



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2026 – 10:20 AM UTC

PDB ID : 2QEX / pdb_00002qex
Title : Negamycin Binds to the Wall of the Nascent Chain Exit Tunnel of the 50S Ribosomal Subunit
Authors : Schroeder, S.J.; Blaha, G.
Deposited on : 2007-06-26
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

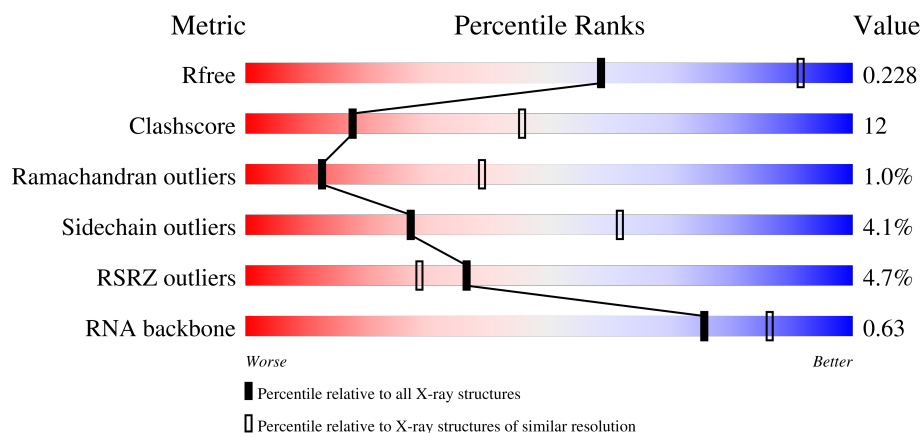
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)
RNA backbone	3983	1120 (3.10-2.70)

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

Mol	Chain	Length	Quality of chain
1	0	2772	
2	9	122	
3	A	240	
4	B	338	

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Mol	Chain	Length	Quality of chain
5	C	246	
6	D	177	
7	E	178	
8	F	120	
9	G	348	
10	H	174	
11	J	145	
12	K	132	
13	L	165	
14	M	196	
15	N	187	
16	O	116	
17	P	149	
18	Q	96	
19	R	155	
20	S	85	
21	T	120	
22	U	67	
23	V	71	
24	W	154	
25	X	92	
26	Y	241	
27	Z	73	
28	1	57	
29	2	50	

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Mol	Chain	Length	Quality of chain
30	3	92	
31	I	162	

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
34	NA	0	8575	-	-	-	X

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99020 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	0	2754	Total	C	N	O	P	0	0	0
			59021	26350	10878	19048	2745			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	9	122	Total	C	N	O	P	0	0	0
			2600	1160	472	847	121			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
9	3073	G	A	conflict	GB 6468293
9	3106	C	U	conflict	GB 6468293

- Molecule 3 is a protein called 50S ribosomal protein L2P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	237	Total	C	N	O	S	0	0	0
			1753	1072	352	324	5			

- Molecule 4 is a protein called 50S ribosomal protein L3P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	337	Total	C	N	O	S	0	0	0
			2625	1616	493	511	5			

- Molecule 5 is a protein called 50S ribosomal protein L4P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	246	Total	C	N	O	S	0	0	0
			1859	1131	344	383	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	73	LEU	GLN	conflict	UNP P12735

- Molecule 6 is a protein called 50S ribosomal protein L5P.

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

- Molecule 7 is a protein called 50S ribosomal protein L6P.

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

- Molecule 8 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	119	Total	C	N	O	S	0	0	0
			890	551	141	197	1			

- Molecule 9 is a protein called Acidic ribosomal protein P0 homolog.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	248	ASP	ALA	conflict	UNP P15825

- Molecule 10 is a protein called 50S ribosomal protein L10e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	160	Total	C	N	O	S	0	0	0
			1266	785	237	238	6			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	164	ASP	-	insertion	UNP P60617
H	165	SER	LYS	conflict	UNP P60617
H	166	SER	VAL	conflict	UNP P60617
H	167	PRO	GLU	conflict	UNP P60617
H	168	ALA	ARG	conflict	UNP P60617
H	?	-	GLU	deletion	UNP P60617
H	?	-	GLU	deletion	UNP P60617
H	?	-	LEU	deletion	UNP P60617
H	?	-	LEU	deletion	UNP P60617
H	170	ASN	ILE	conflict	UNP P60617

- Molecule 11 is a protein called 50S ribosomal protein L13P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	142	Total	C	N	O	S	0	0	0
			1120	696	199	222	3			

- Molecule 12 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	132	Total	C	N	O	S	0	0	0
			992	609	187	192	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	44	LEU	HIS	conflict	UNP P22450

- Molecule 13 is a protein called 50S ribosomal protein L15P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	145	Total	C	N	O		0	0	0
			1118	670	222	226				

- Molecule 14 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	M	194	Total	C	N	O	S	0	0	0
			1559	943	332	283	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	13	GLU	LYS	conflict	UNP P60618
M	194	ALA	GLY	conflict	UNP P60618

- Molecule 15 is a protein called 50S ribosomal protein L18P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	N	186	Total	C	N	O	S	0	0	0
			1445	895	262	286	2			

- Molecule 16 is a protein called 50S ribosomal protein L18e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	O	115	Total	C	N	O		0	0	0
			865	529	161	175				

- Molecule 17 is a protein called 50S ribosomal protein L19e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	P	143	Total	C	N	O		0	0	0
			1136	683	229	224				

- Molecule 18 is a protein called 50S ribosomal protein L21e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Q	95	Total	C	N	O		0	0	0
			735	450	141	144				

- Molecule 19 is a protein called 50S ribosomal protein L22P.

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

- Molecule 20 is a protein called 50S ribosomal protein L23P.

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

- Molecule 21 is a protein called 50S ribosomal protein L24P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	T	119	Total	C	N	O			
			950	568	180	202	0	0	0

- Molecule 22 is a protein called 50S ribosomal protein L24e.

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

- Molecule 23 is a protein called 50S ribosomal protein L29P.

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

- Molecule 24 is a protein called 50S ribosomal protein L30P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	W	154	Total	C	N	O	S			
			1196	737	209	244	6	0	0	0

- Molecule 25 is a protein called 50S ribosomal protein L31e.

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

- Molecule 26 is a protein called 50S ribosomal protein L32e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	Y	142	Total	C	N	O			
			1130	686	228	216	0	0	0

- Molecule 27 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	Z	73	Total	C	N	O	S			
			579	346	116	112	5	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	10	ARG	SER	conflict	UNP P60619

- Molecule 28 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 29 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 30 is a protein called 50S ribosomal protein L44e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 31 is a protein called 50S ribosomal protein L11P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	I	70	Total	C	N	O	S	0	0	0
			519	323	81	114	1			

- Molecule 32 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	108	Total	Mg	0	0
			108	108		
32	9	1	Total	Mg	0	0
			1	1		
32	A	2	Total	Mg	0	0
			2	2		
32	B	1	Total	Mg	0	0
			1	1		
32	K	1	Total	Mg	0	0
			1	1		
32	T	1	Total	Mg	0	0
			1	1		
32	Y	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	3	1	Total	Mg	0	0
			1	1		

- Molecule 33 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 34 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	72	Total	Na	0	0
			72	72		
34	9	3	Total	Na	0	0
			3	3		
34	A	1	Total	Na	0	0
			1	1		
34	C	1	Total	Na	0	0
			1	1		
34	H	1	Total	Na	0	0
			1	1		
34	J	1	Total	Na	0	0
			1	1		
34	L	1	Total	Na	0	0
			1	1		
34	M	1	Total	Na	0	0
			1	1		
34	Q	1	Total	Na	0	0
			1	1		
34	R	3	Total	Na	0	0
			3	3		
34	S	1	Total	Na	0	0
			1	1		

- Molecule 35 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

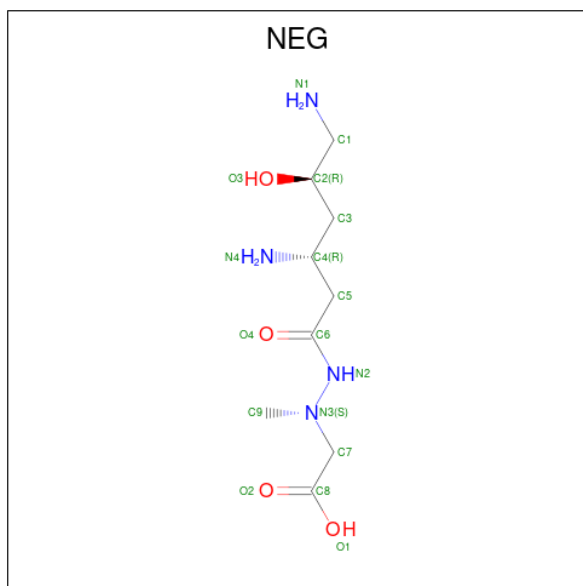
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	10	Total	Cl	0	0
			10	10		
35	A	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	B	1	Total	Cl	0	0
			1	1		
35	J	3	Total	Cl	0	0
			3	3		
35	L	1	Total	Cl	0	0
			1	1		
35	M	1	Total	Cl	0	0
			1	1		
35	N	1	Total	Cl	0	0
			1	1		
35	O	1	Total	Cl	0	0
			1	1		
35	Q	1	Total	Cl	0	0
			1	1		
35	R	1	Total	Cl	0	0
			1	1		
35	3	1	Total	Cl	0	0
			1	1		

- Molecule 36 is NEGAMYCIN (CCD ID: NEG) (formula: $C_9H_{20}N_4O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	0	1	Total	C	N	O	0	0
			17	9	4	4		

- Molecule 37 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	O	1	Total Cd 1 1	0	0
37	U	1	Total Cd 1 1	0	0
37	Z	1	Total Cd 1 1	0	0
37	1	1	Total Cd 1 1	0	0
37	3	1	Total Cd 1 1	0	0

- Molecule 38 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	0	5923	Total O 5923 5923	0	0
38	9	142	Total O 142 142	0	0
38	A	112	Total O 112 112	0	0
38	B	137	Total O 137 137	0	0
38	C	167	Total O 167 167	0	0
38	D	44	Total O 44 44	0	0
38	E	45	Total O 45 45	0	0
38	F	27	Total O 27 27	0	0
38	G	16	Total O 16 16	0	0
38	H	70	Total O 70 70	0	0
38	J	51	Total O 51 51	0	0
38	K	57	Total O 57 57	0	0
38	L	85	Total O 85 85	0	0
38	M	122	Total O 122 122	0	0
38	N	61	Total O 61 61	0	0

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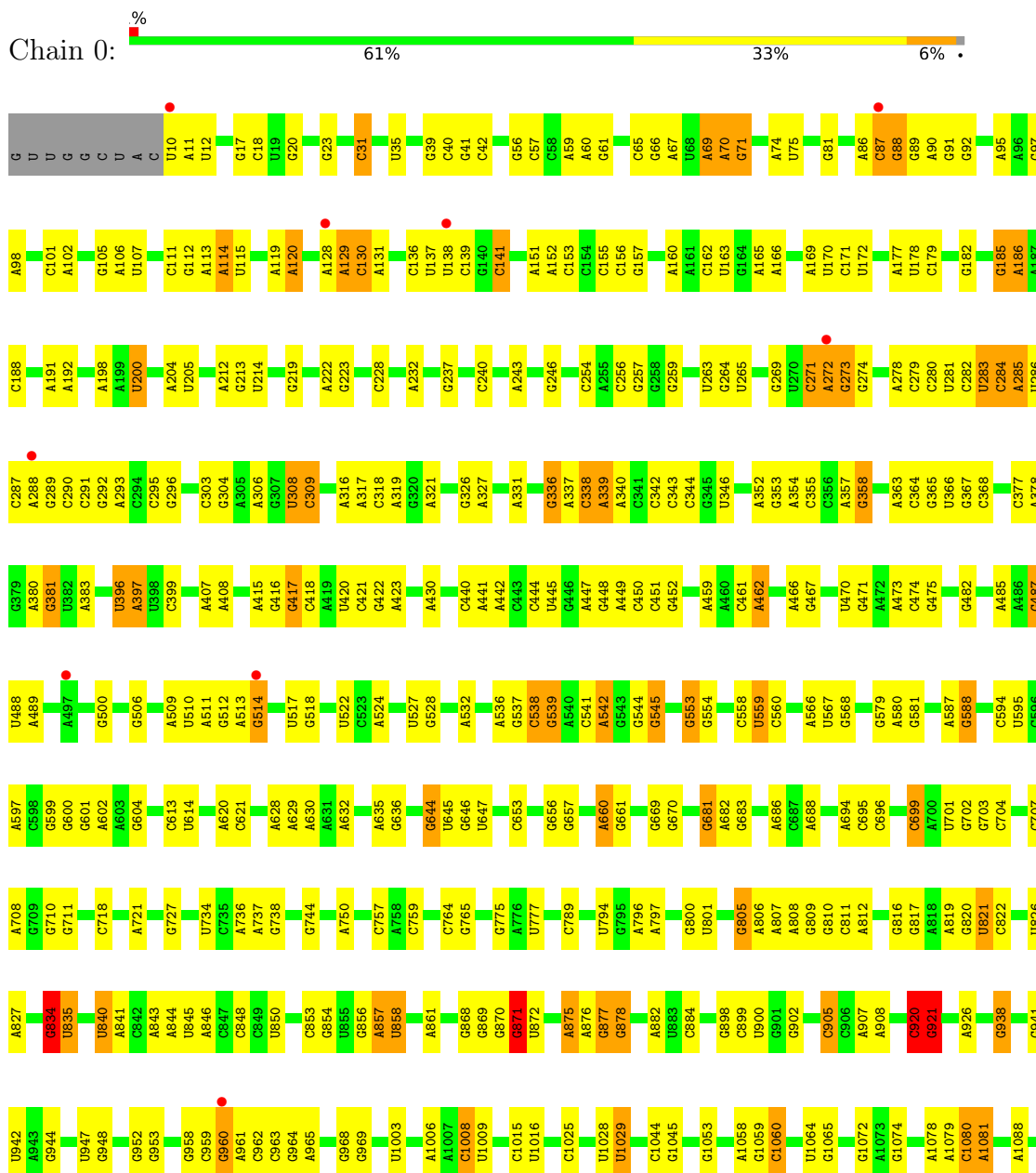
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	O	38	Total 38	O 38	0	0
38	P	63	Total 63	O 63	0	0
38	Q	50	Total 50	O 50	0	0
38	R	85	Total 85	O 85	0	0
38	S	39	Total 39	O 39	0	0
38	T	30	Total 30	O 30	0	0
38	U	28	Total 28	O 28	0	0
38	V	11	Total 11	O 11	0	0
38	W	69	Total 69	O 69	0	0
38	X	24	Total 24	O 24	0	0
38	Y	87	Total 87	O 87	0	0
38	Z	30	Total 30	O 30	0	0
38	1	60	Total 60	O 60	0	0
38	2	36	Total 36	O 36	0	0
38	3	74	Total 74	O 74	0	0
38	I	5	Total 5	O 5	0	0

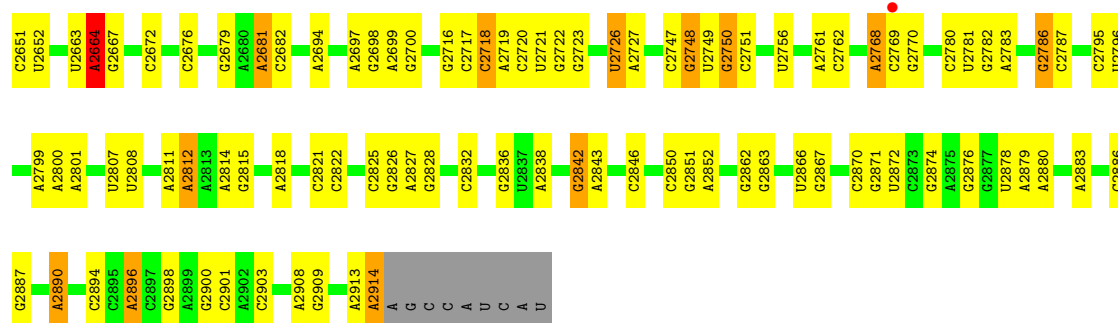
3 Residue-property plots

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

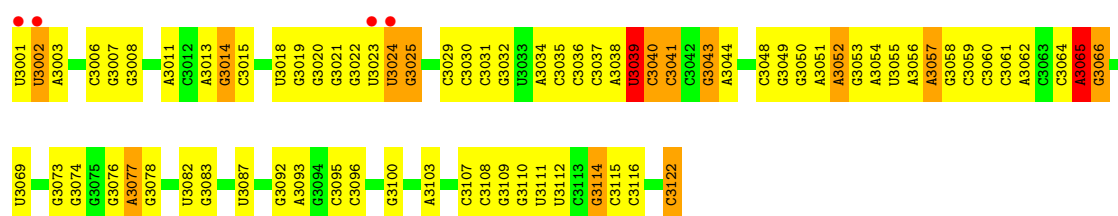
• Molecule 1: 23S ribosomal RNA



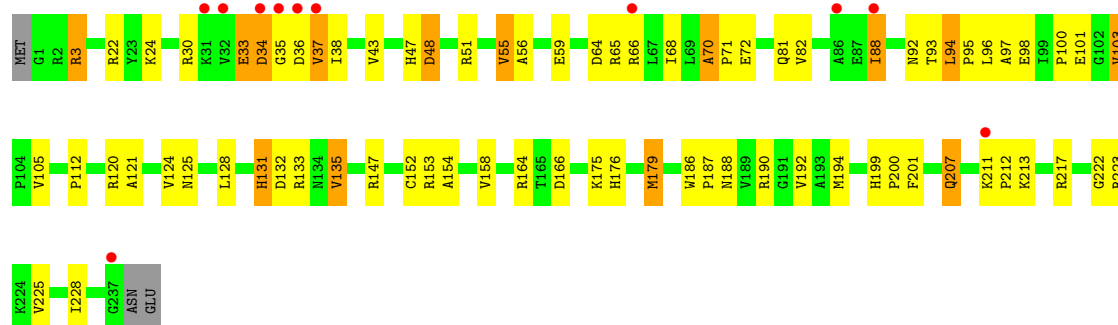
U1097	A1098	G1099	U1109	G1110	U1116	A1117	A1118	G1119	U1120	G1121	U1122	A1123	C1126	C1127	C1128	C1129	U1130	G1131	A1132	G1137	A1150	A1154	G1155	C1156	G1159	G1160	A1161	G1162	U1163	U1164	G1165	A1166	G1167	C1168	U1169	U1170	A1171	G1172	A1173	A1174	G1175	C1176	A1177	G1178	C1179	U1180	A1181	C1182	C1183	U1185	C1186												
U1187	A1188	A1189	G1190	A1191	A1192	A1193	A1194	G1195	G1196	G1197	U1198	A1199	U1200	C1201	A1202	C1203	C1204	U1205	U1206	A1207	C1208	C1209	G1210	G1211	C1212	C1213	C1214	A1215	G1216	G1217	U1218	U1219	G1226	C1229	A1230	A1236	U1237	C1238	G1239	A1242	C1243	U1244	C1245	A1246	A1247	A1248	U1249	C1250	C1253	G1260	A1261	C1262											
U1266	C1267	G1268	G1269	C1273	U1279	C1289	C1290	A1291	G1299	A1300	U1309	U1310	A1313	G1319	U1320	C1321	G1322	A1328	A1329	A1330	U1333	C1334	G1339	A1340	C1342	C1343	G1344	A1352	C1353	A1358	U1359	C1360	G1364	C1365	C1366	A1367	A1368	A1369	G1370	A1371	C1372	A1372	A1372	A1372	A1372	A1372	A1372	A1372															
G1376	C1377	A1378	A1379	A1393	C1394	C1395	C1396	C1397	G1398	A1399	U1407	U1408	G1409	G1410	U1418	U1419	C1420	C1423	A1424	G1430	G1431	G1432	G1441	A1442	U1446	U1447	C1450	C1451	G1452	G1453	U1454	C1455	U1456	C1457	C1462	A1463	C1472	U1473	C1474	C1477	G1481	A1482	C1483	G1484	U1488	A1492																	
C1495	G1496	G1497	U1500	U1503	A1504	C1505	U1506	C1507	C1508	G1512	C1513	G1514	C1515	A1516	U1517	A1518	U1519	G1520	C1521	A1522	G1523	U1524	G1525	A1526	A1527	A1528	G1529	C1537	C1545	G1546	A1547	U1548	C1549	C1550	C1551	C1552	C1553	U1554	G1555	G1556	G1557	C1558	A1559	C1562	G1563	U1568	U1569	A1573	C1574	C1575													
G1576	U1577	A1580	C1584	C1585	G1586	U1587	G1588	G1589	G1592	C1593	C1594	G1595	U1596	A1597	A1598	A1603	G1604	G1605	A1606	A1607	C1613	G1614	A1615	A1624	U1625	A1626	G1627	C1633	G1634	U1635	G1636	A1637	A1641	A1642	U1654	G1655	A1656	A1657	A1658	A1659	G1660	A1661	C1662	G1663	A1664	G1665	C1666	A1667	A1669														
G1670	U1677	A1678	C1679	A1682	G1683	A1684	A1685	C1686	C1687	C1692	G1697	U1698	C1699	A1701	U1702	G1706	G1707	C1714	C1715	A1716	A1717	U1722	G1723	U1724	C1725	G1730	C1731	C1735	A1736	G1739	U1740	U1741	A1742	G1751	G1752	A1755	G1756	A1759	G1760	U1761	C1762	G1763	C1764	A1667	A1669																		
A1767	C1768	C1769	G1773	G1774	G1777	A1778	A1779	U1787	U1788	G1789	C1790	U1791	G1795	A1796	A1797	C1803	G1804	G1805	G1806	U1807	A1808	G1809	G1818	G1819	G1820	A1821	A1822	G1823	G1826	G1827	G1828	A1829	G1834	U1835	A1839	A1840	A1845	C1856	G1867	G1868	U1871	C1872	U1873	U1874	G2001																		
G1877	G1878	U1879	U1883	U1887	C1888	C1889	U1890	G1902	U1903	C1914	A1919	C1920	A1921	A1922	G1925	G1926	C2004	C2005	C2006	C2007	C2008	C2009	A2010	U2011	U2012	G2013	U2016	U2017	A2018	A2019	G2033	U2034	C2047	C2048	C2049	G2050	A2054	G2058	U2059	A2060	U2063	U2064	G2068	G2072	G2073	A2074	A2081	G2090	G2091	G2092	G2093	A2096	A2100	A2101	G2102	U1992	C1993	A1994	U2107	A2108	U2109	G2110	C2114
U2115	U2133	G2134	A2135	G2136	G2237	C2247	C2248	G2251	A2252	G2253	A2254	G2255	A2256	G2257	A2258	G2263	A2264	A2265	A2266	C2269	G2270	G2271	C2272	U2273	A2274	G2275	G2285	G2286	C2287	G2288	U2289	A2291	A2300	A2301	C2309	C2313	G2316	C2317	U2320	A2321	G2323	U2326	A2327	C2328	C2329																		
U2330	C2331	G2338	G2344	A2345	C2346	G2350	C2351	A2354	A2361	A2362	G2363	A2364	A2369	A2372	U2373	A2374	G2375	A2382	G2385	U2386	U2387	C2388	A2401	A2402	G2403	G2404	G2412	A2413	A2414	A2415	G2416	U2419	G2420	U2421	C2423	U2424	A2425	G2426	A2429	U2430	A2433	A2434	U2435	U2436	G2438																		
C2439	G2446	A2447	G2453	A2456	U2457	U2461	G2462	A2465	A2466	A2467	A2468	C2472	C2476	C2477	U2478	A2479	A2483	C2487	A2488	G2489	A2490	C2493	C2498	U2499	C2502	A2503	A2504	G2505	A2506	G2507	C2508	A2509	C2510	A2511	C2515	G2516	G2520	G2524	C2525	C2526	U2527	C2533	C2534																				
U2535	C2536	G2537	A2538	U2541	C2542	G2543	G2544	U2545	U2546	C2552	A2553	C2559	U2563	G2564	C2565	G2570	A2577	G2578	U2586	U2587	G2588	U2589	U2590	C2591	G2592	U2598	A2599	A2600	A2601	G2602	U2607	C2608	G2613	C2614	U2619	U2620	U2621	G2634	A2635	C2636	A2637	U2645	U2648	A2649	U2650																		



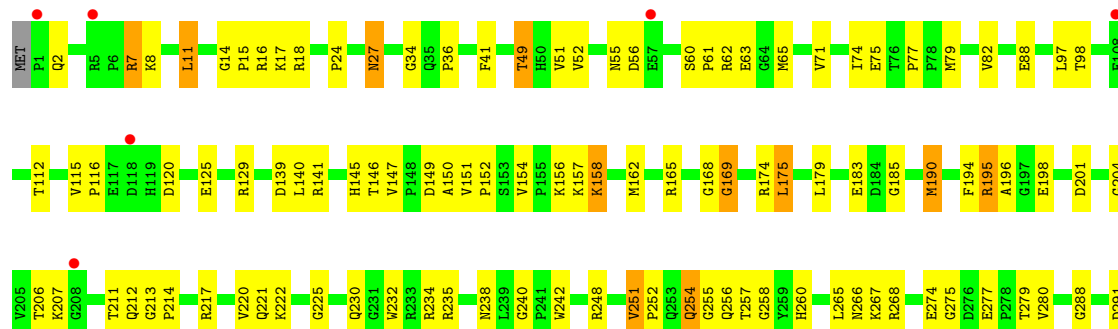
• Molecule 2: 5S ribosomal RNA

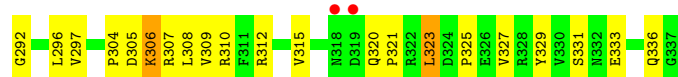


• Molecule 3: 50S ribosomal protein L2P

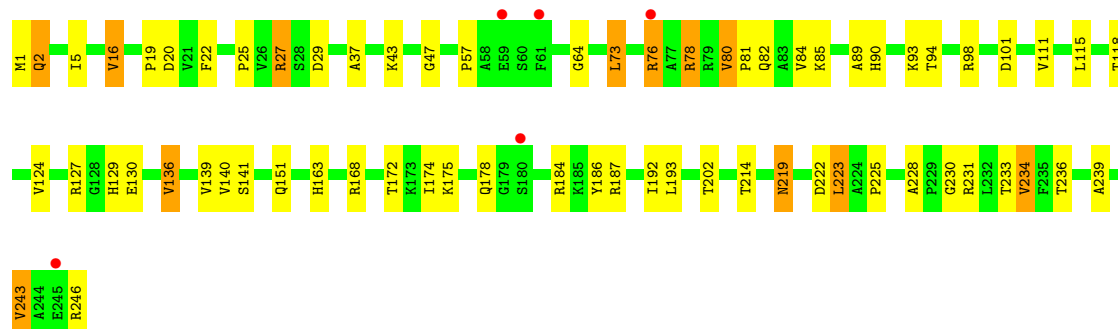
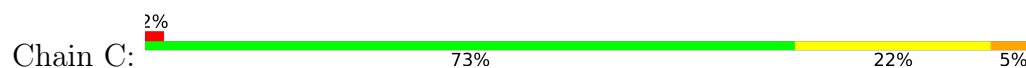


• Molecule 4: 50S ribosomal protein L3P

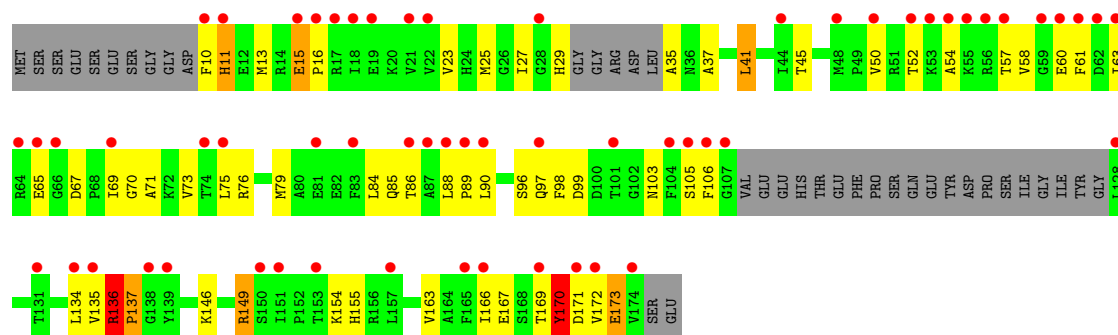




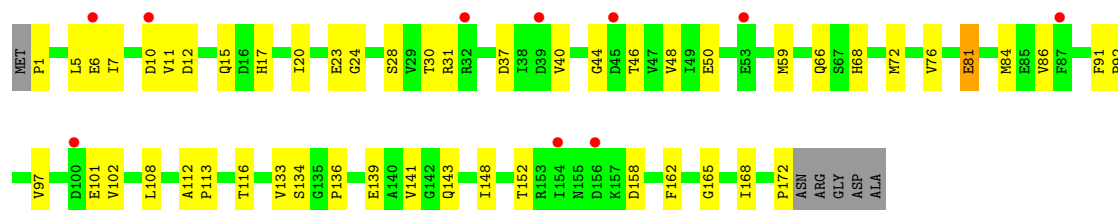
• Molecule 5: 50S ribosomal protein L4P



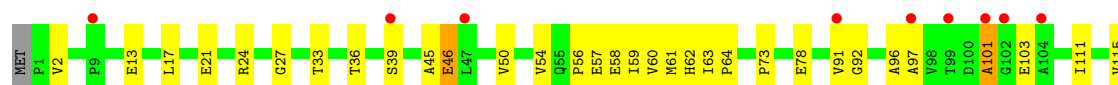
• Molecule 6: 50S ribosomal protein L5P



• Molecule 7: 50S ribosomal protein L6P

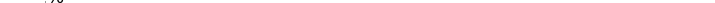


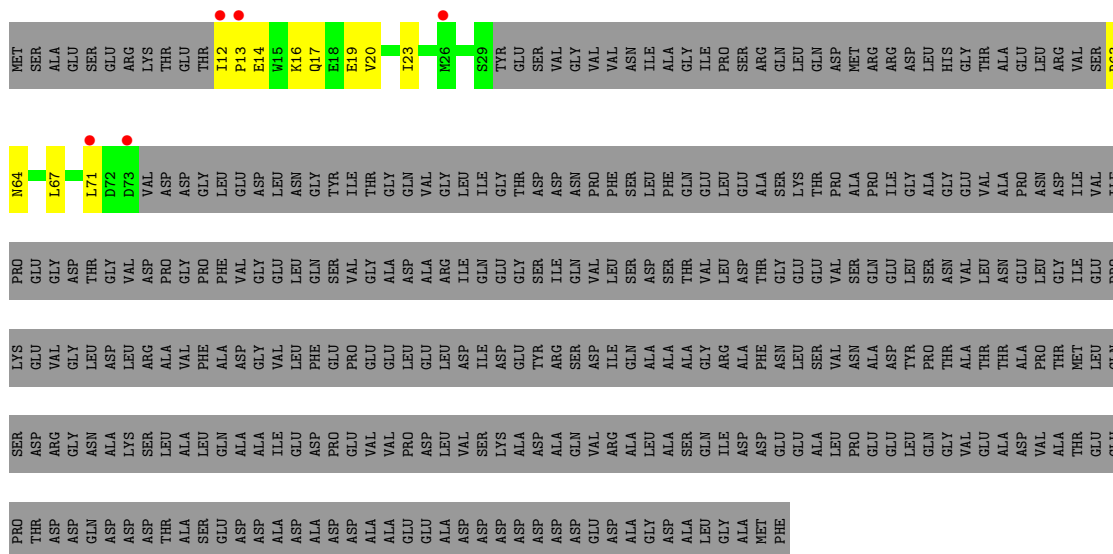
• Molecule 8: 50S ribosomal protein L7Ae



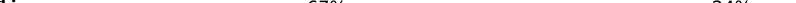
E116	
E117	
L118	
R119	

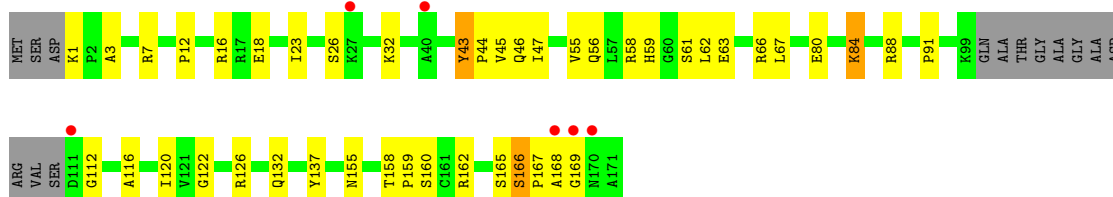
- Molecule 9: Acidic ribosomal protein P0 homolog

Chain G:  %

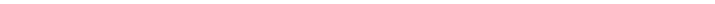


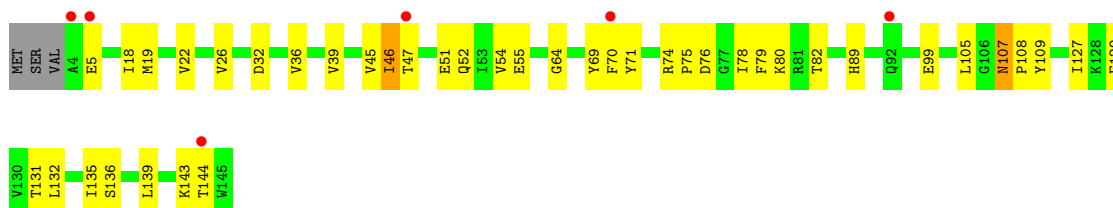
- Molecule 10: 50S ribosomal protein L10e

Chain H: 

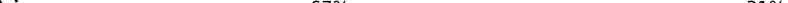


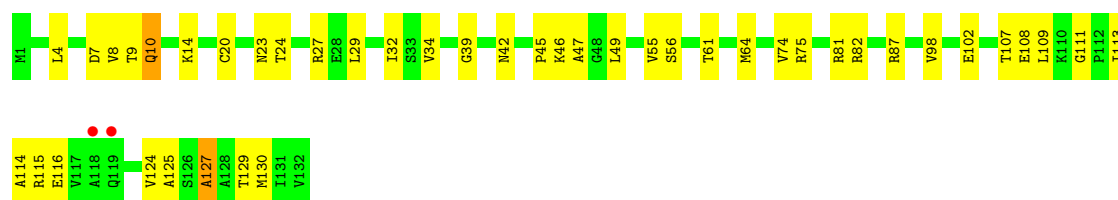
- Molecule 11: 50S ribosomal protein L13P

Chain J:  4% 70% 27% ..

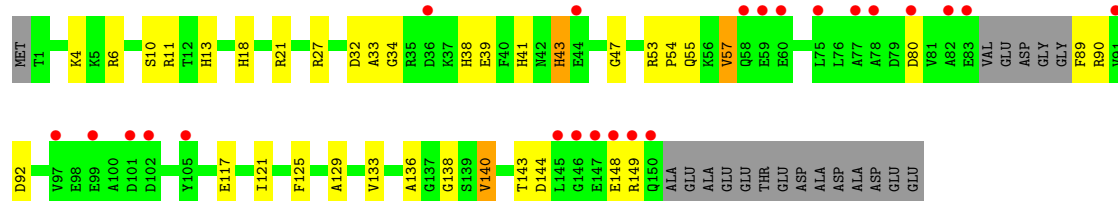


- Molecule 12: 50S ribosomal protein L14P

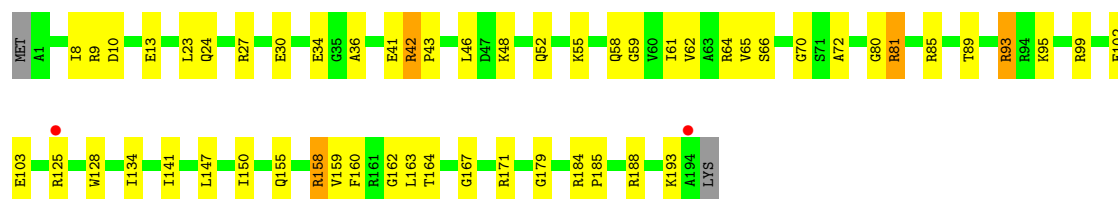
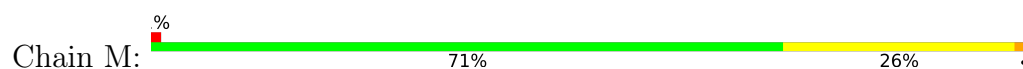
Chain K: 



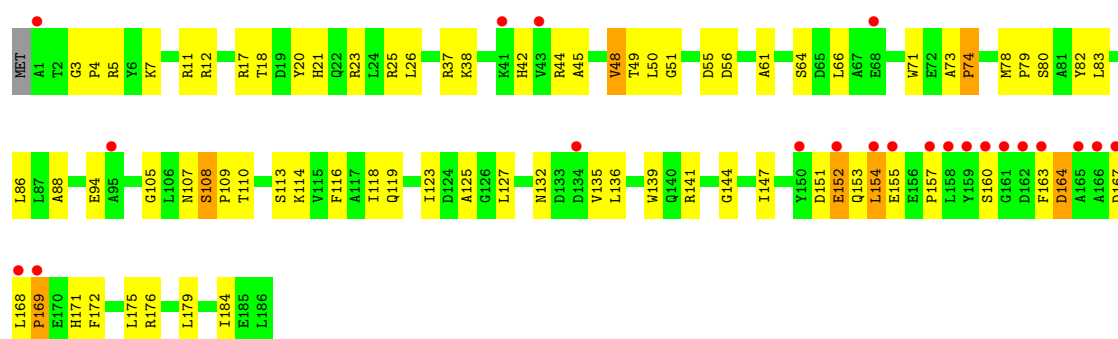
- Molecule 13: 50S ribosomal protein L15P



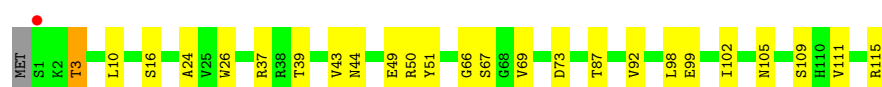
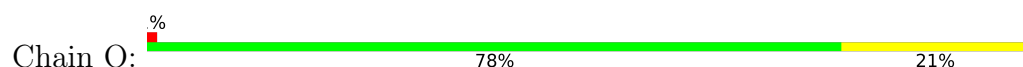
- Molecule 14: 50S ribosomal protein L15e



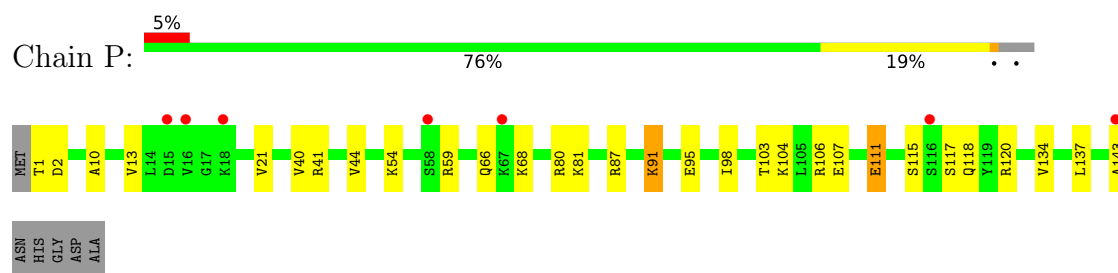
- Molecule 15: 50S ribosomal protein L18P



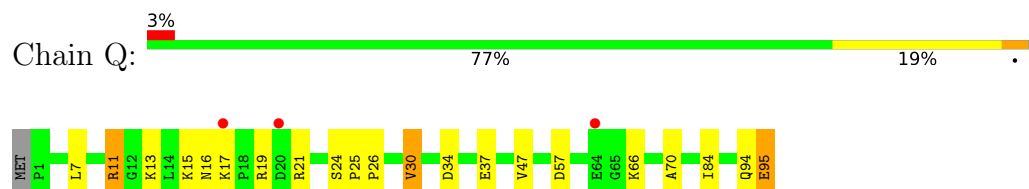
- Molecule 16: 50S ribosomal protein L18e



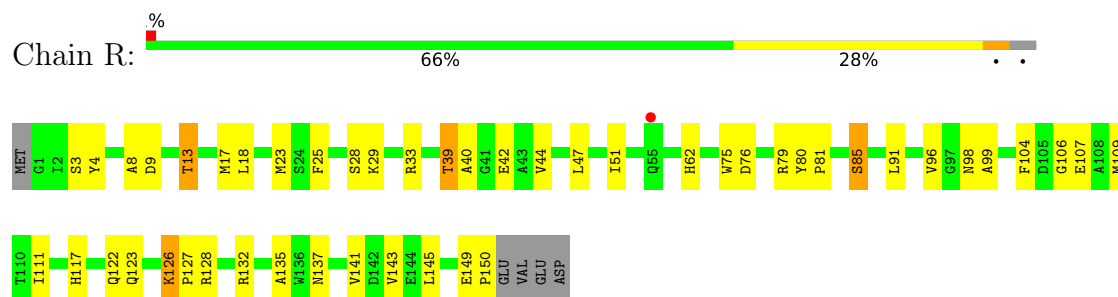
- Molecule 17: 50S ribosomal protein L19e



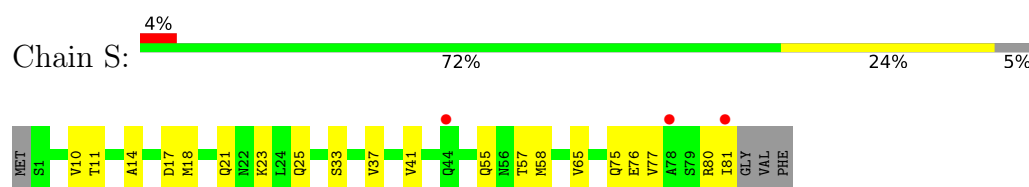
- Molecule 18: 50S ribosomal protein L21e



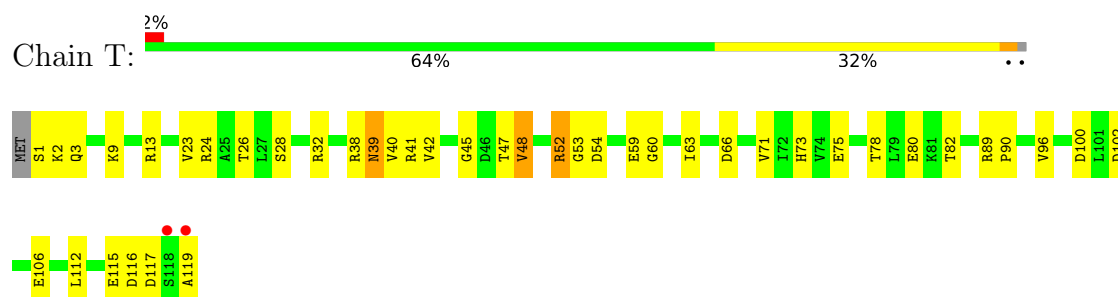
- Molecule 19: 50S ribosomal protein L22P



- Molecule 20: 50S ribosomal protein L23P

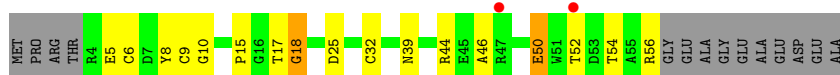


- Molecule 21: 50S ribosomal protein L24P

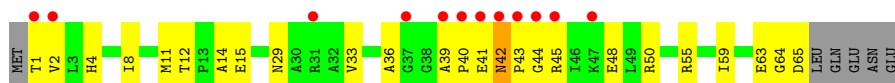


- Molecule 22: 50S ribosomal protein L24e

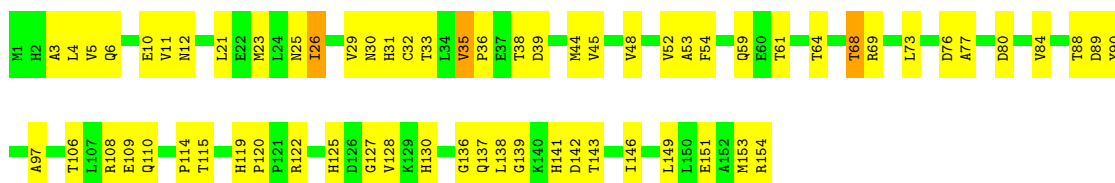




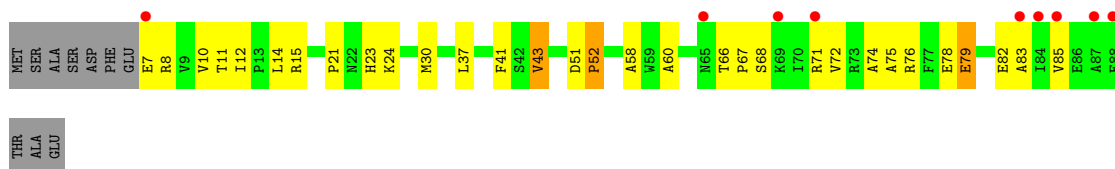
- Molecule 23: 50S ribosomal protein L29P



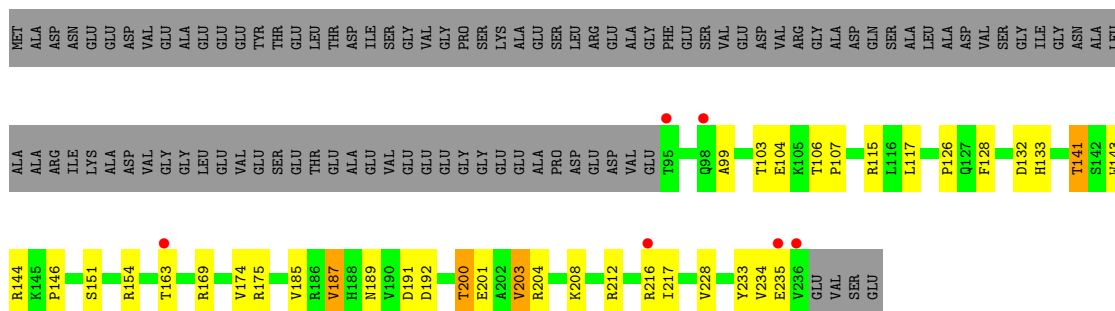
- Molecule 24: 50S ribosomal protein L30P



- Molecule 25: 50S ribosomal protein L31e

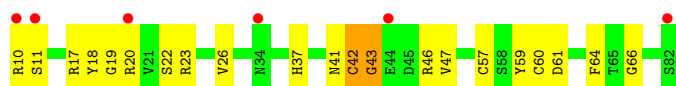


- Molecule 26: 50S ribosomal protein L32e



- Molecule 27: 50S ribosomal protein L37Ae





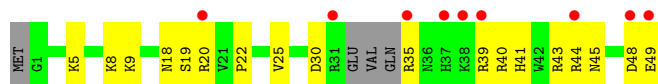
- Molecule 28: 50S ribosomal protein L37e

Chain 1: 74% 25%



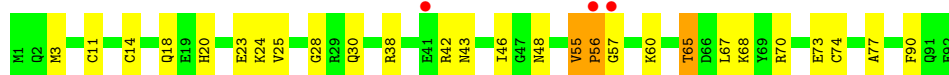
- Molecule 29: 50S ribosomal protein L39e

Chain 2: 18% 56% 36% 8%



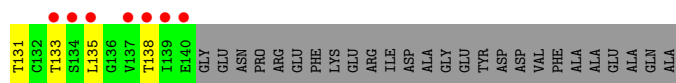
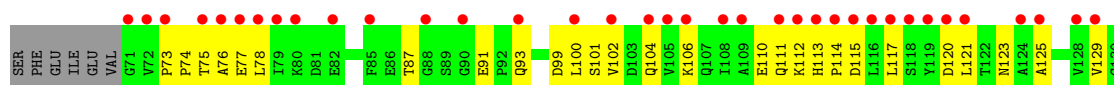
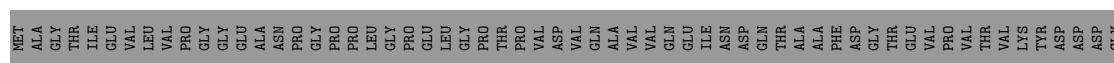
- Molecule 30: 50S ribosomal protein L44e

Chain 3: 3% 71% 26%



- Molecule 31: 50S ribosomal protein L11P

Chain I: 27% 24% 19% 57%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	214.62Å 304.05Å 578.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.92 – 2.90 49.92 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.92-2.90) 93.9 (49.92-2.90)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.42Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.204 , 0.241 0.195 , 0.228	Depositor DCC
R_{free} test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	45.2	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 68.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	99020	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 1MA, NEG, CL, NA, CD, OMU, OMG, MG, UR3, K, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	0	0.40	0/65959	0.60	16/102870 (0.0%)
2	9	0.39	0/2905	0.61	2/4528 (0.0%)
3	A	0.45	0/1786	1.03	14/2408 (0.6%)
4	B	0.41	0/2690	1.02	19/3652 (0.5%)
5	C	0.47	0/1884	1.02	12/2551 (0.5%)
6	D	0.42	0/1111	1.03	9/1498 (0.6%)
7	E	0.41	0/1382	0.90	4/1880 (0.2%)
8	F	0.44	0/901	0.95	1/1224 (0.1%)
9	G	0.40	0/241	0.95	0/324
10	H	0.43	0/1287	1.01	13/1725 (0.8%)
11	J	0.44	0/1136	0.98	4/1530 (0.3%)
12	K	0.44	0/1001	1.02	9/1347 (0.7%)
13	L	0.41	0/1130	0.97	2/1509 (0.1%)
14	M	0.46	0/1583	0.97	7/2119 (0.3%)
15	N	0.39	0/1474	1.07	13/1999 (0.7%)
16	O	0.45	0/874	0.96	3/1181 (0.3%)
17	P	0.43	0/1147	0.90	1/1528 (0.1%)
18	Q	0.45	0/749	1.03	6/1005 (0.6%)
19	R	0.50	0/1172	1.03	8/1578 (0.5%)
20	S	0.39	0/648	0.88	0/875
21	T	0.40	0/958	0.98	6/1289 (0.5%)
22	U	0.43	0/417	0.86	2/562 (0.4%)
23	V	0.41	0/502	1.00	2/675 (0.3%)
24	W	0.50	0/1219	0.98	4/1655 (0.2%)
25	X	0.47	0/664	1.04	5/895 (0.6%)
26	Y	0.47	0/1146	0.95	3/1536 (0.2%)
27	Z	0.42	0/590	0.95	3/787 (0.4%)
28	1	0.48	0/438	0.88	0/578
29	2	0.46	0/401	0.85	0/529
30	3	0.40	0/771	0.91	4/1024 (0.4%)
31	I	0.46	0/526	1.01	4/716 (0.6%)
All	All	0.41	0/98692	0.73	176/147577 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	1	37
2	9	0	2
All	All	1	39

There are no bond length outliers.

All (176) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	15	GLU	CA-C-N	9.32	129.40	119.89
6	D	15	GLU	C-N-CA	9.32	129.40	119.89
14	M	89	THR	N-CA-C	9.05	121.15	111.28
3	A	222	GLY	N-CA-C	-9.00	103.95	113.58
1	0	805	G	C2'-C3'-O3'	7.95	125.62	113.70
13	L	47	GLY	N-CA-C	7.53	121.10	111.09
6	D	136	ARG	CA-C-N	7.35	129.03	119.84
6	D	136	ARG	C-N-CA	7.35	129.03	119.84
3	A	70	ALA	N-CA-C	7.34	120.29	109.42
1	0	1942	A	C5'-C4'-C3'	7.30	126.95	116.00
6	D	170	TYR	N-CA-C	7.17	121.33	112.58
11	J	71	TYR	CA-C-N	7.16	127.16	119.78
11	J	71	TYR	C-N-CA	7.16	127.16	119.78
19	R	141	VAL	N-CA-C	7.16	118.79	108.48
4	B	222	LYS	N-CA-C	-7.09	99.43	110.42
5	C	80	VAL	N-CA-C	7.06	116.73	108.96
6	D	171	ASP	N-CA-C	7.05	117.18	107.73
30	3	55	VAL	CA-C-N	6.98	128.56	119.84
30	3	55	VAL	C-N-CA	6.98	128.56	119.84
16	O	43	VAL	N-CA-C	6.97	117.93	108.17
3	A	48	ASP	CA-C-N	6.95	126.92	119.28
3	A	48	ASP	C-N-CA	6.95	126.92	119.28
15	N	169	PRO	N-CA-C	-6.89	105.24	113.86
3	A	228	ILE	N-CA-C	6.87	117.32	108.12
14	M	13	GLU	N-CA-C	-6.80	103.66	112.23
24	W	69	ARG	N-CA-C	6.74	121.67	113.38
15	N	51	GLY	CA-C-N	6.69	126.94	119.32
15	N	51	GLY	C-N-CA	6.69	126.94	119.32
10	H	55	VAL	N-CA-C	6.62	116.61	108.53
26	Y	143	TRP	N-CA-C	6.61	119.81	109.96

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Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	H	7	ARG	N-CA-C	6.57	118.44	111.28
21	T	3	GLN	CA-C-N	6.57	126.81	119.32
21	T	3	GLN	C-N-CA	6.57	126.81	119.32
15	N	153	GLN	N-CA-C	-6.51	102.63	111.55
4	B	120	ASP	CA-C-N	6.49	126.18	119.82
4	B	120	ASP	C-N-CA	6.49	126.18	119.82
5	C	219	ASN	N-CA-C	6.44	119.70	109.65
1	0	805	G	C4'-C3'-O3'	6.41	122.61	113.00
18	Q	17	LYS	N-CA-C	-6.40	100.90	110.24
2	9	3039	U	N1-C1'-C2'	6.38	121.57	112.00
5	C	175	LYS	N-CA-C	6.37	119.01	110.35
15	N	152	GLU	N-CA-C	-6.37	104.44	111.82
3	A	213	LYS	N-CA-C	6.36	119.20	111.82
24	W	143	THR	N-CA-C	-6.33	104.25	112.23
5	C	90	HIS	CA-C-N	6.33	126.90	120.38
5	C	90	HIS	C-N-CA	6.33	126.90	120.38
10	H	116	ALA	N-CA-C	6.31	120.84	113.20
15	N	48	VAL	N-CA-C	6.31	117.67	108.53
14	M	70	GLY	N-CA-C	6.30	120.78	111.76
12	K	46	LYS	N-CA-C	6.28	119.93	109.95
24	W	68	THR	N-CA-C	6.28	119.06	111.40
15	N	3	GLY	CA-C-N	6.23	125.45	118.97
15	N	3	GLY	C-N-CA	6.23	125.45	118.97
13	L	57	VAL	N-CA-C	-6.21	107.07	113.10
1	0	834	G	C2'-C3'-O3'	-6.17	104.45	113.70
18	Q	84	ILE	N-CA-C	6.16	116.79	108.17
15	N	42	HIS	N-CA-C	6.14	118.53	109.69
4	B	151	VAL	CA-C-N	6.11	126.00	119.28
4	B	151	VAL	C-N-CA	6.11	126.00	119.28
10	H	43	TYR	CA-C-N	6.10	125.50	118.85
10	H	43	TYR	C-N-CA	6.10	125.50	118.85
3	A	135	VAL	N-CA-C	6.08	117.05	108.17
21	T	52	ARG	N-CA-C	6.08	123.74	110.80
1	0	1504	A	N9-C1'-C2'	6.07	121.11	112.00
5	C	228	ALA	CA-C-N	6.05	125.96	119.85
5	C	228	ALA	C-N-CA	6.05	125.96	119.85
15	N	108	SER	CA-C-N	5.98	127.31	119.84
15	N	108	SER	C-N-CA	5.98	127.31	119.84
4	B	157	LYS	N-CA-C	-5.95	106.56	113.88
1	0	1120	U	C5'-C4'-C3'	-5.93	107.11	116.00
8	F	62	HIS	N-CA-C	5.91	118.51	111.71
4	B	158	LYS	CA-C-N	5.90	126.23	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	158	LYS	C-N-CA	5.90	126.23	119.92
27	Z	64	PHE	N-CA-C	5.90	116.88	108.74
10	H	112	GLY	N-CA-C	-5.89	99.22	113.18
1	0	2726	U	N1-C1'-C2'	5.85	120.78	112.00
10	H	122	GLY	N-CA-C	5.82	119.00	110.80
30	3	43	ASN	N-CA-C	5.80	120.22	113.20
4	B	323	LEU	N-CA-C	5.80	118.24	110.35
14	M	193	LYS	N-CA-C	5.80	120.04	111.87
1	0	1979	G	C4'-C3'-O3'	-5.78	104.32	113.00
1	0	2291	A	N9-C1'-C2'	5.78	120.67	112.00
4	B	213	GLY	CA-C-N	5.73	125.86	119.32
4	B	213	GLY	C-N-CA	5.73	125.86	119.32
24	W	25	ASN	N-CA-C	5.73	120.22	113.23
6	D	67	ASP	CA-C-N	5.68	125.69	119.90
6	D	67	ASP	C-N-CA	5.68	125.69	119.90
27	Z	20	ARG	N-CA-C	5.67	117.94	111.02
3	A	56	ALA	N-CA-C	5.61	118.61	109.24
31	I	121	LEU	N-CA-C	-5.61	106.79	113.97
10	H	159	PRO	N-CA-C	5.60	119.06	111.22
7	E	37	ASP	N-CA-C	5.59	119.68	112.86
5	C	192	ILE	N-CA-C	5.56	116.75	109.58
10	H	1	LYS	CA-C-N	5.56	125.46	119.85
10	H	1	LYS	C-N-CA	5.56	125.46	119.85
10	H	160	SER	N-CA-C	-5.54	101.52	110.32
11	J	36	VAL	N-CA-C	5.54	116.45	108.48
23	V	42	ASN	CA-C-N	5.54	126.76	119.84
23	V	42	ASN	C-N-CA	5.54	126.76	119.84
1	0	921	G	N9-C1'-C2'	5.53	120.30	112.00
25	X	12	ILE	N-CA-C	5.52	113.34	107.76
5	C	20	ASP	N-CA-C	5.51	117.29	111.28
18	Q	47	VAL	CA-C-N	5.51	124.86	118.85
18	Q	47	VAL	C-N-CA	5.51	124.86	118.85
5	C	89	ALA	N-CA-C	5.49	117.13	111.03
1	0	920	C	C2'-C3'-O3'	-5.49	105.47	113.70
5	C	186	TYR	N-CA-C	5.48	118.53	110.59
26	Y	175	ARG	N-CA-C	5.47	118.41	110.42
22	U	18	GLY	N-CA-C	5.46	121.35	112.61
31	I	73	PRO	CA-C-N	5.41	126.61	119.84
31	I	73	PRO	C-N-CA	5.41	126.61	119.84
4	B	230	GLN	N-CA-C	5.40	119.92	113.23
25	X	51	ASP	CA-C-N	5.40	126.58	119.84
25	X	51	ASP	C-N-CA	5.40	126.58	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	T	78	THR	N-CA-C	5.39	116.84	109.18
14	M	41	GLU	N-CA-C	5.39	117.15	111.28
15	N	168	LEU	N-CA-C	5.39	120.70	108.74
19	R	79	ARG	N-CA-C	5.35	115.35	108.34
4	B	251	VAL	CA-C-N	5.35	126.52	119.84
4	B	251	VAL	C-N-CA	5.35	126.52	119.84
19	R	122	GLN	N-CA-C	-5.34	100.47	108.96
19	R	123	GLN	N-CA-C	5.34	118.64	110.20
12	K	9	THR	N-CA-C	-5.33	99.08	108.20
16	O	66	GLY	N-CA-C	5.32	125.78	113.18
26	Y	187	VAL	N-CA-C	5.31	115.55	108.11
3	A	207	GLN	N-CA-C	5.30	117.39	108.96
3	A	188	ASN	N-CA-C	5.30	117.05	108.41
6	D	11	HIS	N-CA-C	5.30	117.74	111.33
30	3	60	LYS	N-CA-C	-5.29	102.98	110.29
17	P	111	GLU	N-CA-C	-5.29	106.83	113.28
14	M	42	ARG	CA-C-N	5.28	125.20	119.76
14	M	42	ARG	C-N-CA	5.28	125.20	119.76
1	0	1979	G	N9-C1'-C2'	5.28	119.92	112.00
25	X	60	ALA	N-CA-C	5.28	117.44	111.11
3	A	103	VAL	CA-C-N	5.27	125.52	119.83
3	A	103	VAL	C-N-CA	5.27	125.52	119.83
21	T	89	ARG	CA-C-N	5.25	125.19	119.78
21	T	89	ARG	C-N-CA	5.25	125.19	119.78
12	K	127	ALA	N-CA-C	-5.24	106.41	114.16
1	0	871	G	C5'-C4'-O4'	-5.23	101.95	109.80
2	9	3065	A	N9-C1'-C2'	5.22	119.84	112.00
4	B	266	ASN	N-CA-C	5.22	118.45	111.24
4	B	175	LEU	N-CA-C	-5.22	105.67	111.36
18	Q	24	SER	CA-C-N	5.22	125.76	120.38
18	Q	24	SER	C-N-CA	5.22	125.76	120.38
19	R	126	LYS	CA-C-N	5.21	125.46	119.83
19	R	126	LYS	C-N-CA	5.21	125.46	119.83
1	0	2664	A	N9-C1'-C2'	5.20	119.80	112.00
10	H	88	ARG	N-CA-C	5.20	118.48	112.97
19	R	137	ASN	N-CA-C	5.20	118.16	110.46
3	A	166	ASP	N-CA-C	5.20	117.02	111.36
25	X	79	GLU	N-CA-C	5.19	116.94	111.28
22	U	50	GLU	N-CA-C	5.19	117.68	111.71
7	E	50	GLU	N-CA-C	5.18	117.26	109.23
4	B	147	VAL	CA-C-N	5.17	125.46	119.47
4	B	147	VAL	C-N-CA	5.17	125.46	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	133	ARG	N-CA-C	-5.16	106.83	113.23
4	B	265	LEU	N-CA-C	5.16	117.51	110.55
7	E	17	HIS	CB-CA-C	-5.15	110.66	116.63
12	K	124	VAL	N-CA-C	-5.15	105.83	110.82
7	E	81	GLU	N-CA-C	5.14	116.80	108.26
11	J	89	HIS	N-CA-C	5.14	119.03	112.87
15	N	163	PHE	N-CA-C	-5.14	99.86	110.80
27	Z	18	TYR	N-CA-C	5.13	121.73	110.80
10	H	158	THR	N-CA-C	5.13	121.15	109.81
12	K	61	THR	CA-C-N	5.09	125.12	119.32
12	K	61	THR	C-N-CA	5.09	125.12	119.32
19	R	3	SER	N-CA-C	-5.08	101.65	109.52
16	O	69	VAL	N-CA-C	5.07	115.88	108.53
31	I	110	GLU	N-CA-C	-5.06	108.85	114.62
1	0	129	A	C2'-C3'-O3'	5.05	121.27	113.70
12	K	8	VAL	N-CA-C	5.04	115.39	108.12
12	K	111	GLY	CA-C-N	5.02	125.03	120.21
12	K	111	GLY	C-N-CA	5.02	125.03	120.21
1	0	1358	A	N9-C1'-C2'	5.02	119.52	112.00
5	C	78	ARG	N-CA-C	5.01	116.43	108.96

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	805	G	C3'

All (39) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1078	A	Sidechain
1	0	1237	U	Sidechain
1	0	1304	U	Sidechain
1	0	1309	U	Sidechain
1	0	1340	G	Sidechain
1	0	1359	U	Sidechain
1	0	1368	U	Sidechain
1	0	1376	G	Sidechain
1	0	1430	G	Sidechain
1	0	1684	A	Sidechain
1	0	1777	G	Sidechain
1	0	1829	A	Sidechain
1	0	1839	A	Sidechain

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Mol	Chain	Res	Type	Group
1	0	1867	G	Sidechain
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	1972	U	Sidechain
1	0	1993	C	Sidechain
1	0	2115	U	Sidechain
1	0	23	G	Sidechain
1	0	2313	C	Sidechain
1	0	246	G	Sidechain
1	0	2465	A	Sidechain
1	0	2493	C	Sidechain
1	0	2503	A	Sidechain
1	0	2506	A	Sidechain
1	0	2538	A	Sidechain
1	0	2552	C	Sidechain
1	0	2564	G	Sidechain
1	0	2842	G	Sidechain
1	0	396	U	Sidechain
1	0	462	A	Sidechain
1	0	471	G	Sidechain
1	0	482	G	Sidechain
1	0	518	G	Sidechain
1	0	858	U	Sidechain
1	0	900	U	Sidechain
2	9	3039	U	Sidechain
2	9	3087	U	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59021	0	29810	1022	0
2	9	2600	0	1326	87	0
3	A	1753	0	1766	62	0
4	B	2625	0	2533	91	0
5	C	1859	0	1816	53	0
6	D	1094	0	1085	41	0
7	E	1357	0	1266	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	F	890	0	843	25	0
9	G	240	0	231	12	0
10	H	1266	0	1268	31	0
11	J	1120	0	1098	35	0
12	K	992	0	1031	37	0
13	L	1118	0	1076	33	0
14	M	1559	0	1568	39	0
15	N	1445	0	1401	65	0
16	O	865	0	873	22	0
17	P	1136	0	1123	24	0
18	Q	735	0	729	12	0
19	R	1149	0	1122	34	0
20	S	641	0	605	17	0
21	T	950	0	923	26	0
22	U	410	0	364	18	0
23	V	499	0	511	18	0
24	W	1196	0	1137	57	0
25	X	654	0	653	22	0
26	Y	1130	0	1133	35	0
27	Z	579	0	539	18	0
28	1	431	0	426	19	0
29	2	396	0	413	18	0
30	3	755	0	730	19	0
31	I	519	0	500	31	0
32	0	108	0	0	0	0
32	3	1	0	0	0	0
32	9	1	0	0	0	0
32	A	2	0	0	0	0
32	B	1	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	2	0	0	0	0
34	0	72	0	0	1	0
34	9	3	0	0	0	0
34	A	1	0	0	0	0
34	C	1	0	0	0	0
34	H	1	0	0	0	0
34	J	1	0	0	0	0
34	L	1	0	0	1	0
34	M	1	0	0	0	0
34	Q	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	R	3	0	0	0	0
34	S	1	0	0	0	0
35	0	10	0	0	1	0
35	3	1	0	0	0	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	J	3	0	0	2	0
35	L	1	0	0	0	0
35	M	1	0	0	1	0
35	N	1	0	0	1	0
35	O	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	1	0	0	0	0
36	0	17	0	19	5	0
37	1	1	0	0	0	0
37	3	1	0	0	1	0
37	O	1	0	0	0	0
37	U	1	0	0	0	0
37	Z	1	0	0	0	0
38	0	5923	0	0	177	0
38	1	60	0	0	2	0
38	2	36	0	0	3	0
38	3	74	0	0	6	0
38	9	142	0	0	14	0
38	A	112	0	0	7	0
38	B	137	0	0	14	0
38	C	167	0	0	10	0
38	D	44	0	0	5	0
38	E	45	0	0	3	0
38	F	27	0	0	2	0
38	G	16	0	0	1	0
38	H	70	0	0	5	0
38	I	5	0	0	2	0
38	J	51	0	0	3	0
38	K	57	0	0	4	0
38	L	85	0	0	11	0
38	M	122	0	0	2	0
38	N	61	0	0	7	0
38	O	38	0	0	5	0
38	P	63	0	0	1	0
38	Q	50	0	0	1	0
38	R	85	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	S	39	0	0	4	0
38	T	30	0	0	1	0
38	U	28	0	0	1	0
38	V	11	0	0	1	0
38	W	69	0	0	3	0
38	X	24	0	0	2	0
38	Y	87	0	0	7	0
38	Z	30	0	0	2	0
All	All	99020	0	59918	1861	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 12.

All (1861) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1160:G:C5'	1:0:1161:A:H5'	1.70	1.22
1:0:871:G:C8	1:0:871:G:H5'	1.81	1.14
2:9:3006:C:H5''	15:N:37:ARG:NH1	1.63	1.12
1:0:871:G:H5'	1:0:871:G:H8	1.10	1.11
1:0:656:G:H5'	16:O:3:THR:HG22	1.18	1.10
1:0:541:C:H2'	1:0:542:A:H5''	1.32	1.09
2:9:3006:C:H5''	15:N:37:ARG:HH12	0.94	1.09
1:0:1160:G:H5'	1:0:1161:A:C5'	1.82	1.07
1:0:1242:A:H5'	11:J:82:THR:HG23	1.33	1.05
10:H:46:GLN:HB3	10:H:167:PRO:HD2	1.38	1.05
2:9:3056:A:H2'	2:9:3057:A:H5''	1.40	1.03
1:0:1559:A:H1'	38:O:5694:HOH:O	1.58	1.02
1:0:2717:C:H2'	1:0:2718:C:H5''	1.41	1.02
1:0:2812:A:H2	1:0:2814:A:H62	1.05	1.02
2:9:3076:G:H3'	2:9:3077:A:H5''	1.41	1.01
2:9:3029:C:H2'	2:9:3030:C:H5'	1.43	1.00
1:0:2533:C:H5'	1:0:2533:C:H6	1.26	0.99
1:0:1474:C:H6	1:0:1474:C:H5'	1.21	0.98
12:K:10:GLN:HE21	12:K:10:GLN:H	1.07	0.98
1:0:282:C:H1'	1:0:368:C:N4	1.78	0.98
1:0:541:C:C2'	1:0:542:A:H5''	1.94	0.98
1:0:2672:C:H1'	38:B:8925:HOH:O	1.62	0.98
10:H:166:SER:HB2	10:H:167:PRO:HD3	1.45	0.97
1:0:2533:C:H5'	1:0:2533:C:C6	1.98	0.97
1:0:271:C:H41	1:0:378:A:H2	1.07	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:871:G:H8	1:0:871:G:C5'	1.79	0.96
1:0:2717:C:C2'	1:0:2718:C:H5''	1.95	0.96
1:0:1372:A:H3'	38:0:7013:HOH:O	1.64	0.95
1:0:1160:G:H5'	1:0:1161:A:H5'	0.96	0.95
1:0:1751:G:H2'	1:0:1752:G:H5''	1.45	0.95
25:X:43:VAL:HG13	25:X:76:ARG:HH12	1.31	0.95
1:0:542:A:H5'	1:0:542:A:H8	1.30	0.95
1:0:1189:A:H1'	1:0:1209:C:O4'	1.66	0.94
21:T:71:VAL:HG11	21:T:90:PRO:HB3	1.46	0.94
1:0:2506:A:HO2'	1:0:2507:G:H8	1.14	0.94
1:0:558:C:C2'	1:0:559:U:H5''	1.98	0.94
1:0:559:U:H6	1:0:559:U:H5'	1.31	0.94
1:0:656:G:H5'	16:O:3:THR:CG2	1.98	0.94
1:0:558:C:H2'	1:0:559:U:H5''	1.50	0.93
26:Y:187:VAL:HG23	26:Y:192:ASP:HB2	1.49	0.93
1:0:282:C:O2'	1:0:283:U:H5'	1.68	0.93
10:H:3:ALA:HA	10:H:58:ARG:HH12	1.33	0.93
1:0:1667:A:H8	1:0:1667:A:H5'	1.31	0.92
1:0:2489:G:H1'	38:0:7099:HOH:O	1.67	0.92
1:0:2291:A:C8	1:0:2309:C:H5'	2.05	0.91
1:0:2559:C:H4'	38:0:7080:HOH:O	1.71	0.91
1:0:156:C:H5''	14:M:171:ARG:HD3	1.51	0.91
30:3:74:CYS:HG	37:3:8704:CD:CD	0.91	0.91
1:0:1474:C:H5'	1:0:1474:C:C6	2.06	0.90
19:R:8:ALA:HB1	19:R:13:THR:HG21	1.53	0.90
1:0:962:C:H1'	15:N:5:ARG:NH1	1.87	0.89
1:0:2783:A:H3'	38:0:5060:HOH:O	1.73	0.89
24:W:137:GLN:HE21	24:W:141:HIS:HE1	1.18	0.89
4:B:162:MET:SD	4:B:310:ARG:HD3	2.13	0.89
1:0:545:G:H5'	1:0:545:G:H8	1.37	0.88
1:0:1441:G:H1'	38:0:7584:HOH:O	1.72	0.88
24:W:21:LEU:HD22	24:W:26:ILE:HD11	1.56	0.87
1:0:69:A:H5'	1:0:69:A:H8	1.39	0.87
1:0:1329:A:H2	38:0:4515:HOH:O	1.58	0.87
1:0:1666:C:O2'	1:0:1667:A:H5''	1.74	0.86
1:0:2694:A:H4'	7:E:91:PHE:CE1	2.10	0.86
12:K:29:LEU:HB3	12:K:55:VAL:HG11	1.57	0.86
4:B:62:ARG:HA	4:B:65:MET:HE3	1.57	0.86
1:0:182:G:H5'	38:0:4986:HOH:O	1.74	0.85
1:0:214:U:H5'	38:0:5968:HOH:O	1.76	0.85
1:0:2004:U:H4'	38:0:5134:HOH:O	1.77	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1701:A:H4'	1:0:1702:U:H5''	1.57	0.84
1:0:1835:U:H5	1:0:1840:A:N7	1.74	0.84
1:0:2769:C:C2'	1:0:2770:G:H5'	2.08	0.84
1:0:1118:A:C8	1:0:1118:A:H3'	2.13	0.83
1:0:1919:A:H4'	38:0:4681:HOH:O	1.75	0.83
1:0:2908:A:H2'	1:0:2909:G:O4'	1.77	0.83
1:0:272:A:H5'	1:0:273:G:OP2	1.77	0.83
1:0:544:G:H2'	1:0:545:G:H5''	1.60	0.83
1:0:1450:C:H4'	1:0:1451:C:OP2	1.76	0.83
2:9:3056:A:C2'	2:9:3057:A:H5''	2.09	0.83
1:0:2533:C:H6	1:0:2533:C:C5'	1.90	0.83
1:0:1165:G:H4'	1:0:1174:A:O2'	1.79	0.83
1:0:1979:G:H2'	38:0:3110:HOH:O	1.78	0.83
6:D:134:LEU:HD11	6:D:166:ILE:HD11	1.61	0.83
23:V:12:THR:HG22	23:V:15:GLU:HG3	1.60	0.82
1:0:69:A:H5'	1:0:69:A:C8	2.14	0.82
24:W:149:LEU:HG	24:W:153:MET:HE2	1.62	0.82
1:0:1118:A:H3'	1:0:1118:A:H8	1.43	0.82
1:0:1206:U:H5'	1:0:1206:U:H6	1.42	0.82
1:0:1116:U:O2'	1:0:1118:A:H2	1.62	0.82
1:0:380:A:H2'	38:0:7050:HOH:O	1.79	0.81
1:0:656:G:H3'	16:O:37:ARG:HH12	1.45	0.81
2:9:3049:G:H5''	38:9:4707:HOH:O	1.80	0.81
1:0:1205:U:H2'	1:0:1206:U:C5'	2.11	0.81
24:W:5:VAL:HG11	24:W:153:MET:HE1	1.63	0.81
19:R:99:ALA:HB1	19:R:109:MET:HE1	1.61	0.80
1:0:2756:U:H3	1:0:2896:A:H2	1.28	0.80
17:P:115:SER:H	17:P:118:GLN:NE2	1.80	0.80
1:0:506:G:H22	1:0:509:A:H5'	1.47	0.80
1:0:558:C:H2'	1:0:559:U:C5'	2.12	0.80
1:0:711:G:H1'	38:0:6919:HOH:O	1.81	0.80
1:0:962:C:H1'	15:N:5:ARG:HH12	1.47	0.80
1:0:1180:U:H1'	38:0:3053:HOH:O	1.81	0.80
4:B:55:ASN:HB3	4:B:63:GLU:HA	1.63	0.80
1:0:1205:U:H2'	1:0:1206:U:H5''	1.62	0.80
3:A:211:LYS:HB3	3:A:212:PRO:HD2	1.64	0.80
11:J:107:ASN:HD22	11:J:109:TYR:H	1.27	0.80
1:0:1189:A:H3'	38:0:7501:HOH:O	1.82	0.79
1:0:2851:G:O2'	1:0:2852:A:H5'	1.82	0.79
1:0:2896:A:H5''	38:0:5925:HOH:O	1.82	0.79
2:9:3006:C:C5'	15:N:37:ARG:NH1	2.43	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:870:G:H2'	1:0:871:G:H5''	1.63	0.79
2:9:3092:G:H2'	2:9:3093:A:C8	2.17	0.79
1:0:656:G:C5'	16:O:3:THR:HG22	2.09	0.78
1:0:2526:C:O2'	1:0:2527:U:H5'	1.83	0.78
15:N:71:TRP:CE3	15:N:175:LEU:HD22	2.18	0.78
2:9:3029:C:C2'	2:9:3030:C:H5'	2.14	0.78
1:0:681:G:N3	1:0:681:G:H5'	1.98	0.78
1:0:2508:C:H2'	38:0:6580:HOH:O	1.83	0.78
5:C:139:VAL:HG13	38:C:8641:HOH:O	1.82	0.78
7:E:20:ILE:HD11	7:E:40:VAL:HG11	1.64	0.78
1:0:871:G:C8	1:0:871:G:C5'	2.57	0.78
1:0:542:A:H5'	1:0:542:A:C8	2.17	0.78
1:0:2769:C:O2'	1:0:2770:G:H5'	1.83	0.78
1:0:926:A:H4'	13:L:39:GLU:HG2	1.65	0.77
17:P:59:ARG:HH22	17:P:66:GLN:HE22	1.31	0.77
1:0:1185:U:H5'	38:0:7289:HOH:O	1.84	0.77
1:0:1527:A:H1'	1:0:1528:A:C8	2.20	0.77
1:0:877:G:H5'	1:0:878:G:OP1	1.85	0.77
1:0:2426:G:H1'	38:0:5918:HOH:O	1.84	0.77
1:0:2502:C:C2'	1:0:2503:A:H5'	2.14	0.77
1:0:111:C:O2'	28:1:20:ARG:HG2	1.83	0.77
1:0:848:C:H5'	38:0:7096:HOH:O	1.84	0.77
3:A:153:ARG:HB2	3:A:153:ARG:HH11	1.49	0.77
4:B:212:GLN:HB2	4:B:257:THR:HG21	1.67	0.77
1:0:1603:A:H5'	1:0:1605:G:O4'	1.85	0.77
1:0:2506:A:O2'	1:0:2507:G:H8	1.68	0.76
24:W:137:GLN:HE21	24:W:141:HIS:CE1	2.01	0.76
1:0:130:C:H2'	38:0:9977:HOH:O	1.85	0.76
1:0:1116:U:HO2'	1:0:1118:A:H2	0.81	0.76
1:0:1666:C:H2'	1:0:1667:A:H5'	1.68	0.76
4:B:36:PRO:HA	4:B:168:GLY:HA3	1.67	0.76
1:0:1328:A:OP1	26:Y:169:ARG:HD2	1.86	0.76
24:W:4:LEU:HD22	24:W:52:VAL:HG21	1.68	0.75
30:3:25:VAL:HG22	30:3:68:LYS:HG3	1.67	0.75
3:A:88:ILE:HD13	3:A:100:PRO:HD3	1.68	0.75
5:C:127:ARG:NH2	5:C:225:PRO:HG2	2.01	0.75
1:0:541:C:H2'	1:0:542:A:C5'	2.15	0.75
26:Y:189:ASN:HD22	26:Y:191:ASP:H	1.34	0.75
1:0:1667:A:H5'	1:0:1667:A:C8	2.21	0.75
1:0:2851:G:C2'	1:0:2852:A:H5'	2.17	0.75
38:0:5050:HOH:O	12:K:39:GLY:HA2	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1377:C:H1'	38:0:3564:HOH:O	1.87	0.74
1:0:2694:A:H4'	7:E:91:PHE:HE1	1.50	0.74
1:0:1166:A:H61	1:0:1180:U:H3	1.33	0.74
1:0:2780:C:H1'	7:E:143:GLN:HE21	1.50	0.74
1:0:1446:U:H2'	20:S:55:GLN:NE2	2.03	0.73
1:0:2361:A:H5'	38:0:8824:HOH:O	1.87	0.73
1:0:2799:A:H4'	38:0:7080:HOH:O	1.88	0.73
1:0:587:A:H5''	38:0:7109:HOH:O	1.88	0.73
1:0:2890:A:H1'	22:U:56:ARG:NH2	2.03	0.73
24:W:52:VAL:HG22	24:W:53:ALA:H	1.53	0.73
1:0:1175:G:H1'	1:0:1193:A:H2'	1.69	0.73
1:0:2507:G:H2'	1:0:2510:C:H42	1.53	0.73
26:Y:141:THR:HG23	38:Y:8167:HOH:O	1.88	0.73
11:J:107:ASN:HD21	11:J:109:TYR:HB2	1.53	0.73
1:0:289:G:N2	1:0:363:A:C2	2.57	0.73
1:0:1119:G:N2	1:0:1246:A:C2	2.57	0.73
2:9:3006:C:C5'	15:N:37:ARG:HH12	1.88	0.73
1:0:544:G:C2'	1:0:545:G:H5''	2.19	0.73
1:0:1172:G:H5''	38:0:7084:HOH:O	1.89	0.72
1:0:2004:U:H2'	1:0:2004:U:O2	1.87	0.72
1:0:1751:G:C2'	1:0:1752:G:H5''	2.19	0.72
4:B:238:ASN:HD22	4:B:240:GLY:H	1.38	0.72
9:G:67:LEU:O	9:G:71:LEU:HG	1.89	0.72
1:0:545:G:H5'	1:0:545:G:C8	2.22	0.72
38:0:3566:HOH:O	21:T:9:LYS:HD3	1.88	0.72
1:0:656:G:H3'	16:O:37:ARG:NH1	2.03	0.72
1:0:1183:C:H2'	38:0:6073:HOH:O	1.90	0.72
8:F:58:GLU:HA	8:F:61:MET:HE2	1.71	0.72
1:0:1701:A:H5'	38:0:6109:HOH:O	1.90	0.71
1:0:1973:A:H5'	1:0:1973:A:H8	1.54	0.71
1:0:2716:G:H5''	4:B:206:THR:HG21	1.71	0.71
1:0:1266:U:H4'	26:Y:115:ARG:HH21	1.53	0.71
1:0:2769:C:H2'	1:0:2770:G:H5'	1.70	0.71
1:0:1162:G:H1'	31:I:117:LEU:CD1	2.20	0.71
1:0:1184:C:H1'	38:0:7289:HOH:O	1.90	0.71
1:0:2748:G:H5'	38:0:7362:HOH:O	1.91	0.71
2:9:3014:G:H5'	2:9:3014:G:H8	1.56	0.71
1:0:952:G:H4'	38:0:6557:HOH:O	1.89	0.70
1:0:1615:A:H5'	38:0:4007:HOH:O	1.90	0.70
12:K:10:GLN:H	12:K:10:GLN:NE2	1.85	0.70
38:0:7249:HOH:O	23:V:42:ASN:HB3	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3069:U:OP1	15:N:4:PRO:HG3	1.91	0.70
5:C:140:VAL:HB	38:C:8644:HOH:O	1.91	0.70
7:E:97:VAL:HG12	38:E:4191:HOH:O	1.91	0.70
6:D:154:LYS:H	6:D:154:LYS:HD2	1.57	0.70
38:0:4667:HOH:O	11:J:47:THR:HB	1.91	0.70
1:0:1641:A:H2'	1:0:1642:A:H5'	1.73	0.70
1:0:1116:U:H3	1:0:1246:A:H62	1.36	0.70
1:0:1441:G:O2'	1:0:1442:A:H5'	1.91	0.70
4:B:221:GLN:HE22	12:K:42:ASN:HD22	1.40	0.70
10:H:56:GLN:NE2	10:H:126:ARG:HE	1.89	0.70
1:0:2135:A:O2'	1:0:2136:G:H5'	1.92	0.69
1:0:2664:A:H8	1:0:2664:A:OP1	1.74	0.69
2:9:3051:A:H5'	15:N:160:SER:HB3	1.73	0.69
12:K:81:ARG:HB2	12:K:87:ARG:NH1	2.07	0.69
1:0:381:G:H5''	38:0:4148:HOH:O	1.91	0.69
1:0:1507:C:H4'	38:S:8524:HOH:O	1.92	0.69
4:B:190:MET:HE2	4:B:194:PHE:CD1	2.28	0.69
1:0:2679:G:H2'	1:0:2681:A:OP2	1.92	0.69
3:A:48:ASP:HB3	38:A:8899:HOH:O	1.92	0.69
1:0:506:G:H22	1:0:509:A:C5'	2.06	0.69
1:0:513:A:N3	38:0:3468:HOH:O	2.24	0.69
1:0:2505:G:O2'	1:0:2506:A:H5'	1.91	0.69
1:0:1130:U:H5'	38:0:7493:HOH:O	1.93	0.69
1:0:958:G:O2'	1:0:959:C:H5'	1.93	0.69
1:0:2878:U:H2'	1:0:2879:A:O4'	1.93	0.69
4:B:195:ARG:HG2	4:B:323:LEU:HD22	1.74	0.69
10:H:3:ALA:HA	10:H:58:ARG:NH1	2.07	0.69
10:H:166:SER:CB	10:H:167:PRO:HD3	2.23	0.69
12:K:98:VAL:CG1	12:K:102:GLU:HA	2.23	0.69
1:0:308:U:H5'	1:0:309:C:OP1	1.92	0.69
1:0:870:G:OP2	3:A:3:ARG:HD3	1.92	0.69
1:0:1377:C:H5'	1:0:1377:C:H6	1.56	0.69
11:J:107:ASN:ND2	11:J:109:TYR:H	1.90	0.69
1:0:1669:A:H2'	1:0:1670:G:C8	2.28	0.68
23:V:12:THR:HG23	23:V:14:ALA:H	1.57	0.68
1:0:1120:U:H5'	1:0:1121:G:OP2	1.92	0.68
1:0:2578:G:H5'	1:0:2578:G:H8	1.57	0.68
4:B:8:LYS:HG3	4:B:220:VAL:HG12	1.73	0.68
1:0:271:C:N4	1:0:378:A:C2	2.58	0.68
1:0:2502:C:H2'	1:0:2503:A:H5'	1.76	0.68
1:0:2769:C:H2'	1:0:2770:G:C5'	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:74:A:H2'	1:0:75:U:H6	1.58	0.68
1:0:1163:G:H5'	31:I:115:ASP:O	1.92	0.68
1:0:2812:A:C2	1:0:2814:A:N6	2.59	0.68
1:0:65:C:O2'	1:0:66:G:H5'	1.94	0.68
1:0:2054:A:N3	19:R:128:ARG:NH2	2.42	0.68
10:H:166:SER:HB2	10:H:167:PRO:CD	2.23	0.68
25:X:43:VAL:CG1	25:X:76:ARG:HH12	2.06	0.68
29:2:41:HIS:H	29:2:45:ASN:HD22	1.40	0.68
14:M:99:ARG:HD2	14:M:167:GLY:HA2	1.74	0.68
14:M:24:GLN:HE21	14:M:27:ARG:HH11	1.41	0.68
14:M:164:THR:HG23	14:M:167:GLY:H	1.57	0.68
1:0:119:A:H2'	1:0:120:A:H5''	1.76	0.67
1:0:2533:C:C6	1:0:2533:C:C5'	2.73	0.67
1:0:282:C:H1'	1:0:368:C:H42	1.60	0.67
1:0:1537:C:H1'	38:0:6414:HOH:O	1.94	0.67
13:L:143:THR:HG22	13:L:144:ASP:H	1.58	0.67
2:9:3031:C:H1'	38:9:1137:HOH:O	1.95	0.67
4:B:267:LYS:HD3	38:B:8828:HOH:O	1.93	0.67
22:U:9:CYS:HA	22:U:52:THR:HG23	1.76	0.67
23:V:1:THR:HG23	23:V:2:VAL:H	1.57	0.67
1:0:699:C:H5'	38:0:3831:HOH:O	1.93	0.67
6:D:50:VAL:O	6:D:71:ALA:HA	1.95	0.67
1:0:1118:A:H62	1:0:1244:U:H3	1.41	0.67
8:F:96:ALA:HA	38:F:3111:HOH:O	1.94	0.67
1:0:559:U:H6	1:0:559:U:C5'	2.07	0.67
8:F:21:GLU:O	8:F:24:ARG:HG2	1.95	0.67
12:K:81:ARG:HB2	12:K:87:ARG:HH11	1.59	0.67
1:0:1679:C:H5'	38:0:9137:HOH:O	1.95	0.67
1:0:1701:A:H5''	1:0:1702:U:H3'	1.76	0.67
2:9:3076:G:C3'	2:9:3077:A:H5''	2.23	0.67
1:0:1167:G:H4'	31:I:135:LEU:HD21	1.77	0.67
1:0:1253:C:H4'	38:0:6300:HOH:O	1.94	0.67
15:N:48:VAL:CG1	15:N:55:ASP:HB3	2.24	0.67
1:0:1508:C:H5'	20:S:21:GLN:NE2	2.10	0.66
1:0:1878:G:H2'	38:0:3072:HOH:O	1.95	0.66
2:9:3054:A:O2'	2:9:3055:U:H5'	1.95	0.66
12:K:74:VAL:HG11	12:K:113:ILE:HG12	1.76	0.66
15:N:37:ARG:HH21	15:N:105:GLY:CA	2.08	0.66
31:I:78:LEU:HD12	31:I:112:LYS:NZ	2.09	0.66
1:0:31:C:H2'	38:0:7508:HOH:O	1.95	0.66
1:0:1163:G:H5''	31:I:115:ASP:HB3	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2717:C:H2'	1:0:2718:C:C5'	2.22	0.66
1:0:1921:A:O2'	1:0:1922:A:H5'	1.95	0.66
38:0:7279:HOH:O	4:B:211:THR:HG21	1.95	0.66
12:K:109:LEU:HD13	12:K:113:ILE:HD11	1.78	0.66
1:0:74:A:H2'	1:0:75:U:C6	2.32	0.65
1:0:2507:G:H2'	1:0:2510:C:N4	2.11	0.65
1:0:1940:C:H4'	38:0:7170:HOH:O	1.96	0.65
11:J:75:PRO:HG2	11:J:105:LEU:HD21	1.77	0.65
24:W:4:LEU:HD23	24:W:54:PHE:HB3	1.79	0.65
29:2:40:ARG:HA	29:2:45:ASN:HD22	1.61	0.65
1:0:1377:C:H5'	1:0:1377:C:C6	2.30	0.65
1:0:2256:G:H2'	1:0:2257:G:H5'	1.78	0.65
4:B:248:ARG:O	4:B:251:VAL:HG22	1.97	0.65
4:B:254:GLN:HG2	4:B:255:GLY:N	2.11	0.65
7:E:6:GLU:HA	7:E:46:THR:HG22	1.79	0.65
11:J:19:MET:HE3	11:J:132:LEU:HD11	1.78	0.65
13:L:143:THR:HG22	13:L:144:ASP:N	2.11	0.65
15:N:144:GLY:O	15:N:147:ILE:HG22	1.95	0.65
24:W:125:HIS:HD2	24:W:127:GLY:H	1.43	0.65
1:0:794:U:H3	1:0:819:A:H61	1.44	0.65
1:0:2498:C:O2'	1:0:2499:U:H5'	1.97	0.65
1:0:200:U:H2'	38:0:3257:HOH:O	1.97	0.65
1:0:905:C:H4'	26:Y:144:ARG:NH1	2.12	0.65
1:0:1636:G:O2'	1:0:1637:A:H5'	1.97	0.65
2:9:3058:G:H1'	38:9:3839:HOH:O	1.96	0.65
1:0:1119:G:H8	11:J:52:GLN:HE22	1.45	0.65
2:9:3002:U:H4'	38:9:5321:HOH:O	1.95	0.65
7:E:24:GLY:HA3	7:E:76:VAL:HB	1.79	0.65
1:0:1393:A:H2'	1:0:1394:C:C6	2.32	0.65
3:A:153:ARG:HB2	3:A:153:ARG:NH1	2.11	0.65
4:B:232:TRP:HD1	4:B:235:ARG:HD2	1.60	0.65
5:C:5:ILE:HD11	5:C:16:VAL:HG22	1.78	0.65
14:M:80:GLY:O	14:M:81:ARG:HD3	1.97	0.65
1:0:1205:U:C2'	1:0:1206:U:H5''	2.27	0.64
1:0:1525:G:H5'	1:0:1526:A:OP2	1.97	0.64
24:W:6:GLN:HB2	24:W:26:ILE:HD12	1.79	0.64
30:3:38:ARG:HB3	30:3:42:ARG:HH12	1.62	0.64
1:0:2420:G:O2'	1:0:2421:G:H5'	1.95	0.64
3:A:199:HIS:HD2	3:A:201:PHE:H	1.45	0.64
1:0:2608:C:H3'	38:0:7627:HOH:O	1.96	0.64
5:C:236:THR:HG22	5:C:239:ALA:CB	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:661:G:C5	1:0:686:A:C2	2.86	0.64
1:0:1474:C:H6	1:0:1474:C:C5'	2.03	0.64
1:0:1189:A:O2'	1:0:1208:C:H2'	1.97	0.64
1:0:1162:G:H1'	31:I:117:LEU:HD12	1.79	0.64
23:V:8:ILE:HA	23:V:11:MET:HE3	1.80	0.64
1:0:1364:G:H1'	38:0:4628:HOH:O	1.98	0.64
2:9:3061:C:H2'	2:9:3062:A:H8	1.62	0.64
1:0:420:U:H2'	1:0:421:C:C6	2.33	0.64
1:0:2256:G:C2'	1:0:2257:G:H5'	2.28	0.64
1:0:944:G:C8	24:W:23:MET:HE1	2.33	0.63
3:A:55:VAL:HG22	3:A:68:ILE:O	1.98	0.63
1:0:2346:C:H6	1:0:2346:C:O5'	1.80	0.63
2:9:3024:U:H3'	2:9:3025:G:C5'	2.28	0.63
6:D:25:MET:HE2	6:D:41:LEU:HG	1.81	0.63
1:0:559:U:H5'	1:0:559:U:C6	2.24	0.63
1:0:1528:A:H2'	1:0:1529:G:O4'	1.98	0.63
1:0:2676:C:H4'	11:J:70:PHE:CE1	2.34	0.63
20:S:37:VAL:O	20:S:41:VAL:HG23	1.98	0.63
24:W:21:LEU:HD22	24:W:26:ILE:CD1	2.28	0.63
1:0:290:C:N3	1:0:363:A:C2	2.67	0.63
8:F:91:VAL:HG12	8:F:92:GLY:H	1.64	0.63
1:0:1834:C:H2'	1:0:1840:A:N6	2.13	0.63
8:F:91:VAL:HG12	8:F:92:GLY:N	2.13	0.63
24:W:64:THR:O	24:W:68:THR:HG22	1.99	0.63
26:Y:189:ASN:HD21	26:Y:191:ASP:HB2	1.63	0.63
1:0:450:C:OP1	5:C:184:ARG:NH2	2.31	0.63
4:B:18:ARG:HE	4:B:256:GLN:NE2	1.97	0.63
19:R:39:THR:HG22	19:R:42:GLU:H	1.63	0.63
1:0:1058:A:H2'	1:0:1060:C:H5''	1.81	0.63
1:0:2667:G:H1'	1:0:2914:A:N3	2.14	0.63
19:R:25:PHE:CE2	19:R:29:LYS:HE2	2.34	0.63
1:0:87:C:C2	29:2:30:ASP:OD2	2.52	0.62
1:0:285:A:H2'	1:0:286:U:O4'	1.98	0.62
1:0:960:G:H3'	1:0:960:G:N3	2.14	0.62
38:0:5288:HOH:O	9:G:12:ILE:HG23	1.99	0.62
28:1:37:CYS:SG	28:1:39:PHE:HB2	2.39	0.62
1:0:2256:G:H2'	1:0:2257:G:C5'	2.29	0.62
1:0:2768:A:O2'	1:0:2769:C:H5'	1.99	0.62
34:0:8503:NA:NA	38:0:9254:HOH:O	1.73	0.62
24:W:21:LEU:HD21	24:W:48:VAL:HG11	1.80	0.62
1:0:42:C:H3'	38:0:3992:HOH:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:407:A:H2'	1:0:408:A:C8	2.35	0.62
1:0:1174:A:C5	1:0:1201:C:H4'	2.34	0.62
3:A:199:HIS:CD2	3:A:201:PHE:H	2.16	0.62
14:M:24:GLN:NE2	14:M:27:ARG:HH11	1.97	0.62
1:0:1634:G:H2'	1:0:1635:U:C6	2.34	0.62
1:0:1666:C:H2'	1:0:1667:A:C5'	2.29	0.62
4:B:232:TRP:CD1	4:B:235:ARG:HD2	2.34	0.62
6:D:65:GLU:HA	38:D:6752:HOH:O	1.99	0.62
1:0:155:C:OP2	14:M:188:ARG:HD3	2.00	0.62
1:0:380:A:OP2	14:M:9:ARG:HD2	1.98	0.62
1:0:1524:U:OP1	1:0:1524:U:H4'	2.00	0.62
1:0:1839:A:H3'	38:0:9460:HOH:O	1.99	0.62
21:T:9:LYS:HE3	21:T:13:ARG:NH1	2.13	0.62
1:0:905:C:H4'	26:Y:144:ARG:HH11	1.64	0.62
1:0:1150:A:C2	9:G:20:VAL:HG21	2.35	0.62
1:0:1552:G:H2'	1:0:1553:C:C6	2.35	0.62
1:0:1667:A:H2'	1:0:1668:U:C6	2.34	0.62
1:0:1835:U:C5	1:0:1840:A:N7	2.62	0.62
1:0:694:A:H1'	38:0:3628:HOH:O	1.98	0.62
1:0:1053:G:OP1	10:H:12:PRO:HG3	1.99	0.62
9:G:16:LYS:O	9:G:20:VAL:HG23	2.00	0.62
1:0:1209:C:H2'	1:0:1210:G:H8	1.65	0.62
1:0:1588:G:C6	1:0:1589:G:N1	2.67	0.62
1:0:2826:G:C6	1:0:2913:A:N6	2.68	0.62
6:D:99:ASP:HB3	6:D:103:ASN:H	1.64	0.62
1:0:558:C:O2'	1:0:559:U:H5''	2.00	0.61
12:K:98:VAL:HG11	12:K:102:GLU:HA	1.81	0.61
26:Y:187:VAL:HG23	26:Y:192:ASP:CB	2.27	0.61
26:Y:200:THR:HG22	26:Y:201:GLU:HG3	1.81	0.61
29:2:40:ARG:HA	29:2:45:ASN:ND2	2.15	0.61
1:0:2526:C:C6	1:0:2526:C:H5'	2.36	0.61
5:C:115:LEU:HD13	5:C:223:LEU:HD21	1.82	0.61
1:0:346:U:H4'	38:0:6669:HOH:O	2.00	0.61
1:0:1165:G:H1'	1:0:1174:A:H1'	1.80	0.61
12:K:29:LEU:HB3	12:K:55:VAL:CG1	2.30	0.61
13:L:92:ASP:HA	13:L:121:ILE:HB	1.80	0.61
1:0:902:G:N7	13:L:18:HIS:HD2	1.98	0.61
1:0:2827:A:H2'	1:0:2828:G:O4'	1.99	0.61
1:0:59:A:H5'	38:0:4160:HOH:O	1.99	0.61
24:W:88:THR:HG23	24:W:110:GLN:HB3	1.82	0.61
1:0:396:U:H1'	38:0:7448:HOH:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:653:C:H5''	38:0:7746:HOH:O	1.99	0.61
26:Y:126:PRO:HG2	26:Y:128:PHE:CE1	2.36	0.61
1:0:1666:C:C2'	1:0:1667:A:C5'	2.78	0.61
1:0:2586:U:H3	1:0:2592:G:H22	1.47	0.61
5:C:1:MET:HG2	5:C:2:GLN:H	1.65	0.61
5:C:236:THR:HG22	5:C:239:ALA:HB2	1.83	0.61
19:R:39:THR:HG23	19:R:107:GLU:O	2.00	0.61
1:0:396:U:O2'	1:0:418:C:H4'	2.00	0.61
1:0:399:C:H5'	14:M:179:GLY:O	2.01	0.61
1:0:1080:C:H4'	1:0:1081:A:OP1	1.99	0.61
1:0:2320:U:H4'	1:0:2321:A:O4'	2.00	0.61
3:A:125:ASN:HB3	3:A:158:VAL:HG12	1.82	0.61
17:P:13:VAL:HG21	17:P:41:ARG:HG2	1.82	0.61
25:X:43:VAL:HG13	25:X:76:ARG:NH1	2.11	0.61
1:0:20:G:H21	19:R:117:HIS:HD2	1.48	0.60
1:0:1206:U:H2'	1:0:1207:A:O4'	2.00	0.60
1:0:1666:C:C2'	1:0:1667:A:H5''	2.29	0.60
2:9:3014:G:H5'	2:9:3014:G:C8	2.35	0.60
6:D:146:LYS:NZ	15:N:107:ASN:HD21	1.99	0.60
1:0:290:C:O2'	1:0:291:C:H5'	2.00	0.60
1:0:1701:A:H4'	1:0:1702:U:C5'	2.30	0.60
1:0:2373:U:H1'	38:0:4592:HOH:O	2.00	0.60
12:K:32:ILE:HD11	12:K:56:SER:HB3	1.82	0.60
1:0:2421:G:H1'	38:0:4611:HOH:O	2.00	0.60
15:N:113:SER:HB2	38:N:8854:HOH:O	2.00	0.60
1:0:2414:A:H2'	1:0:2415:A:C8	2.37	0.60
2:9:3122:C:H5	38:9:2536:HOH:O	1.82	0.60
24:W:137:GLN:NE2	24:W:141:HIS:HE1	1.93	0.60
1:0:475:G:OP1	5:C:73:LEU:HD22	2.00	0.60
1:0:962:C:C1'	15:N:5:ARG:NH1	2.64	0.60
12:K:10:GLN:HE21	12:K:10:GLN:N	1.90	0.60
15:N:114:LYS:O	15:N:118:ILE:HG13	2.01	0.60
16:O:105:ASN:HD21	16:O:109:SER:H	1.49	0.60
30:3:70:ARG:HG2	30:3:77:ALA:HB2	1.83	0.60
1:0:130:C:H5'	38:0:5042:HOH:O	2.01	0.60
1:0:1926:G:H2'	1:0:1927:A:C8	2.37	0.60
2:9:3064:C:H2'	2:9:3065:A:H5'	1.84	0.60
26:Y:133:HIS:HD2	38:Y:8161:HOH:O	1.84	0.60
1:0:2329:C:O2'	1:0:2330:U:H5'	2.01	0.60
4:B:74:ILE:HD13	4:B:309:VAL:HG21	1.82	0.60
8:F:39:SER:HB3	8:F:45:ALA:HB2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:14:LYS:HB2	12:K:45:PRO:HG2	1.84	0.60
1:0:1167:G:H4'	31:I:135:LEU:CD2	2.31	0.60
1:0:2908:A:C2'	1:0:2909:G:H5'	2.31	0.60
15:N:37:ARG:HD3	35:N:8807:CL:CL	2.38	0.60
1:0:542:A:H8	1:0:542:A:C5'	2.08	0.60
1:0:1377:C:H6	1:0:1377:C:C5'	2.15	0.60
2:9:3092:G:H2'	2:9:3093:A:H8	1.64	0.60
4:B:125:GLU:O	4:B:129:ARG:HG3	2.00	0.60
1:0:278:A:H2'	1:0:279:C:O4'	2.02	0.60
1:0:1279:U:O2	1:0:1279:U:H2'	2.02	0.60
1:0:1624:A:H5'	1:0:1626:A:O4'	2.02	0.60
1:0:1819:G:H5'	38:0:4544:HOH:O	2.02	0.60
1:0:2252:A:C5	1:0:2253:G:H1'	2.37	0.60
34:L:8580:NA:NA	38:L:8831:HOH:O	1.73	0.59
15:N:37:ARG:HH21	15:N:105:GLY:HA3	1.67	0.59
31:I:113:HIS:N	31:I:114:PRO:HD2	2.17	0.59
11:J:107:ASN:HD22	11:J:107:ASN:C	2.10	0.59
26:Y:189:ASN:HD22	26:Y:191:ASP:N	1.99	0.59
29:2:35:ARG:HB2	38:2:2691:HOH:O	2.01	0.59
1:0:1562:C:H3'	1:0:1563:G:C8	2.38	0.59
23:V:39:ALA:N	23:V:40:PRO:HD2	2.17	0.59
1:0:1299:G:H5'	38:0:3895:HOH:O	2.02	0.59
2:9:3024:U:H3'	2:9:3025:G:H5'	1.82	0.59
10:H:84:LYS:HB2	10:H:84:LYS:NZ	2.18	0.59
1:0:282:C:O2'	1:0:283:U:C5'	2.48	0.59
8:F:63:ILE:HB	8:F:64:PRO:HD3	1.84	0.59
13:L:138:GLY:HA3	38:L:8854:HOH:O	2.01	0.59
22:U:46:ALA:HB1	22:U:52:THR:HG21	1.85	0.59
20:S:81:ILE:HG12	38:S:8541:HOH:O	2.03	0.59
1:0:2346:C:O2'	6:D:52:THR:HG21	2.03	0.59
4:B:320:GLN:HE21	4:B:321:PRO:HD3	1.67	0.59
29:2:19:SER:HB3	38:2:4479:HOH:O	2.03	0.59
1:0:510:U:O3'	36:0:8823:NEG:H31	2.03	0.59
4:B:312:ARG:HD3	4:B:315:VAL:HG13	1.83	0.59
1:0:2316:G:H4'	38:0:5918:HOH:O	2.03	0.59
2:9:3029:C:H5	38:N:8842:HOH:O	1.84	0.59
1:0:797:A:C4'	27:Z:10:ARG:N	2.65	0.59
15:N:80:SER:HB2	38:N:8833:HOH:O	2.02	0.59
1:0:1181:A:H2'	1:0:1182:C:H5'	1.85	0.58
1:0:1523:G:C5	1:0:1524:U:C4	2.91	0.58
2:9:3055:U:H4'	2:9:3056:A:C8	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:75:LEU:HD22	6:D:79:MET:HB3	1.85	0.58
20:S:77:VAL:O	20:S:80:ARG:HG2	2.02	0.58
22:U:44:ARG:HB3	38:U:3805:HOH:O	2.01	0.58
2:9:3048:C:H4'	15:N:141:ARG:HH21	1.69	0.58
18:Q:34:ASP:O	18:Q:37:GLU:HB2	2.03	0.58
19:R:96:VAL:HG13	19:R:106:GLY:HA3	1.85	0.58
3:A:200:PRO:HG2	3:A:225:VAL:HG21	1.85	0.58
7:E:133:VAL:HG12	7:E:141:VAL:HG13	1.85	0.58
11:J:76:ASP:HA	38:J:5907:HOH:O	2.03	0.58
21:T:112:LEU:HD23	21:T:119:ALA:HB3	1.85	0.58
1:0:2635:A:O2'	1:0:2636:C:H5'	2.03	0.58
38:0:5484:HOH:O	3:A:192:VAL:HB	2.03	0.58
2:9:3029:C:H2'	2:9:3030:C:C5'	2.26	0.58
4:B:217:ARG:HG3	4:B:257:THR:HG22	1.85	0.58
13:L:148:GLU:HA	38:L:8871:HOH:O	2.02	0.58
1:0:420:U:H2'	1:0:421:C:H6	1.69	0.58
3:A:97:ALA:HA	3:A:131:HIS:NE2	2.19	0.58
1:0:364:C:H2'	1:0:365:G:O4'	2.04	0.58
1:0:960:G:N3	1:0:960:G:C2'	2.66	0.58
24:W:80:ASP:O	24:W:84:VAL:HG23	2.02	0.58
1:0:1165:G:O2'	1:0:1174:A:H4'	2.02	0.58
1:0:2825:C:H4'	1:0:2826:G:O5'	2.04	0.58
17:P:59:ARG:NH2	17:P:66:GLN:HE22	2.00	0.58
26:Y:146:PRO:O	26:Y:154:ARG:HG3	2.04	0.58
1:0:1587:U:H2'	1:0:1588:G:O4'	2.04	0.58
1:0:2291:A:N9	1:0:2309:C:H5'	2.19	0.58
30:3:65:THR:HG22	30:3:67:LEU:HG	1.85	0.58
1:0:621:C:H5'	26:Y:132:ASP:OD2	2.04	0.58
1:0:2908:A:O5'	1:0:2908:A:H8	1.87	0.58
24:W:38:THR:HG22	24:W:39:ASP:N	2.19	0.58
31:I:78:LEU:HD12	31:I:112:LYS:HZ2	1.69	0.58
1:0:1174:A:C6	1:0:1201:C:H4'	2.39	0.57
1:0:1528:A:H62	1:0:1663:G:H21	1.52	0.57
24:W:88:THR:HG22	24:W:90:TYR:HD1	1.68	0.57
1:0:1603:A:H5''	1:0:1605:G:H5'	1.86	0.57
14:M:99:ARG:CD	14:M:167:GLY:HA2	2.33	0.57
24:W:52:VAL:HG22	24:W:53:ALA:N	2.19	0.57
26:Y:235:GLU:CD	26:Y:235:GLU:H	2.12	0.57
1:0:1396:C:H4'	17:P:2:ASP:OD1	2.05	0.57
1:0:1778:A:H2'	1:0:1779:A:H5'	1.86	0.57
1:0:271:C:N4	1:0:378:A:H2	1.89	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:447:A:OP1	21:T:2:LYS:HG2	2.04	0.57
1:0:500:G:H21	19:R:98:ASN:HD21	1.53	0.57
1:0:1130:U:H2'	1:0:1131:G:O4'	2.05	0.57
1:0:2815:G:N7	11:J:80:LYS:NZ	2.52	0.57
1:0:2005:G:H3'	1:0:2005:G:OP2	2.04	0.57
1:0:2256:G:O2'	1:0:2257:G:H5'	2.04	0.57
1:0:2415:A:C2	15:N:25:ARG:HB3	2.39	0.57
1:0:2890:A:C4	22:U:56:ARG:CZ	2.88	0.57
1:0:2908:A:H2'	1:0:2909:G:C4'	2.33	0.57
38:0:6598:HOH:O	15:N:4:PRO:HD2	2.04	0.57
8:F:36:THR:HG23	8:F:97:ALA:HB2	1.87	0.57
15:N:169:PRO:O	15:N:172:PHE:HB3	2.05	0.57
19:R:18:LEU:HG	19:R:91:LEU:HD13	1.87	0.57
1:0:1181:A:C2'	1:0:1182:C:H5'	2.35	0.57
1:0:1187:U:H2'	38:0:6725:HOH:O	2.03	0.57
1:0:1205:U:H2'	1:0:1206:U:H5'	1.84	0.57
1:0:1249:U:H5	38:0:7333:HOH:O	1.87	0.57
1:0:812:A:H1'	38:0:3773:HOH:O	2.03	0.57
1:0:870:G:C2'	1:0:871:G:H5''	2.33	0.57
1:0:1242:A:H5'	11:J:82:THR:CG2	2.20	0.57
1:0:1731:C:H1'	38:0:6270:HOH:O	2.05	0.57
14:M:66:SER:HB3	14:M:128:TRP:CD1	2.40	0.57
1:0:470:U:O2'	28:1:16:HIS:HD2	1.88	0.57
1:0:517:U:OP2	36:0:8823:NEG:O4	2.23	0.57
1:0:1162:G:H1'	31:I:117:LEU:HD11	1.85	0.57
1:0:1559:A:OP2	1:0:1559:A:H8	1.87	0.57
1:0:2064:U:H5'	1:0:2652:U:O3'	2.05	0.57
3:A:105:VAL:CG1	3:A:154:ALA:HB1	2.35	0.57
7:E:101:GLU:HB2	7:E:116:THR:O	2.04	0.57
1:0:1878:G:H5''	38:0:9612:HOH:O	2.05	0.56
1:0:2874:G:H3'	38:0:9391:HOH:O	2.03	0.56
27:Z:46:ARG:HD3	27:Z:59:TYR:HB2	1.86	0.56
1:0:1181:A:N1	1:0:1192:A:O2'	2.37	0.56
1:0:1687:C:O2	28:1:9:GLY:HA2	2.05	0.56
1:0:2717:C:O2'	1:0:2718:C:H5''	2.04	0.56
1:0:2846:C:H4'	38:0:4908:HOH:O	2.04	0.56
2:9:3002:U:OP2	2:9:3003:A:H5'	2.05	0.56
15:N:175:LEU:HD11	38:N:8835:HOH:O	2.05	0.56
28:1:25:LYS:HD2	29:2:49:GLU:H	1.69	0.56
1:0:630:A:H1'	38:0:5640:HOH:O	2.04	0.56
1:0:797:A:H4'	27:Z:10:ARG:N	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1170:U:H1'	1:0:1172:G:N7	2.20	0.56
1:0:1669:A:H2'	1:0:1670:G:H8	1.68	0.56
1:0:1699:C:H4'	38:0:6264:HOH:O	2.03	0.56
2:9:3078:G:N2	2:9:3103:A:OP2	2.36	0.56
10:H:120:ILE:H	10:H:120:ILE:HD12	1.69	0.56
24:W:88:THR:HG22	24:W:89:ASP:H	1.70	0.56
1:0:1189:A:H1'	1:0:1209:C:C1'	2.35	0.56
4:B:212:GLN:HB2	4:B:257:THR:CG2	2.36	0.56
1:0:2374:A:H2'	1:0:2375:G:C8	2.40	0.56
10:H:56:GLN:HE21	10:H:126:ARG:HE	1.54	0.56
12:K:20:CYS:HB2	12:K:29:LEU:HG	1.88	0.56
1:0:2787:C:H5	38:0:4466:HOH:O	1.88	0.56
3:A:153:ARG:HH11	3:A:153:ARG:CB	2.18	0.56
4:B:179:LEU:O	4:B:183:GLU:HG2	2.05	0.56
11:J:19:MET:HE2	11:J:79:PHE:HA	1.87	0.56
23:V:55:ARG:O	23:V:59:ILE:HG12	2.05	0.56
1:0:960:G:N3	1:0:960:G:H2'	2.20	0.56
1:0:1119:G:H2'	11:J:52:GLN:NE2	2.20	0.56
1:0:1819:G:H2'	1:0:1820:G:H4'	1.85	0.56
1:0:2769:C:C2'	1:0:2770:G:C5'	2.83	0.56
7:E:11:VAL:HG12	7:E:12:ASP:N	2.20	0.56
27:Z:37:HIS:HB2	27:Z:47:VAL:HB	1.88	0.56
1:0:281:U:H2'	1:0:282:C:O4'	2.05	0.56
1:0:1741:U:O2'	1:0:2723:G:H4'	2.06	0.56
12:K:74:VAL:HG13	12:K:113:ILE:HG23	1.88	0.56
15:N:132:ASN:O	15:N:135:VAL:HG12	2.05	0.56
18:Q:66:LYS:HB2	18:Q:70:ALA:O	2.06	0.56
24:W:115:THR:HG23	38:W:5420:HOH:O	2.05	0.56
1:0:1500:U:P	17:P:41:ARG:HH22	2.29	0.56
1:0:1552:G:H2'	1:0:1553:C:H6	1.70	0.56
1:0:1641:A:C2'	1:0:1642:A:H5'	2.36	0.56
1:0:1654:U:H2'	3:A:47:HIS:HD2	1.70	0.56
13:L:136:ALA:HB3	38:L:8872:HOH:O	2.05	0.56
19:R:40:ALA:O	19:R:44:VAL:HG23	2.06	0.56
1:0:447:A:P	21:T:1:SER:HB2	2.47	0.55
2:9:3001:U:O3'	2:9:3003:A:H5''	2.06	0.55
2:9:3107:C:H5	38:9:3167:HOH:O	1.89	0.55
1:0:2563:U:H2'	1:0:2565:C:O5'	2.06	0.55
36:0:8823:NEG:N4	36:0:8823:NEG:O3	2.39	0.55
6:D:23:VAL:HG21	6:D:45:THR:HG21	1.88	0.55
1:0:264:G:H1'	1:0:265:U:H5	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:560:C:H42	1:0:597:A:H61	1.53	0.55
2:9:3064:C:C2'	2:9:3065:A:H5'	2.37	0.55
20:S:33:SER:O	20:S:37:VAL:HG23	2.06	0.55
1:0:451:C:O2'	1:0:452:G:H5'	2.06	0.55
1:0:2453:G:H5''	38:L:8842:HOH:O	2.07	0.55
8:F:33:THR:HG21	8:F:59:ILE:O	2.07	0.55
9:G:12:ILE:HG22	9:G:17:GLN:NE2	2.22	0.55
1:0:1319:G:H1'	38:0:4524:HOH:O	2.07	0.55
3:A:95:PRO:HG2	3:A:98:GLU:HG2	1.88	0.55
20:S:57:THR:HG23	38:S:8534:HOH:O	2.05	0.55
25:X:30:MET:HE1	25:X:58:ALA:HB3	1.87	0.55
1:0:1126:C:O5'	1:0:1126:C:H6	1.89	0.55
1:0:1787:C:H4'	1:0:2883:A:O4'	2.06	0.55
1:0:10:U:H3'	38:0:3147:HOH:O	2.07	0.55
1:0:280:C:H2'	1:0:281:U:O4'	2.06	0.55
1:0:1551:C:O2	1:0:1634:G:N2	2.37	0.55
1:0:2851:G:H2'	1:0:2852:A:H5'	1.87	0.55
4:B:307:ARG:HH11	4:B:307:ARG:HG3	1.71	0.55
7:E:11:VAL:HG12	7:E:12:ASP:H	1.71	0.55
25:X:21:PRO:HG2	25:X:24:LYS:HD3	1.87	0.55
1:0:288:A:H61	1:0:364:C:H42	1.54	0.55
2:9:3061:C:H2'	2:9:3062:A:C8	2.41	0.55
3:A:72:GLU:HG3	27:Z:66:GLY:HA2	1.88	0.55
10:H:56:GLN:HE21	10:H:126:ARG:HG2	1.72	0.55
1:0:1167:G:H2'	1:0:1168:C:O4'	2.07	0.55
1:0:1172:G:H1'	38:0:4805:HOH:O	2.06	0.55
1:0:1192:A:H3'	1:0:1193:A:H5'	1.88	0.55
1:0:2649:A:H5'	1:0:2649:A:H8	1.72	0.55
14:M:147:LEU:O	14:M:150:ILE:HG22	2.07	0.55
15:N:73:ALA:HB1	15:N:74:PRO:HD2	1.88	0.55
1:0:512:G:O3'	1:0:513:A:H8	1.90	0.55
1:0:944:G:H21	24:W:44:MET:HE2	1.72	0.55
2:9:3039:U:H1'	2:9:3044:A:H61	1.71	0.55
9:G:63:ARG:O	9:G:67:LEU:HG	2.06	0.55
14:M:102:GLU:OE1	14:M:164:THR:HG21	2.06	0.55
1:0:90:A:H2'	1:0:91:G:O4'	2.07	0.54
1:0:644:G:H5'	1:0:644:G:N3	2.21	0.54
1:0:1291:A:H2	38:0:5120:HOH:O	1.90	0.54
4:B:150:ALA:O	4:B:152:PRO:HD3	2.07	0.54
5:C:25:PRO:HG2	38:C:8522:HOH:O	2.07	0.54
1:0:204:A:H2'	1:0:205:U:H5'	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:U:39:ASN:ND2	22:U:44:ARG:HH11	2.04	0.54
30:3:3:MET:O	30:3:90:PHE:HA	2.08	0.54
10:H:66:ARG:HD3	38:H:8582:HOH:O	2.06	0.54
1:0:737:A:H2'	1:0:738:G:O4'	2.07	0.54
18:Q:26:PRO:O	18:Q:30:VAL:HG23	2.08	0.54
23:V:29:ASN:O	23:V:33:VAL:HG23	2.08	0.54
1:0:1902:G:O2'	1:0:1903:U:H5'	2.08	0.54
1:0:524:A:H5''	19:R:29:LYS:HD3	1.90	0.54
1:0:941:G:C5	1:0:942:U:C4	2.96	0.54
1:0:1684:A:H1'	29:2:43:ARG:HH22	1.71	0.54
1:0:2001:G:O2'	1:0:2002:C:H5'	2.08	0.54
38:0:4562:HOH:O	15:N:21:HIS:HD2	1.91	0.54
3:A:95:PRO:HA	3:A:153:ARG:HA	1.90	0.54
7:E:84:MET:HE1	7:E:148:ILE:CD1	2.37	0.54
1:0:363:A:O2'	1:0:364:C:H5'	2.08	0.54
1:0:1925:G:O2'	1:0:1926:G:H5'	2.08	0.54
3:A:82:VAL:HG13	3:A:93:THR:HB	1.90	0.54
10:H:46:GLN:HB3	10:H:167:PRO:CD	2.26	0.54
1:0:61:G:H1'	38:0:5570:HOH:O	2.07	0.54
1:0:711:G:C2	1:0:718:C:C2	2.96	0.54
1:0:1183:C:N4	1:0:1184:C:H41	2.06	0.54
23:V:1:THR:HG23	23:V:2:VAL:N	2.23	0.54
1:0:105:G:O2'	1:0:106:A:H5'	2.08	0.54
1:0:657:G:OP1	5:C:27:ARG:NH2	2.37	0.54
1:0:1418:U:C4	20:S:58:MET:HE2	2.43	0.54
1:0:1562:C:O2	1:0:1562:C:H2'	2.08	0.54
1:0:1819:G:H2'	1:0:1820:G:C5'	2.38	0.54
1:0:1973:A:H5'	1:0:1973:A:C8	2.40	0.54
12:K:24:THR:HB	12:K:64:MET:HE2	1.89	0.54
15:N:154:LEU:O	15:N:155:GLU:HB3	2.08	0.54
1:0:1515:A:H2'	1:0:1516:C:C6	2.43	0.54
1:0:2300:A:H4'	1:0:2301:A:O5'	2.08	0.54
24:W:21:LEU:HD21	24:W:48:VAL:CG1	2.38	0.54
1:0:1118:A:C8	1:0:1118:A:C3'	2.76	0.53
1:0:1766:U:O2	1:0:1778:A:H5'	2.08	0.53
1:0:2270:G:H4'	3:A:223:ARG:NH1	2.22	0.53
1:0:2401:A:H2'	1:0:2402:A:C8	2.43	0.53
1:0:2781:U:H2'	1:0:2782:G:H5'	1.90	0.53
5:C:236:THR:HA	38:C:8644:HOH:O	2.08	0.53
1:0:1177:A:H8	1:0:1177:A:O5'	1.90	0.53
5:C:101:ASP:HA	38:C:8642:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:233:THR:HG22	5:C:234:VAL:N	2.23	0.53
10:H:46:GLN:HG3	10:H:137:TYR:CE2	2.42	0.53
28:1:21:ARG:HD2	28:1:37:CYS:SG	2.48	0.53
1:0:750:A:O3'	5:C:101:ASP:HB2	2.08	0.53
1:0:1165:G:O2'	1:0:1174:A:C4'	2.57	0.53
1:0:1321:A:H2'	1:0:1322:G:C8	2.44	0.53
1:0:2718:C:H6	1:0:2718:C:H5'	1.73	0.53
1:0:2721:U:H4'	12:K:87:ARG:HG3	1.89	0.53
17:P:143:ALA:HA	38:P:5521:HOH:O	2.07	0.53
25:X:41:PHE:CZ	25:X:74:ALA:HB3	2.42	0.53
26:Y:106:THR:HG23	26:Y:107:PRO:HD2	1.90	0.53
1:0:321:A:H1'	38:0:6859:HOH:O	2.07	0.53
1:0:635:A:H2'	1:0:636:G:H5''	1.89	0.53
1:0:797:A:H5'	27:Z:10:ARG:N	2.22	0.53
1:0:2649:A:H5'	1:0:2649:A:C8	2.44	0.53
1:0:2870:C:H2'	1:0:2871:G:H8	1.73	0.53
1:0:613:C:H2'	1:0:614:U:H6	1.72	0.53
1:0:1667:A:H2'	1:0:1668:U:H6	1.73	0.53
1:0:2435:U:H1'	38:0:5260:HOH:O	2.09	0.53
1:0:2699:A:H2'	1:0:2700:G:O4'	2.08	0.53
11:J:75:PRO:HD3	11:J:136:SER:OG	2.08	0.53
15:N:86:LEU:HD12	15:N:125:ALA:HB2	1.91	0.53
1:0:259:G:H21	14:M:58:GLN:NE2	2.07	0.53
3:A:36:ASP:C	3:A:38:ILE:H	2.17	0.53
4:B:162:MET:HE1	4:B:308:LEU:HD21	1.91	0.53
6:D:58:VAL:CG1	6:D:60:GLU:HG2	2.38	0.53
9:G:19:GLU:O	9:G:23:ILE:HG13	2.08	0.53
16:O:73:ASP:HA	16:O:92:VAL:O	2.08	0.53
28:1:10:LYS:HG3	38:1:2979:HOH:O	2.08	0.53
29:2:5:LYS:O	29:2:9:LYS:HG3	2.08	0.53
1:0:947:U:H2'	1:0:948:G:C8	2.44	0.53
1:0:1562:C:N4	38:0:5694:HOH:O	2.40	0.53
1:0:1596:U:H2'	1:0:1598:A:OP2	2.09	0.53
1:0:1634:G:H2'	1:0:1635:U:H6	1.73	0.53
1:0:1736:A:H1'	38:0:7406:HOH:O	2.08	0.53
1:0:1739:G:O2'	1:0:1740:U:H5'	2.07	0.53
4:B:154:VAL:CG1	4:B:156:LYS:HG2	2.37	0.53
4:B:214:PRO:HD2	38:B:8822:HOH:O	2.08	0.53
6:D:86:THR:O	6:D:90:LEU:HG	2.08	0.53
9:G:23:ILE:HD13	9:G:67:LEU:HD23	1.90	0.53
1:0:282:C:H1'	1:0:368:C:H41	1.67	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2004:U:O2	1:0:2004:U:C2'	2.57	0.53
2:9:3020:G:O2'	2:9:3021:G:H5'	2.08	0.53
7:E:15:GLN:HG3	7:E:20:ILE:HG12	1.91	0.53
24:W:108:ARG:HG3	24:W:114:PRO:HG3	1.91	0.53
1:0:119:A:H2'	1:0:120:A:C5'	2.38	0.53
1:0:841:A:OP2	19:R:128:ARG:HD2	2.08	0.53
1:0:1677:U:OP2	29:2:8:LYS:NZ	2.42	0.53
1:0:2073:G:OP2	1:0:2490:A:H5'	2.09	0.53
14:M:164:THR:CG2	14:M:167:GLY:H	2.22	0.53
16:O:37:ARG:HG3	38:O:3002:HOH:O	2.09	0.53
1:0:256:C:H2'	1:0:257:G:O4'	2.09	0.53
1:0:462:A:H2'	38:0:4714:HOH:O	2.09	0.53
1:0:545:G:H8	1:0:545:G:C5'	2.17	0.53
21:T:63:ILE:HD11	21:T:75:GLU:HB2	1.90	0.53
1:0:292:G:H2'	1:0:358:G:N2	2.24	0.52
1:0:447:A:OP2	21:T:1:SER:HB2	2.09	0.52
1:0:1594:C:OP2	17:P:120:ARG:HD2	2.09	0.52
1:0:2526:C:H5'	1:0:2526:C:H6	1.73	0.52
1:0:645:U:OP2	13:L:4:LYS:HE3	2.09	0.52
1:0:1768:C:H2'	1:0:1769:C:O4'	2.09	0.52
1:0:2866:U:C5	22:U:50:GLU:HB2	2.44	0.52
3:A:51:ARG:HB2	38:A:8899:HOH:O	2.09	0.52
23:V:4:HIS:HB3	38:V:6622:HOH:O	2.09	0.52
1:0:1226:G:H5'	38:0:4363:HOH:O	2.10	0.52
1:0:1625:U:H6	1:0:1625:U:H3'	1.73	0.52
1:0:1717:A:H5''	17:P:54:LYS:HB2	1.90	0.52
1:0:2364:A:H5''	18:Q:15:LYS:HD3	1.91	0.52
24:W:88:THR:HB	38:W:6679:HOH:O	2.08	0.52
25:X:37:LEU:HD13	25:X:85:VAL:HG21	1.92	0.52
1:0:1074:G:H4'	1:0:1260:G:C6	2.43	0.52
1:0:1244:U:OP1	11:J:18:ILE:HD13	2.09	0.52
15:N:48:VAL:HG11	15:N:55:ASP:HB3	1.90	0.52
1:0:1171:A:H2'	1:0:1172:G:H5'	1.91	0.52
27:Z:10:ARG:HA	38:Z:8715:HOH:O	2.09	0.52
1:0:1218:U:H2'	1:0:1219:U:C6	2.45	0.52
1:0:1370:G:O5'	19:R:62:HIS:HB3	2.09	0.52
5:C:236:THR:CG2	5:C:239:ALA:H	2.23	0.52
8:F:46:GLU:O	8:F:73:PRO:HD2	2.09	0.52
31:I:125:ALA:O	31:I:129:VAL:HG23	2.10	0.52
1:0:1548:U:O2'	1:0:1549:C:H5'	2.09	0.52
1:0:2133:U:H5'	38:0:4024:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2900:G:H2'	1:0:2901:C:O4'	2.10	0.52
25:X:78:GLU:HG2	25:X:79:GLU:H	1.74	0.52
26:Y:126:PRO:HG2	26:Y:128:PHE:CZ	2.44	0.52
1:0:303:C:H2'	1:0:304:G:O4'	2.10	0.52
1:0:1044:C:H5''	38:0:8844:HOH:O	2.09	0.52
1:0:1163:G:N1	1:0:1184:C:N4	2.58	0.52
1:0:1167:G:C4'	31:I:135:LEU:HD21	2.39	0.52
2:9:3100:G:H3'	38:9:7426:HOH:O	2.10	0.52
4:B:274:GLU:HA	4:B:292:GLY:O	2.09	0.52
1:0:308:U:C4	1:0:342:C:H1'	2.45	0.52
1:0:845:U:H2'	38:0:9017:HOH:O	2.08	0.52
1:0:2134:G:C6	1:0:2258:A:C8	2.98	0.52
18:Q:94:GLN:HG2	18:Q:95:GLU:N	2.23	0.52
1:0:39:G:N2	1:0:444:C:C2	2.78	0.52
1:0:1477:C:H5'	1:0:1868:G:C5'	2.40	0.52
1:0:2756:U:N3	1:0:2896:A:H2	2.01	0.52
3:A:81:GLN:HB2	3:A:92:ASN:ND2	2.25	0.52
30:3:11:CYS:HB2	30:3:20:HIS:CE1	2.45	0.52
1:0:926:A:O2'	13:L:41:HIS:HD2	1.93	0.51
1:0:1266:U:H4'	26:Y:115:ARG:NH2	2.23	0.51
7:E:84:MET:HG2	7:E:168:ILE:HA	1.92	0.51
15:N:49:THR:HG22	15:N:56:ASP:HB2	1.92	0.51
1:0:1702:U:H5'	38:0:3239:HOH:O	2.11	0.51
1:0:1805:G:H2'	1:0:1806:G:H8	1.73	0.51
1:0:2862:G:H4'	4:B:336:GLN:O	2.09	0.51
23:V:59:ILE:O	23:V:63:GLU:HG2	2.10	0.51
26:Y:189:ASN:HA	26:Y:217:ILE:HD11	1.91	0.51
1:0:968:G:O2'	1:0:969:G:H5'	2.10	0.51
1:0:2520:G:H5'	10:H:61:SER:OG	2.10	0.51
3:A:36:ASP:O	3:A:38:ILE:N	2.43	0.51
3:A:105:VAL:HG11	3:A:154:ALA:HB1	1.92	0.51
1:0:1202:A:H2'	1:0:1203:G:C5'	2.41	0.51
1:0:1205:U:C2'	1:0:1206:U:C5'	2.84	0.51
1:0:1741:U:H5'	1:0:1742:A:OP1	2.11	0.51
1:0:2326:U:H2'	1:0:2327:A:C8	2.46	0.51
11:J:64:GLY:HA3	35:J:8821:CL:CL	2.48	0.51
13:L:133:VAL:HA	38:L:8872:HOH:O	2.10	0.51
21:T:24:ARG:HH21	21:T:39:ASN:HD22	1.57	0.51
27:Z:46:ARG:CD	27:Z:59:TYR:HB2	2.40	0.51
1:0:11:A:H5'	1:0:12:U:OP2	2.10	0.51
1:0:1201:C:H2'	1:0:1202:A:H5'	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2387:U:H2'	1:0:2388:C:C6	2.45	0.51
1:0:2717:C:OP1	4:B:207:LYS:HG3	2.11	0.51
24:W:4:LEU:HB2	24:W:33:THR:HG22	1.93	0.51
25:X:72:VAL:HG22	25:X:85:VAL:HG12	1.91	0.51
1:0:317:A:OP1	21:T:52:ARG:O	2.29	0.51
1:0:1118:A:H8	1:0:1119:G:H5''	1.76	0.51
2:9:3039:U:H3'	2:9:3040:C:H5''	1.93	0.51
8:F:13:GLU:OE2	8:F:78:GLU:HG2	2.10	0.51
10:H:162:ARG:HD2	38:H:8583:HOH:O	2.09	0.51
15:N:164:ASP:CG	15:N:167:ASP:HA	2.36	0.51
1:0:136:C:H2'	1:0:137:U:O4'	2.11	0.51
1:0:1484:G:H2'	38:0:8919:HOH:O	2.09	0.51
4:B:201:ASP:HB2	4:B:312:ARG:HD2	1.93	0.51
6:D:88:LEU:HB2	6:D:89:PRO:HD3	1.92	0.51
9:G:12:ILE:N	9:G:13:PRO:HD3	2.26	0.51
28:1:8:GLN:HE22	28:1:11:LYS:NZ	2.09	0.51
1:0:820:G:O2'	1:0:856:G:H4'	2.11	0.51
1:0:1181:A:H2'	1:0:1182:C:C5'	2.41	0.51
1:0:1200:A:H3'	38:0:5585:HOH:O	2.10	0.51
1:0:2270:G:H4'	3:A:223:ARG:HH12	1.75	0.51
4:B:16:ARG:NE	38:B:8854:HOH:O	2.39	0.51
16:O:37:ARG:NH1	38:O:5650:HOH:O	2.44	0.51
1:0:106:A:H2'	1:0:107:U:O4'	2.11	0.51
1:0:544:G:C3'	1:0:545:G:H5''	2.41	0.51
1:0:1520:G:H2'	1:0:1521:C:C6	2.46	0.51
1:0:1992:U:H2'	1:0:1994:A:OP2	2.11	0.51
1:0:2019:A:H5'	38:0:4370:HOH:O	2.10	0.51
4:B:280:VAL:HG13	4:B:333:GLU:O	2.11	0.51
6:D:103:ASN:ND2	6:D:134:LEU:H	2.09	0.51
9:G:12:ILE:HG22	9:G:17:GLN:HE21	1.76	0.51
20:S:17:ASP:HB3	20:S:23:LYS:HB2	1.92	0.51
1:0:1159:G:H1	1:0:1208:C:H42	1.58	0.51
1:0:1576:G:H2'	1:0:1577:U:O4'	2.11	0.51
1:0:1965:C:O5'	1:0:1965:C:H6	1.94	0.51
1:0:2135:A:C2'	1:0:2136:G:H5'	2.40	0.51
18:Q:11:ARG:HD3	38:Q:5620:HOH:O	2.10	0.51
1:0:204:A:C2'	1:0:205:U:H5'	2.41	0.50
3:A:192:VAL:CG1	3:A:207:GLN:HB3	2.41	0.50
4:B:41:PHE:CD1	4:B:79:MET:HE2	2.46	0.50
4:B:305:ASP:O	4:B:306:LYS:HB2	2.11	0.50
4:B:329:TYR:CE2	22:U:15:PRO:HG2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1064:U:H2'	1:0:1065:G:C8	2.47	0.50
1:0:1175:G:C5	1:0:1193:A:C2	2.99	0.50
1:0:2338:G:H1'	6:D:105:SER:OG	2.11	0.50
1:0:2419:U:H5''	1:0:2420:G:H5'	1.93	0.50
1:0:2502:C:H4'	10:H:155:ASN:ND2	2.26	0.50
1:0:2505:G:C2'	1:0:2506:A:H5'	2.40	0.50
3:A:96:LEU:HD22	3:A:128:LEU:HD13	1.93	0.50
5:C:5:ILE:HD11	5:C:16:VAL:CG2	2.41	0.50
20:S:10:VAL:HG11	23:V:36:ALA:HA	1.92	0.50
1:0:850:U:H3'	38:0:6635:HOH:O	2.10	0.50
1:0:960:G:N3	1:0:960:G:C3'	2.74	0.50
2:9:3039:U:C2'	2:9:3040:C:OP1	2.59	0.50
13:L:149:ARG:HB2	38:L:8840:HOH:O	2.11	0.50
24:W:4:LEU:O	24:W:32:CYS:HA	2.11	0.50
1:0:682:A:H2'	1:0:683:G:O4'	2.11	0.50
1:0:1025:C:H5'	24:W:23:MET:O	2.11	0.50
1:0:2010:A:H2'	38:0:5787:HOH:O	2.11	0.50
1:0:2350:G:H2'	1:0:2351:C:H6	1.76	0.50
1:0:2515:C:H2'	1:0:2516:G:O4'	2.11	0.50
4:B:88:GLU:HB3	4:B:97:LEU:HD12	1.92	0.50
1:0:522:U:O2'	1:0:1366:C:H5'	2.10	0.50
1:0:2676:C:H4'	11:J:70:PHE:HE1	1.75	0.50
2:9:3038:A:H2	2:9:3043:G:H5''	1.76	0.50
24:W:31:HIS:HB3	38:W:5420:HOH:O	2.11	0.50
31:I:102:VAL:HG12	31:I:106:LYS:HE3	1.94	0.50
1:0:1625:U:H3'	1:0:1625:U:C6	2.47	0.50
16:O:105:ASN:HD21	16:O:109:SER:N	2.10	0.50
1:0:1180:U:H4'	31:I:91:GLU:HG2	1.93	0.50
1:0:1845:A:OP2	3:A:190:ARG:NH1	2.45	0.50
1:0:2429:A:H2'	1:0:2430:A:C8	2.47	0.50
1:0:289:G:N2	1:0:364:C:C2	2.79	0.50
1:0:721:A:H5''	16:O:51:TYR:CE2	2.47	0.50
1:0:820:G:H5'	1:0:821:U:H5'	1.93	0.50
1:0:960:G:H8	38:0:5800:HOH:O	1.94	0.50
1:0:1198:U:C6	1:0:1200:A:OP2	2.64	0.50
1:0:2886:C:O2'	1:0:2887:G:H5'	2.12	0.50
22:U:52:THR:HG22	22:U:54:THR:N	2.26	0.50
25:X:76:ARG:HH11	25:X:76:ARG:HG3	1.75	0.50
1:0:88:G:H2'	1:0:89:G:C8	2.46	0.50
1:0:106:A:H1'	38:0:9311:HOH:O	2.12	0.50
1:0:156:C:H5''	14:M:171:ARG:CD	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:661:G:C6	1:0:686:A:C2	2.99	0.50
1:0:920:C:H5''	1:0:921:G:O5'	2.12	0.50
1:0:1557:G:O2'	1:0:1558:C:H5'	2.12	0.50
6:D:84:LEU:C	6:D:86:THR:H	2.19	0.50
8:F:118:LEU:O	8:F:119:ARG:HB3	2.12	0.50
14:M:30:GLU:O	14:M:34:GLU:HG3	2.10	0.50
23:V:64:GLY:O	23:V:65:ASP:HB2	2.12	0.50
1:0:1209:C:H2'	1:0:1210:G:C8	2.46	0.49
1:0:1289:C:O2'	1:0:1290:G:H5'	2.11	0.49
1:0:1568:G:O2'	1:0:1569:U:H5'	2.12	0.49
1:0:1588:G:C6	1:0:1589:G:C6	3.00	0.49
1:0:2416:G:O2'	15:N:25:ARG:HG2	2.12	0.49
1:0:2591:C:H2'	1:0:2592:G:O4'	2.12	0.49
1:0:2908:A:H2'	1:0:2909:G:C5'	2.41	0.49
17:P:134:VAL:O	17:P:137:LEU:HB3	2.12	0.49
27:Z:42:CYS:SG	27:Z:43:GLY:N	2.84	0.49
1:0:960:G:H4'	38:0:7254:HOH:O	2.11	0.49
2:9:3003:A:H2	2:9:3021:G:N3	2.10	0.49
22:U:6:CYS:HB2	22:U:32:CYS:HB3	1.95	0.49
28:1:1:THR:HA	38:1:435:HOH:O	2.11	0.49
1:0:95:A:H5''	1:0:97:G:O4'	2.13	0.49
1:0:1304:U:H2'	1:0:1305:C:C6	2.47	0.49
1:0:1931:A:H2'	1:0:1932:G:H5'	1.94	0.49
1:0:2781:U:C2'	1:0:2782:G:H5'	2.42	0.49
7:E:81:GLU:HG2	7:E:134:SER:HB3	1.94	0.49
24:W:125:HIS:CD2	24:W:127:GLY:H	2.26	0.49
24:W:125:HIS:NE2	24:W:128:VAL:HG13	2.27	0.49
1:0:475:G:H5'	5:C:73:LEU:CD2	2.42	0.49
1:0:920:C:H4'	1:0:921:G:C2	2.46	0.49
1:0:1764:C:H2'	1:0:1765:G:O4'	2.12	0.49
2:9:3073:G:H2'	2:9:3074:G:C8	2.48	0.49
11:J:18:ILE:O	11:J:22:VAL:HG23	2.12	0.49
25:X:7:GLU:HG3	25:X:74:ALA:O	2.12	0.49
1:0:120:A:H2'	1:0:120:A:N3	2.27	0.49
1:0:517:U:P	36:0:8823:NEG:HN41	2.35	0.49
1:0:1342:C:C2'	1:0:1343:C:H5'	2.42	0.49
1:0:2100:A:H4'	5:C:64:GLY:O	2.12	0.49
5:C:57:PRO:HG2	5:C:73:LEU:HD13	1.94	0.49
19:R:99:ALA:HB1	19:R:109:MET:CE	2.38	0.49
1:0:1174:A:H3'	1:0:1176:C:OP2	2.12	0.49
1:0:1545:C:H2'	1:0:1546:G:O4'	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:304:PRO:HD2	4:B:307:ARG:NE	2.28	0.49
31:I:93:GLN:HE21	31:I:133:THR:CG2	2.26	0.49
1:O:308:U:C2	21:T:52:ARG:NH2	2.81	0.49
1:O:1097:A:H5''	24:W:125:HIS:CE1	2.47	0.49
1:O:1166:A:C6	1:O:1181:A:C2	3.01	0.49
1:O:2263:G:H1'	38:O:6449:HOH:O	2.12	0.49
1:O:2781:U:H1'	7:E:139:GLU:OE2	2.12	0.49
38:9:5071:HOH:O	15:N:20:TYR:HE2	1.95	0.49
4:B:145:HIS:HD2	4:B:146:THR:O	1.96	0.49
6:D:146:LYS:HZ3	15:N:107:ASN:HD21	1.61	0.49
10:H:169:GLY:HA3	38:H:8590:HOH:O	2.12	0.49
12:K:4:LEU:HD22	12:K:116:GLU:HB3	1.95	0.49
17:P:80:ARG:HG2	17:P:87:ARG:CZ	2.43	0.49
19:R:33:ARG:NH1	38:R:8842:HOH:O	2.41	0.49
1:O:1166:A:H2'	1:O:1166:A:N3	2.28	0.49
1:O:1520:G:C6	1:O:1521:C:N4	2.81	0.49
2:9:3049:G:O2'	2:9:3050:G:H5'	2.12	0.49
6:D:166:ILE:HB	38:D:6326:HOH:O	2.13	0.49
8:F:101:ALA:HA	38:F:5413:HOH:O	2.11	0.49
1:O:263:U:O4'	8:F:59:ILE:HD13	2.13	0.49
1:O:1594:C:O2'	1:O:1607:A:H4'	2.13	0.49
38:O:9642:HOH:O	4:B:252:PRO:HD3	2.12	0.49
2:9:3110:G:C5	2:9:3111:U:C5	3.01	0.49
4:B:140:LEU:HD12	4:B:174:ARG:HG3	1.94	0.49
12:K:125:ALA:C	12:K:127:ALA:H	2.20	0.49
14:M:59:GLY:HA3	14:M:141:ILE:HD11	1.95	0.49
15:N:83:LEU:HD13	15:N:175:LEU:HD23	1.94	0.49
25:X:10:VAL:HG12	25:X:11:THR:N	2.28	0.49
1:O:254:C:O2	1:O:254:C:H2'	2.11	0.49
1:O:694:A:H2'	1:O:695:C:H5'	1.94	0.49
1:O:1165:G:O2'	1:O:1166:A:OP1	2.28	0.49
11:J:74:ARG:NH1	11:J:144:THR:HG21	2.28	0.49
20:S:76:GLU:HB3	38:S:8549:HOH:O	2.13	0.49
1:O:415:A:O2'	1:O:416:G:H5'	2.13	0.48
1:O:944:G:H21	24:W:44:MET:CE	2.26	0.48
1:O:1453:G:H2'	1:O:1454:U:O4'	2.12	0.48
1:O:1528:A:H62	1:O:1663:G:N2	2.10	0.48
11:J:99:GLU:HA	38:J:7377:HOH:O	2.13	0.48
26:Y:99:ALA:HB2	26:Y:233:TYR:CE2	2.48	0.48
26:Y:212:ARG:HD2	38:Y:8180:HOH:O	2.12	0.48
31:I:120:ASP:HB2	31:I:123:ASN:HD22	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:51:VAL:HG23	4:B:329:TYR:O	2.13	0.48
5:C:93:LYS:O	5:C:98:ARG:NH2	2.46	0.48
8:F:117:GLU:C	8:F:119:ARG:H	2.21	0.48
24:W:130:HIS:O	24:W:136:GLY:HA3	2.13	0.48
1:O:875:A:C2	3:A:194:MET:HG2	2.48	0.48
1:O:2372:A:H2'	1:O:2373:U:C6	2.48	0.48
2:9:3092:G:C6	2:9:3093:A:N6	2.81	0.48
7:E:84:MET:HE1	7:E:148:ILE:HD12	1.95	0.48
1:O:440:C:H2'	1:O:441:A:C8	2.47	0.48
1:O:1238:C:H5''	1:O:1239:G:OP2	2.14	0.48
1:O:1497:G:H4'	1:O:1627:G:O2'	2.13	0.48
1:O:1508:C:H5'	20:S:21:GLN:HE22	1.77	0.48
1:O:2836:G:O2'	1:O:2838:A:N7	2.46	0.48
10:H:165:SER:OG	10:H:168:ALA:HB3	2.13	0.48
20:S:57:THR:HG22	20:S:58:MET:N	2.28	0.48
1:O:178:U:H2'	1:O:179:C:H6	1.78	0.48
1:O:1217:G:H2'	1:O:1218:U:C6	2.48	0.48
1:O:2385:G:H2'	1:O:2386:U:C6	2.48	0.48
15:N:73:ALA:HB1	15:N:74:PRO:CD	2.43	0.48
15:N:139:TRP:HA	15:N:139:TRP:CE3	2.49	0.48
26:Y:189:ASN:ND2	26:Y:191:ASP:H	2.06	0.48
31:I:78:LEU:HD12	31:I:112:LYS:HZ1	1.78	0.48
1:O:843:A:C2	1:O:846:A:C8	3.02	0.48
1:O:1185:U:H5''	31:I:123:ASN:HB3	1.96	0.48
1:O:1202:A:H2'	1:O:1203:G:O4'	2.14	0.48
1:O:1641:A:H2'	1:O:1642:A:C5'	2.42	0.48
1:O:1657:A:H2'	1:O:1658:A:C8	2.48	0.48
1:O:2870:C:H2'	1:O:2871:G:C8	2.48	0.48
5:C:37:ALA:HB2	38:C:8572:HOH:O	2.12	0.48
12:K:34:VAL:HG22	12:K:47:ALA:HB2	1.95	0.48
1:O:316:A:N3	1:O:336:G:O2'	2.45	0.48
1:O:699:C:C2	1:O:744:G:C2	3.02	0.48
1:O:1218:U:H2'	1:O:1219:U:H6	1.78	0.48
1:O:2372:A:H2'	1:O:2373:U:H6	1.79	0.48
2:9:3065:A:N6	2:9:3112:U:C6	2.81	0.48
2:9:3114:G:O6	15:N:11:ARG:HD3	2.14	0.48
8:F:2:VAL:HG22	8:F:57:GLU:OE1	2.14	0.48
8:F:58:GLU:HB3	14:M:8:ILE:HG23	1.96	0.48
29:2:41:HIS:N	29:2:45:ASN:HD22	2.09	0.48
1:O:128:A:C8	1:O:128:A:H3'	2.49	0.48
1:O:352:A:H2'	1:O:353:G:C8	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:566:A:H2'	1:0:567:U:O4'	2.14	0.48
5:C:118:THR:O	5:C:136:VAL:HG13	2.14	0.48
1:0:1299:G:O6	13:L:6:ARG:HD3	2.13	0.48
1:0:2010:A:C2'	38:0:5787:HOH:O	2.61	0.48
17:P:107:GLU:O	17:P:111:GLU:HG3	2.13	0.48
29:2:20:ARG:HB3	38:2:5444:HOH:O	2.12	0.48
1:0:240:C:O2	1:0:240:C:H2'	2.14	0.47
1:0:489:A:C8	21:T:82:THR:HG22	2.49	0.47
1:0:1398:G:H2'	1:0:1399:A:C8	2.48	0.47
1:0:1759:A:N3	1:0:1818:C:H2'	2.29	0.47
1:0:354:A:H2'	1:0:355:C:H6	1.79	0.47
1:0:407:A:H8	38:0:4289:HOH:O	1.97	0.47
1:0:1192:A:H3'	1:0:1193:A:C5'	2.44	0.47
1:0:1202:A:C2'	1:0:1203:G:H5'	2.44	0.47
38:0:9771:HOH:O	5:C:78:ARG:HD3	2.13	0.47
5:C:27:ARG:HG3	5:C:29:ASP:OD1	2.15	0.47
6:D:106:PHE:HB2	38:D:5198:HOH:O	2.14	0.47
25:X:14:LEU:HD12	25:X:67:PRO:O	2.14	0.47
31:I:75:THR:C	31:I:77:GLU:H	2.22	0.47
1:0:326:G:O2'	1:0:327:A:H5'	2.14	0.47
1:0:366:U:O2'	1:0:367:G:H5'	2.14	0.47
1:0:2570:G:H5''	38:0:4744:HOH:O	2.15	0.47
3:A:186:TRP:CG	3:A:187:PRO:HA	2.50	0.47
4:B:154:VAL:HG12	4:B:156:LYS:HG2	1.95	0.47
4:B:221:GLN:HE22	12:K:42:ASN:ND2	2.09	0.47
7:E:31:ARG:HH12	7:E:68:HIS:CD2	2.31	0.47
11:J:45:VAL:HG21	11:J:129:PHE:CD1	2.49	0.47
13:L:13:HIS:HB3	38:L:8895:HOH:O	2.14	0.47
15:N:44:ARG:HG3	15:N:45:ALA:N	2.29	0.47
1:0:92:G:H5'	38:0:7249:HOH:O	2.13	0.47
1:0:232:A:H4'	38:0:5909:HOH:O	2.12	0.47
1:0:1201:C:H5''	38:0:6062:HOH:O	2.13	0.47
1:0:1871:U:O4'	1:0:1873:G:C8	2.67	0.47
1:0:2251:G:H2'	1:0:2252:A:C8	2.49	0.47
1:0:2578:G:H5'	1:0:2578:G:C8	2.43	0.47
3:A:100:PRO:HG2	3:A:103:VAL:HG21	1.96	0.47
26:Y:189:ASN:ND2	26:Y:191:ASP:HB2	2.29	0.47
1:0:775:G:OP1	28:1:16:HIS:HE1	1.97	0.47
1:0:1202:A:H2'	1:0:1203:G:H5'	1.97	0.47
1:0:1450:C:C4'	1:0:1451:C:OP2	2.56	0.47
4:B:51:VAL:CG2	4:B:327:VAL:HG13	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:155:GLN:O	14:M:158:ARG:HG2	2.13	0.47
15:N:61:ALA:HB3	15:N:88:ALA:HB2	1.94	0.47
29:2:41:HIS:HD2	29:2:44:ARG:H	1.62	0.47
30:3:18:GLN:HB3	38:3:8816:HOH:O	2.13	0.47
1:0:422:G:O2'	1:0:423:A:H5'	2.14	0.47
1:0:2382:A:H5'	38:3:8835:HOH:O	2.14	0.47
1:0:2524:G:H21	1:0:2526:C:N4	2.13	0.47
2:9:3014:G:H2'	2:9:3015:C:H5'	1.97	0.47
38:9:5071:HOH:O	15:N:23:ARG:HD3	2.13	0.47
4:B:268:ARG:HH21	4:B:325:PRO:HG3	1.80	0.47
4:B:275:GLY:O	4:B:291:ASP:HA	2.14	0.47
13:L:129:ALA:O	13:L:133:VAL:HG23	2.15	0.47
28:1:25:LYS:HD2	29:2:49:GLU:N	2.29	0.47
31:I:93:GLN:HE21	31:I:133:THR:HG21	1.80	0.47
1:0:56:G:H5''	23:V:50:ARG:NH1	2.30	0.47
1:0:397:A:O2'	1:0:417:G:N3	2.45	0.47
1:0:968:G:H1'	10:H:32:LYS:HD2	1.97	0.47
1:0:1160:G:H5''	1:0:1161:A:H5'	1.81	0.47
1:0:1187:U:HO2'	1:0:1188:A:H8	1.60	0.47
1:0:2252:A:H2'	1:0:2253:G:O4'	2.15	0.47
1:0:2716:G:C5'	4:B:206:THR:HG21	2.44	0.47
2:9:3003:A:OP2	2:9:3025:G:N2	2.47	0.47
2:9:3034:A:H2'	2:9:3035:C:O4'	2.14	0.47
6:D:23:VAL:CG2	6:D:73:VAL:HB	2.44	0.47
6:D:136:ARG:HD2	6:D:155:HIS:O	2.15	0.47
7:E:10:ASP:HA	38:E:3707:HOH:O	2.14	0.47
9:G:64:ASN:HD22	9:G:64:ASN:N	2.13	0.47
10:H:80:GLU:HA	38:H:8585:HOH:O	2.14	0.47
11:J:51:GLU:O	11:J:55:GLU:HG3	2.15	0.47
17:P:115:SER:H	17:P:118:GLN:HE21	1.56	0.47
21:T:73:HIS:HB3	38:T:6320:HOH:O	2.15	0.47
1:0:1206:U:H6	1:0:1206:U:C5'	2.19	0.47
1:0:2247:C:H2'	1:0:2248:C:H6	1.79	0.47
1:0:2415:A:H2'	1:0:2416:G:H5'	1.95	0.47
1:0:2502:C:O2'	1:0:2503:A:H5'	2.13	0.47
8:F:56:PRO:HG2	14:M:43:PRO:O	2.15	0.47
23:V:44:GLY:O	23:V:48:GLU:HG2	2.14	0.47
27:Z:22:SER:O	27:Z:26:VAL:HG23	2.15	0.47
1:0:282:C:C2'	1:0:283:U:H5'	2.44	0.47
1:0:579:G:H2'	1:0:580:A:C8	2.50	0.47
1:0:1060:C:H6	1:0:1060:C:H5'	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1423:C:O2'	1:0:1424:A:H5'	2.15	0.47
1:0:1878:G:O2'	1:0:1879:U:P	2.72	0.47
1:0:1972:U:H2'	1:0:1973:A:C5'	2.45	0.47
1:0:2016:U:H2'	1:0:2017:U:C6	2.50	0.47
1:0:2768:A:H2'	1:0:2769:C:O4'	2.15	0.47
1:0:2832:C:H5	38:0:7037:HOH:O	1.97	0.47
1:0:2890:A:C1'	22:U:56:ARG:NH2	2.76	0.47
1:0:2908:A:O2'	1:0:2909:G:H5'	2.14	0.47
1:0:319:A:H4'	1:0:338:C:C5	2.50	0.47
1:0:542:A:C8	1:0:542:A:C5'	2.91	0.47
1:0:2866:U:H4'	1:0:2867:G:H5'	1.97	0.47
38:0:6557:HOH:O	18:Q:13:LYS:HE2	2.15	0.47
2:9:3110:G:C5	2:9:3111:U:C6	3.03	0.47
38:9:4707:HOH:O	15:N:147:ILE:HB	2.15	0.47
5:C:124:VAL:HA	5:C:230:GLY:O	2.15	0.47
5:C:129:HIS:CE1	5:C:231:ARG:HA	2.51	0.47
15:N:78:MET:HB2	15:N:79:PRO:HD3	1.97	0.47
26:Y:103:THR:HG22	26:Y:104:GLU:OE2	2.15	0.47
1:0:383:A:C2	1:0:407:A:C4	3.03	0.46
1:0:1181:A:C2	1:0:1192:A:C8	3.03	0.46
1:0:1197:G:H1'	1:0:1203:G:N2	2.29	0.46
1:0:1249:U:H2'	1:0:1250:C:C6	2.50	0.46
1:0:1878:G:O2'	1:0:1879:U:C6	2.65	0.46
1:0:2403:C:H2'	1:0:2404:G:O5'	2.15	0.46
1:0:2467:A:O2'	1:0:2468:A:H2'	2.16	0.46
26:Y:117:LEU:N	26:Y:174:VAL:HG21	2.30	0.46
1:0:130:C:O2'	1:0:131:A:N7	2.49	0.46
1:0:138:U:OP2	1:0:139:C:H5	1.99	0.46
1:0:273:G:H2'	1:0:274:G:O4'	2.15	0.46
1:0:1165:G:O2'	1:0:1174:A:C1'	2.63	0.46
1:0:1714:C:O2'	1:0:1715:C:H5'	2.15	0.46
1:0:1878:G:H1'	38:0:5948:HOH:O	2.15	0.46
2:9:3053:G:N2	6:D:13:MET:HE2	2.30	0.46
15:N:7:LYS:HE3	18:Q:21:ARG:O	2.16	0.46
24:W:88:THR:HG22	24:W:90:TYR:CD1	2.50	0.46
1:0:488:U:H2'	38:0:3825:HOH:O	2.15	0.46
1:0:958:G:H2'	1:0:959:C:H6	1.81	0.46
1:0:1191:A:H2'	1:0:1193:A:H5'	1.96	0.46
1:0:1761:U:H2'	1:0:1762:C:C6	2.50	0.46
1:0:2064:U:H5'	1:0:2652:U:H4'	1.96	0.46
38:0:6511:HOH:O	21:T:38:ARG:NH1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3003:A:C2	2:9:3021:G:N3	2.83	0.46
6:D:167:GLU:C	6:D:169:THR:H	2.24	0.46
10:H:47:ILE:HG12	10:H:165:SER:HA	1.96	0.46
17:P:91:LYS:O	17:P:95:GLU:HG3	2.14	0.46
22:U:17:THR:HG22	22:U:18:GLY:N	2.29	0.46
31:I:75:THR:HG21	38:I:5331:HOH:O	2.15	0.46
1:0:113:A:OP2	1:0:114:A:H2'	2.15	0.46
1:0:417:G:P	38:0:7241:HOH:O	2.74	0.46
1:0:517:U:OP1	36:0:8823:NEG:N4	2.48	0.46
1:0:807:A:H2'	1:0:808:A:O4'	2.16	0.46
1:0:840:U:H2'	19:R:128:ARG:NH1	2.31	0.46
38:0:7244:HOH:O	3:A:22:ARG:HD3	2.15	0.46
3:A:192:VAL:HG13	38:A:8852:HOH:O	2.15	0.46
19:R:9:ASP:O	19:R:13:THR:HB	2.14	0.46
22:U:6:CYS:C	22:U:8:TYR:H	2.24	0.46
28:1:25:LYS:O	28:1:25:LYS:HG2	2.15	0.46
1:0:568:G:OP2	24:W:122:ARG:HD3	2.14	0.46
1:0:1029:U:O2'	1:0:1273:C:OP1	2.33	0.46
1:0:1119:G:H2'	11:J:52:GLN:HE22	1.79	0.46
1:0:1174:A:H5'	38:0:4245:HOH:O	2.15	0.46
5:C:76:ARG:HG2	5:C:78:ARG:NH1	2.30	0.46
24:W:88:THR:HG23	24:W:110:GLN:HE21	1.80	0.46
26:Y:235:GLU:CD	26:Y:235:GLU:N	2.73	0.46
1:0:222:A:H2'	1:0:223:G:O4'	2.14	0.46
1:0:816:G:C6	1:0:817:G:N1	2.83	0.46
1:0:1592:G:O2'	1:0:1593:C:O5'	2.31	0.46
1:0:1665:G:O2'	1:0:1666:C:H5'	2.16	0.46
1:0:2488:A:H61	1:0:2534:C:H42	1.64	0.46
4:B:51:VAL:HG22	4:B:52:VAL:N	2.30	0.46
5:C:239:ALA:O	5:C:243:VAL:HB	2.16	0.46
15:N:71:TRP:HE3	15:N:175:LEU:HD22	1.78	0.46
23:V:39:ALA:N	23:V:40:PRO:CD	2.78	0.46
24:W:88:THR:CG2	24:W:90:TYR:HD1	2.28	0.46
27:Z:23:ARG:NH1	38:Z:8704:HOH:O	2.48	0.46
30:3:14:CYS:SG	30:3:74:CYS:SG	3.13	0.46
30:3:70:ARG:HB3	38:3:8875:HOH:O	2.14	0.46
1:0:287:C:H6	1:0:287:C:O5'	1.99	0.46
6:D:163:VAL:HA	38:D:6326:HOH:O	2.15	0.46
31:I:113:HIS:H	31:I:114:PRO:HD2	1.79	0.46
1:0:283:U:H5	1:0:284:C:N4	2.13	0.46
1:0:669:G:O2'	1:0:670:G:H5'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2107:U:O2'	1:0:2108:A:H5'	2.15	0.46
15:N:37:ARG:HG3	15:N:37:ARG:HH11	1.81	0.46
28:1:8:GLN:HE22	28:1:11:LYS:HZ2	1.64	0.46
30:3:55:VAL:HB	30:3:56:PRO:HD2	1.98	0.46
31:I:78:LEU:HD13	31:I:111:GLN:OE1	2.16	0.46
1:0:789:C:H1'	1:0:827:A:C2	2.51	0.46
1:0:1173:A:C2	1:0:1177:A:C8	3.04	0.46
1:0:1447:U:H3'	1:0:1506:U:O2	2.16	0.46
1:0:1790:C:H2'	1:0:1791:U:H6	1.81	0.46
1:0:2421:G:H3'	1:0:2422:U:H5''	1.98	0.46
3:A:33:GLU:H	3:A:33:GLU:CD	2.23	0.46
11:J:46:ILE:HA	38:J:1123:HOH:O	2.16	0.46
12:K:74:VAL:CG1	12:K:113:ILE:HG12	2.42	0.46
31:I:99:ASP:OD1	31:I:138:THR:HB	2.16	0.46
1:0:157:G:H4'	14:M:95:LYS:HE3	1.98	0.46
1:0:1003:U:H5''	38:0:9447:HOH:O	2.16	0.46
2:9:3056:A:C3'	2:9:3057:A:H5''	2.46	0.46
3:A:132:ASP:HB3	3:A:135:VAL:H	1.81	0.46
11:J:127:ILE:HG22	35:J:8801:CL:CL	2.52	0.46
19:R:132:ARG:NH1	38:R:8885:HOH:O	2.48	0.46
24:W:125:HIS:HD2	24:W:127:GLY:N	2.13	0.46
1:0:57:C:H5''	38:0:6585:HOH:O	2.15	0.45
1:0:553:G:H5'	38:0:3311:HOH:O	2.15	0.45
1:0:1193:A:C2	1:0:1194:A:N6	2.83	0.45
1:0:1371:U:H4'	38:0:7664:HOH:O	2.16	0.45
1:0:1495:C:H1'	1:0:1573:A:H1'	1.99	0.45
2:9:3013:A:H3'	2:9:3014:G:H5'	1.98	0.45
2:9:3065:A:C2'	2:9:3066:G:OP2	2.63	0.45
3:A:121:ALA:O	3:A:124:VAL:HG22	2.15	0.45
3:A:212:PRO:HB2	38:A:8855:HOH:O	2.15	0.45
10:H:45:VAL:HG13	10:H:168:ALA:HB2	1.99	0.45
13:L:90:ARG:NH2	13:L:121:ILE:HD11	2.31	0.45
13:L:143:THR:CG2	13:L:144:ASP:N	2.79	0.45
1:0:834:G:H4'	1:0:835:U:OP2	2.16	0.45
1:0:1118:A:C8	1:0:1119:G:H5''	2.51	0.45
1:0:1313:A:H5'	26:Y:208:LYS:O	2.16	0.45
1:0:1568:G:H2'	1:0:1569:U:O4'	2.16	0.45
1:0:1819:G:H2'	1:0:1820:G:C4'	2.47	0.45
1:0:1902:G:H2'	1:0:1903:U:O4'	2.15	0.45
1:0:2081:A:H4'	11:J:69:TYR:CE1	2.50	0.45
2:9:3040:C:H2'	2:9:3041:C:OP1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:5:LEU:HD21	7:E:66:GLN:HG3	1.97	0.45
1:0:1200:A:H4'	38:0:7164:HOH:O	2.15	0.45
1:0:1330:A:H5''	38:Y:8192:HOH:O	2.15	0.45
1:0:1456:C:H2'	1:0:1457:U:C6	2.51	0.45
1:0:1625:U:C6	1:0:1625:U:C3'	2.99	0.45
38:0:9767:HOH:O	25:X:23:HIS:HD2	1.98	0.45
1:0:120:A:H5'	28:1:20:ARG:HH21	1.82	0.45
1:0:1177:A:O5'	1:0:1177:A:C8	2.68	0.45
1:0:1947:G:N2	1:0:1966:U:C2	2.84	0.45
1:0:2598:U:O2	1:0:2600:A:H8	2.00	0.45
1:0:2676:C:H4'	11:J:70:PHE:CD1	2.52	0.45
3:A:35:GLY:O	3:A:36:ASP:HB3	2.15	0.45
4:B:112:THR:OG1	4:B:158:LYS:HG3	2.16	0.45
14:M:184:ARG:HG3	14:M:185:PRO:HA	1.98	0.45
27:Z:57:CYS:SG	27:Z:59:TYR:HB3	2.56	0.45
1:0:462:A:H3'	38:0:4714:HOH:O	2.17	0.45
1:0:857:A:H4'	3:A:176:HIS:CD2	2.52	0.45
1:0:1342:C:O2'	1:0:1343:C:H5'	2.16	0.45
1:0:1462:C:H2'	1:0:1463:A:C8	2.52	0.45
1:0:2050:G:H5''	19:R:80:TYR:O	2.17	0.45
10:H:26:SER:HA	10:H:59:HIS:HD2	1.82	0.45
13:L:43:HIS:HD2	38:L:8830:HOH:O	1.99	0.45
21:T:45:GLY:HA3	21:T:102:ASP:HB2	1.98	0.45
26:Y:203:VAL:HG12	26:Y:228:VAL:HG22	1.99	0.45
1:0:340:A:C8	1:0:340:A:O5'	2.69	0.45
1:0:920:C:H5'	1:0:921:G:C4	2.52	0.45
1:0:1183:C:H2'	1:0:1183:C:O2	2.17	0.45
1:0:1735:C:OP2	4:B:234:ARG:HG3	2.16	0.45
1:0:1931:A:C2'	1:0:1932:G:H5'	2.47	0.45
1:0:2506:A:O2'	1:0:2507:G:O5'	2.34	0.45
1:0:2587:OMU:H2'	1:0:2589:U:OP2	2.16	0.45
3:A:105:VAL:HG11	3:A:154:ALA:CB	2.46	0.45
6:D:149:ARG:NH1	38:D:3066:HOH:O	2.48	0.45
21:T:48:VAL:O	21:T:59:GLU:HG3	2.16	0.45
1:0:377:C:H5	38:0:3123:HOH:O	1.99	0.45
1:0:821:U:H4'	27:Z:17:ARG:HH12	1.80	0.45
1:0:926:A:O2'	13:L:41:HIS:CD2	2.70	0.45
1:0:1165:G:O2'	1:0:1174:A:H1'	2.16	0.45
1:0:1211:G:H2'	1:0:1212:C:H6	1.81	0.45
2:9:3018:U:H2'	2:9:3019:G:H8	1.82	0.45
2:9:3108:C:O2'	2:9:3109:G:H5'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:17:LYS:O	4:B:260:HIS:HD2	1.98	0.45
5:C:127:ARG:CZ	5:C:225:PRO:HG2	2.46	0.45
6:D:86:THR:C	6:D:89:PRO:HD2	2.42	0.45
7:E:20:ILE:O	7:E:30:THR:HA	2.17	0.45
23:V:39:ALA:C	23:V:41:GLU:H	2.24	0.45
26:Y:216:ARG:HD2	38:Y:8151:HOH:O	2.17	0.45
1:O:601:G:O2'	1:O:602:A:H5'	2.17	0.45
1:O:2060:A:H4'	38:Y:8159:HOH:O	2.16	0.45
1:O:2502:C:H2'	1:O:2503:A:C5'	2.44	0.45
1:O:2664:A:OP1	1:O:2664:A:C8	2.63	0.45
11:J:135:ILE:O	11:J:139:LEU:HG	2.16	0.45
1:O:131:A:OP2	1:O:141:C:H5	2.00	0.45
1:O:710:G:OP1	16:O:24:ALA:HB3	2.17	0.45
1:O:871:G:H4'	38:O:4242:HOH:O	2.16	0.45
1:O:877:G:C5'	1:O:878:G:OP1	2.61	0.45
1:O:1160:G:H5'	1:O:1161:A:C4'	2.43	0.45
1:O:1213:C:O2'	1:O:1214:G:H5'	2.16	0.45
1:O:1420:C:H2'	1:O:1420:C:O2	2.16	0.45
1:O:1573:A:N7	1:O:1574:C:C2	2.85	0.45
1:O:1706:G:C6	1:O:1707:G:N1	2.84	0.45
38:O:5092:HOH:O	4:B:254:GLN:NE2	2.50	0.45
4:B:141:ARG:HG2	4:B:165:ARG:HA	1.99	0.45
1:O:660:A:H4'	1:O:661:G:O5'	2.17	0.45
1:O:1514:C:O2'	1:O:1515:A:H5'	2.17	0.45
1:O:2438:G:H2'	1:O:2439:C:C6	2.51	0.45
4:B:75:GLU:C	4:B:77:PRO:HD3	2.42	0.45
13:L:125:PHE:CE1	13:L:140:VAL:HG13	2.52	0.45
14:M:72:ALA:HB2	14:M:93:ARG:HG2	1.99	0.45
19:R:23:MET:HE3	19:R:28:SER:OG	2.17	0.45
19:R:104:PHE:HB3	19:R:109:MET:HE2	1.99	0.45
25:X:7:GLU:HA	25:X:74:ALA:O	2.17	0.45
1:O:2720:C:O2	12:K:87:ARG:NH2	2.50	0.44
6:D:57:THR:HG23	6:D:63:ILE:HG22	1.98	0.44
7:E:20:ILE:CD1	7:E:40:VAL:HG11	2.40	0.44
10:H:43:TYR:HA	10:H:44:PRO:HD3	1.79	0.44
13:L:34:GLY:HA3	13:L:38:HIS:CE1	2.52	0.44
15:N:82:TYR:OH	15:N:176:ARG:NH1	2.50	0.44
16:O:39:THR:O	16:O:115:ARG:NH2	2.50	0.44
19:R:75:TRP:CG	19:R:76:ASP:H	2.34	0.44
1:O:1008:C:H5''	10:H:16:ARG:HH12	1.82	0.44
1:O:1170:U:O2'	1:O:1172:G:N7	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1481:G:H2'	1:0:1482:A:O4'	2.16	0.44
3:A:81:GLN:HB2	3:A:92:ASN:HD22	1.81	0.44
3:A:103:VAL:O	3:A:105:VAL:HG23	2.17	0.44
5:C:236:THR:HG21	38:C:8567:HOH:O	2.17	0.44
13:L:54:PRO:HG2	13:L:57:VAL:CG2	2.47	0.44
19:R:106:GLY:HA2	19:R:109:MET:HE3	1.99	0.44
20:S:18:MET:HE3	20:S:75:GLN:HA	1.97	0.44
21:T:47:THR:HB	21:T:100:ASP:HB3	1.99	0.44
26:Y:185:VAL:HG12	38:Y:8152:HOH:O	2.17	0.44
1:0:272:A:H3'	38:0:7352:HOH:O	2.17	0.44
1:0:319:A:H4'	1:0:338:C:C4	2.53	0.44
1:0:1613:C:H2'	1:0:1614:G:O4'	2.16	0.44
1:0:2252:A:H2'	1:0:2253:G:H5'	1.98	0.44
1:0:2421:G:H3'	1:0:2422:U:C5'	2.48	0.44
1:0:2842:G:H2'	1:0:2843:A:H5'	2.00	0.44
3:A:94:LEU:HD12	3:A:98:GLU:HB2	1.99	0.44
4:B:27:ASN:HD22	4:B:27:ASN:H	1.66	0.44
4:B:304:PRO:HD2	4:B:307:ARG:HE	1.82	0.44
6:D:10:PHE:CG	6:D:11:HIS:N	2.85	0.44
6:D:35:ALA:C	6:D:37:ALA:H	2.26	0.44
11:J:74:ARG:O	11:J:78:ILE:HG12	2.17	0.44
22:U:5:GLU:HG3	22:U:10:GLY:O	2.17	0.44
1:0:101:C:H2'	1:0:102:A:H8	1.83	0.44
1:0:907:A:H2'	1:0:908:A:H8	1.82	0.44
1:0:963:C:H2'	1:0:964:G:C8	2.53	0.44
1:0:1805:G:H2'	1:0:1806:G:C8	2.52	0.44
1:0:2424:U:H1'	18:Q:7:LEU:HD12	1.99	0.44
1:0:2446:G:H2'	1:0:2447:A:C8	2.52	0.44
1:0:2801:A:H2'	1:0:2801:A:N3	2.32	0.44
2:9:3052:A:H2'	2:9:3053:G:O4'	2.17	0.44
1:0:10:U:O4	1:0:532:A:OP2	2.36	0.44
1:0:213:G:HO2'	1:0:214:U:P	2.40	0.44
1:0:343:C:O2'	1:0:344:C:H5'	2.17	0.44
1:0:702:G:N2	1:0:727:G:H1'	2.31	0.44
1:0:703:G:O2'	1:0:704:C:H5'	2.18	0.44
1:0:899:C:H5'	38:0:3019:HOH:O	2.16	0.44
1:0:2769:C:H2'	1:0:2770:G:O4'	2.18	0.44
19:R:29:LYS:HD2	38:R:8839:HOH:O	2.17	0.44
22:U:52:THR:HG22	22:U:54:THR:H	1.83	0.44
24:W:29:VAL:O	24:W:30:ASN:HB2	2.17	0.44
1:0:281:U:O2'	1:0:282:C:H5'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:840:U:C2	1:0:2648:U:O4	2.70	0.44
1:0:1154:A:H2'	1:0:1155:G:H8	1.81	0.44
1:0:1183:C:H42	1:0:1184:C:H41	1.65	0.44
1:0:1586:G:O2'	1:0:1587:U:H5'	2.17	0.44
1:0:2472:C:O2'	1:0:2634:G:H4'	2.17	0.44
3:A:88:ILE:O	3:A:88:ILE:HG22	2.17	0.44
5:C:236:THR:HG22	5:C:239:ALA:H	1.81	0.44
21:T:41:ARG:NH1	21:T:42:VAL:O	2.50	0.44
31:I:113:HIS:N	31:I:114:PRO:CD	2.80	0.44
1:0:545:G:C8	1:0:545:G:C5'	2.98	0.44
1:0:558:C:C2'	1:0:559:U:C5'	2.78	0.44
14:M:48:LYS:HE3	14:M:52:GLN:NE2	2.33	0.44
19:R:81:PRO:O	19:R:85:SER:HB2	2.18	0.44
25:X:78:GLU:HG2	25:X:79:GLU:N	2.32	0.44
28:1:8:GLN:NE2	28:1:11:LYS:NZ	2.66	0.44
1:0:57:C:H42	1:0:89:G:H1	1.65	0.44
1:0:81:G:N3	1:0:98:A:C2	2.86	0.44
1:0:169:A:H5''	38:0:9502:HOH:O	2.17	0.44
1:0:172:U:H5'	38:0:3982:HOH:O	2.16	0.44
1:0:430:A:H8	1:0:430:A:O5'	2.01	0.44
1:0:1589:G:H4'	38:0:6684:HOH:O	2.18	0.44
1:0:1874:U:H2'	3:A:120:ARG:HG3	1.99	0.44
1:0:2511:A:H5'	1:0:2511:A:H8	1.82	0.44
1:0:2722:G:H4'	38:K:5029:HOH:O	2.18	0.44
1:0:2818:A:H2	38:B:8925:HOH:O	2.00	0.44
38:0:4993:HOH:O	4:B:260:HIS:HE1	2.01	0.44
8:F:111:ILE:O	8:F:115:VAL:HG23	2.18	0.44
10:H:23:ILE:HA	10:H:120:ILE:HG21	1.99	0.44
15:N:49:THR:CG2	15:N:56:ASP:HB2	2.47	0.44
19:R:47:LEU:O	19:R:51:ILE:HG13	2.18	0.44
21:T:26:THR:HA	21:T:39:ASN:HB3	1.99	0.44
24:W:61:THR:HG23	24:W:151:GLU:HG3	2.00	0.44
1:0:11:A:H2'	1:0:11:A:N3	2.33	0.44
1:0:70:A:H4'	1:0:71:G:O5'	2.18	0.44
1:0:707:C:C2	1:0:708:A:C8	3.05	0.44
1:0:1217:G:C2	1:0:1218:U:C2	3.06	0.44
4:B:24:PRO:CG	4:B:204:GLY:HA2	2.48	0.44
7:E:11:VAL:HG13	7:E:76:VAL:HG21	2.00	0.44
7:E:91:PHE:HA	7:E:92:PRO:HD3	1.85	0.44
12:K:23:ASN:HD21	12:K:107:THR:HB	1.82	0.44
14:M:64:ARG:HD2	38:M:8879:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1559:A:OP2	1:0:1559:A:C8	2.69	0.43
1:0:1761:U:H5'	17:P:81:LYS:O	2.18	0.43
1:0:2330:U:H4'	1:0:2331:C:OP1	2.18	0.43
38:9:4350:HOH:O	18:Q:25:PRO:HB2	2.17	0.43
13:L:143:THR:CG2	13:L:144:ASP:H	2.27	0.43
15:N:12:ARG:HD3	15:N:18:THR:OG1	2.18	0.43
30:3:70:ARG:HD3	38:3:8875:HOH:O	2.18	0.43
1:0:711:G:N2	1:0:718:C:C2	2.86	0.43
1:0:941:G:C6	1:0:942:U:C4	3.07	0.43
1:0:1472:C:O5'	1:0:1472:C:H6	2.00	0.43
1:0:1515:A:H2'	1:0:1516:C:H6	1.83	0.43
1:0:2896:A:N3	1:0:2896:A:H2'	2.33	0.43
2:9:3037:C:H4'	15:N:110:THR:HG23	1.99	0.43
2:9:3059:C:H6	2:9:3059:C:O5'	2.01	0.43
4:B:195:ARG:HG3	4:B:196:ALA:N	2.33	0.43
5:C:1:MET:HG2	5:C:2:GLN:NE2	2.33	0.43
6:D:135:VAL:HG22	6:D:136:ARG:H	1.83	0.43
6:D:146:LYS:NZ	15:N:107:ASN:ND2	2.65	0.43
12:K:55:VAL:HG12	12:K:56:SER:N	2.32	0.43
15:N:108:SER:HA	15:N:109:PRO:HD3	1.73	0.43
16:O:44:ASN:CG	16:O:67:SER:HB2	2.43	0.43
24:W:59:GLN:HE22	24:W:97:ALA:CB	2.30	0.43
30:3:73:GLU:HB3	38:3:8863:HOH:O	2.18	0.43
1:0:86:A:C2	29:2:25:VAL:HG13	2.53	0.43
1:0:407:A:H5'	38:0:5854:HOH:O	2.18	0.43
1:0:757:C:OP1	13:L:27:ARG:HD2	2.18	0.43
1:0:1310:U:OP2	5:C:168:ARG:NH1	2.50	0.43
1:0:2253:G:N2	1:0:2254:G:C4	2.86	0.43
1:0:2323:G:H5'	38:0:6847:HOH:O	2.17	0.43
1:0:2456:A:H2'	1:0:2457:U:C6	2.54	0.43
5:C:140:VAL:HG12	5:C:141:SER:N	2.33	0.43
9:G:63:ARG:N	38:G:2569:HOH:O	2.50	0.43
1:0:1132:A:N6	1:0:1229:C:H2'	2.34	0.43
1:0:1268:C:H2'	1:0:1269:G:H8	1.83	0.43
1:0:2478:U:O2'	1:0:2479:A:H5'	2.18	0.43
1:0:2546:U:H4'	38:0:4855:HOH:O	2.19	0.43
1:0:2842:G:C2'	1:0:2843:A:H5'	2.49	0.43
2:9:3095:C:O2'	2:9:3096:C:H5'	2.18	0.43
14:M:66:SER:HB3	14:M:128:TRP:NE1	2.32	0.43
24:W:3:ALA:O	24:W:54:PHE:HA	2.19	0.43
1:0:111:C:H2'	1:0:112:G:C5'	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:514:G:H5'	38:0:6921:HOH:O	2.17	0.43
1:0:1328:A:C8	26:Y:169:ARG:HD3	2.53	0.43
4:B:16:ARG:NH1	38:B:8911:HOH:O	2.51	0.43
22:U:52:THR:CG2	22:U:54:THR:HB	2.49	0.43
25:X:75:ALA:O	25:X:83:ALA:HA	2.19	0.43
1:0:926:A:C4'	13:L:39:GLU:HG2	2.42	0.43
1:0:1370:G:H5''	38:R:8851:HOH:O	2.18	0.43
1:0:1474:C:C6	1:0:1474:C:C5'	2.88	0.43
1:0:1550:A:C2	1:0:1636:G:C2	3.06	0.43
1:0:2613:G:O2'	1:0:2614:C:H5'	2.19	0.43
38:0:5239:HOH:O	3:A:164:ARG:NE	2.52	0.43
38:0:9363:HOH:O	30:3:46:ILE:HB	2.18	0.43
11:J:107:ASN:HA	11:J:108:PRO:HD2	1.94	0.43
13:L:54:PRO:HG2	13:L:57:VAL:HG21	1.99	0.43
23:V:8:ILE:HA	23:V:11:MET:CE	2.48	0.43
25:X:82:GLU:HB3	38:X:5564:HOH:O	2.17	0.43
1:0:293:A:H5''	1:0:357:A:N1	2.34	0.43
1:0:338:C:H4'	5:C:174:ILE:CD1	2.49	0.43
1:0:1333:U:H2'	1:0:1334:C:C6	2.54	0.43
1:0:2271:G:H4'	1:0:2272:G:OP1	2.18	0.43
2:9:3006:C:OP1	15:N:37:ARG:NH1	2.51	0.43
2:9:3013:A:H3'	2:9:3014:G:C5'	2.48	0.43
2:9:3014:G:C2'	2:9:3015:C:H5'	2.49	0.43
4:B:41:PHE:HB3	4:B:190:MET:HE3	2.01	0.43
4:B:307:ARG:HD2	38:B:8943:HOH:O	2.19	0.43
5:C:219:ASN:HB2	38:C:8590:HOH:O	2.18	0.43
13:L:125:PHE:CZ	13:L:140:VAL:HG13	2.54	0.43
14:M:81:ARG:HG3	14:M:85:ARG:HB2	2.01	0.43
16:O:49:GLU:HG2	38:O:5191:HOH:O	2.18	0.43
17:P:103:THR:HA	17:P:106:ARG:NH1	2.34	0.43
26:Y:234:VAL:HG12	26:Y:235:GLU:N	2.32	0.43
1:0:35:U:H5'	5:C:47:GLY:O	2.19	0.43
1:0:290:C:H1'	38:0:5931:HOH:O	2.18	0.43
1:0:475:G:H5'	5:C:73:LEU:HD23	2.00	0.43
1:0:599:G:O2'	1:0:600:G:H5'	2.19	0.43
1:0:734:U:H2'	1:0:736:A:OP2	2.18	0.43
1:0:958:G:H2'	1:0:959:C:C6	2.54	0.43
1:0:1119:G:N2	1:0:1246:A:H2	2.11	0.43
1:0:1506:U:H6	1:0:1506:U:H5'	1.84	0.43
1:0:2269:C:C2'	1:0:2270:G:H5'	2.48	0.43
1:0:2274:A:O2'	1:0:2275:G:H5'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2577:A:H5'	38:0:7569:HOH:O	2.18	0.43
1:0:2786:G:H5'	38:0:4466:HOH:O	2.19	0.43
2:9:3014:G:H2'	2:9:3015:C:C5'	2.49	0.43
4:B:267:LYS:HA	38:B:8828:HOH:O	2.17	0.43
15:N:82:TYR:CD2	15:N:82:TYR:C	2.97	0.43
16:O:10:LEU:HD13	16:O:99:GLU:HG3	1.99	0.43
31:I:101:SER:OG	31:I:104:GLN:HG3	2.19	0.43
1:0:938:G:H4'	38:0:5242:HOH:O	2.18	0.43
1:0:1803:C:H2'	1:0:1804:A:C8	2.54	0.43
1:0:2607:U:C4	4:B:242:TRP:CZ2	3.07	0.43
1:0:2879:A:H2'	1:0:2880:A:O4'	2.19	0.43
2:9:3031:C:H2'	2:9:3032:G:O4'	2.19	0.43
2:9:3052:A:O2'	2:9:3053:G:H5'	2.19	0.43
3:A:101:GLU:HG2	38:A:8871:HOH:O	2.19	0.43
1:0:165:A:H5''	13:L:33:ALA:HB2	2.00	0.43
1:0:185:G:H4'	1:0:186:A:OP1	2.19	0.43
1:0:316:A:H5'	21:T:54:ASP:OD2	2.19	0.43
1:0:1289:C:H3'	38:0:6233:HOH:O	2.18	0.43
1:0:1588:G:C5	1:0:1589:G:C6	3.07	0.43
1:0:1773:G:N2	1:0:1774:G:C8	2.86	0.43
1:0:1878:G:H4'	38:0:3939:HOH:O	2.19	0.43
1:0:1887:U:O5'	1:0:1887:U:H6	2.02	0.43
1:0:1972:U:H2'	1:0:1973:A:H5''	2.01	0.43
1:0:2694:A:C4'	7:E:91:PHE:CE1	2.94	0.43
35:0:8812:CL:CL	38:0:4953:HOH:O	2.59	0.43
2:9:3039:U:H1'	2:9:3044:A:N6	2.34	0.43
4:B:7:ARG:NH1	4:B:11:LEU:HD21	2.33	0.43
8:F:58:GLU:CD	14:M:27:ARG:HH22	2.25	0.43
13:L:55:GLN:HG3	38:L:8882:HOH:O	2.18	0.43
29:2:22:PRO:HG2	29:2:25:VAL:HG23	2.01	0.43
1:0:178:U:H2'	1:0:179:C:C6	2.54	0.42
1:0:764:C:H2'	1:0:765:G:O4'	2.19	0.42
1:0:964:G:H2'	1:0:965:A:O4'	2.19	0.42
1:0:1160:G:H2'	38:0:5461:HOH:O	2.18	0.42
1:0:1299:G:N2	38:0:4515:HOH:O	2.51	0.42
1:0:1795:G:H2'	1:0:1796:A:O4'	2.18	0.42
1:0:1878:G:O2'	1:0:1879:U:OP2	2.37	0.42
1:0:2011:A:H5'	1:0:2013:G:H1'	1.99	0.42
1:0:2768:A:H2'	1:0:2769:C:C6	2.54	0.42
1:0:2781:U:H2'	1:0:2782:G:C5'	2.49	0.42
1:0:2795:C:O2'	1:0:2796:U:H5'	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:193:LEU:HD22	5:C:222:ASP:O	2.19	0.42
6:D:170:TYR:CD1	6:D:170:TYR:N	2.87	0.42
7:E:158:ASP:O	7:E:162:PHE:HD1	2.01	0.42
16:O:50:ARG:HD2	16:O:51:TYR:CE1	2.54	0.42
28:1:8:GLN:NE2	28:1:11:LYS:HZ2	2.16	0.42
1:0:111:C:C2'	1:0:112:G:H5'	2.49	0.42
1:0:188:C:H5''	14:M:163:LEU:HD21	2.00	0.42
1:0:291:C:H2'	1:0:292:G:O4'	2.19	0.42
1:0:636:G:H1'	1:0:2058:G:C4	2.54	0.42
1:0:844:A:C6	1:0:882:A:C6	3.07	0.42
1:0:947:U:H2'	1:0:948:G:H8	1.82	0.42
1:0:1127:C:C5	1:0:1128:U:C4	3.07	0.42
1:0:1211:G:H2'	1:0:1212:C:C6	2.53	0.42
1:0:1516:C:H2'	1:0:1517:U:C6	2.54	0.42
1:0:2316:G:O2'	1:0:2462:G:O6	2.36	0.42
1:0:2748:G:H1'	38:0:7722:HOH:O	2.19	0.42
3:A:101:GLU:OE2	3:A:131:HIS:HB2	2.20	0.42
4:B:24:PRO:HG2	4:B:204:GLY:HA2	2.00	0.42
6:D:172:VAL:HG12	6:D:173:GLU:N	2.34	0.42
8:F:54:VAL:HG12	8:F:56:PRO:O	2.19	0.42
12:K:34:VAL:CG2	12:K:47:ALA:HB2	2.48	0.42
12:K:75:ARG:NH1	38:K:4172:HOH:O	2.51	0.42
15:N:64:SER:C	15:N:66:LEU:H	2.26	0.42
24:W:137:GLN:NE2	24:W:141:HIS:CE1	2.78	0.42
27:Z:10:ARG:HG3	27:Z:11:SER:H	1.83	0.42
27:Z:19:GLY:O	27:Z:23:ARG:HG2	2.18	0.42
1:0:352:A:H2'	1:0:353:G:H8	1.83	0.42
1:0:354:A:H2'	1:0:355:C:C6	2.54	0.42
1:0:441:A:H1'	1:0:442:A:N7	2.34	0.42
1:0:466:A:H2'	1:0:467:G:O4'	2.19	0.42
1:0:553:G:P	26:Y:204:ARG:HH22	2.43	0.42
1:0:807:A:H2'	1:0:808:A:C8	2.54	0.42
1:0:1519:U:H2'	1:0:1520:G:C8	2.55	0.42
1:0:1573:A:H2'	1:0:1574:C:O4'	2.19	0.42
1:0:1730:G:H4'	1:0:1731:C:H6	1.83	0.42
2:9:3013:A:O2'	2:9:3014:G:H5''	2.19	0.42
3:A:65:ARG:C	3:A:66:ARG:HG3	2.43	0.42
12:K:87:ARG:NH1	38:K:4066:HOH:O	2.52	0.42
1:0:318:C:H5'	1:0:339:A:C2	2.53	0.42
1:0:449:A:N7	5:C:43:LYS:HG2	2.35	0.42
1:0:459:A:H4'	38:0:9264:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:646:G:H2'	1:0:647:U:C6	2.54	0.42
1:0:1187:U:O2'	1:0:1188:A:C8	2.71	0.42
1:0:1661:A:C8	38:0:5036:HOH:O	2.57	0.42
1:0:1706:G:C6	1:0:1707:G:C6	3.07	0.42
1:0:2487:C:H5	38:0:4719:HOH:O	2.03	0.42
3:A:207:GLN:HA	38:A:8852:HOH:O	2.19	0.42
6:D:58:VAL:HG12	6:D:60:GLU:HG2	2.01	0.42
7:E:152:THR:HG21	7:E:165:GLY:HA2	2.01	0.42
7:E:172:PRO:HB3	38:E:6931:HOH:O	2.18	0.42
12:K:115:ARG:HG3	12:K:116:GLU:N	2.33	0.42
14:M:159:VAL:HG12	35:M:8818:CL:CL	2.57	0.42
24:W:11:VAL:O	24:W:12:ASN:HB2	2.19	0.42
1:0:796:A:C2	1:0:797:A:C4	3.08	0.42
1:0:1098:A:H2'	1:0:1099:G:O4'	2.19	0.42
1:0:1156:C:O5'	1:0:1156:C:H6	2.03	0.42
1:0:1755:A:H2'	1:0:1756:G:O4'	2.19	0.42
1:0:1789:G:H2'	1:0:1790:C:O5'	2.19	0.42
1:0:2807:U:H2'	1:0:2808:U:H6	1.84	0.42
1:0:2863:G:C2	1:0:2894:C:O2	2.73	0.42
2:9:3035:C:H5''	38:9:4078:HOH:O	2.19	0.42
12:K:130:MET:SD	22:U:25:ASP:O	2.78	0.42
1:0:541:C:C3'	1:0:542:A:H5''	2.47	0.42
1:0:1523:G:H2'	1:0:1524:U:C6	2.55	0.42
1:0:2090:G:H2'	1:0:2091:G:C8	2.54	0.42
1:0:2786:G:H3'	1:0:2787:C:H6	1.83	0.42
2:9:3044:A:O4'	6:D:76:ARG:NE	2.52	0.42
2:9:3115:C:C4	2:9:3116:C:C5	3.07	0.42
5:C:111:VAL:HB	38:C:8521:HOH:O	2.19	0.42
10:H:63:GLU:O	10:H:67:LEU:HB2	2.20	0.42
12:K:27:ARG:HD2	38:K:4747:HOH:O	2.20	0.42
15:N:119:GLN:O	15:N:123:ILE:HG13	2.20	0.42
24:W:4:LEU:HD22	24:W:52:VAL:CG2	2.45	0.42
24:W:106:THR:OG1	24:W:109:GLU:HG3	2.20	0.42
24:W:122:ARG:HH21	24:W:154:ARG:N	2.17	0.42
1:0:101:C:H2'	1:0:102:A:C8	2.54	0.42
1:0:111:C:O2'	1:0:112:G:H5'	2.19	0.42
1:0:213:G:H2'	38:0:6305:HOH:O	2.20	0.42
1:0:820:G:OP1	27:Z:17:ARG:NH2	2.53	0.42
1:0:1307:A:H2'	1:0:1308:A:C8	2.55	0.42
1:0:1503:U:H2'	1:0:1504:A:O4'	2.19	0.42
1:0:1730:G:H4'	1:0:1731:C:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2054:A:H4'	19:R:135:ALA:O	2.19	0.42
38:0:4909:HOH:O	3:A:22:ARG:HG2	2.20	0.42
3:A:179:MET:HG2	3:A:186:TRP:CG	2.55	0.42
4:B:139:ASP:HB3	38:B:8849:HOH:O	2.20	0.42
13:L:53:ARG:NH2	13:L:57:VAL:HG12	2.35	0.42
15:N:151:ASP:HB3	38:N:8824:HOH:O	2.20	0.42
16:O:26:TRP:HB2	38:O:3062:HOH:O	2.20	0.42
25:X:8:ARG:NH1	38:X:2479:HOH:O	2.52	0.42
1:0:243:A:H61	1:0:269:G:H1'	1.85	0.42
1:0:1164:U:OP1	31:I:74:PRO:HA	2.19	0.42
1:0:1170:U:H5	38:0:6824:HOH:O	2.03	0.42
1:0:1343:C:H2'	1:0:1344:G:O5'	2.20	0.42
1:0:1377:C:C6	1:0:1377:C:C5'	2.98	0.42
1:0:1787:C:OP1	17:P:68:LYS:HE2	2.20	0.42
1:0:1889:C:H2'	1:0:1890:U:O4'	2.20	0.42
1:0:1976:G:O2'	1:0:1977:U:H5'	2.20	0.42
1:0:2093:G:H5''	38:0:9291:HOH:O	2.19	0.42
1:0:2265:U:H2'	1:0:2266:A:C8	2.54	0.42
3:A:112:PRO:HD3	3:A:152:CYS:SG	2.60	0.42
4:B:62:ARG:CA	4:B:65:MET:HE3	2.41	0.42
5:C:19:PRO:HG2	5:C:22:PHE:CE1	2.55	0.42
5:C:233:THR:HG22	5:C:234:VAL:H	1.83	0.42
6:D:54:ALA:HB2	6:D:69:ILE:CD1	2.50	0.42
16:O:98:LEU:O	16:O:102:ILE:HG13	2.20	0.42
24:W:128:VAL:O	24:W:138:LEU:HD11	2.20	0.42
1:0:91:G:N2	1:0:92:G:H1'	2.34	0.42
1:0:162:C:H2'	1:0:163:U:H5'	2.02	0.42
1:0:448:G:H5''	38:0:4017:HOH:O	2.18	0.42
1:0:588:G:O6	24:W:154:ARG:NH1	2.53	0.42
38:0:5186:HOH:O	17:P:117:SER:HB2	2.19	0.42
5:C:246:ARG:NE	38:C:8617:HOH:O	2.52	0.42
7:E:68:HIS:O	7:E:72:MET:HG3	2.20	0.42
14:M:162:GLY:HA2	38:M:8819:HOH:O	2.20	0.42
19:R:149:GLU:HA	19:R:150:PRO:HD3	1.86	0.42
24:W:119:HIS:CD2	24:W:120:PRO:HD2	2.54	0.42
31:I:131:THR:O	31:I:131:THR:HG22	2.19	0.42
1:0:420:U:O4'	1:0:1920:C:C4	2.73	0.42
1:0:1155:G:H2'	1:0:1156:C:C6	2.54	0.42
1:0:1209:C:O2'	1:0:1210:G:H5'	2.19	0.42
1:0:1523:G:C6	1:0:1524:U:O4	2.73	0.42
1:0:1584:C:O2'	1:0:1585:C:H5'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1790:C:H2'	1:0:1791:U:C6	2.55	0.42
1:0:2288:G:H2'	1:0:2289:G:O4'	2.19	0.42
1:0:2748:G:N2	38:0:4977:HOH:O	2.52	0.42
3:A:37:VAL:HG22	38:A:8891:HOH:O	2.20	0.42
7:E:162:PHE:CD1	7:E:162:PHE:N	2.87	0.42
8:F:50:VAL:HG13	8:F:60:VAL:HG11	2.02	0.42
15:N:171:HIS:CE1	38:N:8861:HOH:O	2.73	0.42
24:W:139:GLY:O	24:W:141:HIS:HD2	2.03	0.42
29:2:20:ARG:HG3	29:2:39:ARG:HH21	1.85	0.42
30:3:14:CYS:SG	38:3:8863:HOH:O	2.62	0.42
30:3:23:GLU:HG2	30:3:24:LYS:N	2.34	0.42
1:0:177:A:H2'	1:0:178:U:O4'	2.20	0.41
1:0:306:A:P	21:T:38:ARG:HH21	2.42	0.41
1:0:445:U:C1'	38:0:7159:HOH:O	2.66	0.41
1:0:527:U:H2'	1:0:528:G:C8	2.54	0.41
1:0:1079:A:N1	1:0:2068:G:O2'	2.50	0.41
1:0:1186:C:C4	1:0:1187:U:C4	3.08	0.41
1:0:1198:U:H1'	1:0:1201:C:H5	1.85	0.41
1:0:2553:A:H2'	1:0:2553:A:N3	2.35	0.41
1:0:2590:U:H2'	1:0:2591:C:H5'	2.00	0.41
3:A:70:ALA:HA	3:A:71:PRO:HD3	1.80	0.41
4:B:115:VAL:HA	4:B:116:PRO:HD3	1.83	0.41
4:B:198:GLU:HA	38:B:8947:HOH:O	2.19	0.41
4:B:297:VAL:HB	38:B:8900:HOH:O	2.19	0.41
5:C:1:MET:HG2	5:C:2:GLN:N	2.34	0.41
5:C:130:GLU:HG2	5:C:168:ARG:HD3	2.01	0.41
7:E:23:GLU:HG2	7:E:28:SER:CB	2.49	0.41
17:P:10:ALA:O	17:P:13:VAL:HG12	2.20	0.41
19:R:33:ARG:NH2	38:R:8832:HOH:O	2.53	0.41
21:T:28:SER:O	21:T:32:ARG:HG3	2.19	0.41
28:1:28:HIS:CD2	28:1:30:LYS:HB2	2.55	0.41
1:0:1015:C:H2'	1:0:1016:U:C6	2.55	0.41
1:0:1154:A:H2'	1:0:1155:G:C8	2.55	0.41
1:0:1165:G:C4'	1:0:1174:A:O2'	2.59	0.41
1:0:1409:G:C2	1:0:1410:G:C8	3.08	0.41
1:0:1574:C:H2'	1:0:1575:C:C6	2.55	0.41
4:B:36:PRO:HG3	4:B:169:GLY:H	1.84	0.41
27:Z:60:CYS:O	27:Z:61:ASP:HB2	2.20	0.41
1:0:69:A:H8	1:0:69:A:C5'	2.22	0.41
1:0:1028:U:H1'	38:0:3455:HOH:O	2.20	0.41
1:0:1236:A:H2'	1:0:1237:U:O4'	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1379:A:H1'	38:0:9505:HOH:O	2.20	0.41
1:0:2047:C:H2'	1:0:2048:C:H6	1.85	0.41
1:0:2871:G:H2'	1:0:2872:U:C6	2.55	0.41
38:0:7193:HOH:O	12:K:45:PRO:HB2	2.20	0.41
38:0:9350:HOH:O	17:P:81:LYS:HG2	2.19	0.41
4:B:225:GLY:HA3	38:B:8864:HOH:O	2.19	0.41
29:2:48:ASP:O	29:2:49:GLU:HB2	2.20	0.41
1:0:128:A:C8	1:0:128:A:C3'	3.03	0.41
1:0:137:U:C5	1:0:139:C:N4	2.88	0.41
1:0:295:C:C2'	1:0:296:G:H5'	2.51	0.41
1:0:826:U:O5'	1:0:826:U:H6	2.03	0.41
1:0:1123:A:C2	1:0:1129:C:H4'	2.55	0.41
1:0:1500:U:OP2	17:P:41:ARG:NH2	2.52	0.41
1:0:1603:A:C5'	1:0:1605:G:H5'	2.50	0.41
1:0:2898:G:H4'	4:B:288:GLY:HA2	2.03	0.41
2:9:3036:C:C5	2:9:3037:C:C5	3.09	0.41
4:B:139:ASP:HB2	38:B:8830:HOH:O	2.20	0.41
12:K:82:ARG:HH11	12:K:82:ARG:HG3	1.86	0.41
20:S:11:THR:H	20:S:14:ALA:HB3	1.86	0.41
21:T:115:GLU:HG3	21:T:116:ASP:N	2.36	0.41
26:Y:151:SER:HB3	26:Y:154:ARG:HB2	2.01	0.41
1:0:365:G:C6	1:0:366:U:C4	3.09	0.41
1:0:474:C:O3'	5:C:73:LEU:HD21	2.19	0.41
1:0:800:G:H2'	1:0:801:U:C6	2.56	0.41
1:0:1119:G:C6	1:0:1244:U:C5	3.08	0.41
1:0:1189:A:C3'	38:0:7501:HOH:O	2.56	0.41
1:0:1504:A:H5'	38:0:4246:HOH:O	2.19	0.41
1:0:2329:C:H2'	1:0:2330:U:C6	2.55	0.41
1:0:2533:C:C6	1:0:2533:C:C4'	3.03	0.41
3:A:43:VAL:HG21	3:A:59:GLU:HG3	2.01	0.41
4:B:82:VAL:O	4:B:82:VAL:HG12	2.20	0.41
11:J:22:VAL:O	11:J:26:VAL:HG23	2.21	0.41
31:I:99:ASP:O	31:I:100:LEU:HD23	2.21	0.41
1:0:40:C:O2'	1:0:41:G:H5'	2.20	0.41
1:0:169:A:H1'	30:3:48:ASN:ND2	2.36	0.41
1:0:489:A:C8	21:T:82:THR:CG2	3.04	0.41
1:0:821:U:H2'	1:0:822:C:H6	1.86	0.41
1:0:853:C:H2'	1:0:854:G:O4'	2.20	0.41
1:0:1261:A:H3'	1:0:1262:C:C6	2.55	0.41
1:0:1950:G:H2'	1:0:1951:G:C8	2.56	0.41
1:0:2435:U:OP1	30:3:28:GLY:HA3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2543:G:H2'	1:0:2544:G:O4'	2.21	0.41
3:A:94:LEU:HD23	3:A:94:LEU:N	2.35	0.41
4:B:14:GLY:HA2	4:B:15:PRO:C	2.45	0.41
10:H:45:VAL:HA	10:H:167:PRO:O	2.19	0.41
15:N:175:LEU:HD21	38:N:8835:HOH:O	2.20	0.41
19:R:126:LYS:HA	19:R:127:PRO:HD3	1.92	0.41
1:0:243:A:H61	1:0:269:G:C1'	2.33	0.41
1:0:629:A:C2	1:0:2074:A:C2	3.09	0.41
1:0:876:A:N3	1:0:876:A:H2'	2.35	0.41
1:0:1168:C:H5	38:0:7319:HOH:O	2.04	0.41
38:0:3886:HOH:O	4:B:27:ASN:HB2	2.19	0.41
2:9:3110:G:C2'	2:9:3111:U:H5'	2.51	0.41
4:B:49:THR:HG21	4:B:331:SER:O	2.21	0.41
6:D:96:SER:C	6:D:98:PHE:H	2.28	0.41
14:M:134:ILE:HG23	14:M:141:ILE:HD13	2.02	0.41
25:X:10:VAL:O	25:X:71:ARG:HA	2.21	0.41
1:0:485:A:O2'	1:0:487:G:H5'	2.21	0.41
1:0:810:G:H2'	1:0:811:C:C6	2.55	0.41
1:0:1159:G:C2	1:0:1160:G:H1'	2.55	0.41
1:0:1159:G:H2'	1:0:1160:G:O4'	2.20	0.41
1:0:1396:C:H1'	17:P:1:THR:O	2.21	0.41
1:0:1512:G:H4'	38:0:4479:HOH:O	2.19	0.41
1:0:1819:G:C2'	1:0:1820:G:H5'	2.50	0.41
1:0:1976:G:H1'	1:0:2005:G:N2	2.34	0.41
1:0:2362:A:H2'	1:0:2363:G:C8	2.56	0.41
1:0:2598:U:O2	1:0:2600:A:C8	2.74	0.41
1:0:2663:U:C4	1:0:2664:A:C6	3.08	0.41
1:0:2697:A:H2'	1:0:2698:G:O4'	2.20	0.41
1:0:2748:G:H2'	38:0:7362:HOH:O	2.19	0.41
2:9:3110:G:C6	2:9:3111:U:C5	3.09	0.41
16:O:26:TRP:HA	16:O:26:TRP:CE3	2.55	0.41
17:P:40:VAL:O	17:P:44:VAL:HG23	2.20	0.41
21:T:59:GLU:HG2	21:T:60:GLY:N	2.35	0.41
31:I:74:PRO:HG2	31:I:77:GLU:CD	2.46	0.41
1:0:138:U:H5''	1:0:139:C:OP2	2.20	0.41
1:0:160:A:C4	1:0:177:A:C2	3.09	0.41
1:0:797:A:C5'	27:Z:10:ARG:N	2.84	0.41
1:0:1119:G:H8	11:J:52:GLN:NE2	2.14	0.41
1:0:1687:C:H1'	28:1:8:GLN:O	2.21	0.41
1:0:1826:C:O2'	1:0:1827:G:H5'	2.21	0.41
1:0:2285:G:O2'	1:0:2286:G:H5'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2488:A:H2	38:0:7099:HOH:O	2.03	0.41
2:9:3011:A:P	18:Q:19:ARG:HH21	2.44	0.41
2:9:3059:C:H2'	2:9:3060:C:C6	2.55	0.41
2:9:3059:C:H2'	2:9:3060:C:H6	1.86	0.41
3:A:135:VAL:HG21	3:A:147:ARG:HB3	2.03	0.41
4:B:234:ARG:NH1	38:B:8913:HOH:O	2.52	0.41
4:B:305:ASP:O	4:B:306:LYS:CB	2.69	0.41
5:C:80:VAL:HA	5:C:81:PRO:HD3	1.99	0.41
5:C:82:GLN:OE1	5:C:82:GLN:N	2.44	0.41
6:D:58:VAL:HG11	6:D:60:GLU:HG2	2.02	0.41
7:E:40:VAL:HA	7:E:48:VAL:O	2.20	0.41
8:F:17:LEU:O	8:F:21:GLU:HG3	2.20	0.41
8:F:91:VAL:CG1	8:F:92:GLY:N	2.82	0.41
14:M:36:ALA:O	14:M:65:VAL:HA	2.21	0.41
14:M:99:ARG:O	14:M:103:GLU:HG3	2.21	0.41
24:W:149:LEU:CG	24:W:153:MET:HE2	2.43	0.41
25:X:78:GLU:CG	25:X:79:GLU:H	2.33	0.41
1:0:17:G:H2'	1:0:18:C:H6	1.86	0.41
1:0:538:C:H5''	1:0:539:G:C8	2.56	0.41
1:0:1008:C:H2'	1:0:1009:U:C6	2.55	0.41
1:0:1268:C:H2'	1:0:1269:G:C8	2.55	0.41
1:0:1339:G:C6	1:0:1340:G:N1	2.89	0.41
1:0:2600:A:H2'	1:0:2601:A:O4'	2.21	0.41
1:0:2821:C:H2'	1:0:2822:C:C6	2.55	0.41
2:9:3078:G:H5'	38:9:4932:HOH:O	2.20	0.41
4:B:71:VAL:HG11	4:B:296:LEU:HD22	2.03	0.41
4:B:258:GLY:H	4:B:260:HIS:CE1	2.38	0.41
5:C:84:VAL:HG12	5:C:85:LYS:HG2	2.03	0.41
6:D:15:GLU:HA	6:D:16:PRO:HD3	1.71	0.41
6:D:52:THR:HB	6:D:70:GLY:H	1.85	0.41
11:J:45:VAL:HG22	11:J:46:ILE:N	2.35	0.41
15:N:164:ASP:OD1	15:N:167:ASP:HA	2.21	0.41
16:O:16:SER:HB3	38:O:6661:HOH:O	2.21	0.41
16:O:26:TRP:HA	16:O:26:TRP:HE3	1.86	0.41
1:0:69:A:C8	1:0:69:A:C5'	2.97	0.40
1:0:152:A:O2'	1:0:153:C:H5'	2.21	0.40
1:0:536:A:H3'	38:0:4877:HOH:O	2.20	0.40
1:0:861:A:H4'	1:0:1697:G:H4'	2.03	0.40
1:0:1173:A:H4'	1:0:1174:A:C8	2.56	0.40
1:0:1202:A:O2'	1:0:1203:G:H5'	2.21	0.40
1:0:1207:A:C8	1:0:1208:C:C5	3.09	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1822:A:O2'	1:0:1823:G:H5'	2.21	0.40
1:0:2012:U:C2'	1:0:2013:G:OP1	2.69	0.40
2:9:3030:C:OP1	6:D:137:PRO:O	2.39	0.40
2:9:3082:U:H2'	2:9:3083:G:C8	2.56	0.40
4:B:274:GLU:HG3	4:B:292:GLY:C	2.45	0.40
7:E:112:ALA:HA	7:E:113:PRO:HD3	1.88	0.40
25:X:37:LEU:O	25:X:41:PHE:HB2	2.21	0.40
1:0:1419:U:H2'	1:0:1685:A:C2	2.56	0.40
1:0:1446:U:C2'	20:S:55:GLN:NE2	2.80	0.40
1:0:1914:C:C2	1:0:1926:G:N2	2.89	0.40
1:0:2114:C:O2'	1:0:2115:U:H5'	2.21	0.40
1:0:2374:A:H2'	1:0:2375:G:H8	1.86	0.40
1:0:2456:A:H2'	1:0:2457:U:H6	1.87	0.40
38:0:7301:HOH:O	14:M:55:LYS:HE2	2.20	0.40
2:9:3035:C:H2'	15:N:141:ARG:HH12	1.86	0.40
3:A:30:ARG:HG3	3:A:66:ARG:NH1	2.36	0.40
3:A:105:VAL:HG12	3:A:154:ALA:HB1	2.02	0.40
4:B:140:LEU:HD13	4:B:175:LEU:HA	2.02	0.40
13:L:89:PHE:N	38:L:8870:HOH:O	2.55	0.40
15:N:175:LEU:O	15:N:179:LEU:HG	2.20	0.40
31:I:87:THR:HG22	38:I:5128:HOH:O	2.20	0.40
1:0:170:U:H2'	1:0:171:C:H5'	2.01	0.40
1:0:1193:A:H2	1:0:1194:A:N6	2.18	0.40
1:0:1603:A:C5'	1:0:1605:G:O4'	2.64	0.40
1:0:1883:U:H5'	1:0:2012:U:OP2	2.21	0.40
1:0:2092:G:H2'	1:0:2613:G:OP1	2.22	0.40
1:0:2890:A:H1'	22:U:56:ARG:HH21	1.83	0.40
4:B:60:SER:HA	4:B:61:PRO:HD3	1.81	0.40
7:E:1:PRO:HG2	7:E:59:MET:SD	2.61	0.40
14:M:42:ARG:HA	14:M:43:PRO:HD3	1.88	0.40
15:N:37:ARG:HH11	15:N:37:ARG:CG	2.34	0.40
15:N:116:PHE:HB3	15:N:136:LEU:HD23	2.03	0.40
17:P:104:LYS:HD2	17:P:104:LYS:HA	1.92	0.40
19:R:111:ILE:HG23	19:R:145:LEU:CD1	2.51	0.40
19:R:111:ILE:HG23	19:R:145:LEU:HD11	2.02	0.40
24:W:38:THR:HG22	24:W:39:ASP:H	1.86	0.40
1:0:74:A:O2'	1:0:75:U:H5'	2.21	0.40
1:0:212:A:O4'	1:0:214:U:C6	2.75	0.40
1:0:228:C:H5'	38:0:5233:HOH:O	2.20	0.40
1:0:594:C:C4	1:0:595:U:C4	3.10	0.40
1:0:695:C:H2'	1:0:696:C:C6	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:699:C:C6	1:0:744:G:O4'	2.74	0.40
1:0:1246:A:C4	1:0:1248:A:C8	3.09	0.40
1:0:1555:G:O2'	1:0:1556:G:H5'	2.22	0.40
1:0:1659:A:H2'	1:0:1660:G:O4'	2.21	0.40
1:0:1808:C:O2'	1:0:1809:G:H5'	2.21	0.40
1:0:2326:U:H4'	1:0:2412:G:C4'	2.52	0.40
1:0:2433:A:H4'	30:3:30:GLN:NE2	2.36	0.40
1:0:2461:U:O2	1:0:2466:G:H1'	2.21	0.40
1:0:2750:G:H2'	1:0:2751:C:C6	2.57	0.40
5:C:243:VAL:O	5:C:243:VAL:HG13	2.20	0.40
8:F:27:GLY:HA3	8:F:101:ALA:O	2.21	0.40
12:K:107:THR:C	12:K:108:GLU:HG3	2.46	0.40
13:L:117:GLU:HG3	13:L:117:GLU:O	2.21	0.40
14:M:61:ILE:HG22	14:M:62:VAL:N	2.34	0.40
19:R:4:TYR:CE1	19:R:17:MET:HE2	2.56	0.40
20:S:25:GLN:HG2	20:S:65:VAL:HG22	2.04	0.40
24:W:35:VAL:HA	24:W:36:PRO:HD3	1.83	0.40
1:0:120:A:OP1	28:1:32:LYS:NZ	2.47	0.40
1:0:553:G:H2'	1:0:554:G:H5'	2.04	0.40
1:0:1131:G:C6	1:0:1230:A:C4	3.09	0.40
1:0:1204:C:H1'	38:0:4575:HOH:O	2.20	0.40
1:0:2256:G:C6	1:0:2257:G:C4	3.09	0.40
1:0:2650:U:O2'	1:0:2651:C:H5'	2.21	0.40
2:9:3008:G:P	38:9:5071:HOH:O	2.79	0.40
4:B:36:PRO:CA	4:B:168:GLY:HA3	2.46	0.40
10:H:91:PRO:HG2	38:H:8570:HOH:O	2.20	0.40
12:K:113:ILE:HG22	12:K:114:ALA:N	2.36	0.40
13:L:10:SER:O	13:L:11:ARG:HB3	2.21	0.40
14:M:159:VAL:HG13	14:M:160:PHE:N	2.37	0.40
18:Q:25:PRO:HA	18:Q:26:PRO:HD3	1.83	0.40
21:T:40:VAL:HG22	21:T:41:ARG:N	2.36	0.40
24:W:122:ARG:NH2	24:W:154:ARG:HB3	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	235/240 (98%)	215 (92%)	16 (7%)	4 (2%)	7	26
4	B	335/338 (99%)	307 (92%)	23 (7%)	5 (2%)	8	28
5	C	244/246 (99%)	220 (90%)	22 (9%)	2 (1%)	16	44
6	D	134/177 (76%)	108 (81%)	22 (16%)	4 (3%)	3	14
7	E	170/178 (96%)	161 (95%)	7 (4%)	2 (1%)	10	34
8	F	117/120 (98%)	105 (90%)	11 (9%)	1 (1%)	14	41
9	G	25/348 (7%)	25 (100%)	0	0	100	100
10	H	156/174 (90%)	144 (92%)	11 (7%)	1 (1%)	21	51
11	J	140/145 (97%)	132 (94%)	6 (4%)	2 (1%)	9	30
12	K	130/132 (98%)	125 (96%)	5 (4%)	0	100	100
13	L	141/165 (86%)	120 (85%)	19 (14%)	2 (1%)	9	30
14	M	192/196 (98%)	184 (96%)	8 (4%)	0	100	100
15	N	184/187 (98%)	163 (89%)	18 (10%)	3 (2%)	7	27
16	O	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
17	P	141/149 (95%)	139 (99%)	2 (1%)	0	100	100
18	Q	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
19	R	148/155 (96%)	140 (95%)	8 (5%)	0	100	100
20	S	79/85 (93%)	71 (90%)	8 (10%)	0	100	100
21	T	117/120 (98%)	109 (93%)	7 (6%)	1 (1%)	14	41
22	U	51/67 (76%)	48 (94%)	3 (6%)	0	100	100
23	V	63/71 (89%)	59 (94%)	4 (6%)	0	100	100
24	W	152/154 (99%)	147 (97%)	3 (2%)	2 (1%)	9	32
25	X	80/92 (87%)	71 (89%)	7 (9%)	2 (2%)	4	17
26	Y	140/241 (58%)	139 (99%)	1 (1%)	0	100	100
27	Z	71/73 (97%)	61 (86%)	7 (10%)	3 (4%)	2	9
28	1	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
29	2	42/50 (84%)	42 (100%)	0	0	100	100
30	3	90/92 (98%)	85 (94%)	4 (4%)	1 (1%)	11	36
31	I	68/162 (42%)	50 (74%)	17 (25%)	1 (2%)	8	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3705/4426 (84%)	3419 (92%)	250 (7%)	36 (1%)	12	39

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	37	VAL
8	F	101	ALA
15	N	154	LEU
15	N	184	ILE
24	W	77	ALA
27	Z	42	CYS
4	B	34	GLY
6	D	173	GLU
11	J	5	GLU
15	N	164	ASP
21	T	53	GLY
30	3	57	GLY
3	A	34	ASP
6	D	97	GLN
10	H	166	SER
11	J	143	LYS
24	W	76	ASP
31	I	76	ALA
3	A	24	LYS
4	B	169	GLY
4	B	185	GLY
5	C	178	GLN
13	L	21	ARG
13	L	80	ASP
4	B	2	GLN
4	B	306	LYS
5	C	163	HIS
6	D	85	GLN
27	Z	41	ASN
25	X	68	SER
3	A	88	ILE
6	D	27	ILE
7	E	44	GLY
25	X	52	PRO
7	E	136	PRO
27	Z	43	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	179/182 (98%)	169 (94%)	10 (6%)	19	50
4	B	282/283 (100%)	270 (96%)	12 (4%)	26	60
5	C	193/193 (100%)	178 (92%)	15 (8%)	11	35
6	D	117/148 (79%)	110 (94%)	7 (6%)	17	47
7	E	152/156 (97%)	148 (97%)	4 (3%)	40	73
8	F	93/94 (99%)	91 (98%)	2 (2%)	45	77
9	G	27/283 (10%)	26 (96%)	1 (4%)	30	64
10	H	132/141 (94%)	128 (97%)	4 (3%)	36	70
11	J	118/121 (98%)	112 (95%)	6 (5%)	21	53
12	K	106/106 (100%)	102 (96%)	4 (4%)	29	64
13	L	113/127 (89%)	110 (97%)	3 (3%)	39	73
14	M	158/160 (99%)	151 (96%)	7 (4%)	25	59
15	N	149/150 (99%)	140 (94%)	9 (6%)	17	47
16	O	93/94 (99%)	90 (97%)	3 (3%)	34	68
17	P	113/117 (97%)	110 (97%)	3 (3%)	39	73
18	Q	79/80 (99%)	74 (94%)	5 (6%)	16	45
19	R	117/122 (96%)	113 (97%)	4 (3%)	32	66
20	S	71/74 (96%)	71 (100%)	0	100	100
21	T	105/106 (99%)	97 (92%)	8 (8%)	12	36
22	U	44/53 (83%)	44 (100%)	0	100	100
23	V	51/57 (90%)	49 (96%)	2 (4%)	28	63
24	W	130/130 (100%)	123 (95%)	7 (5%)	20	51
25	X	66/74 (89%)	62 (94%)	4 (6%)	17	46
26	Y	120/196 (61%)	116 (97%)	4 (3%)	33	67
27	Z	60/60 (100%)	60 (100%)	0	100	100
28	1	46/47 (98%)	46 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	2	42/46 (91%)	41 (98%)	1 (2%)	43	75
30	3	79/79 (100%)	77 (98%)	2 (2%)	42	74
31	I	58/130 (45%)	58 (100%)	0	100	100
All	All	3093/3609 (86%)	2966 (96%)	127 (4%)	27	61

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	3	ARG
3	A	33	GLU
3	A	34	ASP
3	A	55	VAL
3	A	64	ASP
3	A	94	LEU
3	A	131	HIS
3	A	175	LYS
3	A	179	MET
3	A	217	ARG
4	B	7	ARG
4	B	11	LEU
4	B	27	ASN
4	B	49	THR
4	B	56	ASP
4	B	98	THR
4	B	149	ASP
4	B	190	MET
4	B	195	ARG
4	B	254	GLN
4	B	277	GLU
4	B	279	THR
5	C	2	GLN
5	C	16	VAL
5	C	27	ARG
5	C	73	LEU
5	C	76	ARG
5	C	94	THR
5	C	136	VAL
5	C	151	GLN
5	C	172	THR
5	C	187	ARG
5	C	202	THR

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Mol	Chain	Res	Type
5	C	214	THR
5	C	223	LEU
5	C	234	VAL
5	C	243	VAL
6	D	29	HIS
6	D	41	LEU
6	D	61	PHE
6	D	136	ARG
6	D	137	PRO
6	D	149	ARG
6	D	170	TYR
7	E	7	ILE
7	E	86	VAL
7	E	102	VAL
7	E	108	LEU
8	F	46	GLU
8	F	103	GLU
9	G	14	GLU
10	H	18	GLU
10	H	62	LEU
10	H	84	LYS
10	H	132	GLN
11	J	32	ASP
11	J	39	VAL
11	J	46	ILE
11	J	54	VAL
11	J	107	ASN
11	J	131	THR
12	K	7	ASP
12	K	10	GLN
12	K	49	LEU
12	K	129	THR
13	L	32	ASP
13	L	43	HIS
13	L	140	VAL
14	M	10	ASP
14	M	23	LEU
14	M	46	LEU
14	M	81	ARG
14	M	93	ARG
14	M	125	ARG
14	M	158	ARG

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Mol	Chain	Res	Type
15	N	17	ARG
15	N	26	LEU
15	N	38	LYS
15	N	50	LEU
15	N	74	PRO
15	N	94	GLU
15	N	127	LEU
15	N	152	GLU
15	N	157	PRO
16	O	3	THR
16	O	87	THR
16	O	111	VAL
17	P	21	VAL
17	P	91	LYS
17	P	98	ILE
18	Q	11	ARG
18	Q	16	ASN
18	Q	30	VAL
18	Q	57	ASP
18	Q	95	GLU
19	R	13	THR
19	R	39	THR
19	R	85	SER
19	R	143	VAL
21	T	23	VAL
21	T	39	ASN
21	T	48	VAL
21	T	66	ASP
21	T	80	GLU
21	T	96	VAL
21	T	106	GLU
21	T	117	ASP
23	V	43	PRO
23	V	45	ARG
24	W	10	GLU
24	W	26	ILE
24	W	35	VAL
24	W	45	VAL
24	W	73	LEU
24	W	142	ASP
24	W	146	ILE
25	X	15	ARG

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Mol	Chain	Res	Type
25	X	43	VAL
25	X	52	PRO
25	X	66	THR
26	Y	141	THR
26	Y	163	THR
26	Y	200	THR
26	Y	203	VAL
29	2	18	ASN
30	3	56	PRO
30	3	65	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (103) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	5	GLN
3	A	47	HIS
3	A	81	GLN
3	A	92	ASN
3	A	188	ASN
3	A	199	HIS
4	B	27	ASN
4	B	145	HIS
4	B	221	GLN
4	B	238	ASN
4	B	256	GLN
4	B	260	HIS
4	B	320	GLN
5	C	2	GLN
5	C	69	HIS
5	C	129	HIS
5	C	151	GLN
5	C	178	GLN
6	D	103	ASN
6	D	133	ASN
6	D	158	ASN
7	E	66	GLN
7	E	96	ASN
7	E	119	HIS
7	E	143	GLN
8	F	80	GLN
9	G	17	GLN
9	G	64	ASN

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Mol	Chain	Res	Type
10	H	31	HIS
10	H	46	GLN
10	H	56	GLN
10	H	59	HIS
10	H	72	HIS
10	H	92	HIS
10	H	128	GLN
11	J	52	GLN
11	J	107	ASN
11	J	142	ASN
12	K	10	GLN
13	L	18	HIS
13	L	41	HIS
13	L	42	ASN
14	M	24	GLN
14	M	52	GLN
14	M	58	GLN
14	M	137	ASN
15	N	21	HIS
15	N	93	GLN
15	N	107	ASN
15	N	132	ASN
15	N	140	GLN
15	N	153	GLN
17	P	50	GLN
17	P	66	GLN
17	P	118	GLN
18	Q	16	ASN
18	Q	40	HIS
18	Q	67	GLN
19	R	22	GLN
19	R	61	GLN
19	R	94	ASN
19	R	98	ASN
19	R	117	HIS
19	R	122	GLN
20	S	21	GLN
20	S	51	GLN
20	S	55	GLN
21	T	37	GLN
21	T	39	ASN
21	T	64	ASN

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Mol	Chain	Res	Type
21	T	73	HIS
21	T	95	ASN
22	U	39	ASN
22	U	48	ASN
23	V	29	ASN
23	V	42	ASN
23	V	60	GLN
24	W	25	ASN
24	W	28	HIS
24	W	49	ASN
24	W	59	GLN
24	W	110	GLN
24	W	119	HIS
24	W	125	HIS
24	W	141	HIS
25	X	23	HIS
26	Y	119	GLN
26	Y	133	HIS
26	Y	134	HIS
26	Y	149	GLN
26	Y	188	HIS
26	Y	189	ASN
28	1	8	GLN
28	1	16	HIS
28	1	28	HIS
29	2	18	ASN
29	2	41	HIS
29	2	45	ASN
30	3	30	GLN
30	3	48	ASN
31	I	93	GLN
31	I	104	GLN
31	I	123	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2772 (99%)	242 (8%)	28 (1%)
2	9	121/122 (99%)	17 (14%)	1 (0%)
All	All	2866/2894 (99%)	259 (9%)	29 (1%)

All (259) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	60	A
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G
1	0	87	C
1	0	88	G
1	0	114	A
1	0	115	U
1	0	120	A
1	0	130	C
1	0	141	C
1	0	151	A
1	0	166	A
1	0	185	G
1	0	186	A
1	0	191	A
1	0	192	A
1	0	198	A
1	0	200	U
1	0	219	G
1	0	237	G
1	0	271	C
1	0	272	A
1	0	273	G
1	0	283	U
1	0	284	C
1	0	285	A
1	0	308	U
1	0	309	C
1	0	331	A
1	0	336	G
1	0	337	A
1	0	338	C
1	0	339	A
1	0	358	G
1	0	381	G
1	0	397	A
1	0	417	G
1	0	461	C
1	0	473	A
1	0	487	G

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Mol	Chain	Res	Type
1	0	511	A
1	0	514	G
1	0	537	G
1	0	538	C
1	0	539	G
1	0	542	A
1	0	545	G
1	0	553	G
1	0	559	U
1	0	581	G
1	0	588	G
1	0	604	G
1	0	620	A
1	0	632	A
1	0	644	G
1	0	660	A
1	0	688	A
1	0	701	U
1	0	759	C
1	0	777	U
1	0	805	G
1	0	806	A
1	0	809	G
1	0	821	U
1	0	835	U
1	0	840	U
1	0	857	A
1	0	858	U
1	0	868	G
1	0	869	G
1	0	871	G
1	0	872	U
1	0	875	A
1	0	877	G
1	0	878	G
1	0	884	C
1	0	898	G
1	0	905	C
1	0	920	C
1	0	921	G
1	0	938	G
1	0	953	G

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Mol	Chain	Res	Type
1	0	960	G
1	0	961	A
1	0	1006	A
1	0	1008	C
1	0	1029	U
1	0	1045	G
1	0	1059	G
1	0	1060	C
1	0	1072	G
1	0	1081	A
1	0	1088	A
1	0	1109	U
1	0	1110	G
1	0	1119	G
1	0	1130	U
1	0	1137	G
1	0	1164	U
1	0	1166	A
1	0	1174	A
1	0	1175	G
1	0	1185	U
1	0	1192	A
1	0	1193	A
1	0	1206	U
1	0	1208	C
1	0	1216	G
1	0	1237	U
1	0	1238	C
1	0	1239	G
1	0	1279	U
1	0	1289	C
1	0	1342	C
1	0	1353	C
1	0	1360	C
1	0	1377	C
1	0	1378	G
1	0	1407	A
1	0	1451	C
1	0	1474	C
1	0	1488	U
1	0	1492	A
1	0	1505	U

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Mol	Chain	Res	Type
1	0	1506	U
1	0	1524	U
1	0	1525	G
1	0	1526	A
1	0	1559	A
1	0	1580	A
1	0	1592	G
1	0	1603	A
1	0	1625	U
1	0	1626	A
1	0	1633	C
1	0	1634	G
1	0	1656	A
1	0	1667	A
1	0	1682	A
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1701	A
1	0	1722	U
1	0	1723	G
1	0	1725	C
1	0	1730	G
1	0	1731	C
1	0	1752	G
1	0	1778	A
1	0	1779	A
1	0	1798	C
1	0	1819	G
1	0	1820	G
1	0	1829	A
1	0	1856	C
1	0	1873	G
1	0	1879	U
1	0	1919	A
1	0	1942	A
1	0	1965	C
1	0	1971	G
1	0	1973	A
1	0	1974	G
1	0	1978	A
1	0	1979	G

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Mol	Chain	Res	Type
1	0	1980	U
1	0	1996	U
1	0	2004	U
1	0	2006	C
1	0	2008	U
1	0	2011	A
1	0	2012	U
1	0	2013	G
1	0	2033	G
1	0	2034	U
1	0	2063	U
1	0	2064	U
1	0	2072	G
1	0	2073	G
1	0	2074	A
1	0	2096	A
1	0	2101	A
1	0	2102	G
1	0	2110	G
1	0	2258	A
1	0	2271	G
1	0	2272	G
1	0	2317	C
1	0	2321	A
1	0	2354	A
1	0	2369	A
1	0	2422	U
1	0	2462	G
1	0	2465	A
1	0	2467	A
1	0	2476	C
1	0	2483	A
1	0	2507	G
1	0	2511	A
1	0	2526	C
1	0	2527	U
1	0	2533	C
1	0	2537	G
1	0	2541	U
1	0	2553	A
1	0	2564	G
1	0	2589	U

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Mol	Chain	Res	Type
1	0	2601	A
1	0	2602	G
1	0	2608	C
1	0	2613	G
1	0	2634	G
1	0	2645	U
1	0	2649	A
1	0	2650	U
1	0	2664	A
1	0	2681	A
1	0	2682	C
1	0	2718	C
1	0	2719	A
1	0	2726	U
1	0	2727	A
1	0	2747	C
1	0	2748	G
1	0	2749	U
1	0	2750	G
1	0	2762	C
1	0	2768	A
1	0	2786	G
1	0	2800	A
1	0	2811	A
1	0	2812	A
1	0	2850	C
1	0	2876	G
1	0	2890	A
1	0	2896	A
1	0	2903	C
1	0	2914	A
2	9	3002	U
2	9	3007	G
2	9	3014	G
2	9	3022	G
2	9	3023	U
2	9	3024	U
2	9	3025	G
2	9	3039	U
2	9	3040	C
2	9	3041	C
2	9	3043	G

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Mol	Chain	Res	Type
2	9	3052	A
2	9	3057	A
2	9	3066	G
2	9	3077	A
2	9	3114	G
2	9	3122	C

All (29) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	69	A
1	0	129	A
1	0	338	C
1	0	681	G
1	0	699	C
1	0	805	G
1	0	834	G
1	0	857	A
1	0	871	G
1	0	877	G
1	0	1080	C
1	0	1237	U
1	0	1352	A
1	0	1377	C
1	0	1450	C
1	0	1474	C
1	0	1506	U
1	0	1684	A
1	0	1685	A
1	0	1942	A
1	0	2011	A
1	0	2467	A
1	0	2526	C
1	0	2536	C
1	0	2649	A
1	0	2718	C
1	0	2726	U
1	0	2761	A
2	9	3065	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	UR3	0	2619	1	19,22,23	0.39	0	26,32,35	0.78	1 (3%)
1	OMG	0	2588	1	23,26,27	0.32	0	32,38,41	0.43	0
1	OMU	0	2587	1	19,22,23	0.24	0	25,31,34	0.44	0
1	PSU	0	2621	1	18,21,22	1.52	2 (11%)	21,30,33	1.34	3 (14%)
1	1MA	0	628	1	21,25,26	0.74	1 (4%)	30,37,40	0.66	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UR3	0	2619	1	-	0/7/25/26	0/2/2/2
1	OMG	0	2588	1	-	0/9/27/28	0/3/3/3
1	OMU	0	2587	1	-	0/9/27/28	0/2/2/2
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	1MA	0	628	1	-	2/7/25/26	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C2-N1	4.94	1.43	1.36
1	0	2621	PSU	C6-C5	2.98	1.38	1.35
1	0	628	1MA	C6-N6	2.48	1.34	1.28

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	C6-C5-C4	3.22	120.34	118.17
1	0	2621	PSU	C6-N1-C2	-3.19	119.73	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	O2-C2-N1	2.99	125.87	122.79
1	0	2619	UR3	C4-N3-C2	2.91	126.92	124.58
1	0	628	1MA	N1-C2-N3	2.76	129.27	126.00

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	0	628	1MA	C2'-C1'-N9-C8
1	0	628	1MA	C2'-C1'-N9-C4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 232 ligands modelled in this entry, 231 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	NEG	0	8823	32	14,16,16	1.49	1 (7%)	12,20,20	0.75	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	NEG	0	8823	32	-	5/18/18/18	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	0	8823	NEG	N2-N3	-4.77	1.36	1.41

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	0	8823	NEG	N3-C7-C8-O1
36	0	8823	NEG	N3-C7-C8-O2
36	0	8823	NEG	C6-N2-N3-C7
36	0	8823	NEG	C2-C3-C4-N4
36	0	8823	NEG	C8-C7-N3-N2

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	0	8823	NEG	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	0	2749/2772 (99%)	-0.32	36 (1%) 75 67	19, 42, 86, 144	0
2	9	122/122 (100%)	0.16	4 (3%) 49 40	35, 59, 83, 147	0
3	A	237/240 (98%)	0.33	11 (4%) 37 29	25, 46, 78, 99	0
4	B	337/338 (99%)	0.34	8 (2%) 59 50	26, 50, 75, 85	0
5	C	246/246 (100%)	0.27	5 (2%) 65 56	22, 44, 66, 75	0
6	D	140/177 (79%)	1.91	59 (42%) 0 0	54, 94, 118, 126	0
7	E	172/178 (96%)	0.66	10 (5%) 29 22	40, 63, 83, 88	0
8	F	119/120 (99%)	0.80	9 (7%) 20 16	42, 67, 89, 100	0
9	G	29/348 (8%)	1.47	5 (17%) 4 3	73, 89, 96, 98	0
10	H	160/174 (91%)	0.54	6 (3%) 44 36	36, 56, 86, 95	0
11	J	142/145 (97%)	0.30	6 (4%) 40 32	32, 47, 68, 89	0
12	K	132/132 (100%)	0.13	2 (1%) 72 64	29, 45, 67, 78	0
13	L	145/165 (87%)	0.89	23 (15%) 5 4	23, 62, 102, 114	0
14	M	194/196 (98%)	0.13	2 (1%) 79 73	30, 40, 55, 63	0
15	N	186/187 (99%)	0.88	22 (11%) 9 7	37, 59, 103, 114	0
16	O	115/116 (99%)	0.43	1 (0%) 81 75	35, 51, 67, 76	0
17	P	143/149 (95%)	0.48	7 (4%) 35 27	36, 51, 63, 72	0
18	Q	95/96 (98%)	0.24	3 (3%) 50 41	33, 44, 56, 70	0
19	R	150/155 (96%)	0.14	1 (0%) 84 79	30, 43, 64, 79	0
20	S	81/85 (95%)	0.47	3 (3%) 45 37	43, 58, 78, 80	0
21	T	119/120 (99%)	0.47	2 (1%) 69 61	41, 54, 77, 95	0
22	U	53/67 (79%)	0.26	2 (3%) 44 36	37, 50, 70, 77	0
23	V	65/71 (91%)	1.13	12 (18%) 3 3	51, 72, 106, 114	0
24	W	154/154 (100%)	0.27	0 100 100	33, 47, 63, 73	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	X	82/92 (89%)	0.76	9 (10%) 10 9	43, 56, 81, 96	0
26	Y	142/241 (58%)	0.25	6 (4%) 40 32	25, 42, 64, 84	0
27	Z	73/73 (100%)	0.62	6 (8%) 17 14	45, 57, 74, 93	0
28	1	56/57 (98%)	-0.22	0 100 100	28, 32, 39, 48	0
29	2	46/50 (92%)	1.07	9 (19%) 3 2	34, 60, 93, 102	0
30	3	92/92 (100%)	0.39	3 (3%) 49 40	32, 51, 64, 75	0
31	I	70/162 (43%)	2.53	43 (61%) 0 0	101, 115, 127, 129	0
All	All	6646/7320 (90%)	0.17	315 (4%) 36 28	19, 48, 93, 147	0

All (315) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	V	1	THR	7.5
15	N	161	GLY	6.6
14	M	194	ALA	5.9
6	D	57	THR	5.9
6	D	10	PHE	5.9
25	X	88	GLU	5.7
31	I	79	ILE	5.5
6	D	63	ILE	5.4
26	Y	235	GLU	5.3
31	I	72	VAL	5.2
4	B	1	PRO	5.2
13	L	60	GLU	5.2
31	I	109	ALA	5.2
15	N	154	LEU	5.1
6	D	87	ALA	5.0
23	V	40	PRO	5.0
31	I	133	THR	5.0
29	2	49	GLU	4.9
15	N	166	ALA	4.8
13	L	99	GLU	4.8
31	I	117	LEU	4.7
23	V	39	ALA	4.7
23	V	2	VAL	4.6
1	0	10	U	4.5
31	I	105	VAL	4.4
23	V	43	PRO	4.4
20	S	81	ILE	4.4
7	E	53	GLU	4.4

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Mol	Chain	Res	Type	RSRZ
2	9	3002	U	4.3
6	D	88	LEU	4.3
23	V	41	GLU	4.3
6	D	107	GLY	4.2
15	N	167	ASP	4.1
31	I	75	THR	4.1
9	G	71	LEU	4.1
6	D	135	VAL	4.0
30	3	41	GLU	4.0
15	N	168	LEU	4.0
13	L	102	ASP	4.0
31	I	124	ALA	4.0
12	K	119	GLN	4.0
29	2	48	ASP	3.9
15	N	160	SER	3.9
31	I	137	VAL	3.9
31	I	76	ALA	3.9
9	G	12	ILE	3.9
6	D	66	GLY	3.8
2	9	3001	U	3.8
7	E	45	ASP	3.8
31	I	121	LEU	3.8
17	P	18	LYS	3.7
6	D	18	ILE	3.7
29	2	35	ARG	3.7
31	I	111	GLN	3.7
6	D	55	LYS	3.7
3	A	37	VAL	3.7
6	D	166	ILE	3.7
6	D	11	HIS	3.6
7	E	154	ILE	3.6
15	N	152	GLU	3.6
6	D	174	VAL	3.6
31	I	118	SER	3.6
31	I	119	TYR	3.6
27	Z	20	ARG	3.5
8	F	39	SER	3.5
5	C	180	SER	3.5
13	L	44	GLU	3.5
1	0	2344	G	3.5
1	0	2637	A	3.5
6	D	90	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
6	D	17	ARG	3.5
1	0	1525	G	3.4
6	D	171	ASP	3.4
7	E	100	ASP	3.4
10	H	111	ASP	3.4
15	N	134	ASP	3.4
25	X	87	ALA	3.4
6	D	134	LEU	3.4
31	I	134	SER	3.4
1	0	960	G	3.4
31	I	139	ILE	3.3
11	J	4	ALA	3.3
13	L	150	GLN	3.3
31	I	138	THR	3.3
17	P	143	ALA	3.3
6	D	22	VAL	3.3
6	D	150	SER	3.3
13	L	78	ALA	3.2
1	0	2769	C	3.2
31	I	106	LYS	3.2
25	X	83	ALA	3.2
7	E	6	GLU	3.2
17	P	116	SER	3.2
1	0	1199	A	3.1
6	D	56	ARG	3.1
31	I	88	GLY	3.1
31	I	115	ASP	3.1
8	F	99	THR	3.1
13	L	82	ALA	3.0
13	L	105	TYR	3.0
31	I	90	GLY	3.0
3	A	237	GLY	3.0
13	L	146	GLY	3.0
13	L	148	GLU	3.0
1	0	1172	G	3.0
2	9	3024	U	3.0
25	X	85	VAL	3.0
6	D	128	LEU	2.9
31	I	71	GLY	2.9
31	I	100	LEU	2.9
29	2	20	ARG	2.9
29	2	39	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	0	1171	A	2.9
13	L	36	ASP	2.9
29	2	37	HIS	2.9
13	L	97	VAL	2.9
6	D	104	PHE	2.9
6	D	52	THR	2.9
31	I	113	HIS	2.9
31	I	108	ILE	2.9
31	I	93	GLN	2.9
6	D	89	PRO	2.9
15	N	169	PRO	2.9
15	N	165	ALA	2.9
25	X	71	ARG	2.9
31	I	116	LEU	2.9
6	D	138	GLY	2.8
1	0	1196	C	2.8
18	Q	17	LYS	2.8
6	D	54	ALA	2.8
1	0	2345	A	2.8
15	N	157	PRO	2.8
6	D	53	LYS	2.8
15	N	158	LEU	2.8
6	D	131	THR	2.8
27	Z	11	SER	2.8
6	D	19	GLU	2.8
23	V	45	ARG	2.8
6	D	106	PHE	2.8
6	D	157	LEU	2.8
10	H	168	ALA	2.7
20	S	78	ALA	2.7
31	I	125	ALA	2.7
1	0	138	U	2.7
4	B	318	ASN	2.7
7	E	10	ASP	2.7
15	N	162	ASP	2.7
6	D	153	THR	2.7
6	D	59	GLY	2.7
19	R	55	GLN	2.7
5	C	245	GLU	2.7
31	I	140	GLU	2.7
31	I	128	VAL	2.7
31	I	129	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
6	D	165	PHE	2.7
13	L	77	ALA	2.7
25	X	84	ILE	2.7
1	0	272	A	2.7
11	J	144	THR	2.7
31	I	77	GLU	2.7
1	0	1181	A	2.7
17	P	15	ASP	2.7
31	I	80	LYS	2.6
31	I	85	PHE	2.6
23	V	37	GLY	2.6
23	V	44	GLY	2.6
6	D	65	GLU	2.6
7	E	39	ASP	2.6
31	I	78	LEU	2.6
1	0	514	G	2.6
29	2	31	ARG	2.6
29	2	44	ARG	2.6
31	I	135	LEU	2.6
26	Y	98	GLN	2.6
6	D	83	PHE	2.6
1	0	128	A	2.6
31	I	73	PRO	2.6
31	I	114	PRO	2.6
1	0	1951	G	2.6
13	L	145	LEU	2.6
6	D	75	LEU	2.6
7	E	156	ASP	2.6
9	G	73	ASP	2.6
15	N	159	TYR	2.5
30	3	57	GLY	2.5
6	D	62	ASP	2.5
1	0	1197	G	2.5
25	X	7	GLU	2.5
27	Z	44	GLU	2.5
1	0	1161	A	2.5
31	I	120	ASP	2.5
9	G	26	MET	2.5
8	F	102	GLY	2.5
15	N	155	GLU	2.5
11	J	92	GLN	2.5
15	N	1	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	0	497	A	2.5
1	0	1626	A	2.5
4	B	208	GLY	2.4
13	L	59	GLU	2.4
15	N	150	TYR	2.4
1	0	87	C	2.4
13	L	101	ASP	2.4
3	A	32	VAL	2.4
22	U	52	THR	2.4
27	Z	34	ASN	2.4
13	L	149	ARG	2.4
1	0	1162	G	2.4
1	0	2237	G	2.4
15	N	68	GLU	2.4
1	0	1198	U	2.4
6	D	69	ILE	2.4
1	0	1177	A	2.4
6	D	105	SER	2.4
20	S	44	GLN	2.4
30	3	56	PRO	2.4
8	F	91	VAL	2.3
14	M	125	ARG	2.3
1	0	1178	G	2.3
10	H	169	GLY	2.3
3	A	34	ASP	2.3
10	H	40	ALA	2.3
13	L	58	GLN	2.3
23	V	31	ARG	2.3
3	A	86	ALA	2.3
4	B	108	GLU	2.3
5	C	59	GLU	2.3
6	D	81	GLU	2.3
6	D	44	ILE	2.3
1	0	1173	A	2.3
2	9	3023	U	2.3
15	N	95	ALA	2.3
6	D	64	ARG	2.3
1	0	1169	U	2.3
1	0	1964	U	2.3
8	F	104	ALA	2.2
31	I	82	GLU	2.2
25	X	69	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
6	D	172	VAL	2.2
21	T	118	SER	2.2
31	I	102	VAL	2.2
8	F	101	ALA	2.2
25	X	65	ASN	2.2
3	A	36	ASP	2.2
3	A	35	GLY	2.2
1	0	1929	G	2.2
21	T	119	ALA	2.2
10	H	170	ASN	2.2
26	Y	216	ARG	2.2
31	I	104	GLN	2.2
1	0	1182	C	2.2
6	D	21	VAL	2.2
26	Y	236	VAL	2.2
6	D	169	THR	2.2
26	Y	163	THR	2.2
7	E	87	PHE	2.2
29	2	38	LYS	2.2
31	I	112	LYS	2.2
1	0	288	A	2.2
6	D	16	PRO	2.2
9	G	13	PRO	2.2
10	H	27	LYS	2.2
17	P	67	LYS	2.2
6	D	61	PHE	2.2
8	F	47	LEU	2.2
4	B	57	GLU	2.2
6	D	60	GLU	2.2
4	B	319	ASP	2.1
15	N	41	LYS	2.1
13	L	75	LEU	2.1
3	A	66	ARG	2.1
6	D	50	VAL	2.1
26	Y	95	THR	2.1
27	Z	10	ARG	2.1
6	D	97	GLN	2.1
6	D	86	THR	2.1
22	U	47	ARG	2.1
3	A	88	ILE	2.1
13	L	83	GLU	2.1
13	L	147	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	0	1701	A	2.1
17	P	58	SER	2.1
3	A	31	LYS	2.1
3	A	211	LYS	2.1
13	L	91	VAL	2.1
17	P	16	VAL	2.1
8	F	9	PRO	2.1
5	C	76	ARG	2.1
7	E	32	ARG	2.1
6	D	15	GLU	2.1
6	D	48	MET	2.0
16	O	1	SER	2.0
23	V	47	LYS	2.0
27	Z	82	SER	2.0
15	N	43	VAL	2.0
5	C	61	PHE	2.0
11	J	70	PHE	2.0
1	0	1561	U	2.0
6	D	101	THR	2.0
4	B	118	ASP	2.0
12	K	118	ALA	2.0
13	L	80	ASP	2.0
11	J	5	GLU	2.0
18	Q	64	GLU	2.0
6	D	139	TYR	2.0
4	B	5	ARG	2.0
23	V	42	ASN	2.0
6	D	28	GLY	2.0
15	N	163	PHE	2.0
6	D	151	ILE	2.0
6	D	74	THR	2.0
8	F	97	ALA	2.0
11	J	47	THR	2.0
18	Q	20	ASP	2.0
1	0	1160	G	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	UR3	0	2619	21/22	0.96	0.08	32,34,35,37	0
1	OMG	0	2588	24/25	0.97	0.07	26,32,34,36	0
1	1MA	0	628	23/24	0.97	0.07	26,29,30,31	0
1	PSU	0	2621	20/21	0.97	0.07	23,27,32,33	0
1	OMU	0	2587	21/22	0.98	0.06	29,31,33,36	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	NA	9	8551	1/1	0.52	0.25	95,95,95,95	0
34	NA	0	8571	1/1	0.59	0.19	46,46,46,46	0
32	MG	0	8050	1/1	0.67	0.10	66,66,66,66	0
32	MG	0	8063	1/1	0.67	0.20	89,89,89,89	0
34	NA	0	8584	1/1	0.72	0.15	68,68,68,68	0
34	NA	0	8569	1/1	0.72	0.33	63,63,63,63	0
34	NA	0	8574	1/1	0.74	0.35	73,73,73,73	0
34	NA	S	8512	1/1	0.76	0.18	62,62,62,62	0
32	MG	0	8106	1/1	0.77	0.18	63,63,63,63	0
34	NA	0	8575	1/1	0.78	0.41	52,52,52,52	0
34	NA	0	8566	1/1	0.79	0.25	74,74,74,74	0
34	NA	0	8577	1/1	0.79	0.32	70,70,70,70	0
34	NA	0	8582	1/1	0.79	0.20	88,88,88,88	0
32	MG	0	8082	1/1	0.81	0.18	65,65,65,65	0
34	NA	H	8522	1/1	0.81	0.32	71,71,71,71	0
32	MG	9	8095	1/1	0.81	0.14	55,55,55,55	0
34	NA	0	8562	1/1	0.82	0.28	65,65,65,65	0
32	MG	0	8108	1/1	0.82	0.11	66,66,66,66	0
32	MG	0	8024	1/1	0.82	0.36	80,80,80,80	0
34	NA	0	8507	1/1	0.82	0.15	54,54,54,54	0
34	NA	0	8557	1/1	0.82	0.20	49,49,49,49	0
34	NA	0	8558	1/1	0.82	0.29	68,68,68,68	0
34	NA	0	8585	1/1	0.83	0.32	59,59,59,59	0
34	NA	0	8563	1/1	0.83	0.21	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	0	8092	1/1	0.83	0.12	66,66,66,66	0
32	MG	0	8087	1/1	0.83	0.14	61,61,61,61	0
32	MG	T	8073	1/1	0.84	0.17	63,63,63,63	0
32	MG	0	8094	1/1	0.84	0.27	66,66,66,66	0
34	NA	0	8539	1/1	0.84	0.11	30,30,30,30	0
34	NA	0	8555	1/1	0.84	0.27	81,81,81,81	0
32	MG	A	8066	1/1	0.84	0.18	47,47,47,47	0
33	K	0	8401	1/1	0.85	0.26	78,78,78,78	0
34	NA	9	8583	1/1	0.85	0.11	63,63,63,63	0
37	CD	O	8705	1/1	0.85	0.33	187,187,187,187	0
34	NA	0	8567	1/1	0.86	0.21	51,51,51,51	0
34	NA	0	8511	1/1	0.86	0.09	46,46,46,46	0
34	NA	0	8516	1/1	0.87	0.13	45,45,45,45	0
32	MG	0	8076	1/1	0.87	0.10	44,44,44,44	0
34	NA	9	8552	1/1	0.87	0.13	47,47,47,47	0
34	NA	0	8578	1/1	0.87	0.33	49,49,49,49	0
34	NA	0	8581	1/1	0.87	0.06	38,38,38,38	0
34	NA	R	8586	1/1	0.87	0.29	29,29,29,29	0
32	MG	0	8102	1/1	0.87	0.10	70,70,70,70	0
34	NA	0	8513	1/1	0.87	0.11	46,46,46,46	0
34	NA	0	8565	1/1	0.88	0.38	52,52,52,52	0
34	NA	Q	8548	1/1	0.88	0.11	43,43,43,43	0
34	NA	0	8559	1/1	0.88	0.31	48,48,48,48	0
34	NA	0	8554	1/1	0.88	0.15	39,39,39,39	0
34	NA	0	8535	1/1	0.88	0.15	39,39,39,39	0
34	NA	0	8520	1/1	0.89	0.17	35,35,35,35	0
34	NA	0	8530	1/1	0.89	0.07	33,33,33,33	0
32	MG	0	8110	1/1	0.89	0.12	54,54,54,54	0
32	MG	0	8114	1/1	0.89	0.10	41,41,41,41	0
34	NA	0	8573	1/1	0.89	0.08	56,56,56,56	0
32	MG	0	8043	1/1	0.89	0.19	61,61,61,61	0
35	CL	0	8805	1/1	0.89	0.11	58,58,58,58	0
35	CL	J	8802	1/1	0.89	0.08	58,58,58,58	0
36	NEG	0	8823	17/17	0.89	0.22	68,72,82,83	0
34	NA	0	8502	1/1	0.89	0.15	51,51,51,51	0
35	CL	A	8809	1/1	0.90	0.17	71,71,71,71	0
34	NA	A	8545	1/1	0.90	0.10	57,57,57,57	0
34	NA	0	8529	1/1	0.90	0.06	56,56,56,56	0
34	NA	0	8540	1/1	0.90	0.07	43,43,43,43	0
32	MG	0	8047	1/1	0.91	0.12	72,72,72,72	0
34	NA	0	8527	1/1	0.91	0.13	46,46,46,46	0
32	MG	0	8090	1/1	0.91	0.15	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	NA	0	8568	1/1	0.91	0.18	61,61,61,61	0
32	MG	0	8070	1/1	0.91	0.06	34,34,34,34	0
35	CL	L	8810	1/1	0.91	0.13	54,54,54,54	0
34	NA	0	8532	1/1	0.91	0.10	34,34,34,34	0
34	NA	0	8564	1/1	0.91	0.16	50,50,50,50	0
34	NA	0	8541	1/1	0.92	0.12	47,47,47,47	0
35	CL	0	8815	1/1	0.92	0.12	61,61,61,61	0
35	CL	0	8817	1/1	0.92	0.09	59,59,59,59	0
35	CL	0	8820	1/1	0.92	0.09	36,36,36,36	0
35	CL	0	8822	1/1	0.92	0.24	71,71,71,71	0
34	NA	0	8501	1/1	0.92	0.08	51,51,51,51	0
34	NA	0	8579	1/1	0.92	0.14	46,46,46,46	0
34	NA	R	8537	1/1	0.92	0.07	35,35,35,35	0
32	MG	0	8044	1/1	0.92	0.08	33,33,33,33	0
34	NA	0	8561	1/1	0.92	0.23	61,61,61,61	0
34	NA	C	8504	1/1	0.93	0.08	41,41,41,41	0
34	NA	0	8549	1/1	0.93	0.11	45,45,45,45	0
32	MG	0	8111	1/1	0.93	0.10	50,50,50,50	0
32	MG	0	8113	1/1	0.93	0.07	49,49,49,49	0
34	NA	0	8515	1/1	0.93	0.09	33,33,33,33	0
32	MG	0	8041	1/1	0.93	0.08	54,54,54,54	0
32	MG	0	8096	1/1	0.93	0.11	52,52,52,52	0
34	NA	0	8524	1/1	0.93	0.19	45,45,45,45	0
32	MG	0	8099	1/1	0.93	0.07	42,42,42,42	0
32	MG	0	8101	1/1	0.93	0.15	71,71,71,71	0
32	MG	0	8085	1/1	0.93	0.12	48,48,48,48	0
32	MG	0	8072	1/1	0.93	0.11	55,55,55,55	0
32	MG	0	8064	1/1	0.93	0.08	28,28,28,28	0
32	MG	0	8080	1/1	0.93	0.10	48,48,48,48	0
35	CL	R	8806	1/1	0.93	0.10	52,52,52,52	0
34	NA	0	8508	1/1	0.93	0.14	36,36,36,36	0
34	NA	0	8510	1/1	0.93	0.14	22,22,22,22	0
32	MG	0	8117	1/1	0.94	0.09	45,45,45,45	0
32	MG	0	8057	1/1	0.94	0.07	29,29,29,29	0
32	MG	0	8088	1/1	0.94	0.04	22,22,22,22	0
32	MG	0	8060	1/1	0.94	0.09	43,43,43,43	0
32	MG	0	8045	1/1	0.94	0.09	51,51,51,51	0
34	NA	0	8518	1/1	0.94	0.10	40,40,40,40	0
32	MG	0	8046	1/1	0.94	0.06	45,45,45,45	0
34	NA	0	8550	1/1	0.94	0.10	40,40,40,40	0
32	MG	0	8052	1/1	0.94	0.17	77,77,77,77	0
35	CL	B	8819	1/1	0.94	0.20	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	NA	0	8525	1/1	0.94	0.14	71,71,71,71	0
34	NA	0	8572	1/1	0.94	0.20	68,68,68,68	0
35	CL	N	8807	1/1	0.94	0.11	57,57,57,57	0
35	CL	O	8808	1/1	0.94	0.13	66,66,66,66	0
35	CL	Q	8811	1/1	0.94	0.13	58,58,58,58	0
32	MG	0	8098	1/1	0.94	0.16	31,31,31,31	0
34	NA	0	8528	1/1	0.94	0.08	39,39,39,39	0
32	MG	0	8086	1/1	0.94	0.06	46,46,46,46	0
34	NA	0	8570	1/1	0.95	0.37	64,64,64,64	0
34	NA	0	8544	1/1	0.95	0.04	14,14,14,14	0
34	NA	R	8538	1/1	0.95	0.08	55,55,55,55	0
34	NA	0	8521	1/1	0.95	0.23	43,43,43,43	0
34	NA	0	8506	1/1	0.95	0.12	52,52,52,52	0
32	MG	0	8093	1/1	0.95	0.06	43,43,43,43	0
35	CL	0	8812	1/1	0.95	0.09	40,40,40,40	0
35	CL	0	8813	1/1	0.95	0.08	55,55,55,55	0
32	MG	0	8103	1/1	0.95	0.15	77,77,77,77	0
34	NA	0	8556	1/1	0.95	0.13	54,54,54,54	0
32	MG	0	8035	1/1	0.95	0.06	36,36,36,36	0
32	MG	0	8053	1/1	0.95	0.10	50,50,50,50	0
32	MG	0	8089	1/1	0.95	0.08	32,32,32,32	0
32	MG	Y	8109	1/1	0.95	0.08	36,36,36,36	0
34	NA	0	8533	1/1	0.95	0.12	22,22,22,22	0
35	CL	J	8821	1/1	0.95	0.10	60,60,60,60	0
34	NA	0	8534	1/1	0.95	0.13	41,41,41,41	0
32	MG	0	8075	1/1	0.95	0.06	57,57,57,57	0
34	NA	0	8536	1/1	0.95	0.07	38,38,38,38	0
34	NA	0	8517	1/1	0.95	0.06	24,24,24,24	0
32	MG	0	8112	1/1	0.95	0.06	38,38,38,38	0
32	MG	0	8051	1/1	0.95	0.08	40,40,40,40	0
34	NA	0	8543	1/1	0.95	0.07	32,32,32,32	0
32	MG	0	8083	1/1	0.96	0.07	40,40,40,40	0
35	CL	0	8803	1/1	0.96	0.08	52,52,52,52	0
32	MG	0	8091	1/1	0.96	0.06	53,53,53,53	0
33	K	0	8402	1/1	0.96	0.06	49,49,49,49	0
35	CL	M	8818	1/1	0.96	0.08	36,36,36,36	0
32	MG	0	8081	1/1	0.96	0.06	34,34,34,34	0
32	MG	K	8069	1/1	0.96	0.05	54,54,54,54	0
34	NA	0	8523	1/1	0.96	0.20	56,56,56,56	0
34	NA	0	8514	1/1	0.96	0.11	37,37,37,37	0
32	MG	0	8097	1/1	0.96	0.08	35,35,35,35	0
34	NA	0	8526	1/1	0.96	0.13	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	0	8048	1/1	0.97	0.06	48,48,48,48	0
34	NA	0	8560	1/1	0.97	0.07	44,44,44,44	0
35	CL	J	8801	1/1	0.97	0.09	54,54,54,54	0
34	NA	0	8509	1/1	0.97	0.05	23,23,23,23	0
32	MG	0	8104	1/1	0.97	0.08	67,67,67,67	0
34	NA	0	8553	1/1	0.97	0.07	32,32,32,32	0
32	MG	B	8055	1/1	0.97	0.04	43,43,43,43	0
32	MG	0	8023	1/1	0.97	0.10	39,39,39,39	0
34	NA	0	8576	1/1	0.97	0.08	24,24,24,24	0
32	MG	0	8059	1/1	0.97	0.06	38,38,38,38	0
34	NA	0	8531	1/1	0.97	0.05	35,35,35,35	0
35	CL	3	8804	1/1	0.97	0.04	42,42,42,42	0
34	NA	M	8547	1/1	0.97	0.06	35,35,35,35	0
32	MG	0	8067	1/1	0.97	0.07	52,52,52,52	0
32	MG	0	8100	1/1	0.98	0.11	37,37,37,37	0
32	MG	0	8042	1/1	0.98	0.03	35,35,35,35	0
32	MG	0	8019	1/1	0.98	0.04	26,26,26,26	0
32	MG	0	8039	1/1	0.98	0.17	43,43,43,43	0
32	MG	0	8115	1/1	0.98	0.03	41,41,41,41	0
32	MG	0	8116	1/1	0.98	0.05	47,47,47,47	0
34	NA	0	8542	1/1	0.98	0.14	1,1,1,1	0
32	MG	0	8056	1/1	0.98	0.04	42,42,42,42	0
34	NA	0	8505	1/1	0.98	0.08	36,36,36,36	0
32	MG	0	8032	1/1	0.98	0.05	29,29,29,29	0
35	CL	0	8814	1/1	0.98	0.07	46,46,46,46	0
32	MG	0	8058	1/1	0.98	0.04	32,32,32,32	0
35	CL	0	8816	1/1	0.98	0.16	57,57,57,57	0
32	MG	0	8071	1/1	0.98	0.06	62,62,62,62	0
34	NA	J	8546	1/1	0.98	0.05	27,27,27,27	0
32	MG	0	8037	1/1	0.99	0.03	38,38,38,38	0
32	MG	0	8011	1/1	0.99	0.03	23,23,23,23	0
32	MG	0	8107	1/1	0.99	0.06	36,36,36,36	0
32	MG	0	8040	1/1	0.99	0.03	46,46,46,46	0
32	MG	0	8012	1/1	0.99	0.03	30,30,30,30	0
32	MG	0	8014	1/1	0.99	0.03	34,34,34,34	0
34	NA	0	8519	1/1	0.99	0.07	21,21,21,21	0
32	MG	0	8077	1/1	0.99	0.03	30,30,30,30	0
32	MG	0	8015	1/1	0.99	0.03	34,34,34,34	0
32	MG	0	8017	1/1	0.99	0.03	25,25,25,25	0
32	MG	0	8018	1/1	0.99	0.06	26,26,26,26	0
32	MG	0	8004	1/1	0.99	0.04	23,23,23,23	0
32	MG	0	8020	1/1	0.99	0.04	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	0	8021	1/1	0.99	0.03	37,37,37,37	0
32	MG	A	8065	1/1	0.99	0.07	37,37,37,37	0
32	MG	0	8049	1/1	0.99	0.09	30,30,30,30	0
32	MG	0	8022	1/1	0.99	0.04	40,40,40,40	0
32	MG	0	8005	1/1	0.99	0.04	32,32,32,32	0
32	MG	0	8006	1/1	0.99	0.06	32,32,32,32	0
32	MG	0	8025	1/1	0.99	0.02	32,32,32,32	0
32	MG	3	8078	1/1	0.99	0.05	11,11,11,11	0
32	MG	0	8054	1/1	0.99	0.05	24,24,24,24	0
32	MG	0	8027	1/1	0.99	0.04	39,39,39,39	0
32	MG	0	8028	1/1	0.99	0.03	39,39,39,39	0
32	MG	0	8029	1/1	0.99	0.02	36,36,36,36	0
34	NA	0	8503	1/1	0.99	0.12	1,1,1,1	0
32	MG	0	8031	1/1	0.99	0.03	33,33,33,33	0
32	MG	0	8008	1/1	0.99	0.03	27,27,27,27	0
32	MG	0	8061	1/1	0.99	0.04	30,30,30,30	0
32	MG	0	8034	1/1	0.99	0.04	15,15,15,15	0
32	MG	0	8009	1/1	0.99	0.04	31,31,31,31	0
32	MG	0	8036	1/1	0.99	0.03	29,29,29,29	0
32	MG	0	8068	1/1	0.99	0.05	54,54,54,54	0
37	CD	Z	8703	1/1	0.99	0.03	63,63,63,63	0
37	CD	1	8702	1/1	0.99	0.04	55,55,55,55	0
32	MG	0	8084	1/1	1.00	0.06	42,42,42,42	0
32	MG	0	8030	1/1	1.00	0.03	20,20,20,20	0
32	MG	0	8002	1/1	1.00	0.02	27,27,27,27	0
32	MG	0	8016	1/1	1.00	0.06	19,19,19,19	0
32	MG	0	8033	1/1	1.00	0.02	21,21,21,21	0
32	MG	0	8010	1/1	1.00	0.04	13,13,13,13	0
32	MG	0	8074	1/1	1.00	0.02	28,28,28,28	0
32	MG	0	8003	1/1	1.00	0.02	29,29,29,29	0
32	MG	0	8026	1/1	1.00	0.05	32,32,32,32	0
32	MG	0	8007	1/1	1.00	0.05	9,9,9,9	0
32	MG	0	8079	1/1	1.00	0.02	27,27,27,27	0
32	MG	0	8038	1/1	1.00	0.03	21,21,21,21	0
32	MG	0	8062	1/1	1.00	0.12	5,5,5,5	0
32	MG	0	8013	1/1	1.00	0.02	26,26,26,26	0
37	CD	U	8701	1/1	1.00	0.02	63,63,63,63	0
32	MG	0	8001	1/1	1.00	0.02	25,25,25,25	0
34	NA	L	8580	1/1	1.00	0.12	1,1,1,1	0
37	CD	3	8704	1/1	1.00	0.03	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.