41
1:A:2460:A:OP1	31:4:60:LYS:HB2	2.21	0.41
1:A:1023:C:O2'	1:A:1024:G:H5'	2.21	0.41
1:A:1059:G:C8	1:A:2491:G:H4'	2.55	0.41
1:A:1161:A:O5'	1:A:1161:A:C8	2.73	0.41
1:A:1749:U:O2	1:A:1751:G:C8	2.74	0.41
1:A:1795:G:H2'	1:A:1796:A:O4'	2.21	0.41
1:A:840:U:C2	1:A:2648:U:O4	2.73	0.41
1:A:2880:A:H2'	1:A:2881:C:O4'	2.20	0.41
1:A:64:G:H2'	1:A:65:C:O4'	2.21	0.41
1:A:2837:U:H1'	5:D:307:ARG:HH12	1.85	0.41
6:E:40:ALA:CB	6:E:100:LEU:HD12	2.51	0.41
7:F:163:VAL:HA	38:F:6326:HOH:O	2.20	0.41
7:F:60:GLU:O	7:F:62:ASP:N	2.53	0.41
8:G:158:ASP:OD1	8:G:160:ARG:HB2	2.20	0.41
9:H:4:VAL:HG13	9:H:76:PHE:CD1	2.55	0.41
10:I:65:THR:O	10:I:69:ARG:HB2	2.20	0.41
11:J:26:LYS:CD	11:J:28:ILE:HB	2.51	0.41
24:W:27:LEU:HA	24:W:49:LEU:HD13	2.02	0.41
29:2:5:THR:N	29:2:6:PRO:HD2	2.35	0.41
30:3:36:ASN:HB3	30:3:39:ARG:NE	2.36	0.41
1:A:1383:U:H2'	1:A:1384:C:C6	2.56	0.41
1:A:1616:A:H5''	1:A:1617:C:OP1	2.20	0.41
1:A:1767:A:O2'	1:A:1768:C:H5'	2.21	0.41
1:A:1916:C:C2	1:A:1924:A:C2	3.08	0.41
1:A:2134:G:C6	1:A:2258:A:C8	3.09	0.41
1:A:2445:U:H2'	1:A:2446:G:H8	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2651:C:H2'	1:A:2652:U:O4'	2.20	0.41
1:A:2825:C:H4'	1:A:2826:G:O5'	2.20	0.41
1:A:328:U:O4'	6:E:202:THR:HG22	2.20	0.41
1:A:333:G:O2'	1:A:334:G:H5'	2.21	0.41
1:A:470:U:O2'	29:2:16:HIS:CD2	2.73	0.41
1:A:697:G:H4'	1:A:730:G:O3'	2.21	0.41
1:A:731:U:OP2	38:A:3515:HOH:O	2.22	0.41
5:D:144:THR:CG2	5:D:145:HIS:N	2.83	0.41
5:D:168:GLY:H	5:D:174:ARG:HD3	1.83	0.41
6:E:114:ALA:HB1	6:E:223:LEU:HB3	2.02	0.41
1:A:1352:A:N1	6:E:48:SER:HB3	2.35	0.41
7:F:35:ALA:C	7:F:37:ALA:N	2.74	0.41
7:F:94:ALA:O	7:F:95:THR:O	2.38	0.41
8:G:149:GLU:OE1	8:G:168:ILE:HG12	2.21	0.41
11:J:31:PHE:CD2	11:J:85:ILE:HG23	2.56	0.41
14:M:72:ASN:OD1	14:M:75:LEU:HD12	2.21	0.41
25:X:130:HIS:O	25:X:136:GLY:HA3	2.20	0.41
27:Z:109:LEU:HA	38:Z:8576:HOH:O	2.21	0.41
28:1:39:CYS:SG	28:1:47:LEU:CD2	2.85	0.41
29:2:29:THR:O	29:2:32:LYS:NZ	2.53	0.41
29:2:31:LYS:O	29:2:32:LYS:HB2	2.21	0.41
1:A:1477:C:H5'	1:A:1868:G:C5'	2.50	0.41
1:A:1603:A:H5'	1:A:1605:G:C4'	2.49	0.41
1:A:1880:C:C2	1:A:1881:A:C8	3.09	0.41
1:A:316:A:N3	1:A:336:G:O2'	2.49	0.41
1:A:397:A:P	38:A:3833:HOH:O	2.78	0.41
1:A:920:C:H4'	1:A:921:G:N2	2.35	0.41
1:A:1855:G:O6	4:C:141:PRO:HG2	2.21	0.41
7:F:146:LYS:HE2	16:O:107:ASN:ND2	2.36	0.41
11:J:132:PHE:O	11:J:133:ILE:HD13	2.20	0.41
11:J:1:LYS:HA	11:J:2:PRO:HD3	1.81	0.41
1:A:688:A:H62	14:M:111:ALA:HB2	1.85	0.41
15:N:43:PRO:HG3	15:N:62:VAL:HG21	2.03	0.41
16:O:110:THR:HB	16:O:113:SER:OG	2.20	0.41
18:Q:115:SER:HG	18:Q:118:GLN:HG3	1.83	0.41
22:U:40:VAL:HA	22:U:119:ALA:O	2.21	0.41
24:W:12:THR:HG23	24:W:14:ALA:H	1.85	0.41
25:X:154:ARG:HE	25:X:154:ARG:HB3	1.64	0.41
26:Y:78:GLU:CG	26:Y:79:GLU:N	2.72	0.41
27:Z:116:LEU:HD23	27:Z:116:LEU:HA	1.82	0.41
28:1:46:LYS:O	28:1:57:CYS:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1566:C:O2'	1:A:1567:A:H5'	2.21	0.41
1:A:1706:G:C6	1:A:1707:G:C6	3.08	0.41
1:A:1969:A:N7	1:A:1970:G:C6	2.88	0.41
1:A:2473:U:O3'	1:A:2474:A:H3'	2.20	0.41
1:A:2506:A:H1'	38:A:5515:HOH:O	2.21	0.41
1:A:2839:C:O5'	1:A:2839:C:H6	2.04	0.41
1:A:151:A:C2	1:A:442:A:C8	3.09	0.41
1:A:861:A:H2'	1:A:862:U:C6	2.55	0.41
4:C:231:LYS:O	4:C:232:ARG:HB3	2.21	0.41
6:E:142:ASP:OD1	6:E:237:GLU:HB3	2.21	0.41
7:F:57:THR:HA	7:F:63:ILE:HA	2.01	0.41
13:L:37:TYR:CE2	13:L:45:PRO:HA	2.55	0.41
25:X:122:ARG:HG2	25:X:122:ARG:NH1	2.27	0.41
31:4:42:ARG:HH11	31:4:42:ARG:CG	2.33	0.41
1:A:10:U:O4	1:A:532:A:OP2	2.38	0.41
1:A:1162:G:N3	1:A:1162:G:H2'	2.36	0.41
1:A:1166:A:H2'	1:A:1166:A:N3	2.35	0.41
1:A:1218:U:H2'	1:A:1219:U:H6	1.85	0.41
1:A:123:U:O2'	1:A:124:C:H5'	2.21	0.41
1:A:1463:A:H2'	1:A:1464:U:C6	2.56	0.41
1:A:154:C:O2'	1:A:155:C:H5'	2.20	0.41
1:A:1609:C:H2'	1:A:1610:G:C8	2.56	0.41
1:A:2257:G:H4'	1:A:2259:C:C2	2.56	0.41
1:A:2398:A:H2'	1:A:2399:G:O4'	2.21	0.41
1:A:2501:G:H1'	38:A:4029:HOH:O	2.20	0.41
1:A:2834:G:C4	1:A:2847:G:N2	2.89	0.41
1:A:951:A:O2'	1:A:952:G:H5'	2.21	0.41
1:A:79:G:H22	1:A:97:G:H1'	1.86	0.41
4:C:165:THR:O	4:C:165:THR:CG2	2.69	0.41
4:C:217:ARG:NH1	4:C:217:ARG:CG	2.84	0.41
5:D:14:GLY:HA3	38:D:8609:HOH:O	2.20	0.41
7:F:99:ASP:HB2	7:F:103:ASN:H	1.86	0.41
8:G:154:ILE:HG13	8:G:156:ASP:OD1	2.21	0.41
9:H:115:VAL:O	9:H:118:LEU:N	2.54	0.41
11:J:129:ASN:HD22	11:J:129:ASN:N	2.18	0.41
11:J:26:LYS:HD2	11:J:28:ILE:CG1	2.50	0.41
1:A:1003:U:O2	11:J:90:PHE:CZ	2.73	0.41
25:X:122:ARG:CG	25:X:122:ARG:NH1	2.83	0.41
1:A:1121:G:H21	1:A:1248:A:C4'	2.34	0.41
1:A:1345:A:H2'	1:A:1346:U:C6	2.56	0.41
1:A:1656:A:H2'	1:A:1657:A:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2462:G:O6	31:4:61:PRO:HG3	2.20	0.41
1:A:2786:G:O2'	1:A:2787:C:H5'	2.21	0.41
1:A:453:A:H4'	1:A:455:A:N7	2.36	0.41
1:A:658:C:O2'	1:A:662:U:OP1	2.34	0.41
4:C:179:MET:HG2	4:C:186:TRP:CG	2.56	0.41
6:E:118:THR:HG22	6:E:137:PRO:HB3	2.03	0.41
7:F:67:ASP:N	7:F:67:ASP:OD1	2.54	0.41
1:A:1151:G:OP1	10:I:63:ARG:NH1	2.54	0.41
14:M:125:PHE:CE1	14:M:140:VAL:HG13	2.56	0.41
38:A:9692:HOH:O	14:M:4:LYS:HG3	2.21	0.41
15:N:169:ARG:NH1	38:N:8576:HOH:O	2.54	0.41
38:B:8525:HOH:O	16:O:107:ASN:HB3	2.21	0.41
17:P:35:LYS:HD3	38:P:3360:HOH:O	2.20	0.41
38:B:8386:HOH:O	19:R:25:PRO:HB3	2.20	0.41
19:R:25:PRO:HA	19:R:26:PRO:HD3	1.86	0.41
19:R:40:HIS:CE1	19:R:94:GLN:HA	2.56	0.41
1:A:21:G:H5''	20:S:1:GLY:O	2.21	0.41
21:T:10:VAL:HG11	24:W:36:ALA:HA	2.02	0.41
22:U:14:ALA:HA	22:U:15:PRO:HD3	1.93	0.41
1:A:1191:A:N1	1:A:1206:U:O4	2.54	0.40
1:A:1611:G:O2'	1:A:1612:A:H5'	2.22	0.40
1:A:164:G:C6	1:A:165:A:C5	3.08	0.40
1:A:2047:C:H5'	38:A:9316:HOH:O	2.21	0.40
1:A:2090:G:H2'	1:A:2091:G:C8	2.56	0.40
1:A:243:A:H61	1:A:269:G:H1'	1.86	0.40
1:A:2588:G:H2'	1:A:2589:U:H4'	2.03	0.40
1:A:2846:C:OP1	5:D:158:LYS:HD3	2.21	0.40
1:A:506:G:N2	1:A:509:A:C5'	2.71	0.40
1:A:593:A:N7	38:A:3887:HOH:O	2.53	0.40
1:A:724:G:O2'	1:A:725:C:H5'	2.21	0.40
1:A:78:G:C6	1:A:79:G:C6	3.09	0.40
1:A:1861:C:H4'	4:C:6:GLY:O	2.21	0.40
5:D:222:LYS:HE2	38:D:8547:HOH:O	2.21	0.40
5:D:265:LEU:CD2	5:D:316:ARG:HD3	2.51	0.40
5:D:60:SER:C	5:D:62:ARG:H	2.23	0.40
6:E:120:ASP:OD1	6:E:120:ASP:C	2.60	0.40
6:E:127:ARG:NH2	6:E:225:PRO:O	2.53	0.40
7:F:168:SER:OG	7:F:168:SER:O	2.35	0.40
8:G:132:THR:HB	38:G:2227:HOH:O	2.21	0.40
11:J:113:ALA:N	11:J:114:PRO:CD	2.84	0.40
11:J:26:LYS:HD2	11:J:28:ILE:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:62:GLU:OE2	11:J:66:VAL:CG2	2.69	0.40
15:N:97:ILE:CD1	15:N:127:LYS:HD2	2.51	0.40
17:P:49:GLU:HB2	17:P:70:LEU:HD12	2.03	0.40
20:S:106:GLY:HA2	20:S:109:MET:CE	2.48	0.40
22:U:55:PHE:O	22:U:56:ALA:C	2.59	0.40
26:Y:30:MET:CE	26:Y:58:ALA:HB3	2.52	0.40
38:A:8866:HOH:O	29:2:1:THR:HA	2.20	0.40
1:A:1498:G:O2'	1:A:1499:U:H5'	2.21	0.40
1:A:1594:C:C2	1:A:1601:G:C2	3.09	0.40
1:A:1850:U:H2'	1:A:1851:G:C8	2.56	0.40
1:A:1886:A:C5'	38:1:8405:HOH:O	2.69	0.40
1:A:2004:U:H2'	1:A:2005:G:OP1	2.21	0.40
1:A:2364:A:H5''	19:R:15:LYS:HD3	2.03	0.40
1:A:2590:U:H2'	1:A:2591:C:H5'	2.03	0.40
1:A:2620:U:O4	36:5:76:PPU:CA	2.69	0.40
1:A:2649:A:H5'	1:A:2649:A:H8	1.86	0.40
1:A:2868:C:H2'	1:A:2869:G:O4'	2.21	0.40
1:A:329:A:C5	1:A:347:A:C2	3.10	0.40
1:A:585:C:H6	38:A:5555:HOH:O	2.04	0.40
1:A:587:A:H5''	38:A:6745:HOH:O	2.19	0.40
1:A:88:G:H2'	1:A:89:G:C8	2.55	0.40
1:A:958:G:O2'	1:A:959:C:H5'	2.21	0.40
2:B:3050:G:OP1	16:O:147:ILE:CD1	2.68	0.40
2:B:3078:G:O2'	2:B:3079:U:OP2	2.39	0.40
4:C:105:VAL:HG11	4:C:154:ALA:CB	2.51	0.40
5:D:265:LEU:HD21	5:D:316:ARG:HD3	2.02	0.40
6:E:85:LYS:CE	38:E:8328:HOH:O	2.67	0.40
9:H:66:LEU:HD12	9:H:66:LEU:HA	1.85	0.40
11:J:14:TYR:HB2	38:J:8353:HOH:O	2.21	0.40
11:J:35:ASN:HD21	11:J:80:ASN:HA	1.83	0.40
15:N:137:ASP:HA	15:N:142:LYS:HE3	2.03	0.40
24:W:57:LYS:HA	24:W:60:GLN:HE21	1.85	0.40
25:X:151:GLU:O	25:X:154:ARG:HB3	2.20	0.40
26:Y:14:LEU:HD12	26:Y:67:PRO:O	2.21	0.40
1:A:138:U:OP2	1:A:139:C:H5	2.04	0.40
1:A:1517:U:C2	1:A:1670:G:N2	2.89	0.40
1:A:1815:A:H4'	1:A:2751:C:O4'	2.22	0.40
1:A:2355:G:H5''	1:A:2356:A:OP2	2.22	0.40
1:A:2541:U:O2'	1:A:2542:C:H5'	2.21	0.40
1:A:39:G:C2	1:A:444:C:C2	3.10	0.40
1:A:590:A:H2'	1:A:591:A:O4'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:860:U:C2'	38:A:5151:HOH:O	2.69	0.40
2:B:3034:A:H2'	2:B:3035:C:O4'	2.21	0.40
38:A:3897:HOH:O	4:C:11:ARG:CZ	2.70	0.40
1:A:1309:U:OP2	6:E:189:PRO:HA	2.21	0.40
7:F:128:LEU:N	38:F:5495:HOH:O	2.54	0.40
7:F:48:MET:HA	7:F:49:PRO:HD3	1.81	0.40
11:J:31:PHE:HE2	11:J:87:LYS:O	2.04	0.40
11:J:35:ASN:ND2	11:J:79:ALA:O	2.54	0.40
14:M:107:LYS:HD2	14:M:124:ASP:OD2	2.21	0.40
15:N:69:LYS:HD3	15:N:124:GLY:O	2.21	0.40
18:Q:143:ALA:CA	38:Q:197:HOH:O	2.70	0.40
22:U:101:LEU:HD13	22:U:112:LEU:HD11	2.03	0.40
27:Z:144:ARG:NH1	38:Z:8581:HOH:O	2.51	0.40
29:2:25:LYS:CD	30:3:49:GLU:H	2.33	0.40
1:A:1816:C:H2'	1:A:1817:U:O4'	2.21	0.40
1:A:1972:U:H2'	1:A:1973:A:C5'	2.49	0.40
1:A:2011:A:H4'	1:A:2012:U:O5'	2.22	0.40
1:A:220:C:C4'	38:A:5208:HOH:O	2.69	0.40
1:A:2255:A:H2'	1:A:2256:G:O4'	2.21	0.40
1:A:2481:G:C3'	1:A:2482:G:H5''	2.51	0.40
1:A:2533:C:O2'	1:A:2534:C:H5'	2.21	0.40
1:A:269:G:C2	1:A:270:U:O4	2.73	0.40
1:A:682:A:H2'	1:A:683:G:O4'	2.21	0.40
1:A:690:G:H4'	1:A:741:C:O2	2.22	0.40
1:A:2821:C:H4'	5:D:116:PRO:HB3	2.03	0.40
5:D:16:ARG:NH1	38:D:8617:HOH:O	2.53	0.40
5:D:224:LYS:O	5:D:227:HIS:HB2	2.22	0.40
5:D:279:THR:OG1	5:D:290:VAL:HB	2.22	0.40
6:E:123:LEU:HA	6:E:123:LEU:HD23	1.92	0.40
6:E:80:VAL:HA	6:E:81:PRO:HD3	1.94	0.40
1:A:1235:G:C1'	12:K:63:ILE:HG23	2.51	0.40
13:L:66:ARG:HG2	13:L:66:ARG:HH11	1.86	0.40
16:O:37:ARG:CZ	38:O:8534:HOH:O	2.69	0.40
16:O:5:ARG:HG3	19:R:18:PRO:HB3	2.02	0.40
17:P:59:VAL:CG2	17:P:111:VAL:HG23	2.52	0.40
17:P:63:LYS:HG3	17:P:80:ASP:O	2.22	0.40
18:Q:131:PHE:CD1	18:Q:137:LEU:HD13	2.56	0.40
27:Z:189:ASN:ND2	27:Z:189:ASN:C	2.70	0.40
31:4:70:ARG:HD3	38:4:8537:HOH:O	2.21	0.40
1:A:101:C:O2'	1:A:102:A:H5'	2.21	0.40
1:A:1215:A:O3'	1:A:1216:G:C4'	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1252:A:H2'	1:A:1253:C:O4'	2.21	0.40
1:A:1316:G:H1'	1:A:1340:G:N2	2.37	0.40
1:A:2123:A:P	15:N:89:ASN:ND2	2.95	0.40
1:A:2269:C:C2'	1:A:2270:G:H5'	2.51	0.40
1:A:2554:U:C6	1:A:2577:A:N6	2.90	0.40
1:A:299:U:C5'	38:A:6794:HOH:O	2.60	0.40
1:A:382:U:C5	1:A:406:G:C2	3.09	0.40
1:A:545:G:H2'	1:A:546:C:O4'	2.21	0.40
1:A:853:C:H2'	1:A:854:G:O4'	2.21	0.40
1:A:953:G:H2'	38:A:7145:HOH:O	2.22	0.40
2:B:3058:G:H3'	2:B:3059:C:C6	2.56	0.40
5:D:215:VAL:HA	5:D:220:VAL:HG22	2.02	0.40
6:E:3:ALA:N	6:E:16:VAL:O	2.53	0.40
6:E:7:ASP:O	6:E:9:ASP:N	2.55	0.40
1:A:2348:C:C5'	7:F:22:VAL:HG21	2.51	0.40
7:F:51:ARG:HA	38:F:7636:HOH:O	2.22	0.40
8:G:108:LEU:HD11	8:G:164:ASP:HB2	2.04	0.40
10:I:23:ILE:CD1	10:I:67:LEU:HD23	2.41	0.40
11:J:73:GLN:OE1	11:J:73:GLN:CA	2.69	0.40
14:M:72:ASN:HB2	38:M:8585:HOH:O	2.21	0.40
15:N:77:PHE:O	15:N:77:PHE:CD1	2.75	0.40
16:O:114:LYS:O	16:O:117:ALA:HB3	2.21	0.40
16:O:167:ASP:O	16:O:168:LEU:HD23	2.22	0.40
18:Q:16:VAL:CG1	18:Q:17:GLY:N	2.85	0.40
38:L:1387:HOH:O	23:V:20:MET:HE1	2.22	0.40
1:A:1266:U:H4'	27:Z:115:ARG:HH21	1.85	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	
4	C	235/239 (98%)	202 (86%)	29 (12%)	4 (2%)	9	36
5	D	335/337 (99%)	299 (89%)	28 (8%)	8 (2%)	6	27
6	E	244/246 (99%)	222 (91%)	21 (9%)	1 (0%)	34	70
7	F	134/176 (76%)	93 (69%)	29 (22%)	12 (9%)	1	3
8	G	170/177 (96%)	158 (93%)	11 (6%)	1 (1%)	25	61
9	H	117/119 (98%)	100 (86%)	14 (12%)	3 (3%)	5	25
10	I	25/348 (7%)	23 (92%)	1 (4%)	1 (4%)	3	15
11	J	152/167 (91%)	130 (86%)	17 (11%)	5 (3%)	4	19
12	K	140/145 (97%)	129 (92%)	6 (4%)	5 (4%)	3	17
13	L	130/132 (98%)	118 (91%)	10 (8%)	2 (2%)	10	39
14	M	141/164 (86%)	122 (86%)	18 (13%)	1 (1%)	22	58
15	N	192/194 (99%)	173 (90%)	18 (9%)	1 (0%)	29	66
16	O	184/186 (99%)	163 (89%)	13 (7%)	8 (4%)	2	14
17	P	113/115 (98%)	107 (95%)	6 (5%)	0	100	100
18	Q	141/148 (95%)	135 (96%)	5 (4%)	1 (1%)	22	58
19	R	93/95 (98%)	85 (91%)	5 (5%)	3 (3%)	4	20
20	S	148/154 (96%)	135 (91%)	12 (8%)	1 (1%)	22	58
21	T	79/84 (94%)	74 (94%)	5 (6%)	0	100	100
22	U	117/119 (98%)	110 (94%)	7 (6%)	0	100	100
23	V	51/66 (77%)	47 (92%)	4 (8%)	0	100	100
24	W	63/70 (90%)	58 (92%)	3 (5%)	2 (3%)	4	20
25	X	152/154 (99%)	143 (94%)	7 (5%)	2 (1%)	12	43
26	Y	80/91 (88%)	71 (89%)	6 (8%)	3 (4%)	3	16
27	Z	140/240 (58%)	138 (99%)	2 (1%)	0	100	100
28	1	71/73 (97%)	63 (89%)	6 (8%)	2 (3%)	5	23
29	2	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
30	3	42/48 (88%)	42 (100%)	0	0	100	100
31	4	90/92 (98%)	84 (93%)	4 (4%)	2 (2%)	6	29
All	All	3633/4235 (86%)	3276 (90%)	289 (8%)	68 (2%)	8	33

All (68) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	D	139	ASP
7	F	93	LEU
7	F	95	THR
7	F	137	PRO
7	F	173	GLU
9	H	101	ALA
11	J	162	SER
14	M	80	ASP
16	O	154	LEU
16	O	162	ASP
16	O	164	ASP
16	O	183	ASP
26	Y	87	ALA
4	C	34	ASP
5	D	34	GLY
5	D	169	GLY
6	E	8	LEU
7	F	36	ASN
11	J	138	PRO
11	J	164	ALA
12	K	5	GLU
12	K	143	LYS
13	L	119	GLN
16	O	167	ASP
18	Q	116	SER
19	R	89	ALA
24	W	43	PRO
25	X	77	ALA
28	1	81	LYS
31	4	57	GLY
4	C	132	ASP
5	D	184	ASP
7	F	16	PRO
7	F	20	LYS
7	F	61	PHE
7	F	171	ASP
8	G	44	GLY
11	J	40	PRO
12	K	76	ASP
15	N	140	ALA
16	O	181	ASP
25	X	49	ASN
26	Y	77	PHE

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Mol	Chain	Res	Type
31	4	56	PRO
4	C	62	ASP
5	D	107	SER
7	F	11	HIS
7	F	96	SER
7	F	170	TYR
10	I	72	ASP
13	L	126	SER
26	Y	78	GLU
5	D	2	GLN
5	D	185	GLY
9	H	64	PRO
12	K	7	ASP
12	K	50	GLU
16	O	68	GLU
16	O	155	GLU
4	C	37	VAL
9	H	61	MET
19	R	18	PRO
19	R	54	PRO
24	W	40	PRO
11	J	72	VAL
20	S	106	GLY
28	1	41	VAL
5	D	5	ARG

### 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	
4	C	179/181 (99%)	167 (93%)	12 (7%)	16	47
5	D	282/282 (100%)	264 (94%)	18 (6%)	17	49
6	E	193/193 (100%)	176 (91%)	17 (9%)	10	34
7	F	117/147 (80%)	107 (92%)	10 (8%)	10	36
8	G	152/155 (98%)	148 (97%)	4 (3%)	46	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	H	92/92 (100%)	91 (99%)	1 (1%)	73	90
10	I	27/283 (10%)	27 (100%)	0	100	100
11	J	122/122 (100%)	110 (90%)	12 (10%)	8	29
12	K	118/121 (98%)	107 (91%)	11 (9%)	9	31
13	L	106/106 (100%)	103 (97%)	3 (3%)	43	75
14	M	112/126 (89%)	108 (96%)	4 (4%)	35	68
15	N	166/166 (100%)	157 (95%)	9 (5%)	22	55
16	O	149/149 (100%)	143 (96%)	6 (4%)	31	66
17	P	93/93 (100%)	89 (96%)	4 (4%)	29	64
18	Q	113/116 (97%)	110 (97%)	3 (3%)	44	75
19	R	79/79 (100%)	75 (95%)	4 (5%)	24	57
20	S	117/121 (97%)	113 (97%)	4 (3%)	37	70
21	T	71/73 (97%)	70 (99%)	1 (1%)	67	86
22	U	105/105 (100%)	102 (97%)	3 (3%)	42	74
23	V	44/52 (85%)	42 (96%)	2 (4%)	27	62
24	W	51/56 (91%)	49 (96%)	2 (4%)	32	66
25	X	130/130 (100%)	121 (93%)	9 (7%)	15	46
26	Y	66/73 (90%)	61 (92%)	5 (8%)	13	41
27	Z	120/195 (62%)	112 (93%)	8 (7%)	16	47
28	1	56/56 (100%)	50 (89%)	6 (11%)	6	24
29	2	46/46 (100%)	46 (100%)	0	100	100
30	3	42/44 (96%)	41 (98%)	1 (2%)	49	78
31	4	79/79 (100%)	73 (92%)	6 (8%)	13	41
All	All	3027/3441 (88%)	2862 (94%)	165 (6%)	21	55

All (165) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	C	3	ARG
4	C	33	GLU
4	C	36	ASP
4	C	55	VAL
4	C	68	ILE
4	C	69	LEU

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Mol	Chain	Res	Type
4	C	94	LEU
4	C	120	ARG
4	C	131	HIS
4	C	153	ARG
4	C	179	MET
4	C	217	ARG
5	D	7	ARG
5	D	11	LEU
5	D	27	ASN
5	D	33	ASP
5	D	63	GLU
5	D	97	LEU
5	D	98	THR
5	D	103	ASP
5	D	162	MET
5	D	195	ARG
5	D	245	SER
5	D	251	VAL
5	D	254	GLN
5	D	256	GLN
5	D	264	GLU
5	D	304	PRO
5	D	307	ARG
5	D	312	ARG
6	E	2	GLN
6	E	27	ARG
6	E	67	GLN
6	E	76	ARG
6	E	91	PRO
6	E	94	THR
6	E	101	ASP
6	E	115	LEU
6	E	136	VAL
6	E	187	ARG
6	E	214	THR
6	E	222	ASP
6	E	223	LEU
6	E	234	VAL
6	E	236	THR
6	E	240	LEU
6	E	246	ARG
7	F	24	HIS

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Mol	Chain	Res	Type
7	F	50	VAL
7	F	61	PHE
7	F	99	ASP
7	F	100	ASP
7	F	131	THR
7	F	133	ASN
7	F	136	ARG
7	F	137	PRO
7	F	149	ARG
8	G	7	ILE
8	G	54	ASP
8	G	102	VAL
8	G	164	ASP
9	H	12	LEU
11	J	1	LYS
11	J	59	ASN
11	J	61	LEU
11	J	72	VAL
11	J	73	GLN
11	J	82	LYS
11	J	85	ILE
11	J	86	ARG
11	J	94	ARG
11	J	142	VAL
11	J	150	LYS
11	J	166	ASN
12	K	46	ILE
12	K	52	GLN
12	K	74	ARG
12	K	76	ASP
12	K	79	PHE
12	K	107	ASN
12	K	112	ASP
12	K	120	SER
12	K	125	SER
12	K	127	ILE
12	K	131	THR
13	L	7	ASP
13	L	10	GLN
13	L	98	VAL
14	M	30	ARG
14	M	35	ARG

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Mol	Chain	Res	Type
14	M	80	ASP
14	M	117	GLU
15	N	38	VAL
15	N	46	LEU
15	N	68	ARG
15	N	81	ARG
15	N	87	MET
15	N	93	ARG
15	N	99	ARG
15	N	136	PRO
15	N	164	THR
16	O	26	LEU
16	O	47	LEU
16	O	127	LEU
16	O	128	ASP
16	O	152	GLU
16	O	163	PHE
17	P	3	THR
17	P	28	ASP
17	P	98	LEU
17	P	111	VAL
18	Q	52	LYS
18	Q	91	LYS
18	Q	98	ILE
19	R	11	ARG
19	R	16	ASN
19	R	57	ASP
19	R	95	GLU
20	S	13	THR
20	S	39	THR
20	S	82	GLU
20	S	132	ARG
21	T	10	VAL
22	U	39	ASN
22	U	48	VAL
22	U	73	HIS
23	V	9	CYS
23	V	32	CYS
24	W	43	PRO
24	W	65	ASP
25	X	4	LEU
25	X	35	VAL

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Mol	Chain	Res	Type
25	X	52	VAL
25	X	73	LEU
25	X	120	PRO
25	X	122	ARG
25	X	142	ASP
25	X	146	ILE
25	X	154	ARG
26	Y	15	ARG
26	Y	27	ASP
26	Y	44	ASP
26	Y	52	PRO
26	Y	72	VAL
27	Z	154	ARG
27	Z	163	THR
27	Z	172	THR
27	Z	186	ARG
27	Z	189	ASN
27	Z	200	THR
27	Z	203	VAL
27	Z	235	GLU
28	1	11	THR
28	1	32	LYS
28	1	42	CYS
28	1	60	CYS
28	1	64	ILE
28	1	68	CYS
30	3	18	ASN
31	4	3	MET
31	4	14	CYS
31	4	42	ARG
31	4	56	PRO
31	4	65	THR
31	4	74	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

Mol	Chain	Res	Type
4	C	47	HIS
4	C	92	ASN
4	C	127	GLN
4	C	199	HIS
5	D	27	ASN

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Mol	Chain	Res	Type
5	D	145	HIS
5	D	221	GLN
5	D	238	ASN
5	D	256	GLN
5	D	260	HIS
5	D	332	ASN
6	E	2	GLN
6	E	39	GLN
6	E	129	HIS
7	F	85	GLN
7	F	103	ASN
7	F	133	ASN
8	G	106	ASN
8	G	143	GLN
10	I	17	GLN
10	I	64	ASN
11	J	35	ASN
11	J	55	GLN
11	J	58	HIS
11	J	59	ASN
11	J	69	ASN
11	J	74	ASN
11	J	91	HIS
11	J	129	ASN
11	J	130	HIS
11	J	166	ASN
12	K	52	GLN
12	K	107	ASN
13	L	10	GLN
14	M	18	HIS
14	M	41	HIS
14	M	58	GLN
14	M	116	HIS
15	N	26	HIS
15	N	58	GLN
15	N	89	ASN
15	N	176	GLN
16	O	93	GLN
16	O	107	ASN
16	O	119	GLN
16	O	140	GLN
16	O	153	GLN

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Mol	Chain	Res	Type
18	Q	50	GLN
18	Q	66	GLN
18	Q	73	HIS
18	Q	118	GLN
19	R	16	ASN
19	R	40	HIS
20	S	61	GLN
20	S	94	ASN
20	S	98	ASN
20	S	113	HIS
20	S	117	HIS
20	S	123	GLN
21	T	53	ASN
22	U	39	ASN
22	U	73	HIS
23	V	39	ASN
23	V	48	ASN
24	W	60	GLN
25	X	27	HIS
25	X	28	HIS
25	X	87	HIS
25	X	110	GLN
25	X	119	HIS
25	X	125	HIS
25	X	141	HIS
26	Y	23	HIS
27	Z	134	HIS
27	Z	149	GLN
27	Z	189	ASN
28	1	70	GLN
29	2	8	GLN
29	2	16	HIS
29	2	28	HIS
30	3	16	ASN
30	3	18	ASN
30	3	37	HIS
30	3	41	HIS
30	3	45	ASN
31	4	30	GLN
31	4	48	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2747/2922 (94%)	248 (9%)	36 (1%)
2	B	121/122 (99%)	18 (14%)	5 (4%)
3	5	1/2 (50%)	0	0
All	All	2869/3046 (94%)	266 (9%)	41 (1%)

All (266) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	11	A
1	A	31	C
1	A	60	A
1	A	67	A
1	A	69	A
1	A	70	A
1	A	71	G
1	A	87	C
1	A	88	G
1	A	114	A
1	A	115	U
1	A	120	A
1	A	130	C
1	A	139	C
1	A	141	C
1	A	151	A
1	A	166	A
1	A	169	A
1	A	186	A
1	A	191	A
1	A	192	A
1	A	200	U
1	A	219	G
1	A	237	G
1	A	271	C
1	A	272	A
1	A	273	G
1	A	283	U
1	A	284	C
1	A	285	A
1	A	308	U
1	A	309	C
1	A	318	C
1	A	336	G
1	A	337	A

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Mol	Chain	Res	Type
1	A	345	G
1	A	358	G
1	A	381	G
1	A	397	A
1	A	417	G
1	A	461	C
1	A	487	G
1	A	498	A
1	A	510	U
1	A	511	A
1	A	514	G
1	A	537	G
1	A	538	C
1	A	539	G
1	A	542	A
1	A	545	G
1	A	553	G
1	A	559	U
1	A	588	G
1	A	604	G
1	A	620	A
1	A	632	A
1	A	644	G
1	A	660	A
1	A	688	A
1	A	701	U
1	A	717	C
1	A	759	C
1	A	777	U
1	A	809	G
1	A	821	U
1	A	835	U
1	A	840	U
1	A	857	A
1	A	858	U
1	A	868	G
1	A	869	G
1	A	871	G
1	A	872	U
1	A	875	A
1	A	877	G
1	A	878	G

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Mol	Chain	Res	Type
1	A	882	A
1	A	884	C
1	A	885	G
1	A	898	G
1	A	905	C
1	A	920	C
1	A	921	G
1	A	923	A
1	A	953	G
1	A	960	G
1	A	961	A
1	A	1006	A
1	A	1008	C
1	A	1029	U
1	A	1045	G
1	A	1059	G
1	A	1060	C
1	A	1072	G
1	A	1081	A
1	A	1088	A
1	A	1109	U
1	A	1110	G
1	A	1119	G
1	A	1130	U
1	A	1137	G
1	A	1161	A
1	A	1162	G
1	A	1164	U
1	A	1165	G
1	A	1166	A
1	A	1171	A
1	A	1174	A
1	A	1175	G
1	A	1177	A
1	A	1185	U
1	A	1192	A
1	A	1193	A
1	A	1206	U
1	A	1208	C
1	A	1216	G
1	A	1237	U
1	A	1238	C

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Mol	Chain	Res	Type
1	A	1239	G
1	A	1279	U
1	A	1289	C
1	A	1342	C
1	A	1353	C
1	A	1360	C
1	A	1377	C
1	A	1380	U
1	A	1407	A
1	A	1409	G
1	A	1451	C
1	A	1474	C
1	A	1485	A
1	A	1488	U
1	A	1505	U
1	A	1506	U
1	A	1524	U
1	A	1525	G
1	A	1526	A
1	A	1528	A
1	A	1564	C
1	A	1580	A
1	A	1592	G
1	A	1625	U
1	A	1626	A
1	A	1633	C
1	A	1634	G
1	A	1656	A
1	A	1667	A
1	A	1682	A
1	A	1684	A
1	A	1685	A
1	A	1692	C
1	A	1701	A
1	A	1710	A
1	A	1722	U
1	A	1723	G
1	A	1725	C
1	A	1731	C
1	A	1737	A
1	A	1752	G
1	A	1778	A

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Mol	Chain	Res	Type
1	A	1798	C
1	A	1820	G
1	A	1829	A
1	A	1856	C
1	A	1879	U
1	A	1904	A
1	A	1919	A
1	A	1942	A
1	A	1971	G
1	A	1973	A
1	A	1974	G
1	A	1978	A
1	A	1979	G
1	A	1980	U
1	A	1982	C
1	A	1996	U
1	A	2004	U
1	A	2006	C
1	A	2008	U
1	A	2011	A
1	A	2012	U
1	A	2013	G
1	A	2033	G
1	A	2034	U
1	A	2064	U
1	A	2072	G
1	A	2073	G
1	A	2074	A
1	A	2096	A
1	A	2101	A
1	A	2102	G
1	A	2110	G
1	A	2238	A
1	A	2258	A
1	A	2271	G
1	A	2272	G
1	A	2317	C
1	A	2321	A
1	A	2346	C
1	A	2354	A
1	A	2361	A
1	A	2369	A

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Mol	Chain	Res	Type
1	A	2422	U
1	A	2462	G
1	A	2466	G
1	A	2467	A
1	A	2469	A
1	A	2476	C
1	A	2480	G
1	A	2483	A
1	A	2507	G
1	A	2511	A
1	A	2533	C
1	A	2537	G
1	A	2541	U
1	A	2553	A
1	A	2564	G
1	A	2589	U
1	A	2590	U
1	A	2601	A
1	A	2602	G
1	A	2608	C
1	A	2613	G
1	A	2638	G
1	A	2649	A
1	A	2664	A
1	A	2681	A
1	A	2682	C
1	A	2726	U
1	A	2747	C
1	A	2748	G
1	A	2749	U
1	A	2750	G
1	A	2762	C
1	A	2768	A
1	A	2786	G
1	A	2792	A
1	A	2800	A
1	A	2811	A
1	A	2812	A
1	A	2825	C
1	A	2840	A
1	A	2850	C
1	A	2876	G

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Mol	Chain	Res	Type
1	A	2890	A
1	A	2896	A
1	A	2914	A
2	B	3002	U
2	B	3003	A
2	B	3007	G
2	B	3014	G
2	B	3022	G
2	B	3023	U
2	B	3024	U
2	B	3025	G
2	B	3026	C
2	B	3041	C
2	B	3043	G
2	B	3044	A
2	B	3052	A
2	B	3057	A
2	B	3066	G
2	B	3077	A
2	B	3114	G
2	B	3122	C

All (41) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	10	U
1	A	69	A
1	A	129	A
1	A	284	C
1	A	338	C
1	A	603	A
1	A	644	G
1	A	699	C
1	A	716	G
1	A	834	G
1	A	857	A
1	A	871	G
1	A	877	G
1	A	898	G
1	A	1080	C
1	A	1164	U
1	A	1237	U

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Mol	Chain	Res	Type
1	A	1246	A
1	A	1352	A
1	A	1377	C
1	A	1450	C
1	A	1563	G
1	A	1685	A
1	A	1856	C
1	A	1942	A
1	A	1979	G
1	A	2011	A
1	A	2313	C
1	A	2466	G
1	A	2467	A
1	A	2526	C
1	A	2536	C
1	A	2649	A
1	A	2718	C
1	A	2761	A
1	A	2791	U
2	B	3023	U
2	B	3024	U
2	B	3043	G
2	B	3065	A
2	B	3103	A

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 233 ligands modelled in this entry, 232 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
36	PPU	5	76	3	32,40,41	2.22	12 (37%)	33,57,60	1.72	6 (18%)

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
36	PPU	5	76	3	-	2/21/43/44	0/4/4/4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	76	PPU	CB-CG	4.78	1.62	1.51
36	5	76	PPU	C-N3'	4.39	1.43	1.34
36	5	76	PPU	C10-N6	-4.04	1.36	1.45
36	5	76	PPU	CE2-CD2	-3.75	1.31	1.38
36	5	76	PPU	O-C	3.58	1.30	1.23
36	5	76	PPU	C9-N6	-3.56	1.37	1.45
36	5	76	PPU	CD1-CG	-3.50	1.31	1.38
36	5	76	PPU	CE1-CD1	-3.00	1.33	1.38
36	5	76	PPU	CE1-CZ	2.42	1.43	1.38
36	5	76	PPU	O2'-C2'	-2.41	1.37	1.43
36	5	76	PPU	CA-N	2.33	1.61	1.48
36	5	76	PPU	C2-N1	2.31	1.38	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	76	PPU	CA-C-N3'	-4.23	110.28	116.15
36	5	76	PPU	C3'-N3'-C	-4.06	117.09	123.21
36	5	76	PPU	CG-CB-CA	-3.92	105.98	114.13
36	5	76	PPU	CM-OC-CZ	3.20	124.45	117.51
36	5	76	PPU	O4'-C1'-C2'	2.99	111.29	106.93
36	5	76	PPU	CE2-CZ-CE1	-2.15	116.86	120.18

There are no chirality outliers.

All (2) torsion outliers are listed below:

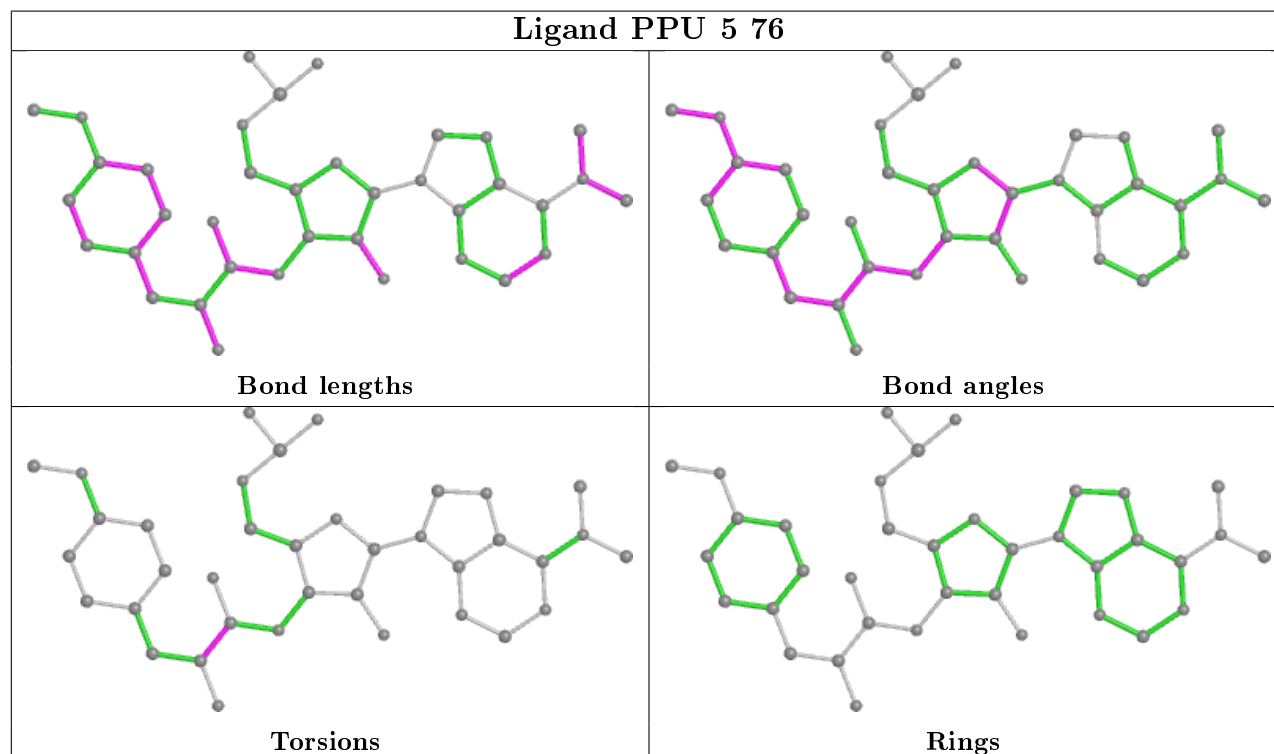
Mol	Chain	Res	Type	Atoms
36	5	76	PPU	O-C-CA-CB
36	5	76	PPU	N3'-C-CA-CB

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	5	76	PPU	4	0

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	A	2754/2922 (94%)	0.09	83 (3%) 50 31	19, 45, 94, 144	0
2	B	122/122 (100%)	0.48	6 (4%) 29 17	33, 67, 97, 147	0
3	5	2/2 (100%)	2.10	1 (50%) 0 0	65, 65, 65, 87	0
4	C	237/239 (99%)	0.59	26 (10%) 5 3	30, 62, 97, 109	0
5	D	337/337 (100%)	0.18	6 (1%) 68 48	22, 50, 77, 89	0
6	E	246/246 (100%)	0.06	5 (2%) 65 45	20, 44, 69, 78	0
7	F	140/176 (79%)	2.16	66 (47%) 0 0	65, 101, 122, 128	0
8	G	172/177 (97%)	0.94	17 (9%) 7 4	38, 62, 84, 89	0
9	H	119/119 (100%)	0.96	24 (20%) 1 0	51, 76, 99, 107	0
10	I	29/348 (8%)	2.38	17 (58%) 0 0	66, 87, 95, 99	0
11	J	156/167 (93%)	0.76	16 (10%) 6 3	35, 59, 82, 89	0
12	K	142/145 (97%)	0.08	2 (1%) 75 57	32, 44, 67, 78	0
13	L	132/132 (100%)	0.26	2 (1%) 73 54	33, 49, 75, 82	0
14	M	145/164 (88%)	1.29	40 (27%) 0 0	26, 79, 106, 111	0
15	N	194/194 (100%)	0.63	22 (11%) 5 3	28, 47, 106, 118	0
16	O	186/186 (100%)	1.10	35 (18%) 1 0	46, 73, 112, 125	0
17	P	115/115 (100%)	0.26	1 (0%) 84 69	36, 53, 68, 72	0
18	Q	143/148 (96%)	0.56	8 (5%) 24 13	34, 53, 76, 85	0
19	R	95/95 (100%)	0.21	3 (3%) 47 29	36, 47, 63, 82	0
20	S	150/154 (97%)	-0.00	0 100 100	26, 40, 61, 72	0
21	T	81/84 (96%)	0.52	4 (4%) 29 17	44, 62, 82, 88	0
22	U	119/119 (100%)	0.82	11 (9%) 9 5	40, 55, 84, 104	0
23	V	53/66 (80%)	2.37	29 (54%) 0 0	77, 92, 100, 108	0
24	W	65/70 (92%)	1.43	21 (32%) 0 0	46, 76, 111, 115	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	X	154/154 (100%)	0.08	0 100 100	28, 42, 59, 70	0
26	Y	82/91 (90%)	0.71	10 (12%) 4 2	37, 53, 77, 91	0
27	Z	142/240 (59%)	0.17	6 (4%) 36 21	25, 41, 64, 82	0
28	1	73/73 (100%)	5.61	53 (72%) 0 0	93, 115, 125, 127	0
29	2	56/56 (100%)	-0.25	0 100 100	22, 32, 40, 45	0
30	3	46/48 (95%)	0.88	7 (15%) 2 1	34, 63, 96, 105	0
31	4	92/92 (100%)	8.87	92 (100%) 0 0	110, 125, 133, 136	0
All	All	6579/7281 (90%)	0.56	613 (9%) 8 5	19, 52, 105, 147	0

All (613) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
31	4	82	GLY	29.1
28	1	11	THR	19.9
31	4	37	ASP	18.9
31	4	83	TRP	18.6
31	4	62	THR	17.9
28	1	26	VAL	16.0
31	4	11	CYS	15.0
31	4	1	MET	14.9
28	1	20	LEU	13.7
31	4	38	ARG	13.6
31	4	31	THR	13.1
28	1	15	GLY	13.1
31	4	20	HIS	13.1
31	4	10	TYR	13.0
31	4	14	CYS	13.0
31	4	91	GLN	12.9
28	1	12	GLY	12.8
31	4	39	GLN	12.6
31	4	71	CYS	12.4
31	4	76	LYS	12.3
31	4	33	MET	12.1
31	4	35	TRP	12.0
28	1	30	GLU	12.0
15	N	71	SER	11.8
31	4	36	ILE	11.7
24	W	1	THR	11.6
28	1	19	GLY	11.6
28	1	34	LYS	11.6

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Mol	Chain	Res	Type	RSRZ
31	4	78	HIS	11.5
28	1	23	ARG	11.2
31	4	44	SER	11.2
31	4	34	LYS	11.1
31	4	22	VAL	11.0
31	4	41	GLU	10.9
28	1	14	PHE	10.8
31	4	4	PRO	10.7
31	4	85	ALA	10.6
28	1	16	PRO	10.6
28	1	31	ILE	10.6
31	4	9	THR	10.4
31	4	59	ASP	10.3
31	4	65	THR	10.3
31	4	84	ARG	10.2
31	4	16	GLU	10.2
28	1	22	ILE	10.1
31	4	18	GLN	10.0
31	4	15	ASN	10.0
31	4	67	LEU	10.0
28	1	39	CYS	10.0
31	4	27	SER	9.6
31	4	86	GLY	9.6
31	4	23	GLU	9.6
31	4	17	HIS	9.6
28	1	35	LYS	9.6
31	4	68	LYS	9.5
15	N	89	ASN	9.5
28	1	28	ASP	9.4
31	4	74	CYS	9.4
28	1	44	PHE	9.3
31	4	3	MET	9.1
31	4	13	HIS	9.1
31	4	42	ARG	9.0
28	1	45	LYS	9.0
31	4	77	ALA	9.0
2	B	3001	U	8.8
31	4	60	LYS	8.8
31	4	8	ASN	8.6
31	4	88	LEU	8.6
28	1	33	HIS	8.5
31	4	32	GLY	8.5

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Mol	Chain	Res	Type	RSRZ
31	4	2	GLN	8.5
31	4	21	GLU	8.2
28	1	25	ARG	8.1
31	4	81	GLU	8.1
7	F	69	ILE	8.1
28	1	24	VAL	8.0
31	4	61	PRO	8.0
15	N	80	GLY	7.9
7	F	57	THR	7.9
31	4	43	ASN	7.7
28	1	32	LYS	7.7
31	4	56	PRO	7.6
31	4	51	LYS	7.6
28	1	18	TYR	7.5
7	F	63	ILE	7.5
31	4	47	GLY	7.3
15	N	78	ASN	7.2
28	1	42	CYS	7.2
31	4	80	ARG	7.1
28	1	57	CYS	7.0
28	1	27	ALA	7.0
31	4	75	GLY	7.0
31	4	12	PRO	7.0
31	4	6	ARG	7.0
31	4	30	GLN	6.9
28	1	10	ARG	6.9
28	1	29	VAL	6.8
31	4	63	LYS	6.7
31	4	69	TYR	6.7
28	1	21	LYS	6.7
15	N	70	GLY	6.7
31	4	19	GLU	6.6
31	4	53	SER	6.5
10	I	27	ILE	6.5
28	1	43	GLY	6.4
31	4	45	GLY	6.4
1	A	735	C	6.2
31	4	58	GLY	6.1
28	1	13	ARG	6.1
31	4	90	PHE	6.0
31	4	72	GLY	6.0
7	F	56	ARG	6.0

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Mol	Chain	Res	Type	RSRZ
31	4	52	PHE	6.0
16	O	179	LEU	5.9
31	4	46	ILE	5.9
31	4	70	ARG	5.8
28	1	41	VAL	5.8
31	4	40	ARG	5.8
31	4	48	ASN	5.8
1	A	1198	U	5.8
31	4	92	GLU	5.8
14	M	44	GLU	5.7
31	4	26	ARG	5.7
7	F	10	PHE	5.7
7	F	66	GLY	5.6
14	M	36	ASP	5.6
14	M	60	GLU	5.6
23	V	52	THR	5.6
15	N	81	ARG	5.5
15	N	83	SER	5.5
28	1	17	ARG	5.4
16	O	162	ASP	5.4
15	N	77	PHE	5.4
31	4	66	ASP	5.3
16	O	186	LEU	5.3
14	M	42	ASN	5.3
28	1	38	LYS	5.3
16	O	138	ASP	5.2
2	B	3025	G	5.2
15	N	90	ARG	5.2
31	4	55	VAL	5.2
23	V	48	ASN	5.1
28	1	40	PRO	5.1
1	A	1173	A	5.1
23	V	54	THR	5.1
31	4	87	ARG	5.0
22	U	119	ALA	5.0
16	O	184	ILE	5.0
11	J	83	PHE	5.0
16	O	160	SER	5.0
30	3	36	ASN	5.0
31	4	89	GLU	5.0
28	1	37	HIS	5.0
30	3	39	ARG	5.0

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Mol	Chain	Res	Type	RSRZ
10	I	23	ILE	4.9
7	F	87	ALA	4.9
24	W	39	ALA	4.9
7	F	64	ARG	4.9
1	A	1177	A	4.8
7	F	27	ILE	4.8
7	F	88	LEU	4.8
1	A	1171	A	4.8
23	V	55	ALA	4.8
31	4	29	ARG	4.8
14	M	133	VAL	4.8
23	V	51	TRP	4.7
31	4	28	GLY	4.7
31	4	49	ASP	4.7
15	N	72	SER	4.7
15	N	88	VAL	4.6
23	V	9	CYS	4.6
31	4	64	LYS	4.6
15	N	74	ARG	4.6
31	4	5	ARG	4.6
28	1	79	VAL	4.5
7	F	25	MET	4.5
16	O	163	PHE	4.5
15	N	82	ARG	4.5
26	Y	88	GLU	4.4
15	N	75	THR	4.4
14	M	34	GLY	4.4
14	M	80	ASP	4.4
31	4	24	LYS	4.4
7	F	75	LEU	4.4
28	1	53	GLY	4.4
31	4	73	GLU	4.3
7	F	90	LEU	4.3
14	M	46	LEU	4.3
28	1	47	LEU	4.3
28	1	58	GLY	4.3
15	N	73	ARG	4.3
31	4	79	LEU	4.3
16	O	167	ASP	4.2
1	A	1199	A	4.2
1	A	1951	G	4.2
2	B	3002	U	4.2

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Mol	Chain	Res	Type	RSRZ
7	F	166	ILE	4.2
7	F	61	PHE	4.1
28	1	55	TRP	4.1
9	H	106	THR	4.1
8	G	45	ASP	4.1
11	J	135	TRP	4.1
16	O	147	ILE	4.1
4	C	37	VAL	4.1
28	1	36	LYS	4.1
23	V	53	ASP	4.0
31	4	50	GLY	4.0
21	T	81	ILE	4.0
23	V	46	ALA	4.0
1	A	2237	G	4.0
14	M	47	GLY	4.0
14	M	45	PRO	4.0
23	V	47	ARG	4.0
28	1	46	LYS	3.9
16	O	159	TYR	3.9
28	1	82	ALA	3.9
7	F	86	THR	3.9
7	F	26	GLY	3.9
31	4	7	PHE	3.9
14	M	130	ARG	3.9
7	F	96	SER	3.9
19	R	95	GLU	3.9
23	V	11	THR	3.9
7	F	47	GLN	3.8
7	F	134	LEU	3.8
23	V	6	CYS	3.8
7	F	44	ILE	3.8
10	I	26	MET	3.8
7	F	18	ILE	3.8
28	1	59	HIS	3.8
28	1	80	MET	3.8
31	4	57	GLY	3.8
16	O	185	GLU	3.8
1	A	1172	G	3.8
7	F	58	VAL	3.7
16	O	80	SER	3.7
16	O	78	MET	3.7
7	F	92	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
7	F	83	PHE	3.7
1	A	282	C	3.6
18	Q	137	LEU	3.6
14	M	124	ASP	3.6
7	F	93	LEU	3.6
14	M	73	VAL	3.6
10	I	15	TRP	3.6
18	Q	110	ASP	3.6
9	H	107	VAL	3.6
16	O	172	PHE	3.6
24	W	40	PRO	3.6
1	A	1181	A	3.6
10	I	20	VAL	3.5
8	G	100	ASP	3.5
14	M	104	ASP	3.5
9	H	19	ALA	3.5
7	F	49	PRO	3.5
7	F	171	ASP	3.5
1	A	1175	G	3.5
9	H	16	ALA	3.4
24	W	61	GLY	3.4
4	C	82	VAL	3.4
15	N	87	MET	3.4
4	C	60	PHE	3.4
10	I	65	THR	3.4
3	5	74	C	3.4
14	M	106	VAL	3.4
23	V	39	ASN	3.4
10	I	67	LEU	3.4
24	W	8	ILE	3.4
4	C	91	GLY	3.4
7	F	130	VAL	3.4
7	F	11	HIS	3.4
4	C	36	ASP	3.4
9	H	17	LEU	3.3
24	W	37	GLY	3.3
14	M	105	TYR	3.3
23	V	43	GLY	3.3
2	B	3122	C	3.3
14	M	38	HIS	3.3
14	M	59	GLU	3.3
1	A	970	U	3.3

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Mol	Chain	Res	Type	RSRZ
23	V	49	LEU	3.3
5	D	1	PRO	3.3
10	I	71	LEU	3.3
4	C	38	ILE	3.3
28	1	60	CYS	3.3
14	M	43	HIS	3.3
1	A	736	A	3.2
8	G	108	LEU	3.2
23	V	40	ALA	3.2
6	E	135	GLU	3.2
24	W	38	GLY	3.2
16	O	139	TRP	3.2
7	F	170	TYR	3.2
14	M	81	VAL	3.2
15	N	79	LYS	3.2
23	V	50	GLU	3.2
1	A	2345	A	3.2
11	J	146	TRP	3.2
7	F	84	LEU	3.2
9	H	119	ARG	3.2
11	J	139	ASP	3.2
7	F	24	HIS	3.1
22	U	112	LEU	3.1
28	1	56	MET	3.1
7	F	62	ASP	3.1
1	A	1947	G	3.1
14	M	123	ASP	3.1
2	B	3023	U	3.1
1	A	1169	U	3.1
1	A	2004	U	3.1
9	H	22	VAL	3.1
4	C	85	ASP	3.1
7	F	65	GLU	3.1
1	A	1163	G	3.1
10	I	66	LEU	3.1
14	M	41	HIS	3.1
23	V	56	ARG	3.1
24	W	52	ALA	3.1
1	A	1182	C	3.1
27	Z	108	ASP	3.1
9	H	44	SER	3.1
7	F	54	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
24	W	3	LEU	3.1
22	U	116	ASP	3.1
1	A	1948	G	3.1
4	C	237	GLY	3.1
16	O	74	PRO	3.1
16	O	75	THR	3.1
4	C	133	ARG	3.0
9	H	26	THR	3.0
1	A	1170	U	3.0
30	3	35	ARG	3.0
16	O	127	LEU	3.0
16	O	158	LEU	3.0
1	A	1190	G	3.0
14	M	140	VAL	3.0
4	C	96	LEU	3.0
23	V	13	ILE	3.0
8	G	22	VAL	3.0
7	F	68	PRO	3.0
18	Q	116	SER	3.0
9	H	20	LEU	2.9
4	C	31	LYS	2.9
11	J	36	ASN	2.9
1	A	1168	C	2.9
1	A	1202	A	2.9
7	F	50	VAL	2.9
14	M	48	LYS	2.9
14	M	118	LEU	2.9
7	F	23	VAL	2.9
9	H	102	GLY	2.9
23	V	36	CYS	2.9
26	Y	7	GLU	2.9
15	N	68	ARG	2.9
26	Y	82	GLU	2.9
1	A	2344	G	2.9
1	A	1162	G	2.9
7	F	22	VAL	2.9
4	C	84	VAL	2.9
22	U	37	GLN	2.9
11	J	35	ASN	2.9
23	V	12	ASP	2.9
7	F	51	ARG	2.9
15	N	86	MET	2.9

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Mol	Chain	Res	Type	RSRZ
7	F	28	GLY	2.8
14	M	89	PHE	2.8
9	H	98	VAL	2.8
21	T	77	VAL	2.8
1	A	1200	A	2.8
14	M	102	ASP	2.8
16	O	175	LEU	2.8
7	F	85	GLN	2.8
11	J	81	TYR	2.8
7	F	43	GLU	2.8
1	A	2239	C	2.8
1	A	960	G	2.8
8	G	131	LEU	2.8
11	J	70	ARG	2.8
7	F	128	LEU	2.8
7	F	17	ARG	2.8
9	H	15	ASP	2.8
26	Y	80	GLU	2.8
1	A	281	U	2.8
31	4	25	VAL	2.8
7	F	45	THR	2.8
24	W	62	GLU	2.7
7	F	159	PRO	2.7
26	Y	10	VAL	2.7
1	A	1525	G	2.7
15	N	76	ARG	2.7
22	U	27	LEU	2.7
1	A	2637	A	2.7
1	A	1180	U	2.7
23	V	29	THR	2.7
1	A	1000	C	2.7
4	C	80	LEU	2.7
7	F	67	ASP	2.7
10	I	24	VAL	2.7
16	O	155	GLU	2.7
24	W	2	VAL	2.7
10	I	68	GLU	2.7
22	U	42	VAL	2.7
7	F	42	GLY	2.7
9	H	101	ALA	2.7
1	A	1192	A	2.6
1	A	2238	A	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	2433	A	2.6
9	H	18	GLU	2.6
30	3	37	HIS	2.6
1	A	806	A	2.6
1	A	1929	G	2.6
1	A	1950	G	2.6
1	A	280	C	2.6
23	V	4	ARG	2.6
1	A	1913	C	2.6
1	A	2508	C	2.6
8	G	129	GLU	2.6
16	O	142	THR	2.6
16	O	178	THR	2.5
27	Z	235	GLU	2.5
14	M	37	LYS	2.5
9	H	103	ALA	2.5
22	U	99	THR	2.5
1	A	10	U	2.5
4	C	64	ASP	2.5
23	V	45	GLU	2.5
24	W	11	MET	2.5
24	W	41	GLU	2.5
10	I	69	ARG	2.5
4	C	58	VAL	2.5
18	Q	1	THR	2.5
9	H	90	GLU	2.5
28	1	62	TYR	2.5
14	M	69	ILE	2.5
23	V	22	VAL	2.5
1	A	1925	G	2.5
1	A	2250	G	2.5
30	3	48	ASP	2.5
4	C	62	ASP	2.5
11	J	32	ASP	2.5
1	A	1167	G	2.5
7	F	80	ALA	2.5
16	O	81	ALA	2.5
10	I	63	ARG	2.5
7	F	55	LYS	2.5
1	A	2249	G	2.5
23	V	33	SER	2.4
23	V	44	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1166	A	2.4
1	A	1626	A	2.4
7	F	71	ALA	2.4
5	D	329	TYR	2.4
24	W	59	ILE	2.4
1	A	368	C	2.4
27	Z	98	GLN	2.4
1	A	138	U	2.4
1	A	1165	G	2.4
8	G	6	GLU	2.4
16	O	68	GLU	2.4
31	4	54	LYS	2.4
21	T	49	VAL	2.4
22	U	40	VAL	2.4
22	U	117	ASP	2.4
24	W	63	GLU	2.4
4	C	128	LEU	2.4
9	H	75	ILE	2.4
9	H	49	PHE	2.4
11	J	142	VAL	2.4
27	Z	234	VAL	2.4
7	F	73	VAL	2.4
8	G	1	PRO	2.4
14	M	108	VAL	2.4
8	G	43	ASP	2.4
5	D	117	GLU	2.4
22	U	80	GLU	2.4
1	A	1185	U	2.4
1	A	285	A	2.4
14	M	120	LEU	2.4
30	3	44	ARG	2.4
1	A	1204	C	2.4
1	A	1949	G	2.3
1	A	130	C	2.3
16	O	157	PRO	2.3
24	W	45	ARG	2.3
10	I	64	ASN	2.3
7	F	70	GLY	2.3
26	Y	85	VAL	2.3
4	C	112	PRO	2.3
11	J	114	PRO	2.3
14	M	39	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
18	Q	141	ILE	2.3
30	3	49	GLU	2.3
7	F	158	ASN	2.3
1	A	1527	A	2.3
4	C	129	LEU	2.3
7	F	102	GLY	2.3
7	F	89	PRO	2.3
8	G	85	GLU	2.3
10	I	13	PRO	2.3
26	Y	74	ALA	2.3
5	D	169	GLY	2.3
18	Q	120	ARG	2.3
8	G	95	VAL	2.3
13	L	119	GLN	2.3
4	C	88	ILE	2.3
24	W	6	GLN	2.3
4	C	135	VAL	2.3
14	M	101	ASP	2.3
16	O	83	LEU	2.3
4	C	99	ILE	2.3
8	G	20	ILE	2.3
11	J	85	ILE	2.3
19	R	75	ILE	2.3
7	F	81	GLU	2.3
22	U	118	SER	2.3
11	J	84	ARG	2.3
23	V	10	GLY	2.3
1	A	1665	G	2.3
1	A	1971	G	2.3
9	H	47	LEU	2.2
14	M	40	PHE	2.2
21	T	45	TYR	2.2
16	O	115	VAL	2.2
24	W	9	ARG	2.2
1	A	2507	G	2.2
2	B	3024	U	2.2
9	H	100	ASP	2.2
23	V	8	TYR	2.2
1	A	999	C	2.2
4	C	65	ARG	2.2
1	A	2252	A	2.2
8	G	10	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1195	G	2.2
14	M	129	ALA	2.2
1	A	284	C	2.2
1	A	283	U	2.2
1	A	1279	U	2.2
9	H	28	ALA	2.2
24	W	4	HIS	2.2
28	1	61	GLY	2.2
8	G	87	PHE	2.2
27	Z	226	ILE	2.2
17	P	51	TYR	2.2
16	O	71	TRP	2.2
5	D	104	GLU	2.2
9	H	71	GLY	2.2
28	1	51	GLY	2.2
23	V	41	ASP	2.2
18	Q	77	ALA	2.2
1	A	1189	A	2.2
1	A	1919	A	2.2
11	J	163	PRO	2.2
1	A	805	G	2.2
15	N	152	ARG	2.2
1	A	1967	U	2.2
24	W	46	ILE	2.2
28	1	54	ILE	2.2
6	E	244	ALA	2.2
12	K	8	ALA	2.2
26	Y	72	VAL	2.2
8	G	118	ILE	2.1
28	1	49	ARG	2.1
7	F	15	GLU	2.1
14	M	35	ARG	2.1
16	O	143	ARG	2.1
24	W	7	GLU	2.1
1	A	601	G	2.1
16	O	150	TYR	2.1
18	Q	114	LEU	2.1
1	A	2432	C	2.1
15	N	165	SER	2.1
7	F	156	ARG	2.1
26	Y	77	PHE	2.1
14	M	99	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
8	G	73	PHE	2.1
6	E	132	ASP	2.1
16	O	152	GLU	2.1
13	L	21	ALA	2.1
1	A	737	A	2.1
7	F	13	MET	2.1
6	E	245	GLU	2.1
16	O	180	LEU	2.1
4	C	34	ASP	2.1
6	E	101	ASP	2.1
16	O	151	ASP	2.1
12	K	39	VAL	2.1
14	M	90	ARG	2.1
8	G	46	THR	2.1
1	A	370	G	2.1
7	F	16	PRO	2.1
1	A	128	A	2.1
1	A	1188	A	2.1
4	C	110	SER	2.1
7	F	104	PHE	2.1
27	Z	97	LEU	2.1
7	F	153	THR	2.1
1	A	1161	A	2.0
1	A	1184	C	2.0
14	M	150	GLN	2.0
1	A	1193	A	2.0
11	J	34	GLY	2.0
11	J	79	ALA	2.0
19	R	81	GLU	2.0
4	C	111	SER	2.0
5	D	183	GLU	2.0
1	A	1174	A	2.0
14	M	114	VAL	2.0
16	O	176	ARG	2.0
10	I	12	ILE	2.0
10	I	72	ASP	2.0
7	F	52	THR	2.0
26	Y	76	ARG	2.0
9	H	12	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates 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( $\text{\AA}^2$ )	Q<0.9
34	NA	A	8384	1/1	0.14	0.75	82,82,82,82	0
32	MG	A	8049	1/1	0.33	0.69	95,95,95,95	0
32	MG	A	8076	1/1	0.34	0.17	79,79,79,79	0
32	MG	A	8024	1/1	0.37	0.60	110,110,110,110	0
34	NA	T	8312	1/1	0.39	0.57	80,80,80,80	0
35	CL	4	8504	1/1	0.40	0.36	101,101,101,101	0
35	CL	M	8510	1/1	0.41	0.43	97,97,97,97	0
34	NA	A	8382	1/1	0.47	0.52	79,79,79,79	0
34	NA	A	8329	1/1	0.53	0.35	61,61,61,61	0
34	NA	A	8340	1/1	0.53	0.59	58,58,58,58	0
34	NA	A	8371	1/1	0.53	0.60	54,54,54,54	0
34	NA	A	8365	1/1	0.56	0.55	46,46,46,46	0
34	NA	B	8351	1/1	0.56	0.39	75,75,75,75	0
34	NA	A	8363	1/1	0.58	0.78	48,48,48,48	0
32	MG	1	8105	1/1	0.59	0.72	58,58,58,58	0
32	MG	A	8102	1/1	0.62	1.13	135,135,135,135	0
34	NA	S	8386	1/1	0.62	0.53	70,70,70,70	0
34	NA	S	8337	1/1	0.64	0.25	52,52,52,52	0
34	NA	A	8372	1/1	0.65	0.54	80,80,80,80	0
34	NA	B	8383	1/1	0.69	0.94	77,77,77,77	0
34	NA	R	8348	1/1	0.69	0.21	57,57,57,57	0
34	NA	A	8373	1/1	0.70	0.27	54,54,54,54	0
32	MG	A	8114	1/1	0.70	1.03	124,124,124,124	0
34	NA	A	8328	1/1	0.71	0.57	47,47,47,47	0
34	NA	A	8385	1/1	0.72	0.34	46,46,46,46	0
37	CD	1	8403	1/1	0.73	0.31	203,203,203,203	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
34	NA	A	8381	1/1	0.73	0.16	46,46,46,46	0
32	MG	A	8092	1/1	0.74	0.47	91,91,91,91	0
37	CD	4	8404	1/1	0.74	0.42	203,203,203,203	0
34	NA	A	8310	1/1	0.76	0.53	40,40,40,40	0
34	NA	A	8357	1/1	0.76	0.10	49,49,49,49	0
32	MG	A	8113	1/1	0.76	0.32	54,54,54,54	0
34	NA	A	8326	1/1	0.76	0.64	60,60,60,60	0
34	NA	A	8307	1/1	0.77	0.64	58,58,58,58	0
34	NA	A	8327	1/1	0.77	0.20	40,40,40,40	0
34	NA	A	8352	1/1	0.78	0.33	39,39,39,39	0
34	NA	4	8369	1/1	0.79	0.33	66,66,66,66	0
35	CL	A	8522	1/1	0.79	0.62	83,83,83,83	0
34	NA	A	8368	1/1	0.79	0.24	56,56,56,56	0
35	CL	K	8502	1/1	0.80	0.19	71,71,71,71	0
34	NA	A	8332	1/1	0.80	0.46	68,68,68,68	0
32	MG	A	8093	1/1	0.80	0.23	44,44,44,44	0
34	NA	A	8319	1/1	0.80	0.15	44,44,44,44	0
35	CL	D	8519	1/1	0.81	0.40	70,70,70,70	0
34	NA	A	8355	1/1	0.82	0.62	64,64,64,64	0
32	MG	D	8055	1/1	0.82	0.15	81,81,81,81	0
34	NA	A	8374	1/1	0.82	0.65	60,60,60,60	0
34	NA	A	8301	1/1	0.82	0.14	31,31,31,31	0
32	MG	A	8045	1/1	0.82	0.13	50,50,50,50	0
35	CL	R	8511	1/1	0.83	0.38	67,67,67,67	0
32	MG	A	8046	1/1	0.83	0.10	53,53,53,53	0
35	CL	C	8509	1/1	0.83	0.32	86,86,86,86	0
32	MG	B	8095	1/1	0.83	0.08	72,72,72,72	0
34	NA	A	8378	1/1	0.84	0.55	52,52,52,52	0
34	NA	A	8303	1/1	0.84	0.36	51,51,51,51	0
32	MG	A	8089	1/1	0.84	0.22	82,82,82,82	0
34	NA	J	8322	1/1	0.84	0.37	72,72,72,72	0
32	MG	U	8073	1/1	0.84	0.21	48,48,48,48	0
34	NA	A	8377	1/1	0.85	0.33	86,86,86,86	0
32	MG	A	8088	1/1	0.85	0.15	65,65,65,65	0
34	NA	A	8356	1/1	0.85	0.81	57,57,57,57	0
32	MG	A	8085	1/1	0.85	0.16	95,95,95,95	0
35	CL	A	8505	1/1	0.85	0.25	74,74,74,74	0
32	MG	A	8115	1/1	0.85	0.09	59,59,59,59	0
34	NA	K	8346	1/1	0.86	0.19	37,37,37,37	0
34	NA	A	8354	1/1	0.86	0.38	51,51,51,51	0
35	CL	K	8516	1/1	0.86	0.27	61,61,61,61	0
32	MG	A	8101	1/1	0.87	0.10	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
34	NA	A	8341	1/1	0.87	0.17	55,55,55,55	0
35	CL	O	8507	1/1	0.87	0.23	65,65,65,65	0
32	MG	A	8099	1/1	0.88	0.24	68,68,68,68	0
34	NA	A	8353	1/1	0.88	0.22	53,53,53,53	0
34	NA	A	8316	1/1	0.88	0.21	45,45,45,45	0
32	MG	A	8064	1/1	0.88	0.24	24,24,24,24	0
34	NA	A	8358	1/1	0.89	0.45	105,105,105,105	0
32	MG	Z	8109	1/1	0.89	0.15	38,38,38,38	0
34	NA	A	8364	1/1	0.89	0.34	54,54,54,54	0
32	MG	A	8051	1/1	0.89	0.11	86,86,86,86	0
32	MG	A	8103	1/1	0.89	0.23	45,45,45,45	0
34	NA	A	8302	1/1	0.90	0.20	31,31,31,31	0
34	NA	N	8347	1/1	0.90	0.11	24,24,24,24	0
35	CL	A	8503	1/1	0.90	0.24	57,57,57,57	0
34	NA	A	8335	1/1	0.90	0.26	57,57,57,57	0
34	NA	A	8366	1/1	0.90	0.43	47,47,47,47	0
34	NA	A	8375	1/1	0.90	0.26	55,55,55,55	0
32	MG	A	8112	1/1	0.90	0.21	57,57,57,57	0
32	MG	A	8071	1/1	0.90	0.07	93,93,93,93	0
34	NA	A	8308	1/1	0.90	0.15	63,63,63,63	0
35	CL	N	8518	1/1	0.90	0.19	46,46,46,46	0
32	MG	A	8116	1/1	0.91	0.16	55,55,55,55	0
34	NA	E	8304	1/1	0.91	0.14	25,25,25,25	0
34	NA	A	8311	1/1	0.91	0.13	31,31,31,31	0
32	MG	A	8047	1/1	0.91	0.16	31,31,31,31	0
35	CL	S	8506	1/1	0.91	0.20	60,60,60,60	0
32	MG	A	8053	1/1	0.91	0.19	41,41,41,41	0
35	CL	K	8501	1/1	0.91	0.17	58,58,58,58	0
36	PPU	5	76	37/38	0.91	0.27	60,64,69,71	0
35	CL	A	8515	1/1	0.91	0.31	68,68,68,68	0
34	NA	A	8370	1/1	0.91	0.32	52,52,52,52	0
32	MG	A	8041	1/1	0.92	0.17	55,55,55,55	0
35	CL	Z	8520	1/1	0.92	0.15	35,35,35,35	0
34	NA	J	8309	1/1	0.92	0.18	42,42,42,42	0
32	MG	A	8104	1/1	0.92	0.20	52,52,52,52	0
34	NA	A	8306	1/1	0.92	0.62	44,44,44,44	0
32	MG	A	8016	1/1	0.92	0.13	36,36,36,36	0
34	NA	A	8331	1/1	0.92	0.15	76,76,76,76	0
34	NA	A	8324	1/1	0.92	0.25	51,51,51,51	0
33	K	A	8202	1/1	0.92	0.15	89,89,89,89	0
32	MG	A	8108	1/1	0.92	0.06	53,53,53,53	0
34	NA	A	8362	1/1	0.92	0.20	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	4	8078	1/1	0.93	0.19	74,74,74,74	0
32	MG	A	8063	1/1	0.93	0.11	85,85,85,85	0
32	MG	A	8059	1/1	0.93	0.10	47,47,47,47	0
32	MG	A	8106	1/1	0.93	0.20	76,76,76,76	0
32	MG	A	8090	1/1	0.93	0.19	70,70,70,70	0
34	NA	A	8333	1/1	0.93	0.08	33,33,33,33	0
32	MG	A	8027	1/1	0.93	0.05	54,54,54,54	0
32	MG	A	8096	1/1	0.93	0.07	51,51,51,51	0
34	NA	M	8380	1/1	0.93	0.17	65,65,65,65	0
34	NA	A	8336	1/1	0.93	0.10	49,49,49,49	0
35	CL	K	8521	1/1	0.93	0.24	60,60,60,60	0
32	MG	A	8082	1/1	0.93	0.16	56,56,56,56	0
32	MG	A	8094	1/1	0.93	0.17	65,65,65,65	0
34	NA	A	8325	1/1	0.94	0.25	40,40,40,40	0
32	MG	A	8013	1/1	0.94	0.11	42,42,42,42	0
34	NA	A	8339	1/1	0.94	0.09	30,30,30,30	0
34	NA	A	8359	1/1	0.94	0.45	60,60,60,60	0
34	NA	A	8361	1/1	0.94	0.45	62,62,62,62	0
32	MG	A	8035	1/1	0.94	0.06	48,48,48,48	0
32	MG	A	8062	1/1	0.94	0.14	49,49,49,49	0
32	MG	A	8043	1/1	0.94	0.10	32,32,32,32	0
37	CD	P	8405	1/1	0.94	0.07	89,89,89,89	0
34	NA	A	8350	1/1	0.94	0.16	37,37,37,37	0
34	NA	A	8313	1/1	0.94	0.10	74,74,74,74	0
32	MG	A	8077	1/1	0.94	0.06	32,32,32,32	0
34	NA	A	8342	1/1	0.94	0.14	28,28,28,28	0
34	NA	A	8349	1/1	0.94	0.23	67,67,67,67	0
34	NA	A	8323	1/1	0.94	0.22	45,45,45,45	0
32	MG	A	8042	1/1	0.94	0.17	34,34,34,34	0
32	MG	A	8075	1/1	0.94	0.12	45,45,45,45	0
32	MG	A	8056	1/1	0.94	0.15	56,56,56,56	0
34	NA	A	8344	1/1	0.94	0.07	27,27,27,27	0
32	MG	A	8008	1/1	0.94	0.08	42,42,42,42	0
34	NA	A	8334	1/1	0.94	0.09	46,46,46,46	0
34	NA	A	8330	1/1	0.94	0.20	35,35,35,35	0
32	MG	A	8100	1/1	0.94	0.14	79,79,79,79	0
34	NA	A	8321	1/1	0.94	0.42	48,48,48,48	0
32	MG	A	8079	1/1	0.94	0.07	48,48,48,48	0
35	CL	A	8514	1/1	0.94	0.27	50,50,50,50	0
32	MG	A	8057	1/1	0.94	0.17	46,46,46,46	0
32	MG	A	8066	1/1	0.94	0.16	65,65,65,65	0
32	MG	A	8010	1/1	0.94	0.05	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	8070	1/1	0.95	0.78	69,69,69,69	0
32	MG	A	8060	1/1	0.95	0.19	44,44,44,44	0
32	MG	A	8034	1/1	0.95	0.05	36,36,36,36	0
32	MG	A	8087	1/1	0.95	0.09	49,49,49,49	0
34	NA	C	8345	1/1	0.95	0.12	35,35,35,35	0
32	MG	A	8044	1/1	0.95	0.15	54,54,54,54	0
32	MG	A	8004	1/1	0.95	0.07	53,53,53,53	0
32	MG	A	8052	1/1	0.95	0.08	51,51,51,51	0
34	NA	U	8343	1/1	0.95	0.09	27,27,27,27	0
32	MG	A	8050	1/1	0.95	0.10	52,52,52,52	0
34	NA	A	8317	1/1	0.95	0.06	32,32,32,32	0
32	MG	A	8039	1/1	0.95	0.05	51,51,51,51	0
34	NA	A	8314	1/1	0.95	0.10	43,43,43,43	0
34	NA	A	8320	1/1	0.95	0.23	42,42,42,42	0
32	MG	A	8097	1/1	0.95	0.20	32,32,32,32	0
32	MG	A	8018	1/1	0.95	0.08	42,42,42,42	0
32	MG	A	8081	1/1	0.95	0.08	39,39,39,39	0
32	MG	A	8030	1/1	0.95	0.12	34,34,34,34	0
32	MG	A	8029	1/1	0.95	0.10	38,38,38,38	0
32	MG	A	8068	1/1	0.95	0.11	46,46,46,46	0
32	MG	A	8028	1/1	0.96	0.07	37,37,37,37	0
35	CL	Z	8517	1/1	0.96	0.31	61,61,61,61	0
34	NA	A	8379	1/1	0.96	0.24	48,48,48,48	0
34	NA	A	8338	1/1	0.96	0.09	44,44,44,44	0
32	MG	A	8058	1/1	0.96	0.08	39,39,39,39	0
32	MG	A	8040	1/1	0.96	0.13	100,100,100,100	0
32	MG	C	8065	1/1	0.96	0.13	68,68,68,68	0
34	NA	A	8360	1/1	0.96	0.73	61,61,61,61	0
32	MG	A	8091	1/1	0.96	0.10	67,67,67,67	0
37	CD	V	8401	1/1	0.96	0.15	129,129,129,129	0
32	MG	A	8061	1/1	0.96	0.06	45,45,45,45	0
32	MG	A	8023	1/1	0.96	0.12	45,45,45,45	0
35	CL	A	8513	1/1	0.96	0.12	56,56,56,56	0
32	MG	A	8072	1/1	0.96	0.07	53,53,53,53	0
34	NA	A	8367	1/1	0.96	0.14	43,43,43,43	0
32	MG	A	8067	1/1	0.96	0.14	41,41,41,41	0
32	MG	A	8003	1/1	0.97	0.07	23,23,23,23	0
32	MG	A	8111	1/1	0.97	0.07	61,61,61,61	0
33	K	A	8201	1/1	0.97	0.24	71,71,71,71	0
32	MG	A	8009	1/1	0.97	0.06	32,32,32,32	0
32	MG	A	8012	1/1	0.97	0.10	44,44,44,44	0
32	MG	A	8032	1/1	0.97	0.06	34,34,34,34	0

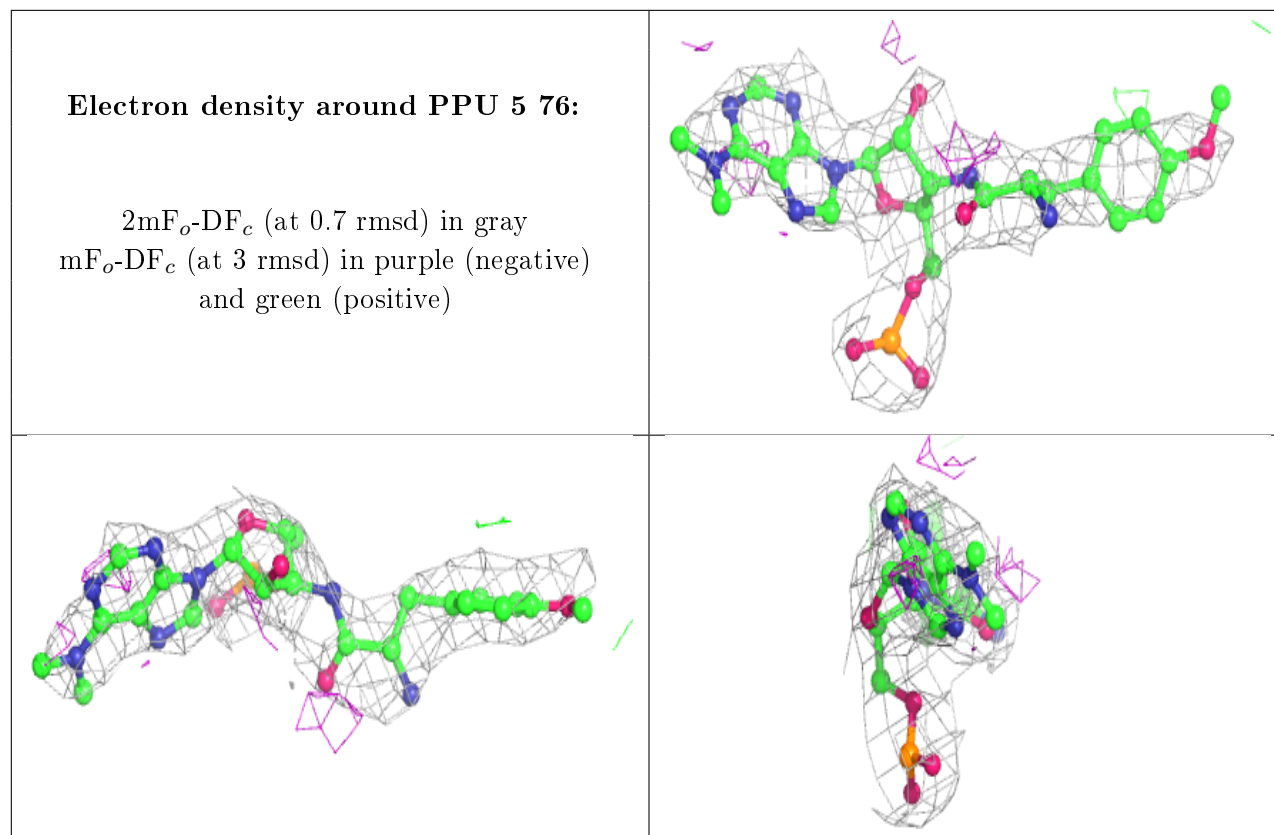
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	8001	1/1	0.97	0.09	33,33,33,33	0
32	MG	A	8017	1/1	0.97	0.05	35,35,35,35	0
35	CL	A	8512	1/1	0.97	0.10	31,31,31,31	0
32	MG	A	8031	1/1	0.97	0.04	32,32,32,32	0
32	MG	A	8054	1/1	0.97	0.06	33,33,33,33	0
32	MG	A	8037	1/1	0.97	0.09	43,43,43,43	0
32	MG	A	8006	1/1	0.97	0.09	57,57,57,57	0
32	MG	A	8038	1/1	0.97	0.05	33,33,33,33	0
32	MG	A	8021	1/1	0.97	0.11	32,32,32,32	0
32	MG	A	8083	1/1	0.97	0.08	37,37,37,37	0
34	NA	A	8318	1/1	0.97	0.28	43,43,43,43	0
32	MG	A	8074	1/1	0.97	0.05	42,42,42,42	0
32	MG	A	8014	1/1	0.97	0.07	20,20,20,20	0
32	MG	A	8117	1/1	0.97	0.08	33,33,33,33	0
32	MG	A	8002	1/1	0.97	0.05	36,36,36,36	0
32	MG	A	8048	1/1	0.97	0.07	33,33,33,33	0
32	MG	A	8022	1/1	0.97	0.05	32,32,32,32	0
32	MG	A	8033	1/1	0.97	0.12	25,25,25,25	0
32	MG	A	8110	1/1	0.97	0.07	30,30,30,30	0
32	MG	A	8007	1/1	0.97	0.03	28,28,28,28	0
34	NA	A	8315	1/1	0.98	0.16	43,43,43,43	0
32	MG	A	8107	1/1	0.98	0.06	36,36,36,36	0
32	MG	L	8069	1/1	0.98	0.09	81,81,81,81	0
35	CL	P	8508	1/1	0.98	0.32	82,82,82,82	0
34	NA	A	8305	1/1	0.98	0.09	27,27,27,27	0
32	MG	A	8020	1/1	0.98	0.05	46,46,46,46	0
34	NA	A	8376	1/1	0.98	0.17	79,79,79,79	0
32	MG	A	8015	1/1	0.98	0.05	50,50,50,50	0
32	MG	A	8098	1/1	0.98	0.18	33,33,33,33	0
32	MG	A	8084	1/1	0.98	0.05	50,50,50,50	0
32	MG	A	8036	1/1	0.98	0.06	38,38,38,38	0
32	MG	A	8005	1/1	0.99	0.07	38,38,38,38	0
32	MG	A	8011	1/1	0.99	0.13	24,24,24,24	0
32	MG	A	8019	1/1	0.99	0.07	30,30,30,30	0
32	MG	A	8086	1/1	0.99	0.09	49,49,49,49	0
32	MG	A	8026	1/1	0.99	0.05	33,33,33,33	0
32	MG	A	8080	1/1	0.99	0.06	35,35,35,35	0
37	CD	2	8402	1/1	0.99	0.07	57,57,57,57	0
32	MG	A	8025	1/1	0.99	0.06	40,40,40,40	0

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

orientation to approximate a three-dimensional view.



## 6.5 Other polymers ⓘ

There are no such residues in this entry.