



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 05:14 AM UTC

PDB ID : 5DM7 / pdb_00005dm7
Title : Crystal structure of the 50S ribosomal subunit from *Deinococcus radiodurans* in complex with hygromycin A
Authors : Kaminishi, T.; Schedlbauer, A.; Ochoa-Lizarralde, B.; Connell, S.R.; Fucini, P.
Deposited on : 2015-09-08
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

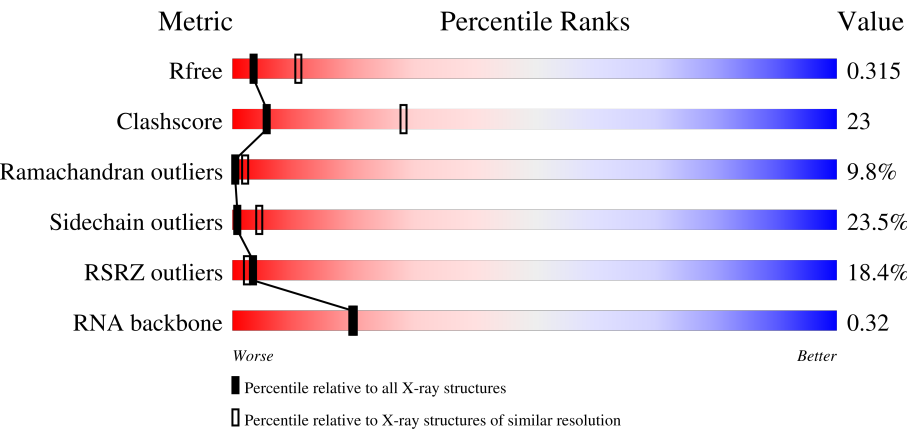
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)
RNA backbone	3983	1109 (3.20-2.80)

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	224	
2	A	274	
3	B	205	

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Mol	Chain	Length	Quality of chain
4	C	197	
5	D	177	
6	E	171	
7	F	144	
8	G	142	
9	H	134	
10	I	141	
11	J	136	
12	K	113	
13	L	104	
14	M	109	
15	N	117	
16	O	94	
17	P	127	
18	Q	93	
19	R	110	
20	S	175	
21	T	84	
22	U	72	
23	V	66	
24	W	55	
25	Z	57	
26	1	54	
27	2	47	
28	3	65	

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Mol	Chain	Length	Quality of chain
29	X	2881	
30	Y	122	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	MG	X	6001	-	-	-	X
31	MG	X	6003	-	-	-	X
31	MG	X	6006	-	-	-	X
31	MG	X	6010	-	-	-	X
31	MG	X	6013	-	-	-	X
31	MG	X	6018	-	-	-	X
31	MG	X	6022	-	-	-	X
31	MG	X	6025	-	-	-	X
31	MG	X	6027	-	-	-	X
31	MG	X	6031	-	-	-	X
31	MG	X	6033	-	-	-	X
31	MG	X	6035	-	-	-	X
31	MG	X	6042	-	-	-	X
31	MG	X	6045	-	-	-	X
31	MG	X	6046	-	-	-	X
31	MG	X	6048	-	-	-	X
31	MG	X	6049	-	-	-	X
31	MG	X	6051	-	-	-	X
31	MG	X	6052	-	-	-	X
31	MG	X	6053	-	-	-	X
31	MG	X	6054	-	-	-	X
31	MG	X	6057	-	-	-	X
31	MG	X	6060	-	-	-	X
31	MG	X	6062	-	-	-	X
31	MG	X	6072	-	-	-	X
31	MG	X	6074	-	-	-	X
31	MG	X	6076	-	-	-	X
31	MG	X	6082	-	-	-	X
31	MG	X	6087	-	-	-	X
31	MG	X	6089	-	-	-	X
31	MG	X	6090	-	-	-	X
31	MG	X	6091	-	-	-	X
31	MG	X	6092	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	MG	X	6099	-	-	-	X
31	MG	X	6100	-	-	-	X
31	MG	X	6101	-	-	-	X
31	MG	X	6105	-	-	-	X
31	MG	X	6114	-	-	-	X
31	MG	X	6116	-	-	-	X
31	MG	X	6117	-	-	-	X
31	MG	X	6123	-	-	-	X
31	MG	X	6124	-	-	-	X
31	MG	X	6125	-	-	-	X
31	MG	X	6127	-	-	-	X
31	MG	X	6129	-	-	-	X
31	MG	X	6132	-	-	-	X
31	MG	X	6133	-	-	-	X
31	MG	X	6135	-	-	-	X
31	MG	X	6141	-	-	-	X
31	MG	X	6142	-	-	-	X
31	MG	X	6147	-	-	-	X
31	MG	X	6149	-	-	-	X
31	MG	X	6150	-	-	-	X
31	MG	X	6151	-	-	-	X
31	MG	X	6153	-	-	-	X
31	MG	X	6154	-	-	-	X
31	MG	X	6155	-	-	-	X
31	MG	X	6157	-	-	-	X
31	MG	X	6159	-	-	-	X
31	MG	X	6160	-	-	-	X
31	MG	X	6162	-	-	-	X
31	MG	X	6167	-	-	-	X
31	MG	X	6168	-	-	-	X
31	MG	X	6169	-	-	-	X
31	MG	X	6170	-	-	-	X
31	MG	X	6175	-	-	-	X
31	MG	X	6177	-	-	-	X
31	MG	Y	201	-	-	-	X
31	MG	Y	203	-	-	-	X
31	MG	Y	204	-	-	-	X

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 89361 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 protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	224	Total	C	N	O	S	0	0	0
			1651	1031	302	313	5			

- Molecule 2 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	274	Total	C	N	O	S	0	0	0
			2107	1313	423	368	3			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	LYS	ARG	conflict	UNP Q9RXJ9
A	25	ALA	THR	conflict	UNP Q9RXJ9
A	270	LEU	ILE	conflict	UNP Q9RXJ9

- Molecule 3 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	205	Total	C	N	O	S	0	0	0
			1540	965	295	272	8			

- Molecule 4 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	197	Total	C	N	O	S	0	0	0
			1507	935	287	283	2			

- Molecule 5 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	177	Total	C	N	O	S	0	0	0
			1401	892	247	255	7			

- Molecule 6 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	171	Total	C	N	O	S	0	0	0
			1287	812	237	237	1			

- Molecule 7 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	F	144	Total	C	N	O	S	0	0	0
			1048	663	183	197	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	2	ARG	LYS	conflict	UNP Q9RSS7
F	3	ARG	LYS	conflict	UNP Q9RSS7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	G	142	Total	C	N	O	S	0	0	0
			1115	704	209	199	3			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	I	141	Total	C	N	O	0	0	0
			1068	655	216	197			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	136	Total	C	N	O	S	0	0	0
			1091	696	202	186	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	113	Total	C	N	O	S	0	0	0
			879	541	178	158	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	L	104	Total	C	N	O	0	0	0
			778	476	159	143			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	26	LYS	ARG	conflict	UNP Q9RSL2

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	M	109	Total	C	N	O	0	0	0
			867	540	171	156			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	?	-	LEU	deletion	UNP Q9RWB4
M	?	-	ARG	deletion	UNP Q9RWB4
M	?	-	GLU	deletion	UNP Q9RWB4
M	?	-	LEU	deletion	UNP Q9RWB4

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	O	94	Total	C	N	O	0	0	0
			742	465	139	138			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Q	93	Total	C	N	O	S	0	0	0
			727	458	136	131	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	R	110	Total	C	N	O	S	0	0	0
			826	513	160	152	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	175	Total	C	N	O	S	0	0	0
			1346	849	236	255	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	T	84	Total	C	N	O	S	0	0	0
			626	393	122	110	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	U	72	Total	C	N	O	0	0	0
			553	341	116	96			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	67	ILE	LEU	conflict	UNP Q9RRG8

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	V	66	Total	C	N	O	S	0	0	0
			534	327	107	97	3			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Z	57	Total	C	N	O	S	0	0	0
			453	278	93	77	5			

- Molecule 26 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1	54	Total	C	N	O	S	0	0	0
			404	256	73	74	1			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	0	ALA	-	insertion	UNP Q9RSS4
1	1	ALA	-	insertion	UNP Q9RSS4
1	3	GLY	LYS	conflict	UNP Q9RSS4
1	4	ALA	ASP	conflict	UNP Q9RSS4
1	5	ALA	GLY	conflict	UNP Q9RSS4
1	45	ALA	LYS	conflict	UNP Q9RSS4
1	46	HIS	LYS	conflict	UNP Q9RSS4
1	47	VAL	HIS	conflict	UNP Q9RSS4
1	49	PHE	VAL	conflict	UNP Q9RSS4
1	50	ALA	PHE	conflict	UNP Q9RSS4
1	51	ALA	-	insertion	UNP Q9RSS4
1	52	ALA	-	insertion	UNP Q9RSS4
1	53	ALA	-	insertion	UNP Q9RSS4

- Molecule 27 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	2	47	Total	C	N	O	S	0	0	0
			393	235	92	64	2			

- Molecule 28 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	3	65	Total	C	N	O	S	0	0	0
			509	320	104	80	5			

- Molecule 29 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	X	2780	Total	C	N	O	P	0	0	0
			59673	26617	11011	19265	2780			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1526	U	UNK	conflict	GB 11612676

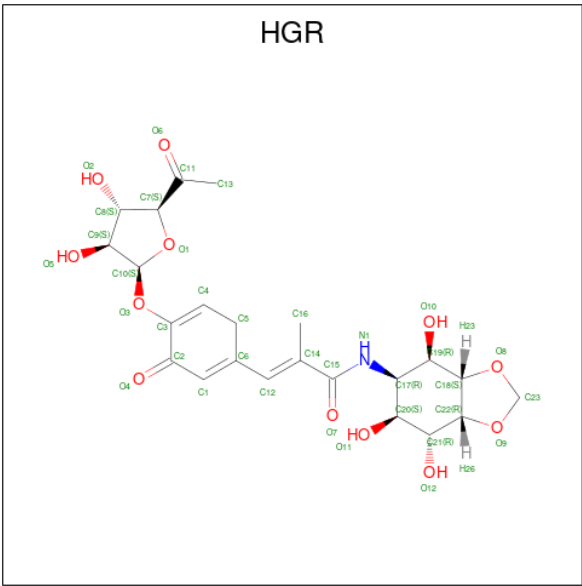
- Molecule 30 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	Y	122	Total	C	N	O	P	0	0	0
			2601	1161	476	842	122			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	A	1	Total	Mg	0	0
			1	1		
31	H	1	Total	Mg	0	0
			1	1		
31	M	1	Total	Mg	0	0
			1	1		
31	N	1	Total	Mg	0	0
			1	1		
31	X	177	Total	Mg	0	0
			177	177		
31	Y	5	Total	Mg	0	0
			5	5		

- Molecule 32 is Hygromycin A (CCD ID: HGR) (formula: C₂₃H₂₉NO₁₂).

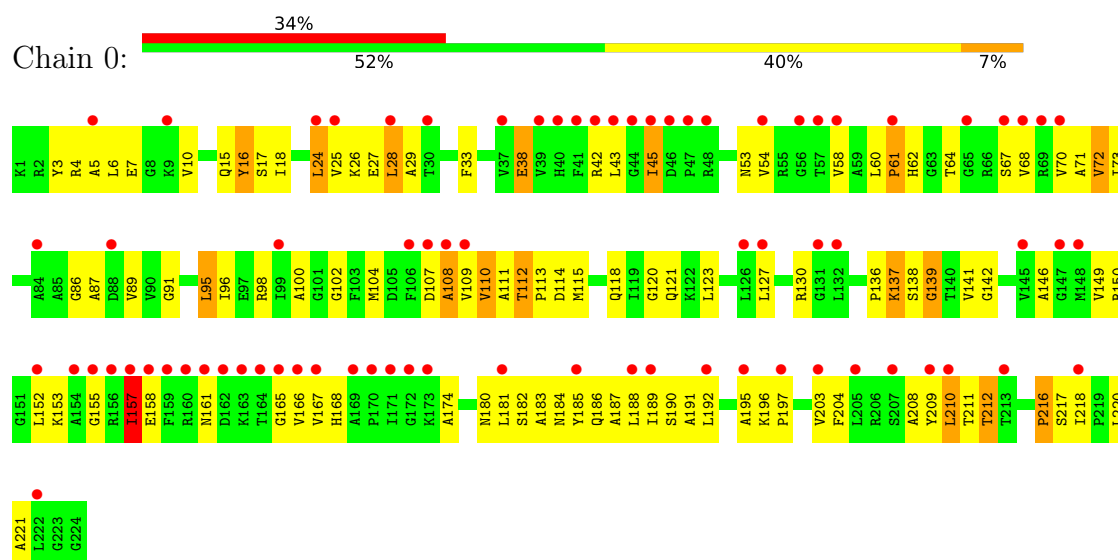


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	X	1	Total	C	N	O	0	0
			36	23	1	12		

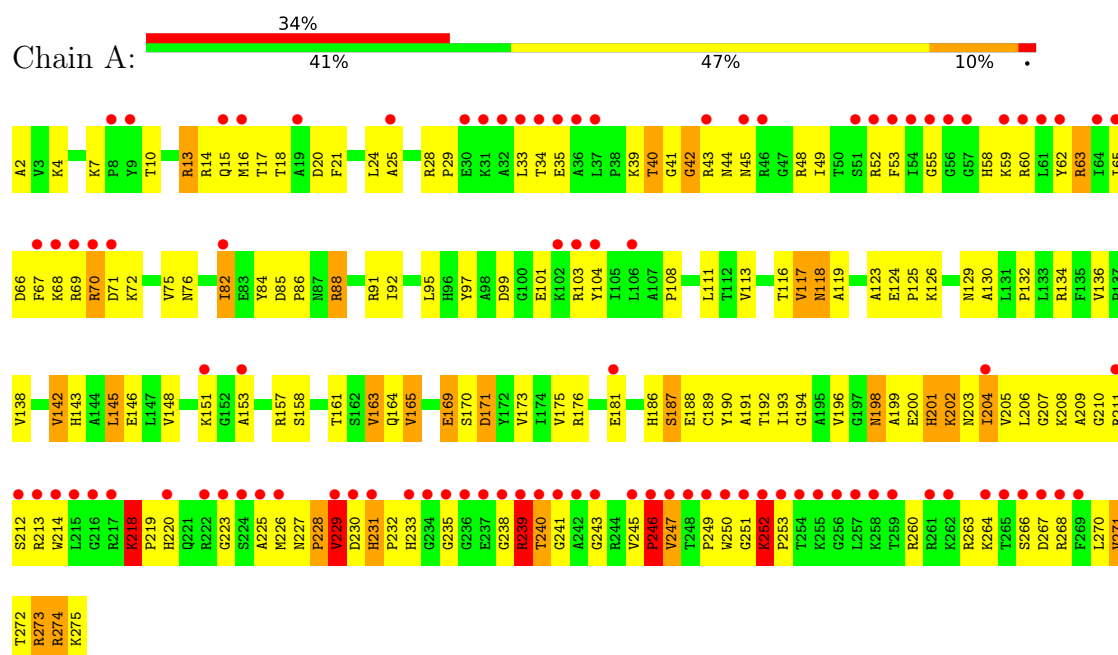
3 Residue-property plots [i](#)

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

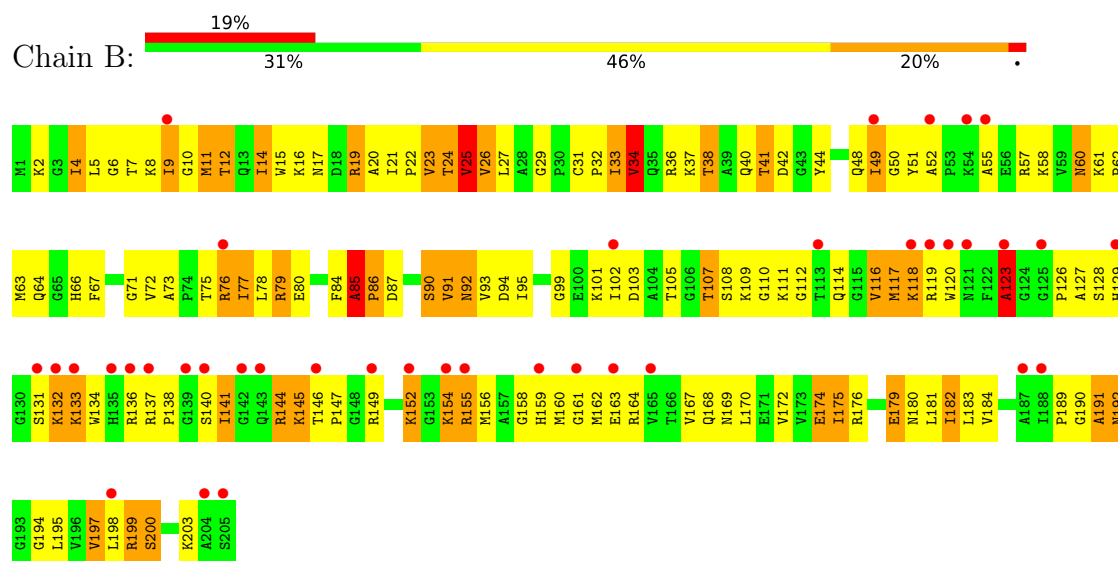
• Molecule 1: 50S ribosomal protein L1



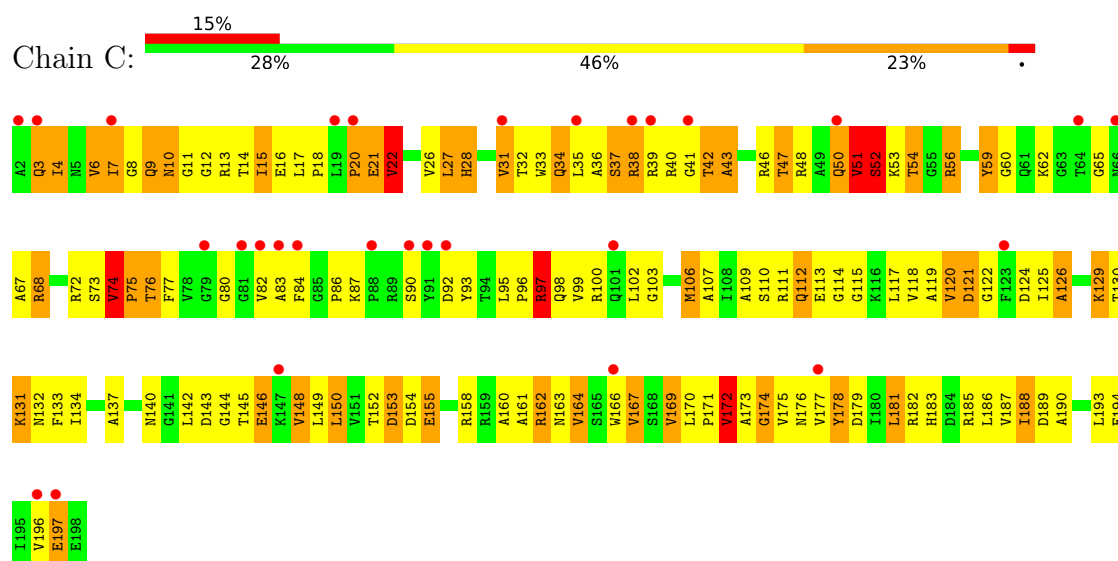
• Molecule 2: 50S ribosomal protein L2



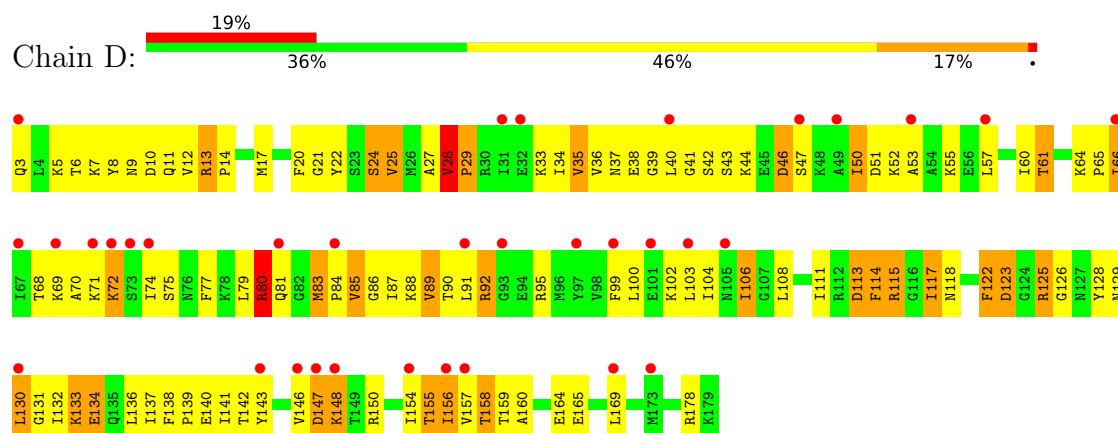
• Molecule 3: 50S ribosomal protein L3



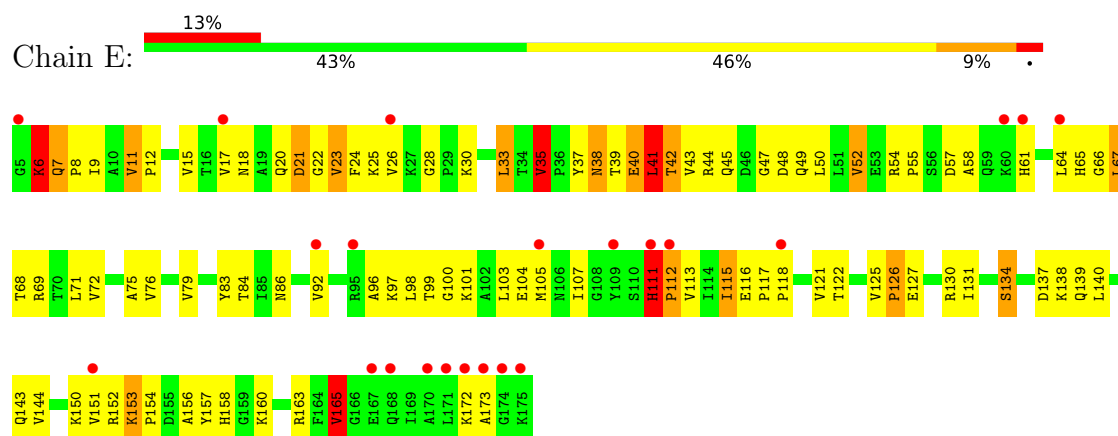
• Molecule 4: 50S ribosomal protein L4



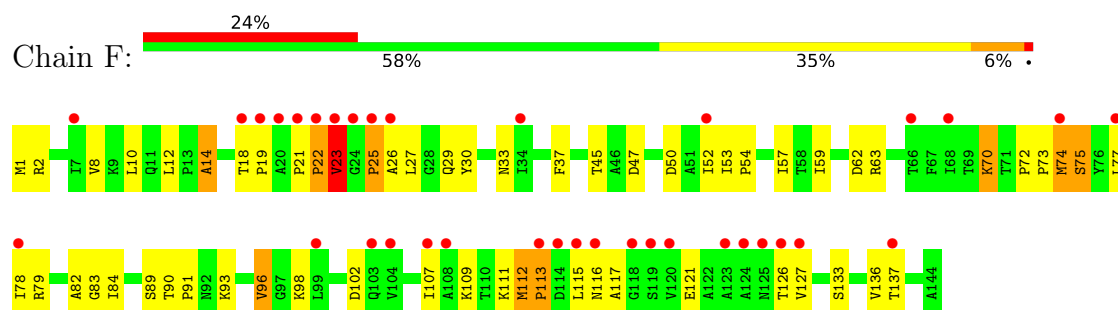
• Molecule 5: 50S ribosomal protein L5



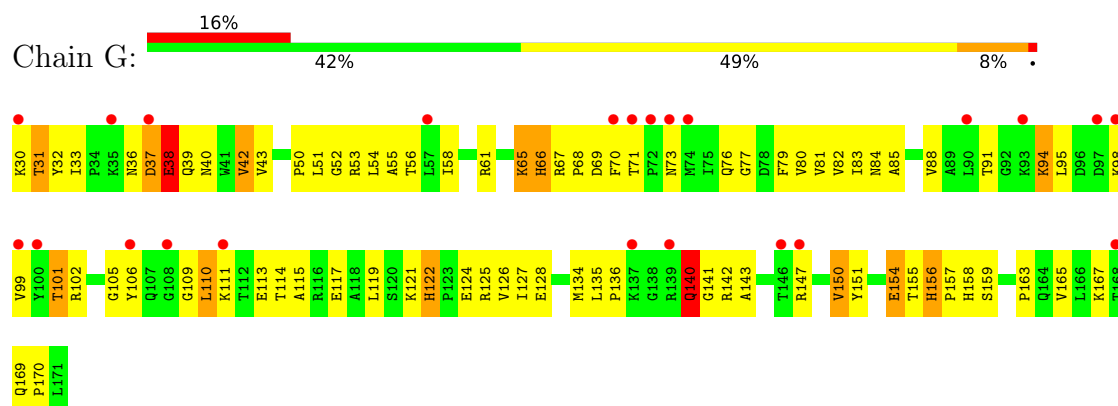
• Molecule 6: 50S ribosomal protein L6



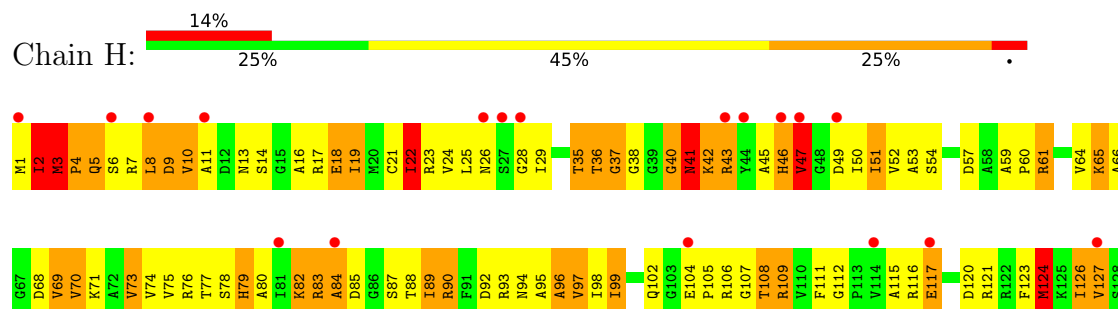
• Molecule 7: 50S ribosomal protein L11

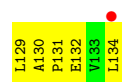


• Molecule 8: 50S ribosomal protein L13

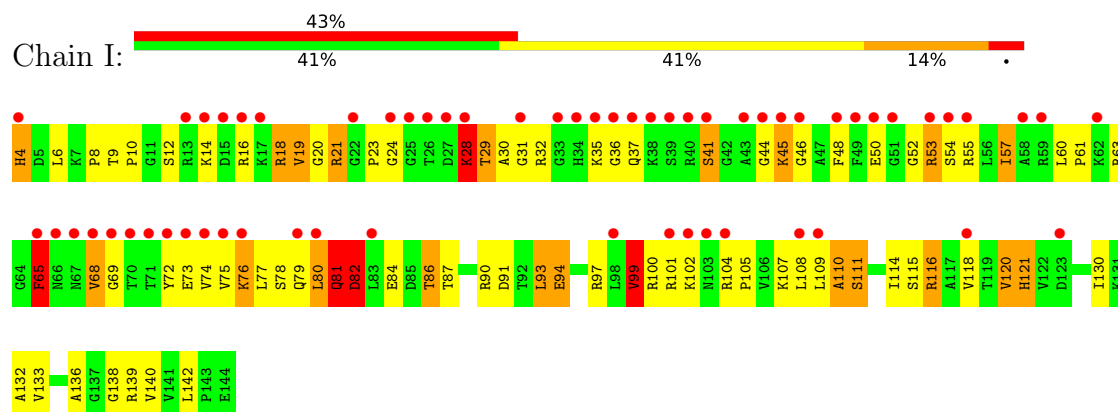


• Molecule 9: 50S ribosomal protein L14

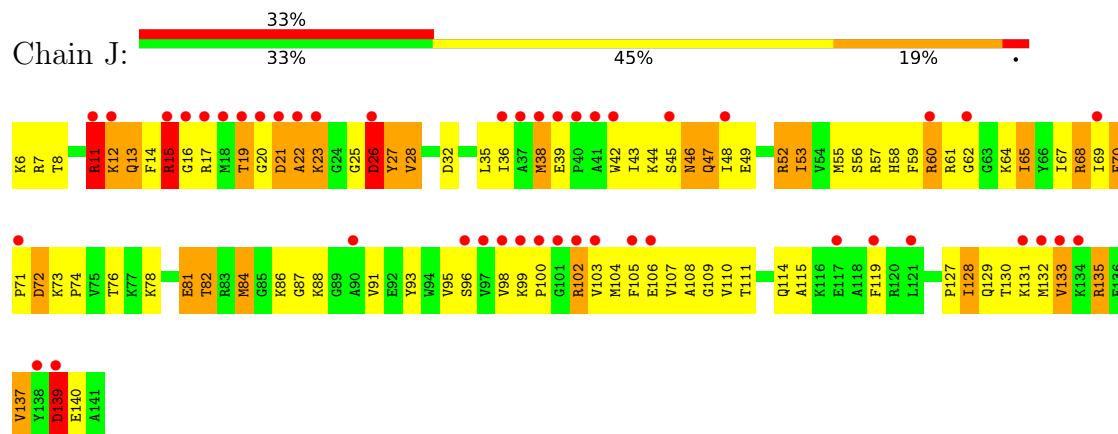




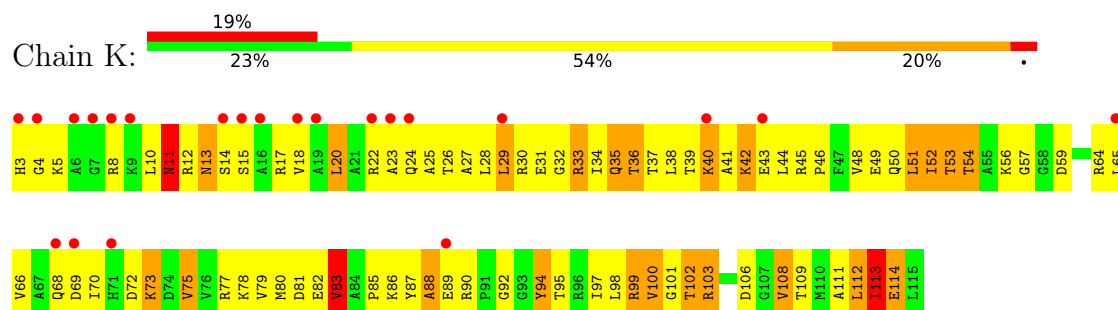
• Molecule 10: 50S ribosomal protein L15



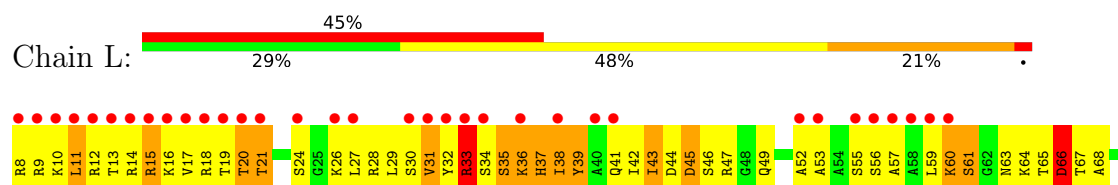
• Molecule 11: 50S ribosomal protein L16

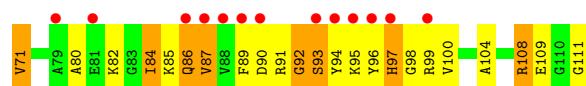


• Molecule 12: 50S ribosomal protein L17



• Molecule 13: 50S ribosomal protein L18





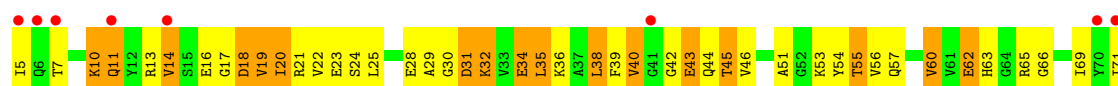
• Molecule 14: 50S ribosomal protein L19



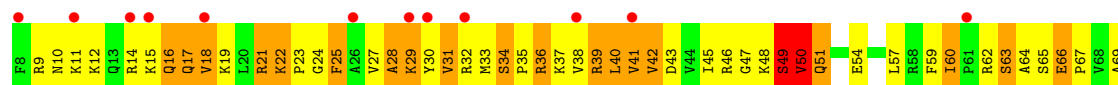
• Molecule 15: 50S ribosomal protein L20



• Molecule 16: 50S ribosomal protein L21

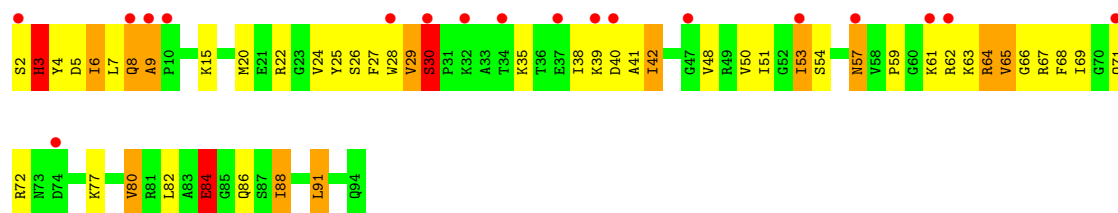


• Molecule 17: 50S ribosomal protein L22

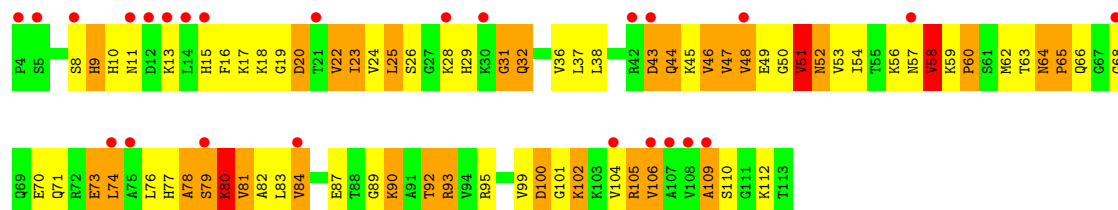


• Molecule 18: 50S ribosomal protein L23

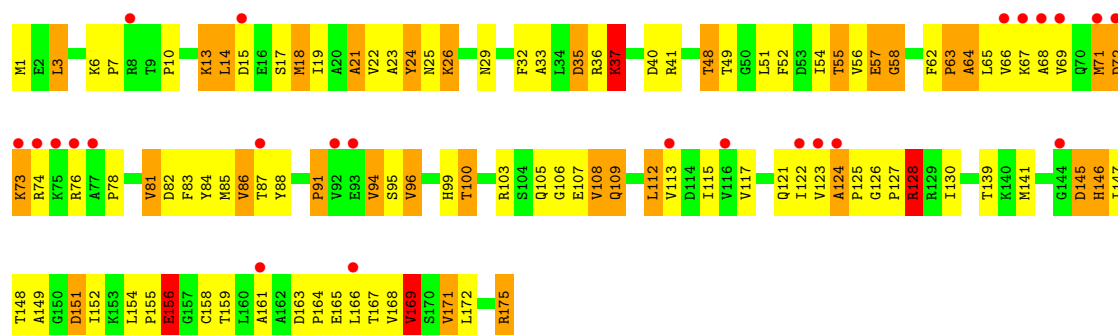




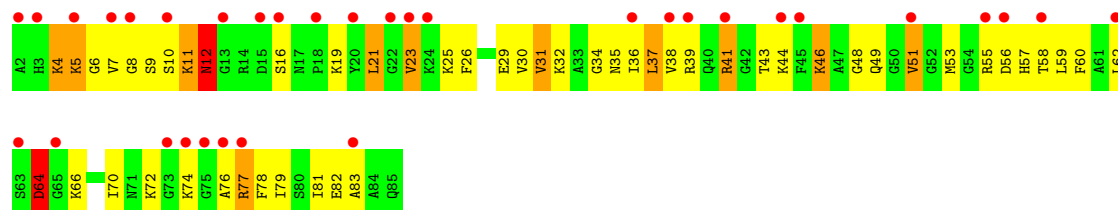
• Molecule 19: 50S ribosomal protein L24



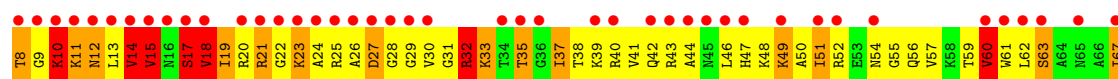
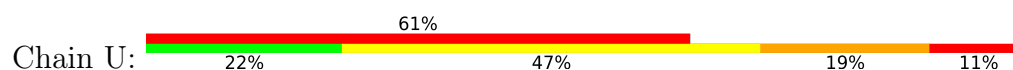
• Molecule 20: 50S ribosomal protein L25

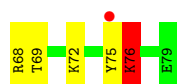


• Molecule 21: 50S ribosomal protein L27

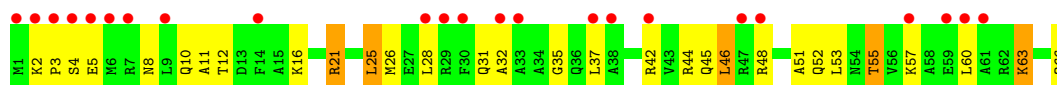


• Molecule 22: 50S ribosomal protein L28





- Molecule 23: 50S ribosomal protein L29



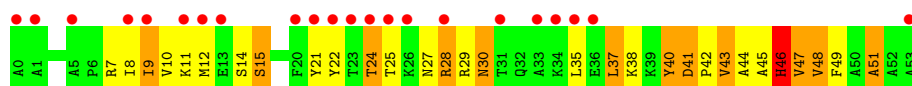
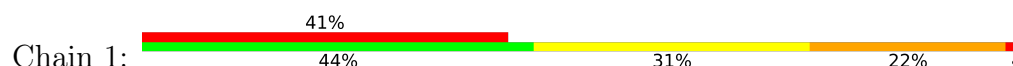
- Molecule 24: 50S ribosomal protein L30



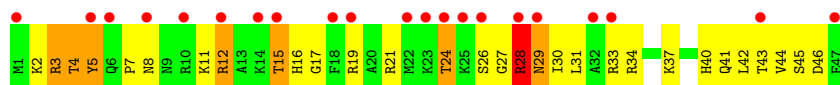
- Molecule 25: 50S ribosomal protein L32



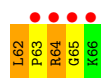
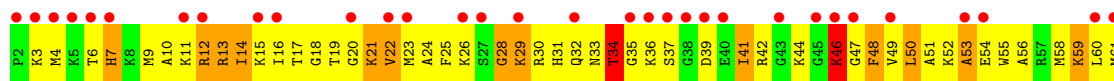
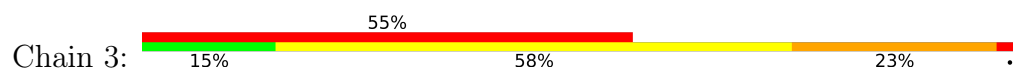
- Molecule 26: 50S ribosomal protein L33



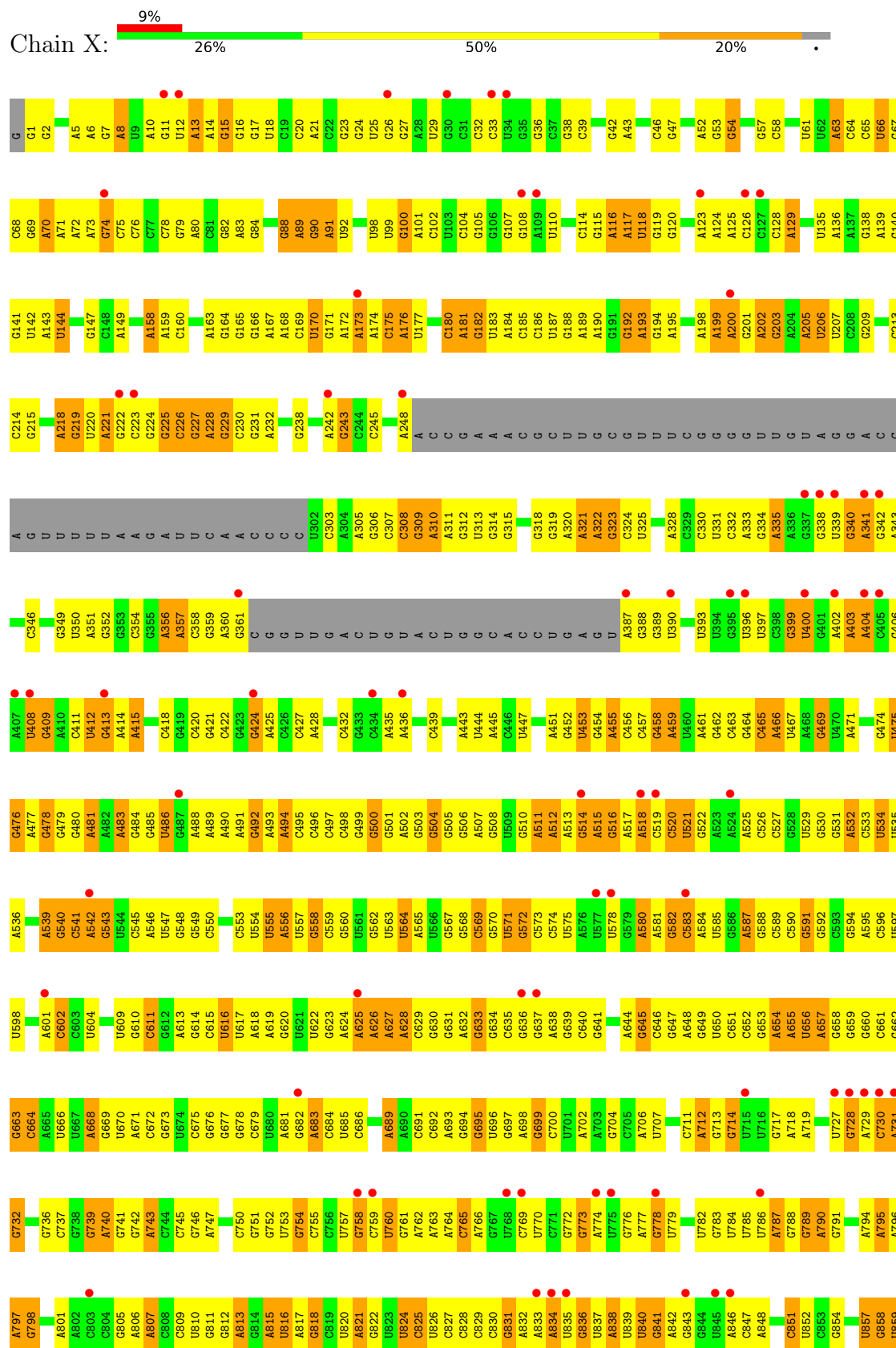
- Molecule 27: 50S ribosomal protein L34



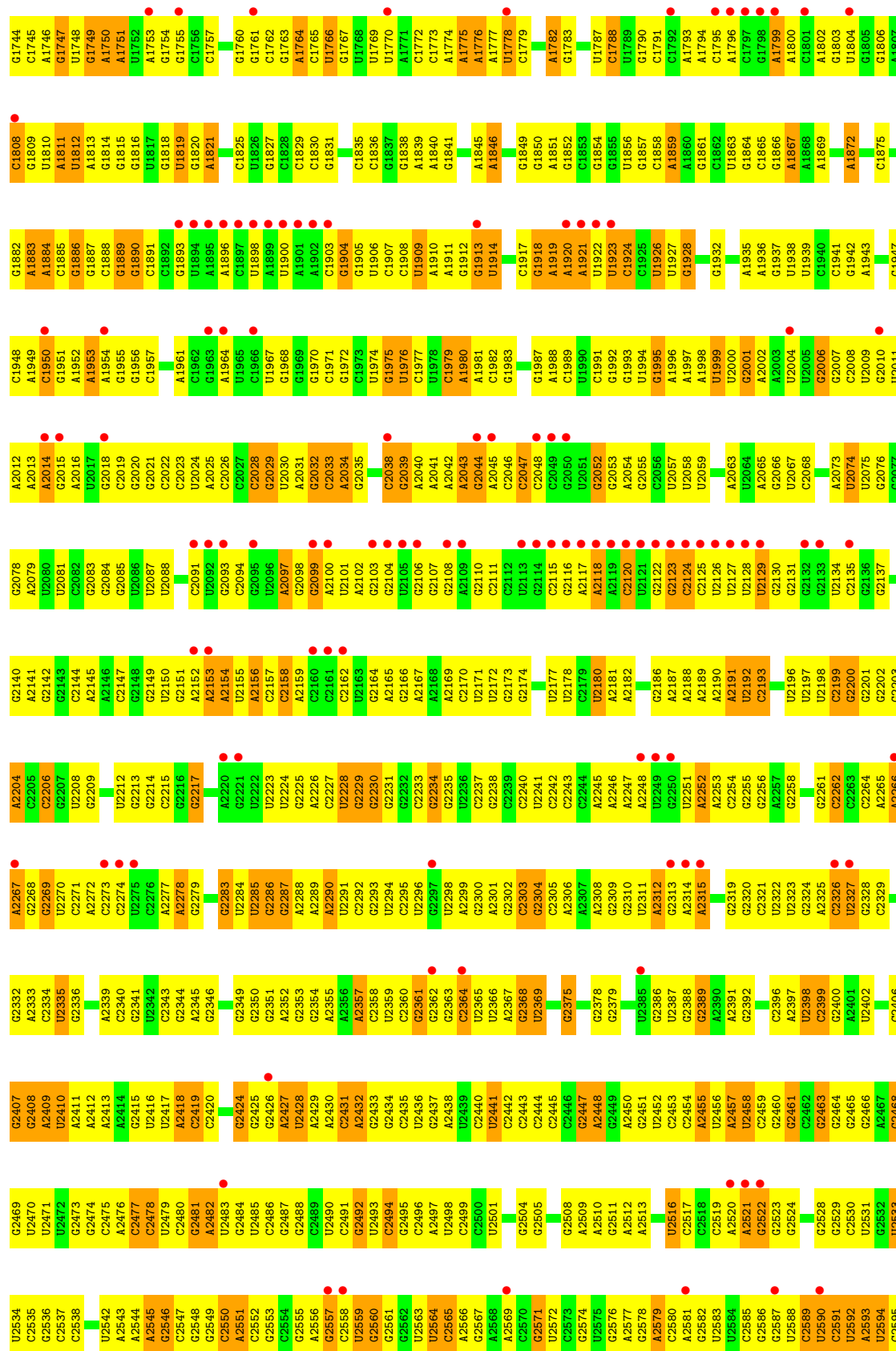
- Molecule 28: 50S ribosomal protein L35

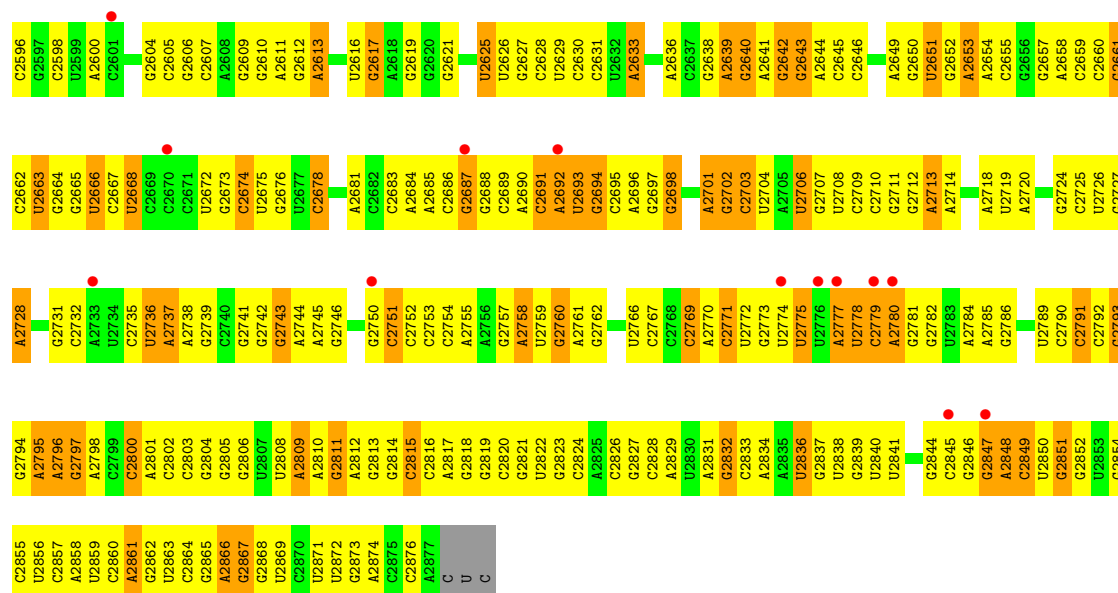


- Molecule 29: 23S ribosomal RNA

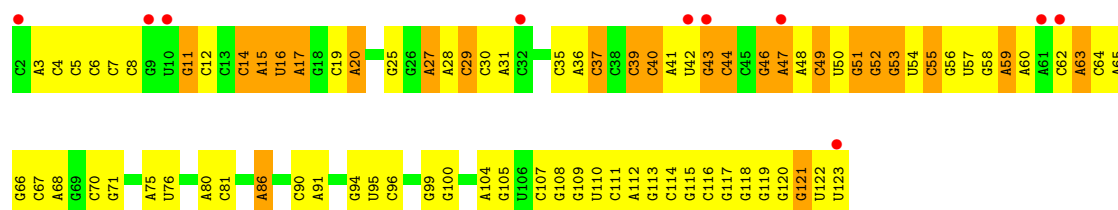


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A1607	U1608	A1609	A1610	A1611	U1612	C1616	C1617	U1618	U1619	U1620	C1620	G1621	G1622	C1623	A1624	A1625	A1626	C1627	C1628	A1629	A1630	C1631	C1632	C1633	G1634	A1636	C1639	G1642	A1643	U1651	G1652	C1653	G1654	C1655	A1656	U1657	A1658	C1659	U1660	C1661	C1663	G1664	C1665	C1666	A1667	C1668	U1669	C1692	A1693	C1696	U1697	C1698	A1699	C1700	C1701	C1702	C1703	G1704	U1705	A1706	A1707	U1708	U1709	U1710	G1711	G1712	G1713	A1714	A1715	G1716	A1717	A1718	G1719	G1720	G1721	G1722	U1723	C1724	C1725	C1726	C1727	A1728	U1733	C1734	G1735	C1736	G1737	U1738	G1741	G1742	C1743
G1533	A1534	A1535			U1539	C1540	G1541	U1542	G1543	A1544	G1545	U1548	C1549	C1550	U1551	C1552	G1553	C1554	A1555	A1556	G1557		A1560	G1561	G1562	U1563	U1564		A1567	A1568	A1569	C1570	G1571	C1572	G1573	A1574	C1575	U1578	C1579	C1580	C1581	A1582		A1585	A1586	U1591	U1592	C1593		U1600	U1601	C1602	A1603	A1604	A1605	C1606																																			
U1461	C1462	A1463	A1464	C1465	C1466	U1467	A1468	U1469	C1470	G1471		A1474	U1475	G1476	C1477	U1478	C1479	G1480	U1481	C1482	G1483	G1484	U1485		U1490	C1491		G1494	G1495	C1496	C1497	U1498	A1499	U1500		G1503	G1504	U1505	C1506	A1507	G1508	A1509	A1510	A1511	A1512	U1513		C1517	C1518	C1522	A1523	C1524	A1525	U1526	G1527	C1528	C1529	U1530																																	
C1385	A1386		A1391	C1392	G1393	G1394	A1395	C1396	A1397	G1398		G1401	U1402	U1403	C1404	A1405	A1406	G1407	U1408	U1409	G1483	C1411	C1412	U1413	G1414		G1419	A1420		U1424	G1425	U1426	G1427	G1428	A1429	G1430		A1433	G1434	G1435	G1436	A1437	C1438	G1439	G1440	A1441	C1442		A1445		C1451	U1452	A1453	U1454	C1455		U1458	U1459	G1460																																
A1315	A1318		C1319	A1320	A1321	G1322	G1323	G1324	U1325	U1326		U1329	G1330	G1331	G1332	G1333	A1334	A1335	G1336	G1337	G1338	U1339	C1340	G1341	U1342	C1343	C1344	G1345	C1346	C1347	C1348	U1349	G1350	G1351	G1352	A1353	A1354	G1359	G1360		U1365	A1366	A1367	G1368	G1369	U1370	G1371		G1374	C1375		U1378	A1379	C1380	G1381	C1382	G1383	C1384																																	
A1250	G1251	C1252	C1253	A1254	A1255	C1256	U1257	G1258	A1259	A1260	C1261	U1262	G1263	C1264	G1265	G1266	A1267	U1268	G1269	C1270	C1271	G1272	C1273	C1274	A1275	G1276	G1277	A1278	G1279	U1280	A1281	C1282	G1283	G1284	A1285	U1286	A1287	A1288	A1289	A1290	G1291		G1296	A1297	G1298	A1299	A1300	U1301	C1302	U1303		U1307	C1308	G1309	C1310	G1311	G1312	U1313	A1314																																
A1188	G1189		A1192	G1193	U1194	U1195	G1196	U1197	C1198	U1199	G1200	U1201	U1202	A1203	G1204	G1205	G1206	G1207	A1208	C1209	G1210	U1211	U1212	U1213	C1214	A1215		C1218	C1219	G1220	C1221	G1222	C1223	A1224	G1225	G1226	A1227	G1228	C1229	C1230	A1231		C1236	G1237	A1238	A1239	G1240	G1241	A1242	G1243	U1244	G1245	G1246	U1247	G1248	G1249																																			
G1118	U1119		G1121	A1122	G1123	U1124	G1125		G1128	A1129	U1130	G1131	C1132	G1133	G1134	C1135	G1136	A1137	A1138	A1139	U1140	U1141	G1142	A1143	U1144	C1145	G1146	G1147	G1148	G1149	C1150	U1151	C1152	A1153	A1154	G1155	U1156	G1157	A1158		A1162	C1163	C1164	G1165	A1166	A1167	G1168	C1169	G1174	A1175	U1176	U1177	C1178	A1179	C1185	G1186	U1187																																		
A1055	U1056	A1057	G1058	A1059	C1060	A1061	G1062	C1063	A1064	U1065	G1066	U1067	A1068	G1069	U1070	U1071	U1072	G1073	G1074	U1075	U1076	U1077	A1078	G1079	A1080	A1081	G1082	C1083	A1084	G1085	C1086	C1087	C1088	C1089	C1090	C1091	U1092		A1096	A1097	G1098	A1099	U1100	U1101	G1102	C1103	G1104		A1107	U1108	A1109	G1110	C1111	U1112	C1113	A1114	C1115	U1116	G1117																																
A991	A992	C993	A994	A995	C996	C997	C998	A999	U1000	A1001	C1002	C1003	A1004	U1005	C1006	A1007	G1008	C1009	U1010	A1011	A1012	G1013	G1014	U1015	C1016	C1017	G1018	A995	U1019	A1020	A1021	A1022	U1023	G1024	C992	C993	A964	G965	A966	C967	C968	U969	A970	A971	C972	U973	U974	A975	C976	G980	C981	C982	A983	A984	G985	A986	U987	G988																																	
C927	G928	A929	C930	C931	G932	C933	G934	C935	A936	C937	C938	G939	G940	U941	U942	U943	A944	C945	U946	C947	C948	G949	G950	G951	A952	G953	U954	A955	A956	G957	G958	C959	U960	G961	C962	G963	A964	G965	A966	C967	C968	U969	A970	A971	C972	U973	U974	A975	C976	G980	C981	C982	A983	A984	G985	A986	U987	G988																																	
U860	C861	A862	C863	C864	A865	U866	C867	U868	C869	C870	U871	C872	U873	A874	C875	A876	C877	C878	A879	C880	G887	G888	A891	G	G	G	G	G	G	G	G	C	C	U	A	C	C	A	G	C	U	U	A	A	C	A911	A912	A913	C914	C915	U916	U919	G920	A921	A922	A923	C924	U925	C926																																





● Molecule 30: 5S ribosomal RNA



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	169.82Å 411.54Å 695.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.02 – 3.00 57.02 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.9 (57.02-3.00) 76.2 (57.02-3.00)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.27 (at 3.01Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.284 , 0.326 0.269 , 0.315	Depositor DCC
R_{free} test set	22814 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	67.3	Xtriage
Anisotropy	0.451	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 38.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	89361	wwPDB-VP
Average B, all atoms (Å ²)	142.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% 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: HGR, MG

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	0.41	0/1674	0.84	3/2257 (0.1%)
2	A	0.51	0/2149	1.03	13/2890 (0.4%)
3	B	0.85	0/1568	1.32	15/2105 (0.7%)
4	C	0.65	0/1530	1.16	11/2070 (0.5%)
5	D	0.49	0/1420	1.02	10/1903 (0.5%)
6	E	0.52	0/1309	1.06	12/1771 (0.7%)
7	F	0.47	0/1067	0.97	3/1446 (0.2%)
8	G	0.57	0/1139	1.22	10/1539 (0.6%)
9	H	0.97	1/1007 (0.1%)	1.50	15/1352 (1.1%)
10	I	0.62	0/1082	1.14	5/1448 (0.3%)
11	J	0.81	1/1114 (0.1%)	1.28	13/1486 (0.9%)
12	K	1.06	0/887	1.47	12/1188 (1.0%)
13	L	0.74	1/784 (0.1%)	1.11	3/1045 (0.3%)
14	M	0.95	0/880	1.51	15/1179 (1.3%)
15	N	0.79	1/994 (0.1%)	1.16	4/1323 (0.3%)
16	O	0.62	0/751	1.09	6/1000 (0.6%)
17	P	0.94	1/1027 (0.1%)	1.43	15/1373 (1.1%)
18	Q	0.58	0/738	0.98	3/988 (0.3%)
19	R	0.76	1/836 (0.1%)	1.28	7/1121 (0.6%)
20	S	0.58	0/1371	1.04	6/1862 (0.3%)
21	T	0.62	0/634	1.03	3/838 (0.4%)
22	U	0.74	0/557	1.30	6/741 (0.8%)
23	V	0.50	0/538	0.92	0/714
24	W	0.70	0/426	1.32	5/568 (0.9%)
25	Z	0.84	0/465	1.35	6/622 (1.0%)
26	1	0.70	0/411	1.14	4/554 (0.7%)
27	2	0.59	0/397	1.08	5/521 (1.0%)
28	3	0.65	0/516	1.09	2/673 (0.3%)
29	X	0.45	0/66826	0.52	0/104247
30	Y	0.36	0/2907	0.47	0/4529
All	All	0.53	6/97004 (0.0%)	0.74	212/145353 (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
3	B	0	1
9	H	0	1
10	I	0	1
13	L	0	1
14	M	0	2
19	R	0	1
All	All	0	7

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	R	58	VAL	CA-CB	6.75	1.63	1.54
11	J	19	THR	CA-C	6.35	1.60	1.53
13	L	31	VAL	CA-CB	6.24	1.62	1.54
15	N	47	TYR	C-O	5.44	1.30	1.24
9	H	2	ILE	CA-CB	-5.11	1.48	1.54
17	P	28	ALA	CA-CB	-5.01	1.46	1.52

All (212) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	M	42	GLY	N-CA-C	-15.96	96.79	111.95
8	G	71	THR	CA-C-N	12.54	132.22	119.56
8	G	71	THR	C-N-CA	12.54	132.22	119.56
14	M	3	THR	N-CA-C	-12.07	89.56	109.24
24	W	23	LEU	N-CA-C	-10.12	101.50	114.04
22	U	33	LYS	N-CA-C	-9.94	97.94	111.96
4	C	188	ILE	N-CA-C	9.36	119.96	110.23
14	M	35	VAL	CB-CA-C	-9.24	99.13	111.15
4	C	74	VAL	CA-C-N	9.17	131.31	119.84
4	C	74	VAL	C-N-CA	9.17	131.31	119.84
9	H	37	GLY	N-CA-C	9.07	122.31	112.33
6	E	111	HIS	CA-C-N	8.88	130.95	119.84
6	E	111	HIS	C-N-CA	8.88	130.95	119.84
12	K	83	VAL	N-CA-C	8.49	118.47	110.74
3	B	191	ALA	N-CA-C	8.34	121.08	110.24
19	R	47	VAL	N-CA-C	8.32	120.14	107.99
17	P	17	GLN	N-CA-C	8.22	120.02	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	K	111	ALA	N-CA-C	8.15	121.26	108.79
24	W	12	ARG	CA-C-N	8.09	129.96	119.84
24	W	12	ARG	C-N-CA	8.09	129.96	119.84
3	B	85	ALA	CA-C-N	8.05	129.90	119.84
3	B	85	ALA	C-N-CA	8.05	129.90	119.84
11	J	42	TRP	N-CA-C	-8.04	97.15	109.85
3	B	179	GLU	N-CA-C	-8.01	93.75	110.80
19	R	80	LYS	N-CA-C	-7.73	102.89	114.64
9	H	49	ASP	N-CA-C	-7.70	99.12	110.52
17	P	66	GLU	CA-C-N	-7.65	111.08	119.19
17	P	66	GLU	C-N-CA	-7.65	111.08	119.19
20	S	21	ALA	N-CA-C	7.61	120.93	108.99
17	P	22	LYS	CA-C-N	7.60	129.33	119.84
17	P	22	LYS	C-N-CA	7.60	129.33	119.84
25	Z	33	CYS	CA-C-N	7.58	129.31	119.84
25	Z	33	CYS	C-N-CA	7.58	129.31	119.84
3	B	90	SER	N-CA-C	7.55	121.23	108.02
22	U	17	SER	CA-C-N	7.41	135.03	121.70
22	U	17	SER	C-N-CA	7.41	135.03	121.70
11	J	28	VAL	N-CA-C	7.39	114.12	106.21
17	P	51	GLN	N-CA-C	-7.34	102.25	112.45
9	H	109	ARG	N-CA-C	7.25	116.83	108.49
5	D	28	VAL	CA-C-N	7.12	128.74	119.84
5	D	28	VAL	C-N-CA	7.12	128.74	119.84
17	P	34	SER	CA-C-N	7.04	128.64	119.84
17	P	34	SER	C-N-CA	7.04	128.64	119.84
3	B	25	VAL	CB-CA-C	-7.03	102.45	110.96
12	K	108	VAL	CB-CA-C	-6.99	101.13	110.98
2	A	231	HIS	CA-C-N	6.97	128.55	119.84
2	A	231	HIS	C-N-CA	6.97	128.55	119.84
10	I	21	ARG	N-CA-C	6.96	119.71	111.02
9	H	102	GLN	N-CA-C	-6.95	104.46	114.12
26	1	47	VAL	N-CA-C	6.92	118.24	111.67
10	I	28	LYS	CB-CA-C	-6.90	107.58	115.79
7	F	75	SER	N-CA-C	-6.89	104.86	112.72
27	2	40	HIS	N-CA-C	-6.88	103.23	111.69
5	D	13	ARG	CA-C-N	-6.87	113.11	120.94
5	D	13	ARG	C-N-CA	-6.87	113.11	120.94
2	A	252	LYS	CA-C-N	6.85	128.41	119.84
2	A	252	LYS	C-N-CA	6.85	128.41	119.84
1	0	189	ILE	N-CA-C	-6.77	105.89	111.91
9	H	65	LYS	N-CA-C	6.63	120.17	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	K	112	LEU	N-CA-C	-6.59	98.66	109.40
12	K	35	GLN	N-CA-C	-6.56	98.50	109.07
19	R	109	ALA	N-CA-C	-6.51	102.50	112.99
14	M	42	GLY	CA-C-O	-6.50	118.00	122.22
20	S	115	ILE	N-CA-C	6.43	113.09	106.21
14	M	80	VAL	CB-CA-C	-6.42	103.09	110.73
12	K	77	ARG	N-CA-C	-6.41	104.29	111.28
11	J	87	GLY	N-CA-C	6.40	119.20	110.69
19	R	51	VAL	N-CA-C	6.40	122.65	109.34
27	2	19	ARG	N-CA-C	-6.39	104.31	111.28
24	W	52	GLU	N-CA-C	-6.38	100.12	110.20
2	A	245	VAL	CA-C-N	6.37	127.81	119.84
2	A	245	VAL	C-N-CA	6.37	127.81	119.84
16	O	38	LEU	N-CA-C	-6.35	106.11	114.31
6	E	163	ARG	N-CA-C	6.35	118.72	109.07
2	A	28	ARG	CA-C-N	6.34	127.77	119.84
2	A	28	ARG	C-N-CA	6.34	127.77	119.84
9	H	14	SER	N-CA-C	-6.31	103.62	113.02
11	J	70	PHE	CA-C-N	6.30	127.72	119.84
11	J	70	PHE	C-N-CA	6.30	127.72	119.84
7	F	37	PHE	N-CA-C	-6.26	107.49	114.62
12	K	113	ILE	N-CA-C	-6.24	99.14	108.12
12	K	15	SER	N-CA-C	-6.23	103.79	112.45
11	J	139	ASP	N-CA-C	-6.20	105.37	113.12
11	J	109	GLY	N-CA-C	-6.19	106.69	115.30
14	M	3	THR	CA-C-N	-6.16	114.57	122.77
14	M	3	THR	C-N-CA	-6.16	114.57	122.77
4	C	74	VAL	N-CA-C	6.15	114.93	107.61
9	H	112	GLY	CA-C-N	-6.15	114.40	120.98
9	H	112	GLY	C-N-CA	-6.15	114.40	120.98
19	R	28	LYS	N-CA-C	-6.13	105.93	113.41
4	C	197	GLU	N-CA-C	-6.08	104.29	111.03
16	O	43	GLU	N-CA-C	6.08	118.61	110.35
22	U	11	LYS	N-CA-C	-6.07	101.43	110.23
6	E	21	ASP	CB-CA-C	-6.06	108.98	117.23
3	B	77	ILE	N-CA-C	6.04	116.82	108.12
14	M	93	ILE	N-CA-C	-6.01	103.50	110.05
4	C	120	VAL	N-CA-C	5.98	116.48	107.75
2	A	42	GLY	N-CA-C	-5.97	106.28	114.64
2	A	171	ASP	N-CA-C	-5.97	105.81	114.12
17	P	39	ARG	N-CA-C	-5.97	104.78	111.28
15	N	102	GLU	CA-C-N	5.96	127.29	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	102	GLU	C-N-CA	5.96	127.29	119.84
27	2	3	ARG	N-CA-C	5.96	119.37	110.14
28	3	48	PHE	N-CA-C	5.95	117.58	108.42
9	H	95	ALA	N-CA-C	5.94	118.32	108.99
25	Z	37	HIS	N-CA-C	5.92	117.84	110.91
26	1	24	THR	N-CA-C	5.89	115.79	108.19
22	U	60	VAL	N-CA-C	5.87	121.55	109.34
10	I	80	LEU	N-CA-C	-5.86	104.85	112.23
12	K	75	VAL	N-CA-C	5.85	116.04	110.42
3	B	107	THR	N-CA-C	-5.83	101.39	110.42
11	J	19	THR	N-CA-C	5.80	115.67	108.19
21	T	44	LYS	N-CA-C	-5.79	105.11	111.82
6	E	127	GLU	CA-C-N	5.78	127.07	119.84
6	E	127	GLU	C-N-CA	5.78	127.07	119.84
19	R	92	THR	CB-CA-C	-5.77	103.58	111.95
16	O	39	PHE	N-CA-C	5.74	117.73	108.32
13	L	86	GLN	N-CA-C	5.74	118.82	109.24
16	O	86	HIS	N-CA-C	5.73	117.83	108.55
28	3	59	LYS	N-CA-C	-5.73	104.73	110.97
12	K	72	ASP	N-CA-C	5.69	118.91	109.46
3	B	50	GLY	N-CA-C	5.65	119.54	110.90
8	G	36	ASN	N-CA-C	5.65	118.37	109.39
25	Z	57	VAL	N-CA-C	-5.64	100.86	109.78
16	O	62	GLU	N-CA-C	5.64	117.10	108.42
8	G	122	HIS	CA-C-N	5.63	125.15	119.19
8	G	122	HIS	C-N-CA	5.63	125.15	119.19
17	P	115	ASN	N-CA-C	5.62	118.61	108.48
4	C	65	GLY	N-CA-C	-5.61	107.44	115.64
17	P	18	VAL	N-CA-C	5.59	120.98	109.34
20	S	64	ALA	N-CA-C	5.59	117.50	108.34
8	G	42	VAL	N-CA-C	5.55	116.17	108.23
11	J	11	ARG	N-CA-C	5.55	122.62	110.80
5	D	114	PHE	N-CA-C	5.55	116.63	107.20
8	G	105	GLY	N-CA-C	-5.55	108.08	114.69
8	G	32	TYR	N-CA-C	5.53	117.74	108.23
10	I	36	GLY	N-CA-C	-5.52	106.00	111.85
11	J	58	HIS	N-CA-C	5.50	117.28	111.28
8	G	126	VAL	N-CA-C	-5.49	106.34	111.45
17	P	122	SER	N-CA-C	5.49	118.40	108.69
17	P	46	ARG	N-CA-C	5.47	118.40	110.42
7	F	21	PRO	N-CA-C	5.46	117.36	110.70
1	0	149	VAL	N-CA-C	-5.45	105.66	113.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	H	108	THR	N-CA-C	-5.44	106.69	113.38
8	G	101	THR	N-CA-C	5.42	117.59	107.99
27	2	5	TYR	N-CA-C	5.41	117.81	107.75
13	L	92	GLY	N-CA-C	-5.38	100.42	113.18
10	I	37	GLN	N-CA-C	-5.37	106.23	112.89
3	B	34	VAL	N-CA-C	5.37	120.50	109.34
3	B	15	TRP	N-CA-C	5.37	117.71	109.07
4	C	4	ILE	N-CA-C	5.36	116.94	109.55
9	H	96	ALA	N-CA-C	5.36	117.12	109.14
25	Z	25	LEU	N-CA-C	5.35	117.98	110.23
6	E	125	VAL	CA-C-N	5.34	126.51	119.84
6	E	125	VAL	C-N-CA	5.34	126.51	119.84
4	C	6	VAL	N-CA-C	5.33	120.42	109.34
14	M	90	GLN	N-CA-C	5.32	117.28	108.13
20	S	163	ASP	CA-C-N	5.31	126.48	119.84
20	S	163	ASP	C-N-CA	5.31	126.48	119.84
4	C	3	GLN	N-CA-C	5.31	117.15	108.76
12	K	18	VAL	N-CA-C	5.31	115.45	110.30
2	A	218	LYS	CA-C-N	5.28	125.58	119.93
2	A	218	LYS	C-N-CA	5.28	125.58	119.93
24	W	34	VAL	N-CA-C	5.28	115.88	108.17
9	H	41	ASN	N-CA-C	5.27	122.03	110.80
17	P	60	ILE	N-CA-C	-5.27	103.78	108.95
5	D	83	MET	CA-C-N	5.27	126.43	119.84
5	D	83	MET	C-N-CA	5.27	126.43	119.84
26	1	41	ASP	CA-C-N	5.27	126.42	119.84
26	1	41	ASP	C-N-CA	5.27	126.42	119.84
15	N	23	GLY	N-CA-C	-5.25	108.39	115.21
6	E	35	VAL	CA-C-N	5.24	126.39	119.84
6	E	35	VAL	C-N-CA	5.24	126.39	119.84
5	D	138	PHE	CA-C-N	5.23	126.07	120.47
5	D	138	PHE	C-N-CA	5.23	126.07	120.47
9	H	99	ILE	N-CA-C	5.23	116.24	108.65
22	U	51	ILE	N-CA-C	5.23	114.28	106.85
19	R	58	VAL	CB-CA-C	5.22	119.86	111.29
11	J	15	ARG	N-CA-C	5.20	121.89	110.80
14	M	81	PHE	CA-C-N	5.20	126.34	119.84
14	M	81	PHE	C-N-CA	5.20	126.34	119.84
16	O	95	ILE	N-CA-C	5.20	116.23	108.54
5	D	24	SER	N-CA-C	5.19	116.18	108.60
18	Q	6	ILE	N-CA-C	5.19	115.81	110.36
11	J	22	ALA	N-CA-C	5.19	117.21	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	H	3	MET	CA-C-N	5.18	126.32	119.84
9	H	3	MET	C-N-CA	5.18	126.32	119.84
3	B	174	GLU	N-CA-C	5.18	117.87	109.06
3	B	123	ALA	N-CA-C	5.18	121.83	110.80
11	J	21	ASP	N-CA-C	5.18	121.83	110.80
6	E	52	VAL	CB-CA-C	-5.16	105.07	111.32
14	M	26	ASP	CA-C-N	-5.14	114.94	122.19
14	M	26	ASP	C-N-CA	-5.14	114.94	122.19
27	2	28	ARG	N-CA-C	-5.14	104.94	111.11
17	P	67	PRO	N-CA-C	-5.13	106.84	113.57
13	L	66	ASP	N-CA-C	-5.12	105.77	112.23
15	N	84	LYS	N-CA-C	-5.12	107.16	113.41
3	B	23	VAL	N-CA-C	5.11	115.26	108.11
21	T	12	ASN	N-CA-C	5.11	112.97	108.78
3	B	9	ILE	CB-CA-C	-5.07	105.55	111.94
12	K	97	ILE	N-CA-C	5.06	116.00	108.46
4	C	54	THR	N-CA-C	5.05	121.56	110.80
6	E	6	LYS	N-CA-C	5.05	117.38	108.75
25	Z	54	GLY	N-CA-C	-5.04	101.22	113.18
18	Q	30	SER	CA-C-N	5.03	126.13	119.84
18	Q	30	SER	C-N-CA	5.03	126.13	119.84
1	O	210	LEU	N-CA-C	5.03	115.95	108.86
2	A	164	GLN	N-CA-C	5.03	116.61	108.41
21	T	12	ASN	CA-C-O	5.02	120.85	117.94
20	S	81	VAL	N-CA-C	5.02	115.50	108.17
14	M	28	ARG	CA-C-N	5.00	124.93	119.78
14	M	28	ARG	C-N-CA	5.00	124.93	119.78

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	85	ALA	Peptide
9	H	36	THR	Peptide
10	I	52	GLY	Peptide
13	L	87	VAL	Peptide
14	M	108	LYS	Peptide
14	M	2	GLN	Peptide
19	R	105	ARG	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	1651	0	1693	52	0
2	A	2107	0	2190	135	0
3	B	1540	0	1600	122	0
4	C	1507	0	1525	118	0
5	D	1401	0	1481	85	0
6	E	1287	0	1336	53	0
7	F	1048	0	1088	36	0
8	G	1115	0	1144	54	0
9	H	997	0	1046	83	0
10	I	1068	0	1103	69	0
11	J	1091	0	1125	71	0
12	K	879	0	930	82	0
13	L	778	0	820	58	0
14	M	867	0	890	68	0
15	N	978	0	1020	99	0
16	O	742	0	756	39	0
17	P	1014	0	1096	85	0
18	Q	727	0	753	31	0
19	R	826	0	881	65	0
20	S	1346	0	1372	72	0
21	T	626	0	655	39	0
22	U	553	0	604	52	0
23	V	534	0	558	13	0
24	W	424	0	470	24	0
25	Z	453	0	455	51	0
26	1	404	0	416	26	0
27	2	393	0	420	24	0
28	3	509	0	565	62	0
29	X	59673	0	30060	1976	0
30	Y	2601	0	1327	92	0
31	A	1	0	0	0	0
31	H	1	0	0	0	0
31	M	1	0	0	0	0
31	N	1	0	0	0	0
31	X	177	0	0	1	0
31	Y	5	0	0	0	0
32	X	36	0	29	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	89361	0	59408	3390	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 23.

All (3390) 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)
3:B:14:ILE:HB	14:M:20:HIS:HD2	1.16	1.11
12:K:79:VAL:HA	12:K:83:VAL:HG13	1.35	1.06
29:X:1225:G:H1'	29:X:1250:A:H61	1.21	1.03
29:X:517:A:H5''	29:X:518:A:H5'	1.37	1.02
29:X:2690:A:OP1	29:X:2692:A:OP2	1.78	0.99
29:X:2550:C:H5''	29:X:2551:A:H5'	1.42	0.98
22:U:21:ARG:HH12	29:X:400:U:H5'	1.28	0.98
15:N:48:ARG:HD2	29:X:1167:A:H61	1.27	0.97
29:X:320:A:N3	29:X:340:G:O2'	1.96	0.97
10:I:21:ARG:NH2	29:X:596:C:OP2	1.99	0.96
29:X:2796:A:H2'	29:X:2797:G:H8	1.30	0.96
29:X:623:G:O2'	29:X:626:A:N6	1.99	0.95
29:X:1230:C:H2'	29:X:1231:A:H8	1.31	0.94
3:B:14:ILE:HB	14:M:20:HIS:CD2	2.03	0.93
28:3:29:LYS:NZ	29:X:2398:U:OP2	2.01	0.93
25:Z:19:ARG:NH2	29:X:1277:G:OP1	2.02	0.92
14:M:25:PRO:HB3	14:M:93:ILE:HD11	1.53	0.91
29:X:2796:A:H2'	29:X:2797:G:C8	2.05	0.91
14:M:82:PRO:O	14:M:84:ALA:N	2.04	0.90
29:X:646:C:O2'	29:X:650:U:OP1	1.90	0.90
11:J:19:THR:HG22	11:J:20:GLY:H	1.37	0.89
12:K:36:THR:OG1	29:X:1291:G:OP1	1.91	0.89
17:P:31:VAL:HG11	17:P:124:ILE:HD11	1.54	0.89
8:G:140:GLN:HG3	29:X:567:G:H5'	1.55	0.88
29:X:2083:G:H1	29:X:2172:U:H3	1.21	0.88
14:M:42:GLY:O	14:M:44:ARG:N	2.08	0.87
24:W:43:MET:HE1	29:X:940:G:H21	1.38	0.87
28:3:34:THR:OG1	29:X:2399:C:OP1	1.92	0.86
3:B:75:THR:HG22	3:B:77:ILE:H	1.38	0.86
10:I:21:ARG:HA	29:X:824:U:H2'	1.55	0.86
6:E:22:GLY:HA3	6:E:39:THR:HG22	1.56	0.86
14:M:29:PRO:HD3	14:M:57:ILE:HD11	1.57	0.86
29:X:320:A:N6	29:X:1223:G:O2'	2.08	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:578:U:O2'	29:X:994:A:N1	2.08	0.86
12:K:53:THR:OG1	29:X:2815:C:OP1	1.92	0.85
24:W:25:LEU:HD22	24:W:30:ASP:HB3	1.57	0.85
17:P:49:SER:O	17:P:51:GLN:N	2.08	0.85
29:X:834:A:H1'	29:X:955:G:H5'	1.58	0.85
29:X:1230:C:H2'	29:X:1231:A:C8	2.12	0.84
29:X:1919:A:H2	29:X:1926:U:H3	1.24	0.84
13:L:18:ARG:NH2	29:X:2271:C:OP2	2.10	0.84
29:X:469:G:N2	29:X:481:A:OP2	2.08	0.84
29:X:1989:C:O2'	29:X:2798:A:N3	2.11	0.84
29:X:2821:G:H2'	29:X:2822:U:C6	2.12	0.83
12:K:11:ASN:HD22	12:K:11:ASN:H	1.25	0.83
29:X:841:G:H2'	29:X:842:A:C8	2.13	0.83
29:X:1202:U:H2'	29:X:1203:A:H8	1.44	0.83
22:U:17:SER:HB2	22:U:18:VAL:HB	1.60	0.83
27:2:43:THR:HG22	27:2:45:SER:H	1.41	0.83
29:X:2352:A:H2'	29:X:2353:G:C8	2.14	0.82
27:2:46:ASP:OD1	29:X:125:A:N6	2.13	0.82
29:X:1983:G:N2	29:X:2668:U:O4	2.10	0.82
29:X:2522:G:H2'	29:X:2523:G:C8	2.14	0.82
20:S:141:MET:HG2	20:S:145:ASP:HB2	1.62	0.81
29:X:693:A:H2'	29:X:694:G:H8	1.45	0.81
29:X:1060:C:H42	29:X:2731:G:H1	1.26	0.81
24:W:40:VAL:HA	24:W:43:MET:HE3	1.62	0.81
15:N:37:GLN:HA	15:N:40:LEU:HD12	1.60	0.81
12:K:13:ASN:O	12:K:17:ARG:NH2	2.14	0.81
29:X:1244:U:H2'	29:X:1245:G:H8	1.45	0.81
29:X:1909:U:OP2	29:X:1912:G:N1	2.13	0.80
29:X:2668:U:O2	29:X:2693:U:H5''	1.82	0.80
29:X:1681:A:N6	29:X:1975:G:O6	2.14	0.80
29:X:2543:A:OP1	29:X:2627:G:O2'	1.97	0.80
3:B:189:PRO:HA	29:X:2659:C:H5'	1.61	0.80
15:N:49:ASP:HA	15:N:52:ASN:HB2	1.61	0.80
28:3:64:ARG:NH2	29:X:219:G:OP1	2.15	0.80
3:B:111:LYS:NZ	29:X:2704:U:OP1	2.13	0.80
29:X:1336:G:H2'	29:X:1337:G:H5'	1.63	0.79
29:X:652:C:H42	29:X:657:A:H61	1.28	0.79
29:X:1674:C:H2'	29:X:1675:C:C6	2.17	0.79
29:X:698:A:OP1	29:X:699:G:N2	2.15	0.79
29:X:2309:G:N2	29:X:2365:U:O2	2.16	0.79
29:X:1573:G:H3'	29:X:1574:A:H5''	1.61	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:79:G:H2'	29:X:80:A:H8	1.48	0.79
22:U:48:LYS:HG2	22:U:49:LYS:H	1.48	0.79
17:P:109:ARG:NH1	29:X:760:U:O2'	2.15	0.79
29:X:833:A:N3	29:X:954:U:O2'	2.15	0.79
29:X:2118:A:N6	29:X:2140:G:O6	2.15	0.79
11:J:26:ASP:OD1	11:J:26:ASP:N	2.14	0.78
2:A:60:ARG:HD3	2:A:86:PRO:HB2	1.65	0.78
29:X:312:G:HO2'	29:X:313:U:H6	1.31	0.78
12:K:103:ARG:HH21	12:K:108:VAL:HB	1.48	0.78
2:A:16:MET:HG3	2:A:207:GLY:HA3	1.65	0.78
29:X:546:A:H2'	29:X:547:U:H6	1.49	0.78
29:X:2303:C:H5''	29:X:2304:G:H5''	1.66	0.78
26:I:45:ALA:HB1	29:X:2350:G:H4'	1.66	0.78
14:M:69:ARG:HD2	14:M:78:GLU:HG2	1.64	0.78
11:J:38:MET:HE2	11:J:131:LYS:HB2	1.66	0.78
16:O:46:VAL:HG13	16:O:51:ALA:HB2	1.66	0.78
17:P:32:ARG:NH1	17:P:120:ARG:O	2.16	0.78
29:X:1164:C:H2'	29:X:1165:G:C8	2.18	0.78
5:D:75:SER:H	5:D:79:LEU:HD22	1.49	0.77
4:C:150:LEU:HA	4:C:187:VAL:HB	1.64	0.77
17:P:15:LYS:NZ	29:X:512:A:O2'	2.12	0.77
17:P:28:ALA:HB2	17:P:71:VAL:HG21	1.66	0.77
8:G:151:TYR:HH	8:G:158:HIS:HE2	1.30	0.77
9:H:64:VAL:HG22	9:H:106:ARG:HH21	1.48	0.77
10:I:28:LYS:HB3	10:I:29:THR:HG23	1.67	0.77
2:A:157:ARG:NH1	29:X:1810:U:OP2	2.18	0.77
29:X:226:C:H4'	29:X:227:G:H5''	1.66	0.77
29:X:2283:G:H22	29:X:2291:U:H3	1.32	0.77
29:X:2772:U:H2'	29:X:2773:G:H8	1.48	0.77
14:M:60:SER:HA	14:M:64:LYS:HB2	1.64	0.77
20:S:67:LYS:HD2	20:S:84:TYR:HB2	1.66	0.77
22:U:32:ARG:H	22:U:32:ARG:NE	1.81	0.77
17:P:117:ILE:HD11	29:X:1995:G:H4'	1.66	0.77
29:X:7:G:H2'	29:X:8:A:H8	1.50	0.77
29:X:1097:A:O2'	29:X:1098:G:N7	2.17	0.77
4:C:26:VAL:HB	4:C:106:MET:HE1	1.65	0.77
8:G:88:VAL:HG21	8:G:127:ILE:HD11	1.67	0.77
29:X:2494:C:H42	29:X:2548:G:H1	1.30	0.77
3:B:6:GLY:HA3	3:B:27:LEU:O	1.85	0.77
2:A:69:ARG:HH12	2:A:192:THR:HG22	1.50	0.77
29:X:2418:A:H4'	29:X:2419:C:C5'	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:102:GLU:OE1	16:O:13:ARG:NH2	2.18	0.76
30:Y:40:C:O2	30:Y:50:U:O2'	2.01	0.76
29:X:1770:U:H5	29:X:1775:A:N7	1.83	0.76
29:X:1674:C:H2'	29:X:1675:C:H6	1.49	0.76
17:P:81:HIS:O	17:P:83:ASP:N	2.18	0.76
27:2:12:ARG:NH1	29:X:476:G:OP1	2.19	0.76
25:Z:15:LYS:O	25:Z:18:MET:N	2.18	0.76
29:X:1058:G:O2'	29:X:1120:C:N4	2.19	0.76
3:B:78:LEU:O	3:B:79:ARG:NE	2.17	0.76
10:I:28:LYS:O	10:I:30:ALA:N	2.19	0.76
6:E:107:ILE:O	6:E:152:ARG:NH1	2.19	0.76
29:X:693:A:H2'	29:X:694:G:C8	2.20	0.76
29:X:857:U:H3'	29:X:858:G:C8	2.21	0.76
11:J:32:ASP:H	11:J:108:ALA:HB2	1.51	0.76
20:S:25:ASN:HA	20:S:85:MET:HB2	1.68	0.76
5:D:111:ILE:HG12	5:D:137:ILE:HD12	1.65	0.75
19:R:37:LEU:HD11	19:R:49:GLU:HG3	1.68	0.75
29:X:1225:G:H1'	29:X:1250:A:N6	1.98	0.75
29:X:1104:G:H21	29:X:1109:A:H62	1.33	0.75
21:T:25:LYS:HB2	21:T:37:LEU:HA	1.67	0.75
29:X:2629:U:H2'	29:X:2630:C:H6	1.52	0.75
16:O:14:VAL:HG11	16:O:95:ILE:HG13	1.69	0.74
17:P:15:LYS:HB3	29:X:512:A:H4'	1.67	0.74
9:H:22:ILE:HD11	29:X:1935:A:C6	2.22	0.74
5:D:14:PRO:HA	5:D:17:MET:HB2	1.68	0.74
29:X:43:A:H61	29:X:447:U:H3	1.36	0.74
15:N:12:ARG:NH1	29:X:1229:C:OP2	2.21	0.74
19:R:15:HIS:CD2	19:R:16:PHE:HD2	2.06	0.74
29:X:867:G:H1	29:X:935:C:H42	1.32	0.74
14:M:93:ILE:HD12	14:M:93:ILE:H	1.52	0.74
29:X:455:A:H2	29:X:1258:G:N3	1.85	0.74
29:X:1437:A:H2'	29:X:1438:G:H8	1.52	0.74
30:Y:4:C:N4	30:Y:121:G:O6	2.18	0.74
29:X:2543:A:H5'	29:X:2627:G:H4'	1.69	0.74
29:X:2789:U:H3	29:X:2861:A:H61	1.36	0.74
15:N:74:MET:HE2	15:N:110:VAL:HG13	1.70	0.74
29:X:2672:U:H2'	29:X:2673:G:H8	1.52	0.74
5:D:131:GLY:HA2	5:D:154:ILE:H	1.52	0.73
13:L:39:TYR:OH	30:Y:118:G:N3	2.21	0.73
29:X:205:A:H2'	29:X:206:U:H5'	1.68	0.73
29:X:2639:A:N3	29:X:2639:A:H5"	2.02	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:38:GLU:HB3	5:D:87:ILE:HB	1.70	0.73
17:P:109:ARG:NH2	29:X:1996:A:N3	2.37	0.73
29:X:517:A:C5'	29:X:518:A:H5'	2.18	0.73
7:F:73:PRO:O	7:F:75:SER:N	2.20	0.73
29:X:333:A:H5'	29:X:351:A:H1'	1.70	0.73
29:X:2417:U:O2'	29:X:2419:C:OP1	2.06	0.73
29:X:2811:G:H2'	29:X:2812:A:C8	2.23	0.73
5:D:92:ARG:NH2	30:Y:47:A:OP1	2.21	0.73
8:G:151:TYR:OH	8:G:158:HIS:NE2	2.21	0.73
12:K:81:ASP:O	12:K:85:PRO:HG3	1.88	0.73
5:D:60:ILE:HG22	5:D:140:GLU:HB2	1.70	0.73
10:I:130:ILE:HG12	10:I:140:VAL:HG21	1.70	0.73
29:X:692:C:H2'	29:X:693:A:H8	1.54	0.73
29:X:2550:C:H5''	29:X:2551:A:C5'	2.18	0.73
17:P:62:ARG:HH11	25:Z:25:LEU:HD11	1.53	0.73
19:R:16:PHE:CE2	19:R:81:VAL:HG11	2.23	0.73
19:R:93:ARG:NH2	29:X:312:G:OP2	2.19	0.73
29:X:1479:G:H2'	29:X:1480:G:C8	2.24	0.72
29:X:1726:C:O2'	29:X:2834:A:N3	2.21	0.72
2:A:201:HIS:O	2:A:203:ASN:N	2.21	0.72
29:X:402:A:N7	29:X:2392:G:O2'	2.22	0.72
29:X:2270:U:O2'	29:X:2353:G:N3	2.21	0.72
29:X:421:G:H2'	29:X:422:C:H6	1.54	0.72
29:X:2611:A:H61	29:X:2766:U:H3	1.36	0.72
2:A:108:PRO:HB3	2:A:143:HIS:HE1	1.53	0.72
23:V:51:ALA:O	23:V:55:THR:OG1	2.08	0.72
13:L:89:PHE:O	13:L:91:ARG:NH2	2.22	0.72
29:X:834:A:H5'	29:X:835:U:H6	1.53	0.72
9:H:22:ILE:HG22	9:H:52:VAL:HG12	1.70	0.72
15:N:48:ARG:NH2	29:X:987:G:OP1	2.22	0.72
29:X:488:A:H2'	29:X:489:A:C8	2.25	0.72
29:X:2014:A:C6	29:X:2477:C:H1'	2.25	0.72
2:A:17:THR:OG1	2:A:205:VAL:N	2.22	0.72
3:B:84:PHE:CD2	3:B:86:PRO:HD3	2.25	0.72
9:H:21:CYS:SG	9:H:22:ILE:N	2.62	0.72
2:A:239:ARG:HG3	29:X:2569:A:H5''	1.72	0.72
28:3:52:LYS:O	28:3:54:GLU:N	2.23	0.72
29:X:1164:C:H2'	29:X:1165:G:H8	1.53	0.72
12:K:87:TYR:CD1	12:K:90:ARG:HD2	2.25	0.72
24:W:5:LEU:HB2	24:W:25:LEU:HD13	1.71	0.72
29:X:46:C:H2'	29:X:47:G:H8	1.52	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2336:G:N2	29:X:2339:A:OP2	2.22	0.72
2:A:39:LYS:NZ	2:A:58:HIS:H	1.88	0.71
9:H:47:VAL:HG23	9:H:77:THR:HG23	1.72	0.71
10:I:63:ARG:NH1	29:X:2396:C:OP1	2.22	0.71
20:S:54:ILE:HB	20:S:62:PHE:HB2	1.70	0.71
29:X:1437:A:H2'	29:X:1438:G:C8	2.25	0.71
29:X:2522:G:H2'	29:X:2523:G:H8	1.54	0.71
15:N:26:GLY:O	15:N:28:ARG:N	2.23	0.71
20:S:148:THR:HB	20:S:165:GLU:HA	1.71	0.71
12:K:3:HIS:O	12:K:5:LYS:N	2.21	0.71
15:N:111:ASP:O	15:N:115:ASN:ND2	2.22	0.71
19:R:77:HIS:HD2	29:X:339:U:H4'	1.55	0.71
29:X:1333:G:C2	29:X:1342:U:H5''	2.26	0.71
29:X:2761:A:H5''	29:X:2762:G:H5'	1.72	0.71
19:R:22:VAL:HG11	19:R:81:VAL:HG22	1.70	0.71
7:F:75:SER:O	7:F:79:ARG:NH1	2.23	0.71
12:K:10:LEU:O	12:K:12:ARG:N	2.24	0.71
29:X:789:G:N1	29:X:2055:G:OP1	2.17	0.71
30:Y:25:G:H1	30:Y:62:C:H42	1.37	0.71
22:U:31:GLY:HA2	22:U:32:ARG:HH11	1.56	0.70
29:X:1030:U:H3	29:X:1153:A:N6	1.89	0.70
29:X:1505:U:H1'	29:X:1506:C:H2'	1.73	0.70
29:X:2665:G:C2	29:X:2704:U:O2	2.44	0.70
4:C:148:VAL:HG13	4:C:185:ARG:HB3	1.73	0.70
29:X:542:A:OP1	29:X:570:G:N2	2.24	0.70
29:X:1212:U:H2'	29:X:1213:U:C6	2.26	0.70
29:X:1997:A:H2'	29:X:1998:A:C8	2.26	0.70
28:3:13:ARG:NH2	29:X:227:G:OP2	2.24	0.70
29:X:713:G:H22	29:X:745:C:H5	1.38	0.70
29:X:870:C:N4	29:X:871:U:O4	2.25	0.70
29:X:2013:A:H4'	29:X:2014:A:C8	2.26	0.70
15:N:37:GLN:HG3	29:X:1265:G:H1	1.55	0.70
24:W:35:SER:O	24:W:37:THR:N	2.22	0.70
29:X:2418:A:H4'	29:X:2419:C:H5''	1.74	0.70
3:B:176:ARG:HH21	14:M:16:ILE:HA	1.54	0.70
12:K:90:ARG:NH1	29:X:2855:C:O2'	2.25	0.70
25:Z:33:CYS:O	25:Z:35:GLN:N	2.23	0.70
29:X:1662:G:H5''	29:X:1663:C:H5'	1.71	0.70
29:X:1939:U:H1'	29:X:2531:U:OP1	1.90	0.70
20:S:74:ARG:HH22	30:Y:94:G:H5''	1.54	0.70
29:X:992:A:N1	29:X:2010:G:O2'	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1053:G:H1	29:X:1124:U:H3	1.38	0.70
29:X:2387:U:H2'	29:X:2388:G:C8	2.27	0.70
8:G:169:GLN:HG2	8:G:170:PRO:HD2	1.73	0.70
13:L:44:ASP:O	13:L:46:SER:N	2.24	0.70
19:R:100:ASP:HB3	19:R:101:GLY:HA3	1.74	0.70
29:X:2123:G:N2	29:X:2134:U:O2	2.25	0.70
5:D:39:GLY:HA2	5:D:86:GLY:HA2	1.74	0.69
29:X:1267:A:H5''	29:X:1268:U:H5''	1.72	0.69
29:X:2378:G:H1	29:X:2396:C:H42	1.40	0.69
3:B:110:GLY:HA2	3:B:161:GLY:HA3	1.74	0.69
30:Y:64:C:H2'	30:Y:65:A:C8	2.27	0.69
1:O:42:ARG:HH22	1:O:209:TYR:HB2	1.56	0.69
29:X:172:A:H5''	29:X:173:A:OP2	1.92	0.69
29:X:1937:G:O2'	29:X:1939:U:O4	2.10	0.69
2:A:274:ARG:NH2	29:X:1788:C:OP2	2.24	0.69
4:C:111:ARG:HH11	4:C:181:LEU:HA	1.56	0.69
5:D:50:ILE:HG22	5:D:87:ILE:HD11	1.74	0.69
14:M:104:LEU:HA	14:M:106:TYR:CE2	2.27	0.69
29:X:2187:A:H2	29:X:2198:U:H3	1.38	0.69
29:X:2775:U:O2'	29:X:2778:U:OP2	2.08	0.69
2:A:198:ASN:O	2:A:200:GLU:N	2.26	0.69
10:I:86:THR:OG1	10:I:116:ARG:NH1	2.26	0.69
29:X:57:G:N2	29:X:68:C:O2	2.24	0.69
29:X:2845:C:N4	29:X:2846:G:O6	2.25	0.69
30:Y:27:A:OP2	30:Y:27:A:H8	1.75	0.69
6:E:143:GLN:HG3	29:X:2725:C:H1'	1.74	0.69
10:I:60:LEU:O	28:3:13:ARG:NH1	2.26	0.69
11:J:22:ALA:HB2	11:J:99:LYS:HB2	1.74	0.69
11:J:65:ILE:HA	11:J:107:VAL:HG12	1.74	0.69
11:J:15:ARG:HG2	11:J:74:PRO:HD2	1.75	0.69
22:U:31:GLY:HA2	22:U:32:ARG:NH1	2.08	0.69
23:V:2:LYS:NZ	29:X:76:C:OP1	2.17	0.69
29:X:711:C:O2'	29:X:747:A:N6	2.25	0.69
12:K:3:HIS:N	29:X:2795:A:H4'	2.08	0.69
21:T:34:GLY:HA3	29:X:2332:G:H1'	1.75	0.69
29:X:877:G:H1	29:X:924:C:H42	1.39	0.69
10:I:75:VAL:HG22	10:I:99:VAL:HG11	1.75	0.68
29:X:1185:C:H2'	29:X:1186:G:H2'	1.74	0.68
2:A:243:GLY:HA3	29:X:2576:G:H5'	1.74	0.68
4:C:72:ARG:HE	4:C:77:PHE:HE2	1.41	0.68
12:K:29:LEU:HD13	12:K:79:VAL:HB	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:33:ARG:HE	13:L:38:ILE:HG21	1.57	0.68
17:P:50:VAL:HB	17:P:91:PHE:HA	1.75	0.68
29:X:796:A:H4'	29:X:2567:G:H4'	1.75	0.68
30:Y:5:C:N3	30:Y:120:G:N2	2.37	0.68
17:P:85:MET:HE2	17:P:130:GLU:HG3	1.73	0.68
8:G:109:GLY:O	8:G:111:LYS:N	2.26	0.68
9:H:23:ARG:HG3	9:H:24:VAL:H	1.57	0.68
9:H:69:VAL:HG12	9:H:70:VAL:H	1.58	0.68
15:N:54:LYS:NZ	29:X:1006:C:OP2	2.27	0.68
29:X:1043:A:H2	29:X:1133:G:H22	1.39	0.68
1:O:208:ALA:HB3	1:O:220:LEU:HB2	1.75	0.68
29:X:511:A:O2'	29:X:512:A:OP1	2.09	0.68
29:X:1255:A:H2'	29:X:1256:C:H6	1.59	0.68
29:X:2032:G:N2	29:X:2598:C:O2	2.24	0.68
9:H:134:LEU:HA	14:M:48:GLN:HE22	1.59	0.68
26:1:15:SER:OG	26:1:48:VAL:O	2.12	0.68
2:A:161:THR:H	2:A:196:VAL:HB	1.59	0.68
3:B:132:LYS:NZ	29:X:2590:U:OP1	2.27	0.68
4:C:47:THR:H	4:C:50:GLN:HG3	1.58	0.68
28:3:29:LYS:HZ3	28:3:41:ILE:HG23	1.59	0.68
29:X:33:C:N4	29:X:458:G:O2'	2.27	0.68
29:X:1116:U:H2'	29:X:1117:G:C8	2.29	0.68
15:N:92:ARG:NH2	29:X:1009:C:OP2	2.26	0.67
29:X:796:A:OP1	29:X:1778:U:O2'	2.12	0.67
29:X:1556:A:H2'	29:X:1557:G:H8	1.58	0.67
29:X:1850:G:O4'	29:X:1867:A:N6	2.26	0.67
29:X:2690:A:OP1	29:X:2692:A:P	2.52	0.67
29:X:79:G:H2'	29:X:80:A:C8	2.28	0.67
29:X:654:A:O2'	29:X:655:A:OP1	2.12	0.67
29:X:2485:U:O2	32:X:6178:HGR:H23	1.93	0.67
8:G:142:ARG:NH2	29:X:539:A:OP2	2.24	0.67
14:M:102:ALA:O	14:M:103:LYS:NZ	2.26	0.67
29:X:198:A:N1	29:X:242:A:O2'	2.26	0.67
29:X:677:G:O2'	29:X:952:A:OP2	2.12	0.67
29:X:580:A:H4'	29:X:581:A:OP1	1.95	0.67
29:X:2440:C:H2'	29:X:2441:U:H6	1.58	0.67
2:A:173:VAL:HG23	2:A:187:SER:HB3	1.76	0.67
4:C:62:LYS:NZ	29:X:2043:A:H3'	2.10	0.67
29:X:2043:A:H1'	29:X:2481:G:C1'	2.24	0.67
4:C:129:LYS:HB3	4:C:132:ASN:ND2	2.10	0.67
29:X:1401:G:H1	29:X:1412:C:H42	1.40	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1407:G:O6	29:X:1408:A:N6	2.28	0.67
29:X:2225:G:H2'	29:X:2226:A:H8	1.58	0.67
29:X:219:G:N2	29:X:231:G:H2'	2.10	0.67
29:X:1507:A:H2'	29:X:1508:G:C8	2.30	0.67
29:X:2816:C:C2	29:X:2852:G:N2	2.63	0.67
4:C:62:LYS:HZ1	29:X:2043:A:H3'	1.60	0.67
4:C:112:GLN:HA	4:C:117:LEU:HG	1.76	0.67
1:O:104:MET:SD	1:O:130:ARG:NH1	2.68	0.67
20:S:1:MET:HG3	20:S:52:PHE:HD2	1.60	0.67
16:O:35:LEU:HD23	16:O:36:LYS:H	1.60	0.67
29:X:168:A:H2'	29:X:169:C:C6	2.30	0.67
2:A:55:GLY:HA3	2:A:218:LYS:HG3	1.77	0.66
4:C:4:ILE:HG22	4:C:13:ARG:HH12	1.60	0.66
9:H:25:LEU:HD22	9:H:52:VAL:HG23	1.77	0.66
28:3:58:MET:HA	28:3:61:MET:HG3	1.76	0.66
29:X:1686:A:OP2	31:X:6021:MG:MG	1.38	0.66
29:X:546:A:H2'	29:X:547:U:C6	2.28	0.66
29:X:1301:U:O2'	29:X:1664:G:N2	2.29	0.66
29:X:1679:U:O2	29:X:2666:U:H5''	1.94	0.66
20:S:3:LEU:HG	20:S:32:PHE:CD1	2.30	0.66
29:X:403:A:H4'	29:X:404:A:H5'	1.76	0.66
29:X:1195:U:H2'	29:X:1196:G:C8	2.30	0.66
29:X:2873:G:H2'	29:X:2874:A:C8	2.29	0.66
10:I:68:VAL:HG13	10:I:69:GLY:H	1.60	0.66
12:K:31:GLU:O	12:K:33:ARG:N	2.25	0.66
15:N:24:PHE:HB2	15:N:29:SER:HB3	1.76	0.66
21:T:46:LYS:HE2	21:T:77:ARG:H	1.60	0.66
27:2:8:ASN:HB3	27:2:11:LYS:HB3	1.77	0.66
29:X:474:G:N2	29:X:477:A:OP2	2.28	0.66
29:X:1454:U:H2'	29:X:1455:C:H6	1.61	0.66
29:X:2241:U:H2'	29:X:2242:C:H6	1.61	0.66
29:X:2791:C:C2	29:X:2806:G:N2	2.63	0.66
30:Y:64:C:H2'	30:Y:65:A:H8	1.60	0.66
2:A:274:ARG:HH22	29:X:1788:C:P	2.18	0.66
29:X:2826:C:H2'	29:X:2827:G:O4'	1.95	0.66
11:J:68:ARG:O	11:J:102:ARG:NH2	2.29	0.66
29:X:1030:U:H3	29:X:1153:A:H62	1.44	0.66
1:O:127:LEU:HD23	1:O:130:ARG:HG3	1.76	0.66
7:F:96:VAL:HB	7:F:136:VAL:HG12	1.75	0.66
9:H:40:GLY:HA3	29:X:2545:A:H61	1.61	0.66
24:W:39:ALA:O	29:X:864:C:O2'	2.14	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1697:U:O2'	29:X:1754:G:N7	2.25	0.66
29:X:2226:A:H2'	29:X:2227:C:H6	1.61	0.66
3:B:119:ARG:HG2	3:B:120:TRP:CD1	2.31	0.66
16:O:22:VAL:HG12	16:O:23:GLU:H	1.60	0.66
29:X:1223:G:H4'	29:X:1224:A:H5''	1.78	0.66
29:X:1624:A:H1'	29:X:1626:A:OP2	1.96	0.66
26:1:14:SER:HB2	26:1:47:VAL:HG11	1.77	0.66
29:X:639:G:HO2'	29:X:661:C:HO2'	1.43	0.66
29:X:1454:U:H2'	29:X:1455:C:C6	2.30	0.66
29:X:2450:A:N6	29:X:2455:A:O2'	2.29	0.66
29:X:2690:A:P	29:X:2692:A:OP2	2.54	0.66
12:K:46:PRO:O	12:K:50:GLN:HG3	1.96	0.65
15:N:13:ARG:NH1	29:X:1264:C:H5''	2.11	0.65
1:O:212:THR:O	29:X:2106:G:N2	2.28	0.65
4:C:9:GLN:O	4:C:10:ASN:ND2	2.16	0.65
7:F:12:LEU:HD22	7:F:18:THR:HG21	1.78	0.65
26:1:7:ARG:NH2	29:X:2265:A:OP2	2.28	0.65
29:X:1753:A:H8	29:X:1753:A:O5'	1.78	0.65
29:X:1856:U:OP1	29:X:2389:G:O2'	2.12	0.65
10:I:90:ARG:HB2	10:I:93:LEU:HB2	1.76	0.65
15:N:66:ASN:HA	15:N:76:TYR:HB2	1.77	0.65
29:X:335:A:N6	29:X:349:G:O2'	2.28	0.65
29:X:573:C:H2'	29:X:574:C:H6	1.59	0.65
29:X:1482:U:O4'	29:X:1562:G:N2	2.30	0.65
5:D:37:ASN:OD1	29:X:2291:U:O2'	2.13	0.65
6:E:28:GLY:HA3	6:E:79:VAL:HB	1.78	0.65
14:M:40:ARG:HB3	14:M:40:ARG:HH11	1.59	0.65
17:P:90:LEU:HD11	17:P:128:VAL:HB	1.76	0.65
7:F:112:MET:HG3	7:F:113:PRO:HD3	1.77	0.65
12:K:20:LEU:O	12:K:22:ARG:N	2.29	0.65
29:X:1467:U:O2	29:X:1468:A:N6	2.30	0.65
29:X:421:G:H1	29:X:432:C:H42	1.44	0.65
29:X:1005:U:O2'	29:X:1007:A:OP1	2.10	0.65
29:X:1359:G:O6	29:X:1616:C:N4	2.27	0.65
5:D:36:VAL:HB	5:D:89:VAL:HG23	1.79	0.65
12:K:108:VAL:HG12	12:K:109:THR:O	1.96	0.65
2:A:238:GLY:O	2:A:240:THR:OG1	2.13	0.65
6:E:45:GLN:NE2	6:E:47:GLY:O	2.30	0.65
26:1:29:ARG:O	26:1:30:ASN:ND2	2.30	0.65
29:X:2191:A:H5''	29:X:2192:U:H5	1.61	0.65
1:O:152:LEU:HD23	1:O:157:ILE:HD12	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:206:LEU:HB2	29:X:1782:A:O3'	1.97	0.65
12:K:11:ASN:HD22	12:K:11:ASN:N	1.92	0.65
29:X:1255:A:H2'	29:X:1256:C:C6	2.32	0.65
4:C:164:VAL:HB	4:C:167:VAL:HG22	1.79	0.65
11:J:81:GLU:HB3	21:T:4:LYS:HE2	1.80	0.65
12:K:87:TYR:HD1	12:K:90:ARG:HD2	1.62	0.65
29:X:510:G:H22	29:X:513:A:H5'	1.61	0.65
29:X:1140:A:O2'	29:X:2494:C:O2	2.14	0.65
2:A:225:ALA:HB1	29:X:795:A:O2'	1.98	0.64
7:F:115:LEU:O	7:F:117:ALA:N	2.24	0.64
29:X:2410:U:O2	29:X:2412:A:H8	1.79	0.64
11:J:23:LYS:O	20:S:73:LYS:NZ	2.29	0.64
13:L:16:LYS:NZ	13:L:90:ASP:OD1	2.29	0.64
18:Q:66:GLY:O	18:Q:68:PHE:N	2.29	0.64
19:R:58:VAL:HA	29:X:494:A:H5'	1.79	0.64
2:A:223:GLY:HA2	2:A:226:MET:HG3	1.77	0.64
29:X:876:A:H2'	29:X:877:G:C8	2.33	0.64
8:G:124:GLU:HB3	8:G:150:VAL:HB	1.80	0.64
11:J:52:ARG:HG3	11:J:67:ILE:HD11	1.79	0.64
12:K:73:LYS:H	12:K:73:LYS:CE	2.10	0.64
13:L:33:ARG:HG2	13:L:99:ARG:HG3	1.79	0.64
29:X:104:C:H2'	29:X:105:G:H8	1.62	0.64
23:V:2:LYS:HE2	23:V:52:GLN:NE2	2.12	0.64
29:X:746:G:N7	29:X:774:A:C6	2.66	0.64
29:X:1981:A:HO2'	29:X:2704:U:HO2'	1.40	0.64
30:Y:16:U:H1'	30:Y:109:G:H21	1.62	0.64
29:X:2691:C:O2'	29:X:2692:A:O5'	2.13	0.64
29:X:7:G:H2'	29:X:8:A:C8	2.33	0.64
29:X:10:A:H2'	29:X:11:G:H8	1.63	0.64
29:X:531:G:H2'	29:X:532:A:H8	1.61	0.64
29:X:540:G:N2	29:X:2006:G:OP1	2.27	0.64
29:X:1838:G:H2'	29:X:1839:A:C8	2.33	0.64
29:X:2099:G:OP2	29:X:2149:G:O2'	2.14	0.64
18:Q:29:VAL:HG12	18:Q:30:SER:H	1.63	0.64
29:X:794:A:H2	29:X:1767:G:N3	1.96	0.64
29:X:2299:A:N6	29:X:2312:A:O2'	2.30	0.64
22:U:28:GLY:O	22:U:30:VAL:N	2.30	0.64
26:1:38:LYS:HG2	26:1:48:VAL:HG22	1.80	0.64
29:X:14:A:C6	29:X:536:A:C2	2.86	0.64
29:X:2775:U:H4'	29:X:2777:A:H3'	1.79	0.64
3:B:51:TYR:N	3:B:75:THR:HG21	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:149:ARG:O	29:X:2035:G:H1'	1.98	0.64
6:E:137:ASP:OD1	6:E:138:LYS:N	2.30	0.64
13:L:90:ASP:OD2	13:L:91:ARG:N	2.31	0.64
15:N:6:THR:HG21	15:N:10:ARG:HB2	1.80	0.64
29:X:88:G:H5''	29:X:89:A:H5''	1.79	0.64
29:X:1237:G:O2'	29:X:1238:A:H5'	1.97	0.64
29:X:1279:G:O2'	29:X:1995:G:O6	2.06	0.64
29:X:2617:G:O2'	29:X:2755:A:N1	2.31	0.64
29:X:1090:C:N4	29:X:1099:A:OP1	2.28	0.63
29:X:1116:U:H2'	29:X:1117:G:H8	1.60	0.63
29:X:1366:A:H2'	29:X:1367:A:C8	2.32	0.63
1:O:10:VAL:HG21	1:O:216:PRO:HG2	1.80	0.63
10:I:18:ARG:NH2	29:X:1263:G:N7	2.47	0.63
11:J:82:THR:HG23	21:T:4:LYS:HG3	1.81	0.63
29:X:2040:A:H2'	29:X:2041:A:C8	2.33	0.63
29:X:104:C:H2'	29:X:105:G:C8	2.33	0.63
2:A:134:ARG:HB3	2:A:187:SER:HB2	1.79	0.63
4:C:173:ALA:O	4:C:175:VAL:N	2.32	0.63
29:X:1393:G:O2'	29:X:1585:A:N6	2.31	0.63
29:X:2278:A:H61	29:X:2296:U:H3	1.45	0.63
10:I:90:ARG:O	10:I:121:HIS:ND1	2.32	0.63
27:2:5:TYR:HE1	29:X:699:G:C8	2.17	0.63
29:X:942:U:H2'	29:X:943:U:H6	1.63	0.63
29:X:1329:U:H2'	29:X:1330:G:H8	1.63	0.63
29:X:1429:A:C6	29:X:1600:U:H4'	2.34	0.63
4:C:126:ALA:HB3	4:C:132:ASN:ND2	2.14	0.63
28:3:22:VAL:HG13	28:3:55:TRP:CD1	2.33	0.63
29:X:5:A:H2'	29:X:6:A:C8	2.33	0.63
29:X:2043:A:H1'	29:X:2481:G:O4'	1.97	0.63
29:X:2736:U:H4'	29:X:2737:A:OP1	1.99	0.63
10:I:16:ARG:HH22	29:X:598:U:P	2.22	0.63
12:K:11:ASN:H	12:K:11:ASN:ND2	1.95	0.63
20:S:68:ALA:HB3	20:S:82:ASP:HB2	1.80	0.63
5:D:34:ILE:HG22	5:D:91:LEU:HB2	1.79	0.63
15:N:50:ARG:HA	15:N:53:LYS:HE2	1.81	0.63
21:T:56:ASP:HB2	21:T:58:THR:OG1	1.99	0.63
29:X:89:A:H4'	29:X:90:G:O5'	1.97	0.63
29:X:1507:A:H2'	29:X:1508:G:H8	1.62	0.63
2:A:71:ASP:HB3	2:A:103:ARG:HH12	1.64	0.62
9:H:76:ARG:O	9:H:94:ASN:HA	1.98	0.62
17:P:93:LYS:HD3	17:P:94:GLU:HG3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:23:ILE:HA	19:R:32:GLN:O	1.98	0.62
29:X:1705:U:O4'	29:X:1718:A:N6	2.32	0.62
7:F:90:THR:HB	29:X:1087:C:H1'	1.80	0.62
3:B:102:ILE:N	3:B:170:LEU:O	2.31	0.62
13:L:37:HIS:HE1	13:L:39:TYR:CD1	2.18	0.62
29:X:652:C:N4	29:X:657:A:H61	1.95	0.62
29:X:858:G:O2'	29:X:859:U:OP2	2.17	0.62
29:X:2191:A:OP1	29:X:2193:C:N4	2.32	0.62
29:X:2674:C:H2'	29:X:2675:U:C6	2.33	0.62
2:A:123:ALA:HB1	2:A:129:ASN:HD22	1.64	0.62
6:E:17:VAL:HG22	6:E:26:VAL:HG13	1.81	0.62
15:N:3:ARG:HB3	29:X:1261:G:C5	2.34	0.62
29:X:2102:A:O4'	29:X:2155:U:O2'	2.17	0.62
29:X:2240:C:O2	29:X:2258:G:N2	2.19	0.62
29:X:2369:U:H3'	29:X:2369:U:H6	1.64	0.62
10:I:94:GLU:N	10:I:97:ARG:HH11	1.97	0.62
28:3:25:PHE:HA	28:3:47:GLY:HA2	1.80	0.62
29:X:160:C:O2'	29:X:445:A:N3	2.31	0.62
29:X:1703:C:H2'	29:X:1704:G:O4'	1.99	0.62
3:B:27:LEU:HD23	3:B:29:GLY:H	1.64	0.62
26:1:46:HIS:HD2	29:X:2350:G:O2'	1.83	0.62
29:X:334:G:OP1	29:X:349:G:N2	2.32	0.62
29:X:2640:G:H2'	29:X:2641:A:C8	2.35	0.62
7:F:62:ASP:OD1	7:F:63:ARG:NH1	2.32	0.62
22:U:23:LYS:HD2	22:U:35:THR:HG21	1.81	0.62
29:X:421:G:H2'	29:X:422:C:C6	2.34	0.62
29:X:1454:U:H3	29:X:1567:A:H61	1.47	0.62
29:X:1654:A:H4'	29:X:2690:A:O2'	2.00	0.62
3:B:132:LYS:O	3:B:134:TRP:N	2.33	0.62
9:H:124:MET:O	9:H:127:VAL:HG12	1.99	0.62
14:M:104:LEU:HA	14:M:106:TYR:HE2	1.64	0.62
25:Z:14:SER:O	25:Z:18:MET:HG3	2.00	0.62
29:X:427:C:H2'	29:X:428:A:C8	2.34	0.62
29:X:494:A:H3'	29:X:495:C:H6	1.65	0.62
29:X:2285:U:H5'	29:X:2286:G:C8	2.35	0.62
19:R:84:VAL:HG22	19:R:89:GLY:HA2	1.80	0.62
28:3:17:THR:OG1	28:3:18:GLY:N	2.33	0.62
29:X:1642:G:H5''	29:X:1643:A:OP1	2.00	0.62
29:X:2033:C:N4	29:X:2034:A:N1	2.48	0.62
30:Y:68:A:N6	30:Y:111:C:OP2	2.33	0.62
13:L:27:LEU:HD13	13:L:84:ILE:HG23	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:170:U:N3	29:X:180:C:O2	2.32	0.61
29:X:1192:A:H2'	29:X:1193:G:H8	1.63	0.61
2:A:63:ARG:HH21	2:A:86:PRO:HD3	1.65	0.61
4:C:149:LEU:HD21	4:C:170:LEU:HD12	1.82	0.61
29:X:555:U:C2	29:X:1243:G:C2	2.88	0.61
29:X:753:U:H2'	29:X:754:G:C8	2.34	0.61
29:X:1790:G:N2	29:X:1811:A:OP2	2.31	0.61
29:X:2186:G:H2'	29:X:2187:A:C8	2.36	0.61
9:H:2:ILE:N	9:H:45:ALA:O	2.27	0.61
29:X:1030:U:O2	29:X:1155:G:N2	2.33	0.61
29:X:1066:G:H1	29:X:1115:C:H42	1.48	0.61
11:J:43:ILE:O	11:J:95:VAL:HA	2.00	0.61
19:R:51:VAL:HG13	19:R:73:GLU:HB3	1.81	0.61
19:R:93:ARG:NH2	29:X:311:A:O5'	2.33	0.61
29:X:510:G:N2	29:X:513:A:H5'	2.16	0.61
9:H:51:ILE:HD11	9:H:53:ALA:HB2	1.81	0.61
29:X:98:U:O2	29:X:100:G:N1	2.33	0.61
29:X:759:C:OP1	29:X:761:G:H4'	2.01	0.61
29:X:1511:A:N1	29:X:1512:A:N6	2.48	0.61
4:C:67:ALA:HA	29:X:1268:U:C5	2.35	0.61
9:H:41:ASN:HB2	29:X:2654:A:H5'	1.83	0.61
17:P:94:GLU:HB2	17:P:127:ILE:HB	1.83	0.61
29:X:1608:U:H2'	29:X:1609:G:C8	2.36	0.61
3:B:12:THR:OG1	14:M:17:GLU:OE1	2.18	0.61
17:P:111:ARG:HG2	29:X:764:A:O4'	2.01	0.61
29:X:220:U:H2'	29:X:221:A:H8	1.65	0.61
2:A:142:VAL:HG23	2:A:193:ILE:HA	1.82	0.61
3:B:55:ALA:H	3:B:58:LYS:NZ	1.97	0.61
8:G:67:ARG:O	8:G:70:PHE:HB2	2.01	0.61
16:O:55:THR:OG1	16:O:56:VAL:N	2.33	0.61
17:P:98:ASP:OD1	29:X:23:G:N2	2.29	0.61
18:Q:2:SER:OG	18:Q:3:HIS:N	2.32	0.61
29:X:1770:U:H6	29:X:1775:A:H62	1.49	0.61
19:R:25:LEU:HD11	19:R:82:ALA:HB2	1.83	0.61
29:X:511:A:HO2'	29:X:512:A:P	2.24	0.61
16:O:40:VAL:HG12	16:O:42:GLY:H	1.66	0.61
19:R:68:GLY:N	29:X:494:A:O2'	2.33	0.61
29:X:90:G:H5''	29:X:91:A:OP2	2.01	0.61
29:X:926:C:H42	30:Y:104:A:H5'	1.66	0.61
29:X:2672:U:H2'	29:X:2673:G:C8	2.35	0.61
13:L:104:ALA:O	13:L:108:ARG:N	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:18:LEU:HA	15:N:21:ALA:HB3	1.83	0.60
22:U:20:ARG:NE	29:X:393:U:OP1	2.34	0.60
24:W:43:MET:HE2	29:X:864:C:H1'	1.83	0.60
29:X:653:G:H21	29:X:656:U:H3	1.49	0.60
29:X:761:G:C8	29:X:763:A:C8	2.89	0.60
29:X:836:G:H2'	29:X:837:U:C6	2.36	0.60
29:X:2201:G:H2'	29:X:2202:G:H8	1.66	0.60
2:A:210:GLY:HA2	29:X:777:A:H5'	1.82	0.60
3:B:26:VAL:HG12	3:B:182:ILE:HB	1.82	0.60
9:H:16:ALA:CB	9:H:98:ILE:HD11	2.31	0.60
29:X:174:A:N6	29:X:2409:A:O2'	2.33	0.60
29:X:588:G:O2'	29:X:2002:A:OP1	2.14	0.60
29:X:761:G:C8	29:X:763:A:N7	2.69	0.60
29:X:1863:U:H2'	29:X:1864:G:C8	2.34	0.60
1:O:123:LEU:HB3	1:O:127:LEU:HB2	1.84	0.60
3:B:189:PRO:HA	29:X:2659:C:C5'	2.31	0.60
4:C:40:ARG:NH2	29:X:39:C:O2	2.32	0.60
4:C:133:PHE:HB2	4:C:160:ALA:HB1	1.82	0.60
12:K:46:PRO:HB3	29:X:2814:G:H5'	1.82	0.60
29:X:1690:U:O2'	29:X:1691:G:OP1	2.18	0.60
9:H:8:LEU:HD23	9:H:8:LEU:H	1.64	0.60
12:K:106:ASP:N	29:X:1300:A:N7	2.49	0.60
19:R:83:LEU:O	19:R:92:THR:OG1	2.20	0.60
20:S:127:PRO:HA	20:S:130:ILE:HD11	1.82	0.60
22:U:51:ILE:HG23	22:U:59:THR:HA	1.83	0.60
29:X:531:G:H2'	29:X:532:A:C8	2.35	0.60
29:X:957:G:H2'	29:X:958:G:H8	1.66	0.60
29:X:2208:U:H2'	29:X:2209:G:H8	1.66	0.60
29:X:2038:C:H2'	29:X:2483:U:H4'	1.82	0.60
29:X:2246:A:H61	29:X:2251:U:H3	1.48	0.60
30:Y:6:C:H2'	30:Y:7:C:C6	2.36	0.60
5:D:72:LYS:HG3	5:D:81:GLN:HG3	1.83	0.60
11:J:36:ILE:HG12	11:J:103:VAL:HG13	1.83	0.60
12:K:11:ASN:OD1	29:X:1669:A:N6	2.35	0.60
20:S:167:THR:OG1	29:X:888:G:H4'	2.01	0.60
29:X:490:A:N3	29:X:492:G:H5''	2.17	0.60
29:X:505:G:H8	29:X:505:G:O5'	1.84	0.60
29:X:1982:C:OP1	29:X:2703:C:O2'	2.19	0.60
29:X:2639:A:H3'	29:X:2640:G:C8	2.37	0.60
29:X:330:C:H2'	29:X:331:U:H6	1.67	0.60
29:X:691:C:H2'	29:X:692:C:H6	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Y:17:A:OP1	30:Y:110:U:O2'	2.13	0.60
5:D:34:ILE:HG13	5:D:156:ILE:HG23	1.83	0.60
9:H:40:GLY:CA	29:X:2545:A:H61	2.14	0.60
13:L:19:THR:O	13:L:21:THR:N	2.34	0.60
17:P:24:GLY:O	17:P:127:ILE:HA	2.01	0.60
4:C:142:LEU:HB3	4:C:166:TRP:HH2	1.66	0.60
5:D:35:VAL:HG11	29:X:2293:G:H5'	1.83	0.60
6:E:137:ASP:OD1	6:E:139:GLN:N	2.35	0.60
29:X:2579:A:H2'	29:X:2580:C:C6	2.37	0.60
9:H:38:GLY:O	29:X:2627:G:H1'	2.01	0.60
17:P:63:SER:HB2	29:X:1993:G:H5''	1.83	0.60
20:S:91:PRO:HG3	20:S:126:GLY:H	1.66	0.60
20:S:154:LEU:HD22	20:S:158:CYS:HB2	1.83	0.60
26:1:22:TYR:OH	29:X:2326:C:O2'	2.20	0.60
29:X:633:G:C2	29:X:634:G:C8	2.90	0.60
29:X:1479:G:H2'	29:X:1480:G:H8	1.66	0.60
29:X:1681:A:N3	29:X:2706:U:C2	2.69	0.60
29:X:1992:G:O2'	29:X:1993:G:H5'	2.02	0.60
29:X:2277:A:C2	29:X:2278:A:H1'	2.36	0.60
6:E:83:TYR:CE1	6:E:138:LYS:HB2	2.37	0.59
11:J:84:MET:HE1	29:X:970:A:H62	1.67	0.59
13:L:87:VAL:HG21	13:L:108:ARG:HH12	1.67	0.59
22:U:51:ILE:O	22:U:52:ARG:NH2	2.33	0.59
29:X:70:A:H4'	29:X:71:A:H5''	1.84	0.59
29:X:389:G:H1	29:X:411:C:H42	1.50	0.59
29:X:825:C:H2'	29:X:826:U:H6	1.67	0.59
29:X:1556:A:H2'	29:X:1557:G:C8	2.35	0.59
2:A:208:LYS:HB2	29:X:742:G:C5	2.37	0.59
20:S:105:GLN:O	20:S:109:GLN:NE2	2.35	0.59
25:Z:19:ARG:HA	29:X:2029:G:H5'	1.84	0.59
28:3:33:ASN:O	28:3:35:GLY:N	2.35	0.59
6:E:17:VAL:HG13	6:E:26:VAL:HG22	1.82	0.59
11:J:39:GLU:HB2	11:J:128:ILE:HG22	1.83	0.59
29:X:1701:C:C2	29:X:1722:G:N2	2.69	0.59
5:D:113:ASP:HB3	5:D:115:ARG:HH12	1.65	0.59
7:F:89:SER:HA	29:X:1075:C:H4'	1.84	0.59
12:K:20:LEU:O	12:K:23:ALA:N	2.36	0.59
21:T:23:VAL:HB	21:T:38:VAL:HG22	1.83	0.59
29:X:451:A:H2'	29:X:452:G:C8	2.37	0.59
29:X:663:G:H2'	29:X:664:C:H4'	1.84	0.59
29:X:1117:G:H2'	29:X:1118:G:H8	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2013:A:H4'	29:X:2014:A:H8	1.66	0.59
2:A:33:LEU:HD13	2:A:104:TYR:HD2	1.66	0.59
2:A:273:ARG:HB2	2:A:275:LYS:HE2	1.85	0.59
7:F:54:PRO:HG2	7:F:70:LYS:HB2	1.83	0.59
11:J:72:ASP:OD2	11:J:72:ASP:N	2.35	0.59
12:K:37:THR:HB	12:K:40:LYS:HG3	1.85	0.59
19:R:77:HIS:O	19:R:79:SER:N	2.35	0.59
29:X:388:G:OP1	29:X:406:G:OP1	2.20	0.59
29:X:1504:G:N2	29:X:1517:C:O2	2.35	0.59
1:O:113:PRO:HG3	1:O:142:GLY:HA2	1.84	0.59
4:C:131:LYS:HA	4:C:134:ILE:HD12	1.85	0.59
9:H:75:VAL:HG22	9:H:96:ALA:HA	1.84	0.59
11:J:47:GLN:OE1	11:J:127:PRO:HD3	2.01	0.59
14:M:16:ILE:O	14:M:18:GLN:N	2.32	0.59
14:M:82:PRO:C	14:M:84:ALA:H	2.09	0.59
29:X:118:U:H4'	29:X:119:G:H5''	1.83	0.59
29:X:129:A:H61	29:X:142:U:H3	1.50	0.59
29:X:1909:U:H5''	29:X:1911:A:OP2	2.02	0.59
29:X:2791:C:O2	29:X:2858:A:O2'	2.19	0.59
2:A:70:ARG:NH1	2:A:146:GLU:OE2	2.35	0.59
3:B:9:ILE:HD11	3:B:27:LEU:HB2	1.83	0.59
5:D:37:ASN:ND2	29:X:2291:U:O2	2.35	0.59
19:R:19:GLY:H	19:R:36:VAL:HB	1.68	0.59
29:X:575:U:O2'	29:X:822:G:OP2	2.20	0.59
29:X:1053:G:N2	29:X:1124:U:O2	2.29	0.59
29:X:1322:G:HO2'	29:X:1627:C:HO2'	1.51	0.59
29:X:2821:G:H2'	29:X:2822:U:H6	1.64	0.59
1:O:174:ALA:HA	1:O:181:LEU:HD21	1.83	0.59
2:A:263:ARG:NH1	29:X:2206:C:OP1	2.35	0.59
29:X:627:A:H2'	29:X:628:A:C8	2.38	0.59
29:X:2180:U:H2'	29:X:2203:G:H1	1.67	0.59
15:N:33:ARG:HB3	29:X:1265:G:C2	2.38	0.59
29:X:712:A:H2'	29:X:713:G:O4'	2.03	0.59
29:X:1827:G:H1'	29:X:1914:U:C2	2.38	0.59
29:X:2088:U:H3	29:X:2167:A:H61	1.50	0.59
29:X:2559:U:H5''	29:X:2560:G:OP2	2.03	0.59
29:X:2792:C:C2	29:X:2805:G:N2	2.71	0.59
13:L:38:ILE:HD12	13:L:39:TYR:H	1.67	0.59
18:Q:35:LYS:HD2	18:Q:53:ILE:HD13	1.85	0.59
25:Z:38:GLY:O	25:Z:39:LYS:HG2	2.01	0.59
26:1:35:LEU:HB3	26:1:51:ALA:HB2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Y:25:G:H1	30:Y:62:C:N4	2.01	0.59
1:0:15:GLN:HB3	1:0:221:ALA:HB2	1.85	0.58
1:0:136:PRO:HA	1:0:141:VAL:HG11	1.84	0.58
1:0:138:SER:OG	1:0:139:GLY:N	2.34	0.58
19:R:77:HIS:CD2	29:X:339:U:H4'	2.37	0.58
29:X:82:G:N2	29:X:100:G:H1'	2.18	0.58
29:X:641:G:N2	29:X:644:A:OP2	2.34	0.58
29:X:1465:G:N2	29:X:1466:C:C2	2.71	0.58
3:B:4:ILE:HG12	3:B:5:LEU:H	1.67	0.58
4:C:84:PHE:CE1	29:X:596:C:H5'	2.38	0.58
12:K:92:GLY:HA2	12:K:94:TYR:CE2	2.38	0.58
19:R:26:SER:HB2	29:X:321:A:H5'	1.85	0.58
29:X:455:A:C2	29:X:1258:G:N3	2.68	0.58
29:X:1326:U:H4'	29:X:1345:G:H4'	1.85	0.58
29:X:1679:U:H2'	29:X:1680:U:O4'	2.02	0.58
29:X:2516:U:H2'	29:X:2517:C:C6	2.37	0.58
8:G:140:GLN:HG3	29:X:567:G:C5'	2.30	0.58
9:H:115:ALA:O	9:H:117:GLU:N	2.36	0.58
20:S:103:ARG:HH22	20:S:107:GLU:HB3	1.67	0.58
23:V:32:ALA:HA	23:V:37:LEU:HB2	1.84	0.58
29:X:548:G:H1	29:X:564:U:H3	1.50	0.58
29:X:970:A:N3	29:X:2436:U:O2'	2.33	0.58
29:X:1100:G:H5'	29:X:1101:U:OP2	2.04	0.58
4:C:125:ILE:HD12	4:C:133:PHE:HA	1.85	0.58
8:G:31:THR:OG1	29:X:1006:C:N3	2.37	0.58
18:Q:88:ILE:HD11	18:Q:91:LEU:HB2	1.85	0.58
23:V:42:ARG:NH1	23:V:45:GLN:OE1	2.36	0.58
29:X:243:G:H1	29:X:439:C:H42	1.50	0.58
29:X:930:A:H4'	30:Y:100:G:N3	2.18	0.58
29:X:958:G:H2'	29:X:959:C:C6	2.38	0.58
10:I:77:LEU:O	10:I:79:GLN:N	2.37	0.58
12:K:3:HIS:O	12:K:3:HIS:CD2	2.56	0.58
15:N:31:GLN:NE2	29:X:589:C:H4'	2.18	0.58
15:N:91:ASN:HD22	15:N:93:LYS:HB3	1.69	0.58
29:X:1117:G:H2'	29:X:1118:G:C8	2.38	0.58
29:X:1655:C:H5''	29:X:2689:C:H1'	1.85	0.58
29:X:1815:G:H2'	29:X:1816:G:H8	1.68	0.58
29:X:2226:A:H2'	29:X:2227:C:C6	2.37	0.58
5:D:128:TYR:HB3	5:D:156:ILE:HD12	1.84	0.58
6:E:150:LYS:NZ	29:X:2741:G:H21	2.00	0.58
11:J:16:GLY:O	11:J:73:LYS:NZ	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:32:TYR:O	13:L:34:SER:N	2.36	0.58
19:R:8:SER:OG	19:R:9:HIS:N	2.36	0.58
26:1:42:PRO:HG3	29:X:2327:U:O2'	2.03	0.58
29:X:622:U:H2'	29:X:623:G:C8	2.38	0.58
29:X:2418:A:H4'	29:X:2419:C:H5'	1.84	0.58
29:X:2633:A:N1	29:X:2644:A:H5''	2.17	0.58
13:L:43:ILE:HG22	13:L:45:ASP:H	1.69	0.58
14:M:70:LYS:NZ	14:M:72:SER:OG	2.37	0.58
15:N:83:LEU:HD22	15:N:88:ILE:HD12	1.85	0.58
28:3:64:ARG:HH21	29:X:219:G:P	2.26	0.58
29:X:2565:C:H2'	29:X:2566:A:C8	2.39	0.58
13:L:49:GLN:HG2	30:Y:116:C:H4'	1.86	0.58
17:P:41:VAL:HG11	17:P:65:SER:HA	1.84	0.58
29:X:1035:G:C6	29:X:1036:G:C6	2.92	0.58
29:X:1040:A:C8	29:X:1041:G:C8	2.92	0.58
29:X:1124:U:H2'	29:X:1125:G:C8	2.39	0.58
29:X:1298:G:C6	29:X:1342:U:C6	2.92	0.58
29:X:1621:C:O2	29:X:1626:A:O2'	2.20	0.58
29:X:1921:A:O2'	29:X:1922:U:H5'	2.03	0.58
29:X:2625:U:O5'	29:X:2625:U:H6	1.87	0.58
10:I:75:VAL:HG12	10:I:108:LEU:HD13	1.85	0.58
14:M:31:ASP:OD1	14:M:96:ARG:HA	2.04	0.58
22:U:48:LYS:HE3	29:X:2074:U:H1'	1.85	0.58
29:X:1033:G:N2	29:X:1034:U:O4	2.28	0.58
1:0:182:SER:HA	1:0:185:TYR:HB3	1.86	0.58
14:M:106:TYR:CE1	29:X:1745:C:H5'	2.39	0.58
15:N:3:ARG:HB3	29:X:1261:G:C4	2.39	0.58
21:T:53:MET:HG2	21:T:57:HIS:HA	1.86	0.58
29:X:834:A:H5'	29:X:835:U:C6	2.38	0.58
4:C:86:PRO:HD3	29:X:1261:G:C8	2.38	0.57
9:H:90:ARG:NH2	14:M:78:GLU:OE1	2.37	0.57
9:H:97:VAL:HG11	9:H:126:ILE:HD13	1.86	0.57
14:M:46:ARG:HG2	14:M:47:SER:H	1.68	0.57
15:N:58:ARG:O	15:N:62:ILE:HG13	2.04	0.57
20:S:123:VAL:HG23	20:S:161:ALA:HB2	1.84	0.57
24:W:2:LYS:HB3	24:W:54:GLN:HB2	1.87	0.57
29:X:333:A:H5'	29:X:351:A:C1'	2.33	0.57
29:X:501:G:H2'	29:X:502:A:O4'	2.04	0.57
29:X:2531:U:H2'	29:X:2533:U:OP2	2.04	0.57
30:Y:58:G:H4'	30:Y:59:A:H5''	1.84	0.57
2:A:62:TYR:HE1	29:X:1808:C:H3'	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:66:ILE:HD11	30:Y:43:G:H2'	1.85	0.57
6:E:66:GLY:HA3	29:X:2728:A:H4'	1.86	0.57
15:N:59:ARG:HH22	29:X:1019:U:H4'	1.69	0.57
16:O:71:ILE:HB	16:O:84:THR:OG1	2.04	0.57
25:Z:3:LYS:HD2	29:X:2556:A:H4'	1.84	0.57
29:X:219:G:O2'	29:X:231:G:O6	2.19	0.57
29:X:484:G:H2'	29:X:485:G:H8	1.69	0.57
29:X:622:U:H2'	29:X:623:G:H8	1.68	0.57
29:X:836:G:N2	29:X:847:C:O2	2.37	0.57
29:X:936:A:H2'	29:X:937:C:C6	2.40	0.57
29:X:1281:A:H2'	29:X:1282:A:C8	2.40	0.57
29:X:1608:U:H2'	29:X:1609:G:H8	1.68	0.57
29:X:2198:U:H3'	29:X:2199:C:H4'	1.85	0.57
29:X:2424:G:H2'	29:X:2425:G:H8	1.69	0.57
1:O:187:ALA:HA	1:O:190:SER:HB3	1.86	0.57
9:H:25:LEU:CD2	9:H:52:VAL:HG23	2.34	0.57
11:J:11:ARG:NH2	11:J:72:ASP:HB2	2.19	0.57
19:R:58:VAL:HG13	19:R:60:PRO:HD2	1.85	0.57
28:3:7:HIS:HD2	28:3:61:MET:HE2	1.68	0.57
29:X:548:G:C2	29:X:549:G:C8	2.91	0.57
29:X:992:A:H5''	29:X:993:C:OP2	2.04	0.57
29:X:1067:G:H1'	29:X:1114:A:H61	1.69	0.57
29:X:1072:U:N3	29:X:1080:A:OP1	2.38	0.57
29:X:1336:G:C2'	29:X:1337:G:H5'	2.32	0.57
29:X:2391:A:C8	29:X:2392:G:C8	2.91	0.57
2:A:210:GLY:HA3	29:X:777:A:OP1	2.04	0.57
8:G:33:ILE:HG21	29:X:548:G:H5'	1.84	0.57
11:J:27:TYR:HB3	11:J:137:VAL:HB	1.85	0.57
19:R:106:VAL:O	19:R:112:LYS:HB2	2.04	0.57
29:X:668:A:H4'	29:X:669:G:H5'	1.85	0.57
29:X:2197:U:H2'	29:X:2198:U:C6	2.38	0.57
16:O:34:GLU:HG3	16:O:57:GLN:HA	1.86	0.57
17:P:31:VAL:HG12	17:P:122:SER:O	2.05	0.57
17:P:59:PHE:HD1	25:Z:30:LEU:HD11	1.70	0.57
29:X:691:C:H2'	29:X:692:C:C6	2.39	0.57
2:A:108:PRO:HB3	2:A:143:HIS:CE1	2.36	0.57
10:I:77:LEU:C	10:I:79:GLN:H	2.12	0.57
13:L:37:HIS:CE1	13:L:39:TYR:HD1	2.23	0.57
29:X:1464:A:H61	29:X:1477:C:H42	1.50	0.57
30:Y:39:C:H5''	30:Y:40:C:C5	2.39	0.57
3:B:92:ASN:OD1	3:B:92:ASN:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:8:GLY:H	4:C:121:ASP:HB3	1.70	0.57
15:N:6:THR:O	15:N:8:ILE:N	2.35	0.57
16:O:32:LYS:NZ	16:O:57:GLN:HB3	2.20	0.57
20:S:63:PRO:HB2	20:S:86:VAL:HG22	1.87	0.57
29:X:308:C:H2'	29:X:309:G:C8	2.40	0.57
29:X:485:G:C6	29:X:520:C:N4	2.73	0.57
29:X:497:C:O2	29:X:505:G:N2	2.38	0.57
2:A:142:VAL:HA	2:A:194:GLY:H	1.69	0.57
5:D:5:LYS:HA	5:D:8:TYR:CD2	2.40	0.57
5:D:126:GLY:O	5:D:160:ALA:HB3	2.04	0.57
6:E:83:TYR:O	6:E:134:SER:OG	2.20	0.57
8:G:84:ASN:ND2	8:G:154:GLU:OE1	2.34	0.57
17:P:80:LEU:HD11	17:P:87:GLU:HB2	1.87	0.57
27:2:12:ARG:HD2	27:2:44:VAL:HG11	1.87	0.57
29:X:1787:U:H2'	29:X:1788:C:H6	1.70	0.57
29:X:1981:A:H4'	29:X:2704:U:O2'	2.03	0.57
2:A:211:ARG:HD2	2:A:214:TRP:CZ3	2.40	0.57
2:A:260:ARG:NH2	2:A:267:ASP:OD1	2.24	0.57
12:K:24:GLN:HB3	12:K:44:LEU:HD22	1.87	0.57
15:N:24:PHE:CE1	29:X:543:G:H5'	2.40	0.57
29:X:958:G:H2'	29:X:959:C:H6	1.70	0.57
29:X:1071:U:H4'	29:X:1072:U:H5'	1.86	0.57
29:X:1192:A:H2'	29:X:1193:G:C8	2.40	0.57
29:X:2124:C:N4	29:X:2125:C:N3	2.53	0.57
29:X:2354:G:N2	29:X:2357:A:OP2	2.34	0.57
29:X:2691:C:H2'	29:X:2694:G:H5''	1.85	0.57
1:0:53:ASN:ND2	1:0:161:ASN:OD1	2.37	0.57
15:N:50:ARG:O	15:N:53:LYS:HG2	2.04	0.57
17:P:31:VAL:HG11	17:P:124:ILE:CD1	2.33	0.57
29:X:533:C:H5''	29:X:550:C:O2'	2.05	0.57
28:3:24:ALA:O	28:3:48:PHE:N	2.33	0.56
29:X:654:A:H2'	29:X:655:A:C8	2.39	0.56
29:X:1458:A:H5''	29:X:1459:U:OP2	2.05	0.56
29:X:1529:C:H2'	29:X:1530:U:C6	2.40	0.56
29:X:1982:C:H2'	29:X:1983:G:O4'	2.05	0.56
4:C:189:ASP:OD1	4:C:190:ALA:N	2.37	0.56
24:W:13:PRO:HG2	24:W:16:GLN:HB2	1.87	0.56
28:3:28:GLY:HA3	28:3:32:GLN:OE1	2.06	0.56
29:X:602:C:H42	29:X:678:G:H1	1.52	0.56
29:X:874:A:H2'	29:X:875:G:O4'	2.05	0.56
29:X:1845:A:H2'	29:X:1846:A:C8	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1935:A:C6	29:X:1936:A:N1	2.73	0.56
29:X:2048:C:H5''	29:X:2231:G:H1'	1.86	0.56
1:O:73:ILE:HG12	1:O:95:LEU:HB3	1.86	0.56
3:B:141:ILE:HD12	29:X:2035:G:C8	2.40	0.56
3:B:144:ARG:HD3	29:X:2551:A:C8	2.41	0.56
3:B:152:LYS:HB3	8:G:106:TYR:CE1	2.41	0.56
14:M:100:ARG:NH2	29:X:1744:G:OP1	2.34	0.56
19:R:43:ASP:OD2	19:R:43:ASP:N	2.38	0.56
22:U:20:ARG:HB3	22:U:43:ARG:NH2	2.20	0.56
28:3:3:LYS:HA	29:X:602:C:H1'	1.88	0.56
29:X:340:G:H4'	29:X:341:A:OP2	2.06	0.56
29:X:837:U:H2'	29:X:838:A:C8	2.39	0.56
29:X:1002:C:H5'	29:X:1200:G:OP2	2.05	0.56
29:X:1793:A:H2'	29:X:1794:A:C8	2.40	0.56
29:X:2197:U:H2'	29:X:2198:U:C5	2.40	0.56
29:X:2251:U:H5''	29:X:2252:A:OP1	2.05	0.56
30:Y:16:U:O2'	30:Y:17:A:OP2	2.21	0.56
5:D:69:LYS:NZ	30:Y:43:G:H1	2.04	0.56
8:G:95:LEU:HA	8:G:115:ALA:HB3	1.88	0.56
14:M:69:ARG:NH2	14:M:108:LYS:HA	2.20	0.56
15:N:37:GLN:HG3	29:X:1265:G:N1	2.20	0.56
17:P:27:VAL:HG22	17:P:125:THR:OG1	2.05	0.56
17:P:36:ARG:NH1	25:Z:20:ARG:HH21	2.04	0.56
4:C:97:ARG:NH2	29:X:630:G:N7	2.53	0.56
21:T:46:LYS:HZ3	21:T:76:ALA:HA	1.70	0.56
29:X:16:G:H2'	29:X:17:G:H8	1.71	0.56
29:X:52:A:H5''	29:X:53:G:OP2	2.05	0.56
29:X:224:G:H4'	29:X:399:G:C4	2.41	0.56
29:X:858:G:H8	29:X:858:G:OP2	1.87	0.56
29:X:1863:U:H2'	29:X:1864:G:H8	1.70	0.56
29:X:2605:C:H2'	29:X:2606:G:H8	1.70	0.56
29:X:2662:C:C2'	29:X:2663:U:H5'	2.35	0.56
2:A:48:ARG:HH21	29:X:791:G:H5'	1.70	0.56
3:B:7:THR:HG23	3:B:194:GLY:O	2.06	0.56
3:B:109:LYS:HG2	3:B:191:ALA:HB2	1.87	0.56
8:G:51:LEU:HD12	8:G:88:VAL:HG11	1.87	0.56
28:3:7:HIS:CD2	28:3:61:MET:HE2	2.41	0.56
28:3:56:ALA:HA	28:3:59:LYS:HG3	1.88	0.56
29:X:1329:U:H2'	29:X:1330:G:C8	2.40	0.56
29:X:1909:U:P	29:X:1912:G:H1	2.26	0.56
29:X:1956:G:H2'	29:X:1957:C:C6	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1989:C:O5'	29:X:1989:C:H6	1.88	0.56
2:A:142:VAL:HG23	2:A:193:ILE:HD13	1.86	0.56
3:B:2:LYS:HA	3:B:84:PHE:HE1	1.70	0.56
3:B:107:THR:O	3:B:190:GLY:HA3	2.05	0.56
29:X:33:C:H41	29:X:458:G:HO2'	1.52	0.56
29:X:840:U:H4'	29:X:841:G:C8	2.41	0.56
29:X:2129:U:H2'	29:X:2130:G:H8	1.70	0.56
29:X:2308:A:H2'	29:X:2309:G:C8	2.40	0.56
4:C:158:ARG:O	4:C:161:ALA:N	2.39	0.56
8:G:136:PRO:O	8:G:141:GLY:HA3	2.06	0.56
13:L:11:LEU:HD21	29:X:2273:C:OP1	2.06	0.56
29:X:1016:C:H1'	29:X:1023:U:N3	2.20	0.56
4:C:188:ILE:HB	4:C:189:ASP:O	2.05	0.56
11:J:12:LYS:O	11:J:13:GLN:HB2	2.05	0.56
12:K:73:LYS:H	12:K:73:LYS:HE2	1.71	0.56
20:S:3:LEU:HB2	20:S:33:ALA:O	2.06	0.56
26:1:9:ILE:HA	26:1:25:THR:HG22	1.87	0.56
29:X:10:A:H2'	29:X:11:G:C8	2.40	0.56
29:X:628:A:H2'	29:X:629:C:C6	2.40	0.56
29:X:692:C:H2'	29:X:693:A:C8	2.37	0.56
29:X:1383:C:H3'	29:X:1384:G:H8	1.71	0.56
29:X:1736:C:H2'	29:X:1737:G:C8	2.41	0.56
2:A:52:ARG:HG2	2:A:53:PHE:CD2	2.41	0.56
15:N:94:VAL:O	15:N:98:ILE:HG12	2.06	0.56
21:T:9:SER:HB3	29:X:2235:G:O2'	2.05	0.56
22:U:22:GLY:C	22:U:39:LYS:HZ3	2.13	0.56
25:Z:7:PRO:HA	29:X:2594:U:C2	2.42	0.56
29:X:415:A:H61	29:X:435:A:H61	1.54	0.56
29:X:806:A:OP2	29:X:2054:A:O2'	2.24	0.56
29:X:861:G:H22	29:X:943:U:H1'	1.69	0.56
29:X:861:G:N3	29:X:944:A:H1'	2.21	0.56
29:X:995:A:P	29:X:996:C:H41	2.28	0.56
29:X:1426:U:H3	29:X:1605:A:H61	1.54	0.56
29:X:1656:U:OP1	29:X:2688:G:N2	2.39	0.56
29:X:1707:A:H3'	29:X:1708:C:H6	1.71	0.56
29:X:1856:U:H3	29:X:1861:G:H1	1.52	0.56
29:X:2225:G:H2'	29:X:2226:A:C8	2.40	0.56
29:X:2387:U:H2'	29:X:2388:G:H8	1.70	0.56
4:C:146:GLU:O	4:C:166:TRP:HE3	1.90	0.55
13:L:37:HIS:HD2	30:Y:29:C:O3'	1.89	0.55
14:M:38:LYS:HZ2	14:M:89:ASN:HB2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:60:ILE:HD11	25:Z:28:PRO:HD3	1.88	0.55
22:U:30:VAL:O	22:U:32:ARG:NH1	2.39	0.55
29:X:1077:U:O2'	29:X:1079:G:N7	2.28	0.55
29:X:1342:U:O5'	29:X:1343:C:H5	1.87	0.55
29:X:1690:U:H6	29:X:1690:U:H3'	1.72	0.55
29:X:2434:G:H2'	29:X:2435:C:C6	2.41	0.55
29:X:2516:U:H2'	29:X:2517:C:H6	1.70	0.55
2:A:227:ASN:CG	29:X:797:A:H5''	2.31	0.55
5:D:13:ARG:HB2	5:D:14:PRO:HD3	1.88	0.55
5:D:85:VAL:HG23	29:X:2291:U:H5'	1.88	0.55
9:H:2:ILE:HD12	9:H:6:SER:OG	2.06	0.55
16:O:66:GLY:O	16:O:87:ARG:HD2	2.06	0.55
20:S:69:VAL:HG22	20:S:81:VAL:HG22	1.88	0.55
29:X:1244:U:H2'	29:X:1245:G:C8	2.36	0.55
29:X:2198:U:C2	29:X:2199:C:H1'	2.41	0.55
2:A:142:VAL:HG21	2:A:191:ALA:HB1	1.89	0.55
15:N:19:LYS:NZ	29:X:1233:A:OP1	2.36	0.55
15:N:61:TRP:O	15:N:65:ILE:HG13	2.05	0.55
16:O:28:GLU:O	16:O:30:GLY:N	2.39	0.55
20:S:151:ASP:OD2	20:S:151:ASP:N	2.37	0.55
29:X:165:G:O2'	29:X:1378:A:N6	2.39	0.55
29:X:568:G:H2'	29:X:569:C:O4'	2.07	0.55
29:X:652:C:N3	29:X:658:G:N2	2.54	0.55
29:X:810:U:H2'	29:X:811:G:O4'	2.06	0.55
2:A:246:PRO:HG2	29:X:1884:A:O2'	2.07	0.55
16:O:23:GLU:O	16:O:25:LEU:N	2.38	0.55
19:R:58:VAL:HA	29:X:494:A:H4'	1.87	0.55
22:U:54:ASN:O	22:U:56:GLN:N	2.39	0.55
29:X:1975:G:N2	29:X:1979:C:O2'	2.37	0.55
29:X:2031:A:H2'	29:X:2032:G:H5''	1.89	0.55
29:X:2234:G:H2'	29:X:2235:G:O4'	2.07	0.55
29:X:2586:G:H2'	29:X:2587:G:O4'	2.05	0.55
1:O:68:VAL:HG22	1:O:153:LYS:HA	1.89	0.55
2:A:43:ARG:HA	2:A:48:ARG:O	2.06	0.55
2:A:208:LYS:HB2	29:X:742:G:C6	2.41	0.55
8:G:94:LYS:O	8:G:98:LYS:N	2.31	0.55
8:G:125:ARG:NH1	29:X:2619:G:OP1	2.36	0.55
15:N:13:ARG:O	15:N:16:LYS:HB2	2.06	0.55
28:3:52:LYS:O	28:3:55:TRP:N	2.39	0.55
29:X:877:G:H1	29:X:924:C:N4	2.03	0.55
29:X:1283:C:H5''	29:X:1284:G:H5'	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1325:U:H4'	29:X:1326:U:O5'	2.05	0.55
29:X:1819:U:H2'	29:X:1820:G:O4'	2.06	0.55
29:X:2443:C:H42	29:X:2465:G:H1	1.52	0.55
18:Q:2:SER:C	18:Q:4:TYR:H	2.15	0.55
28:3:33:ASN:HB3	29:X:2398:U:H5''	1.89	0.55
29:X:495:C:H2'	29:X:496:C:C6	2.42	0.55
29:X:1550:C:H2'	29:X:1553:G:H1	1.71	0.55
29:X:2328:G:O6	29:X:2361:G:N2	2.30	0.55
5:D:99:PHE:HA	5:D:102:LYS:HD2	1.88	0.55
19:R:23:ILE:HG13	19:R:31:GLY:HA2	1.88	0.55
29:X:774:A:H8	29:X:774:A:O5'	1.90	0.55
29:X:1710:U:H3	29:X:1821:A:H61	1.55	0.55
29:X:1922:U:OP1	29:X:2583:U:O2'	2.25	0.55
29:X:2546:G:H2'	29:X:2547:C:C6	2.42	0.55
30:Y:41:A:O2'	30:Y:48:A:N1	2.35	0.55
1:0:123:LEU:HD13	1:0:127:LEU:HD12	1.87	0.55
5:D:92:ARG:NH2	30:Y:46:G:H3'	2.22	0.55
8:G:61:ARG:HD3	8:G:66:HIS:CE1	2.42	0.55
29:X:2277:A:H2'	29:X:2278:A:O4'	2.07	0.55
29:X:2604:G:H2'	29:X:2605:C:O4'	2.07	0.55
10:I:65:PHE:HA	28:3:12:ARG:HD2	1.89	0.55
11:J:78:LYS:NZ	11:J:84:MET:HG3	2.22	0.55
14:M:63:ARG:HD3	29:X:2661:G:H4'	1.88	0.55
21:T:21:LEU:HD11	21:T:41:ARG:NE	2.21	0.55
21:T:64:ASP:OD1	21:T:64:ASP:N	2.40	0.55
25:Z:17:ASP:HB3	29:X:16:G:OP1	2.07	0.55
27:2:12:ARG:CD	27:2:44:VAL:HG11	2.36	0.55
29:X:518:A:H5''	29:X:518:A:H8	1.71	0.55
29:X:974:U:H2'	29:X:975:C:C6	2.42	0.55
29:X:1108:U:H3'	29:X:1109:A:C8	2.41	0.55
29:X:1221:C:C2	29:X:1222:G:C8	2.95	0.55
29:X:1484:G:H2'	29:X:1485:U:C6	2.42	0.55
29:X:2053:G:H2'	29:X:2054:A:C8	2.41	0.55
1:0:38:GLU:HB2	1:0:211:THR:HB	1.88	0.55
3:B:84:PHE:HD2	3:B:86:PRO:HD3	1.71	0.55
13:L:64:LYS:HZ3	30:Y:53:G:H5''	1.72	0.55
20:S:168:VAL:HG12	20:S:169:VAL:H	1.71	0.55
24:W:17:VAL:O	24:W:20:VAL:N	2.40	0.55
25:Z:3:LYS:HB2	29:X:2590:U:O2	2.07	0.55
29:X:68:C:H2'	29:X:69:G:C8	2.41	0.55
29:X:713:G:O5'	29:X:713:G:H8	1.90	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:751:G:H2'	29:X:752:G:C8	2.41	0.55
29:X:2145:A:H4'	29:X:2155:U:H5''	1.89	0.55
3:B:22:PRO:HB3	29:X:2661:G:C2	2.42	0.54
3:B:134:TRP:CD1	3:B:137:ARG:HB2	2.42	0.54
9:H:4:PRO:O	9:H:5:GLN:HB2	2.07	0.54
13:L:19:THR:HG21	13:L:28:ARG:HD3	1.88	0.54
15:N:10:ARG:HG3	15:N:13:ARG:HH22	1.72	0.54
26:1:12:MET:HE2	26:1:37:LEU:HB2	1.87	0.54
29:X:562:G:H2'	29:X:563:U:O4'	2.07	0.54
29:X:618:A:H2'	29:X:619:A:C8	2.43	0.54
29:X:1988:A:O2'	29:X:2032:G:OP1	2.17	0.54
30:Y:7:C:H2'	30:Y:8:C:H6	1.72	0.54
2:A:39:LYS:HZ1	2:A:58:HIS:H	1.53	0.54
3:B:116:VAL:HG11	3:B:138:PRO:HB3	1.89	0.54
5:D:24:SER:OG	30:Y:57:U:O3'	2.15	0.54
5:D:65:PRO:HA	5:D:89:VAL:HG13	1.89	0.54
10:I:90:ARG:HD2	10:I:93:LEU:HG	1.88	0.54
18:Q:84:GLU:OE2	18:Q:86:GLN:NE2	2.40	0.54
20:S:26:LYS:HE3	30:Y:107:C:H4'	1.89	0.54
21:T:12:ASN:OD1	21:T:12:ASN:N	2.40	0.54
26:1:37:LEU:HG	29:X:2323:U:O2'	2.06	0.54
27:2:37:LYS:HG2	29:X:469:G:C8	2.41	0.54
29:X:165:G:H2'	29:X:166:G:O4'	2.08	0.54
29:X:313:U:H2'	29:X:314:G:H8	1.72	0.54
29:X:1773:C:O4'	29:X:2588:U:C2	2.60	0.54
13:L:85:LYS:HD2	13:L:86:GLN:HG2	1.89	0.54
29:X:867:G:H1	29:X:935:C:N4	2.02	0.54
29:X:1298:G:C6	29:X:1342:U:C5	2.95	0.54
29:X:1987:G:C5	29:X:1988:A:C8	2.96	0.54
29:X:2482:A:H4'	29:X:2483:U:OP1	2.06	0.54
29:X:2605:C:H2'	29:X:2606:G:C8	2.43	0.54
4:C:117:LEU:HD22	4:C:188:ILE:HD11	1.88	0.54
24:W:19:THR:HG23	24:W:43:MET:HG2	1.88	0.54
29:X:1818:G:H2'	29:X:1819:U:H6	1.71	0.54
29:X:2030:U:H2'	29:X:2031:A:C8	2.42	0.54
29:X:2495:G:N2	29:X:2548:G:H1'	2.23	0.54
29:X:2574:G:N2	29:X:2577:A:OP2	2.39	0.54
29:X:2779:C:H2'	29:X:2780:A:H8	1.72	0.54
30:Y:86:A:C2	30:Y:96:C:N3	2.76	0.54
2:A:145:LEU:HD22	2:A:163:VAL:HG11	1.90	0.54
3:B:57:ARG:NH2	29:X:2809:A:H5'	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:108:SER:OG	3:B:162:MET:N	2.41	0.54
5:D:117:ILE:HG21	5:D:130:LEU:HD21	1.89	0.54
6:E:96:ALA:HA	6:E:104:GLU:O	2.08	0.54
14:M:106:TYR:CD2	14:M:106:TYR:N	2.75	0.54
18:Q:2:SER:O	18:Q:4:TYR:N	2.34	0.54
29:X:510:G:H2'	29:X:511:A:H3'	1.88	0.54
29:X:573:C:H2'	29:X:574:C:C6	2.41	0.54
29:X:659:G:H2'	29:X:660:G:C8	2.41	0.54
29:X:1296:G:N2	29:X:1299:A:H5'	2.23	0.54
29:X:1974:U:H2'	29:X:1975:G:H5'	1.89	0.54
1:O:112:THR:HB	1:O:115:MET:HB2	1.89	0.54
8:G:31:THR:HG21	15:N:61:TRP:HE1	1.71	0.54
10:I:100:ARG:C	10:I:101:ARG:HD2	2.33	0.54
14:M:40:ARG:HB3	14:M:40:ARG:NH1	2.21	0.54
16:O:18:ASP:N	16:O:18:ASP:OD1	2.39	0.54
16:O:78:VAL:HG23	16:O:80:TYR:H	1.73	0.54
27:2:34:ARG:HD3	29:X:478:G:OP2	2.07	0.54
29:X:854:G:H1'	29:X:949:G:H22	1.71	0.54
29:X:932:G:H2'	29:X:933:G:C8	2.42	0.54
29:X:1385:C:H2'	29:X:1386:A:O4'	2.08	0.54
29:X:2285:U:H5	29:X:2290:A:C6	2.26	0.54
29:X:2660:C:C4	29:X:2704:U:C5	2.95	0.54
3:B:164:ARG:O	29:X:2753:C:H5''	2.08	0.54
3:B:175:ILE:HG12	3:B:182:ILE:HD11	1.90	0.54
13:L:80:ALA:HB2	13:L:111:GLY:O	2.08	0.54
20:S:49:THR:HG21	20:S:96:VAL:HG13	1.89	0.54
29:X:588:G:H1	29:X:1274:C:H42	1.55	0.54
29:X:706:A:H2'	29:X:707:U:O4'	2.08	0.54
29:X:994:A:N7	29:X:995:A:C6	2.76	0.54
29:X:1353:A:H3'	29:X:1354:A:C8	2.42	0.54
29:X:2557:G:H2'	29:X:2558:C:C6	2.43	0.54
5:D:64:LYS:HD3	30:Y:44:C:H4'	1.90	0.54
10:I:61:PRO:HG2	28:3:25:PHE:HB2	1.89	0.54
17:P:45:ILE:HD11	17:P:57:LEU:HG	1.90	0.54
29:X:597:U:H2'	29:X:598:U:C6	2.42	0.54
29:X:1818:G:H2'	29:X:1819:U:C6	2.43	0.54
2:A:260:ARG:HH22	2:A:266:SER:HB2	1.72	0.54
29:X:521:U:O4	29:X:522:G:N2	2.41	0.54
29:X:2594:U:H2'	29:X:2595:C:H6	1.73	0.54
8:G:106:TYR:CD2	29:X:2621:G:H5'	2.42	0.54
14:M:8:ASN:HA	29:X:2851:G:OP1	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:V:21:ARG:HG3	23:V:46:LEU:HD23	1.89	0.54
29:X:24:G:H2'	29:X:25:U:C6	2.43	0.54
29:X:1542:G:H2'	29:X:1543:G:C8	2.43	0.54
29:X:2433:G:H2'	29:X:2434:G:H8	1.73	0.54
29:X:2819:G:H2'	29:X:2820:C:H6	1.73	0.54
5:D:74:ILE:HA	5:D:79:LEU:HB2	1.90	0.53
6:E:41:LEU:HG	6:E:54:ARG:HA	1.90	0.53
11:J:78:LYS:HZ2	11:J:84:MET:HG3	1.73	0.53
18:Q:64:ARG:HB2	18:Q:69:ILE:HD13	1.90	0.53
18:Q:65:VAL:HG23	29:X:63:A:H1'	1.88	0.53
19:R:13:LYS:NZ	29:X:349:G:OP1	2.30	0.53
25:Z:45:ILE:HD13	25:Z:57:VAL:HG22	1.90	0.53
29:X:525:A:H2'	29:X:526:C:H5'	1.90	0.53
29:X:555:U:H5'	29:X:556:A:C2	2.43	0.53
29:X:1324:G:OP2	29:X:1324:G:N2	2.29	0.53
29:X:1329:U:H5'	29:X:1405:A:H1'	1.89	0.53
3:B:105:THR:HB	3:B:197:VAL:HG13	1.90	0.53
12:K:66:VAL:HG21	12:K:80:MET:HE1	1.89	0.53
17:P:11:LYS:HG3	17:P:14:ARG:NH2	2.22	0.53
20:S:52:PHE:N	20:S:64:ALA:O	2.32	0.53
28:3:56:ALA:O	28:3:60:LEU:HG	2.08	0.53
29:X:957:G:H2'	29:X:958:G:C8	2.43	0.53
29:X:1359:G:H2'	29:X:1360:G:H8	1.73	0.53
29:X:2245:A:H4'	29:X:2246:A:C2	2.43	0.53
2:A:124:GLU:C	2:A:126:LYS:H	2.17	0.53
4:C:130:THR:HG21	29:X:331:U:H2'	1.90	0.53
10:I:35:LYS:HE2	29:X:820:U:P	2.48	0.53
19:R:48:VAL:HG13	19:R:50:GLY:H	1.72	0.53
20:S:55:THR:O	20:S:55:THR:OG1	2.23	0.53
22:U:21:ARG:HH21	22:U:23:LYS:HG2	1.72	0.53
25:Z:36:CYS:SG	25:Z:49:CYS:N	2.73	0.53
29:X:163:A:H2'	29:X:164:G:C8	2.43	0.53
29:X:175:C:O2'	29:X:176:A:H5'	2.08	0.53
9:H:132:GLU:HB2	14:M:73:PHE:CE1	2.44	0.53
12:K:34:ILE:O	12:K:112:LEU:HA	2.08	0.53
14:M:106:TYR:N	14:M:106:TYR:HD2	2.07	0.53
15:N:24:PHE:HB3	15:N:28:ARG:HB3	1.89	0.53
15:N:104:GLU:O	15:N:107:LYS:HB3	2.09	0.53
16:O:32:LYS:HZ3	16:O:57:GLN:HB3	1.73	0.53
21:T:32:LYS:HB3	21:T:35:ASN:OD1	2.09	0.53
28:3:36:LYS:HB3	28:3:41:ILE:HG13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:651:C:H2'	29:X:652:C:C6	2.44	0.53
29:X:1840:A:H2'	29:X:1841:G:O4'	2.09	0.53
29:X:2081:U:H3	29:X:2174:G:H1	1.55	0.53
29:X:2310:G:C6	29:X:2311:U:C5	2.97	0.53
29:X:2490:U:H2'	29:X:2491:C:O4'	2.09	0.53
3:B:11:MET:HG2	3:B:24:THR:OG1	2.09	0.53
3:B:176:ARG:NH2	14:M:16:ILE:HA	2.20	0.53
4:C:74:VAL:HG12	4:C:76:THR:H	1.74	0.53
7:F:74:MET:HE3	7:F:77:LEU:HB2	1.90	0.53
8:G:110:LEU:HD22	29:X:1142:G:H4'	1.91	0.53
11:J:111:THR:HG22	11:J:114:GLN:HG3	1.91	0.53
20:S:103:ARG:NH2	20:S:107:GLU:HB3	2.22	0.53
29:X:548:G:N2	29:X:564:U:O2	2.33	0.53
29:X:645:G:H2'	29:X:646:C:C6	2.43	0.53
29:X:839:U:OP1	29:X:2408:G:OP1	2.26	0.53
29:X:1770:U:C2	29:X:1774:A:N7	2.77	0.53
29:X:2200:G:H2'	29:X:2201:G:C8	2.43	0.53
29:X:2451:G:H2'	29:X:2454:C:H42	1.74	0.53
29:X:2726:U:O2	29:X:2739:G:N2	2.41	0.53
4:C:33:TRP:HD1	4:C:93:TYR:CE1	2.27	0.53
4:C:67:ALA:HA	29:X:1268:U:C6	2.44	0.53
4:C:68:ARG:NH2	29:X:2043:A:N6	2.55	0.53
4:C:106:MET:O	4:C:110:SER:OG	2.15	0.53
12:K:27:ALA:O	12:K:30:ARG:N	2.42	0.53
12:K:83:VAL:HG23	12:K:87:TYR:CE2	2.43	0.53
15:N:54:LYS:NZ	29:X:1005:U:H3'	2.24	0.53
29:X:310:A:N3	29:X:330:C:O2'	2.40	0.53
29:X:493:A:OP2	29:X:517:A:N6	2.28	0.53
29:X:1007:A:H2'	29:X:1008:G:H8	1.71	0.53
29:X:1020:A:N7	29:X:1021:A:C6	2.76	0.53
29:X:1430:G:O2'	29:X:1603:A:N3	2.41	0.53
29:X:1699:A:H61	29:X:1723:U:H3	1.57	0.53
29:X:2198:U:H3'	29:X:2199:C:C4'	2.38	0.53
29:X:2375:G:C2	29:X:2400:G:C2	2.96	0.53
29:X:2820:C:C2	29:X:2821:G:C8	2.97	0.53
3:B:147:PRO:HG2	3:B:149:ARG:HG2	1.90	0.53
13:L:63:ASN:HB3	13:L:66:ASP:HB2	1.91	0.53
22:U:20:ARG:HD2	22:U:43:ARG:NH1	2.23	0.53
25:Z:36:CYS:SG	25:Z:48:ASN:HB2	2.49	0.53
29:X:186:C:H2'	29:X:187:U:O4'	2.09	0.53
29:X:218:A:N1	29:X:232:A:H5''	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:513:A:C6	29:X:516:G:C6	2.97	0.53
29:X:1340:C:H2'	29:X:1341:G:C8	2.44	0.53
29:X:1662:G:H5''	29:X:1663:C:C5'	2.38	0.53
29:X:2084:G:H2'	29:X:2085:G:C8	2.43	0.53
8:G:50:PRO:HG3	29:X:1152:C:C5	2.44	0.53
8:G:122:HIS:ND1	8:G:122:HIS:O	2.39	0.53
9:H:35:THR:HG21	29:X:2628:C:O3'	2.09	0.53
13:L:64:LYS:NZ	30:Y:53:G:H5''	2.24	0.53
19:R:100:ASP:HB3	19:R:101:GLY:CA	2.38	0.53
29:X:571:U:O2'	29:X:581:A:H8	1.91	0.53
29:X:1069:G:H2'	29:X:1070:G:H8	1.73	0.53
29:X:1436:G:O3'	29:X:1508:G:O2'	2.27	0.53
29:X:1495:G:H2'	29:X:1496:G:C8	2.44	0.53
29:X:1991:C:H2'	29:X:1992:G:C8	2.44	0.53
29:X:2369:U:H3'	29:X:2369:U:C6	2.43	0.53
29:X:2769:C:H1'	29:X:2866:A:H2	1.73	0.53
29:X:2817:A:C2	29:X:2851:G:C2	2.96	0.53
2:A:229:VAL:HG11	29:X:797:A:C4	2.43	0.53
3:B:99:GLY:N	3:B:172:VAL:O	2.42	0.53
4:C:62:LYS:HZ2	29:X:2043:A:H5'	1.73	0.53
5:D:74:ILE:HG12	5:D:80:ARG:O	2.09	0.53
9:H:82:LYS:NZ	9:H:82:LYS:HB3	2.24	0.53
12:K:39:THR:O	12:K:42:LYS:N	2.42	0.53
15:N:91:ASN:HB3	15:N:94:VAL:HG23	1.91	0.53
17:P:97:VAL:HG22	17:P:124:ILE:HG23	1.89	0.53
19:R:44:GLN:HG2	19:R:77:HIS:HE1	1.72	0.53
22:U:32:ARG:H	22:U:32:ARG:HE	1.54	0.53
27:2:12:ARG:HD3	29:X:699:G:O6	2.09	0.53
29:X:500:G:H5''	29:X:501:G:OP2	2.09	0.53
29:X:937:C:H1'	29:X:939:C:H41	1.74	0.53
29:X:1692:C:C5	29:X:1693:A:N7	2.77	0.53
29:X:2750:G:H8	29:X:2750:G:O5'	1.92	0.53
1:0:157:ILE:HD13	1:0:157:ILE:H	1.73	0.53
3:B:145:LYS:HB2	29:X:2551:A:N7	2.24	0.53
4:C:34:GLN:HE21	29:X:627:A:P	2.31	0.53
7:F:115:LEU:HD22	7:F:126:THR:HG21	1.91	0.53
10:I:23:PRO:HD2	29:X:826:U:OP1	2.08	0.53
10:I:87:THR:OG1	10:I:97:ARG:NH2	2.41	0.53
13:L:35:SER:OG	30:Y:30:C:OP1	2.10	0.53
15:N:13:ARG:HH12	29:X:1264:C:P	2.30	0.53
19:R:58:VAL:HA	29:X:494:A:C5'	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:149:ALA:HB3	20:S:164:PRO:HA	1.91	0.53
28:3:15:LYS:HE3	28:3:23:MET:HE3	1.90	0.53
29:X:307:C:C2'	29:X:308:C:H5'	2.38	0.53
29:X:359:G:H2'	29:X:360:A:C8	2.43	0.53
29:X:1104:G:N3	29:X:1110:G:N2	2.56	0.53
29:X:1924:C:N4	29:X:1948:C:OP2	2.42	0.53
29:X:2098:G:O2'	29:X:2154:A:N6	2.42	0.53
3:B:16:LYS:HB2	3:B:21:ILE:HD11	1.92	0.52
8:G:37:ASP:HB2	8:G:38:GLU:HG3	1.91	0.52
11:J:115:ALA:O	11:J:119:PHE:HB2	2.09	0.52
13:L:35:SER:OG	13:L:36:LYS:N	2.37	0.52
15:N:11:ARG:O	15:N:15:LYS:HG3	2.08	0.52
21:T:26:PHE:CE1	29:X:870:C:H1'	2.44	0.52
22:U:17:SER:CB	22:U:18:VAL:HB	2.36	0.52
29:X:220:U:H2'	29:X:221:A:C8	2.43	0.52
29:X:1728:A:H61	29:X:1738:U:H3	1.57	0.52
29:X:1794:A:N6	29:X:1806:G:O2'	2.42	0.52
29:X:2038:C:H2'	29:X:2483:U:C4'	2.40	0.52
29:X:2262:C:C5	29:X:2368:G:H2'	2.45	0.52
29:X:2606:G:H21	29:X:2761:A:H2	1.56	0.52
1:O:112:THR:HG22	1:O:113:PRO:HD2	1.91	0.52
6:E:103:LEU:HD21	6:E:131:ILE:HD13	1.91	0.52
9:H:2:ILE:O	9:H:45:ALA:N	2.43	0.52
15:N:6:THR:O	15:N:9:VAL:HG23	2.10	0.52
19:R:59:LYS:N	19:R:60:PRO:HD2	2.24	0.52
22:U:51:ILE:HA	22:U:59:THR:O	2.09	0.52
25:Z:10:LYS:HB2	29:X:2000:U:O2	2.09	0.52
29:X:218:A:H61	29:X:232:A:H3'	1.74	0.52
29:X:627:A:C6	29:X:628:A:C6	2.96	0.52
29:X:670:U:H2'	29:X:671:A:C8	2.44	0.52
29:X:2630:C:H2'	29:X:2631:C:C6	2.44	0.52
6:E:99:THR:O	6:E:101:LYS:N	2.40	0.52
9:H:16:ALA:HB2	9:H:98:ILE:HD11	1.91	0.52
21:T:39:ARG:HH21	29:X:2334:C:H1'	1.73	0.52
28:3:17:THR:HG21	28:3:21:LYS:HG3	1.90	0.52
29:X:16:G:O2'	29:X:17:G:H5'	2.10	0.52
29:X:2651:U:C2	29:X:2652:G:C8	2.98	0.52
9:H:38:GLY:HA2	29:X:2627:G:N3	2.24	0.52
9:H:54:SER:HA	9:H:69:VAL:HA	1.91	0.52
10:I:86:THR:HG1	10:I:116:ARG:HH11	1.56	0.52
14:M:55:ILE:O	14:M:103:LYS:O	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:73:PHE:O	14:M:75:GLU:N	2.42	0.52
17:P:40:LEU:HA	17:P:43:ASP:OD2	2.08	0.52
22:U:22:GLY:O	22:U:39:LYS:HG3	2.09	0.52
29:X:24:G:H2'	29:X:25:U:H6	1.73	0.52
29:X:58:C:H1'	29:X:72:A:H2'	1.91	0.52
29:X:490:A:H4'	29:X:491:A:OP1	2.09	0.52
29:X:529:U:C2	29:X:530:G:C8	2.98	0.52
29:X:1030:U:N3	29:X:1031:C:H5	2.06	0.52
29:X:1672:A:H3'	29:X:1673:C:C6	2.44	0.52
29:X:1686:A:H5''	29:X:1687:C:OP2	2.09	0.52
29:X:2707:G:H2'	29:X:2708:U:H6	1.74	0.52
10:I:114:ILE:HG21	10:I:132:ALA:O	2.09	0.52
11:J:49:GLU:O	11:J:53:ILE:HG13	2.10	0.52
11:J:100:PRO:HG2	20:S:74:ARG:HH11	1.74	0.52
13:L:89:PHE:HZ	13:L:100:VAL:HG22	1.74	0.52
18:Q:15:LYS:NZ	29:X:1353:A:OP1	2.38	0.52
20:S:155:PRO:O	20:S:156:GLU:HB3	2.10	0.52
29:X:812:G:H3'	29:X:813:A:H2'	1.91	0.52
29:X:1222:G:O2'	29:X:1250:A:N1	2.42	0.52
29:X:1282:A:O5'	29:X:1282:A:H8	1.92	0.52
29:X:1774:A:H5'	29:X:2587:G:H4'	1.90	0.52
29:X:2001:G:C6	29:X:2002:A:C6	2.97	0.52
30:Y:16:U:O2'	30:Y:17:A:P	2.67	0.52
10:I:93:LEU:HB3	10:I:97:ARG:NH1	2.24	0.52
29:X:483:A:H3'	29:X:484:G:H5'	1.91	0.52
29:X:1903:C:H5'	29:X:1904:G:OP2	2.09	0.52
29:X:2779:C:H2'	29:X:2780:A:C8	2.45	0.52
9:H:70:VAL:HG21	9:H:106:ARG:NH1	2.25	0.52
11:J:84:MET:HE2	29:X:967:G:H4'	1.92	0.52
12:K:54:THR:HG22	12:K:66:VAL:HG23	1.90	0.52
13:L:15:ARG:HH21	29:X:2272:A:P	2.32	0.52
13:L:60:LYS:HG2	13:L:61:SER:H	1.74	0.52
26:1:21:TYR:OH	29:X:2397:A:N3	2.43	0.52
29:X:739:G:O2'	29:X:740:A:OP2	2.27	0.52
29:X:1238:A:O2'	29:X:1239:A:O4'	2.25	0.52
29:X:2198:U:C3'	29:X:2199:C:H4'	2.39	0.52
11:J:19:THR:HG22	11:J:20:GLY:N	2.16	0.52
13:L:65:THR:OG1	30:Y:52:G:OP1	2.25	0.52
23:V:31:GLN:O	23:V:35:GLY:N	2.43	0.52
25:Z:3:LYS:HA	29:X:2556:A:O2'	2.10	0.52
29:X:501:G:H2'	29:X:502:A:C8	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1744:G:C2	29:X:1747:G:C2	2.98	0.52
29:X:2230:G:H5''	29:X:2231:G:OP2	2.09	0.52
29:X:2791:C:N3	29:X:2806:G:N2	2.57	0.52
30:Y:39:C:H5''	30:Y:40:C:C6	2.45	0.52
2:A:250:TRP:CE2	29:X:1796:A:H5''	2.45	0.52
4:C:84:PHE:HE1	29:X:596:C:H5'	1.75	0.52
7:F:133:SER:OG	29:X:1073:G:N3	2.43	0.52
10:I:20:GLY:HA3	10:I:21:ARG:NH1	2.24	0.52
11:J:59:PHE:CD2	11:J:110:VAL:HG11	2.44	0.52
25:Z:5:PRO:HG3	29:X:2593:A:C8	2.45	0.52
29:X:242:A:H1'	29:X:243:G:H1'	1.91	0.52
29:X:1234:C:H42	29:X:1241:G:H1	1.58	0.52
29:X:1323:G:H1'	29:X:1627:C:H5'	1.91	0.52
29:X:1462:C:O2'	29:X:1560:A:N3	2.32	0.52
29:X:1533:G:H2'	29:X:1534:A:C8	2.44	0.52
29:X:1578:U:H2'	29:X:1579:G:H8	1.75	0.52
29:X:1889:G:O2'	29:X:1890:G:H5''	2.09	0.52
2:A:238:GLY:O	2:A:240:THR:N	2.43	0.52
4:C:51:VAL:O	4:C:53:LYS:N	2.43	0.52
10:I:18:ARG:HH22	29:X:1262:U:H2'	1.74	0.52
22:U:27:ASP:O	22:U:32:ARG:HD3	2.10	0.52
29:X:13:A:O2'	29:X:15:G:N7	2.43	0.52
29:X:1065:A:H2'	29:X:1066:G:C8	2.45	0.52
29:X:1194:U:H2'	29:X:1195:U:C6	2.45	0.52
29:X:1905:G:H8	29:X:1905:G:OP2	1.92	0.52
29:X:1982:C:H4'	29:X:2703:C:O2	2.09	0.52
29:X:2551:A:H5''	29:X:2553:G:H4'	1.91	0.52
29:X:2579:A:H2'	29:X:2580:C:C5	2.44	0.52
29:X:2676:G:C2	29:X:2690:A:C2	2.98	0.52
30:Y:59:A:H5'	30:Y:60:A:OP2	2.09	0.52
2:A:48:ARG:NH2	29:X:791:G:H5'	2.25	0.51
4:C:18:PRO:HB2	4:C:106:MET:HG3	1.92	0.51
7:F:2:ARG:NH2	7:F:29:GLN:O	2.43	0.51
18:Q:28:TRP:CZ3	18:Q:77:LYS:HB2	2.45	0.51
19:R:46:VAL:N	19:R:76:LEU:O	2.44	0.51
29:X:1278:A:H5'	29:X:1280:U:H1'	1.91	0.51
29:X:1533:G:H2'	29:X:1534:A:H8	1.74	0.51
29:X:2120:C:N4	29:X:2137:G:O6	2.42	0.51
29:X:2308:A:N6	29:X:2365:U:O4	2.39	0.51
30:Y:15:A:N1	30:Y:71:G:O2'	2.33	0.51
2:A:124:GLU:O	2:A:126:LYS:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:231:HIS:CG	2:A:232:PRO:HD2	2.45	0.51
7:F:107:ILE:HG21	7:F:127:VAL:HG11	1.92	0.51
8:G:81:VAL:HG11	8:G:156:HIS:CD2	2.45	0.51
13:L:37:HIS:CE1	13:L:39:TYR:CD1	2.96	0.51
15:N:3:ARG:HG2	29:X:457:C:H5''	1.92	0.51
15:N:90:LEU:HD13	15:N:95:LEU:HD21	1.92	0.51
29:X:826:U:H2'	29:X:827:C:C6	2.45	0.51
29:X:1548:U:H3	29:X:1555:A:H61	1.57	0.51
29:X:1673:C:C2	29:X:1674:C:C5	2.98	0.51
4:C:130:THR:HG23	29:X:332:C:H5''	1.92	0.51
29:X:915:C:H2'	29:X:916:U:C6	2.45	0.51
29:X:1354:A:H2'	29:X:1410:U:O2	2.10	0.51
29:X:1441:A:H4'	29:X:1442:C:O5'	2.09	0.51
29:X:2859:U:C5	29:X:2860:C:C2	2.98	0.51
1:O:61:PRO:HG2	1:O:184:ASN:HA	1.91	0.51
17:P:12:LYS:NZ	29:X:319:G:N7	2.41	0.51
17:P:48:LYS:O	17:P:50:VAL:N	2.37	0.51
22:U:21:ARG:NH1	29:X:400:U:H5'	2.12	0.51
22:U:38:THR:HG22	29:X:2412:A:H2	1.75	0.51
29:X:389:G:H1	29:X:411:C:N4	2.08	0.51
29:X:1662:G:OP1	29:X:1663:C:H5'	2.10	0.51
29:X:2340:C:H2'	29:X:2341:G:O4'	2.11	0.51
2:A:14:ARG:HG3	2:A:15:GLN:H	1.76	0.51
2:A:85:ASP:HB2	2:A:92:ILE:HD13	1.93	0.51
14:M:10:GLY:O	14:M:13:LEU:HB2	2.11	0.51
19:R:95:ARG:HH22	19:R:109:ALA:HA	1.75	0.51
23:V:25:LEU:HA	23:V:28:LEU:HD12	1.92	0.51
27:2:7:PRO:HB2	29:X:1322:G:H4'	1.93	0.51
28:3:29:LYS:O	28:3:30:ARG:HD3	2.11	0.51
28:3:64:ARG:HD2	29:X:220:U:H5'	1.92	0.51
29:X:854:G:H1'	29:X:949:G:N2	2.26	0.51
29:X:929:A:H2	30:Y:81:C:O2	1.93	0.51
29:X:1334:A:H2'	29:X:1335:A:O4'	2.11	0.51
29:X:1681:A:O5'	29:X:1681:A:C8	2.63	0.51
29:X:1685:A:N6	29:X:1693:A:H61	2.09	0.51
29:X:2440:C:H2'	29:X:2441:U:C6	2.42	0.51
3:B:112:GLY:O	3:B:159:HIS:HA	2.10	0.51
3:B:134:TRP:HA	3:B:137:ARG:HD3	1.93	0.51
4:C:149:LEU:HD11	4:C:170:LEU:HG	1.92	0.51
4:C:174:GLY:HA3	29:X:626:A:C4	2.45	0.51
9:H:83:ARG:CZ	9:H:89:ILE:HD11	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:22:ARG:HD3	12:K:69:ASP:HA	1.93	0.51
20:S:56:VAL:O	20:S:58:GLY:N	2.39	0.51
21:T:16:SER:OG	29:X:2241:U:OP2	2.20	0.51
29:X:67:G:H2'	29:X:68:C:H6	1.76	0.51
29:X:556:A:H4'	29:X:558:G:H21	1.76	0.51
29:X:1680:U:H4'	29:X:2666:U:OP1	2.10	0.51
29:X:2144:C:O2'	29:X:2156:A:H1'	2.10	0.51
29:X:2494:C:O2	29:X:2549:G:C2	2.63	0.51
29:X:2528:G:C2	29:X:2529:G:N7	2.79	0.51
29:X:2607:C:H1'	29:X:2761:A:C2	2.46	0.51
29:X:2665:G:N2	29:X:2704:U:O2	2.43	0.51
1:O:71:ALA:HB3	1:O:109:VAL:HG22	1.93	0.51
3:B:144:ARG:HD3	29:X:2551:A:N7	2.25	0.51
3:B:174:GLU:HB3	3:B:183:LEU:HD12	1.93	0.51
11:J:86:LYS:HZ3	21:T:6:GLY:HA2	1.76	0.51
14:M:106:TYR:HE1	29:X:1745:C:H5'	1.75	0.51
17:P:9:ARG:NH2	29:X:318:G:OP1	2.43	0.51
22:U:46:LEU:HB2	29:X:2209:G:H4'	1.92	0.51
29:X:227:G:C6	29:X:228:A:C6	2.98	0.51
29:X:942:U:H2'	29:X:943:U:C6	2.46	0.51
29:X:1578:U:H2'	29:X:1579:G:C8	2.46	0.51
29:X:2097:A:H61	29:X:2102:A:N6	2.09	0.51
29:X:2477:C:O2'	29:X:2478:C:H5'	2.11	0.51
29:X:2542:U:O2	29:X:2544:A:H8	1.93	0.51
29:X:2867:G:OP2	29:X:2867:G:H8	1.92	0.51
2:A:201:HIS:C	2:A:203:ASN:H	2.19	0.51
4:C:193:LEU:HA	4:C:196:VAL:HG22	1.93	0.51
11:J:28:VAL:HB	11:J:135:ARG:HA	1.93	0.51
13:L:39:TYR:OH	30:Y:118:G:H1'	2.10	0.51
24:W:35:SER:O	24:W:37:THR:OG1	2.28	0.51
28:3:22:VAL:HG22	28:3:50:LEU:HD23	1.91	0.51
29:X:959:C:H2'	29:X:960:U:C6	2.45	0.51
29:X:1764:A:H2'	29:X:1765:C:H5'	1.92	0.51
29:X:1851:A:H3'	29:X:1852:G:H8	1.75	0.51
30:Y:7:C:H2'	30:Y:8:C:C6	2.45	0.51
2:A:24:LEU:HD22	2:A:82:ILE:O	2.11	0.51
5:D:129:ASN:HA	5:D:155:THR:HA	1.93	0.51
7:F:12:LEU:HD21	7:F:23:VAL:HG22	1.93	0.51
14:M:2:GLN:N	29:X:2795:A:H61	2.09	0.51
15:N:31:GLN:HB3	29:X:590:C:OP1	2.11	0.51
19:R:44:GLN:HG2	19:R:77:HIS:CE1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:914:C:H2'	29:X:915:C:C6	2.46	0.51
29:X:1478:U:H2'	29:X:1479:G:H8	1.75	0.51
29:X:1889:G:H1	29:X:1908:C:H5''	1.76	0.51
29:X:2629:U:H2'	29:X:2630:C:C6	2.40	0.51
5:D:27:ALA:HB2	30:Y:59:A:H1'	1.91	0.51
7:F:10:LEU:HD22	7:F:27:LEU:HD21	1.92	0.51
11:J:26:ASP:HA	11:J:103:VAL:HG23	1.93	0.51
12:K:8:ARG:HB2	12:K:43:GLU:OE1	2.11	0.51
20:S:17:SER:HA	20:S:36:ARG:HH22	1.75	0.51
23:V:63:LYS:HG2	23:V:66:GLN:NE2	2.25	0.51
29:X:1683:G:H1	29:X:1977:C:N4	2.08	0.51
29:X:2447:G:HO2'	29:X:2448:A:H8	1.57	0.51
29:X:2847:G:C2	29:X:2848:A:N6	2.79	0.51
5:D:115:ARG:HB2	5:D:178:ARG:HG3	1.93	0.50
5:D:117:ILE:HG22	5:D:118:ASN:H	1.76	0.50
7:F:90:THR:OG1	7:F:93:LYS:HB2	2.10	0.50
10:I:101:ARG:O	10:I:102:LYS:HB2	2.11	0.50
12:K:28:LEU:HD23	12:K:48:VAL:HG11	1.92	0.50
25:Z:7:PRO:HB3	29:X:2594:U:H1'	1.93	0.50
27:2:37:LYS:O	29:X:469:G:H2'	2.11	0.50
28:3:33:ASN:C	28:3:35:GLY:H	2.18	0.50
29:X:1211:G:C2	29:X:1212:U:C5	2.98	0.50
29:X:1231:A:N6	29:X:1245:G:O6	2.44	0.50
29:X:1281:A:OP1	29:X:1989:C:OP1	2.28	0.50
29:X:1707:A:H3'	29:X:1708:C:C6	2.46	0.50
29:X:1971:C:H2'	29:X:1972:G:O4'	2.11	0.50
29:X:2283:G:N2	29:X:2291:U:H3	2.05	0.50
29:X:2695:C:H2'	29:X:2696:A:H8	1.76	0.50
4:C:72:ARG:NE	4:C:77:PHE:HE2	2.07	0.50
19:R:18:LYS:HA	19:R:36:VAL:CG1	2.40	0.50
25:Z:18:MET:HE2	29:X:2028:C:H5'	1.92	0.50
29:X:522:G:OP1	29:X:1247:U:O2'	2.27	0.50
29:X:640:C:H4'	29:X:660:G:H21	1.75	0.50
29:X:967:G:H2'	29:X:968:C:H2'	1.93	0.50
29:X:1039:A:N6	29:X:1137:A:OP1	2.35	0.50
29:X:1468:A:N7	29:X:2681:A:N6	2.59	0.50
4:C:189:ASP:CG	4:C:190:ALA:H	2.19	0.50
5:D:10:ASP:HA	5:D:13:ARG:HG3	1.94	0.50
7:F:54:PRO:HD3	7:F:73:PRO:HD3	1.94	0.50
11:J:88:LYS:HG3	29:X:966:A:H5''	1.92	0.50
12:K:52:ILE:HG21	12:K:94:TYR:CG	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:103:ARG:NH2	12:K:108:VAL:HB	2.24	0.50
15:N:48:ARG:CD	29:X:1167:A:H61	2.13	0.50
29:X:503:G:H2'	29:X:504:G:O4'	2.11	0.50
29:X:653:G:H2'	29:X:654:A:H3'	1.93	0.50
29:X:1238:A:H2'	29:X:1239:A:C8	2.46	0.50
30:Y:16:U:HO2'	30:Y:17:A:P	2.34	0.50
30:Y:39:C:H5'	30:Y:40:C:OP2	2.11	0.50
4:C:179:ASP:O	4:C:182:ARG:HB3	2.11	0.50
6:E:45:GLN:HG2	6:E:47:GLY:H	1.77	0.50
8:G:52:GLY:O	8:G:55:ALA:HB3	2.12	0.50
12:K:103:ARG:CZ	12:K:106:ASP:OD2	2.59	0.50
17:P:37:LYS:NZ	29:X:1995:G:OP2	2.41	0.50
20:S:37:LYS:O	20:S:41:ARG:HG2	2.12	0.50
21:T:41:ARG:HE	21:T:41:ARG:HA	1.77	0.50
29:X:125:A:H5''	29:X:126:C:O4'	2.11	0.50
29:X:213:C:H2'	29:X:214:C:H6	1.75	0.50
29:X:661:C:H2'	29:X:662:G:C8	2.46	0.50
29:X:866:U:H2'	29:X:867:G:C8	2.45	0.50
29:X:1856:U:H2'	29:X:1857:G:C8	2.46	0.50
29:X:1991:C:H2'	29:X:1992:G:H8	1.77	0.50
29:X:2425:G:H2'	29:X:2480:C:H5	1.76	0.50
29:X:2563:U:HO2'	29:X:2564:U:H5	1.58	0.50
29:X:2595:C:H2'	29:X:2596:C:H6	1.76	0.50
29:X:2659:C:C2	29:X:2660:C:C5	3.00	0.50
30:Y:36:A:N6	30:Y:46:G:O2'	2.44	0.50
1:O:150:ARG:HG2	1:O:153:LYS:HD2	1.92	0.50
3:B:8:LYS:HG2	3:B:192:ASN:HD22	1.76	0.50
6:E:150:LYS:HZ1	29:X:2741:G:H21	1.60	0.50
10:I:72:TYR:HE2	10:I:105:PRO:HB2	1.76	0.50
11:J:44:LYS:O	11:J:47:GLN:N	2.44	0.50
12:K:98:LEU:HD23	12:K:99:ARG:NH2	2.27	0.50
17:P:81:HIS:HD1	17:P:82:ASN:N	2.10	0.50
17:P:106:LEU:HA	17:P:115:ASN:O	2.11	0.50
19:R:20:ASP:O	19:R:36:VAL:HG23	2.11	0.50
29:X:46:C:H2'	29:X:47:G:C8	2.41	0.50
29:X:872:G:O2'	29:X:928:G:O6	2.30	0.50
29:X:991:A:C4	29:X:1146:G:O4'	2.64	0.50
29:X:2630:C:H2'	29:X:2631:C:H6	1.76	0.50
29:X:2649:A:H2'	29:X:2650:G:O4'	2.11	0.50
2:A:40:THR:O	2:A:40:THR:OG1	2.26	0.50
4:C:46:ARG:HB3	4:C:50:GLN:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:67:LEU:HD11	29:X:2738:A:C5	2.47	0.50
6:E:158:HIS:NE2	29:X:2638:G:OP1	2.45	0.50
8:G:157:PRO:HG2	8:G:158:HIS:CE1	2.47	0.50
9:H:115:ALA:C	9:H:117:GLU:H	2.18	0.50
10:I:57:ILE:HD12	28:3:61:MET:SD	2.52	0.50
17:P:39:ARG:NH2	29:X:527:C:O2'	2.44	0.50
29:X:98:U:H4'	29:X:100:G:C8	2.45	0.50
29:X:1142:G:H1'	29:X:1143:A:C8	2.47	0.50
29:X:1353:A:H3'	29:X:1354:A:H8	1.76	0.50
2:A:40:THR:O	2:A:42:GLY:N	2.44	0.50
2:A:208:LYS:HD2	29:X:742:G:C8	2.47	0.50
3:B:146:THR:HG23	29:X:1141:U:C5	2.47	0.50
9:H:1:MET:SD	9:H:79:HIS:NE2	2.84	0.50
9:H:43:ARG:HH21	29:X:1979:C:P	2.34	0.50
16:O:92:ALA:C	16:O:93:ILE:HD12	2.37	0.50
29:X:5:A:H2'	29:X:6:A:H8	1.73	0.50
29:X:513:A:OP1	29:X:514:G:N2	2.39	0.50
29:X:2230:G:H3'	29:X:2231:G:H8	1.76	0.50
29:X:2407:G:H4'	29:X:2408:G:C4	2.47	0.50
2:A:202:LYS:HB2	29:X:1812:U:C2	2.46	0.50
2:A:219:PRO:HG3	29:X:794:A:C8	2.46	0.50
22:U:21:ARG:O	22:U:39:LYS:HD2	2.11	0.50
29:X:61:U:H3	29:X:91:A:H2	1.58	0.50
29:X:1742:G:C2	29:X:1743:C:N3	2.80	0.50
29:X:2291:U:H2'	29:X:2292:C:H6	1.77	0.50
30:Y:35:C:H2'	30:Y:36:A:C8	2.47	0.50
2:A:18:THR:HG21	29:X:1581:C:H5''	1.92	0.50
3:B:11:MET:O	29:X:2661:G:H5'	2.12	0.50
13:L:67:THR:HG22	13:L:71:VAL:HG12	1.94	0.50
15:N:33:ARG:HB3	29:X:1265:G:N2	2.27	0.50
26:1:27:ASN:C	26:1:29:ARG:H	2.20	0.50
29:X:12:U:O2	29:X:12:U:H2'	2.12	0.50
29:X:79:G:N2	29:X:104:C:O2	2.45	0.50
29:X:525:A:C2'	29:X:526:C:H5'	2.42	0.50
29:X:746:G:O6	29:X:774:A:C8	2.65	0.50
29:X:787:A:O2'	29:X:788:G:O4'	2.24	0.50
29:X:1030:U:OP1	29:X:1046:U:O2'	2.21	0.50
3:B:2:LYS:HZ3	3:B:95:ILE:HA	1.77	0.49
10:I:16:ARG:NH2	29:X:598:U:OP2	2.44	0.49
10:I:50:GLU:HA	29:X:846:A:C4'	2.42	0.49
11:J:53:ILE:O	11:J:57:ARG:HG2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:99:ARG:H	12:K:99:ARG:NE	2.10	0.49
17:P:39:ARG:O	17:P:42:VAL:HG12	2.11	0.49
18:Q:53:ILE:HG12	18:Q:54:SER:N	2.27	0.49
20:S:100:THR:HG21	20:S:113:VAL:HG11	1.93	0.49
22:U:9:GLY:H	22:U:14:VAL:HG22	1.77	0.49
25:Z:4:HIS:ND1	25:Z:4:HIS:O	2.45	0.49
29:X:668:A:H2'	29:X:668:A:OP2	2.12	0.49
29:X:1354:A:H5''	29:X:1410:U:O2	2.11	0.49
29:X:1815:G:H2'	29:X:1816:G:C8	2.46	0.49
29:X:2410:U:O2	29:X:2412:A:C8	2.63	0.49
29:X:2587:G:H8	29:X:2587:G:O5'	1.95	0.49
29:X:2642:G:H2'	29:X:2643:G:O4'	2.12	0.49
4:C:152:THR:HA	4:C:189:ASP:OD2	2.12	0.49
12:K:102:THR:O	12:K:103:ARG:HB2	2.12	0.49
19:R:99:VAL:HB	19:R:105:ARG:HD2	1.93	0.49
24:W:26:ARG:NH1	29:X:1197:U:H5''	2.28	0.49
28:3:36:LYS:HB2	28:3:37:SER:HA	1.94	0.49
29:X:224:G:OP2	29:X:226:C:N4	2.44	0.49
29:X:513:A:C6	29:X:515:A:C6	3.00	0.49
29:X:580:A:N3	29:X:582:G:C8	2.80	0.49
29:X:991:A:N6	29:X:992:A:N6	2.60	0.49
29:X:1017:C:H2'	29:X:1018:C:H6	1.76	0.49
29:X:1830:C:H4'	29:X:1831:G:C8	2.47	0.49
29:X:2180:U:H2'	29:X:2203:G:N1	2.27	0.49
4:C:72:ARG:NH1	29:X:1271:C:OP1	2.32	0.49
5:D:8:TYR:O	5:D:12:VAL:HG23	2.12	0.49
11:J:15:ARG:HG3	11:J:73:LYS:HG3	1.93	0.49
12:K:83:VAL:O	12:K:86:LYS:HB2	2.11	0.49
14:M:48:GLN:HG2	14:M:49:ALA:H	1.76	0.49
20:S:66:VAL:HG22	20:S:83:PHE:HE1	1.77	0.49
20:S:149:ALA:HA	20:S:152:ILE:HD13	1.94	0.49
22:U:23:LYS:HB3	22:U:37:ILE:HG22	1.95	0.49
28:3:33:ASN:O	28:3:36:LYS:HA	2.13	0.49
29:X:974:U:H2'	29:X:975:C:H6	1.77	0.49
29:X:1428:G:N2	29:X:1601:U:O4'	2.45	0.49
29:X:1451:C:O2'	29:X:1533:G:H4'	2.10	0.49
29:X:1542:G:H2'	29:X:1543:G:H8	1.76	0.49
29:X:1872:A:N1	29:X:2213:G:H1'	2.27	0.49
29:X:2273:C:H2'	29:X:2274:C:C6	2.47	0.49
1:O:58:VAL:HG13	1:O:191:ALA:HB3	1.94	0.49
3:B:9:ILE:HD11	3:B:27:LEU:CB	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:92:ARG:HD3	30:Y:47:A:H8	1.77	0.49
6:E:153:LYS:HG3	6:E:154:PRO:HD2	1.94	0.49
7:F:78:ILE:HD11	7:F:107:ILE:HD11	1.93	0.49
9:H:10:VAL:HG22	9:H:19:ILE:HG22	1.94	0.49
10:I:4:HIS:C	10:I:4:HIS:CD2	2.90	0.49
10:I:31:GLY:O	29:X:1204:G:H5''	2.12	0.49
22:U:50:ALA:HB3	22:U:62:LEU:HB3	1.93	0.49
26:1:38:LYS:HB2	29:X:2323:U:H2'	1.94	0.49
29:X:358:C:H2'	29:X:359:G:H5'	1.95	0.49
29:X:464:G:H2'	29:X:465:C:C6	2.48	0.49
29:X:583:C:C5	29:X:2016:A:H4'	2.47	0.49
29:X:1326:U:O3'	29:X:1345:G:H5'	2.13	0.49
29:X:1669:A:H2	29:X:1989:C:N3	2.10	0.49
29:X:1681:A:C2	29:X:2706:U:C2	3.00	0.49
29:X:2511:G:H2'	29:X:2512:A:O4'	2.12	0.49
29:X:2837:G:H2'	29:X:2838:U:H6	1.77	0.49
30:Y:63:A:H2'	30:Y:64:C:H6	1.77	0.49
2:A:4:LYS:NZ	29:X:1581:C:OP1	2.40	0.49
3:B:159:HIS:NE2	29:X:2797:G:OP1	2.45	0.49
4:C:176:ASN:OD1	4:C:179:ASP:N	2.41	0.49
7:F:73:PRO:HB3	29:X:1071:U:OP1	2.13	0.49
9:H:42:LYS:HA	29:X:2653:A:O3'	2.13	0.49
10:I:50:GLU:HA	29:X:846:A:H4'	1.94	0.49
14:M:55:ILE:HD11	14:M:67:THR:HG21	1.93	0.49
25:Z:16:ARG:HG3	29:X:1277:G:OP1	2.12	0.49
28:3:32:GLN:OE1	28:3:44:LYS:HE2	2.12	0.49
29:X:54:G:C2	29:X:114:C:C2	2.99	0.49
29:X:78:C:H2'	29:X:79:G:H8	1.77	0.49
29:X:206:U:O2	29:X:206:U:H2'	2.11	0.49
29:X:1174:G:C2	29:X:1175:A:N7	2.80	0.49
29:X:1313:U:O2	29:X:1642:G:N1	2.46	0.49
29:X:2661:G:O6	29:X:2708:U:H1'	2.13	0.49
29:X:2802:C:H2'	29:X:2803:C:H6	1.76	0.49
11:J:19:THR:CG2	11:J:20:GLY:H	2.16	0.49
13:L:37:HIS:CD2	30:Y:29:C:O3'	2.65	0.49
17:P:29:LYS:HB2	29:X:503:G:H4'	1.95	0.49
20:S:23:ALA:HA	20:S:83:PHE:HB2	1.94	0.49
25:Z:7:PRO:O	29:X:1999:U:O2'	2.25	0.49
29:X:356:A:H2'	29:X:357:A:N7	2.26	0.49
29:X:457:C:H2'	29:X:458:G:H5''	1.93	0.49
29:X:564:U:H2'	29:X:565:A:C8	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:712:A:H5'	29:X:712:A:H8	1.75	0.49
29:X:1660:G:C6	29:X:1661:C:C5	3.01	0.49
29:X:1913:G:N2	29:X:1914:U:O4	2.38	0.49
29:X:1919:A:C2	29:X:1928:G:C8	3.00	0.49
29:X:2140:G:H2'	29:X:2140:G:N3	2.27	0.49
4:C:95:LEU:HD12	4:C:96:PRO:CD	2.42	0.49
25:Z:49:CYS:SG	25:Z:51:TYR:HB2	2.53	0.49
29:X:661:C:H2'	29:X:662:G:H8	1.77	0.49
29:X:754:G:H2'	29:X:755:C:C6	2.47	0.49
29:X:858:G:C8	29:X:858:G:OP2	2.65	0.49
29:X:1299:A:C6	29:X:1302:C:C2	3.01	0.49
29:X:1673:C:H2'	29:X:1674:C:H6	1.78	0.49
29:X:2378:G:H1	29:X:2396:C:N4	2.08	0.49
29:X:2713:A:H2'	29:X:2714:A:H8	1.78	0.49
3:B:133:LYS:NZ	29:X:758:G:OP2	2.28	0.49
12:K:51:LEU:HD13	12:K:70:ILE:HD11	1.95	0.49
18:Q:7:LEU:HD11	18:Q:41:ALA:HB1	1.94	0.49
20:S:106:GLY:HA2	20:S:109:GLN:HE22	1.77	0.49
28:3:46:LYS:HB3	28:3:47:GLY:H	1.40	0.49
29:X:331:U:H4'	29:X:333:A:C8	2.48	0.49
29:X:1099:A:H2'	29:X:1099:A:N3	2.28	0.49
29:X:2097:A:H2'	29:X:2098:G:O4'	2.13	0.49
29:X:2794:G:C6	29:X:2796:A:C2	3.00	0.49
30:Y:30:C:H42	30:Y:58:G:H1	1.58	0.49
3:B:141:ILE:HD11	29:X:2034:A:O4'	2.12	0.49
4:C:33:TRP:HD1	4:C:93:TYR:CZ	2.31	0.49
10:I:72:TYR:HB3	10:I:107:LYS:HB2	1.94	0.49
19:R:17:LYS:HG3	29:X:83:A:H3'	1.95	0.49
26:1:8:ILE:HD12	26:1:28:ARG:NE	2.28	0.49
29:X:171:G:H2'	29:X:172:A:C8	2.48	0.49
29:X:229:G:H2'	29:X:230:C:H6	1.78	0.49
29:X:635:C:O2	29:X:670:U:H4'	2.12	0.49
29:X:1129:A:H2'	29:X:1130:U:O4'	2.13	0.49
29:X:1174:G:C2	29:X:1175:A:C5	3.00	0.49
29:X:1379:A:H2'	29:X:1380:C:C6	2.47	0.49
29:X:1499:A:H2'	29:X:1500:U:C6	2.48	0.49
29:X:1505:U:O2	29:X:1506:C:O2'	2.21	0.49
29:X:1611:U:H2'	29:X:1612:U:C6	2.48	0.49
29:X:1669:A:C2	29:X:1989:C:N3	2.81	0.49
29:X:2034:A:H2	29:X:2035:G:O6	1.95	0.49
29:X:2431:C:H1'	32:X:6178:HGR:C1	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2592:U:H6	29:X:2592:U:H5'	1.78	0.49
2:A:199:ALA:HA	29:X:1812:U:H3	1.77	0.49
4:C:155:GLU:H	4:C:155:GLU:CD	2.21	0.49
8:G:58:ILE:HG12	8:G:80:VAL:HG11	1.94	0.49
9:H:64:VAL:HG13	9:H:68:ASP:OD2	2.13	0.49
15:N:22:LYS:NZ	29:X:1232:U:OP1	2.46	0.49
15:N:60:LEU:HD11	15:N:64:ARG:HE	1.78	0.49
22:U:14:VAL:HB	22:U:15:VAL:H	1.41	0.49
28:3:17:THR:HG21	28:3:21:LYS:CG	2.43	0.49
29:X:399:G:O2'	29:X:400:U:OP1	2.29	0.49
29:X:408:U:H2'	29:X:409:G:C8	2.48	0.49
29:X:820:U:H2'	29:X:821:A:H8	1.78	0.49
29:X:1982:C:H5''	29:X:2703:C:H1'	1.95	0.49
2:A:201:HIS:O	2:A:204:ILE:HG13	2.13	0.48
3:B:175:ILE:HG12	3:B:182:ILE:CD1	2.43	0.48
9:H:10:VAL:HA	9:H:96:ALA:O	2.12	0.48
9:H:21:CYS:SG	9:H:51:ILE:HG13	2.53	0.48
10:I:110:ALA:O	10:I:111:SER:OG	2.26	0.48
11:J:70:PHE:HA	11:J:71:PRO:HD2	1.63	0.48
25:Z:55:ARG:HH21	25:Z:58:LEU:HA	1.77	0.48
29:X:590:C:H2'	29:X:591:G:H8	1.78	0.48
29:X:742:G:H2'	29:X:1766:U:O2	2.13	0.48
29:X:746:G:C8	29:X:774:A:C6	3.00	0.48
29:X:987:G:C2	29:X:988:G:N7	2.80	0.48
29:X:1761:G:C5	29:X:1762:C:C5	3.01	0.48
29:X:1989:C:O5'	29:X:1989:C:C6	2.65	0.48
29:X:2047:C:O2	29:X:2429:A:N6	2.46	0.48
2:A:132:PRO:O	2:A:136:VAL:HG23	2.12	0.48
3:B:22:PRO:HB3	29:X:2661:G:N3	2.28	0.48
4:C:56:ARG:HB2	29:X:810:U:OP1	2.13	0.48
5:D:17:MET:HE2	5:D:25:VAL:HG12	1.94	0.48
21:T:23:VAL:HG11	29:X:870:C:H4'	1.94	0.48
27:2:34:ARG:NH2	27:2:41:GLN:HG3	2.28	0.48
29:X:202:A:C4	29:X:203:G:H1'	2.48	0.48
29:X:625:A:OP2	29:X:625:A:H4'	2.13	0.48
29:X:689:A:H8	29:X:2052:G:H21	1.60	0.48
29:X:966:A:N6	29:X:967:G:C6	2.81	0.48
29:X:1426:U:H3'	29:X:1427:G:H5''	1.95	0.48
29:X:1491:C:N3	29:X:1533:G:N2	2.60	0.48
29:X:1503:G:H2'	29:X:1504:G:C8	2.48	0.48
29:X:1904:G:H2'	29:X:1905:G:O4'	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1917:C:C2'	29:X:1918:G:H5'	2.43	0.48
29:X:2409:A:O2'	29:X:2410:U:O5'	2.25	0.48
2:A:2:ALA:N	2:A:20:ASP:OD1	2.46	0.48
6:E:54:ARG:NE	6:E:57:ASP:OD2	2.37	0.48
13:L:91:ARG:HB2	13:L:94:TYR:HD1	1.78	0.48
16:O:21:ARG:HD3	16:O:90:PHE:CE1	2.48	0.48
19:R:18:LYS:HB2	29:X:84:G:OP2	2.13	0.48
20:S:3:LEU:HD11	20:S:56:VAL:HG22	1.95	0.48
29:X:750:C:H4'	29:X:779:U:O3'	2.14	0.48
29:X:1108:U:H2'	29:X:1109:A:O4'	2.13	0.48
29:X:1919:A:H2	29:X:1926:U:N3	2.02	0.48
29:X:1920:A:N7	29:X:1923:U:H5	2.11	0.48
9:H:83:ARG:O	9:H:85:ASP:N	2.41	0.48
15:N:74:MET:HE3	15:N:79:PHE:HD1	1.78	0.48
17:P:14:ARG:O	17:P:18:VAL:HG22	2.13	0.48
21:T:56:ASP:CG	29:X:2343:C:H5'	2.39	0.48
25:Z:10:LYS:HG3	29:X:1276:U:H1'	1.96	0.48
29:X:306:G:H2'	29:X:307:C:C6	2.49	0.48
29:X:697:G:O2'	29:X:801:A:N7	2.46	0.48
29:X:731:A:H2'	29:X:732:G:H5'	1.94	0.48
29:X:870:C:C4	29:X:871:U:C4	3.02	0.48
29:X:956:A:C4	29:X:2427:A:C2	3.01	0.48
29:X:965:G:O2'	29:X:2253:A:N1	2.34	0.48
29:X:1174:G:C2	29:X:1175:A:C8	3.02	0.48
29:X:1337:G:N2	29:X:1344:C:C2	2.82	0.48
29:X:1469:U:H4'	29:X:1470:G:OP1	2.14	0.48
29:X:2425:G:H2'	29:X:2480:C:C5	2.47	0.48
29:X:2769:C:H1'	29:X:2866:A:C2	2.48	0.48
2:A:243:GLY:HA3	29:X:2576:G:C5'	2.42	0.48
3:B:57:ARG:HH21	29:X:2809:A:H5'	1.78	0.48
3:B:144:ARG:NH1	29:X:2551:A:C4	2.81	0.48
13:L:46:SER:OG	13:L:47:ARG:N	2.47	0.48
24:W:49:HIS:CD2	24:W:50:LEU:HG	2.49	0.48
27:2:11:LYS:HE2	29:X:699:G:H5''	1.96	0.48
29:X:82:G:H21	29:X:83:A:N6	2.11	0.48
29:X:149:A:OP2	29:X:149:A:H8	1.97	0.48
29:X:219:G:H22	29:X:231:G:H2'	1.78	0.48
29:X:647:G:O2'	29:X:649:G:O2'	2.26	0.48
29:X:772:G:H2'	29:X:773:G:H8	1.79	0.48
29:X:1882:G:O2'	29:X:1883:A:OP2	2.27	0.48
29:X:2279:G:H8	29:X:2279:G:O5'	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2498:U:C5	29:X:2520:A:C6	3.02	0.48
29:X:2533:U:H2'	29:X:2534:U:C6	2.48	0.48
29:X:2708:U:H2'	29:X:2709:C:C6	2.48	0.48
29:X:2840:U:C4	29:X:2841:U:C4	3.01	0.48
1:O:16:TYR:CZ	1:O:24:LEU:HD22	2.49	0.48
2:A:76:ASN:HB3	2:A:118:ASN:CG	2.39	0.48
2:A:211:ARG:NE	29:X:1582:A:OP1	2.40	0.48
11:J:46:ASN:OD1	11:J:46:ASN:N	2.34	0.48
15:N:10:ARG:HG3	15:N:13:ARG:NH2	2.28	0.48
15:N:51:ARG:HA	15:N:54:LYS:HD2	1.96	0.48
17:P:93:LYS:HB2	17:P:129:ALA:HB3	1.95	0.48
19:R:25:LEU:CD1	19:R:82:ALA:HB2	2.42	0.48
20:S:147:ILE:HG23	20:S:151:ASP:HB2	1.95	0.48
27:2:30:ILE:HD13	29:X:477:A:H4'	1.95	0.48
29:X:1370:U:H3'	29:X:1371:G:C8	2.48	0.48
29:X:1509:A:H8	29:X:1510:A:C8	2.32	0.48
29:X:2495:G:C6	29:X:2496:C:N4	2.81	0.48
30:Y:65:A:H2'	30:Y:66:G:H8	1.79	0.48
1:O:210:LEU:HB2	1:O:217:SER:HA	1.94	0.48
4:C:142:LEU:HB3	4:C:166:TRP:CH2	2.48	0.48
6:E:7:GLN:H	6:E:8:PRO:CD	2.27	0.48
10:I:55:ARG:NH1	29:X:228:A:OP1	2.35	0.48
12:K:11:ASN:N	12:K:11:ASN:ND2	2.59	0.48
29:X:218:A:H5'	29:X:220:U:O4'	2.12	0.48
29:X:713:G:H2'	29:X:714:G:O4'	2.13	0.48
29:X:1096:A:H1'	29:X:1116:U:H1'	1.95	0.48
29:X:1727:C:O2'	29:X:2833:C:N3	2.43	0.48
29:X:2047:C:H1'	29:X:2429:A:C6	2.49	0.48
29:X:2784:A:C2	29:X:2866:A:C4	3.02	0.48
1:O:10:VAL:HG22	1:O:218:ILE:HD11	1.96	0.48
2:A:52:ARG:CZ	2:A:53:PHE:HE2	2.26	0.48
4:C:137:ALA:HB1	4:C:142:LEU:HD12	1.95	0.48
5:D:52:LYS:HE2	5:D:146:VAL:HB	1.96	0.48
5:D:70:ALA:C	5:D:72:LYS:H	2.21	0.48
5:D:122:PHE:HE2	5:D:130:LEU:N	2.12	0.48
10:I:81:GLN:HB3	10:I:82:ASP:H	1.43	0.48
20:S:24:TYR:O	20:S:26:LYS:NZ	2.42	0.48
29:X:1054:C:H2'	29:X:1055:A:C8	2.49	0.48
29:X:1401:G:H1	29:X:1412:C:N4	2.08	0.48
29:X:2265:A:H4'	29:X:2266:A:O4'	2.14	0.48
3:B:44:TYR:CE1	29:X:2616:U:H5'	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:115:SER:O	10:I:136:ALA:HB1	2.14	0.48
20:S:26:LYS:HD2	30:Y:107:C:O2'	2.14	0.48
24:W:2:LYS:HD2	24:W:32:ARG:O	2.14	0.48
27:2:2:LYS:HG2	27:2:3:ARG:N	2.28	0.48
29:X:174:A:C5	29:X:175:C:C5	3.02	0.48
29:X:341:A:H2'	29:X:341:A:N3	2.29	0.48
29:X:691:C:C2	29:X:692:C:C5	3.01	0.48
29:X:1672:A:C8	29:X:1673:C:C5	3.01	0.48
29:X:1979:C:H4'	29:X:1980:A:OP1	2.14	0.48
29:X:2492:G:H2'	29:X:2493:U:C6	2.48	0.48
11:J:99:LYS:O	11:J:102:ARG:HB3	2.14	0.48
14:M:105:TYR:HD2	29:X:2698:G:H5'	1.79	0.48
21:T:46:LYS:HB3	21:T:78:PHE:CD2	2.49	0.48
24:W:26:ARG:HH12	29:X:1197:U:H5''	1.78	0.48
26:1:40:TYR:CG	26:1:41:ASP:N	2.82	0.48
29:X:187:U:H2'	29:X:188:G:C8	2.48	0.48
29:X:322:A:H3'	29:X:323:G:C8	2.49	0.48
29:X:772:G:H2'	29:X:773:G:C8	2.49	0.48
29:X:1378:A:H2'	29:X:1378:A:N3	2.29	0.48
29:X:1882:G:N7	29:X:1885:C:N4	2.46	0.48
29:X:2345:A:H2'	29:X:2346:G:O4'	2.14	0.48
29:X:2565:C:H2'	29:X:2566:A:H8	1.78	0.48
4:C:20:PRO:C	4:C:21:GLU:HG2	2.39	0.47
4:C:149:LEU:HB2	4:C:183:HIS:ND1	2.29	0.47
6:E:6:LYS:HB3	6:E:6:LYS:HZ3	1.79	0.47
6:E:35:VAL:HB	6:E:37:TYR:CZ	2.49	0.47
9:H:109:ARG:HA	9:H:129:LEU:HD22	1.95	0.47
12:K:88:ALA:O	12:K:90:ARG:N	2.47	0.47
15:N:52:ASN:O	15:N:55:ARG:N	2.47	0.47
16:O:14:VAL:HG13	16:O:20:ILE:HD11	1.96	0.47
22:U:10:LYS:HD3	22:U:11:LYS:H	1.78	0.47
22:U:49:LYS:HB2	22:U:61:TRP:CZ3	2.47	0.47
26:1:11:LYS:HB2	26:1:22:TYR:O	2.14	0.47
29:X:181:A:H2	29:X:182:G:H21	1.61	0.47
29:X:303:C:N3	29:X:359:G:N2	2.44	0.47
29:X:797:A:O2'	29:X:798:G:H8	1.97	0.47
29:X:1658:A:N6	29:X:1659:G:C2	2.83	0.47
29:X:2432:A:H2'	29:X:2433:G:H8	1.79	0.47
29:X:2456:U:H4'	29:X:2458:U:O4	2.14	0.47
29:X:2495:G:C6	29:X:2548:G:C2	3.01	0.47
29:X:2702:G:C2'	29:X:2703:C:H5'	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2707:G:C4	29:X:2708:U:C5	3.02	0.47
29:X:2728:A:C6	29:X:2737:A:N7	2.83	0.47
29:X:2796:A:C6	29:X:2797:G:C6	3.02	0.47
29:X:2813:G:C4	29:X:2814:G:C8	3.02	0.47
1:O:72:VAL:HG13	1:O:110:VAL:HB	1.96	0.47
4:C:119:ALA:HA	4:C:188:ILE:HB	1.95	0.47
9:H:37:GLY:O	29:X:2627:G:O2'	2.32	0.47
12:K:34:ILE:HG13	12:K:113:ILE:HG22	1.97	0.47
13:L:92:GLY:O	13:L:94:TYR:N	2.43	0.47
17:P:11:LYS:NZ	17:P:15:LYS:HE2	2.27	0.47
17:P:18:VAL:O	17:P:19:LYS:HB2	2.14	0.47
21:T:48:GLY:H	21:T:51:VAL:CG2	2.27	0.47
29:X:699:G:H2'	29:X:801:A:N1	2.29	0.47
29:X:998:C:O2'	29:X:1011:A:N3	2.37	0.47
29:X:1606:C:H2'	29:X:1607:A:H8	1.79	0.47
29:X:1606:C:H2'	29:X:1607:A:C8	2.48	0.47
29:X:1987:G:C4	29:X:1988:A:C8	3.02	0.47
29:X:2662:C:C6	29:X:2663:U:H5	2.32	0.47
2:A:44:ASN:HB2	29:X:1804:U:O2'	2.13	0.47
2:A:71:ASP:CG	2:A:103:ARG:HH22	2.22	0.47
3:B:136:ARG:NH1	29:X:1673:C:OP1	2.46	0.47
5:D:70:ALA:HB3	5:D:81:GLN:O	2.14	0.47
9:H:8:LEU:HD23	9:H:8:LEU:N	2.28	0.47
9:H:26:ASN:HB3	9:H:38:GLY:H	1.78	0.47
9:H:85:ASP:CG	9:H:87:SER:H	2.22	0.47
15:N:34:ASN:O	15:N:38:THR:OG1	2.29	0.47
15:N:61:TRP:HZ2	29:X:1006:C:O2	1.96	0.47
17:P:30:TYR:CD1	17:P:123:HIS:HE1	2.32	0.47
25:Z:33:CYS:HB3	25:Z:40:LYS:HB3	1.95	0.47
29:X:617:U:H5''	29:X:630:G:O6	2.14	0.47
29:X:1337:G:C4	29:X:1341:G:O6	2.67	0.47
29:X:1724:C:H42	29:X:1742:G:H1	1.61	0.47
29:X:2367:A:N7	29:X:2368:G:C5	2.83	0.47
29:X:2675:U:H2'	29:X:2676:G:C8	2.49	0.47
3:B:169:ASN:ND2	29:X:2711:G:OP1	2.38	0.47
6:E:97:LYS:HB3	6:E:98:LEU:H	1.49	0.47
7:F:133:SER:HB2	29:X:1099:A:N6	2.29	0.47
12:K:30:ARG:HG2	12:K:31:GLU:OE1	2.14	0.47
12:K:106:ASP:HB3	29:X:1666:G:O2'	2.13	0.47
13:L:30:SER:HB3	13:L:41:GLN:HB2	1.96	0.47
15:N:13:ARG:CZ	29:X:1264:C:H5''	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:91:ASN:HB2	16:O:11:GLN:HB2	1.97	0.47
19:R:77:HIS:O	19:R:80:LYS:HG3	2.15	0.47
21:T:5:LYS:HA	21:T:5:LYS:HE3	1.96	0.47
22:U:19:ILE:HD12	22:U:20:ARG:N	2.29	0.47
25:Z:21:SER:O	25:Z:21:SER:OG	2.32	0.47
28:3:6:THR:HG23	28:3:62:LEU:HB3	1.96	0.47
29:X:536:A:N6	29:X:2605:C:H4'	2.29	0.47
29:X:1309:G:H1	29:X:1661:C:H42	1.62	0.47
29:X:1391:A:O2'	29:X:1392:U:OP2	2.33	0.47
29:X:1452:U:H2'	29:X:1453:A:O4'	2.13	0.47
29:X:2098:G:HO2'	29:X:2154:A:N6	2.12	0.47
29:X:2335:U:H2'	29:X:2336:G:C8	2.50	0.47
29:X:2645:C:H3'	29:X:2646:C:C6	2.49	0.47
29:X:2757:G:H4'	29:X:2758:A:H5''	1.96	0.47
4:C:194:GLU:O	4:C:197:GLU:HB3	2.14	0.47
5:D:104:ILE:HA	5:D:108:LEU:HD12	1.97	0.47
10:I:9:THR:HB	10:I:12:SER:HB2	1.97	0.47
15:N:11:ARG:HH12	29:X:29:U:C4'	2.28	0.47
16:O:10:LYS:H	16:O:10:LYS:HD3	1.80	0.47
17:P:25:PHE:C	17:P:25:PHE:CD2	2.92	0.47
19:R:99:VAL:O	19:R:100:ASP:HB2	2.14	0.47
24:W:35:SER:HB3	29:X:941:U:OP1	2.13	0.47
25:Z:44:HIS:ND1	25:Z:44:HIS:N	2.63	0.47
29:X:553:C:H1'	29:X:556:A:H8	1.79	0.47
29:X:746:G:N7	29:X:774:A:C5	2.83	0.47
29:X:840:U:H4'	29:X:841:G:N7	2.29	0.47
29:X:1909:U:P	29:X:1912:G:H22	2.37	0.47
29:X:1998:A:C8	29:X:1999:U:C5	3.02	0.47
29:X:2158:C:H2'	29:X:2159:A:C8	2.49	0.47
29:X:2827:G:H2'	29:X:2828:C:O4'	2.15	0.47
30:Y:39:C:N4	30:Y:50:U:O2'	2.47	0.47
2:A:227:ASN:OD1	29:X:797:A:H5''	2.14	0.47
5:D:5:LYS:HE2	5:D:104:ILE:HD12	1.96	0.47
5:D:41:GLY:O	5:D:43:SER:N	2.47	0.47
9:H:10:VAL:HG23	9:H:17:ARG:O	2.14	0.47
11:J:14:PHE:CD1	11:J:88:LYS:HD3	2.50	0.47
17:P:81:HIS:ND1	17:P:82:ASN:OD1	2.48	0.47
20:S:94:VAL:HG12	20:S:96:VAL:HG22	1.97	0.47
22:U:20:ARG:HB2	22:U:43:ARG:HD2	1.96	0.47
29:X:717:G:N3	29:X:739:G:N1	2.63	0.47
29:X:1212:U:H2'	29:X:1213:U:H6	1.75	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1463:A:H2'	29:X:1464:A:H8	1.79	0.47
29:X:2033:C:C4	29:X:2034:A:C6	3.03	0.47
29:X:2237:C:O2'	29:X:2406:C:OP2	2.25	0.47
29:X:2594:U:H2'	29:X:2595:C:C6	2.49	0.47
29:X:2658:A:H2'	29:X:2659:C:O4'	2.15	0.47
29:X:2659:C:N4	29:X:2660:C:H41	2.11	0.47
30:Y:19:C:H2'	30:Y:20:A:C8	2.49	0.47
1:O:60:LEU:HB2	1:O:155:GLY:HA2	1.97	0.47
2:A:233:HIS:HE2	2:A:247:VAL:HG12	1.79	0.47
3:B:61:LYS:N	3:B:62:PRO:HD2	2.29	0.47
6:E:11:VAL:HG12	6:E:15:VAL:HG11	1.95	0.47
8:G:33:ILE:CD1	29:X:547:U:H4'	2.45	0.47
8:G:85:ALA:HB1	8:G:127:ILE:HG13	1.96	0.47
8:G:128:GLU:CD	29:X:2760:G:H1	2.23	0.47
9:H:13:ASN:ND2	9:H:109:ARG:HG2	2.30	0.47
11:J:61:ARG:HG2	20:S:175:ARG:H	1.79	0.47
11:J:100:PRO:C	11:J:102:ARG:H	2.22	0.47
12:K:3:HIS:O	12:K:3:HIS:CG	2.68	0.47
12:K:82:GLU:O	12:K:85:PRO:HG2	2.14	0.47
15:N:55:ARG:O	15:N:58:ARG:HB3	2.15	0.47
17:P:90:LEU:HA	17:P:129:ALA:O	2.14	0.47
19:R:16:PHE:CZ	19:R:46:VAL:HG21	2.50	0.47
21:T:37:LEU:HD12	21:T:59:LEU:O	2.14	0.47
22:U:48:LYS:HZ1	29:X:2073:A:H2	1.62	0.47
29:X:176:A:N6	29:X:2413:A:C6	2.83	0.47
29:X:640:C:H5''	29:X:660:G:O2'	2.14	0.47
29:X:1987:G:N7	29:X:1988:A:N7	2.62	0.47
29:X:2044:G:N2	29:X:2046:C:C2	2.83	0.47
29:X:2145:A:H5''	29:X:2155:U:C6	2.49	0.47
29:X:2396:C:H2'	29:X:2397:A:O4'	2.14	0.47
29:X:2612:G:H2'	29:X:2613:A:O4'	2.15	0.47
29:X:2662:C:H2'	29:X:2663:U:H5'	1.95	0.47
29:X:2836:U:O2'	29:X:2837:G:H5'	2.14	0.47
29:X:2871:U:H2'	29:X:2872:U:C6	2.50	0.47
30:Y:5:C:H42	30:Y:120:G:H1	1.63	0.47
30:Y:80:A:H2'	30:Y:81:C:O4'	2.13	0.47
3:B:8:LYS:HG2	3:B:192:ASN:HA	1.96	0.47
4:C:153:ASP:HA	4:C:158:ARG:HH22	1.78	0.47
12:K:73:LYS:H	12:K:73:LYS:HE3	1.77	0.47
13:L:42:ILE:HB	13:L:52:ALA:HB3	1.97	0.47
19:R:58:VAL:C	19:R:60:PRO:HD2	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:V:4:SER:O	23:V:8:ASN:ND2	2.48	0.47
25:Z:18:MET:CE	29:X:2028:C:H5'	2.45	0.47
29:X:389:G:H2'	29:X:390:U:C6	2.50	0.47
29:X:459:A:H5''	29:X:461:A:C5	2.50	0.47
29:X:475:U:C4	29:X:801:A:C5	3.03	0.47
29:X:494:A:H3'	29:X:495:C:C6	2.46	0.47
29:X:981:C:N4	29:X:982:C:N4	2.63	0.47
29:X:1174:G:N3	29:X:1175:A:C8	2.83	0.47
29:X:2087:U:H2'	29:X:2088:U:C6	2.49	0.47
29:X:2474:G:C6	29:X:2475:C:N3	2.82	0.47
29:X:2542:U:C2	29:X:2544:A:OP2	2.67	0.47
29:X:2697:G:H2'	29:X:2698:G:C8	2.49	0.47
29:X:2711:G:H2'	29:X:2712:G:C8	2.50	0.47
1:O:150:ARG:HA	1:O:153:LYS:HB2	1.97	0.47
4:C:39:ARG:HD2	29:X:455:A:N7	2.30	0.47
5:D:22:TYR:HE1	5:D:28:VAL:HG13	1.80	0.47
5:D:57:LEU:HD23	5:D:60:ILE:HD11	1.97	0.47
12:K:8:ARG:HD2	12:K:10:LEU:HD21	1.97	0.47
13:L:37:HIS:HB3	30:Y:30:C:OP1	2.14	0.47
15:N:58:ARG:HH21	15:N:92:ARG:HH12	1.61	0.47
15:N:115:ASN:HA	15:N:118:GLN:OE1	2.15	0.47
17:P:98:ASP:OD2	17:P:98:ASP:N	2.47	0.47
20:S:146:HIS:HB3	20:S:167:THR:HG23	1.97	0.47
21:T:35:ASN:OD1	29:X:2332:G:O2'	2.25	0.47
29:X:116:A:OP2	29:X:117:A:H2'	2.15	0.47
29:X:202:A:C5	29:X:203:G:H1'	2.50	0.47
29:X:828:C:N4	29:X:1206:G:H1	2.13	0.47
29:X:1141:U:H6	29:X:1141:U:O5'	1.98	0.47
29:X:2519:C:O2	29:X:2720:A:H2	1.98	0.47
29:X:2663:U:C2	29:X:2664:G:C8	3.02	0.47
29:X:2796:A:C4	29:X:2797:G:N7	2.83	0.47
4:C:137:ALA:CB	4:C:142:LEU:HD12	2.44	0.47
12:K:24:GLN:HB3	12:K:44:LEU:HD13	1.96	0.47
17:P:47:GLY:H	17:P:92:VAL:HB	1.78	0.47
19:R:90:LYS:C	19:R:92:THR:HG23	2.39	0.47
29:X:587:A:OP1	29:X:1268:U:O2'	2.15	0.47
29:X:649:G:N2	29:X:661:C:H1'	2.30	0.47
29:X:754:G:H2'	29:X:755:C:H6	1.80	0.47
29:X:2487:G:C6	29:X:2561:G:O6	2.68	0.47
29:X:2701:A:H1'	29:X:2848:A:O2'	2.15	0.47
29:X:2789:U:H2'	29:X:2790:C:C6	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2820:C:H42	29:X:2846:G:H1	1.62	0.47
2:A:171:ASP:O	2:A:187:SER:OG	2.27	0.46
4:C:27:LEU:HG	4:C:106:MET:HE3	1.96	0.46
9:H:130:ALA:HA	9:H:131:PRO:HD3	1.81	0.46
22:U:68:ARG:NH1	29:X:413:G:O4'	2.39	0.46
29:X:218:A:H4'	29:X:219:G:OP1	2.14	0.46
29:X:790:A:C2	29:X:791:G:C4	3.03	0.46
29:X:953:G:O2'	29:X:1203:A:N3	2.44	0.46
29:X:1690:U:H3'	29:X:1690:U:C6	2.50	0.46
29:X:2411:A:H8	29:X:2411:A:O5'	1.98	0.46
2:A:163:VAL:HA	2:A:176:ARG:O	2.15	0.46
2:A:209:ALA:O	2:A:210:GLY:C	2.57	0.46
3:B:37:LYS:NZ	3:B:80:GLU:OE2	2.38	0.46
3:B:103:ASP:OD1	3:B:168:GLN:HA	2.14	0.46
4:C:47:THR:N	4:C:50:GLN:HG3	2.28	0.46
5:D:57:LEU:O	5:D:61:THR:HG23	2.15	0.46
8:G:115:ALA:O	8:G:119:LEU:HB2	2.15	0.46
9:H:59:ALA:O	9:H:61:ARG:N	2.48	0.46
10:I:72:TYR:CE2	10:I:105:PRO:HB2	2.50	0.46
12:K:20:LEU:C	12:K:22:ARG:N	2.73	0.46
14:M:20:HIS:O	14:M:62:SER:HB2	2.15	0.46
14:M:82:PRO:C	14:M:84:ALA:N	2.71	0.46
25:Z:52:TYR:HH	29:X:2859:U:H3	1.62	0.46
27:2:15:THR:HG22	27:2:16:HIS:CG	2.50	0.46
29:X:646:C:H2'	29:X:647:G:O4'	2.16	0.46
29:X:991:A:H62	29:X:992:A:N6	2.13	0.46
29:X:1340:C:H2'	29:X:1341:G:O4'	2.16	0.46
29:X:1687:C:C4	29:X:1688:U:C2	3.03	0.46
29:X:1794:A:H5''	29:X:1795:C:OP2	2.15	0.46
29:X:2040:A:H2'	29:X:2041:A:H8	1.76	0.46
29:X:2406:C:H5''	29:X:2407:G:OP1	2.15	0.46
6:E:157:TYR:CE2	29:X:2510:A:H4'	2.50	0.46
8:G:134:MET:HE2	29:X:1148:G:N3	2.30	0.46
17:P:109:ARG:HD2	29:X:761:G:OP2	2.15	0.46
19:R:10:HIS:NE2	29:X:338:G:H1'	2.31	0.46
20:S:26:LYS:HE2	20:S:84:TYR:CE1	2.51	0.46
28:3:23:MET:HA	28:3:49:VAL:HA	1.97	0.46
29:X:402:A:H8	29:X:2392:G:H4'	1.79	0.46
29:X:1153:A:C5	29:X:1155:G:C5	3.03	0.46
29:X:1179:A:C2	29:X:1196:G:C2	3.04	0.46
29:X:1301:U:C2	29:X:1340:C:O2	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1511:A:C6	29:X:1512:A:C6	3.03	0.46
29:X:1715:A:C8	29:X:1717:A:O4'	2.68	0.46
29:X:2505:G:N2	29:X:2517:C:H1'	2.31	0.46
29:X:2802:C:H2'	29:X:2803:C:C6	2.50	0.46
29:X:2859:U:H5	29:X:2860:C:C4	2.33	0.46
2:A:123:ALA:HB1	2:A:129:ASN:ND2	2.29	0.46
2:A:232:PRO:HB2	2:A:233:HIS:CD2	2.50	0.46
4:C:48:ARG:HD2	4:C:75:PRO:HD2	1.97	0.46
5:D:46:ASP:OD2	5:D:46:ASP:N	2.49	0.46
7:F:23:VAL:HA	7:F:26:ALA:HB3	1.98	0.46
8:G:117:GLU:O	8:G:121:LYS:HB2	2.16	0.46
13:L:15:ARG:HD3	13:L:15:ARG:HA	1.38	0.46
21:T:60:PHE:CE2	29:X:2344:G:H4'	2.51	0.46
25:Z:43:HIS:HA	25:Z:52:TYR:OH	2.15	0.46
29:X:223:C:C4	29:X:224:G:N7	2.84	0.46
29:X:471:A:C2	29:X:481:A:C4	3.03	0.46
29:X:518:A:H5''	29:X:518:A:C8	2.50	0.46
29:X:713:G:N2	29:X:745:C:H5	2.09	0.46
29:X:860:U:H5'	29:X:861:G:OP2	2.16	0.46
29:X:1118:G:N1	29:X:1119:U:O2	2.47	0.46
29:X:1513:U:H6	29:X:1593:C:H5''	1.80	0.46
29:X:2151:G:N2	29:X:2154:A:O5'	2.46	0.46
29:X:2229:G:HO2'	29:X:2475:C:P	2.38	0.46
29:X:2455:A:N3	29:X:2460:G:N1	2.54	0.46
14:M:2:GLN:HB3	29:X:2795:A:C2	2.51	0.46
14:M:32:THR:HG22	14:M:94:VAL:HB	1.98	0.46
15:N:44:THR:O	15:N:48:ARG:HG2	2.15	0.46
18:Q:63:LYS:HD2	18:Q:72:ARG:NH2	2.30	0.46
26:1:38:LYS:HD2	29:X:2323:U:OP1	2.15	0.46
29:X:143:A:H2'	29:X:144:U:C6	2.51	0.46
29:X:784:U:H2'	29:X:785:U:H6	1.81	0.46
29:X:828:C:H42	29:X:1206:G:H1	1.64	0.46
29:X:1235:C:H2'	29:X:1236:G:C8	2.51	0.46
29:X:1542:G:N2	29:X:1562:G:H1	2.14	0.46
29:X:1994:U:H2'	29:X:1995:G:C5'	2.45	0.46
29:X:2042:A:C5	29:X:2482:A:C2	3.03	0.46
8:G:38:GLU:OE2	8:G:67:ARG:NH2	2.48	0.46
17:P:74:SER:HA	29:X:498:C:H1'	1.98	0.46
19:R:76:LEU:HD23	19:R:76:LEU:HA	1.69	0.46
28:3:21:LYS:HE2	29:X:661:C:OP1	2.16	0.46
29:X:1:G:H2'	29:X:2:G:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:169:C:H5''	29:X:170:U:OP2	2.15	0.46
29:X:1079:G:N2	29:X:1107:A:O5'	2.49	0.46
29:X:1655:C:O3'	29:X:2688:G:N2	2.48	0.46
29:X:1683:G:H1	29:X:1977:C:H42	1.62	0.46
30:Y:119:G:C6	30:Y:120:G:C5	3.04	0.46
3:B:2:LYS:NZ	3:B:95:ILE:HA	2.30	0.46
3:B:128:SER:OG	29:X:1693:A:H1'	2.15	0.46
9:H:42:LYS:NZ	29:X:2653:A:H5'	2.31	0.46
17:P:27:VAL:HB	29:X:504:G:H4'	1.98	0.46
28:3:7:HIS:O	28:3:10:ALA:N	2.43	0.46
29:X:515:A:H2'	29:X:516:G:H5'	1.97	0.46
29:X:590:C:H2'	29:X:591:G:C8	2.50	0.46
29:X:695:G:H2'	29:X:696:U:C6	2.51	0.46
29:X:1067:G:O2'	29:X:1098:G:O6	2.34	0.46
29:X:1103:C:H2'	29:X:1104:G:O4'	2.15	0.46
29:X:1685:A:O4'	29:X:1686:A:C2	2.68	0.46
29:X:2441:U:H2'	29:X:2442:C:C6	2.50	0.46
4:C:149:LEU:HD22	4:C:179:ASP:HB3	1.98	0.46
5:D:3:GLN:O	5:D:6:THR:OG1	2.17	0.46
9:H:92:ASP:OD2	14:M:69:ARG:NH1	2.48	0.46
12:K:25:ALA:N	12:K:44:LEU:HD11	2.31	0.46
13:L:28:ARG:HH22	30:Y:11:G:H5'	1.81	0.46
17:P:34:SER:HB3	17:P:37:LYS:HG3	1.98	0.46
17:P:60:ILE:CD1	25:Z:28:PRO:HD3	2.46	0.46
19:R:62:MET:HA	19:R:63:THR:HA	1.70	0.46
24:W:16:GLN:O	24:W:20:VAL:HG23	2.15	0.46
29:X:78:C:H2'	29:X:79:G:C8	2.51	0.46
29:X:573:C:O2'	29:X:574:C:H5'	2.16	0.46
29:X:824:U:O2	29:X:1263:G:H3'	2.16	0.46
29:X:861:G:C4	29:X:862:A:C8	3.03	0.46
29:X:1067:G:H5''	29:X:1068:A:O4'	2.15	0.46
29:X:1322:G:O2'	29:X:1627:C:O2'	2.26	0.46
29:X:1495:G:N2	29:X:1529:C:O2	2.29	0.46
29:X:1733:U:H2'	29:X:1734:C:C5	2.50	0.46
29:X:1850:G:N3	29:X:1850:G:H2'	2.30	0.46
29:X:2415:G:H2'	29:X:2416:U:C6	2.51	0.46
29:X:2585:C:H2'	29:X:2586:G:H5'	1.98	0.46
5:D:60:ILE:HG13	5:D:61:THR:HG22	1.98	0.46
5:D:147:ASP:HB2	5:D:148:LYS:H	1.57	0.46
9:H:23:ARG:HG3	9:H:24:VAL:N	2.29	0.46
13:L:57:ALA:HB3	30:Y:119:G:H4'	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:126:GLY:HA3	20:S:128:ARG:NH2	2.31	0.46
29:X:1402:G:H2'	29:X:1403:U:C6	2.51	0.46
29:X:1464:A:C6	29:X:1465:G:C6	3.04	0.46
29:X:1698:C:O2'	29:X:1753:A:N3	2.37	0.46
29:X:1765:C:O5'	29:X:1765:C:H6	1.98	0.46
29:X:2447:G:O2'	29:X:2448:A:H8	1.99	0.46
29:X:2494:C:C2	29:X:2549:G:C2	3.04	0.46
29:X:2695:C:H2'	29:X:2696:A:C8	2.51	0.46
2:A:69:ARG:HD2	2:A:130:ALA:HB2	1.98	0.46
3:B:27:LEU:HD22	3:B:51:TYR:OH	2.15	0.46
5:D:70:ALA:O	5:D:72:LYS:N	2.43	0.46
6:E:117:PRO:HA	6:E:118:PRO:HD2	1.84	0.46
8:G:79:PHE:CE2	8:G:147:ARG:HD3	2.50	0.46
20:S:10:PRO:O	20:S:13:LYS:HG3	2.16	0.46
29:X:38:G:C2	29:X:454:G:C2	3.04	0.46
29:X:119:G:H1	29:X:128:C:H42	1.63	0.46
29:X:194:G:H2'	29:X:195:A:O4'	2.16	0.46
29:X:992:A:H2	29:X:2010:G:N3	2.13	0.46
29:X:1008:G:H1	29:X:1169:C:H42	1.64	0.46
29:X:1017:C:O2'	29:X:1018:C:H5'	2.16	0.46
29:X:1470:G:C2	29:X:1471:G:C8	3.04	0.46
29:X:1661:C:O2	29:X:1661:C:H2'	2.16	0.46
29:X:1669:A:N7	29:X:1670:G:C6	2.84	0.46
29:X:1769:U:H2'	29:X:1775:A:N6	2.31	0.46
29:X:2790:C:H2'	29:X:2791:C:C6	2.51	0.46
3:B:91:VAL:HG12	3:B:92:ASN:H	1.81	0.45
4:C:34:GLN:OE1	4:C:176:ASN:HB2	2.17	0.45
4:C:36:ALA:O	4:C:38:ARG:N	2.49	0.45
5:D:79:LEU:HD21	29:X:2289:A:H2	1.81	0.45
10:I:86:THR:HG1	10:I:116:ARG:NH1	2.13	0.45
12:K:106:ASP:OD2	29:X:1300:A:C8	2.69	0.45
20:S:6:LYS:HA	20:S:32:PHE:HA	1.98	0.45
26:1:21:TYR:CE2	29:X:2378:G:H1'	2.51	0.45
28:3:62:LEU:HD13	28:3:65:GLY:HA2	1.97	0.45
29:X:165:G:H4'	29:X:1378:A:C5	2.51	0.45
29:X:1033:G:H22	29:X:1153:A:H2	1.63	0.45
29:X:1194:U:H2'	29:X:1195:U:H6	1.80	0.45
29:X:1510:A:H2'	29:X:1511:A:O4'	2.16	0.45
29:X:1685:A:H61	29:X:1693:A:H61	1.63	0.45
29:X:1813:A:H2'	29:X:1814:G:H8	1.81	0.45
3:B:38:THR:HG23	3:B:41:THR:OG1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:60:ASN:HB2	3:B:63:MET:HB2	1.98	0.45
3:B:140:SER:HB2	29:X:2557:G:N7	2.31	0.45
4:C:53:LYS:HB2	4:C:73:SER:HB3	1.98	0.45
5:D:92:ARG:HD3	30:Y:47:A:C8	2.50	0.45
13:L:12:ARG:O	13:L:16:LYS:HB2	2.16	0.45
16:O:83:ARG:N	29:X:827:C:OP1	2.45	0.45
19:R:58:VAL:HG13	19:R:60:PRO:CD	2.46	0.45
22:U:8:THR:HA	22:U:13:LEU:HD12	1.98	0.45
27:2:4:THR:O	29:X:700:C:H5'	2.16	0.45
28:3:4:MET:HE2	29:X:679:C:H1'	1.98	0.45
29:X:15:G:C5	29:X:16:G:N7	2.84	0.45
29:X:742:G:H2'	29:X:1766:U:H1'	1.98	0.45
29:X:1670:G:H8	29:X:1670:G:OP2	2.00	0.45
29:X:2227:C:H5''	29:X:2228:U:OP2	2.16	0.45
29:X:2727:G:O6	29:X:2735:C:H5''	2.15	0.45
29:X:2754:C:N4	29:X:2755:A:C5	2.84	0.45
30:Y:54:U:H4'	30:Y:54:U:OP1	2.16	0.45
2:A:39:LYS:NZ	2:A:58:HIS:O	2.34	0.45
5:D:74:ILE:HG23	5:D:80:ARG:HA	1.97	0.45
6:E:38:ASN:OD1	6:E:64:LEU:HD22	2.16	0.45
7:F:25:PRO:HB2	7:F:29:GLN:NE2	2.31	0.45
9:H:9:ASP:OD2	9:H:9:ASP:N	2.48	0.45
14:M:2:GLN:N	29:X:2795:A:N1	2.64	0.45
18:Q:42:ILE:HD12	18:Q:80:VAL:HG21	1.99	0.45
18:Q:62:ARG:HA	18:Q:71:GLN:HA	1.98	0.45
18:Q:91:LEU:HD12	18:Q:91:LEU:HA	1.80	0.45
22:U:24:ALA:C	22:U:26:ALA:H	2.25	0.45
22:U:75:TYR:O	22:U:76:LYS:HB2	2.16	0.45
24:W:21:GLN:C	24:W:23:LEU:H	2.25	0.45
29:X:38:G:H2'	29:X:39:C:H6	1.81	0.45
29:X:314:G:H2'	29:X:315:G:C8	2.52	0.45
29:X:571:U:C2	29:X:581:A:C8	3.05	0.45
29:X:615:C:H1'	29:X:670:U:H1'	1.98	0.45
29:X:628:A:H8	29:X:628:A:O5'	1.99	0.45
29:X:1296:G:N2	29:X:1299:A:OP2	2.49	0.45
29:X:1302:C:O2'	29:X:1303:U:H5'	2.17	0.45
29:X:1336:G:O5'	29:X:1336:G:H8	1.99	0.45
29:X:2235:G:N2	29:X:2254:C:C4	2.85	0.45
29:X:2431:C:H2'	29:X:2432:A:C8	2.51	0.45
29:X:2468:G:C6	29:X:2469:G:C6	3.04	0.45
29:X:2555:G:OP1	29:X:2555:G:H3'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2686:C:C2'	29:X:2687:G:H5'	2.46	0.45
1:O:95:LEU:HD13	1:O:98:ARG:HB2	1.98	0.45
5:D:114:PHE:HE1	5:D:117:ILE:HG13	1.81	0.45
5:D:143:TYR:HA	5:D:146:VAL:HG22	1.98	0.45
8:G:69:ASP:HA	15:N:64:ARG:HH22	1.82	0.45
11:J:69:ILE:HG23	11:J:104:MET:HA	1.99	0.45
13:L:14:ARG:HG2	13:L:15:ARG:HH12	1.82	0.45
17:P:9:ARG:HG3	17:P:10:ASN:H	1.82	0.45
25:Z:36:CYS:HB3	25:Z:49:CYS:HB3	1.55	0.45
29:X:78:C:O2'	29:X:357:A:N3	2.43	0.45
29:X:99:U:H5''	29:X:100:G:N7	2.32	0.45
29:X:158:A:H2	29:X:447:U:H4'	1.81	0.45
29:X:573:C:H2'	29:X:574:C:O4'	2.17	0.45
29:X:602:C:N4	29:X:678:G:H1	2.14	0.45
29:X:1202:U:H2'	29:X:1203:A:C8	2.36	0.45
29:X:1888:C:OP1	29:X:1889:G:H5'	2.14	0.45
29:X:1918:G:H1'	29:X:1947:G:N2	2.31	0.45
29:X:1932:G:N2	29:X:1941:C:C2	2.85	0.45
29:X:2286:G:H3'	29:X:2287:G:H8	1.81	0.45
29:X:2792:C:C2	29:X:2805:G:C2	3.05	0.45
3:B:176:ARG:NE	14:M:16:ILE:HD13	2.31	0.45
4:C:162:ARG:HG3	4:C:169:VAL:HG21	1.98	0.45
5:D:164:GLU:HG3	5:D:165:GLU:HG2	1.98	0.45
6:E:40:GLU:H	6:E:40:GLU:HG3	1.55	0.45
12:K:64:ARG:O	12:K:68:GLN:HG3	2.17	0.45
18:Q:38:ILE:O	18:Q:42:ILE:HG13	2.16	0.45
28:3:58:MET:CA	28:3:61:MET:HG3	2.45	0.45
29:X:42:G:H2'	29:X:43:A:H8	1.81	0.45
29:X:534:U:H2'	29:X:535:U:C6	2.51	0.45
29:X:585:U:H4'	29:X:2481:G:N7	2.31	0.45
29:X:588:G:N2	29:X:1275:A:C4	2.85	0.45
29:X:591:G:C6	29:X:592:G:C6	3.04	0.45
29:X:650:U:H2'	29:X:651:C:C6	2.51	0.45
29:X:1069:G:H2'	29:X:1070:G:C8	2.52	0.45
29:X:1310:C:C2	29:X:1311:C:C5	3.05	0.45
29:X:2523:G:N3	29:X:2524:G:C8	2.85	0.45
1:O:7:GLU:HA	1:O:10:VAL:HB	1.98	0.45
2:A:186:HIS:O	2:A:189:CYS:N	2.47	0.45
3:B:20:ALA:HB2	9:H:85:ASP:O	2.16	0.45
3:B:61:LYS:O	3:B:64:GLN:HB2	2.16	0.45
4:C:148:VAL:HG12	4:C:187:VAL:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:32:ASP:OD2	11:J:135:ARG:NH2	2.40	0.45
12:K:11:ASN:ND2	29:X:1670:G:O6	2.49	0.45
17:P:97:VAL:HG22	17:P:124:ILE:HA	1.99	0.45
20:S:26:LYS:HD3	20:S:26:LYS:N	2.31	0.45
20:S:103:ARG:NH1	20:S:108:VAL:HG22	2.32	0.45
29:X:115:G:OP2	29:X:117:A:O2'	2.29	0.45
29:X:306:G:H2'	29:X:307:C:H6	1.82	0.45
29:X:476:G:H2'	29:X:477:A:C8	2.52	0.45
29:X:1269:G:N3	29:X:1269:G:H2'	2.32	0.45
29:X:1367:A:H2'	29:X:1368:G:O4'	2.16	0.45
29:X:1810:U:H4'	29:X:1813:A:H1'	1.99	0.45
29:X:2007:G:C2	29:X:2023:C:C2	3.05	0.45
29:X:2430:A:OP1	29:X:2476:A:N6	2.49	0.45
29:X:2523:G:C4	29:X:2524:G:C8	3.05	0.45
29:X:2529:G:C4	29:X:2530:C:C5	3.05	0.45
29:X:2837:G:H2'	29:X:2838:U:C6	2.51	0.45
6:E:97:LYS:H	6:E:104:GLU:HB2	1.80	0.45
9:H:64:VAL:HG22	9:H:106:ARG:NH2	2.25	0.45
11:J:11:ARG:HB3	11:J:12:LYS:H	1.41	0.45
20:S:112:LEU:HD12	20:S:113:VAL:H	1.82	0.45
21:T:46:LYS:NZ	21:T:76:ALA:HA	2.31	0.45
21:T:57:HIS:N	21:T:57:HIS:CD2	2.84	0.45
22:U:14:VAL:O	22:U:15:VAL:HG22	2.16	0.45
26:1:46:HIS:CE1	29:X:2351:G:HO2'	2.35	0.45
29:X:311:A:H1'	29:X:330:C:O4'	2.17	0.45
29:X:458:G:H5''	29:X:458:G:H8	1.82	0.45
29:X:2589:C:H4'	29:X:2590:U:H5'	1.99	0.45
29:X:2683:C:H2'	29:X:2684:A:O4'	2.17	0.45
29:X:2792:C:N3	29:X:2805:G:C2	2.84	0.45
1:0:43:LEU:HD12	1:0:167:VAL:HG11	1.99	0.45
3:B:9:ILE:HD12	3:B:9:ILE:N	2.32	0.45
14:M:33:VAL:HG11	14:M:91:VAL:HG12	1.98	0.45
21:T:36:ILE:HD11	29:X:2343:C:O2	2.16	0.45
29:X:491:A:H3'	29:X:492:G:H5''	1.97	0.45
29:X:697:G:C2	29:X:807:A:C2	3.05	0.45
29:X:769:C:C4	29:X:770:U:C4	3.05	0.45
29:X:1029:C:O3'	29:X:1131:G:N2	2.49	0.45
29:X:1298:G:N2	29:X:1341:G:H5'	2.32	0.45
29:X:1628:C:N3	29:X:1629:G:C8	2.85	0.45
29:X:1750:A:H2'	29:X:1751:A:H8	1.81	0.45
29:X:2264:C:H4'	29:X:2267:A:N7	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2302:G:H1	29:X:2311:U:H5	1.65	0.45
29:X:2345:A:C6	29:X:2346:G:C4	3.05	0.45
29:X:2611:A:C2	29:X:2767:C:O2	2.70	0.45
29:X:2819:G:H2'	29:X:2820:C:C6	2.51	0.45
2:A:63:ARG:O	2:A:65:ILE:HG13	2.17	0.45
2:A:69:ARG:HH11	2:A:130:ALA:HB2	1.82	0.45
2:A:76:ASN:HB2	2:A:117:VAL:O	2.17	0.45
2:A:186:HIS:NE2	29:X:2201:G:H5'	2.32	0.45
2:A:218:LYS:HB3	2:A:218:LYS:HE3	1.49	0.45
4:C:3:GLN:O	4:C:12:GLY:HA3	2.17	0.45
4:C:14:THR:HB	4:C:15:ILE:H	1.58	0.45
4:C:172:VAL:HB	4:C:173:ALA:H	1.64	0.45
10:I:63:ARG:HD3	28:3:25:PHE:CE1	2.52	0.45
10:I:80:LEU:HD23	10:I:80:LEU:HA	1.75	0.45
11:J:22:ALA:HB2	11:J:99:LYS:CB	2.46	0.45
11:J:102:ARG:NH1	11:J:103:VAL:O	2.49	0.45
11:J:139:ASP:OD2	11:J:139:ASP:N	2.50	0.45
12:K:51:LEU:CD2	12:K:66:VAL:HG22	2.47	0.45
13:L:99:ARG:H	13:L:99:ARG:HG2	1.52	0.45
14:M:33:VAL:CG1	14:M:91:VAL:HG12	2.46	0.45
24:W:5:LEU:HB2	24:W:25:LEU:CD1	2.43	0.45
29:X:820:U:OP1	29:X:843:G:N2	2.50	0.45
29:X:831:G:N7	29:X:1201:G:C6	2.85	0.45
29:X:1309:G:H1	29:X:1661:C:N4	2.15	0.45
29:X:1478:U:C2	29:X:1479:G:C8	3.05	0.45
29:X:2217:G:H2'	29:X:2217:G:N3	2.32	0.45
29:X:2248:A:N3	29:X:2248:A:H2'	2.30	0.45
29:X:2494:C:N4	29:X:2548:G:H1	2.06	0.45
2:A:40:THR:C	2:A:42:GLY:H	2.24	0.45
2:A:43:ARG:HH21	29:X:704:G:H4'	1.82	0.45
3:B:5:LEU:HD22	3:B:195:LEU:HD11	1.98	0.45
5:D:22:TYR:CE1	5:D:28:VAL:HG13	2.52	0.45
6:E:9:ILE:HD11	6:E:52:VAL:HG23	1.99	0.45
10:I:14:LYS:HD3	29:X:675:C:O2'	2.17	0.45
16:O:35:LEU:HD23	16:O:36:LYS:N	2.28	0.45
19:R:15:HIS:CD2	19:R:16:PHE:CD2	2.96	0.45
22:U:21:ARG:CG	22:U:22:GLY:H	2.30	0.45
29:X:1:G:H1	29:X:2876:C:H42	1.65	0.45
29:X:567:G:H2'	29:X:568:G:C8	2.52	0.45
29:X:1408:A:N1	29:X:1411:C:C2	2.85	0.45
29:X:1713:G:C6	29:X:1714:A:C5	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1775:A:H4'	29:X:1776:A:OP1	2.15	0.45
29:X:2078:G:H2'	29:X:2079:A:C8	2.52	0.45
29:X:2691:C:HO2'	29:X:2692:A:P	2.36	0.45
30:Y:15:A:H4'	30:Y:17:A:H2'	1.99	0.45
2:A:232:PRO:HB2	2:A:233:HIS:HD2	1.82	0.44
4:C:118:VAL:O	4:C:120:VAL:HG23	2.17	0.44
4:C:133:PHE:CE1	4:C:161:ALA:HB2	2.51	0.44
6:E:126:PRO:HG2	6:E:130:ARG:HB2	1.99	0.44
8:G:140:GLN:O	8:G:143:ALA:N	2.50	0.44
10:I:118:VAL:O	10:I:138:GLY:HA3	2.17	0.44
14:M:81:PHE:HA	14:M:82:PRO:HD3	1.74	0.44
14:M:93:ILE:HD12	14:M:93:ILE:N	2.26	0.44
16:O:5:ILE:N	16:O:38:LEU:HD12	2.33	0.44
17:P:91:PHE:CZ	17:P:131:LYS:HG3	2.52	0.44
18:Q:7:LEU:HD21	18:Q:42:ILE:HG12	1.99	0.44
18:Q:8:GLN:O	18:Q:9:ALA:HB2	2.16	0.44
18:Q:64:ARG:HH21	18:Q:69:ILE:HD11	1.82	0.44
28:3:17:THR:HG23	28:3:20:GLY:H	1.82	0.44
29:X:404:A:H1'	29:X:424:G:O4'	2.17	0.44
29:X:452:G:H2'	29:X:453:U:C6	2.51	0.44
29:X:498:C:N4	29:X:499:G:C6	2.85	0.44
29:X:944:A:OP2	29:X:944:A:H8	2.00	0.44
29:X:1236:G:C6	29:X:1240:G:C6	3.05	0.44
29:X:1611:U:H2'	29:X:1612:U:H6	1.82	0.44
29:X:2020:G:H2'	29:X:2021:G:C8	2.52	0.44
29:X:2048:C:H1'	29:X:2428:U:N3	2.32	0.44
29:X:2283:G:H2'	29:X:2283:G:N3	2.32	0.44
29:X:2831:A:H2'	29:X:2832:G:O4'	2.17	0.44
1:O:68:VAL:HG21	1:O:153:LYS:HG2	2.00	0.44
2:A:271:VAL:HG22	2:A:272:THR:HG23	1.98	0.44
3:B:119:ARG:HG2	3:B:120:TRP:NE1	2.33	0.44
4:C:95:LEU:O	4:C:100:ARG:NH1	2.45	0.44
7:F:1:MET:HE2	7:F:2:ARG:HH11	1.82	0.44
10:I:19:VAL:O	10:I:21:ARG:NH1	2.51	0.44
12:K:27:ALA:O	12:K:31:GLU:N	2.49	0.44
15:N:40:LEU:O	15:N:43:ALA:HB3	2.18	0.44
18:Q:62:ARG:HG2	18:Q:71:GLN:HG3	1.98	0.44
20:S:36:ARG:HG2	20:S:40:ASP:OD2	2.17	0.44
22:U:27:ASP:C	22:U:32:ARG:HD3	2.42	0.44
24:W:49:HIS:HD2	24:W:50:LEU:HG	1.82	0.44
25:Z:13:LYS:HD3	29:X:527:C:OP2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:420:C:H2'	29:X:421:G:H8	1.83	0.44
29:X:654:A:HO2'	29:X:655:A:P	2.40	0.44
29:X:1229:C:O5'	29:X:1229:C:H6	2.00	0.44
29:X:1348:C:H2'	29:X:1349:A:C8	2.52	0.44
29:X:1352:G:C6	29:X:1353:A:N6	2.85	0.44
29:X:1787:U:H2'	29:X:1788:C:C6	2.52	0.44
29:X:1882:G:N3	29:X:1882:G:H2'	2.32	0.44
29:X:2034:A:H2'	29:X:2557:G:OP1	2.17	0.44
30:Y:58:G:C4'	30:Y:59:A:H5''	2.47	0.44
2:A:233:HIS:NE2	2:A:247:VAL:HG12	2.33	0.44
4:C:17:LEU:HA	4:C:18:PRO:HD3	1.77	0.44
12:K:54:THR:CG2	12:K:66:VAL:HG23	2.47	0.44
17:P:22:LYS:HA	17:P:23:PRO:HD3	1.56	0.44
28:3:64:ARG:HH21	29:X:219:G:H5'	1.82	0.44
29:X:443:A:H5''	29:X:444:U:OP2	2.18	0.44
29:X:587:A:OP2	29:X:587:A:H8	2.00	0.44
29:X:742:G:H5'	29:X:743:A:H5''	2.00	0.44
29:X:828:C:H2'	29:X:829:C:H6	1.82	0.44
29:X:1067:G:H2'	29:X:1113:C:H41	1.81	0.44
29:X:1142:G:C8	29:X:2008:C:H4'	2.52	0.44
29:X:1174:G:N2	29:X:1175:A:C4	2.85	0.44
29:X:1733:U:H3	29:X:1734:C:H41	1.64	0.44
29:X:1770:U:C5	29:X:1775:A:N7	2.73	0.44
29:X:1815:G:C4	29:X:1816:G:C8	3.06	0.44
29:X:1858:C:H2'	29:X:1859:A:O4'	2.16	0.44
29:X:2241:U:H2'	29:X:2242:C:C6	2.48	0.44
29:X:2375:G:N3	29:X:2400:G:N2	2.65	0.44
29:X:2662:C:H2'	29:X:2663:U:H6	1.82	0.44
30:Y:16:U:O2'	30:Y:110:U:H1'	2.18	0.44
3:B:19:ARG:HH11	9:H:84:ALA:HB1	1.82	0.44
14:M:106:TYR:HD1	29:X:1745:C:H4'	1.83	0.44
15:N:25:TRP:CE3	15:N:25:TRP:C	2.96	0.44
16:O:14:VAL:HG12	16:O:18:ASP:OD2	2.18	0.44
18:Q:9:ALA:O	18:Q:27:PHE:HB3	2.17	0.44
20:S:121:GLN:O	20:S:161:ALA:HB3	2.18	0.44
28:3:21:LYS:HB3	28:3:55:TRP:CH2	2.53	0.44
29:X:526:C:H1'	29:X:1274:C:O2'	2.16	0.44
29:X:619:A:N6	29:X:630:G:O2'	2.51	0.44
29:X:1283:C:H5''	29:X:1284:G:C5'	2.47	0.44
29:X:1359:G:C6	29:X:1617:G:C6	3.05	0.44
29:X:1623:C:H4'	29:X:1624:A:O5'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2022:C:H2'	29:X:2023:C:C6	2.53	0.44
29:X:2067:U:H2'	29:X:2068:C:C6	2.53	0.44
30:Y:30:C:H2'	30:Y:31:A:O4'	2.18	0.44
4:C:68:ARG:NH2	29:X:2043:A:H62	2.16	0.44
4:C:178:TYR:O	4:C:182:ARG:N	2.42	0.44
7:F:109:LYS:HD2	7:F:109:LYS:HA	1.60	0.44
8:G:70:PHE:HA	8:G:76:GLN:OE1	2.18	0.44
8:G:128:GLU:HG3	8:G:150:VAL:HG21	1.99	0.44
9:H:1:MET:O	9:H:2:ILE:HD13	2.17	0.44
11:J:84:MET:HE1	29:X:971:A:H61	1.83	0.44
12:K:38:LEU:O	12:K:41:ALA:HB3	2.18	0.44
12:K:39:THR:O	12:K:41:ALA:N	2.51	0.44
15:N:47:TYR:CE2	15:N:51:ARG:CZ	3.00	0.44
20:S:66:VAL:HG22	20:S:83:PHE:CE1	2.53	0.44
20:S:91:PRO:HG2	20:S:124:ALA:HA	1.99	0.44
21:T:11:LYS:HE2	21:T:11:LYS:HB2	1.61	0.44
29:X:318:G:N1	29:X:321:A:OP2	2.47	0.44
29:X:757:U:H2'	29:X:758:G:O4'	2.17	0.44
29:X:875:G:O2'	30:Y:80:A:N3	2.38	0.44
29:X:1283:C:O5'	29:X:1283:C:H6	1.99	0.44
29:X:1629:G:C6	29:X:1633:C:C6	3.05	0.44
29:X:1724:C:N3	29:X:1747:G:C6	2.85	0.44
29:X:1951:G:O2'	29:X:1952:A:O4'	2.26	0.44
29:X:2011:U:H2'	29:X:2012:A:O4'	2.18	0.44
29:X:2427:A:OP1	29:X:2478:C:OP1	2.35	0.44
29:X:2741:G:C6	29:X:2742:G:N7	2.86	0.44
29:X:2817:A:H2'	29:X:2818:G:O4'	2.16	0.44
30:Y:16:U:O2'	30:Y:110:U:O2	2.34	0.44
30:Y:67:C:N4	30:Y:111:C:O2'	2.43	0.44
2:A:142:VAL:HG12	2:A:163:VAL:O	2.17	0.44
5:D:106:ILE:HB	5:D:139:PRO:HB3	2.00	0.44
14:M:60:SER:O	14:M:63:ARG:NH1	2.51	0.44
15:N:85:ARG:C	15:N:87:ASN:H	2.26	0.44
19:R:51:VAL:HG13	19:R:73:GLU:CB	2.48	0.44
29:X:7:G:C4	29:X:8:A:C8	3.06	0.44
29:X:42:G:H2'	29:X:43:A:C8	2.52	0.44
29:X:223:C:N4	29:X:224:G:O6	2.50	0.44
29:X:389:G:N2	29:X:412:U:H1'	2.32	0.44
29:X:1329:U:O2'	29:X:1330:G:H5'	2.17	0.44
29:X:1819:U:H5'	29:X:1954:A:O3'	2.17	0.44
29:X:1835:C:H2'	29:X:1836:C:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2038:C:O5'	29:X:2039:G:H5''	2.17	0.44
29:X:2039:G:N2	29:X:2040:A:C4	2.86	0.44
29:X:2233:C:C2'	29:X:2234:G:H5'	2.48	0.44
29:X:2290:A:N3	29:X:2290:A:H2'	2.33	0.44
29:X:2800:C:H5''	29:X:2801:A:OP2	2.17	0.44
6:E:7:GLN:H	6:E:8:PRO:HD3	1.82	0.44
6:E:111:HIS:HA	6:E:112:PRO:HD2	1.55	0.44
7:F:111:LYS:HD3	7:F:115:LEU:HG	1.99	0.44
11:J:25:GLY:HA3	29:X:919:U:OP1	2.18	0.44
14:M:42:GLY:C	14:M:44:ARG:H	2.24	0.44
15:N:68:GLY:HA2	15:N:71:LEU:HD12	2.00	0.44
16:O:31:ASP:HB2	16:O:60:VAL:HG21	2.00	0.44
16:O:53:LYS:HG3	16:O:54:TYR:CD1	2.53	0.44
17:P:33:MET:SD	17:P:64:ALA:HB2	2.58	0.44
17:P:75:ALA:HB1	17:P:128:VAL:HG22	1.99	0.44
20:S:18:MET:HA	20:S:35:ASP:HA	1.98	0.44
28:3:42:ARG:HD3	29:X:2328:G:OP2	2.16	0.44
29:X:349:G:H2'	29:X:350:U:C6	2.53	0.44
29:X:387:A:N6	29:X:413:G:O2'	2.51	0.44
29:X:488:A:H8	29:X:488:A:OP1	2.01	0.44
29:X:580:A:C8	29:X:2013:A:N6	2.86	0.44
29:X:1177:U:C2	29:X:1198:C:O2	2.71	0.44
29:X:1310:C:OP1	29:X:2689:C:H4'	2.17	0.44
29:X:1430:G:O2'	29:X:1603:A:H1'	2.18	0.44
29:X:1506:C:H4'	29:X:1507:A:OP1	2.17	0.44
29:X:1653:C:O2'	29:X:1751:A:N3	2.48	0.44
29:X:2793:G:N2	29:X:2804:G:C4	2.86	0.44
1:0:96:ILE:HD11	1:0:118:GLN:HB3	2.00	0.44
1:0:96:ILE:HG23	1:0:123:LEU:HG	2.00	0.44
2:A:29:PRO:HG2	2:A:63:ARG:NH1	2.33	0.44
3:B:7:THR:O	3:B:9:ILE:HD12	2.17	0.44
3:B:55:ALA:H	3:B:58:LYS:HZ2	1.61	0.44
5:D:122:PHE:HB3	5:D:123:ASP:H	1.63	0.44
11:J:12:LYS:HG2	29:X:923:A:N6	2.33	0.44
13:L:9:ARG:O	13:L:11:LEU:N	2.51	0.44
13:L:91:ARG:CG	13:L:92:GLY:H	2.31	0.44
14:M:56:ALA:HB1	14:M:103:LYS:HE3	2.00	0.44
14:M:101:ARG:NH1	29:X:1745:C:OP1	2.47	0.44
20:S:91:PRO:HG3	20:S:126:GLY:N	2.32	0.44
22:U:24:ALA:C	22:U:26:ALA:N	2.76	0.44
28:3:3:LYS:HE3	29:X:219:G:OP2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:3:11:LYS:HB3	28:3:11:LYS:HE2	1.68	0.44
29:X:213:C:H2'	29:X:214:C:C6	2.53	0.44
29:X:464:G:H2'	29:X:465:C:H6	1.83	0.44
29:X:471:A:C2	29:X:481:A:C5	3.06	0.44
29:X:534:U:P	29:X:549:G:H21	2.40	0.44
29:X:790:A:H2'	29:X:791:G:H8	1.83	0.44
29:X:1065:A:H2'	29:X:1066:G:H8	1.82	0.44
29:X:2309:G:H2'	29:X:2310:G:O4'	2.18	0.44
29:X:2571:G:C6	29:X:2572:U:N3	2.86	0.44
29:X:2578:G:C2	29:X:2579:A:C8	3.05	0.44
29:X:2857:C:N3	29:X:2858:A:C8	2.86	0.44
1:0:4:ARG:HG2	1:0:5:ALA:H	1.82	0.44
3:B:5:LEU:HD12	3:B:49:ILE:CD1	2.48	0.44
3:B:10:GLY:O	3:B:25:VAL:HG23	2.18	0.44
3:B:123:ALA:HB2	29:X:2491:C:OP1	2.17	0.44
3:B:199:ARG:H	3:B:199:ARG:HG3	1.65	0.44
10:I:41:SER:OG	29:X:684:C:H3'	2.18	0.44
15:N:91:ASN:ND2	15:N:93:LYS:HB3	2.33	0.44
29:X:65:C:H2'	29:X:66:U:O4'	2.18	0.44
29:X:199:A:O2'	29:X:200:A:O5'	2.29	0.44
29:X:228:A:C5	29:X:229:G:H1'	2.53	0.44
29:X:501:G:H2'	29:X:502:A:H8	1.82	0.44
29:X:1024:G:H2'	29:X:1025:A:C8	2.53	0.44
29:X:1174:G:H2'	29:X:1175:A:H8	1.82	0.44
29:X:1236:G:N2	29:X:1239:A:OP2	2.37	0.44
29:X:1254:G:C2	29:X:1255:A:C5	3.06	0.44
29:X:1642:G:H8	29:X:1642:G:O5'	2.01	0.44
29:X:2508:G:H5''	29:X:2509:A:H5''	2.00	0.44
29:X:2813:G:C5	29:X:2814:G:N7	2.86	0.44
3:B:60:ASN:HB3	3:B:62:PRO:HD2	2.00	0.43
4:C:154:ASP:OD1	4:C:154:ASP:N	2.50	0.43
5:D:92:ARG:CZ	30:Y:46:G:H5''	2.48	0.43
11:J:111:THR:H	11:J:114:GLN:HG3	1.83	0.43
16:O:32:LYS:HB3	16:O:32:LYS:HE3	1.80	0.43
20:S:3:LEU:HD13	20:S:56:VAL:HA	2.00	0.43
28:3:17:THR:HG22	28:3:21:LYS:O	2.18	0.43
28:3:23:MET:HG2	28:3:49:VAL:HG22	1.99	0.43
29:X:567:G:H2'	29:X:568:G:H8	1.83	0.43
29:X:758:G:N2	29:X:766:A:C6	2.86	0.43
29:X:1474:A:H2'	29:X:1474:A:N3	2.32	0.43
29:X:1494:G:O2'	29:X:1574:A:N7	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1600:U:H5''	29:X:1601:U:H5'	1.99	0.43
29:X:1734:C:H2'	29:X:1735:G:H5'	1.99	0.43
29:X:2433:G:C4	29:X:2434:G:C8	3.06	0.43
29:X:2684:A:O5'	29:X:2684:A:H8	2.01	0.43
1:O:110:VAL:HG12	1:O:111:ALA:H	1.83	0.43
1:O:196:LYS:HE2	1:O:204:PHE:CZ	2.53	0.43
3:B:48:GLN:HA	3:B:79:ARG:O	2.19	0.43
5:D:88:LYS:HD3	29:X:2292:C:H5''	1.99	0.43
5:D:158:THR:O	5:D:158:THR:OG1	2.36	0.43
9:H:7:ARG:HD3	9:H:18:GLU:OE2	2.17	0.43
13:L:33:ARG:NH2	13:L:38:ILE:HD13	2.32	0.43
17:P:36:ARG:NH1	25:Z:20:ARG:NH2	2.65	0.43
19:R:24:VAL:HA	19:R:80:LYS:O	2.18	0.43
20:S:19:ILE:HD11	20:S:36:ARG:HG3	2.00	0.43
29:X:312:G:N2	29:X:328:A:H1'	2.32	0.43
29:X:616:U:H4'	29:X:671:A:H4'	1.99	0.43
29:X:818:G:N2	29:X:842:A:OP1	2.51	0.43
29:X:825:C:H2'	29:X:826:U:C6	2.51	0.43
29:X:1146:G:N2	29:X:1147:G:C4	2.86	0.43
29:X:1436:G:O2'	29:X:1508:G:N3	2.51	0.43
29:X:1562:G:H3'	29:X:1563:U:H5'	2.01	0.43
29:X:2269:G:N2	29:X:2322:U:O2'	2.51	0.43
29:X:2273:C:H2'	29:X:2274:C:H6	1.82	0.43
29:X:2407:G:H5''	29:X:2408:G:O5'	2.17	0.43
29:X:2814:G:C2	29:X:2815:C:C2	3.06	0.43
2:A:210:GLY:O	2:A:213:ARG:N	2.50	0.43
4:C:27:LEU:O	4:C:31:VAL:HG23	2.18	0.43
4:C:103:GLY:O	4:C:106:MET:N	2.51	0.43
5:D:129:ASN:HB3	5:D:155:THR:HG22	2.00	0.43
11:J:55:MET:HE1	11:J:105:PHE:CD1	2.52	0.43
15:N:51:ARG:O	15:N:54:LYS:HB2	2.18	0.43
16:O:78:VAL:O	16:O:79:GLN:HB2	2.18	0.43
17:P:81:HIS:C	17:P:83:ASP:H	2.20	0.43
18:Q:29:VAL:HG12	18:Q:30:SER:N	2.32	0.43
22:U:17:SER:OG	22:U:44:ALA:HA	2.18	0.43
24:W:37:THR:CB	29:X:940:G:H5'	2.48	0.43
29:X:851:C:C2	29:X:952:A:C6	3.07	0.43
29:X:1089:C:H1'	29:X:1099:A:H2	1.83	0.43
29:X:1424:U:H2'	29:X:1425:G:O4'	2.18	0.43
29:X:2097:A:H61	29:X:2102:A:H62	1.65	0.43
29:X:2212:U:H2'	29:X:2213:G:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2294:U:H2'	29:X:2295:C:C6	2.53	0.43
29:X:2349:G:C6	29:X:2350:G:C5	3.07	0.43
29:X:2511:G:C5	29:X:2512:A:N7	2.86	0.43
29:X:2678:C:O2	29:X:2688:G:N1	2.52	0.43
2:A:69:ARG:HH22	2:A:192:THR:HG21	1.84	0.43
3:B:129:HIS:CE1	29:X:1692:C:N3	2.86	0.43
4:C:28:HIS:CD2	10:I:8:PRO:HA	2.54	0.43
6:E:25:LYS:HG2	6:E:26:VAL:N	2.32	0.43
7:F:10:LEU:HD21	7:F:57:ILE:HG13	2.00	0.43
7:F:53:ILE:HG12	7:F:72:PRO:HB3	2.00	0.43
9:H:22:ILE:HD11	29:X:1935:A:N6	2.33	0.43
12:K:33:ARG:CB	12:K:114:GLU:HB2	2.49	0.43
15:N:67:ALA:O	15:N:71:LEU:HG	2.18	0.43
19:R:78:ALA:HA	19:R:81:VAL:HB	2.01	0.43
20:S:21:ALA:HB3	20:S:32:PHE:C	2.42	0.43
29:X:82:G:H1	29:X:100:G:HO2'	1.66	0.43
29:X:312:G:O2'	29:X:313:U:H6	1.95	0.43
29:X:350:U:H6	29:X:350:U:O5'	2.01	0.43
29:X:574:C:H4'	29:X:1266:G:C6	2.54	0.43
29:X:714:G:C2	29:X:745:C:C5	3.07	0.43
29:X:717:G:H1'	29:X:739:G:H22	1.84	0.43
29:X:1229:C:H2'	29:X:1230:C:C6	2.52	0.43
29:X:1310:C:H2'	29:X:1311:C:H6	1.84	0.43
29:X:2445:C:H42	29:X:2463:G:H1	1.66	0.43
29:X:2659:C:N3	29:X:2660:C:C5	2.86	0.43
2:A:62:TYR:CE1	29:X:1808:C:H3'	2.51	0.43
4:C:43:ALA:HB2	29:X:456:C:H4'	2.01	0.43
7:F:10:LEU:HD12	7:F:12:LEU:HG	2.00	0.43
10:I:73:GLU:HG3	10:I:105:PRO:O	2.19	0.43
12:K:10:LEU:O	12:K:11:ASN:C	2.61	0.43
15:N:28:ARG:HG2	15:N:38:THR:OG1	2.19	0.43
19:R:54:ILE:HD12	19:R:71:GLN:NE2	2.33	0.43
20:S:49:THR:HG22	20:S:94:VAL:HG13	2.00	0.43
20:S:72:ASP:O	20:S:76:ARG:N	2.49	0.43
25:Z:35:GLN:O	25:Z:37:HIS:N	2.52	0.43
29:X:502:A:H2'	29:X:503:G:O4'	2.19	0.43
29:X:1749:G:N3	29:X:1749:G:H5''	2.34	0.43
29:X:2499:C:C4	29:X:2546:G:C8	3.06	0.43
29:X:2666:U:O2'	29:X:2667:C:H5'	2.18	0.43
3:B:117:MET:O	3:B:118:LYS:C	2.61	0.43
5:D:147:ASP:OD1	5:D:147:ASP:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:8:THR:HG22	11:J:70:PHE:CE2	2.53	0.43
11:J:70:PHE:C	11:J:96:SER:HB2	2.43	0.43
17:P:36:ARG:CZ	25:Z:20:ARG:HH21	2.31	0.43
18:Q:15:LYS:HZ3	29:X:1354:A:H62	1.67	0.43
19:R:58:VAL:HA	29:X:494:A:C4'	2.48	0.43
23:V:11:ALA:HB1	23:V:57:LYS:HD2	2.01	0.43
29:X:26:G:O2'	29:X:27:G:H5'	2.18	0.43
29:X:436:A:N3	29:X:436:A:H2'	2.34	0.43
29:X:539:A:N7	29:X:2025:A:C2	2.87	0.43
29:X:676:G:C5	29:X:677:G:C8	3.07	0.43
29:X:777:A:O2'	29:X:778:G:H5'	2.19	0.43
29:X:783:G:N1	29:X:784:U:C2	2.87	0.43
29:X:1071:U:O4'	29:X:1073:G:H5'	2.18	0.43
29:X:1175:A:H2'	29:X:1176:U:C6	2.54	0.43
29:X:1419:G:H2'	29:X:1420:A:C8	2.53	0.43
29:X:1539:U:O5'	29:X:1539:U:H6	2.02	0.43
29:X:1678:G:C4	29:X:1983:G:N2	2.87	0.43
29:X:1715:A:H8	29:X:1715:A:O5'	2.01	0.43
29:X:1865:C:H2'	29:X:1866:G:O4'	2.19	0.43
29:X:2269:G:N2	29:X:2322:U:H1'	2.34	0.43
29:X:2487:G:C2	29:X:2561:G:C6	3.07	0.43
29:X:2528:G:C2	29:X:2529:G:C8	3.05	0.43
30:Y:25:G:N2	30:Y:62:C:N3	2.52	0.43
30:Y:86:A:C2	30:Y:96:C:C2	3.07	0.43
4:C:59:TYR:HD1	4:C:60:GLY:N	2.15	0.43
4:C:114:GLY:N	4:C:115:GLY:HA2	2.33	0.43
7:F:22:PRO:HB2	7:F:23:VAL:H	1.61	0.43
10:I:73:GLU:OE2	10:I:104:ARG:HB2	2.19	0.43
19:R:38:LEU:O	19:R:46:VAL:HG23	2.19	0.43
29:X:717:G:N3	29:X:739:G:C2	2.87	0.43
29:X:998:C:O2	29:X:1011:A:H2	2.02	0.43
29:X:1110:G:H8	29:X:1110:G:O5'	2.01	0.43
29:X:1609:G:H2'	29:X:1610:A:O4'	2.18	0.43
29:X:1670:G:H5''	29:X:2797:G:N2	2.33	0.43
1:O:188:LEU:O	1:O:192:LEU:HB2	2.18	0.43
2:A:226:MET:HB3	2:A:230:ASP:HB2	2.01	0.43
3:B:44:TYR:CZ	29:X:2616:U:H5'	2.54	0.43
3:B:55:ALA:H	3:B:58:LYS:HZ1	1.64	0.43
9:H:11:ALA:O	9:H:111:PHE:N	2.46	0.43
11:J:52:ARG:O	11:J:56:SER:HB3	2.18	0.43
12:K:102:THR:HG22	12:K:103:ARG:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:63:GLN:H	15:N:63:GLN:HG2	1.56	0.43
18:Q:57:ASN:OD1	18:Q:57:ASN:N	2.51	0.43
21:T:72:LYS:HD3	30:Y:14:C:H5	1.84	0.43
25:Z:32:GLU:O	25:Z:34:PRO:HD3	2.18	0.43
29:X:330:C:C2	29:X:331:U:C6	3.06	0.43
29:X:444:U:O2'	29:X:445:A:H5'	2.19	0.43
29:X:547:U:H2'	29:X:548:G:C8	2.54	0.43
29:X:649:G:C5	29:X:650:U:C5	3.06	0.43
29:X:655:A:H8	29:X:655:A:O5'	2.01	0.43
29:X:817:A:H5''	29:X:818:G:OP1	2.19	0.43
29:X:1030:U:C4	29:X:1031:C:H5	2.36	0.43
29:X:1210:C:H1'	29:X:1239:A:C4	2.53	0.43
29:X:1339:U:C4'	29:X:1993:G:H21	2.32	0.43
29:X:1402:G:H2'	29:X:1403:U:H6	1.84	0.43
29:X:1527:G:H2'	29:X:1528:C:H6	1.83	0.43
29:X:1723:U:C6	29:X:1748:U:OP2	2.71	0.43
29:X:2021:G:C2	29:X:2022:C:C2	3.07	0.43
29:X:2238:G:C6	29:X:2261:G:O6	2.72	0.43
29:X:2655:C:O2	29:X:2712:G:N2	2.51	0.43
29:X:2662:C:C2	29:X:2663:U:C5	3.07	0.43
30:Y:63:A:H2'	30:Y:64:C:C6	2.53	0.43
2:A:247:VAL:HA	2:A:253:PRO:HA	2.01	0.43
4:C:59:TYR:CD1	4:C:60:GLY:N	2.87	0.43
8:G:68:PRO:O	15:N:64:ARG:HG2	2.19	0.43
10:I:73:GLU:OE2	10:I:101:ARG:HB2	2.19	0.43
14:M:69:ARG:CZ	14:M:108:LYS:HG2	2.48	0.43
15:N:37:GLN:CG	29:X:1265:G:H1	2.27	0.43
17:P:9:ARG:HG3	17:P:10:ASN:N	2.33	0.43
20:S:168:VAL:HG12	20:S:169:VAL:N	2.34	0.43
22:U:38:THR:HG22	29:X:2412:A:C2	2.53	0.43
29:X:167:A:H3'	29:X:168:A:H8	1.84	0.43
29:X:312:G:C4	29:X:313:U:C5	3.06	0.43
29:X:402:A:C8	29:X:2392:G:H4'	2.54	0.43
29:X:578:U:H1'	29:X:958:G:O4'	2.19	0.43
29:X:628:A:H2'	29:X:629:C:H6	1.80	0.43
29:X:1287:A:C2	29:X:1315:A:C2	3.07	0.43
29:X:1299:A:N6	29:X:1302:C:C2	2.87	0.43
29:X:1883:A:H5'	29:X:1953:A:H5'	2.00	0.43
29:X:2006:G:C2	29:X:2024:U:O2	2.72	0.43
29:X:2033:C:H5''	29:X:2034:A:OP2	2.19	0.43
29:X:2043:A:H1'	29:X:2481:G:H1'	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2707:G:H2'	29:X:2708:U:C6	2.53	0.43
2:A:126:LYS:HB3	2:A:126:LYS:HE2	1.81	0.43
4:C:129:LYS:HB3	4:C:132:ASN:HD22	1.83	0.43
4:C:176:ASN:OD1	4:C:178:TYR:HB3	2.19	0.43
12:K:8:ARG:NH1	29:X:1669:A:OP1	2.47	0.43
14:M:2:GLN:HB3	29:X:2795:A:N1	2.33	0.43
15:N:10:ARG:HG3	29:X:1264:C:OP1	2.18	0.43
15:N:31:GLN:HE22	29:X:589:C:H4'	1.83	0.43
15:N:107:LYS:O	15:N:110:VAL:HB	2.19	0.43
17:P:36:ARG:HA	17:P:39:ARG:HD2	2.01	0.43
22:U:8:THR:N	22:U:14:VAL:HG23	2.34	0.43
29:X:225:G:H2'	29:X:226:C:OP1	2.19	0.43
29:X:320:A:C6	29:X:341:A:C6	3.07	0.43
29:X:815:A:C5	29:X:816:U:C5	3.07	0.43
29:X:854:G:H22	29:X:948:C:N4	2.17	0.43
29:X:987:G:C2	29:X:988:G:C5	3.07	0.43
29:X:1021:A:N3	29:X:1164:C:H1'	2.34	0.43
29:X:1321:A:H61	29:X:1624:A:H61	1.66	0.43
29:X:1322:G:H1	29:X:1621:C:H42	1.67	0.43
29:X:2015:G:OP2	29:X:2433:G:O2'	2.36	0.43
29:X:2369:U:C6	29:X:2369:U:C3'	3.02	0.43
29:X:2429:A:OP1	29:X:2476:A:C8	2.71	0.43
29:X:2493:U:H2'	29:X:2494:C:C6	2.54	0.43
29:X:2604:G:C5	29:X:2605:C:C4	3.07	0.43
30:Y:42:U:H3'	30:Y:43:G:H5''	2.01	0.43
2:A:88:ARG:NH1	29:X:1809:G:OP1	2.51	0.42
3:B:34:VAL:HG21	3:B:67:PHE:HE1	1.83	0.42
3:B:52:ALA:O	3:B:76:ARG:N	2.48	0.42
5:D:61:THR:O	5:D:61:THR:OG1	2.37	0.42
6:E:45:GLN:HG3	6:E:49:GLN:O	2.18	0.42
9:H:43:ARG:NH2	29:X:1979:C:OP2	2.49	0.42
11:J:88:LYS:HG2	29:X:967:G:OP1	2.20	0.42
12:K:112:LEU:HD11	25:Z:57:VAL:HG13	2.01	0.42
25:Z:52:TYR:CZ	29:X:2859:U:N3	2.84	0.42
27:2:24:THR:O	27:2:28:ARG:HD3	2.19	0.42
29:X:351:A:H2'	29:X:352:G:H5'	2.01	0.42
29:X:469:G:N2	29:X:480:G:H2'	2.34	0.42
29:X:520:C:H2'	29:X:521:U:O4'	2.19	0.42
29:X:585:U:H4'	29:X:2481:G:C8	2.54	0.42
29:X:815:A:H5''	29:X:816:U:OP2	2.19	0.42
29:X:951:G:H2'	29:X:952:A:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1028:G:C2	29:X:1157:G:C4	3.06	0.42
29:X:1104:G:N2	29:X:1109:A:H62	2.09	0.42
29:X:1287:A:C2	29:X:1315:A:H2	2.37	0.42
29:X:1672:A:H3'	29:X:1673:C:H6	1.84	0.42
29:X:1746:A:H8	29:X:1746:A:O5'	2.02	0.42
29:X:2214:G:H2'	29:X:2215:C:C6	2.54	0.42
29:X:2326:C:H2'	29:X:2327:U:C6	2.54	0.42
29:X:2512:A:H2'	29:X:2513:A:O4'	2.18	0.42
30:Y:55:C:H2'	30:Y:56:G:O4'	2.18	0.42
2:A:67:PHE:HB3	2:A:153:ALA:H	1.84	0.42
2:A:252:LYS:HA	2:A:253:PRO:HD3	1.90	0.42
3:B:23:VAL:HG11	3:B:183:LEU:HB3	2.00	0.42
3:B:33:ILE:HG12	3:B:36:ARG:HH21	1.84	0.42
4:C:22:VAL:HG22	4:C:106:MET:HG2	2.01	0.42
4:C:48:ARG:NH2	29:X:686:C:OP1	2.52	0.42
4:C:102:LEU:HD12	4:C:102:LEU:O	2.18	0.42
6:E:21:ASP:HB3	6:E:22:GLY:H	1.41	0.42
6:E:75:ALA:O	6:E:79:VAL:HG22	2.19	0.42
15:N:9:VAL:O	15:N:12:ARG:HB2	2.20	0.42
19:R:51:VAL:HG22	19:R:52:ASN:N	2.34	0.42
20:S:24:TYR:HB3	20:S:29:ASN:HB2	2.00	0.42
23:V:25:LEU:O	23:V:28:LEU:HB2	2.19	0.42
28:3:4:MET:HE3	28:3:4:MET:HB2	1.73	0.42
28:3:33:ASN:ND2	29:X:2398:U:O5'	2.50	0.42
29:X:1:G:H2'	29:X:2:G:H8	1.83	0.42
29:X:218:A:C6	29:X:232:A:H5''	2.54	0.42
29:X:351:A:N6	29:X:352:G:C2	2.86	0.42
29:X:1088:A:N1	29:X:1099:A:O2'	2.34	0.42
29:X:1142:G:C8	29:X:2008:C:O2'	2.59	0.42
29:X:2432:A:H2'	29:X:2433:G:C8	2.54	0.42
29:X:2595:C:H2'	29:X:2596:C:C6	2.53	0.42
29:X:2660:C:C2	29:X:2704:U:O4	2.72	0.42
4:C:35:LEU:O	4:C:38:ARG:HG3	2.19	0.42
5:D:7:LYS:O	5:D:11:GLN:HG3	2.19	0.42
7:F:126:THR:HA	29:X:1091:C:O2'	2.19	0.42
13:L:8:ARG:HA	13:L:8:ARG:HD2	1.80	0.42
13:L:98:GLY:HA3	30:Y:51:G:OP1	2.19	0.42
15:N:59:ARG:O	15:N:63:GLN:HG2	2.19	0.42
16:O:71:ILE:HG13	29:X:1003:C:O2'	2.19	0.42
16:O:72:ARG:HA	16:O:82:ARG:O	2.19	0.42
17:P:38:VAL:O	17:P:41:VAL:HG23	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:64:ASN:HA	19:R:65:PRO:HD2	1.82	0.42
29:X:746:G:N7	29:X:774:A:N6	2.66	0.42
29:X:782:U:H2'	29:X:783:G:C8	2.54	0.42
29:X:828:C:N3	29:X:1207:G:C2	2.87	0.42
29:X:836:G:H2'	29:X:837:U:H6	1.80	0.42
29:X:1080:A:H4'	29:X:1081:A:H8	1.84	0.42
29:X:1091:C:H2'	29:X:1092:U:C6	2.54	0.42
29:X:1179:A:C2	29:X:1196:G:N1	2.87	0.42
29:X:1381:G:C2'	29:X:1799:A:H61	2.31	0.42
29:X:1674:C:C2	29:X:1675:C:C5	3.07	0.42
29:X:1942:G:H2'	29:X:1943:A:O4'	2.20	0.42
29:X:1950:C:N4	29:X:1951:G:C6	2.88	0.42
29:X:2057:U:C2	29:X:2415:G:C2	3.07	0.42
29:X:2450:A:C4	29:X:2451:G:C8	3.08	0.42
29:X:2543:A:C6	29:X:2544:A:N1	2.88	0.42
29:X:2610:G:O2'	29:X:2785:A:N1	2.48	0.42
30:Y:36:A:H4'	30:Y:37:C:H5	1.84	0.42
2:A:72:LYS:O	2:A:75:VAL:HG12	2.19	0.42
4:C:42:THR:HG21	29:X:454:G:N3	2.33	0.42
8:G:141:GLY:O	8:G:142:ARG:C	2.62	0.42
9:H:115:ALA:C	9:H:117:GLU:N	2.75	0.42
11:J:60:ARG:O	11:J:62:GLY:HA2	2.19	0.42
13:L:65:THR:HG21	30:Y:52:G:OP2	2.19	0.42
16:O:32:LYS:NZ	16:O:34:GLU:OE1	2.51	0.42
16:O:75:LYS:HG3	16:O:80:TYR:HD1	1.84	0.42
25:Z:16:ARG:HD2	25:Z:20:ARG:HH12	1.85	0.42
29:X:587:A:H2'	29:X:588:G:H5''	1.99	0.42
29:X:718:A:H2'	29:X:719:A:C8	2.55	0.42
29:X:887:G:H1	29:X:915:C:H42	1.67	0.42
29:X:1667:A:H5''	29:X:1668:G:OP2	2.20	0.42
29:X:1720:G:C2	29:X:1721:G:C4	3.07	0.42
29:X:1977:C:O2	29:X:1977:C:H2'	2.19	0.42
29:X:2041:A:H8	29:X:2041:A:O5'	2.02	0.42
29:X:2255:G:C2	29:X:2256:G:C8	3.07	0.42
29:X:2691:C:O2	29:X:2692:A:H2'	2.19	0.42
7:F:14:ALA:C	7:F:45:THR:HG21	2.44	0.42
8:G:61:ARG:HA	8:G:66:HIS:CE1	2.54	0.42
10:I:94:GLU:HA	10:I:97:ARG:HE	1.84	0.42
17:P:16:GLN:NE2	29:X:511:A:O2'	2.52	0.42
17:P:30:TYR:H	17:P:123:HIS:CE1	2.37	0.42
21:T:4:LYS:HA	21:T:4:LYS:HD3	1.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:192:G:H4'	29:X:193:A:H4'	2.01	0.42
29:X:303:C:H42	29:X:359:G:H1	1.66	0.42
29:X:681:A:C2	29:X:683:A:C6	3.07	0.42
29:X:752:G:H4'	29:X:753:U:OP1	2.20	0.42
29:X:813:A:O5'	29:X:813:A:H8	2.02	0.42
29:X:816:U:O2'	29:X:817:A:H5'	2.20	0.42
29:X:1672:A:H3'	29:X:1673:C:C5	2.54	0.42
29:X:1699:A:H2'	29:X:1700:C:C6	2.55	0.42
29:X:1811:A:H1'	29:X:1813:A:C6	2.54	0.42
29:X:1830:C:H41	29:X:1882:G:P	2.42	0.42
29:X:2169:A:H2'	29:X:2170:C:C6	2.54	0.42
29:X:2223:U:H2'	29:X:2224:U:O4'	2.20	0.42
29:X:2536:G:O2'	29:X:2537:C:H5'	2.20	0.42
29:X:2543:A:C2	29:X:2626:U:H4'	2.54	0.42
29:X:2564:U:C6	29:X:2564:U:H5'	2.54	0.42
29:X:2720:A:C8	29:X:2743:G:N2	2.87	0.42
29:X:2844:G:C6	29:X:2845:C:N3	2.88	0.42
3:B:146:THR:HG23	29:X:1141:U:H5	1.84	0.42
11:J:78:LYS:HE3	11:J:78:LYS:HB2	1.64	0.42
15:N:64:ARG:O	15:N:67:ALA:HB3	2.19	0.42
17:P:62:ARG:NH1	25:Z:25:LEU:HD11	2.28	0.42
19:R:45:LYS:HA	19:R:76:LEU:O	2.19	0.42
29:X:74:G:OP1	29:X:74:G:H4'	2.20	0.42
29:X:740:A:OP1	29:X:1445:A:O2'	2.30	0.42
29:X:984:A:O4'	29:X:1202:U:C6	2.72	0.42
29:X:1713:G:H21	29:X:1961:A:H5'	1.85	0.42
29:X:1762:C:C2	29:X:1763:G:C8	3.08	0.42
29:X:2706:U:H3'	29:X:2707:G:H8	1.85	0.42
2:A:229:VAL:HG11	29:X:797:A:C5	2.54	0.42
3:B:19:ARG:HA	9:H:84:ALA:O	2.20	0.42
3:B:117:MET:O	3:B:119:ARG:N	2.53	0.42
3:B:203:LYS:NZ	29:X:2712:G:OP1	2.43	0.42
9:H:73:VAL:HG12	9:H:99:ILE:HD13	2.00	0.42
14:M:101:ARG:NH1	29:X:1745:C:P	2.92	0.42
15:N:39:LEU:HA	15:N:42:ALA:HB3	2.01	0.42
21:T:56:ASP:OD1	29:X:2343:C:H5'	2.19	0.42
22:U:72:LYS:HA	22:U:72:LYS:HD3	1.89	0.42
25:Z:6:VAL:O	29:X:2594:U:C4	2.71	0.42
27:2:16:HIS:HD2	29:X:699:G:O6	2.02	0.42
29:X:18:U:H6	29:X:18:U:O5'	2.03	0.42
29:X:389:G:H2'	29:X:390:U:H6	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1298:G:C5	29:X:1342:U:C5	3.08	0.42
29:X:1374:G:O2'	29:X:1375:C:H5'	2.19	0.42
29:X:1541:G:C4	29:X:1542:G:C8	3.07	0.42
29:X:1554:G:H2'	29:X:1555:A:C8	2.54	0.42
29:X:1569:A:N6	29:X:1571:G:H1'	2.35	0.42
29:X:1750:A:C2	29:X:1751:A:C5	3.08	0.42
29:X:2001:G:C6	29:X:2002:A:C5	3.07	0.42
29:X:2849:C:H2'	29:X:2850:U:H6	1.84	0.42
30:Y:7:C:O2	30:Y:119:G:N2	2.52	0.42
1:O:115:MET:HE3	1:O:118:GLN:HE22	1.85	0.42
3:B:41:THR:HB	3:B:42:ASP:OD1	2.20	0.42
4:C:51:VAL:HG11	4:C:80:GLY:C	2.44	0.42
4:C:95:LEU:HD12	4:C:96:PRO:HD2	2.00	0.42
6:E:86:ASN:HB2	6:E:165:VAL:HG22	2.02	0.42
10:I:57:ILE:HG21	28:3:61:MET:HE1	2.02	0.42
11:J:6:LYS:HB3	11:J:7:ARG:H	1.67	0.42
15:N:91:ASN:O	15:N:95:LEU:HG	2.20	0.42
16:O:19:VAL:HG12	16:O:20:ILE:H	1.84	0.42
16:O:95:ILE:HD13	16:O:95:ILE:HA	1.83	0.42
17:P:28:ALA:O	17:P:123:HIS:HA	2.20	0.42
26:1:14:SER:HB3	26:1:49:PHE:CE1	2.54	0.42
27:2:28:ARG:O	27:2:31:LEU:HB2	2.19	0.42
29:X:13:A:N3	29:X:15:G:C6	2.88	0.42
29:X:14:A:N6	29:X:15:G:C2	2.88	0.42
29:X:511:A:C6	29:X:512:A:C2	3.08	0.42
29:X:728:G:H22	29:X:730:C:N4	2.18	0.42
29:X:763:A:C2	29:X:765:C:H4'	2.54	0.42
29:X:790:A:C2	29:X:791:G:C5	3.07	0.42
29:X:946:U:C2	29:X:947:C:C6	3.08	0.42
29:X:1040:A:H2	29:X:2444:C:O2	2.02	0.42
29:X:1135:C:C2	29:X:1136:G:C8	3.08	0.42
29:X:1345:G:N7	29:X:1626:A:C8	2.88	0.42
29:X:1643:A:H61	29:X:1656:U:H3	1.66	0.42
29:X:1693:A:C2	29:X:1976:U:H5'	2.55	0.42
29:X:1733:U:C5	29:X:1735:G:H1'	2.54	0.42
29:X:2019:C:O2'	29:X:2020:G:H5'	2.19	0.42
29:X:2425:G:N2	29:X:2480:C:N3	2.67	0.42
2:A:13:ARG:HA	2:A:13:ARG:HD3	1.44	0.42
2:A:108:PRO:HA	2:A:196:VAL:O	2.20	0.42
2:A:126:LYS:HB2	2:A:129:ASN:OD1	2.20	0.42
2:A:235:GLY:HA3	29:X:2577:A:H5''	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:186:LEU:HG	4:C:188:ILE:HA	2.02	0.42
5:D:34:ILE:HA	5:D:156:ILE:HG23	2.02	0.42
6:E:39:THR:OG1	6:E:40:GLU:N	2.53	0.42
8:G:69:ASP:HA	15:N:64:ARG:NH2	2.33	0.42
9:H:73:VAL:HG21	9:H:123:PHE:CE2	2.55	0.42
9:H:124:MET:HE3	9:H:124:MET:H	1.85	0.42
12:K:27:ALA:HA	12:K:30:ARG:HB3	2.02	0.42
12:K:100:VAL:HG12	12:K:101:GLY:N	2.34	0.42
14:M:56:ALA:CB	14:M:103:LYS:HE3	2.50	0.42
20:S:13:LYS:HB2	20:S:14:LEU:H	1.51	0.42
20:S:48:THR:O	20:S:48:THR:OG1	2.32	0.42
26:1:7:ARG:NH1	26:1:25:THR:O	2.53	0.42
29:X:139:A:H2'	29:X:140:G:C8	2.55	0.42
29:X:541:C:O2'	29:X:572:G:H5''	2.19	0.42
29:X:877:G:N2	29:X:925:U:O2	2.53	0.42
29:X:963:G:H5'	29:X:964:A:OP2	2.20	0.42
29:X:1681:A:O5'	29:X:1681:A:H8	2.01	0.42
29:X:1689:U:C2'	29:X:1690:U:H5'	2.50	0.42
29:X:1699:A:C2	29:X:1700:C:C2	3.08	0.42
29:X:1701:C:C2	29:X:1722:G:C2	3.08	0.42
29:X:2038:C:H6	29:X:2483:U:H5'	1.83	0.42
29:X:2201:G:C4	29:X:2202:G:C8	3.07	0.42
29:X:2310:G:N2	29:X:2364:C:C4	2.87	0.42
29:X:2494:C:H2'	29:X:2495:G:H8	1.85	0.42
29:X:2709:C:H2'	29:X:2710:C:C6	2.55	0.42
29:X:2829:A:C2	29:X:2839:G:C4	3.08	0.42
30:Y:90:C:H2'	30:Y:91:A:O4'	2.20	0.42
3:B:26:VAL:HG11	3:B:198:LEU:HD11	2.01	0.42
3:B:61:LYS:O	3:B:62:PRO:C	2.61	0.42
4:C:7:ILE:HD13	4:C:7:ILE:HA	1.74	0.42
4:C:107:ALA:HB2	4:C:177:VAL:HG13	2.02	0.42
12:K:44:LEU:O	12:K:44:LEU:HG	2.18	0.42
13:L:32:TYR:O	13:L:32:TYR:CG	2.72	0.42
15:N:13:ARG:NH2	29:X:1264:C:OP1	2.50	0.42
17:P:102:THR:HG22	17:P:120:ARG:HA	2.02	0.42
17:P:110:ALA:HB2	29:X:761:G:O5'	2.20	0.42
19:R:24:VAL:HB	19:R:29:HIS:O	2.19	0.42
21:T:66:LYS:HE2	21:T:66:LYS:HB3	1.72	0.42
25:Z:3:LYS:HG3	29:X:2591:C:OP2	2.20	0.42
28:3:33:ASN:C	28:3:35:GLY:N	2.76	0.42
29:X:167:A:C2	29:X:168:A:C4	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:215:G:H1'	29:X:619:A:H1'	2.01	0.42
29:X:457:C:C2'	29:X:458:G:H5''	2.50	0.42
29:X:961:G:C6	29:X:962:C:C4	3.08	0.42
29:X:1016:C:C2	29:X:1154:A:C5	3.08	0.42
29:X:1059:A:O5'	29:X:1059:A:H8	2.03	0.42
29:X:1314:A:H2	29:X:1642:G:N3	2.18	0.42
29:X:1704:G:H1'	29:X:1719:G:N2	2.34	0.42
29:X:2150:U:H2'	29:X:2151:G:C8	2.55	0.42
29:X:2461:G:H2'	29:X:2461:G:N3	2.34	0.42
29:X:2685:A:N1	29:X:2686:C:C2	2.87	0.42
30:Y:48:A:C5	30:Y:49:C:C4	3.07	0.42
2:A:151:LYS:HD3	29:X:2186:G:H4'	2.02	0.41
4:C:28:HIS:NE2	10:I:8:PRO:HB3	2.34	0.41
4:C:153:ASP:HA	4:C:158:ARG:NH2	2.35	0.41
10:I:120:VAL:HG23	10:I:139:ARG:O	2.20	0.41
11:J:131:LYS:HD2	11:J:131:LYS:HA	1.93	0.41
21:T:31:VAL:HG22	21:T:35:ASN:HB2	2.01	0.41
22:U:27:ASP:CA	22:U:32:ARG:HH21	2.33	0.41
25:Z:4:HIS:HD1	25:Z:4:HIS:C	2.28	0.41
28:3:7:HIS:HD2	28:3:61:MET:CE	2.32	0.41
29:X:63:A:O2'	29:X:64:C:H5'	2.19	0.41
29:X:66:U:H2'	29:X:67:G:H8	1.85	0.41
29:X:71:A:O2'	29:X:74:G:N2	2.53	0.41
29:X:76:C:C2	29:X:108:G:C2	3.08	0.41
29:X:198:A:O2'	29:X:243:G:O6	2.35	0.41
29:X:736:G:H2'	29:X:737:C:O4'	2.20	0.41
29:X:824:U:H1'	29:X:1264:C:O4'	2.20	0.41
29:X:830:C:O2	29:X:1205:G:N2	2.53	0.41
29:X:2269:G:H22	29:X:2322:U:H1'	1.85	0.41
29:X:2437:G:C8	29:X:2469:G:C6	3.08	0.41
29:X:2496:C:O2'	29:X:2521:A:N7	2.44	0.41
29:X:2665:G:C6	29:X:2666:U:N3	2.88	0.41
29:X:2770:A:H4'	29:X:2771:C:O5'	2.20	0.41
30:Y:3:A:C6	30:Y:4:C:N4	2.88	0.41
3:B:179:GLU:O	3:B:181:LEU:N	2.53	0.41
5:D:125:ARG:HD2	29:X:2295:C:O4'	2.20	0.41
6:E:68:THR:O	6:E:72:VAL:HG23	2.21	0.41
8:G:39:GLN:HG3	8:G:79:PHE:CE1	2.55	0.41
15:N:33:ARG:HD3	29:X:1265:G:N3	2.35	0.41
15:N:74:MET:CE	15:N:79:PHE:HD1	2.33	0.41
17:P:41:VAL:HG13	17:P:60:ILE:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:112:LEU:O	20:S:171:VAL:HA	2.20	0.41
29:X:198:A:C8	29:X:243:G:C5	3.08	0.41
29:X:632:A:H2'	29:X:633:G:O4'	2.20	0.41
29:X:656:U:C5	29:X:657:A:C4	3.08	0.41
29:X:658:G:H2'	29:X:659:G:H8	1.85	0.41
29:X:753:U:O4'	29:X:1964:A:C4	2.73	0.41
29:X:786:U:H2'	29:X:787:A:H5'	2.02	0.41
29:X:787:A:O2'	29:X:790:A:H1'	2.21	0.41
29:X:1045:G:C6	29:X:1133:G:C2	3.08	0.41
29:X:1298:G:N1	29:X:1342:U:OP1	2.49	0.41
29:X:1302:C:H2'	29:X:1303:U:H6	1.84	0.41
29:X:1407:G:C6	29:X:1408:A:N6	2.89	0.41
29:X:1526:U:H4'	29:X:1527:G:OP1	2.20	0.41
29:X:1920:A:N7	29:X:1923:U:C5	2.88	0.41
29:X:1987:G:C6	29:X:1988:A:C4	3.08	0.41
29:X:2326:C:C5	29:X:2361:G:H1'	2.55	0.41
29:X:2639:A:H3'	29:X:2640:G:H8	1.81	0.41
2:A:231:HIS:ND1	2:A:249:PRO:HA	2.35	0.41
3:B:141:ILE:HD11	29:X:2034:A:C1'	2.50	0.41
3:B:154:LYS:O	3:B:155:ARG:C	2.64	0.41
4:C:17:LEU:HG	4:C:109:ALA:HB2	2.02	0.41
4:C:50:GLN:O	4:C:52:SER:N	2.53	0.41
4:C:112:GLN:C	4:C:114:GLY:H	2.28	0.41
5:D:36:VAL:HG22	5:D:154:ILE:HG13	2.01	0.41
5:D:60:ILE:HG21	5:D:141:ILE:HG12	2.02	0.41
6:E:30:LYS:HB2	6:E:79:VAL:O	2.21	0.41
14:M:8:ASN:O	14:M:9:ARG:C	2.64	0.41
17:P:33:MET:HE1	17:P:64:ALA:HA	2.01	0.41
22:U:67:ILE:HD13	22:U:67:ILE:HA	1.89	0.41
29:X:202:A:N6	29:X:203:G:N3	2.68	0.41
29:X:750:C:N3	29:X:751:G:C8	2.88	0.41
29:X:854:G:H8	29:X:854:G:O5'	2.03	0.41
29:X:1135:C:H2'	29:X:1136:G:H8	1.84	0.41
29:X:1147:G:N2	29:X:1148:G:H1'	2.35	0.41
29:X:1353:A:H4'	29:X:1407:G:H1'	2.02	0.41
29:X:1467:U:H4'	29:X:1468:A:C4	2.54	0.41
29:X:1665:C:C4	29:X:1666:G:N7	2.88	0.41
29:X:1710:U:H4'	29:X:1711:C:OP2	2.20	0.41
29:X:2010:G:C2	29:X:2020:G:C5	3.09	0.41
29:X:2044:G:N7	29:X:2480:C:H4'	2.34	0.41
29:X:2781:G:H2'	29:X:2782:G:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Y:58:G:H4'	30:Y:59:A:O4'	2.21	0.41
30:Y:117:G:H8	30:Y:117:G:O5'	2.03	0.41
2:A:95:LEU:HD23	2:A:95:LEU:HA	1.85	0.41
2:A:260:ARG:NH2	2:A:264:LYS:HD3	2.34	0.41
3:B:101:LYS:HA	3:B:170:LEU:O	2.20	0.41
4:C:77:PHE:CE1	29:X:1270:C:H4'	2.55	0.41
4:C:179:ASP:HA	4:C:182:ARG:HB3	2.02	0.41
5:D:100:LEU:O	5:D:103:LEU:HB3	2.20	0.41
6:E:115:ILE:HD12	6:E:115:ILE:HA	1.83	0.41
12:K:39:THR:C	12:K:41:ALA:N	2.79	0.41
15:N:47:TYR:CZ	15:N:51:ARG:NH2	2.88	0.41
17:P:21:ARG:O	17:P:23:PRO:HD3	2.20	0.41
17:P:57:LEU:HD13	17:P:69:ALA:HA	2.03	0.41
18:Q:20:MET:HG3	18:Q:25:TYR:CE1	2.55	0.41
18:Q:22:ARG:HH12	18:Q:24:VAL:HG21	1.85	0.41
29:X:33:C:N4	29:X:458:G:HO2'	2.13	0.41
29:X:88:G:H5''	29:X:89:A:C5'	2.49	0.41
29:X:841:G:C2	29:X:842:A:N6	2.89	0.41
29:X:980:G:O5'	29:X:980:G:H8	2.03	0.41
29:X:982:C:H2'	29:X:983:G:O4'	2.21	0.41
29:X:1194:U:C4	29:X:1195:U:C4	3.08	0.41
29:X:1243:G:C2	29:X:1244:U:O2	2.73	0.41
29:X:1261:G:H8	29:X:1261:G:O5'	2.04	0.41
29:X:1374:G:H2'	29:X:1375:C:H6	1.85	0.41
29:X:1440:G:C6	29:X:1441:A:C6	3.08	0.41
29:X:1802:A:H3'	29:X:1803:G:H8	1.85	0.41
29:X:1917:C:O2'	29:X:1918:G:H5'	2.19	0.41
29:X:2022:C:H2'	29:X:2023:C:H6	1.85	0.41
29:X:2177:U:H2'	29:X:2178:U:O4'	2.21	0.41
29:X:2311:U:H4'	29:X:2315:A:H62	1.85	0.41
29:X:2332:G:C6	29:X:2344:G:N2	2.88	0.41
29:X:2560:G:H22	29:X:2589:C:H2'	1.85	0.41
1:O:95:LEU:HD22	1:O:98:ARG:HD2	2.02	0.41
2:A:170:SER:HB3	2:A:171:ASP:H	1.67	0.41
2:A:209:ALA:O	2:A:212:SER:N	2.52	0.41
5:D:37:ASN:CG	29:X:2291:U:HO2'	2.24	0.41
5:D:83:MET:HA	5:D:84:PRO:HD3	1.86	0.41
6:E:160:LYS:NZ	29:X:2636:A:O3'	2.52	0.41
9:H:22:ILE:HD12	9:H:22:ILE:HA	1.92	0.41
9:H:79:HIS:CG	9:H:80:ALA:H	2.38	0.41
10:I:14:LYS:O	29:X:675:C:H5'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:32:ARG:HH22	29:X:684:C:P	2.43	0.41
15:N:29:SER:C	15:N:30:LYS:HG2	2.45	0.41
18:Q:68:PHE:CD1	29:X:64:C:H1'	2.54	0.41
19:R:38:LEU:HB3	19:R:47:VAL:HG23	2.03	0.41
20:S:3:LEU:HG	20:S:32:PHE:HD1	1.84	0.41
23:V:48:ARG:HG2	23:V:52:GLN:HE21	1.85	0.41
27:2:21:ARG:O	27:2:27:GLY:HA3	2.21	0.41
29:X:182:G:O2'	29:X:183:U:OP2	2.37	0.41
29:X:184:A:H2'	29:X:185:C:O4'	2.21	0.41
29:X:318:G:N2	29:X:321:A:C8	2.89	0.41
29:X:530:G:O2'	29:X:531:G:H5'	2.21	0.41
29:X:1109:A:H8	29:X:1109:A:O5'	2.02	0.41
29:X:1204:G:H2'	29:X:1205:G:C8	2.55	0.41
29:X:1581:C:O2'	29:X:1582:A:OP2	2.33	0.41
29:X:2325:A:H4'	29:X:2326:C:OP2	2.18	0.41
29:X:2359:U:H2'	29:X:2360:C:C6	2.56	0.41
29:X:2487:G:H2'	29:X:2488:G:O4'	2.21	0.41
1:O:28:LEU:HB3	1:O:216:PRO:HD3	2.02	0.41
2:A:119:ALA:HA	2:A:130:ALA:HB3	2.02	0.41
2:A:231:HIS:CE1	2:A:249:PRO:HA	2.55	0.41
3:B:33:ILE:HG12	3:B:36:ARG:HE	1.85	0.41
4:C:7:ILE:CG2	4:C:122:GLY:HA3	2.51	0.41
6:E:45:GLN:HA	6:E:50:LEU:HA	2.02	0.41
6:E:105:MET:HB2	6:E:113:VAL:O	2.20	0.41
8:G:51:LEU:HD11	8:G:127:ILE:HD13	2.02	0.41
11:J:19:THR:CG2	11:J:20:GLY:N	2.81	0.41
11:J:84:MET:HE2	29:X:967:G:C4'	2.50	0.41
13:L:28:ARG:HH21	13:L:45:ASP:HB3	1.85	0.41
16:O:62:GLU:HG2	16:O:63:HIS:N	2.35	0.41
17:P:19:LYS:N	17:P:19:LYS:HD2	2.35	0.41
17:P:27:VAL:O	29:X:503:G:O2'	2.32	0.41
26:I:27:ASN:ND2	29:X:2264:C:OP1	2.53	0.41
29:X:36:G:N3	29:X:462:G:O2'	2.53	0.41
29:X:205:A:C2'	29:X:206:U:H5'	2.44	0.41
29:X:1066:G:H1	29:X:1115:C:N4	2.15	0.41
29:X:1513:U:C6	29:X:1593:C:H5''	2.56	0.41
29:X:1666:G:C6	29:X:1992:G:O6	2.74	0.41
29:X:1935:A:N6	29:X:1936:A:N1	2.68	0.41
29:X:1994:U:H2'	29:X:1995:G:H5'	2.01	0.41
29:X:2320:G:H2'	29:X:2321:C:O4'	2.20	0.41
29:X:2415:G:H2'	29:X:2416:U:H6	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2604:G:H2'	29:X:2605:C:C6	2.55	0.41
29:X:2801:A:H2'	29:X:2801:A:N3	2.36	0.41
30:Y:104:A:C6	30:Y:105:G:C5	3.09	0.41
2:A:24:LEU:CD1	2:A:84:TYR:HB2	2.50	0.41
2:A:206:LEU:HD23	29:X:1783:G:OP1	2.21	0.41
4:C:178:TYR:O	4:C:179:ASP:C	2.63	0.41
5:D:38:GLU:HG2	5:D:53:ALA:HB1	2.03	0.41
5:D:125:ARG:H	5:D:125:ARG:HG2	1.50	0.41
8:G:33:ILE:HG12	29:X:547:U:O2'	2.21	0.41
8:G:134:MET:O	8:G:135:LEU:HG	2.20	0.41
9:H:1:MET:N	9:H:46:HIS:HB3	2.35	0.41
9:H:3:MET:HE2	9:H:3:MET:HB2	1.86	0.41
9:H:117:GLU:O	9:H:120:ASP:HB2	2.21	0.41
10:I:45:LYS:H	10:I:46:GLY:HA2	1.86	0.41
12:K:99:ARG:H	12:K:99:ARG:HE	1.69	0.41
19:R:44:GLN:HE21	19:R:44:GLN:HB2	1.70	0.41
21:T:41:ARG:NH1	29:X:2366:U:H1'	2.35	0.41
25:Z:55:ARG:NH2	25:Z:58:LEU:HA	2.36	0.41
29:X:315:G:C2	29:X:325:U:O2	2.74	0.41
29:X:790:A:N3	29:X:791:G:C8	2.89	0.41
29:X:797:A:HO2'	29:X:798:G:H8	1.66	0.41
29:X:1340:C:C4	29:X:1341:G:C6	3.08	0.41
29:X:1495:G:H2'	29:X:1496:G:H8	1.84	0.41
29:X:1656:U:O2'	29:X:2678:C:H4'	2.20	0.41
29:X:1750:A:H2'	29:X:1751:A:C8	2.55	0.41
29:X:2151:G:N2	29:X:2153:A:H3'	2.35	0.41
29:X:2292:C:C2	29:X:2293:G:C8	3.09	0.41
29:X:2352:A:C6	29:X:2353:G:C6	3.09	0.41
29:X:2445:C:N3	29:X:2464:G:C2	2.89	0.41
29:X:2494:C:H2'	29:X:2495:G:C8	2.55	0.41
29:X:2728:A:C5	29:X:2737:A:N6	2.89	0.41
1:O:27:GLU:O	1:O:29:ALA:N	2.48	0.41
2:A:204:ILE:HG13	2:A:204:ILE:H	1.64	0.41
6:E:116:GLU:HA	6:E:117:PRO:HD2	1.96	0.41
7:F:2:ARG:NH2	7:F:30:TYR:HA	2.36	0.41
15:N:50:ARG:NH1	29:X:1004:A:OP1	2.42	0.41
17:P:37:LYS:O	17:P:40:LEU:HB2	2.20	0.41
17:P:90:LEU:CD1	17:P:128:VAL:HB	2.47	0.41
19:R:51:VAL:HG21	19:R:74:LEU:O	2.20	0.41
20:S:62:PHE:HB3	20:S:85:MET:SD	2.60	0.41
20:S:172:LEU:HD23	20:S:172:LEU:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:28:ILE:H	24:W:28:ILE:HG13	1.71	0.41
26:1:37:LEU:HD12	26:1:37:LEU:HA	1.80	0.41
28:3:52:LYS:HB3	28:3:53:ALA:H	1.68	0.41
29:X:23:G:C2	29:X:24:G:C8	3.09	0.41
29:X:114:C:O2'	29:X:124:A:N3	2.49	0.41
29:X:140:G:H2'	29:X:141:G:C8	2.56	0.41
29:X:168:A:HO2'	29:X:691:C:HO2'	1.55	0.41
29:X:623:G:N1	29:X:627:A:C6	2.88	0.41
29:X:784:U:H2'	29:X:785:U:C6	2.55	0.41
29:X:1098:G:O6	29:X:1100:G:N2	2.54	0.41
29:X:1716:G:O6	29:X:1754:G:H1'	2.20	0.41
29:X:1787:U:O2'	29:X:1788:C:H5'	2.20	0.41
29:X:1885:C:C2	29:X:1886:G:H1'	2.56	0.41
29:X:1887:G:O2'	29:X:1911:A:N1	2.53	0.41
29:X:2145:A:H5''	29:X:2155:U:H6	1.84	0.41
29:X:2165:A:H2'	29:X:2166:G:C8	2.55	0.41
29:X:2459:C:N4	29:X:2460:G:O6	2.54	0.41
29:X:2751:C:H2'	29:X:2752:C:C6	2.55	0.41
1:0:3:TYR:O	1:0:7:GLU:HB3	2.21	0.41
2:A:186:HIS:O	2:A:188:GLU:N	2.53	0.41
3:B:31:CYS:HA	3:B:32:PRO:HD3	1.75	0.41
3:B:126:PRO:O	3:B:128:SER:N	2.53	0.41
4:C:162:ARG:HH21	29:X:333:A:P	2.44	0.41
4:C:176:ASN:ND2	29:X:626:A:O2'	2.54	0.41
5:D:29:PRO:HB2	5:D:169:LEU:HD13	2.03	0.41
5:D:51:ASP:O	5:D:55:LYS:HG2	2.21	0.41
8:G:109:GLY:O	8:G:110:LEU:C	2.64	0.41
9:H:2:ILE:HB	9:H:45:ALA:HB3	2.02	0.41
9:H:22:ILE:CG2	9:H:52:VAL:HG12	2.45	0.41
9:H:98:ILE:HG22	9:H:99:ILE:N	2.35	0.41
10:I:53:ARG:CG	10:I:54:SER:H	2.34	0.41
10:I:55:ARG:HB3	10:I:57:ILE:HG12	2.03	0.41
10:I:76:LYS:HB2	10:I:76:LYS:HE3	1.93	0.41
11:J:17:ARG:NH2	29:X:969:U:O5'	2.54	0.41
12:K:80:MET:O	12:K:85:PRO:HD3	2.21	0.41
13:L:33:ARG:HB2	13:L:33:ARG:CZ	2.51	0.41
15:N:41:ASN:HB3	15:N:45:TYR:HE2	1.86	0.41
16:O:43:GLU:C	16:O:45:THR:H	2.27	0.41
17:P:50:VAL:O	17:P:54:GLU:HG3	2.21	0.41
21:T:46:LYS:HB2	21:T:77:ARG:O	2.20	0.41
22:U:48:LYS:HE2	22:U:48:LYS:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:71:A:H62	29:X:110:U:H5'	1.85	0.41
29:X:184:A:C6	29:X:185:C:C2	3.09	0.41
29:X:507:A:H2'	29:X:508:G:C8	2.56	0.41
29:X:698:A:C2	29:X:702:A:C5	3.09	0.41
29:X:1047:G:C2	29:X:1131:G:C4	3.09	0.41
29:X:1203:A:N3	29:X:1203:A:H2'	2.35	0.41
29:X:1238:A:O2'	29:X:1239:A:O5'	2.35	0.41
29:X:1300:A:C2	29:X:1301:U:C2	3.09	0.41
29:X:1453:A:H3'	29:X:1454:U:C6	2.55	0.41
29:X:1549:C:H2'	29:X:1550:C:O4'	2.21	0.41
29:X:1554:G:H2'	29:X:1555:A:H8	1.86	0.41
29:X:1724:C:C2	29:X:1747:G:C4	3.09	0.41
29:X:1782:A:N6	29:X:1820:G:O2'	2.54	0.41
29:X:1850:G:O3'	29:X:1851:A:H8	2.04	0.41
29:X:1967:U:H2'	29:X:1968:G:H8	1.86	0.41
29:X:2006:G:H5'	29:X:2596:C:H4'	2.03	0.41
29:X:2038:C:H6	29:X:2038:C:H3'	1.85	0.41
29:X:2230:G:H8	29:X:2230:G:OP2	2.03	0.41
29:X:2265:A:H4'	29:X:2266:A:N9	2.35	0.41
29:X:2411:A:H2'	29:X:2412:A:O4'	2.21	0.41
29:X:2457:A:H3'	29:X:2458:U:H6	1.86	0.41
29:X:2630:C:C2	29:X:2631:C:C5	3.09	0.41
29:X:2662:C:C5	29:X:2663:U:H5	2.39	0.41
1:O:107:ASP:HB3	1:O:108:ALA:H	1.63	0.41
2:A:227:ASN:O	2:A:228:PRO:C	2.63	0.41
2:A:268:ARG:NH2	29:X:2204:A:OP1	2.54	0.41
3:B:2:LYS:HB2	3:B:200:SER:HB3	2.03	0.41
3:B:170:LEU:HA	3:B:170:LEU:HD23	1.48	0.41
4:C:144:GLY:HA2	4:C:166:TRP:CZ2	2.55	0.41
6:E:156:ALA:HB3	29:X:2509:A:H61	1.85	0.41
9:H:59:ALA:HA	9:H:60:PRO:HD3	1.89	0.41
10:I:18:ARG:NH2	29:X:1262:U:C2	2.89	0.41
11:J:15:ARG:HB3	11:J:16:GLY:H	1.45	0.41
11:J:36:ILE:HG23	11:J:103:VAL:HG22	2.03	0.41
13:L:16:LYS:HZ2	13:L:90:ASP:CG	2.25	0.41
15:N:66:ASN:OD1	15:N:70:ARG:HD2	2.21	0.41
18:Q:39:LYS:NZ	18:Q:50:VAL:HG12	2.36	0.41
29:X:459:A:H4'	29:X:461:A:N7	2.35	0.41
29:X:465:C:HO2'	29:X:466:A:P	2.42	0.41
29:X:825:C:O2'	29:X:1239:A:O2'	2.30	0.41
29:X:837:U:H2'	29:X:838:A:H8	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:858:G:H8	29:X:858:G:P	2.44	0.41
29:X:1059:A:H2'	29:X:1060:C:OP1	2.21	0.41
29:X:1330:G:C4	29:X:1331:G:C8	3.09	0.41
29:X:1354:A:P	29:X:1410:U:H3	2.43	0.41
29:X:2229:G:O2'	29:X:2475:C:OP1	2.36	0.41
29:X:2293:G:H2'	29:X:2294:U:C6	2.56	0.41
29:X:2529:G:C6	29:X:2530:C:N4	2.89	0.41
29:X:2662:C:C4	29:X:2663:U:C5	3.09	0.41
1:O:180:ASN:HA	1:O:183:ALA:HB3	2.04	0.40
2:A:99:ASP:HB2	29:X:1506:C:O2	2.21	0.40
2:A:158:SER:O	2:A:196:VAL:HG11	2.20	0.40
3:B:8:LYS:HD3	3:B:190:GLY:O	2.21	0.40
3:B:27:LEU:HD23	3:B:29:GLY:N	2.32	0.40
3:B:114:GLN:HB2	3:B:160:MET:HB2	2.03	0.40
8:G:43:VAL:HG23	8:G:163:PRO:HB2	2.02	0.40
11:J:27:TYR:HA	11:J:137:VAL:HG21	2.03	0.40
14:M:56:ALA:O	14:M:66:PHE:HA	2.21	0.40
14:M:106:TYR:HD2	14:M:106:TYR:H	1.67	0.40
15:N:55:ARG:HD3	29:X:1166:A:H5''	2.04	0.40
16:O:43:GLU:O	16:O:45:THR:N	2.46	0.40
20:S:71:MET:HA	20:S:78:PRO:HA	2.03	0.40
21:T:21:LEU:HD11	21:T:41:ARG:CZ	2.50	0.40
25:Z:19:ARG:HA	29:X:2029:G:C5'	2.51	0.40
27:2:11:LYS:NZ	29:X:699:G:OP1	2.29	0.40
27:2:29:ASN:O	27:2:33:ARG:HG2	2.21	0.40
28:3:4:MET:CE	29:X:679:C:H1'	2.51	0.40
29:X:484:G:C2	29:X:485:G:N7	2.89	0.40
29:X:611:C:O2	29:X:615:C:H4'	2.20	0.40
29:X:869:C:H42	29:X:933:G:H1	1.69	0.40
29:X:1245:G:C2	29:X:1246:G:C8	3.09	0.40
29:X:1413:U:H2'	29:X:1414:G:H8	1.86	0.40
29:X:1659:G:C4	29:X:1660:G:C8	3.09	0.40
29:X:1903:C:O3'	29:X:1904:G:H8	2.04	0.40
29:X:2033:C:N4	29:X:2034:A:C6	2.89	0.40
29:X:2197:U:H2'	29:X:2198:U:H6	1.82	0.40
2:A:24:LEU:HD13	2:A:84:TYR:HB2	2.02	0.40
2:A:53:PHE:CE1	2:A:220:HIS:HA	2.56	0.40
2:A:97:TYR:HB2	2:A:101:GLU:O	2.22	0.40
3:B:144:ARG:NH1	29:X:2551:A:N3	2.70	0.40
5:D:72:LYS:O	5:D:74:ILE:HG13	2.22	0.40
6:E:33:LEU:HD12	6:E:33:LEU:HA	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:91:PRO:HD2	29:X:1087:C:O2	2.21	0.40
8:G:37:ASP:N	8:G:38:GLU:OE1	2.54	0.40
9:H:50:ILE:HG22	9:H:51:ILE:N	2.36	0.40
12:K:51:LEU:HD23	12:K:66:VAL:HG22	2.03	0.40
14:M:106:TYR:HD1	29:X:1745:C:C4'	2.33	0.40
15:N:6:THR:OG1	15:N:10:ARG:NH2	2.54	0.40
15:N:43:ALA:O	15:N:44:THR:C	2.64	0.40
19:R:43:ASP:HB2	19:R:45:LYS:HG3	2.03	0.40
29:X:18:U:O2'	29:X:563:U:OP1	2.33	0.40
29:X:20:C:H2'	29:X:21:A:C8	2.57	0.40
29:X:174:A:C6	29:X:2409:A:N3	2.89	0.40
29:X:193:A:C8	29:X:445:A:C6	3.08	0.40
29:X:614:G:C6	29:X:636:G:C2	3.10	0.40
29:X:762:A:O2'	29:X:1634:A:OP1	2.30	0.40
29:X:815:A:H3'	29:X:816:U:H6	1.87	0.40
29:X:1135:C:C4	29:X:1136:G:N7	2.89	0.40
29:X:1255:A:C4	29:X:1256:C:C5	3.10	0.40
29:X:1477:C:O2'	29:X:2681:A:H1'	2.21	0.40
29:X:1534:A:H2'	29:X:1535:C:C6	2.56	0.40
29:X:1757:C:C2	29:X:1970:G:C2	3.09	0.40
29:X:2011:U:H2'	29:X:2012:A:C8	2.56	0.40
29:X:2065:A:C2	29:X:2066:G:H1'	2.57	0.40
29:X:2528:G:N3	29:X:2529:G:C8	2.90	0.40
29:X:2590:U:O2	29:X:2590:U:H2'	2.21	0.40
29:X:2617:G:N2	29:X:2755:A:H2'	2.36	0.40
29:X:2697:G:H2'	29:X:2698:G:H8	1.86	0.40
30:Y:3:A:H2'	30:Y:4:C:C6	2.57	0.40
2:A:48:ARG:HE	29:X:791:G:H5''	1.86	0.40
2:A:229:VAL:HG13	2:A:230:ASP:OD2	2.20	0.40
2:A:247:VAL:HG22	2:A:251:GLY:C	2.46	0.40
3:B:155:ARG:O	3:B:156:MET:HB3	2.21	0.40
4:C:120:VAL:N	4:C:189:ASP:O	2.43	0.40
5:D:80:ARG:HD3	5:D:83:MET:HB2	2.02	0.40
7:F:63:ARG:HE	7:F:63:ARG:HB2	1.73	0.40
9:H:11:ALA:HB3	9:H:97:VAL:HG23	2.03	0.40
12:K:8:ARG:HB3	12:K:10:LEU:HG	2.03	0.40
14:M:73:PHE:C	14:M:75:GLU:H	2.28	0.40
17:P:59:PHE:CD1	25:Z:30:LEU:HD11	2.52	0.40
17:P:79:ALA:O	17:P:85:MET:HB2	2.21	0.40
19:R:83:LEU:HD23	19:R:83:LEU:HA	1.92	0.40
22:U:51:ILE:O	22:U:52:ARG:HD3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:67:G:H2'	29:X:68:C:C6	2.54	0.40
29:X:189:A:H2'	29:X:190:A:H8	1.85	0.40
29:X:356:A:H2'	29:X:357:A:C8	2.56	0.40
29:X:404:A:C5	29:X:424:G:C2	3.09	0.40
29:X:486:U:O2'	29:X:515:A:H1'	2.21	0.40
29:X:933:G:H4'	29:X:2248:A:C6	2.56	0.40
29:X:963:G:C6	29:X:964:A:N7	2.89	0.40
29:X:965:G:N3	29:X:2253:A:C2	2.90	0.40
29:X:1326:U:H2'	29:X:1626:A:C2	2.56	0.40
29:X:1504:G:C6	29:X:1505:U:O4	2.75	0.40
29:X:1591:U:H2'	29:X:1592:U:C6	2.57	0.40
29:X:1673:C:H2'	29:X:1674:C:C6	2.56	0.40
29:X:2165:A:H2'	29:X:2166:G:H8	1.87	0.40
29:X:2535:C:H2'	29:X:2536:G:C8	2.56	0.40
29:X:2701:A:C2	29:X:2848:A:C4	3.10	0.40
30:Y:120:G:C2	30:Y:121:G:C5	3.09	0.40
1:O:54:VAL:HG13	1:O:195:ALA:HB2	2.03	0.40
3:B:51:TYR:C	3:B:75:THR:HG23	2.46	0.40
4:C:28:HIS:O	4:C:32:THR:HG23	2.21	0.40
5:D:133:LYS:HB2	5:D:134:GLU:H	1.61	0.40
6:E:12:PRO:HG2	6:E:15:VAL:HG13	2.03	0.40
8:G:98:LYS:HB3	8:G:115:ALA:HB2	2.02	0.40
9:H:129:LEU:HD23	9:H:129:LEU:HA	1.89	0.40
10:I:63:ARG:HB3	28:3:25:PHE:CZ	2.56	0.40
11:J:76:THR:HG22	11:J:91:VAL:HA	2.03	0.40
12:K:46:PRO:HA	12:K:49:GLU:HB2	2.02	0.40
12:K:78:LYS:O	12:K:82:GLU:HB2	2.20	0.40
15:N:67:ALA:O	15:N:68:GLY:C	2.64	0.40
16:O:53:LYS:H	16:O:53:LYS:HG2	1.67	0.40
28:3:10:ALA:HB1	28:3:14:ILE:HG13	2.02	0.40
29:X:66:U:H2'	29:X:67:G:C8	2.55	0.40
29:X:572:G:H22	29:X:587:A:H2	1.68	0.40
29:X:695:G:N2	29:X:809:C:C2	2.89	0.40
29:X:746:G:C8	29:X:774:A:N6	2.89	0.40
29:X:836:G:O2'	29:X:837:U:H5'	2.22	0.40
29:X:941:U:H2'	29:X:942:U:C6	2.57	0.40
29:X:1079:G:H8	29:X:1079:G:OP2	2.03	0.40
29:X:1235:C:C2	29:X:1241:G:N2	2.89	0.40
29:X:1272:G:H2'	29:X:1273:G:C8	2.57	0.40
29:X:2039:G:H2'	29:X:2039:G:N3	2.37	0.40
29:X:2320:G:H2'	29:X:2321:C:C6	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2345:A:N6	29:X:2346:G:C2	2.89	0.40
29:X:2559:U:C5	29:X:2560:G:C6	3.10	0.40
29:X:2585:C:C2'	29:X:2586:G:H5'	2.50	0.40
29:X:2666:U:C5	29:X:2667:C:C4	3.09	0.40
29:X:2863:U:N3	29:X:2864:C:C5	2.90	0.40
30:Y:12:C:H42	30:Y:113:G:H1	1.69	0.40
30:Y:35:C:H2'	30:Y:36:A:H8	1.85	0.40
30:Y:94:G:N2	30:Y:95:U:C2	2.89	0.40
1:O:18:ILE:HG12	1:O:185:TYR:HE1	1.85	0.40
3:B:119:ARG:NH1	3:B:158:GLY:HA3	2.36	0.40
9:H:105:PRO:HB2	9:H:107:GLY:H	1.87	0.40
10:I:41:SER:OG	29:X:685:U:OP2	2.33	0.40
14:M:42:GLY:C	14:M:44:ARG:N	2.78	0.40
14:M:96:ARG:HA	14:M:96:ARG:HD2	1.84	0.40
15:N:91:ASN:HD21	29:X:1007:A:H4'	1.86	0.40
15:N:92:ARG:HG2	29:X:1008:G:OP1	2.21	0.40
24:W:11:GLY:HA2	29:X:980:G:O2'	2.22	0.40
29:X:32:C:H2'	29:X:33:C:C6	2.56	0.40
29:X:654:A:O2'	29:X:655:A:P	2.80	0.40
29:X:874:A:C2	29:X:875:G:H1'	2.57	0.40
29:X:947:C:C2	29:X:948:C:C5	3.10	0.40
29:X:955:G:H3'	29:X:955:G:C8	2.57	0.40
29:X:1033:G:N2	29:X:1035:G:N2	2.69	0.40
29:X:1080:A:H4'	29:X:1081:A:C8	2.57	0.40
29:X:1265:G:O2'	29:X:1266:G:C8	2.75	0.40
29:X:1320:A:N6	29:X:1622:G:O2'	2.55	0.40
29:X:1359:G:C5	29:X:1360:G:N7	2.90	0.40
29:X:1503:G:C6	29:X:1504:G:C6	3.09	0.40
29:X:2225:G:C4	29:X:2226:A:C8	3.09	0.40
29:X:2262:C:C6	29:X:2368:G:H2'	2.56	0.40
29:X:2302:G:C6	29:X:2303:C:C4	3.10	0.40
29:X:2309:G:N2	29:X:2365:U:C2	2.88	0.40
29:X:2424:G:H2'	29:X:2425:G:C8	2.51	0.40
29:X:2563:U:H2'	29:X:2564:U:H6	1.85	0.40
29:X:2785:A:C8	29:X:2786:G:C8	3.10	0.40
29:X:2856:U:H2'	29:X:2857:C:H6	1.86	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	
1	O	222/224 (99%)	139 (63%)	58 (26%)	25 (11%)	0	1
2	A	272/274 (99%)	206 (76%)	50 (18%)	16 (6%)	1	7
3	B	203/205 (99%)	152 (75%)	33 (16%)	18 (9%)	0	3
4	C	195/197 (99%)	123 (63%)	50 (26%)	22 (11%)	0	1
5	D	175/177 (99%)	117 (67%)	42 (24%)	16 (9%)	0	2
6	E	169/171 (99%)	119 (70%)	33 (20%)	17 (10%)	0	2
7	F	142/144 (99%)	100 (70%)	27 (19%)	15 (11%)	0	2
8	G	140/142 (99%)	111 (79%)	19 (14%)	10 (7%)	1	4
9	H	132/134 (98%)	96 (73%)	18 (14%)	18 (14%)	0	1
10	I	139/141 (99%)	93 (67%)	30 (22%)	16 (12%)	0	1
11	J	134/136 (98%)	97 (72%)	28 (21%)	9 (7%)	1	5
12	K	111/113 (98%)	81 (73%)	18 (16%)	12 (11%)	0	1
13	L	102/104 (98%)	68 (67%)	18 (18%)	16 (16%)	0	0
14	M	107/109 (98%)	83 (78%)	14 (13%)	10 (9%)	0	2
15	N	115/117 (98%)	90 (78%)	19 (16%)	6 (5%)	1	9
16	O	92/94 (98%)	69 (75%)	13 (14%)	10 (11%)	0	1
17	P	125/127 (98%)	102 (82%)	17 (14%)	6 (5%)	2	11
18	Q	91/93 (98%)	67 (74%)	16 (18%)	8 (9%)	0	3
19	R	108/110 (98%)	63 (58%)	28 (26%)	17 (16%)	0	0
20	S	173/175 (99%)	123 (71%)	32 (18%)	18 (10%)	0	2
21	T	82/84 (98%)	68 (83%)	8 (10%)	6 (7%)	1	4
22	U	70/72 (97%)	39 (56%)	15 (21%)	16 (23%)	0	0
23	V	64/66 (97%)	54 (84%)	9 (14%)	1 (2%)	7	34
24	W	53/55 (96%)	36 (68%)	13 (24%)	4 (8%)	1	4
25	Z	55/57 (96%)	36 (66%)	13 (24%)	6 (11%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	1	52/54 (96%)	31 (60%)	13 (25%)	8 (15%)	0	0
27	2	45/47 (96%)	38 (84%)	6 (13%)	1 (2%)	5	26
28	3	63/65 (97%)	38 (60%)	17 (27%)	8 (13%)	0	1
All	All	3431/3487 (98%)	2439 (71%)	657 (19%)	335 (10%)	0	2

All (335) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	17	SER
1	0	61	PRO
1	0	157	ILE
1	0	216	PRO
2	A	25	ALA
2	A	111	LEU
2	A	202	LYS
3	B	34	VAL
3	B	85	ALA
3	B	86	PRO
3	B	117	MET
3	B	123	ALA
3	B	133	LYS
3	B	180	ASN
4	C	9	GLN
4	C	20	PRO
4	C	51	VAL
4	C	52	SER
4	C	54	THR
4	C	97	ARG
4	C	126	ALA
4	C	172	VAL
4	C	174	GLY
5	D	40	LEU
5	D	134	GLU
6	E	24	PHE
6	E	42	THR
6	E	55	PRO
6	E	58	ALA
6	E	65	HIS
6	E	112	PRO
6	E	126	PRO
6	E	165	VAL

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Mol	Chain	Res	Type
7	F	23	VAL
7	F	50	ASP
7	F	74	MET
7	F	116	ASN
8	G	37	ASP
8	G	66	HIS
8	G	110	LEU
9	H	5	GLN
9	H	29	ILE
9	H	41	ASN
9	H	47	VAL
9	H	61	ARG
9	H	84	ALA
9	H	116	ARG
10	I	29	THR
10	I	78	SER
10	I	82	ASP
10	I	110	ALA
10	I	111	SER
11	J	21	ASP
11	J	23	LYS
11	J	135	ARG
12	K	4	GLY
12	K	11	ASN
12	K	13	ASN
12	K	20	LEU
12	K	32	GLY
12	K	88	ALA
12	K	100	VAL
13	L	10	LYS
13	L	21	THR
13	L	33	ARG
13	L	45	ASP
13	L	53	ALA
14	M	25	PRO
14	M	43	ASN
14	M	83	PHE
15	N	5	LYS
15	N	7	GLY
15	N	27	SER
16	O	24	SER
16	O	29	ALA

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Mol	Chain	Res	Type
17	P	49	SER
17	P	50	VAL
17	P	81	HIS
17	P	82	ASN
17	P	87	GLU
19	R	11	ASN
19	R	51	VAL
19	R	58	VAL
19	R	60	PRO
19	R	78	ALA
19	R	93	ARG
19	R	110	SER
20	S	91	PRO
20	S	124	ALA
20	S	169	VAL
21	T	30	VAL
21	T	64	ASP
21	T	74	LYS
22	U	14	VAL
22	U	15	VAL
22	U	18	VAL
22	U	25	ARG
22	U	55	GLY
22	U	60	VAL
22	U	76	LYS
24	W	36	ASP
24	W	38	PRO
25	Z	34	PRO
26	1	40	TYR
26	1	44	ALA
28	3	53	ALA
1	0	62	HIS
1	0	87	ALA
1	0	100	ALA
1	0	108	ALA
1	0	137	LYS
2	A	41	GLY
2	A	125	PRO
2	A	169	GLU
2	A	239	ARG
3	B	60	ASN
3	B	71	GLY

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Mol	Chain	Res	Type
3	B	118	LYS
4	C	11	GLY
4	C	22	VAL
4	C	37	SER
4	C	43	ALA
4	C	56	ARG
4	C	75	PRO
4	C	178	TYR
5	D	33	LYS
5	D	42	SER
5	D	122	PHE
5	D	132	ILE
5	D	133	LYS
6	E	18	ASN
6	E	100	GLY
6	E	173	ALA
7	F	14	ALA
7	F	22	PRO
7	F	82	ALA
8	G	38	GLU
8	G	77	GLY
8	G	94	LYS
9	H	4	PRO
9	H	22	ILE
9	H	42	LYS
9	H	66	ALA
9	H	69	VAL
9	H	79	HIS
10	I	41	SER
10	I	44	GLY
10	I	57	ILE
10	I	86	THR
10	I	99	VAL
11	J	13	GLN
11	J	26	ASP
11	J	98	VAL
12	K	40	LYS
12	K	103	ARG
13	L	20	THR
13	L	55	SER
13	L	56	SER
13	L	59	LEU

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Mol	Chain	Res	Type
13	L	61	SER
13	L	93	SER
13	L	96	TYR
14	M	16	ILE
14	M	17	GLU
14	M	26	ASP
16	O	16	GLU
18	Q	3	HIS
18	Q	59	PRO
18	Q	61	LYS
18	Q	67	ARG
19	R	25	LEU
19	R	79	SER
20	S	26	LYS
22	U	10	LYS
22	U	29	GLY
22	U	32	ARG
22	U	63	SER
25	Z	36	CYS
26	1	30	ASN
28	3	12	ARG
28	3	34	THR
28	3	51	ALA
1	0	28	LEU
1	0	33	PHE
1	0	45	ILE
1	0	102	GLY
1	0	146	ALA
1	0	203	VAL
2	A	187	SER
2	A	198	ASN
2	A	241	GLY
2	A	246	PRO
3	B	17	ASN
3	B	127	ALA
3	B	155	ARG
4	C	83	ALA
4	C	171	PRO
5	D	71	LYS
5	D	80	ARG
6	E	7	GLN
6	E	41	LEU

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Mol	Chain	Res	Type
6	E	172	LYS
7	F	47	ASP
8	G	65	LYS
8	G	113	GLU
9	H	28	GLY
9	H	71	LYS
10	I	65	PHE
10	I	68	VAL
10	I	81	GLN
11	J	11	ARG
12	K	56	LYS
13	L	26	LYS
14	M	46	ARG
14	M	47	SER
15	N	73	GLY
15	N	103	PRO
16	O	45	THR
18	Q	8	GLN
19	R	20	ASP
19	R	87	GLU
20	S	7	PRO
20	S	14	LEU
20	S	51	LEU
20	S	58	GLY
20	S	63	PRO
20	S	94	VAL
20	S	156	GLU
21	T	83	ALA
22	U	17	SER
22	U	27	ASP
22	U	47	HIS
24	W	17	VAL
24	W	22	ALA
25	Z	21	SER
26	1	28	ARG
26	1	46	HIS
26	1	48	VAL
27	2	17	GLY
28	3	46	LYS
1	0	6	LEU
1	0	139	GLY
1	0	158	GLU

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Mol	Chain	Res	Type
1	0	197	PRO
2	A	45	ASN
3	B	66	HIS
3	B	73	ALA
3	B	144	ARG
3	B	154	LYS
4	C	90	SER
5	D	20	PHE
5	D	35	VAL
5	D	77	PHE
7	F	19	PRO
7	F	25	PRO
7	F	70	LYS
7	F	83	GLY
8	G	140	GLN
10	I	116	ARG
12	K	102	THR
13	L	68	ALA
13	L	97	HIS
14	M	74	GLY
16	O	20	ILE
16	O	40	VAL
16	O	44	GLN
18	Q	84	GLU
19	R	52	ASN
19	R	64	ASN
19	R	102	LYS
20	S	37	LYS
20	S	57	GLU
20	S	88	TYR
20	S	122	ILE
20	S	128	ARG
21	T	8	GLY
23	V	3	PRO
25	Z	24	ALA
2	A	228	PRO
3	B	131	SER
4	C	15	ILE
4	C	27	LEU
4	C	41	GLY
5	D	29	PRO
5	D	44	LYS

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Mol	Chain	Res	Type
6	E	23	VAL
7	F	113	PRO
9	H	70	VAL
9	H	124	MET
11	J	81	GLU
11	J	133	VAL
12	K	57	GLY
16	O	31	ASP
19	R	65	PRO
25	Z	4	HIS
25	Z	20	ARG
26	1	51	ALA
28	3	63	PRO
1	0	67	SER
1	0	120	GLY
2	A	201	HIS
5	D	21	GLY
5	D	113	ASP
6	E	92	VAL
8	G	165	VAL
13	L	84	ILE
16	O	60	VAL
19	R	31	GLY
19	R	100	ASP
20	S	35	ASP
22	U	12	ASN
22	U	41	VAL
1	0	89	VAL
2	A	165	VAL
7	F	52	ILE
10	I	24	GLY
14	M	7	ILE
15	N	88	ILE
20	S	125	PRO
26	1	43	VAL
16	O	17	GLY
18	Q	9	ALA
18	Q	29	VAL
21	T	31	VAL
28	3	16	ILE
1	0	86	GLY
1	0	165	GLY

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Mol	Chain	Res	Type
2	A	229	VAL
9	H	40	GLY
17	P	35	PRO
10	I	10	PRO
28	3	28	GLY
1	0	91	GLY
6	E	76	VAL
7	F	96	VAL

5.3.2 Protein sidechains [i](#)

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	
1	0	167/167 (100%)	147 (88%)	20 (12%)	5	22
2	A	214/214 (100%)	172 (80%)	42 (20%)	1	8
3	B	155/155 (100%)	119 (77%)	36 (23%)	1	4
4	C	157/157 (100%)	109 (69%)	48 (31%)	0	1
5	D	153/153 (100%)	121 (79%)	32 (21%)	1	7
6	E	136/136 (100%)	108 (79%)	28 (21%)	1	7
7	F	107/107 (100%)	97 (91%)	10 (9%)	8	32
8	G	118/118 (100%)	94 (80%)	24 (20%)	1	7
9	H	103/103 (100%)	69 (67%)	34 (33%)	0	1
10	I	108/108 (100%)	85 (79%)	23 (21%)	1	6
11	J	110/110 (100%)	79 (72%)	31 (28%)	0	2
12	K	90/90 (100%)	66 (73%)	24 (27%)	0	3
13	L	74/74 (100%)	50 (68%)	24 (32%)	0	1
14	M	92/92 (100%)	60 (65%)	32 (35%)	0	1
15	N	96/96 (100%)	84 (88%)	12 (12%)	4	20
16	O	75/75 (100%)	58 (77%)	17 (23%)	1	5
17	P	109/109 (100%)	80 (73%)	29 (27%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	Q	75/75 (100%)	57 (76%)	18 (24%)	1	4
19	R	91/91 (100%)	68 (75%)	23 (25%)	0	3
20	S	149/149 (100%)	114 (76%)	35 (24%)	1	4
21	T	62/62 (100%)	38 (61%)	24 (39%)	0	1
22	U	57/57 (100%)	35 (61%)	22 (39%)	0	1
23	V	54/54 (100%)	41 (76%)	13 (24%)	1	4
24	W	48/48 (100%)	37 (77%)	11 (23%)	1	5
25	Z	51/51 (100%)	43 (84%)	8 (16%)	2	13
26	1	38/38 (100%)	31 (82%)	7 (18%)	1	9
27	2	40/40 (100%)	32 (80%)	8 (20%)	1	7
28	3	51/51 (100%)	34 (67%)	17 (33%)	0	1
All	All	2780/2780 (100%)	2128 (76%)	652 (24%)	1	4

All (652) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	16	TYR
1	0	24	LEU
1	0	25	VAL
1	0	26	LYS
1	0	38	GLU
1	0	45	ILE
1	0	64	THR
1	0	70	VAL
1	0	72	VAL
1	0	95	LEU
1	0	110	VAL
1	0	112	THR
1	0	114	ASP
1	0	121	GLN
1	0	137	LYS
1	0	157	ILE
1	0	166	VAL
1	0	168	HIS
1	0	186	GLN
1	0	212	THR
2	A	7	LYS
2	A	10	THR

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Mol	Chain	Res	Type
2	A	13	ARG
2	A	21	PHE
2	A	34	THR
2	A	35	GLU
2	A	40	THR
2	A	49	ILE
2	A	59	LYS
2	A	63	ARG
2	A	66	ASP
2	A	68	LYS
2	A	70	ARG
2	A	82	ILE
2	A	88	ARG
2	A	91	ARG
2	A	113	VAL
2	A	116	THR
2	A	117	VAL
2	A	118	ASN
2	A	138	VAL
2	A	142	VAL
2	A	145	LEU
2	A	148	VAL
2	A	163	VAL
2	A	165	VAL
2	A	169	GLU
2	A	175	VAL
2	A	181	GLU
2	A	190	TYR
2	A	204	ILE
2	A	218	LYS
2	A	229	VAL
2	A	239	ARG
2	A	240	THR
2	A	246	PRO
2	A	247	VAL
2	A	252	LYS
2	A	270	LEU
2	A	271	VAL
2	A	273	ARG
2	A	274	ARG
3	B	4	ILE
3	B	11	MET

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Mol	Chain	Res	Type
3	B	12	THR
3	B	14	ILE
3	B	19	ARG
3	B	24	THR
3	B	25	VAL
3	B	26	VAL
3	B	33	ILE
3	B	38	THR
3	B	40	GLN
3	B	41	THR
3	B	49	ILE
3	B	72	VAL
3	B	76	ARG
3	B	79	ARG
3	B	87	ASP
3	B	90	SER
3	B	91	VAL
3	B	92	ASN
3	B	93	VAL
3	B	94	ASP
3	B	116	VAL
3	B	132	LYS
3	B	141	ILE
3	B	145	LYS
3	B	152	LYS
3	B	163	GLU
3	B	167	VAL
3	B	175	ILE
3	B	182	ILE
3	B	184	VAL
3	B	192	ASN
3	B	197	VAL
3	B	199	ARG
3	B	200	SER
4	C	6	VAL
4	C	7	ILE
4	C	10	ASN
4	C	16	GLU
4	C	21	GLU
4	C	22	VAL
4	C	28	HIS
4	C	31	VAL

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Mol	Chain	Res	Type
4	C	34	GLN
4	C	37	SER
4	C	38	ARG
4	C	42	THR
4	C	47	THR
4	C	50	GLN
4	C	51	VAL
4	C	52	SER
4	C	59	TYR
4	C	68	ARG
4	C	74	VAL
4	C	76	THR
4	C	82	VAL
4	C	87	LYS
4	C	92	ASP
4	C	97	ARG
4	C	98	GLN
4	C	99	VAL
4	C	106	MET
4	C	112	GLN
4	C	113	GLU
4	C	121	ASP
4	C	124	ASP
4	C	129	LYS
4	C	131	LYS
4	C	140	ASN
4	C	143	ASP
4	C	145	THR
4	C	146	GLU
4	C	148	VAL
4	C	150	LEU
4	C	153	ASP
4	C	155	GLU
4	C	162	ARG
4	C	163	ASN
4	C	164	VAL
4	C	167	VAL
4	C	169	VAL
4	C	172	VAL
4	C	181	LEU
5	D	9	ASN
5	D	25	VAL

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Mol	Chain	Res	Type
5	D	28	VAL
5	D	46	ASP
5	D	47	SER
5	D	50	ILE
5	D	61	THR
5	D	66	ILE
5	D	68	THR
5	D	72	LYS
5	D	80	ARG
5	D	85	VAL
5	D	89	VAL
5	D	90	THR
5	D	92	ARG
5	D	95	ARG
5	D	106	ILE
5	D	115	ARG
5	D	117	ILE
5	D	123	ASP
5	D	125	ARG
5	D	130	LEU
5	D	136	LEU
5	D	142	THR
5	D	147	ASP
5	D	148	LYS
5	D	150	ARG
5	D	155	THR
5	D	156	ILE
5	D	157	VAL
5	D	158	THR
5	D	159	THR
6	E	6	LYS
6	E	11	VAL
6	E	20	GLN
6	E	23	VAL
6	E	33	LEU
6	E	35	VAL
6	E	38	ASN
6	E	40	GLU
6	E	41	LEU
6	E	42	THR
6	E	43	VAL
6	E	44	ARG

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Mol	Chain	Res	Type
6	E	48	ASP
6	E	61	HIS
6	E	67	LEU
6	E	69	ARG
6	E	71	LEU
6	E	84	THR
6	E	111	HIS
6	E	115	ILE
6	E	121	VAL
6	E	122	THR
6	E	134	SER
6	E	140	LEU
6	E	144	VAL
6	E	151	VAL
6	E	153	LYS
6	E	165	VAL
7	F	8	VAL
7	F	23	VAL
7	F	33	ASN
7	F	59	ILE
7	F	84	ILE
7	F	98	LYS
7	F	102	ASP
7	F	112	MET
7	F	121	GLU
7	F	137	THR
8	G	30	LYS
8	G	31	THR
8	G	38	GLU
8	G	40	ASN
8	G	42	VAL
8	G	53	ARG
8	G	54	LEU
8	G	56	THR
8	G	65	LYS
8	G	73	ASN
8	G	82	VAL
8	G	83	ILE
8	G	91	THR
8	G	99	VAL
8	G	101	THR
8	G	102	ARG

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Mol	Chain	Res	Type
8	G	114	THR
8	G	140	GLN
8	G	150	VAL
8	G	154	GLU
8	G	155	THR
8	G	156	HIS
8	G	159	SER
8	G	167	LYS
9	H	2	ILE
9	H	3	MET
9	H	8	LEU
9	H	9	ASP
9	H	10	VAL
9	H	18	GLU
9	H	19	ILE
9	H	22	ILE
9	H	35	THR
9	H	36	THR
9	H	41	ASN
9	H	43	ARG
9	H	46	HIS
9	H	47	VAL
9	H	51	ILE
9	H	57	ASP
9	H	65	LYS
9	H	73	VAL
9	H	74	VAL
9	H	78	SER
9	H	82	LYS
9	H	83	ARG
9	H	88	THR
9	H	89	ILE
9	H	90	ARG
9	H	93	ARG
9	H	97	VAL
9	H	104	GLU
9	H	108	THR
9	H	117	GLU
9	H	121	ARG
9	H	124	MET
9	H	126	ILE
9	H	127	VAL

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Mol	Chain	Res	Type
10	I	4	HIS
10	I	6	LEU
10	I	18	ARG
10	I	19	VAL
10	I	28	LYS
10	I	45	LYS
10	I	48	PHE
10	I	53	ARG
10	I	65	PHE
10	I	74	VAL
10	I	76	LYS
10	I	81	GLN
10	I	82	ASP
10	I	84	GLU
10	I	91	ASP
10	I	93	LEU
10	I	94	GLU
10	I	99	VAL
10	I	109	LEU
10	I	120	VAL
10	I	121	HIS
10	I	133	VAL
10	I	142	LEU
11	J	11	ARG
11	J	12	LYS
11	J	15	ARG
11	J	26	ASP
11	J	27	TYR
11	J	35	LEU
11	J	38	MET
11	J	45	SER
11	J	46	ASN
11	J	47	GLN
11	J	48	ILE
11	J	52	ARG
11	J	53	ILE
11	J	60	ARG
11	J	64	LYS
11	J	65	ILE
11	J	68	ARG
11	J	72	ASP
11	J	82	THR

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Mol	Chain	Res	Type
11	J	84	MET
11	J	93	TYR
11	J	102	ARG
11	J	106	GLU
11	J	128	ILE
11	J	129	GLN
11	J	130	THR
11	J	132	MET
11	J	133	VAL
11	J	137	VAL
11	J	139	ASP
11	J	140	GLU
12	K	11	ASN
12	K	14	SER
12	K	26	THR
12	K	29	LEU
12	K	33	ARG
12	K	35	GLN
12	K	36	THR
12	K	42	LYS
12	K	45	ARG
12	K	51	LEU
12	K	52	ILE
12	K	53	THR
12	K	54	THR
12	K	59	ASP
12	K	65	LEU
12	K	73	LYS
12	K	75	VAL
12	K	83	VAL
12	K	89	GLU
12	K	94	TYR
12	K	95	THR
12	K	99	ARG
12	K	113	ILE
12	K	114	GLU
13	L	11	LEU
13	L	13	THR
13	L	15	ARG
13	L	17	VAL
13	L	20	THR
13	L	24	SER

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Mol	Chain	Res	Type
13	L	29	LEU
13	L	31	VAL
13	L	33	ARG
13	L	35	SER
13	L	36	LYS
13	L	37	HIS
13	L	38	ILE
13	L	39	TYR
13	L	43	ILE
13	L	60	LYS
13	L	66	ASP
13	L	71	VAL
13	L	82	LYS
13	L	93	SER
13	L	95	LYS
13	L	97	HIS
13	L	108	ARG
13	L	109	GLU
14	M	2	GLN
14	M	7	ILE
14	M	12	LEU
14	M	13	LEU
14	M	14	ARG
14	M	18	GLN
14	M	21	THR
14	M	23	GLN
14	M	29	PRO
14	M	32	THR
14	M	33	VAL
14	M	35	VAL
14	M	37	THR
14	M	40	ARG
14	M	44	ARG
14	M	51	GLU
14	M	54	VAL
14	M	57	ILE
14	M	60	SER
14	M	62	SER
14	M	63	ARG
14	M	68	VAL
14	M	72	SER
14	M	77	VAL

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Mol	Chain	Res	Type
14	M	78	GLU
14	M	91	VAL
14	M	95	GLU
14	M	96	ARG
14	M	99	VAL
14	M	101	ARG
14	M	103	LYS
14	M	106	TYR
15	N	5	LYS
15	N	9	VAL
15	N	17	VAL
15	N	34	ASN
15	N	63	GLN
15	N	77	SER
15	N	80	ILE
15	N	83	LEU
15	N	93	LYS
15	N	102	GLU
15	N	113	SER
15	N	118	GLN
16	O	7	THR
16	O	10	LYS
16	O	11	GLN
16	O	14	VAL
16	O	18	ASP
16	O	19	VAL
16	O	32	LYS
16	O	34	GLU
16	O	35	LEU
16	O	55	THR
16	O	65	ARG
16	O	69	ILE
16	O	72	ARG
16	O	78	VAL
16	O	81	ARG
16	O	87	ARG
16	O	93	ILE
17	P	16	GLN
17	P	17	GLN
17	P	21	ARG
17	P	25	PHE
17	P	29	LYS

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Mol	Chain	Res	Type
17	P	31	VAL
17	P	36	ARG
17	P	40	LEU
17	P	41	VAL
17	P	42	VAL
17	P	49	SER
17	P	50	VAL
17	P	63	SER
17	P	66	GLU
17	P	84	GLU
17	P	85	MET
17	P	89	ARG
17	P	91	PHE
17	P	93	LYS
17	P	96	TYR
17	P	98	ASP
17	P	103	LEU
17	P	105	ARG
17	P	109	ARG
17	P	115	ASN
17	P	116	ILE
17	P	117	ILE
17	P	124	ILE
17	P	126	ILE
18	Q	3	HIS
18	Q	5	ASP
18	Q	6	ILE
18	Q	26	SER
18	Q	30	SER
18	Q	40	ASP
18	Q	42	ILE
18	Q	48	VAL
18	Q	51	ILE
18	Q	53	ILE
18	Q	57	ASN
18	Q	64	ARG
18	Q	65	VAL
18	Q	80	VAL
18	Q	82	LEU
18	Q	84	GLU
18	Q	88	ILE
18	Q	91	LEU

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Mol	Chain	Res	Type
19	R	9	HIS
19	R	22	VAL
19	R	23	ILE
19	R	32	GLN
19	R	43	ASP
19	R	44	GLN
19	R	46	VAL
19	R	48	VAL
19	R	51	VAL
19	R	53	VAL
19	R	56	LYS
19	R	57	ASN
19	R	66	GLN
19	R	70	GLU
19	R	73	GLU
19	R	74	LEU
19	R	80	LYS
19	R	81	VAL
19	R	84	VAL
19	R	90	LYS
19	R	102	LYS
19	R	104	VAL
19	R	106	VAL
20	S	3	LEU
20	S	13	LYS
20	S	15	ASP
20	S	18	MET
20	S	22	VAL
20	S	24	TYR
20	S	37	LYS
20	S	48	THR
20	S	55	THR
20	S	57	GLU
20	S	65	LEU
20	S	71	MET
20	S	72	ASP
20	S	73	LYS
20	S	86	VAL
20	S	87	THR
20	S	95	SER
20	S	96	VAL
20	S	99	HIS

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Mol	Chain	Res	Type
20	S	100	THR
20	S	108	VAL
20	S	109	GLN
20	S	112	LEU
20	S	117	VAL
20	S	128	ARG
20	S	139	THR
20	S	145	ASP
20	S	146	HIS
20	S	151	ASP
20	S	156	GLU
20	S	159	THR
20	S	166	LEU
20	S	169	VAL
20	S	171	VAL
20	S	175	ARG
21	T	4	LYS
21	T	5	LYS
21	T	7	VAL
21	T	10	SER
21	T	11	LYS
21	T	12	ASN
21	T	19	LYS
21	T	21	LEU
21	T	23	VAL
21	T	29	GLU
21	T	37	LEU
21	T	41	ARG
21	T	43	THR
21	T	46	LYS
21	T	49	GLN
21	T	51	VAL
21	T	55	ARG
21	T	62	LEU
21	T	64	ASP
21	T	70	ILE
21	T	77	ARG
21	T	79	ILE
21	T	81	ILE
21	T	82	GLU
22	U	8	THR
22	U	10	LYS

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Mol	Chain	Res	Type
22	U	12	ASN
22	U	14	VAL
22	U	15	VAL
22	U	18	VAL
22	U	19	ILE
22	U	21	ARG
22	U	23	LYS
22	U	32	ARG
22	U	33	LYS
22	U	35	THR
22	U	37	ILE
22	U	40	ARG
22	U	42	GLN
22	U	49	LYS
22	U	57	VAL
22	U	60	VAL
22	U	63	SER
22	U	67	ILE
22	U	69	THR
22	U	76	LYS
23	V	5	GLU
23	V	10	GLN
23	V	12	THR
23	V	16	LYS
23	V	21	ARG
23	V	25	LEU
23	V	26	MET
23	V	44	ARG
23	V	46	LEU
23	V	53	LEU
23	V	55	THR
23	V	60	LEU
23	V	63	LYS
24	W	3	ILE
24	W	6	VAL
24	W	9	VAL
24	W	10	ILE
24	W	26	ARG
24	W	34	VAL
24	W	37	THR
24	W	46	THR
24	W	51	LEU

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Mol	Chain	Res	Type
24	W	52	GLU
24	W	53	VAL
25	Z	9	LYS
25	Z	25	LEU
25	Z	26	THR
25	Z	34	PRO
25	Z	44	HIS
25	Z	45	ILE
25	Z	48	ASN
25	Z	57	VAL
26	1	9	ILE
26	1	10	VAL
26	1	15	SER
26	1	24	THR
26	1	37	LEU
26	1	43	VAL
26	1	46	HIS
27	2	4	THR
27	2	12	ARG
27	2	15	THR
27	2	24	THR
27	2	26	SER
27	2	28	ARG
27	2	29	ASN
27	2	42	LEU
28	3	7	HIS
28	3	9	MET
28	3	13	ARG
28	3	14	ILE
28	3	19	THR
28	3	21	LYS
28	3	22	VAL
28	3	26	LYS
28	3	29	LYS
28	3	31	HIS
28	3	34	THR
28	3	39	ASP
28	3	41	ILE
28	3	46	LYS
28	3	50	LEU
28	3	62	LEU
28	3	64	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	118	GLN
1	0	186	GLN
2	A	15	GLN
2	A	58	HIS
2	A	118	ASN
2	A	129	ASN
2	A	166	GLN
3	B	17	ASN
3	B	60	ASN
3	B	192	ASN
4	C	34	GLN
4	C	132	ASN
5	D	19	GLN
5	D	171	GLN
6	E	139	GLN
7	F	11	GLN
7	F	29	GLN
7	F	116	ASN
8	G	161	GLN
10	I	66	ASN
13	L	37	HIS
14	M	20	HIS
14	M	48	GLN
15	N	63	GLN
16	O	57	GLN
16	O	89	ASN
17	P	17	GLN
17	P	73	ASN
17	P	123	HIS
18	Q	94	GLN
20	S	46	GLN
20	S	109	GLN
23	V	52	GLN
25	Z	29	ASN
25	Z	37	HIS
25	Z	43	HIS
26	1	30	ASN
26	1	46	HIS
28	3	7	HIS
28	3	33	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
29	X	2776/2881 (96%)	842 (30%)	30 (1%)
30	Y	121/122 (99%)	35 (28%)	1 (0%)
All	All	2897/3003 (96%)	877 (30%)	31 (1%)

All (877) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
29	X	8	A
29	X	13	A
29	X	15	G
29	X	54	G
29	X	63	A
29	X	66	U
29	X	70	A
29	X	73	A
29	X	74	G
29	X	75	C
29	X	88	G
29	X	89	A
29	X	90	G
29	X	91	A
29	X	92	U
29	X	100	G
29	X	101	A
29	X	102	C
29	X	107	G
29	X	116	A
29	X	117	A
29	X	118	U
29	X	120	G
29	X	123	A
29	X	129	A
29	X	135	U
29	X	136	A
29	X	138	G
29	X	144	U
29	X	147	G
29	X	158	A
29	X	159	A
29	X	170	U
29	X	173	A

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Mol	Chain	Res	Type
29	X	175	C
29	X	176	A
29	X	177	U
29	X	180	C
29	X	181	A
29	X	182	G
29	X	192	G
29	X	193	A
29	X	199	A
29	X	200	A
29	X	201	G
29	X	202	A
29	X	203	G
29	X	205	A
29	X	206	U
29	X	207	U
29	X	209	G
29	X	218	A
29	X	219	G
29	X	221	A
29	X	222	G
29	X	225	G
29	X	226	C
29	X	227	G
29	X	228	A
29	X	229	G
29	X	238	G
29	X	243	G
29	X	245	C
29	X	248	A
29	X	305	A
29	X	308	C
29	X	309	G
29	X	310	A
29	X	321	A
29	X	322	A
29	X	323	G
29	X	324	C
29	X	335	A
29	X	340	G
29	X	341	A
29	X	342	G

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Mol	Chain	Res	Type
29	X	343	A
29	X	346	C
29	X	354	C
29	X	356	A
29	X	357	A
29	X	361	G
29	X	396	U
29	X	397	U
29	X	399	G
29	X	400	U
29	X	403	A
29	X	404	A
29	X	408	U
29	X	409	G
29	X	412	U
29	X	413	G
29	X	414	A
29	X	415	A
29	X	418	C
29	X	424	G
29	X	425	A
29	X	453	U
29	X	455	A
29	X	458	G
29	X	459	A
29	X	463	C
29	X	466	A
29	X	467	U
29	X	469	G
29	X	475	U
29	X	476	G
29	X	478	G
29	X	479	G
29	X	481	A
29	X	483	A
29	X	486	U
29	X	492	G
29	X	494	A
29	X	500	G
29	X	504	G
29	X	506	G
29	X	511	A

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Mol	Chain	Res	Type
29	X	512	A
29	X	514	G
29	X	515	A
29	X	516	G
29	X	518	A
29	X	519	C
29	X	520	C
29	X	521	U
29	X	532	A
29	X	534	U
29	X	539	A
29	X	540	G
29	X	541	C
29	X	542	A
29	X	543	G
29	X	545	C
29	X	554	U
29	X	555	U
29	X	556	A
29	X	557	U
29	X	558	G
29	X	559	C
29	X	560	G
29	X	564	U
29	X	569	C
29	X	571	U
29	X	572	G
29	X	580	A
29	X	582	G
29	X	583	C
29	X	584	A
29	X	587	A
29	X	591	G
29	X	594	G
29	X	595	A
29	X	601	A
29	X	602	C
29	X	604	U
29	X	609	U
29	X	610	G
29	X	611	C
29	X	613	A

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Mol	Chain	Res	Type
29	X	616	U
29	X	620	G
29	X	624	A
29	X	625	A
29	X	626	A
29	X	627	A
29	X	628	A
29	X	631	G
29	X	633	G
29	X	637	G
29	X	638	A
29	X	645	G
29	X	648	A
29	X	655	A
29	X	656	U
29	X	657	A
29	X	663	G
29	X	664	C
29	X	666	U
29	X	668	A
29	X	672	C
29	X	673	G
29	X	682	G
29	X	683	A
29	X	689	A
29	X	695	G
29	X	699	G
29	X	712	A
29	X	714	G
29	X	727	U
29	X	728	G
29	X	729	A
29	X	730	C
29	X	731	A
29	X	732	G
29	X	739	G
29	X	740	A
29	X	741	G
29	X	743	A
29	X	754	G
29	X	758	G
29	X	760	U

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Mol	Chain	Res	Type
29	X	765	C
29	X	773	G
29	X	776	G
29	X	778	G
29	X	787	A
29	X	789	G
29	X	790	A
29	X	795	A
29	X	797	A
29	X	798	G
29	X	805	G
29	X	807	A
29	X	815	A
29	X	816	U
29	X	818	G
29	X	821	A
29	X	824	U
29	X	825	C
29	X	831	G
29	X	832	A
29	X	834	A
29	X	836	G
29	X	838	A
29	X	840	U
29	X	841	G
29	X	848	A
29	X	851	C
29	X	852	U
29	X	857	U
29	X	858	G
29	X	859	U
29	X	869	C
29	X	872	G
29	X	879	A
29	X	880	C
29	X	912	A
29	X	914	C
29	X	922	A
29	X	924	C
29	X	926	C
29	X	927	C
29	X	931	G

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Mol	Chain	Res	Type
29	X	937	C
29	X	939	C
29	X	940	G
29	X	943	U
29	X	946	U
29	X	947	C
29	X	950	G
29	X	955	G
29	X	956	A
29	X	957	G
29	X	964	A
29	X	967	G
29	X	969	U
29	X	972	C
29	X	975	C
29	X	976	C
29	X	982	C
29	X	984	A
29	X	985	G
29	X	992	A
29	X	994	A
29	X	1001	A
29	X	1005	U
29	X	1007	A
29	X	1013	G
29	X	1015	U
29	X	1016	C
29	X	1017	C
29	X	1018	C
29	X	1020	A
29	X	1022	A
29	X	1023	U
29	X	1024	G
29	X	1028	G
29	X	1029	C
29	X	1033	G
29	X	1034	U
29	X	1036	G
29	X	1037	U
29	X	1044	U
29	X	1047	G
29	X	1055	A

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Mol	Chain	Res	Type
29	X	1056	U
29	X	1058	G
29	X	1059	A
29	X	1060	C
29	X	1061	A
29	X	1066	G
29	X	1068	A
29	X	1069	G
29	X	1071	U
29	X	1072	U
29	X	1079	G
29	X	1080	A
29	X	1081	A
29	X	1082	G
29	X	1084	A
29	X	1086	C
29	X	1089	C
29	X	1096	A
29	X	1097	A
29	X	1098	G
29	X	1099	A
29	X	1100	G
29	X	1101	U
29	X	1102	G
29	X	1104	G
29	X	1107	A
29	X	1108	U
29	X	1111	C
29	X	1112	U
29	X	1113	C
29	X	1114	A
29	X	1119	U
29	X	1120	C
29	X	1121	G
29	X	1122	A
29	X	1123	G
29	X	1124	U
29	X	1128	G
29	X	1137	A
29	X	1138	A
29	X	1139	A
29	X	1140	A

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Mol	Chain	Res	Type
29	X	1141	U
29	X	1142	G
29	X	1143	A
29	X	1145	C
29	X	1146	G
29	X	1149	G
29	X	1151	U
29	X	1152	C
29	X	1153	A
29	X	1154	A
29	X	1158	A
29	X	1162	A
29	X	1165	G
29	X	1166	A
29	X	1168	G
29	X	1178	C
29	X	1179	A
29	X	1185	C
29	X	1187	A
29	X	1189	G
29	X	1195	U
29	X	1199	U
29	X	1200	G
29	X	1209	G
29	X	1218	C
29	X	1220	G
29	X	1223	G
29	X	1225	G
29	X	1226	A
29	X	1233	A
29	X	1235	C
29	X	1236	G
29	X	1238	A
29	X	1240	G
29	X	1246	G
29	X	1247	U
29	X	1250	A
29	X	1255	A
29	X	1256	C
29	X	1261	G
29	X	1266	G
29	X	1269	G

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Mol	Chain	Res	Type
29	X	1271	C
29	X	1275	A
29	X	1277	G
29	X	1280	U
29	X	1281	A
29	X	1284	G
29	X	1285	A
29	X	1286	U
29	X	1288	A
29	X	1290	A
29	X	1291	G
29	X	1299	A
29	X	1302	C
29	X	1307	U
29	X	1313	U
29	X	1314	A
29	X	1322	G
29	X	1326	U
29	X	1331	G
29	X	1334	A
29	X	1342	U
29	X	1346	C
29	X	1347	C
29	X	1351	G
29	X	1354	A
29	X	1359	G
29	X	1365	U
29	X	1370	U
29	X	1378	A
29	X	1381	G
29	X	1391	A
29	X	1392	U
29	X	1393	G
29	X	1395	A
29	X	1398	G
29	X	1403	U
29	X	1404	C
29	X	1408	A
29	X	1409	U
29	X	1425	G
29	X	1427	G
29	X	1428	G

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Mol	Chain	Res	Type
29	X	1433	A
29	X	1435	G
29	X	1442	C
29	X	1454	U
29	X	1459	U
29	X	1460	G
29	X	1468	A
29	X	1469	U
29	X	1470	G
29	X	1475	U
29	X	1490	U
29	X	1498	G
29	X	1505	U
29	X	1506	C
29	X	1507	A
29	X	1512	A
29	X	1517	C
29	X	1518	C
29	X	1522	C
29	X	1523	A
29	X	1524	C
29	X	1525	A
29	X	1527	G
29	X	1541	G
29	X	1543	G
29	X	1544	A
29	X	1545	G
29	X	1552	C
29	X	1553	G
29	X	1562	G
29	X	1563	U
29	X	1564	U
29	X	1574	A
29	X	1575	C
29	X	1582	A
29	X	1585	A
29	X	1586	A
29	X	1601	U
29	X	1602	G
29	X	1603	A
29	X	1616	C
29	X	1618	U

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Mol	Chain	Res	Type
29	X	1619	A
29	X	1622	G
29	X	1624	A
29	X	1625	A
29	X	1626	A
29	X	1628	C
29	X	1631	C
29	X	1643	A
29	X	1651	U
29	X	1653	C
29	X	1656	U
29	X	1662	G
29	X	1663	C
29	X	1665	C
29	X	1666	G
29	X	1668	G
29	X	1669	A
29	X	1670	G
29	X	1677	C
29	X	1678	G
29	X	1680	U
29	X	1688	U
29	X	1690	U
29	X	1691	G
29	X	1692	C
29	X	1696	C
29	X	1697	U
29	X	1699	A
29	X	1707	A
29	X	1711	C
29	X	1714	A
29	X	1717	A
29	X	1718	A
29	X	1722	G
29	X	1733	U
29	X	1734	C
29	X	1735	G
29	X	1741	G
29	X	1747	G
29	X	1749	G
29	X	1750	A
29	X	1751	A

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Mol	Chain	Res	Type
29	X	1755	G
29	X	1760	G
29	X	1764	A
29	X	1766	U
29	X	1772	C
29	X	1775	A
29	X	1776	A
29	X	1777	A
29	X	1778	U
29	X	1779	C
29	X	1782	A
29	X	1788	C
29	X	1791	C
29	X	1799	A
29	X	1800	A
29	X	1808	C
29	X	1811	A
29	X	1812	U
29	X	1819	U
29	X	1821	A
29	X	1825	C
29	X	1829	C
29	X	1846	A
29	X	1849	G
29	X	1854	G
29	X	1859	A
29	X	1867	A
29	X	1869	A
29	X	1872	A
29	X	1875	C
29	X	1883	A
29	X	1884	A
29	X	1886	G
29	X	1889	G
29	X	1890	G
29	X	1891	C
29	X	1893	G
29	X	1896	A
29	X	1898	U
29	X	1900	U
29	X	1904	G
29	X	1906	U

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Mol	Chain	Res	Type
29	X	1907	C
29	X	1909	U
29	X	1910	A
29	X	1913	G
29	X	1914	U
29	X	1918	G
29	X	1919	A
29	X	1920	A
29	X	1921	A
29	X	1923	U
29	X	1924	C
29	X	1926	U
29	X	1927	U
29	X	1928	G
29	X	1938	U
29	X	1949	A
29	X	1950	C
29	X	1953	A
29	X	1955	G
29	X	1975	G
29	X	1976	U
29	X	1979	C
29	X	1980	A
29	X	1995	G
29	X	1999	U
29	X	2001	G
29	X	2004	U
29	X	2006	G
29	X	2009	U
29	X	2014	A
29	X	2018	G
29	X	2026	C
29	X	2028	C
29	X	2029	G
29	X	2032	G
29	X	2033	C
29	X	2034	A
29	X	2038	C
29	X	2039	G
29	X	2043	A
29	X	2044	G
29	X	2045	A

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Mol	Chain	Res	Type
29	X	2047	C
29	X	2052	G
29	X	2058	U
29	X	2059	U
29	X	2063	A
29	X	2074	U
29	X	2075	U
29	X	2076	G
29	X	2091	C
29	X	2093	G
29	X	2094	C
29	X	2097	A
29	X	2099	G
29	X	2100	A
29	X	2101	U
29	X	2103	G
29	X	2104	G
29	X	2107	G
29	X	2108	G
29	X	2110	G
29	X	2111	C
29	X	2115	C
29	X	2116	G
29	X	2117	A
29	X	2118	A
29	X	2120	C
29	X	2122	G
29	X	2123	G
29	X	2124	C
29	X	2126	U
29	X	2127	U
29	X	2128	U
29	X	2129	U
29	X	2131	G
29	X	2135	C
29	X	2141	A
29	X	2142	G
29	X	2147	C
29	X	2152	A
29	X	2153	A
29	X	2154	A
29	X	2156	A

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Mol	Chain	Res	Type
29	X	2157	C
29	X	2158	C
29	X	2162	C
29	X	2164	G
29	X	2171	U
29	X	2173	G
29	X	2180	U
29	X	2181	A
29	X	2182	A
29	X	2188	A
29	X	2189	A
29	X	2190	A
29	X	2191	A
29	X	2192	U
29	X	2193	C
29	X	2196	U
29	X	2199	C
29	X	2200	G
29	X	2204	A
29	X	2206	C
29	X	2217	G
29	X	2228	U
29	X	2229	G
29	X	2230	G
29	X	2234	G
29	X	2243	C
29	X	2247	A
29	X	2252	A
29	X	2262	C
29	X	2266	A
29	X	2267	A
29	X	2268	G
29	X	2269	G
29	X	2278	A
29	X	2283	G
29	X	2284	U
29	X	2285	U
29	X	2286	G
29	X	2287	G
29	X	2288	A
29	X	2290	A
29	X	2298	U

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Mol	Chain	Res	Type
29	X	2300	G
29	X	2301	A
29	X	2303	C
29	X	2304	G
29	X	2305	C
29	X	2306	A
29	X	2312	A
29	X	2313	G
29	X	2314	A
29	X	2315	A
29	X	2319	G
29	X	2324	G
29	X	2326	C
29	X	2327	U
29	X	2329	C
29	X	2333	A
29	X	2335	U
29	X	2355	A
29	X	2357	A
29	X	2358	C
29	X	2361	G
29	X	2362	G
29	X	2363	G
29	X	2364	C
29	X	2368	G
29	X	2369	U
29	X	2375	G
29	X	2379	G
29	X	2386	G
29	X	2389	G
29	X	2398	U
29	X	2399	C
29	X	2402	U
29	X	2407	G
29	X	2408	G
29	X	2409	A
29	X	2410	U
29	X	2418	A
29	X	2419	C
29	X	2420	C
29	X	2424	G
29	X	2426	G

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Mol	Chain	Res	Type
29	X	2427	A
29	X	2428	U
29	X	2431	C
29	X	2432	A
29	X	2438	A
29	X	2441	U
29	X	2447	G
29	X	2448	A
29	X	2452	U
29	X	2453	C
29	X	2455	A
29	X	2457	A
29	X	2458	U
29	X	2461	G
29	X	2463	G
29	X	2466	G
29	X	2468	G
29	X	2470	U
29	X	2471	U
29	X	2473	G
29	X	2477	C
29	X	2478	C
29	X	2479	U
29	X	2481	G
29	X	2482	A
29	X	2484	G
29	X	2486	C
29	X	2492	G
29	X	2494	C
29	X	2497	A
29	X	2501	U
29	X	2504	G
29	X	2516	U
29	X	2521	A
29	X	2522	G
29	X	2533	U
29	X	2538	C
29	X	2545	A
29	X	2546	G
29	X	2550	C
29	X	2551	A
29	X	2552	C

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Mol	Chain	Res	Type
29	X	2557	G
29	X	2559	U
29	X	2560	G
29	X	2564	U
29	X	2565	C
29	X	2571	G
29	X	2579	A
29	X	2581	A
29	X	2582	G
29	X	2589	C
29	X	2590	U
29	X	2591	C
29	X	2592	U
29	X	2593	A
29	X	2594	U
29	X	2600	A
29	X	2609	G
29	X	2613	A
29	X	2617	G
29	X	2625	U
29	X	2633	A
29	X	2639	A
29	X	2640	G
29	X	2642	G
29	X	2643	G
29	X	2651	U
29	X	2653	A
29	X	2657	G
29	X	2661	G
29	X	2663	U
29	X	2666	U
29	X	2668	U
29	X	2674	C
29	X	2678	C
29	X	2687	G
29	X	2691	C
29	X	2692	A
29	X	2693	U
29	X	2694	G
29	X	2698	G
29	X	2701	A
29	X	2702	G

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Mol	Chain	Res	Type
29	X	2703	C
29	X	2706	U
29	X	2713	A
29	X	2718	A
29	X	2719	U
29	X	2724	G
29	X	2728	A
29	X	2732	C
29	X	2737	A
29	X	2743	G
29	X	2744	A
29	X	2745	A
29	X	2746	G
29	X	2751	C
29	X	2758	A
29	X	2759	U
29	X	2760	G
29	X	2769	C
29	X	2771	C
29	X	2774	U
29	X	2775	U
29	X	2777	A
29	X	2778	U
29	X	2779	C
29	X	2780	A
29	X	2791	C
29	X	2793	G
29	X	2795	A
29	X	2796	A
29	X	2797	G
29	X	2800	C
29	X	2808	U
29	X	2809	A
29	X	2810	A
29	X	2811	G
29	X	2815	C
29	X	2823	G
29	X	2824	C
29	X	2832	G
29	X	2836	U
29	X	2847	G
29	X	2848	A

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Mol	Chain	Res	Type
29	X	2849	C
29	X	2851	G
29	X	2854	G
29	X	2861	A
29	X	2862	G
29	X	2865	G
29	X	2866	A
29	X	2867	G
29	X	2868	G
29	X	2869	U
30	Y	11	G
30	Y	14	C
30	Y	15	A
30	Y	16	U
30	Y	17	A
30	Y	20	A
30	Y	27	A
30	Y	28	A
30	Y	29	C
30	Y	37	C
30	Y	39	C
30	Y	40	C
30	Y	43	G
30	Y	44	C
30	Y	46	G
30	Y	47	A
30	Y	49	C
30	Y	51	G
30	Y	52	G
30	Y	53	G
30	Y	55	C
30	Y	59	A
30	Y	63	A
30	Y	70	C
30	Y	75	A
30	Y	76	U
30	Y	86	A
30	Y	99	G
30	Y	108	G
30	Y	112	A
30	Y	114	C
30	Y	115	G

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Mol	Chain	Res	Type
30	Y	121	G
30	Y	122	U
30	Y	123	U

All (31) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
29	X	459	A
29	X	465	C
29	X	475	U
29	X	511	A
29	X	518	A
29	X	654	A
29	X	655	A
29	X	813	A
29	X	939	C
29	X	940	G
29	X	1000	G
29	X	1123	G
29	X	1138	A
29	X	1225	G
29	X	1506	C
29	X	1526	U
29	X	1601	U
29	X	1602	G
29	X	1690	U
29	X	1715	A
29	X	1777	A
29	X	2044	G
29	X	2228	U
29	X	2550	C
29	X	2551	A
29	X	2592	U
29	X	2736	U
29	X	2758	A
29	X	2823	G
29	X	2854	G
30	Y	16	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 187 ligands modelled in this entry, 186 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	HGR	X	6178	-	39,39,39	1.75	7 (17%)	48,58,58	1.76	9 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	HGR	X	6178	-	-	3/20/79/79	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	X	6178	HGR	C5-C6	-4.13	1.42	1.50
32	X	6178	HGR	C12-C14	4.05	1.43	1.33
32	X	6178	HGR	C3-C2	-3.91	1.41	1.48
32	X	6178	HGR	C12-C6	3.75	1.55	1.44
32	X	6178	HGR	C5-C4	-3.53	1.43	1.49
32	X	6178	HGR	C1-C6	2.93	1.41	1.36
32	X	6178	HGR	C17-N1	2.17	1.49	1.45

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	X	6178	HGR	C10-O3-C3	4.94	126.09	115.41
32	X	6178	HGR	C4-C5-C6	4.28	121.49	112.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	X	6178	HGR	C4-C3-C2	-4.22	118.17	121.81
32	X	6178	HGR	C23-O8-C18	-4.00	100.22	106.31
32	X	6178	HGR	O3-C3-C2	3.26	118.43	112.51
32	X	6178	HGR	O1-C10-C9	-2.76	101.47	104.98
32	X	6178	HGR	O10-C19-C17	2.66	114.88	109.58
32	X	6178	HGR	C1-C2-C3	2.54	120.84	116.06
32	X	6178	HGR	C18-C19-C17	2.01	115.24	110.31

There are no chirality outliers.

All (3) torsion outliers are listed below:

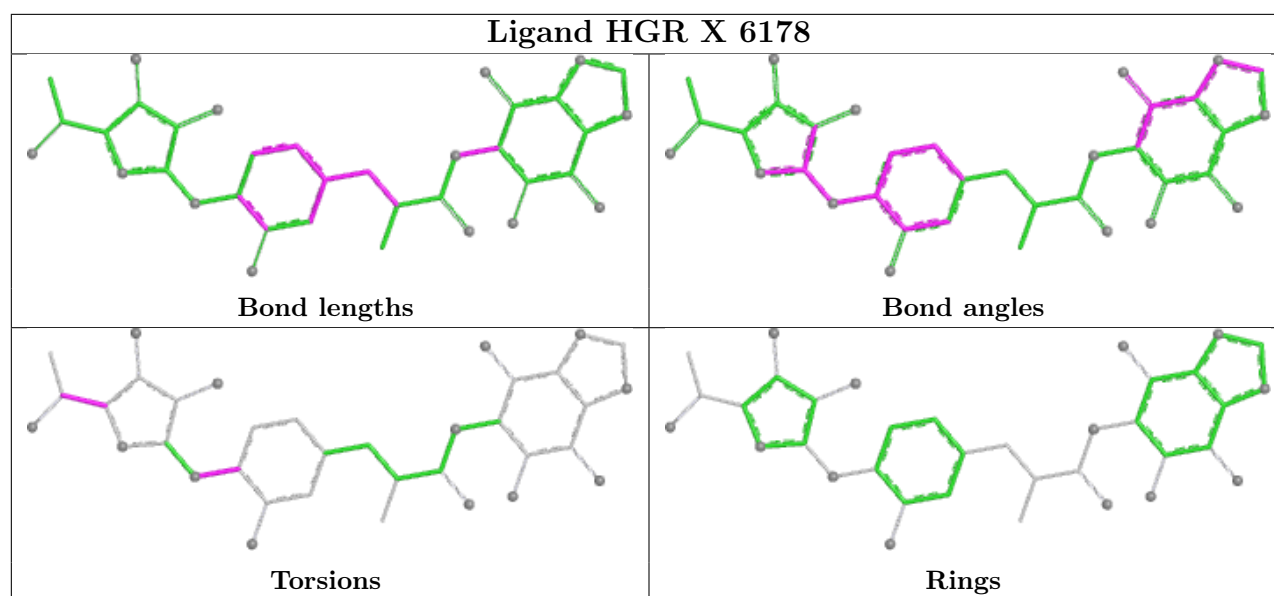
Mol	Chain	Res	Type	Atoms
32	X	6178	HGR	C2-C3-O3-C10
32	X	6178	HGR	C13-C11-C7-O1
32	X	6178	HGR	C13-C11-C7-C8

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	X	6178	HGR	2	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	0	224/224 (100%)	1.70	76 (33%) 1 1	291, 311, 319, 322	0
2	A	274/274 (100%)	1.68	94 (34%) 1 1	108, 151, 172, 185	0
3	B	205/205 (100%)	1.18	39 (19%) 3 2	67, 102, 129, 146	0
4	C	197/197 (100%)	1.09	29 (14%) 6 3	93, 133, 158, 177	0
5	D	177/177 (100%)	1.14	34 (19%) 3 2	165, 183, 200, 214	0
6	E	171/171 (100%)	0.98	22 (12%) 7 5	116, 167, 191, 198	0
7	F	144/144 (100%)	1.40	35 (24%) 2 1	233, 259, 275, 281	0
8	G	142/142 (100%)	1.07	23 (16%) 4 3	87, 125, 139, 169	0
9	H	134/134 (100%)	1.00	19 (14%) 6 4	70, 92, 108, 118	0
10	I	141/141 (100%)	2.00	60 (42%) 0 1	98, 150, 173, 182	0
11	J	136/136 (100%)	1.75	45 (33%) 1 1	107, 126, 156, 159	0
12	K	113/113 (100%)	1.33	22 (19%) 3 2	63, 82, 95, 99	0
13	L	104/104 (100%)	2.14	47 (45%) 0 0	126, 147, 162, 173	0
14	M	109/109 (100%)	0.98	14 (12%) 7 5	72, 89, 117, 147	0
15	N	117/117 (100%)	1.31	30 (25%) 1 1	90, 118, 144, 153	0
16	O	94/94 (100%)	1.06	19 (20%) 3 2	103, 129, 156, 173	0
17	P	127/127 (100%)	0.99	24 (18%) 3 2	81, 96, 120, 180	0
18	Q	93/93 (100%)	1.32	18 (19%) 3 2	108, 137, 160, 176	0
19	R	110/110 (100%)	1.28	25 (22%) 2 1	111, 131, 166, 180	0
20	S	175/175 (100%)	1.13	24 (13%) 6 4	134, 167, 185, 193	0
21	T	84/84 (100%)	1.88	33 (39%) 1 1	111, 130, 148, 171	0
22	U	72/72 (100%)	2.94	44 (61%) 0 0	134, 163, 177, 182	0
23	V	66/66 (100%)	1.98	23 (34%) 1 1	147, 163, 190, 201	0
24	W	55/55 (100%)	1.16	7 (12%) 8 5	112, 124, 142, 157	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Z	57/57 (100%)	1.10	11 (19%) 3 2	82, 97, 120, 130	0
26	1	54/54 (100%)	2.01	22 (40%) 0 1	140, 153, 179, 189	0
27	2	47/47 (100%)	1.87	21 (44%) 0 1	108, 121, 132, 134	0
28	3	65/65 (100%)	2.38	36 (55%) 0 0	115, 132, 143, 153	0
29	X	2780/2881 (96%)	0.73	272 (9%) 13 7	59, 127, 241, 397	0
30	Y	122/122 (100%)	0.77	10 (8%) 17 9	110, 157, 182, 203	0
All	All	6389/6490 (98%)	1.11	1178 (18%) 3 2	59, 134, 276, 397	0

All (1178) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
29	X	2116	G	12.7
22	U	27	ASP	10.9
29	X	2127	U	10.8
30	Y	43	G	10.1
13	L	12	ARG	10.1
29	X	731	A	9.7
22	U	8	THR	9.3
29	X	730	C	8.9
22	U	13	LEU	8.6
20	S	74	ARG	8.2
23	V	3	PRO	8.1
11	J	21	ASP	8.0
29	X	2125	C	7.8
29	X	2115	C	7.7
1	0	159	PHE	7.7
1	0	162	ASP	7.6
23	V	2	LYS	7.5
30	Y	123	U	7.4
13	L	34	SER	7.3
21	T	2	ALA	7.3
5	D	81	GLN	7.3
2	A	265	THR	7.2
10	I	74	VAL	7.1
13	L	94	TYR	7.1
10	I	69	GLY	7.1
10	I	33	GLY	7.0
10	I	67	ASN	7.0
13	L	93	SER	7.0
13	L	9	ARG	7.0

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Mol	Chain	Res	Type	RSRZ
10	I	103	ASN	7.0
13	L	36	LYS	7.0
22	U	26	ALA	6.9
3	B	205	SER	6.9
23	V	6	MET	6.7
13	L	8	ARG	6.6
22	U	16	ASN	6.6
15	N	48	ARG	6.6
11	J	99	LYS	6.5
12	K	69	ASP	6.5
11	J	100	PRO	6.5
10	I	68	VAL	6.5
18	Q	32	LYS	6.5
11	J	22	ALA	6.4
4	C	88	PRO	6.3
29	X	1086	C	6.3
1	O	158	GLU	6.2
20	S	15	ASP	6.2
2	A	32	ALA	6.2
29	X	1901	A	6.2
12	K	22	ARG	6.1
22	U	25	ARG	6.1
2	A	255	LYS	6.1
5	D	72	LYS	6.1
29	X	1900	U	6.1
22	U	15	VAL	6.0
1	O	163	LYS	6.0
6	E	173	ALA	6.0
2	A	35	GLU	6.0
29	X	834	A	6.0
2	A	231	HIS	5.9
20	S	68	ALA	5.9
29	X	1139	A	5.9
29	X	2133	G	5.9
2	A	241	GLY	5.9
29	X	1085	G	5.9
20	S	75	LYS	5.9
2	A	51	SER	5.9
11	J	37	ALA	5.9
29	X	2120	C	5.8
18	Q	62	ARG	5.8
11	J	16	GLY	5.8

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Mol	Chain	Res	Type	RSRZ
20	S	73	LYS	5.8
29	X	2092	U	5.8
28	3	23	MET	5.8
7	F	115	LEU	5.8
29	X	1902	A	5.8
13	L	31	VAL	5.7
29	X	2126	U	5.7
10	I	79	GLN	5.7
14	M	99	VAL	5.7
29	X	2121	U	5.7
28	3	37	SER	5.7
15	N	20	ARG	5.6
16	O	5	ILE	5.6
26	1	23	THR	5.6
13	L	24	SER	5.6
29	X	2776	U	5.6
22	U	12	ASN	5.5
2	A	223	GLY	5.5
21	T	3	HIS	5.4
29	X	1090	C	5.4
29	X	1897	C	5.4
22	U	28	GLY	5.4
29	X	1102	G	5.4
2	A	36	ALA	5.4
12	K	7	GLY	5.4
14	M	53	VAL	5.3
20	S	92	VAL	5.3
20	S	72	ASP	5.3
29	X	2274	C	5.3
16	O	74	TYR	5.3
10	I	45	LYS	5.3
4	C	91	TYR	5.3
13	L	53	ALA	5.3
19	R	43	ASP	5.2
10	I	75	VAL	5.2
2	A	268	ARG	5.2
29	X	1525	A	5.2
22	U	51	ILE	5.1
15	N	53	LYS	5.1
16	O	81	ARG	5.1
11	J	98	VAL	5.1
29	X	1187	A	5.1

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Mol	Chain	Res	Type	RSRZ
18	Q	8	GLN	5.1
28	3	46	LYS	5.1
29	X	2114	G	5.1
28	3	54	GLU	5.1
13	L	40	ALA	5.1
13	L	20	THR	5.0
13	L	33	ARG	5.0
29	X	1899	A	5.0
10	I	66	ASN	5.0
11	J	97	VAL	5.0
29	X	2275	U	5.0
26	1	53	ALA	5.0
29	X	1552	C	5.0
4	C	38	ARG	5.0
29	X	728	G	5.0
11	J	20	GLY	5.0
29	X	2128	U	4.9
19	R	4	PRO	4.9
29	X	1101	U	4.9
2	A	55	GLY	4.9
11	J	23	LYS	4.9
28	3	64	ARG	4.9
2	A	237	GLU	4.8
29	X	2103	G	4.8
26	1	22	TYR	4.8
10	I	37	GLN	4.8
29	X	2124	C	4.8
23	V	1	MET	4.8
29	X	1922	U	4.8
1	0	218	ILE	4.7
22	U	52	ARG	4.7
28	3	12	ARG	4.7
1	0	169	ALA	4.7
28	3	11	LYS	4.7
29	X	1524	C	4.7
2	A	239	ARG	4.7
29	X	1089	C	4.7
21	T	5	LYS	4.7
29	X	2777	A	4.7
19	R	12	ASP	4.6
21	T	74	LYS	4.6
1	0	54	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
30	Y	42	U	4.5
2	A	71	ASP	4.5
5	D	103	LEU	4.5
29	X	1797	C	4.5
2	A	104	TYR	4.5
1	0	43	LEU	4.5
7	F	23	VAL	4.5
11	J	101	GLY	4.5
15	N	57	PHE	4.5
8	G	99	VAL	4.5
2	A	254	THR	4.5
22	U	47	HIS	4.5
22	U	40	ARG	4.5
14	M	106	TYR	4.4
2	A	251	GLY	4.4
24	W	15	ASN	4.4
1	0	25	VAL	4.4
29	X	2109	A	4.4
4	C	2	ALA	4.4
10	I	44	GLY	4.4
23	V	4	SER	4.4
22	U	46	LEU	4.4
20	S	93	GLU	4.3
29	X	2385	U	4.3
21	T	24	LYS	4.3
12	K	68	GLN	4.3
29	X	833	A	4.3
29	X	1753	A	4.3
29	X	984	A	4.3
11	J	26	ASP	4.3
21	T	76	ALA	4.2
11	J	48	ILE	4.2
25	Z	42	SER	4.2
22	U	30	VAL	4.2
26	1	9	ILE	4.2
26	1	33	ALA	4.2
7	F	18	THR	4.2
29	X	2117	A	4.2
29	X	1189	G	4.2
10	I	50	GLU	4.2
28	3	32	GLN	4.2
3	B	54	LYS	4.2

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Mol	Chain	Res	Type	RSRZ
10	I	38	LYS	4.2
16	O	83	ARG	4.2
5	D	3	GLN	4.1
6	E	172	LYS	4.1
22	U	75	TYR	4.1
22	U	43	ARG	4.1
22	U	34	THR	4.1
29	X	1103	C	4.1
2	A	226	MET	4.1
11	J	131	LYS	4.1
16	O	73	LYS	4.1
18	Q	9	ALA	4.1
29	X	1920	A	4.1
21	T	15	ASP	4.1
22	U	10	LYS	4.1
15	N	21	ALA	4.1
14	M	104	LEU	4.0
28	3	45	GLY	4.0
2	A	64	ILE	4.0
29	X	1114	A	4.0
21	T	75	GLY	4.0
1	0	195	ALA	4.0
16	O	80	TYR	4.0
26	1	26	LYS	4.0
29	X	1523	A	4.0
2	A	267	ASP	4.0
13	L	10	LYS	3.9
2	A	61	LEU	3.9
13	L	30	SER	3.9
29	X	2104	G	3.9
4	C	41	GLY	3.9
2	A	250	TRP	3.9
29	X	2774	U	3.9
11	J	117	GLU	3.9
18	Q	37	GLU	3.9
5	D	99	PHE	3.9
17	P	8	PHE	3.9
2	A	242	ALA	3.9
16	O	72	ARG	3.9
27	2	47	GLU	3.9
2	A	262	LYS	3.9
28	3	66	LYS	3.9

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Mol	Chain	Res	Type	RSRZ
9	H	11	ALA	3.9
15	N	39	LEU	3.9
29	X	2015	G	3.9
7	F	24	GLY	3.9
6	E	168	GLN	3.9
7	F	123	ALA	3.9
29	X	601	A	3.8
29	X	774	A	3.8
29	X	715	U	3.8
6	E	111	HIS	3.8
13	L	96	TYR	3.8
2	A	238	GLY	3.8
14	M	30	GLY	3.8
25	Z	56	GLN	3.8
2	A	60	ARG	3.8
29	X	1138	A	3.8
29	X	2108	G	3.8
2	A	56	GLY	3.8
21	T	73	GLY	3.8
10	I	101	ARG	3.8
19	R	42	ARG	3.8
20	S	69	VAL	3.8
2	A	259	THR	3.8
10	I	31	GLY	3.8
10	I	46	GLY	3.8
1	0	205	LEU	3.8
10	I	48	PHE	3.8
29	X	436	A	3.8
29	X	2119	A	3.8
12	K	15	SER	3.7
11	J	139	ASP	3.7
22	U	29	GLY	3.7
28	3	63	PRO	3.7
28	3	6	THR	3.7
22	U	42	GLN	3.7
1	0	171	ILE	3.7
2	A	222	ARG	3.7
11	J	96	SER	3.7
23	V	7	ARG	3.7
5	D	67	ILE	3.7
29	X	1037	U	3.7
29	X	2129	U	3.7

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Mol	Chain	Res	Type	RSRZ
28	3	65	GLY	3.7
26	1	1	ALA	3.7
26	1	5	ALA	3.7
3	B	118	LYS	3.7
18	Q	2	SER	3.7
5	D	32	GLU	3.7
12	K	43	GLU	3.7
16	O	70	TYR	3.7
10	I	104	ARG	3.7
29	X	2049	C	3.7
22	U	23	LYS	3.7
2	A	266	SER	3.6
28	3	16	ILE	3.6
29	X	2152	A	3.6
30	Y	2	C	3.6
13	L	89	PHE	3.6
1	0	166	VAL	3.6
27	2	10	ARG	3.6
2	A	106	LEU	3.6
16	O	79	GLN	3.6
29	X	2313	G	3.6
29	X	2153	A	3.6
22	U	45	ASN	3.6
27	2	29	ASN	3.6
13	L	55	SER	3.6
2	A	230	ASP	3.6
15	N	49	ASP	3.6
22	U	62	LEU	3.6
28	3	3	LYS	3.6
28	3	36	LYS	3.6
1	0	37	VAL	3.6
26	1	0	ALA	3.6
11	J	18	MET	3.6
19	R	15	HIS	3.6
22	U	44	ALA	3.6
29	X	1409	U	3.6
2	A	65	ILE	3.6
10	I	71	THR	3.6
29	X	1921	A	3.5
29	X	2045	A	3.5
29	X	1319	C	3.5
12	K	18	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
26	1	28	ARG	3.5
2	A	68	LYS	3.5
13	L	17	VAL	3.5
1	0	170	PRO	3.5
10	I	58	ALA	3.5
11	J	40	PRO	3.5
29	X	2733	A	3.5
29	X	2132	G	3.5
23	V	59	GLU	3.5
23	V	30	PHE	3.5
2	A	57	GLY	3.5
6	E	5	GLY	3.5
1	0	39	VAL	3.5
4	C	31	VAL	3.5
26	1	11	LYS	3.5
29	X	1188	A	3.5
15	N	2	PRO	3.5
19	R	14	LEU	3.5
29	X	727	U	3.5
3	B	137	ARG	3.5
21	T	20	TYR	3.5
3	B	133	LYS	3.5
13	L	95	LYS	3.5
2	A	220	HIS	3.5
7	F	77	LEU	3.5
27	2	1	MET	3.5
29	X	1526	U	3.5
9	H	127	VAL	3.4
8	G	168	THR	3.4
12	K	3	HIS	3.4
2	A	217	ARG	3.4
29	X	1551	U	3.4
29	X	2557	G	3.4
11	J	36	ILE	3.4
22	U	63	SER	3.4
2	A	215	LEU	3.4
1	0	5	ALA	3.4
3	B	76	ARG	3.4
9	H	43	ARG	3.4
29	X	1091	C	3.4
27	2	22	MET	3.4
1	0	47	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
2	A	62	TYR	3.4
11	J	38	MET	3.4
5	D	31	ILE	3.4
4	C	147	LYS	3.4
6	E	175	LYS	3.4
29	X	1808	C	3.4
30	Y	62	C	3.4
3	B	165	VAL	3.4
14	M	54	VAL	3.4
5	D	173	MET	3.4
12	K	23	ALA	3.4
16	O	41	GLY	3.4
6	E	60	LYS	3.4
15	N	34	ASN	3.3
19	R	11	ASN	3.3
11	J	119	PHE	3.3
3	B	136	ARG	3.3
4	C	19	LEU	3.3
29	X	2161	C	3.3
3	B	123	ALA	3.3
26	1	21	TYR	3.3
29	X	843	G	3.3
1	0	210	LEU	3.3
6	E	64	LEU	3.3
22	U	14	VAL	3.3
2	A	224	SER	3.3
12	K	14	SER	3.3
29	X	2314	A	3.3
10	I	15	ASP	3.3
2	A	261	ARG	3.3
4	C	196	VAL	3.3
2	A	211	ARG	3.3
2	A	213	ARG	3.3
21	T	77	ARG	3.3
29	X	2091	C	3.3
2	A	31	LYS	3.3
13	L	16	LYS	3.3
3	B	52	ALA	3.3
28	3	20	GLY	3.3
7	F	113	PRO	3.3
11	J	17	ARG	3.3
17	P	98	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	0	132	LEU	3.3
6	E	17	VAL	3.3
3	B	163	GLU	3.3
3	B	204	ALA	3.3
1	0	160	ARG	3.2
2	A	253	PRO	3.2
2	A	252	LYS	3.2
10	I	102	LYS	3.2
20	S	87	THR	3.2
2	A	216	GLY	3.2
29	X	222	G	3.2
29	X	2099	G	3.2
7	F	99	LEU	3.2
23	V	37	LEU	3.2
23	V	57	LYS	3.2
13	L	87	VAL	3.2
10	I	72	TYR	3.2
10	I	54	SER	3.2
29	X	413	G	3.2
29	X	424	G	3.2
12	K	71	HIS	3.2
29	X	1252	C	3.2
7	F	68	ILE	3.2
13	L	14	ARG	3.2
22	U	21	ARG	3.2
10	I	36	GLY	3.2
7	F	125	ASN	3.2
13	L	27	LEU	3.2
2	A	53	PHE	3.2
21	T	55	ARG	3.2
29	X	1671	A	3.2
15	N	5	LYS	3.2
19	R	13	LYS	3.2
29	X	1798	G	3.2
12	K	29	LEU	3.2
13	L	81	GLU	3.2
29	X	1801	C	3.2
2	A	229	VAL	3.2
3	B	159	HIS	3.2
10	I	13	ARG	3.2
11	J	19	THR	3.2
8	G	37	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
21	T	44	LYS	3.1
29	X	1434	U	3.1
29	X	1676	U	3.1
29	X	248	A	3.1
29	X	407	A	3.1
29	X	846	A	3.1
15	N	52	ASN	3.1
5	D	143	TYR	3.1
22	U	18	VAL	3.1
29	X	983	G	3.1
29	X	2687	G	3.1
11	J	102	ARG	3.1
1	0	157	ILE	3.1
1	0	9	LYS	3.1
8	G	35	LYS	3.1
22	U	11	LYS	3.1
27	2	25	LYS	3.1
1	0	147	GLY	3.1
29	X	2105	U	3.1
2	A	43	ARG	3.1
28	3	4	MET	3.1
29	X	123	A	3.1
5	D	71	LYS	3.1
29	X	1734	C	3.1
29	X	2779	C	3.1
13	L	11	LEU	3.1
19	R	79	SER	3.1
7	F	127	VAL	3.1
14	M	28	ARG	3.1
6	E	112	PRO	3.1
12	K	9	LYS	3.1
29	X	1923	U	3.1
29	X	2004	U	3.1
29	X	2590	U	3.1
1	0	131	GLY	3.1
19	R	21	THR	3.1
28	3	40	GLU	3.1
29	X	1063	C	3.1
9	H	44	TYR	3.1
1	0	155	GLY	3.1
21	T	22	GLY	3.1
27	2	15	THR	3.1

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Mol	Chain	Res	Type	RSRZ
29	X	729	A	3.1
4	C	20	PRO	3.1
9	H	1	MET	3.1
29	X	2326	C	3.0
3	B	125	GLY	3.0
29	X	1223	G	3.0
30	Y	9	G	3.0
7	F	126	THR	3.0
29	X	2249	U	3.0
8	G	97	ASP	3.0
28	3	60	LEU	3.0
9	H	26	ASN	3.0
1	0	164	THR	3.0
10	I	76	LYS	3.0
11	J	103	VAL	3.0
21	T	58	THR	3.0
27	2	23	LYS	3.0
11	J	106	GLU	3.0
5	D	74	ILE	3.0
7	F	21	PRO	3.0
29	X	778	G	3.0
7	F	104	VAL	3.0
2	A	33	LEU	3.0
19	R	74	LEU	3.0
1	0	69	ARG	3.0
10	I	59	ARG	3.0
21	T	56	ASP	3.0
2	A	59	LYS	3.0
10	I	35	LYS	3.0
10	I	25	GLY	3.0
10	I	49	PHE	3.0
10	I	70	THR	3.0
3	B	120	TRP	3.0
23	V	9	LEU	3.0
29	X	242	A	3.0
29	X	402	A	3.0
15	N	35	ALA	3.0
8	G	111	LYS	3.0
19	R	108	VAL	3.0
1	0	106	PHE	3.0
13	L	19	THR	3.0
1	0	192	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
8	G	72	PRO	2.9
29	X	1553	G	2.9
2	A	245	VAL	2.9
4	C	79	GLY	2.9
6	E	61	HIS	2.9
15	N	9	VAL	2.9
19	R	68	GLY	2.9
21	T	7	VAL	2.9
7	F	52	ILE	2.9
26	1	12	MET	2.9
3	B	113	THR	2.9
23	V	28	LEU	2.9
26	1	24	THR	2.9
12	K	19	ALA	2.9
19	R	5	SER	2.9
6	E	174	GLY	2.9
29	X	637	G	2.9
29	X	1222	G	2.9
29	X	2250	G	2.9
29	X	1954	A	2.9
29	X	2118	A	2.9
7	F	20	ALA	2.9
13	L	57	ALA	2.9
19	R	75	ALA	2.9
29	X	835	U	2.9
1	0	48	ARG	2.9
11	J	15	ARG	2.9
13	L	60	LYS	2.9
26	1	34	LYS	2.9
10	I	26	THR	2.9
27	2	24	THR	2.9
3	B	187	ALA	2.9
26	1	13	GLU	2.9
29	X	1186	G	2.9
29	X	1799	A	2.9
29	X	2692	A	2.9
15	N	47	TYR	2.9
29	X	972	C	2.9
13	L	15	ARG	2.9
1	0	24	LEU	2.9
7	F	78	ILE	2.9
2	A	151	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
10	I	80	LEU	2.9
5	D	101	GLU	2.9
21	T	51	VAL	2.9
29	X	2122	G	2.9
1	0	40	HIS	2.8
2	A	240	THR	2.8
1	0	68	VAL	2.8
1	0	161	ASN	2.8
10	I	62	LYS	2.8
17	P	106	LEU	2.8
1	0	207	SER	2.8
2	A	212	SER	2.8
23	V	38	ALA	2.8
29	X	339	U	2.8
1	0	42	ARG	2.8
11	J	39	GLU	2.8
2	A	204	ILE	2.8
5	D	154	ILE	2.8
5	D	156	ILE	2.8
22	U	9	GLY	2.8
23	V	61	ALA	2.8
2	A	249	PRO	2.8
6	E	26	VAL	2.8
15	N	25	TRP	2.8
1	0	41	PHE	2.8
7	F	107	ILE	2.8
22	U	22	GLY	2.8
1	0	209	TYR	2.8
29	X	975	C	2.8
25	Z	59	ALA	2.8
1	0	67	SER	2.8
5	D	146	VAL	2.8
22	U	65	ASN	2.8
17	P	30	TYR	2.8
29	X	1285	A	2.8
1	0	156	ARG	2.8
15	N	12	ARG	2.8
4	C	101	GLN	2.8
29	X	2670	C	2.8
7	F	120	VAL	2.8
24	W	40	VAL	2.8
29	X	957	G	2.8

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Mol	Chain	Res	Type	RSRZ
1	0	213	THR	2.8
13	L	13	THR	2.8
26	1	31	THR	2.8
27	2	5	TYR	2.7
10	I	34	HIS	2.7
8	G	93	LYS	2.7
27	2	14	LYS	2.7
5	D	157	VAL	2.7
3	B	131	SER	2.7
29	X	514	G	2.7
29	X	955	G	2.7
25	Z	3	LYS	2.7
1	0	108	ALA	2.7
1	0	188	LEU	2.7
10	I	65	PHE	2.7
26	1	8	ILE	2.7
29	X	578	U	2.7
29	X	1019	U	2.7
2	A	236	GLY	2.7
7	F	119	SER	2.7
10	I	24	GLY	2.7
19	R	8	SER	2.7
29	X	524	A	2.7
29	X	921	A	2.7
29	X	33	C	2.7
23	V	33	ALA	2.7
1	0	28	LEU	2.7
21	T	36	ILE	2.7
12	K	4	GLY	2.7
22	U	36	GLY	2.7
18	Q	34	THR	2.7
20	S	67	LYS	2.7
29	X	1796	A	2.7
10	I	43	ALA	2.7
29	X	519	C	2.7
21	T	45	PHE	2.7
21	T	39	ARG	2.7
22	U	49	LYS	2.7
22	U	35	THR	2.7
29	X	2093	G	2.7
29	X	2297	G	2.7
22	U	17	SER	2.7

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Mol	Chain	Res	Type	RSRZ
9	H	114	VAL	2.7
17	P	18	VAL	2.7
29	X	768	U	2.7
23	V	47	ARG	2.6
2	A	256	GLY	2.6
23	V	5	GLU	2.6
26	1	36	GLU	2.6
5	D	49	ALA	2.6
5	D	130	LEU	2.6
9	H	8	LEU	2.6
27	2	12	ARG	2.6
29	X	26	G	2.6
29	X	1249	G	2.6
10	I	17	LYS	2.6
13	L	41	GLN	2.6
2	A	37	LEU	2.6
10	I	98	LEU	2.6
10	I	118	VAL	2.6
3	B	140	SER	2.6
24	W	8	SER	2.6
8	G	106	TYR	2.6
2	A	52	ARG	2.6
3	B	155	ARG	2.6
11	J	11	ARG	2.6
17	P	116	ILE	2.6
13	L	86	GLN	2.6
1	0	57	THR	2.6
4	C	35	LEU	2.6
15	N	54	LYS	2.6
18	Q	39	LYS	2.6
22	U	67	ILE	2.6
15	N	36	PHE	2.6
4	C	50	GLN	2.6
29	X	583	C	2.6
29	X	803	C	2.6
29	X	1792	C	2.6
1	0	56	GLY	2.6
3	B	121	ASN	2.6
21	T	13	GLY	2.6
21	T	65	GLY	2.6
1	0	126	LEU	2.6
20	S	66	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
2	A	258	LYS	2.6
23	V	48	ARG	2.6
29	X	408	U	2.6
15	N	8	ILE	2.6
2	A	67	PHE	2.6
29	X	2522	G	2.6
24	W	13	PRO	2.6
2	A	257	LEU	2.6
15	N	18	LEU	2.6
16	O	14	VAL	2.6
17	P	97	VAL	2.6
22	U	60	VAL	2.6
10	I	14	LYS	2.6
2	A	214	TRP	2.5
2	A	248	THR	2.6
7	F	34	ILE	2.5
2	A	233	HIS	2.5
29	X	1202	U	2.5
3	B	142	GLY	2.5
13	L	59	LEU	2.5
4	C	66	ASN	2.5
10	I	55	ARG	2.5
13	L	26	LYS	2.5
18	Q	40	ASP	2.5
29	X	1913	G	2.5
29	X	2100	A	2.5
2	A	54	ILE	2.5
3	B	132	LYS	2.5
8	G	98	LYS	2.5
10	I	53	ARG	2.5
19	R	107	ALA	2.5
14	M	57	ILE	2.5
29	X	542	A	2.5
29	X	2095	G	2.5
2	A	69	ARG	2.5
17	P	11	LYS	2.5
28	3	38	GLY	2.5
10	I	39	SER	2.5
15	N	63	GLN	2.5
1	0	148	MET	2.5
3	B	129	HIS	2.5
7	F	19	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
28	3	35	GLY	2.5
29	X	387	A	2.5
29	X	404	A	2.5
20	S	123	VAL	2.5
9	H	6	SER	2.5
10	I	41	SER	2.5
29	X	1062	G	2.5
10	I	73	GLU	2.5
29	X	1903	C	2.5
27	2	8	ASN	2.5
29	X	396	U	2.5
25	Z	8	LYS	2.5
9	H	134	LEU	2.5
28	3	7	HIS	2.5
24	W	6	VAL	2.5
6	E	170	ALA	2.4
24	W	22	ALA	2.4
4	C	90	SER	2.4
6	E	167	GLU	2.4
12	K	89	GLU	2.4
29	X	2521	A	2.4
5	D	105	ASN	2.4
20	S	8	ARG	2.4
22	U	61	TRP	2.4
23	V	42	ARG	2.4
10	I	108	LEU	2.4
29	X	636	G	2.4
29	X	1251	G	2.4
29	X	2123	G	2.4
29	X	2587	G	2.4
29	X	2847	G	2.4
21	T	18	PRO	2.4
10	I	4	HIS	2.4
29	X	1770	U	2.4
1	0	109	VAL	2.4
2	A	234	GLY	2.4
28	3	53	ALA	2.4
9	H	81	ILE	2.4
11	J	45	SER	2.4
21	T	63	SER	2.4
4	C	84	PHE	2.4
28	3	26	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
10	I	83	LEU	2.4
25	Z	58	LEU	2.4
7	F	116	ASN	2.4
8	G	73	ASN	2.4
1	O	88	ASP	2.4
2	A	34	THR	2.4
15	N	56	ASP	2.4
17	P	102	THR	2.4
29	X	1895	A	2.4
29	X	2581	A	2.4
1	O	44	GLY	2.4
17	P	107	ILE	2.4
29	X	405	C	2.4
29	X	769	C	2.4
29	X	361	G	2.4
29	X	958	G	2.4
29	X	2327	U	2.4
8	G	74	MET	2.4
2	A	264	LYS	2.4
17	P	29	LYS	2.4
1	O	61	PRO	2.4
7	F	22	PRO	2.4
13	L	21	THR	2.4
18	Q	28	TRP	2.4
19	R	106	VAL	2.4
10	I	22	GLY	2.4
7	F	124	ALA	2.4
29	X	1259	A	2.4
8	G	137	LYS	2.4
10	I	40	ARG	2.4
26	1	35	LEU	2.4
29	X	1396	C	2.4
29	X	1778	U	2.4
15	N	29	SER	2.4
29	X	2044	G	2.4
29	X	2750	G	2.4
25	Z	11	THR	2.4
1	O	107	ASP	2.4
3	B	161	GLY	2.4
2	A	25	ALA	2.4
7	F	26	ALA	2.4
20	S	124	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
24	W	45	LYS	2.4
28	3	29	LYS	2.4
2	A	70	ARG	2.4
27	2	19	ARG	2.4
28	3	61	MET	2.4
8	G	90	LEU	2.4
10	I	109	LEU	2.4
21	T	16	SER	2.4
5	D	84	PRO	2.4
11	J	133	VAL	2.4
13	L	88	VAL	2.4
29	X	577	U	2.4
29	X	1623	C	2.3
1	0	189	ILE	2.3
2	A	82	ILE	2.3
6	E	109	TYR	2.3
11	J	41	ALA	2.3
13	L	79	ALA	2.3
29	X	395	G	2.3
29	X	682	G	2.3
29	X	1284	G	2.3
29	X	1963	G	2.3
1	0	167	VAL	2.3
13	L	56	SER	2.3
14	M	29	PRO	2.3
17	P	61	PRO	2.3
5	D	148	LYS	2.3
28	3	43	GLY	2.3
29	X	1215	A	2.3
29	X	2248	A	2.3
3	B	188	ILE	2.3
6	E	95	ARG	2.3
10	I	16	ARG	2.3
12	K	6	ALA	2.3
13	L	58	ALA	2.3
1	0	185	TYR	2.3
8	G	100	TYR	2.3
8	G	70	PHE	2.3
11	J	121	LEU	2.3
29	X	434	C	2.3
29	X	1214	C	2.3
16	O	6	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
29	X	758	G	2.3
29	X	950	G	2.3
29	X	1554	G	2.3
19	R	30	LYS	2.3
17	P	105	ARG	2.3
2	A	243	GLY	2.3
4	C	166	TRP	2.3
9	H	28	GLY	2.3
18	Q	53	ILE	2.3
2	A	153	ALA	2.3
19	R	109	ALA	2.3
20	S	161	ALA	2.3
25	Z	4	HIS	2.3
11	J	105	PHE	2.3
23	V	14	PHE	2.3
3	B	143	GLN	2.3
14	M	2	GLN	2.3
4	C	177	VAL	2.3
8	G	30	LYS	2.3
16	O	78	VAL	2.3
17	P	41	VAL	2.3
7	F	25	PRO	2.3
11	J	71	PRO	2.3
28	3	2	PRO	2.3
20	S	71	MET	2.3
5	D	73	SER	2.3
1	0	127	LEU	2.3
23	V	60	LEU	2.3
5	D	97	TYR	2.3
4	C	123	PHE	2.3
27	2	18	PHE	2.3
29	X	338	G	2.3
29	X	1228	G	2.3
29	X	2106	G	2.3
2	A	45	ASN	2.3
9	H	49	ASP	2.3
14	M	100	ARG	2.3
19	R	48	VAL	2.3
23	V	29	ARG	2.3
30	Y	47	A	2.3
29	X	786	U	2.3
29	X	1898	U	2.3

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Mol	Chain	Res	Type	RSRZ
7	F	7	ILE	2.3
4	C	81	GLY	2.3
2	A	16	MET	2.3
7	F	108	ALA	2.3
12	K	16	ALA	2.3
21	T	8	GLY	2.3
29	X	1950	C	2.3
29	X	1966	C	2.3
29	X	2135	C	2.3
20	S	166	LEU	2.3
14	M	66	PHE	2.3
3	B	149	ARG	2.3
12	K	8	ARG	2.3
21	T	41	ARG	2.3
29	X	74	G	2.2
29	X	1755	G	2.2
29	X	2221	G	2.2
18	Q	47	GLY	2.2
29	X	200	A	2.2
29	X	2483	U	2.2
1	0	30	THR	2.2
7	F	137	THR	2.2
25	Z	26	THR	2.2
5	D	69	LYS	2.2
12	K	24	GLN	2.2
19	R	84	VAL	2.2
27	2	6	GLN	2.2
2	A	181	GLU	2.2
13	L	90	ASP	2.2
5	D	66	ILE	2.2
2	A	19	ALA	2.2
3	B	139	GLY	2.2
5	D	57	LEU	2.2
5	D	91	LEU	2.2
10	I	51	GLY	2.2
11	J	62	GLY	2.2
23	V	32	ALA	2.2
27	2	32	ALA	2.2
12	K	40	LYS	2.2
17	P	15	LYS	2.2
26	1	25	THR	2.2
29	X	2018	G	2.2

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Mol	Chain	Res	Type	RSRZ
29	X	973	U	2.2
30	Y	10	U	2.2
29	X	2014	A	2.2
4	C	3	GLN	2.2
1	O	45	ILE	2.2
7	F	114	ASP	2.2
29	X	223	C	2.2
2	A	8	PRO	2.2
6	E	105	MET	2.2
6	E	171	LEU	2.2
21	T	83	ALA	2.2
25	Z	13	LYS	2.2
11	J	42	TRP	2.2
4	C	64	THR	2.2
27	2	43	THR	2.2
1	O	58	VAL	2.2
15	N	17	VAL	2.2
9	H	27	SER	2.2
29	X	34	U	2.2
29	X	775	U	2.2
29	X	845	U	2.2
17	P	124	ILE	2.2
14	M	78	GLU	2.2
29	X	11	G	2.2
29	X	1896	A	2.2
30	Y	61	A	2.2
1	O	84	ALA	2.2
2	A	225	ALA	2.2
5	D	53	ALA	2.2
22	U	24	ALA	2.2
1	O	46	ASP	2.2
5	D	147	ASP	2.2
10	I	123	ASP	2.2
19	R	28	LYS	2.2
2	A	46	ARG	2.2
26	1	20	PHE	2.2
29	X	2048	C	2.2
29	X	2558	C	2.2
7	F	66	THR	2.2
8	G	146	THR	2.2
13	L	32	TYR	2.2
2	A	15	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
13	L	38	ILE	2.2
11	J	132	MET	2.2
1	O	65	GLY	2.2
2	A	102	LYS	2.2
10	I	28	LYS	2.2
15	N	23	GLY	2.2
22	U	39	LYS	2.2
29	X	1092	U	2.2
2	A	103	ARG	2.2
4	C	39	ARG	2.2
8	G	147	ARG	2.2
16	O	82	ARG	2.2
27	2	33	ARG	2.2
29	X	1582	A	2.2
29	X	1964	A	2.2
29	X	2267	A	2.2
29	X	2780	A	2.2
29	X	337	G	2.2
29	X	487	G	2.2
29	X	2010	G	2.2
11	J	69	ILE	2.1
14	M	55	ILE	2.1
29	X	127	C	2.1
29	X	2364	C	2.1
30	Y	32	C	2.1
5	D	169	LEU	2.1
8	G	57	LEU	2.1
3	B	55	ALA	2.1
18	Q	30	SER	2.1
7	F	118	GLY	2.1
17	P	32	ARG	2.1
17	P	111	ARG	2.1
18	Q	10	PRO	2.1
2	A	269	PHE	2.1
4	C	92	ASP	2.1
18	Q	74	ASP	2.1
29	X	12	U	2.1
9	H	47	VAL	2.1
20	S	113	VAL	2.1
20	S	122	ILE	2.1
29	X	341	A	2.1
29	X	956	A	2.1

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Mol	Chain	Res	Type	RSRZ
29	X	1318	A	2.1
11	J	134	LYS	2.1
15	N	90	LEU	2.1
21	T	62	LEU	2.1
18	Q	71	GLN	2.1
29	X	965	G	2.1
29	X	1761	G	2.1
1	0	197	PRO	2.1
16	O	77	GLY	2.1
21	T	10	SER	2.1
28	3	47	GLY	2.1
29	X	1795	C	2.1
29	X	2273	C	2.1
29	X	2845	C	2.1
6	E	92	VAL	2.1
6	E	151	VAL	2.1
28	3	49	VAL	2.1
3	B	135	HIS	2.1
13	L	97	HIS	2.1
17	P	123	HIS	2.1
1	0	152	LEU	2.1
3	B	152	LYS	2.1
16	O	75	LYS	2.1
29	X	2113	U	2.1
11	J	60	ARG	2.1
13	L	18	ARG	2.1
13	L	99	ARG	2.1
20	S	76	ARG	2.1
4	C	83	ALA	2.1
9	H	84	ALA	2.1
15	N	4	ALA	2.1
16	O	11	GLN	2.1
2	A	30	GLU	2.1
29	X	173	A	2.1
29	X	2315	A	2.1
15	N	41	ASN	2.1
18	Q	57	ASN	2.1
19	R	57	ASN	2.1
1	0	70	VAL	2.1
21	T	23	VAL	2.1
29	X	2050	G	2.1
29	X	2426	G	2.1

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Mol	Chain	Res	Type	RSRZ
29	X	126	C	2.1
29	X	1115	C	2.1
29	X	2601	C	2.1
10	I	27	ASP	2.1
28	3	15	LYS	2.1
12	K	65	LEU	2.1
3	B	146	THR	2.1
8	G	139	ARG	2.1
11	J	90	ALA	2.1
17	P	26	ALA	2.1
29	X	1639	U	2.1
29	X	1804	U	2.1
1	0	172	GLY	2.1
17	P	132	GLY	2.1
20	S	144	GLY	2.1
4	C	197	GLU	2.1
6	E	118	PRO	2.1
28	3	27	SER	2.1
3	B	154	LYS	2.1
22	U	54	ASN	2.1
29	X	1509	A	2.1
29	X	2266	A	2.1
3	B	102	ILE	2.1
5	D	40	LEU	2.1
27	2	28	ARG	2.1
28	3	39	ASP	2.1
2	A	9	TYR	2.1
29	X	1549	C	2.1
29	X	342	G	2.1
29	X	1324	G	2.1
1	0	165	GLY	2.1
5	D	93	GLY	2.1
1	0	145	VAL	2.0
1	0	203	VAL	2.0
20	S	116	VAL	2.0
28	3	5	LYS	2.0
29	X	390	U	2.0
25	Z	12	SER	2.0
27	2	26	SER	2.0
1	0	181	LEU	2.0
3	B	9	ILE	2.0
16	O	71	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
15	N	61	TRP	2.0
7	F	74	MET	2.0
9	H	46	HIS	2.0
1	O	154	ALA	2.0
11	J	138	TYR	2.0
16	O	7	THR	2.0
20	S	77	ALA	2.0
29	X	991	A	2.0
29	X	2569	A	2.0
2	A	235	GLY	2.0
7	F	103	GLN	2.0
8	G	108	GLY	2.0
1	O	173	LYS	2.0
15	N	46	GLU	2.0
2	A	247	VAL	2.0
4	C	82	VAL	2.0
17	P	38	VAL	2.0
28	3	22	VAL	2.0
29	X	1185	C	2.0
29	X	2038	C	2.0
3	B	119	ARG	2.0
17	P	14	ARG	2.0
29	X	30	G	2.0
29	X	108	G	2.0
29	X	920	G	2.0
29	X	1893	G	2.0
29	X	2362	G	2.0
1	O	99	ILE	2.0
4	C	7	ILE	2.0
5	D	47	SER	2.0
29	X	400	U	2.0
29	X	1894	U	2.0
8	G	71	THR	2.0
13	L	52	ALA	2.0
17	P	96	TYR	2.0
2	A	246	PRO	2.0
11	J	12	LYS	2.0
18	Q	61	LYS	2.0
9	H	104	GLU	2.0
9	H	117	GLU	2.0
19	R	104	VAL	2.0
21	T	38	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
29	X	109	A	2.0
29	X	518	A	2.0
29	X	625	A	2.0
29	X	1250	A	2.0
29	X	2220	A	2.0
29	X	2520	A	2.0
22	U	20	ARG	2.0
1	0	222	LEU	2.0
3	B	198	LEU	2.0
3	B	49	ILE	2.0
29	X	759	C	2.0
29	X	926	C	2.0
29	X	1575	C	2.0
29	X	2160	C	2.0
29	X	2162	C	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	MG	X	6152	1/1	0.06	0.34	158,158,158,158	0
31	MG	X	6135	1/1	0.07	0.82	129,129,129,129	0
31	MG	X	6116	1/1	0.29	0.95	99,99,99,99	0
31	MG	X	6101	1/1	0.32	0.99	138,138,138,138	0
31	MG	X	6103	1/1	0.37	0.27	126,126,126,126	0
31	MG	X	6142	1/1	0.39	0.57	106,106,106,106	0
31	MG	X	6130	1/1	0.45	0.38	132,132,132,132	0
31	MG	X	6177	1/1	0.45	0.53	125,125,125,125	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	MG	X	6125	1/1	0.46	0.55	109,109,109,109	0
31	MG	X	6159	1/1	0.47	0.52	109,109,109,109	0
31	MG	Y	204	1/1	0.47	0.50	116,116,116,116	0
31	MG	X	6137	1/1	0.49	0.40	136,136,136,136	0
31	MG	X	6079	1/1	0.50	0.36	99,99,99,99	0
31	MG	X	6003	1/1	0.51	0.41	72,72,72,72	0
31	MG	X	6100	1/1	0.51	0.47	111,111,111,111	0
31	MG	X	6114	1/1	0.52	0.67	93,93,93,93	0
31	MG	X	6087	1/1	0.53	0.53	85,85,85,85	0
31	MG	X	6051	1/1	0.54	0.45	83,83,83,83	0
31	MG	X	6162	1/1	0.54	0.62	104,104,104,104	0
31	MG	X	6046	1/1	0.55	0.58	76,76,76,76	0
31	MG	X	6176	1/1	0.55	0.37	73,73,73,73	0
31	MG	X	6117	1/1	0.55	0.43	130,130,130,130	0
31	MG	X	6060	1/1	0.55	1.10	80,80,80,80	0
31	MG	X	6006	1/1	0.58	0.66	70,70,70,70	0
31	MG	X	6093	1/1	0.58	0.36	96,96,96,96	0
31	MG	Y	203	1/1	0.58	0.61	96,96,96,96	0
31	MG	X	6132	1/1	0.58	0.52	84,84,84,84	0
31	MG	X	6057	1/1	0.59	0.65	92,92,92,92	0
31	MG	X	6147	1/1	0.60	0.80	93,93,93,93	0
31	MG	X	6022	1/1	0.62	0.48	92,92,92,92	0
31	MG	X	6148	1/1	0.62	0.28	104,104,104,104	0
31	MG	X	6149	1/1	0.62	0.41	99,99,99,99	0
31	MG	X	6029	1/1	0.62	0.35	82,82,82,82	0
31	MG	X	6020	1/1	0.62	0.37	76,76,76,76	0
31	MG	X	6167	1/1	0.63	0.74	97,97,97,97	0
31	MG	X	6175	1/1	0.63	0.54	121,121,121,121	0
31	MG	X	6133	1/1	0.64	0.56	91,91,91,91	0
31	MG	X	6025	1/1	0.64	0.57	76,76,76,76	0
31	MG	X	6018	1/1	0.64	0.52	86,86,86,86	0
31	MG	X	6165	1/1	0.64	0.34	88,88,88,88	0
31	MG	X	6141	1/1	0.64	0.40	87,87,87,87	0
31	MG	Y	205	1/1	0.64	0.40	123,123,123,123	0
31	MG	X	6139	1/1	0.65	0.31	113,113,113,113	0
31	MG	X	6160	1/1	0.65	0.66	108,108,108,108	0
31	MG	X	6170	1/1	0.65	0.40	97,97,97,97	0
31	MG	X	6174	1/1	0.65	0.33	117,117,117,117	0
31	MG	X	6153	1/1	0.65	0.45	114,114,114,114	0
31	MG	X	6076	1/1	0.66	0.41	73,73,73,73	0
31	MG	X	6072	1/1	0.66	0.53	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	MG	X	6096	1/1	0.66	0.26	99,99,99,99	0
31	MG	X	6168	1/1	0.67	0.43	100,100,100,100	0
31	MG	X	6099	1/1	0.67	0.59	120,120,120,120	0
31	MG	X	6052	1/1	0.67	0.49	86,86,86,86	0
31	MG	X	6089	1/1	0.68	0.43	89,89,89,89	0
31	MG	X	6124	1/1	0.68	0.43	100,100,100,100	0
31	MG	X	6123	1/1	0.69	0.40	89,89,89,89	0
31	MG	X	6001	1/1	0.69	0.53	67,67,67,67	0
31	MG	X	6013	1/1	0.69	0.67	76,76,76,76	0
31	MG	X	6073	1/1	0.69	0.24	105,105,105,105	0
31	MG	X	6017	1/1	0.69	0.35	54,54,54,54	0
31	MG	X	6163	1/1	0.70	0.25	82,82,82,82	0
31	MG	X	6048	1/1	0.70	0.42	66,66,66,66	0
31	MG	X	6115	1/1	0.70	0.23	133,133,133,133	0
31	MG	X	6158	1/1	0.70	0.26	76,76,76,76	0
31	MG	X	6106	1/1	0.71	0.39	100,100,100,100	0
31	MG	X	6157	1/1	0.71	0.42	96,96,96,96	0
31	MG	X	6043	1/1	0.71	0.26	106,106,106,106	0
31	MG	X	6049	1/1	0.71	0.56	91,91,91,91	0
31	MG	X	6150	1/1	0.71	0.47	97,97,97,97	0
31	MG	X	6092	1/1	0.71	0.49	97,97,97,97	0
31	MG	X	6156	1/1	0.72	0.28	91,91,91,91	0
31	MG	X	6155	1/1	0.72	0.44	108,108,108,108	0
31	MG	X	6058	1/1	0.73	0.27	70,70,70,70	0
31	MG	X	6120	1/1	0.73	0.32	78,78,78,78	0
31	MG	X	6019	1/1	0.74	0.30	75,75,75,75	0
31	MG	X	6033	1/1	0.74	0.56	76,76,76,76	0
31	MG	X	6112	1/1	0.74	0.24	80,80,80,80	0
31	MG	X	6042	1/1	0.74	0.74	96,96,96,96	0
31	MG	X	6053	1/1	0.75	0.64	85,85,85,85	0
31	MG	X	6127	1/1	0.75	0.44	81,81,81,81	0
31	MG	X	6097	1/1	0.75	0.31	122,122,122,122	0
31	MG	X	6118	1/1	0.75	0.29	82,82,82,82	0
31	MG	X	6091	1/1	0.75	0.41	72,72,72,72	0
31	MG	H	201	1/1	0.75	0.21	104,104,104,104	0
31	MG	X	6074	1/1	0.75	0.48	89,89,89,89	0
31	MG	X	6113	1/1	0.76	0.34	143,143,143,143	0
31	MG	X	6045	1/1	0.76	0.53	94,94,94,94	0
31	MG	X	6140	1/1	0.76	0.23	97,97,97,97	0
31	MG	X	6172	1/1	0.76	0.23	88,88,88,88	0
31	MG	X	6173	1/1	0.76	0.19	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	MG	X	6031	1/1	0.76	0.46	85,85,85,85	0
31	MG	X	6090	1/1	0.77	0.47	72,72,72,72	0
31	MG	X	6068	1/1	0.77	0.29	111,111,111,111	0
31	MG	X	6010	1/1	0.77	0.45	64,64,64,64	0
31	MG	X	6083	1/1	0.77	0.32	83,83,83,83	0
31	MG	X	6024	1/1	0.77	0.25	100,100,100,100	0
31	MG	X	6111	1/1	0.77	0.40	98,98,98,98	0
31	MG	Y	202	1/1	0.77	0.16	130,130,130,130	0
31	MG	A	301	1/1	0.77	0.39	108,108,108,108	0
31	MG	X	6169	1/1	0.77	0.43	91,91,91,91	0
31	MG	X	6134	1/1	0.77	0.13	100,100,100,100	0
31	MG	X	6030	1/1	0.78	0.28	101,101,101,101	0
31	MG	X	6016	1/1	0.78	0.37	74,74,74,74	0
31	MG	Y	201	1/1	0.78	0.45	96,96,96,96	0
31	MG	X	6129	1/1	0.78	0.51	89,89,89,89	0
31	MG	X	6105	1/1	0.78	0.43	86,86,86,86	0
31	MG	X	6011	1/1	0.78	0.29	104,104,104,104	0
31	MG	X	6007	1/1	0.78	0.38	78,78,78,78	0
31	MG	X	6014	1/1	0.79	0.38	99,99,99,99	0
31	MG	X	6146	1/1	0.79	0.24	125,125,125,125	0
31	MG	X	6161	1/1	0.79	0.33	113,113,113,113	0
31	MG	X	6082	1/1	0.79	0.49	105,105,105,105	0
31	MG	X	6055	1/1	0.79	0.33	85,85,85,85	0
31	MG	X	6062	1/1	0.79	1.02	87,87,87,87	0
31	MG	X	6015	1/1	0.79	0.28	74,74,74,74	0
31	MG	X	6002	1/1	0.80	0.23	91,91,91,91	0
31	MG	X	6094	1/1	0.80	0.35	95,95,95,95	0
31	MG	X	6054	1/1	0.80	0.44	79,79,79,79	0
31	MG	X	6151	1/1	0.80	0.50	88,88,88,88	0
31	MG	X	6027	1/1	0.80	0.62	65,65,65,65	0
31	MG	X	6004	1/1	0.80	0.24	93,93,93,93	0
31	MG	X	6154	1/1	0.80	0.49	96,96,96,96	0
31	MG	X	6035	1/1	0.80	0.59	80,80,80,80	0
31	MG	X	6077	1/1	0.81	0.39	80,80,80,80	0
31	MG	X	6143	1/1	0.81	0.49	99,99,99,99	0
31	MG	X	6066	1/1	0.81	0.21	105,105,105,105	0
31	MG	X	6075	1/1	0.81	0.14	85,85,85,85	0
31	MG	X	6126	1/1	0.81	0.34	114,114,114,114	0
31	MG	X	6061	1/1	0.81	0.23	100,100,100,100	0
31	MG	X	6171	1/1	0.82	0.34	118,118,118,118	0
31	MG	X	6144	1/1	0.82	0.35	132,132,132,132	0
31	MG	X	6078	1/1	0.82	0.36	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	MG	X	6104	1/1	0.82	0.42	89,89,89,89	0
31	MG	X	6040	1/1	0.83	0.49	63,63,63,63	0
31	MG	X	6080	1/1	0.83	0.75	82,82,82,82	0
31	MG	X	6085	1/1	0.83	0.42	66,66,66,66	0
31	MG	X	6095	1/1	0.84	0.37	78,78,78,78	0
31	MG	N	201	1/1	0.84	0.26	74,74,74,74	0
31	MG	X	6081	1/1	0.84	0.31	90,90,90,90	0
31	MG	X	6070	1/1	0.84	0.32	69,69,69,69	0
31	MG	X	6023	1/1	0.84	0.42	83,83,83,83	0
31	MG	X	6063	1/1	0.84	0.40	87,87,87,87	0
31	MG	X	6164	1/1	0.84	0.31	86,86,86,86	0
31	MG	X	6039	1/1	0.84	0.19	79,79,79,79	0
31	MG	X	6065	1/1	0.85	0.19	93,93,93,93	0
31	MG	X	6047	1/1	0.85	0.21	79,79,79,79	0
31	MG	X	6138	1/1	0.85	0.23	86,86,86,86	0
31	MG	X	6128	1/1	0.85	0.22	131,131,131,131	0
31	MG	X	6110	1/1	0.85	0.39	84,84,84,84	0
31	MG	X	6145	1/1	0.86	0.25	84,84,84,84	0
31	MG	X	6166	1/1	0.86	0.24	76,76,76,76	0
31	MG	X	6032	1/1	0.86	0.29	86,86,86,86	0
31	MG	X	6084	1/1	0.86	0.22	124,124,124,124	0
31	MG	X	6050	1/1	0.86	0.49	91,91,91,91	0
31	MG	X	6122	1/1	0.86	0.42	84,84,84,84	0
31	MG	X	6059	1/1	0.87	0.27	88,88,88,88	0
31	MG	X	6098	1/1	0.87	0.21	71,71,71,71	0
31	MG	X	6119	1/1	0.87	0.47	89,89,89,89	0
31	MG	X	6037	1/1	0.87	0.52	65,65,65,65	0
31	MG	X	6026	1/1	0.87	0.24	79,79,79,79	0
31	MG	X	6108	1/1	0.87	0.38	108,108,108,108	0
31	MG	X	6028	1/1	0.87	0.22	75,75,75,75	0
31	MG	M	201	1/1	0.88	0.53	71,71,71,71	0
31	MG	X	6131	1/1	0.88	0.35	80,80,80,80	0
31	MG	X	6071	1/1	0.88	0.38	99,99,99,99	0
31	MG	X	6102	1/1	0.88	0.20	98,98,98,98	0
31	MG	X	6069	1/1	0.89	0.30	65,65,65,65	0
31	MG	X	6109	1/1	0.89	0.29	92,92,92,92	0
31	MG	X	6038	1/1	0.89	0.10	82,82,82,82	0
31	MG	X	6136	1/1	0.89	0.35	84,84,84,84	0
31	MG	X	6012	1/1	0.89	0.25	78,78,78,78	0
31	MG	X	6036	1/1	0.90	0.28	70,70,70,70	0
31	MG	X	6064	1/1	0.90	0.50	77,77,77,77	0
31	MG	X	6056	1/1	0.90	0.22	81,81,81,81	0

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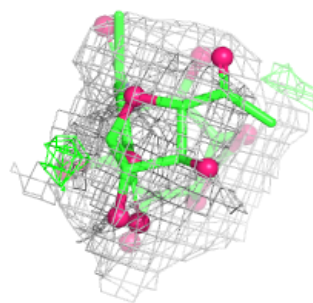
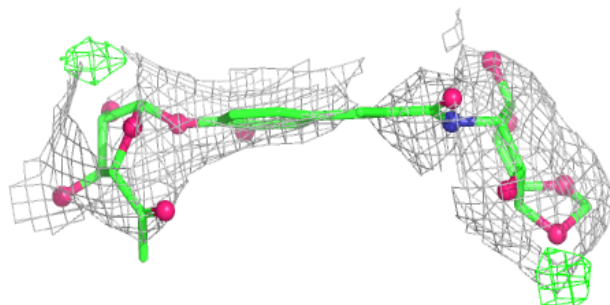
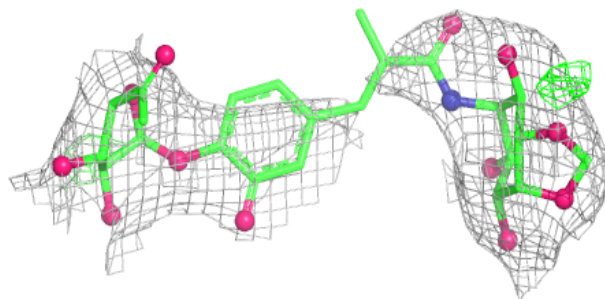
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	MG	X	6044	1/1	0.90	0.28	66,66,66,66	0
31	MG	X	6009	1/1	0.90	0.23	50,50,50,50	0
31	MG	X	6034	1/1	0.91	0.15	69,69,69,69	0
31	MG	X	6041	1/1	0.91	0.33	64,64,64,64	0
31	MG	X	6008	1/1	0.92	0.21	58,58,58,58	0
32	HGR	X	6178	36/36	0.92	0.15	79,99,109,111	0
31	MG	X	6005	1/1	0.93	0.48	58,58,58,58	0
31	MG	X	6021	1/1	0.93	0.15	91,91,91,91	0
31	MG	X	6107	1/1	0.93	0.20	76,76,76,76	0
31	MG	X	6088	1/1	0.94	0.21	88,88,88,88	0
31	MG	X	6121	1/1	0.95	0.65	85,85,85,85	0
31	MG	X	6067	1/1	0.96	0.12	72,72,72,72	0
31	MG	X	6086	1/1	0.97	0.08	104,104,104,104	0

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

Electron density around HGR X 6178:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.