



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 08:03 PM UTC

PDB ID : 1YI2 / pdb_00001yi2
Title : Crystal Structure Of Erythromycin Bound To The G2099A Mutant 50S Ribosomal Subunit Of Haloarcula Marismortui
Authors : Tu, D.; Blaha, G.; Moore, P.B.; Steitz, T.A.
Deposited on : 2005-01-11
Resolution : 2.65 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

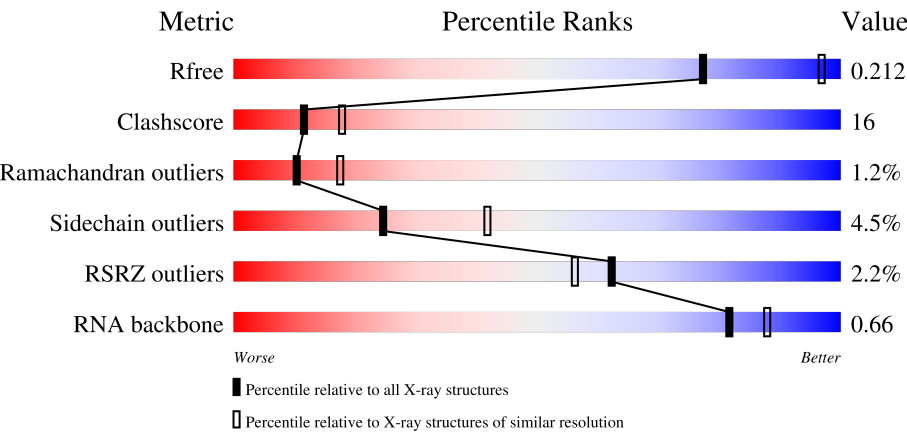
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)
RNA backbone	3983	1090 (2.90-2.42)

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	2922	61%27%5%6%
2	9	122	55%35%8%
3	A	240	61%32%6%
4	B	338	49%46%5%

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Mol	Chain	Length	Quality of chain
5	C	246	
6	D	177	
7	E	178	
8	F	120	
9	G	348	
10	H	177	
11	I	162	
12	J	145	
13	K	132	
14	L	165	
15	M	195	
16	N	187	
17	O	116	
18	P	149	
19	Q	96	
20	R	155	
21	S	85	
22	T	120	
23	U	66	
24	V	71	
25	W	154	
26	X	92	
27	Y	241	
28	Z	83	
29	1	57	

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Mol	Chain	Length	Quality of chain
30	2	50	
31	3	92	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	NA	R	8586	-	-	-	X

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99086 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	2754	Total	C	N	O	P	0	0	0
			59020	26349	10873	19053	2745			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	628	1MA	A	modified residue	GB 55229667
0	2099	A	G	engineered mutation	GB 55229667
0	2587	OMU	U	modified residue	GB 55229667
0	2588	OMG	G	modified residue	GB 55229667
0	2619	UR3	U	modified residue	GB 55229667
0	2621	PSU	U	modified residue	GB 55229667

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	9	122	Total	C	N	O	P	0	0	0
			2599	1160	471	847	121			

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

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

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

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

- Molecule 5 is a protein called 50S ribosomal protein L4E.

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

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

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

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

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

- Molecule 8 is a protein called 50S ribosomal protein L7AE.

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

- Molecule 9 is a protein called ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG.

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

- Molecule 10 is a protein called 50S RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	160	Total	C	N	O	S	0	0	0
			1282	798	240	238	6			

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L11P.

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

- Molecule 15 is a protein called 50S Ribosomal Protein L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	M	194	Total	C	N	O	S	0	0	0
			1558	942	332	283	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	13	GLU	LYS	conflict	GB 55231501

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	Z	73	Total	C	N	O	S	0	0	0
			578	346	116	111	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	10	ARG	SER	conflict	GB 55231162

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

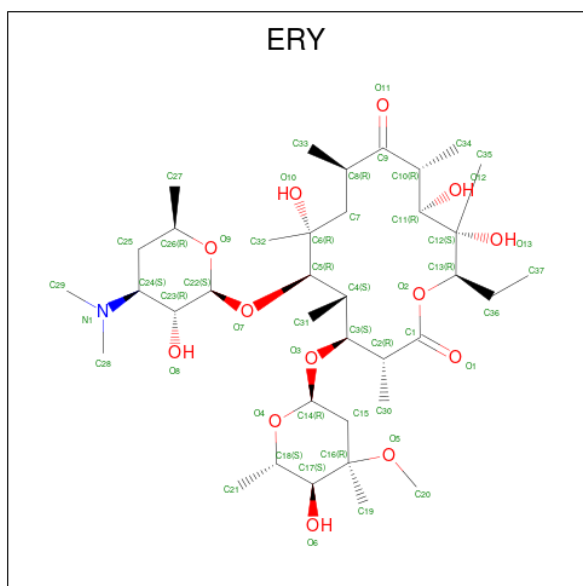
- Molecule 30 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 32 is ERYTHROMYCIN A (CCD ID: ERY) (formula: $C_{37}H_{67}NO_{13}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	0	1	Total	C	N	O	0	0
			51	37	1	13		

- Molecule 33 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	108	Total	Mg	0	0
			108	108		
33	9	1	Total	Mg	0	0
			1	1		
33	A	1	Total	Mg	0	0
			1	1		
33	B	1	Total	Mg	0	0
			1	1		
33	K	1	Total	Mg	0	0
			1	1		
33	T	1	Total	Mg	0	0
			1	1		
33	Y	1	Total	Mg	0	0
			1	1		
33	2	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	3	1	Total	Mg	0	0
			1	1		

- Molecule 34 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	2	Total	K	0	0
			2	2		

- Molecule 35 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	71	Total	Na	0	0
			71	71		
35	9	2	Total	Na	0	0
			2	2		
35	A	1	Total	Na	0	0
			1	1		
35	C	1	Total	Na	0	0
			1	1		
35	H	2	Total	Na	0	0
			2	2		
35	J	1	Total	Na	0	0
			1	1		
35	L	1	Total	Na	0	0
			1	1		
35	M	1	Total	Na	0	0
			1	1		
35	Q	1	Total	Na	0	0
			1	1		
35	R	3	Total	Na	0	0
			3	3		
35	S	1	Total	Na	0	0
			1	1		
35	T	1	Total	Na	0	0
			1	1		

- Molecule 36 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	10	Total	Cl	0	0
			10	10		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	A	1	Total 1	Cl 1	0	0
36	B	1	Total 1	Cl 1	0	0
36	J	3	Total 3	Cl 3	0	0
36	L	1	Total 1	Cl 1	0	0
36	M	1	Total 1	Cl 1	0	0
36	N	1	Total 1	Cl 1	0	0
36	O	1	Total 1	Cl 1	0	0
36	R	1	Total 1	Cl 1	0	0
36	Y	1	Total 1	Cl 1	0	0
36	3	1	Total 1	Cl 1	0	0

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

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

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	0	5869	Total 5869	O 5869	0	0
38	9	138	Total 138	O 138	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	A	121	Total 121	O 121	0	0
38	B	151	Total 151	O 151	0	0
38	C	168	Total 168	O 168	0	0
38	D	50	Total 50	O 50	0	0
38	E	42	Total 42	O 42	0	0
38	F	28	Total 28	O 28	0	0
38	G	19	Total 19	O 19	0	0
38	H	71	Total 71	O 71	0	0
38	I	9	Total 9	O 9	0	0
38	J	55	Total 55	O 55	0	0
38	K	61	Total 61	O 61	0	0
38	L	81	Total 81	O 81	0	0
38	M	124	Total 124	O 124	0	0
38	N	67	Total 67	O 67	0	0
38	O	43	Total 43	O 43	0	0
38	P	66	Total 66	O 66	0	0
38	Q	49	Total 49	O 49	0	0
38	R	80	Total 80	O 80	0	0
38	S	37	Total 37	O 37	0	0
38	T	37	Total 37	O 37	0	0
38	U	27	Total 27	O 27	0	0

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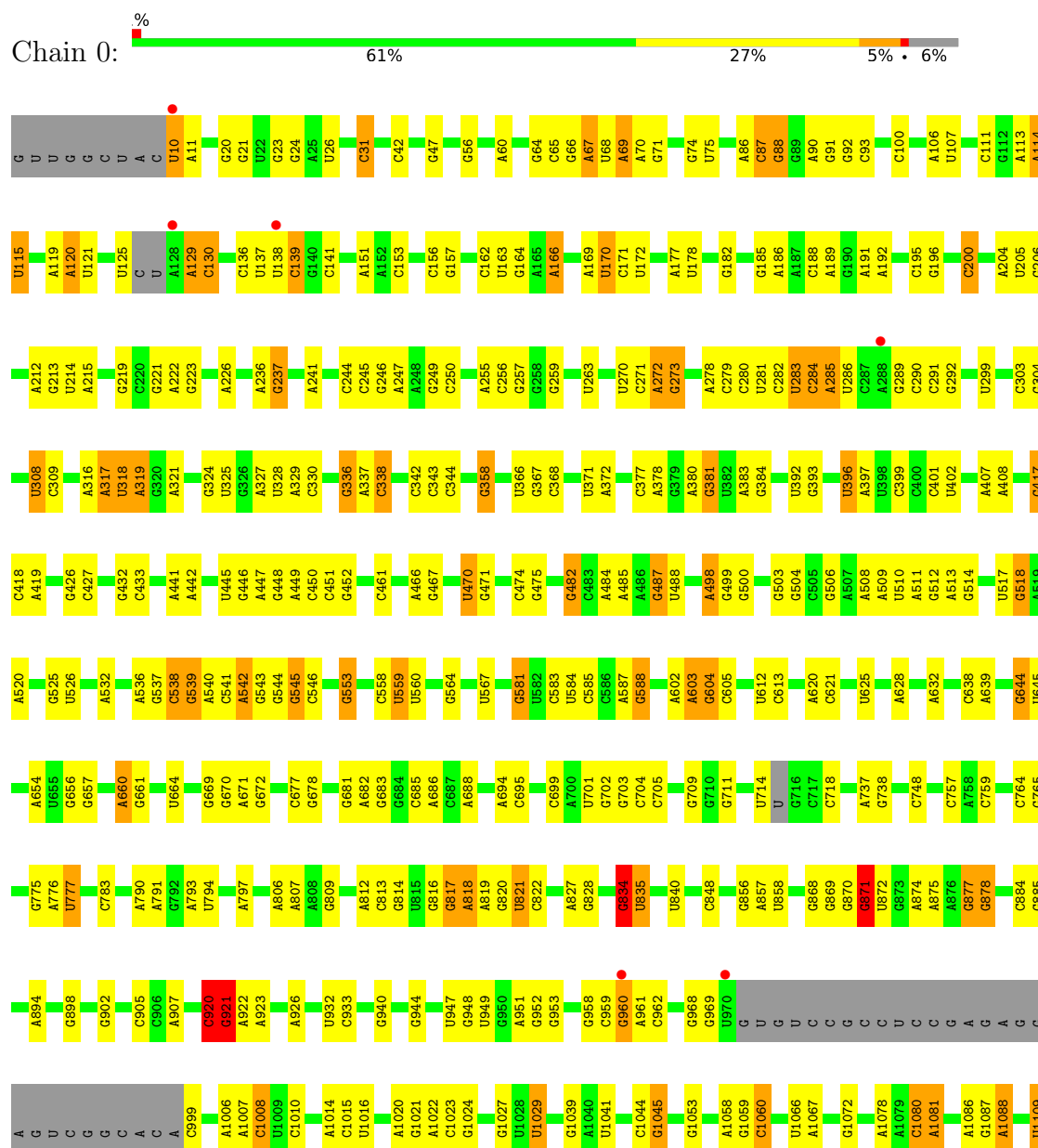
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	V	14	Total 14	O 14	0	0
38	W	73	Total 73	O 73	0	0
38	X	27	Total 27	O 27	0	0
38	Y	94	Total 94	O 94	0	0
38	Z	30	Total 30	O 30	0	0
38	1	54	Total 54	O 54	0	0
38	2	45	Total 45	O 45	0	0
38	3	78	Total 78	O 78	0	0

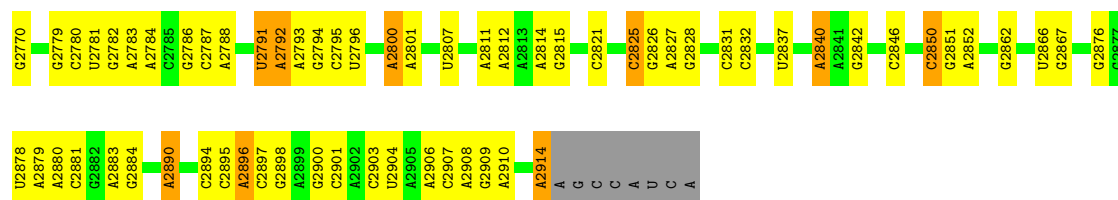
3 Residue-property plots [i](#)

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.

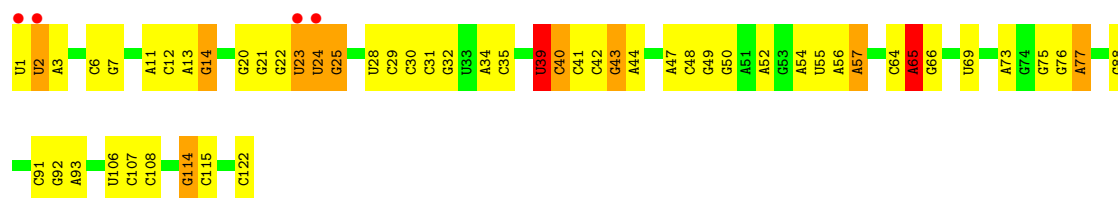
• Molecule 1: 23S Ribosomal RNA



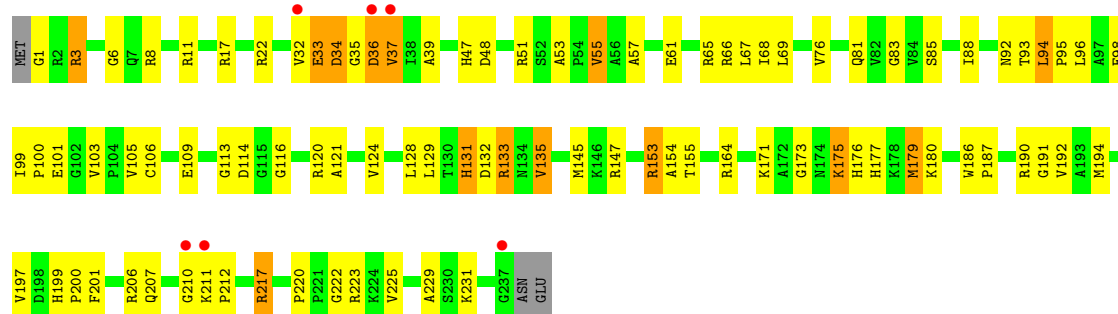
U2652	C2536	U2445	C	G	U2064	C1940	C1798	C1692	G1592	C1462	C1334	U1205	G1110
A2653	G2537	G2446	A	U	U2064	A1941	G1819	C1692	C1593	A1470	C1335	U1206	U1116
A2664	U2541	G2453	G	C	G2072	A1942	C1820	A1701	C1594	C1474	G1340	C1207	A1117
U	C2547	A2456	A	G	G2073	C1943	U1825	U1702	G1595	C1477	C1342	C1209	G1118
G2667	C2548	U2457	U	U	A2074	G1947	C1826	A1711	U1596	C1477	C1343	G1210	A1119
G2668	C2552	G2462	G	G	A2081	G1951	U1826	A1712	A1598	C1477	C1343	U1213	U1120
U2669	A2553	A2465	A	U	A2089	U	A1829	A1717	A1603	A1482	G1351	G1214	G1121
U2671	G2553	G2466	U	C	G2090	A	C1830	A	G1604	C1483	A1352	A1215	A1123
C2676	C2559	A2468	C	A	G2091	C	C1834	U1722	A1606	U1488	C1360	C1229	U1130
U2679	U2563	U2469	U	G	G2092	U	U1835	G1723	A1607	A1494	G1363	A1230	A1132
A2681	G2564	C2472	C	A	G2093	A	A1840	U1724	G1613	C1495	G1363	U1234	G1135
C2682	C2565	C2476	U	G	A2095	C	A1846	C1725	G1614	A1495	U1234	U1234	U1136
A2694	G2570	C2483	A	U	A2096	C	A1847	G1731	A1615	G1497	A1372	U1236	G1137
G2708	C2578	G2480	C	C	A2101	C	G1848	A1733	A1616	U1500	A1375	U1237	G1151
G2709	U2586	U2484	C	C	G2102	U1964	G1849	A1733	A1624	U1503	A1376	C1238	G1159
U2710	U2587	G2485	C	C	A2103	C1965	U1850	C1735	U1625	A1504	U1380	A1242	G1160
U2711	C2588	U2486	G	G	C2104	U1966	G1851	A1736	A1626	U1505	U1244	C1243	A1161
G2712	U2589	U2488	C	C	G2110	G1970	C1852	U1741	G1627	U1506	G1391	U1244	G1162
U2713	C2592	G2489	U	U	U2115	G1971	C1856	A1742	A1630	A1515	A1392	U1246	G1163
G2715	U2592	U2490	A	A	U2116	A1972	A1857	G1751	C1633	U1516	A1393	A1246	G1165
G2716	C2597	C2491	C	C	C2132	G1974	C1861	G1752	G1634	U1524	A1394	C1250	A1166
U2717	U2598	U2492	G	G	A2135	A1978	C1862	C1753	G1635	G1525	G1398	C1251	G1167
C2718	A2601	C2493	G	C	G2136	G1979	G1863	A1755	G1636	A1526	A1399	A1252	C1168
A2719	G2602	C2498	C	C	A	U1980	G1867	G1756	A1641	U1528	A1406	C1253	U1169
G2720	C2603	C2499	A	A	C	U1996	G1868	U1761	A1642	G1529	A1407	A1261	U1170
G2722	A2604	C2502	C	C	U	A1997	G1877	C1762	C1643	U1535	G1415	U1266	A1171
U2724	U2607	A2503	C	C	G	G2000	G1878	C1763	A1653	G1536	G1416	U1267	A1173
G2725	C2608	G2504	A	U	U	G2001	C1879	U1766	U1684	C1537	G1417	C1268	A1174
U2726	C2613	G2505	G	C	C	G2002	C1880	A1767	G1655	U1544	U1419	C1269	G1175
A2727	G2613	U2506	A	G	A	U2003	A1881	C1768	A1656	C1545	U1419	C1273	A1177
C2747	U2619	G2507	C	C	C	U2004	C1882	C1769	A1657	G1552	U1422	A1278	U1180
G2748	U2620	A2508	A	A	A	G2005	U1887	U1771	A1658	C1553	C1423	U1279	A1181
U2749	U2621	C2510	C	C	A	U2008	A1904	C1772	C1666	C1554	A1424	C1287	C1182
G2750	C2629	A2511	A	U	U	A2011	U1905	G1773	C1667	U1555	A1427	U1288	C1183
G2754	G2630	C2515	G	U	G	U2012	A1919	G1774	U1668	U1434	U1289	C1290	U1185
G2755	G2634	G2516	U	U	C	G2013	C1920	A1778	C1675	U1435	U1187	G1290	C1186
U2756	A2635	A2521	A	A	A	C	A1921	A1779	G1676	U1561	C1436	G1295	A1188
G2761	C2636	G2524	A	A	G	G2033	G1925	A1783	C1679	C1562	U1440	G1295	A1189
G2762	A2637	U2525	C	U	C	U2034	C2035	U1784	G1680	U1564	G1441	U1298	A1191
G2763	G2638	C2526	A	A	A	C2036	G1926	U1785	G1681	A1442	A1442	C1299	A1192
C2764	C2765	U2527	U	C	U	U2044	A1927	G1787	A1882	A1573	C1450	U1314	A1193
C2765	A2643	C2326	U	U	A	G2044	C1928	U1788	G1683	A1580	C1451	U1314	A1193
A2766	U2649	C2326	A	A	G	U	G1929	G1789	A1684	A1580	C1451	U1314	A1193
C2767	U2650	C2338	C	C	G	G2050	A1930	U1791	A1685	G1589	G1460	A1328	G1201
A2768	C2654	C2338	C	C	U	A2054	A1931	U1791	C1686	G1589	G1461	A1333	G1203
C2769	C2651	U2535	C	C	A				C1687				C1204



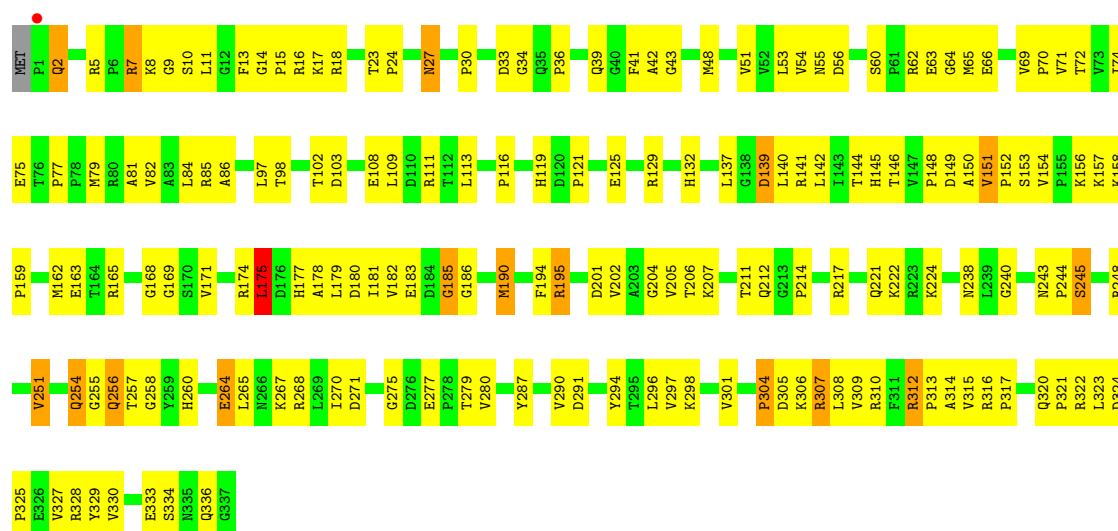
• Molecule 2: 5S Ribosomal RNA



• Molecule 3: 50S ribosomal protein L2P



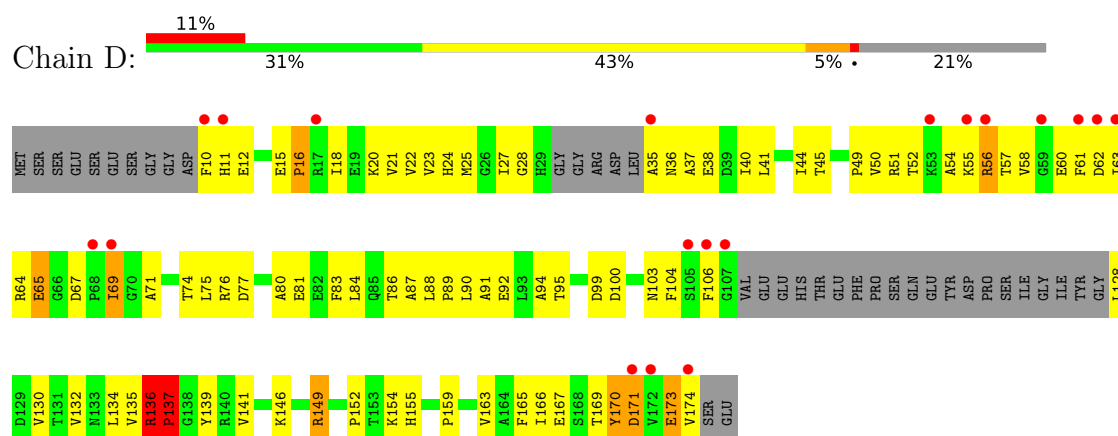
• Molecule 4: 50S ribosomal protein L3P



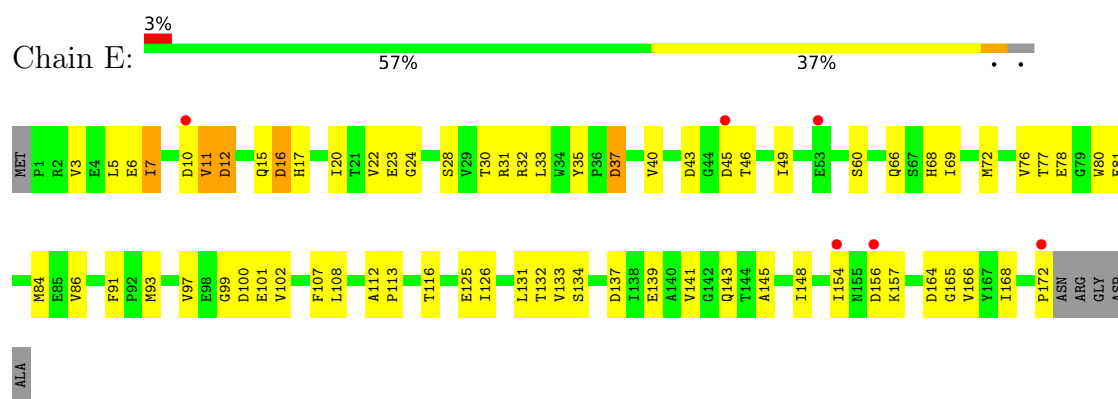
• Molecule 5: 50S ribosomal protein L4E



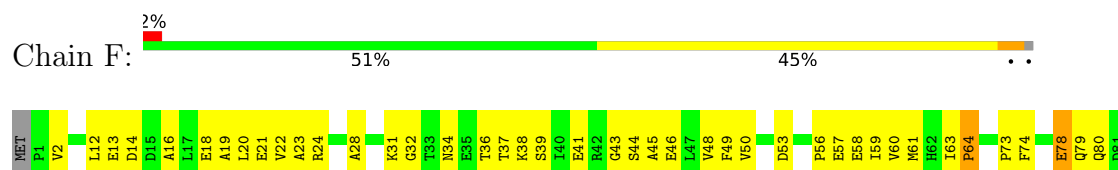
• Molecule 6: 50S ribosomal protein L5P



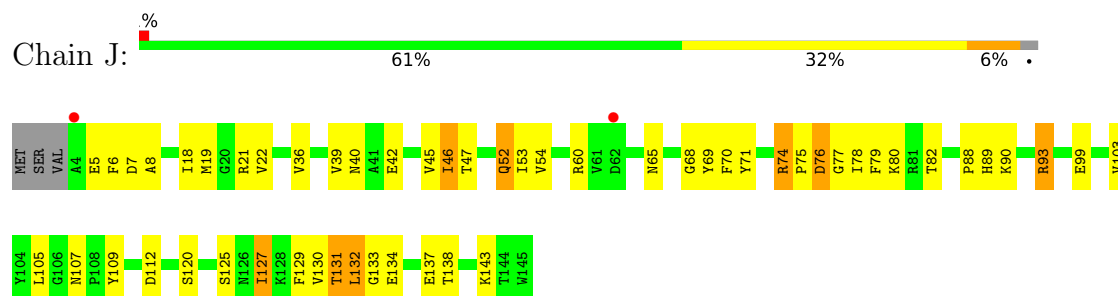
• Molecule 7: 50S ribosomal protein L6P



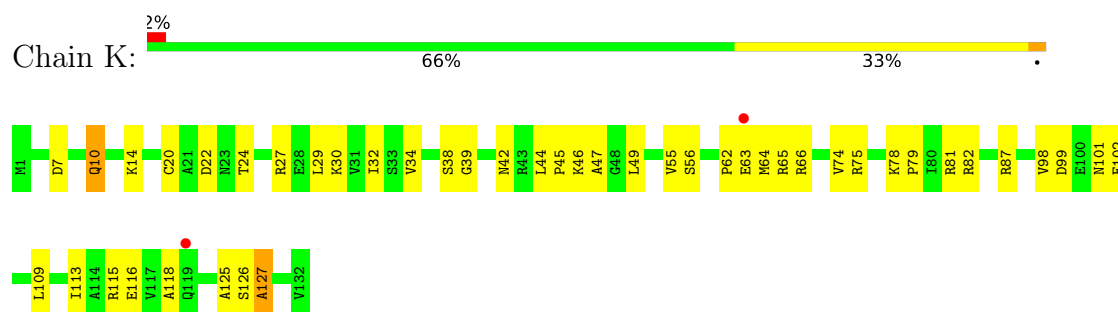
• Molecule 8: 50S ribosomal protein L7AE



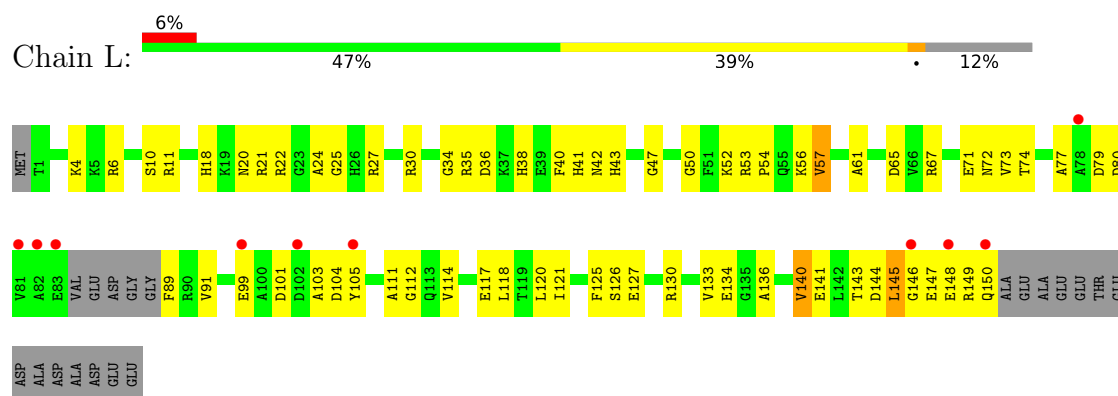
- Molecule 12: 50S ribosomal protein L13P



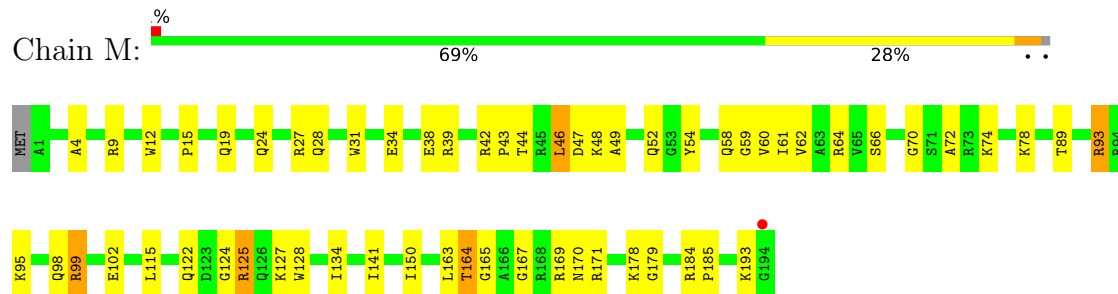
- Molecule 13: 50S ribosomal protein L14P



- Molecule 14: 50S ribosomal protein L15P



- Molecule 15: 50S Ribosomal Protein L15E

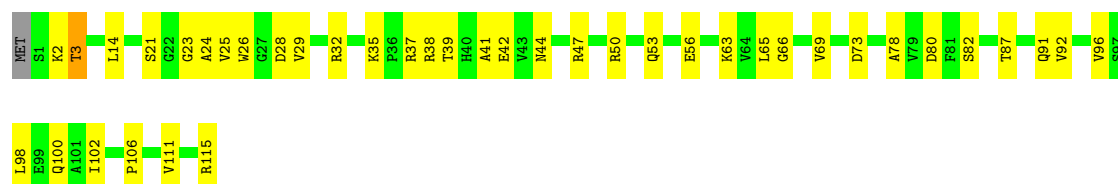


- Molecule 16: 50S ribosomal protein L18P

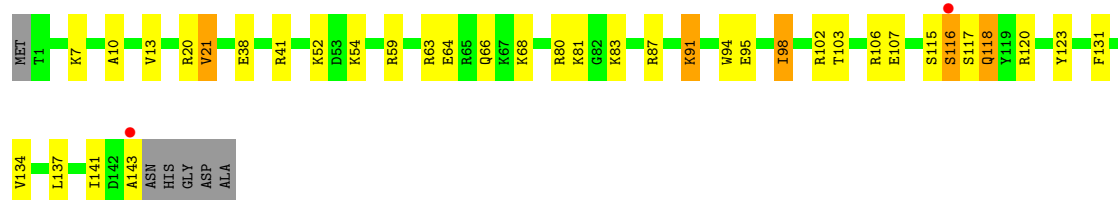




- Molecule 17: 50S ribosomal protein L18e



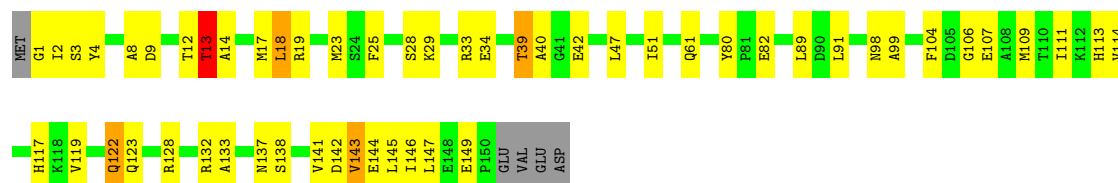
- Molecule 18: 50S ribosomal protein L19E



- Molecule 19: 50S ribosomal protein L21e

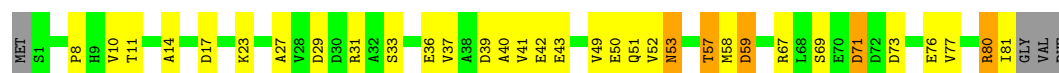


- Molecule 20: 50S ribosomal protein L22P



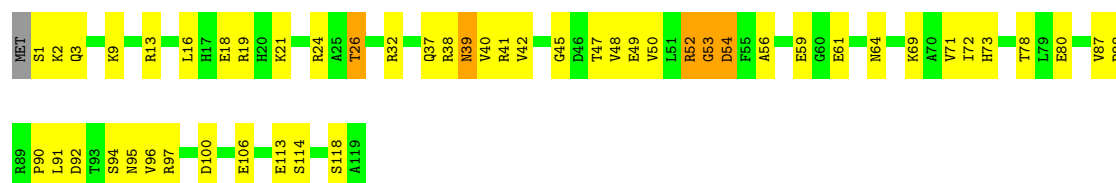
- Molecule 21: 50S ribosomal protein L23P

Chain S: 

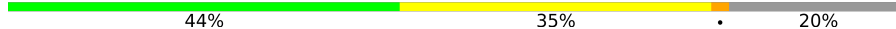


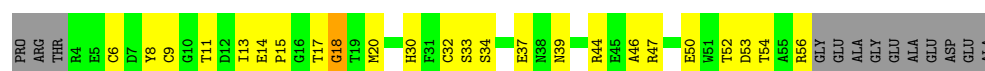
- Molecule 22: 50S ribosomal protein L24P

Chain T: 



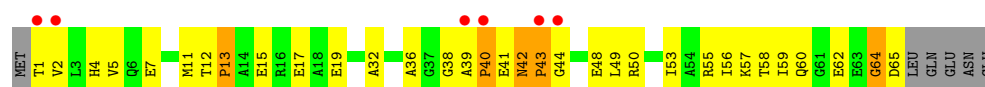
- Molecule 23: 50S ribosomal protein L24E

Chain U: 



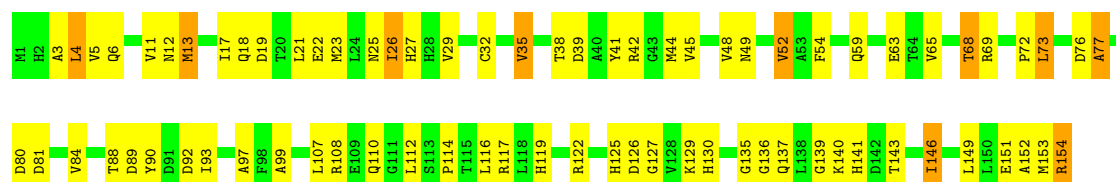
- Molecule 24: 50S ribosomal protein L29P

Chain V: 



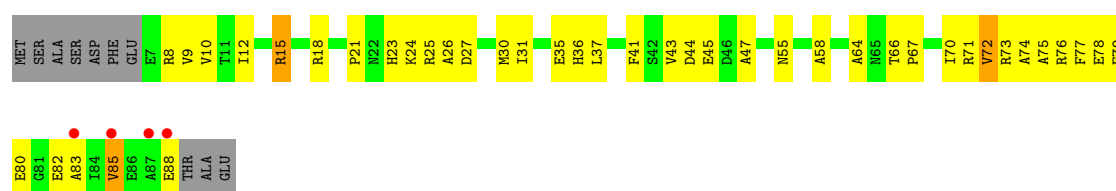
- Molecule 25: 50S ribosomal protein L30P

Chain W: 



- Molecule 26: 50S ribosomal protein L31e

Chain X: 



Chain Y:

Amino Acid	Percentage (%)
MET	0%
ASP	~36%
THR	~41%
VAL	~21%

Chain Z:

Chain 1: 58% 40%

Chain	Met	T1	G1	P6	S7	Q8	G9	K10	K11	K12	H16	R20	R21	C22	G23	E24	K25	H28	T29	K30	K31	K32	G38	F39	A43	K44	R45	E46	
Chain 1	Grey	Yellow	Yellow	Green	Green	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow	Green	Yellow	Yellow	Yellow	Green	Yellow	Yellow	Yellow	Yellow	Green	Yellow	Yellow	Yellow	Yellow	Green

Chain 2:

Category	Value
MET	2%
G1	48%
K5	44%
K9	8%
L11	0%
N18	0%
S19	0%
R20	0%
V21	0%
P22	0%
V25	0%
K28	0%
R31	0%
GLJ	0%
V4L	0%
GLN	0%
R35	0%
K38	0%
R39	0%
R40	0%
H41	0%
M42	0%
R43	0%
R44	0%
M45	0%
P46	0%
T47	0%
D48	0%
E49	0%

Chain 3: 63% 34%

Block	Color
P1	Green
Q2	Green
K3	Green
P4	Green
M15	Green
E16	Green
H17	Green
Q18	Green
V25	Green
G28	Green
R29	Green
Q30	Green
T31	Green
G32	Green
K33	Green
K34	Green
R38	Green
M48	Green
D49	Green
G50	Green
V55	Green
P56	Green
G57	Green
K60	Green
P61	Green
T62	Green
T65	Green
D66	Green
L67	Green
K68	Yellow
Y69	Yellow
R70	Yellow
E73	Yellow
C74	Yellow
A77	Yellow
H78	Yellow
L79	Yellow
R80	Yellow
M83	Yellow
F90	Yellow
Q91	Yellow
E92	Yellow

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	212.44Å 299.99Å 574.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.65 30.00 – 2.65	Depositor EDS
% Data completeness (in resolution range)	94.4 (30.00-2.65) 94.4 (30.00-2.65)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.65Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.176 , 0.214 0.174 , 0.212	Depositor DCC
R_{free} test set	4879 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	52.1	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	99086	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% 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: CL, OMG, K, UR3, CD, MG, OMU, ERY, NA, PSU, 1MA

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	0.37	0/65957	0.61	25/102867 (0.0%)
2	9	0.37	0/2904	0.61	3/4526 (0.1%)
3	A	0.41	0/1786	1.00	5/2408 (0.2%)
4	B	0.40	0/2690	0.98	6/3652 (0.2%)
5	C	0.45	0/1884	0.99	9/2551 (0.4%)
6	D	0.35	0/1111	0.92	7/1498 (0.5%)
7	E	0.38	0/1382	0.89	2/1880 (0.1%)
8	F	0.36	0/901	0.87	0/1224
9	G	0.34	0/241	0.73	0/324
10	H	0.43	0/1302	0.95	4/1743 (0.2%)
11	I	0.38	0/526	0.99	5/716 (0.7%)
12	J	0.42	0/1136	0.95	7/1530 (0.5%)
13	K	0.40	0/1001	1.01	1/1347 (0.1%)
14	L	0.36	0/1130	0.97	6/1509 (0.4%)
15	M	0.40	0/1582	0.92	4/2117 (0.2%)
16	N	0.37	0/1474	1.03	9/1999 (0.5%)
17	O	0.42	0/874	0.93	6/1181 (0.5%)
18	P	0.40	0/1147	0.85	1/1528 (0.1%)
19	Q	0.42	0/749	1.06	4/1005 (0.4%)
20	R	0.44	0/1172	0.95	8/1578 (0.5%)
21	S	0.37	0/648	0.88	3/875 (0.3%)
22	T	0.37	0/958	0.96	5/1289 (0.4%)
23	U	0.37	0/417	0.89	2/562 (0.4%)
24	V	0.37	0/502	0.97	3/675 (0.4%)
25	W	0.47	0/1219	1.00	4/1655 (0.2%)
26	X	0.43	0/664	0.94	1/895 (0.1%)
27	Y	0.44	0/1146	0.92	2/1536 (0.1%)
28	Z	0.38	0/589	0.93	0/787
29	1	0.42	0/438	0.92	1/578 (0.2%)
30	2	0.40	0/401	0.77	0/529
31	3	0.40	0/771	0.89	3/1024 (0.3%)
All	All	0.38	0/98702	0.72	136/147588 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	1	45
2	9	0	2
All	All	1	47

There are no bond length outliers.

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1563	G	C2'-C3'-O3'	13.57	129.85	109.50
16	N	135	VAL	N-CA-C	-10.09	103.32	113.10
1	0	1563	G	C4'-C3'-O3'	8.79	122.58	109.40
19	Q	17	LYS	N-CA-C	-8.70	98.78	109.83
6	D	136	ARG	CA-C-N	8.53	130.50	119.84
6	D	136	ARG	C-N-CA	8.53	130.50	119.84
3	A	222	GLY	N-CA-C	-8.18	104.06	114.37
1	0	1942	A	C5'-C4'-C3'	8.05	128.08	116.00
4	B	175	LEU	N-CA-C	-7.61	102.92	111.14
10	H	163	SER	N-CA-C	-7.57	99.32	110.52
4	B	157	LYS	N-CA-C	-7.48	104.76	114.04
2	9	39	U	N1-C1'-C2'	7.41	123.12	112.00
21	S	27	ALA	N-CA-C	-7.40	96.67	108.73
14	L	145	LEU	N-CA-C	-7.39	103.16	111.14
7	E	11	VAL	N-CA-C	7.29	120.39	109.17
24	V	42	ASN	CA-C-N	6.98	128.57	119.84
24	V	42	ASN	C-N-CA	6.98	128.57	119.84
6	D	100	ASP	N-CA-C	-6.95	104.80	113.28
16	N	14	ARG	N-CA-C	-6.94	103.65	111.07
16	N	169	PRO	N-CA-C	-6.91	105.53	114.03
27	Y	143	TRP	N-CA-C	6.87	120.27	109.96
15	M	70	GLY	N-CA-C	6.82	121.72	112.17
11	I	89	GLU	N-CA-C	-6.81	105.50	113.88
13	K	127	ALA	N-CA-C	-6.80	104.30	114.64
1	0	2291	A	N9-C1'-C2'	6.69	122.04	112.00
15	M	89	THR	N-CA-C	6.64	118.18	111.07
4	B	265	LEU	N-CA-C	6.64	120.31	110.48
20	R	141	VAL	N-CA-C	6.53	117.89	108.48
16	N	153	GLN	N-CA-C	-6.48	104.39	113.20
18	P	118	GLN	N-CA-C	-6.48	104.30	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	W	35	VAL	N-CA-C	6.45	114.92	107.89
20	R	137	ASN	N-CA-C	6.45	120.01	110.46
17	O	24	ALA	N-CA-C	-6.42	106.07	114.04
1	0	920	C	C2'-C3'-O3'	-6.41	104.08	113.70
4	B	222	LYS	N-CA-C	-6.37	100.55	110.42
22	T	54	ASP	N-CA-C	-6.35	105.50	113.18
1	0	1979	G	C4'-C3'-O3'	-6.35	103.48	113.00
12	J	68	GLY	N-CA-C	6.30	120.62	112.18
11	I	116	LEU	N-CA-C	-6.30	104.86	112.54
14	L	47	GLY	N-CA-C	6.27	118.50	111.85
1	0	834	G	C2'-C3'-O3'	-6.24	104.34	113.70
3	A	135	VAL	N-CA-C	6.23	116.83	108.11
25	W	143	THR	N-CA-C	-6.21	104.51	111.28
11	I	86	GLU	CA-C-N	6.21	126.17	120.03
11	I	86	GLU	C-N-CA	6.21	126.17	120.03
19	Q	49	ASN	N-CA-C	6.18	118.50	110.53
22	T	52	ARG	N-CA-C	6.10	123.80	110.80
1	0	1120	U	C5'-C4'-C3'	-6.10	106.84	116.00
6	D	170	TYR	N-CA-C	6.10	120.28	111.56
1	0	2526	C	N1-C1'-C2'	6.08	121.13	112.00
1	0	1819	G	C5'-C4'-C3'	6.06	125.08	116.00
3	A	133	ARG	N-CA-C	-6.05	105.89	113.28
1	0	1979	G	N9-C1'-C2'	6.02	121.03	112.00
5	C	78	ARG	N-CA-C	6.00	116.49	108.38
16	N	51	GLY	CA-C-N	6.00	126.43	119.47
16	N	51	GLY	C-N-CA	6.00	126.43	119.47
14	L	57	VAL	N-CA-C	-5.99	106.48	112.17
1	0	871	G	C5'-C4'-O4'	-5.99	100.82	109.80
16	N	48	VAL	N-CA-C	5.95	117.16	108.53
2	9	65	A	N9-C1'-C2'	5.94	120.91	112.00
21	S	57	THR	N-CA-C	5.92	118.54	110.55
1	0	2726	U	N1-C1'-C2'	5.89	120.84	112.00
2	9	39	U	C4'-C3'-O3'	-5.88	104.19	113.00
10	H	16	ALA	N-CA-C	-5.87	101.60	110.28
16	N	13	ARG	N-CA-C	-5.85	106.27	113.41
1	0	1592	G	N9-C1'-C2'	5.85	120.77	112.00
20	R	122	GLN	N-CA-C	-5.84	99.62	108.67
31	3	55	VAL	CA-C-N	5.84	127.14	119.84
31	3	55	VAL	C-N-CA	5.84	127.14	119.84
5	C	178	GLN	N-CA-C	5.79	120.09	113.19
25	W	68	THR	N-CA-C	5.77	117.65	111.36
5	C	179	GLY	N-CA-C	-5.73	105.84	112.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1504	A	N9-C1'-C2'	5.71	120.57	112.00
4	B	151	VAL	CA-C-N	5.71	125.83	119.32
4	B	151	VAL	C-N-CA	5.71	125.83	119.32
12	J	88	PRO	N-CA-C	-5.67	104.82	112.48
11	I	96	SER	N-CA-C	-5.67	103.44	110.41
29	1	43	ALA	N-CA-C	-5.66	104.73	111.69
23	U	50	GLU	N-CA-C	5.63	118.19	111.71
14	L	117	GLU	N-CA-C	-5.62	100.66	109.25
26	X	12	ILE	N-CA-C	5.60	113.41	107.76
10	H	115	GLY	N-CA-C	-5.60	99.91	113.18
5	C	175	LYS	N-CA-C	5.58	117.49	110.24
12	J	22	VAL	N-CA-C	-5.57	105.19	110.42
5	C	89	ALA	N-CA-C	5.54	117.78	111.02
12	J	112	ASP	N-CA-C	-5.53	100.67	109.96
15	M	74	LYS	N-CA-C	5.52	118.47	109.59
7	E	37	ASP	N-CA-C	5.52	119.59	112.86
17	O	2	LYS	N-CA-C	-5.52	102.32	110.48
15	M	125	ARG	N-CA-C	5.51	119.80	112.30
22	T	3	GLN	CA-C-N	5.50	124.97	119.24
22	T	3	GLN	C-N-CA	5.50	124.97	119.24
20	R	34	GLU	N-CA-C	5.50	117.35	111.36
3	A	48	ASP	CA-C-N	5.48	125.31	119.28
3	A	48	ASP	C-N-CA	5.48	125.31	119.28
1	0	2316	G	C5'-C4'-C3'	-5.47	106.99	115.20
10	H	121	GLY	N-CA-C	5.43	118.31	112.33
17	O	82	SER	N-CA-C	-5.42	103.37	110.53
1	0	921	G	N9-C1'-C2'	5.41	120.12	112.00
6	D	137	PRO	N-CA-C	5.41	123.62	112.47
12	J	36	VAL	N-CA-C	5.41	116.52	108.46
23	U	18	GLY	N-CA-C	5.40	121.25	112.61
20	R	18	LEU	N-CA-C	-5.37	101.13	109.72
14	L	43	HIS	N-CA-C	-5.35	101.17	109.72
20	R	3	SER	N-CA-C	-5.34	101.17	109.24
31	3	67	LEU	N-CA-C	5.34	118.28	109.85
19	Q	68	GLY	N-CA-C	-5.32	102.32	111.47
1	0	129	A	C2'-C3'-O3'	5.32	121.67	113.70
27	Y	183	GLU	N-CA-C	-5.30	101.06	109.76
5	C	167	ASP	N-CA-C	-5.30	105.67	111.82
1	0	206	G	C5'-C4'-C3'	-5.30	108.06	116.00
5	C	20	ASP	N-CA-C	5.28	117.72	111.33
22	T	78	THR	N-CA-C	5.27	117.42	109.41
12	J	71	TYR	CA-C-N	5.27	125.19	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	J	71	TYR	C-N-CA	5.27	125.19	119.76
1	0	2313	C	C5'-C4'-C3'	5.25	123.88	116.00
21	S	59	ASP	N-CA-C	-5.24	106.91	113.72
19	Q	13	LYS	N-CA-C	5.19	118.39	111.75
1	0	1878	G	O4'-C1'-C2'	-5.17	102.43	107.60
1	0	2301	A	N9-C1'-C2'	5.16	119.74	112.00
14	L	20	ASN	N-CA-C	5.16	120.56	110.56
20	R	13	THR	N-CA-C	5.15	117.56	108.75
5	C	192	ILE	N-CA-C	5.13	116.19	109.21
17	O	66	GLY	N-CA-C	5.11	125.29	113.18
17	O	50	ARG	N-CA-C	5.11	116.93	111.36
5	C	186	TYR	N-CA-C	5.10	118.01	110.46
24	V	64	GLY	N-CA-C	-5.10	107.77	115.32
17	O	69	VAL	N-CA-C	5.10	115.82	108.48
1	0	1261	A	N9-C1'-C2'	5.09	119.64	112.00
16	N	42	HIS	N-CA-C	5.09	116.72	109.14
25	W	25	ASN	N-CA-C	5.08	119.06	112.86
6	D	15	GLU	CA-C-N	5.06	126.16	119.84
6	D	15	GLU	C-N-CA	5.06	126.16	119.84
20	R	123	GLN	N-CA-C	5.05	117.75	110.28
1	0	874	A	C4'-C3'-O3'	-5.04	105.44	113.00
1	0	1942	A	C4'-C3'-C2'	-5.04	97.56	102.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1563	G	C3'

All (47) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1039	G	Sidechain
1	0	1078	A	Sidechain
1	0	1340	G	Sidechain
1	0	1342	C	Sidechain
1	0	1351	G	Sidechain
1	0	1377	C	Sidechain
1	0	1417	G	Sidechain
1	0	1653	A	Sidechain
1	0	1681	G	Sidechain
1	0	1682	A	Sidechain
1	0	1829	A	Sidechain

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Mol	Chain	Res	Type	Group
1	0	1835	U	Sidechain
1	0	1845	A	Sidechain
1	0	1848	G	Sidechain
1	0	1861	C	Sidechain
1	0	1863	G	Sidechain
1	0	1867	G	Sidechain
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	1970	G	Sidechain
1	0	1972	U	Sidechain
1	0	221	G	Sidechain
1	0	2315	C	Sidechain
1	0	2316	G	Sidechain
1	0	2412	G	Sidechain
1	0	2465	A	Sidechain
1	0	2493	C	Sidechain
1	0	2503	A	Sidechain
1	0	2506	A	Sidechain
1	0	2526	C	Sidechain
1	0	2552	C	Sidechain
1	0	2564	G	Sidechain
1	0	26	U	Sidechain
1	0	2607	U	Sidechain
1	0	2630	G	Sidechain
1	0	2643	G	Sidechain
1	0	270	U	Sidechain
1	0	2842	G	Sidechain
1	0	396	U	Sidechain
1	0	470	U	Sidechain
1	0	471	G	Sidechain
1	0	482	G	Sidechain
1	0	518	G	Sidechain
1	0	817	G	Sidechain
1	0	818	A	Sidechain
2	9	39	U	Sidechain
2	9	65	A	Sidechain

5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59020	0	29810	812	0
2	9	2599	0	1325	63	0
3	A	1753	0	1766	116	0
4	B	2625	0	2533	178	0
5	C	1859	0	1816	124	0
6	D	1094	0	1085	91	0
7	E	1357	0	1266	79	0
8	F	890	0	843	61	0
9	G	240	0	231	19	0
10	H	1282	0	1292	72	0
11	I	519	0	500	61	0
12	J	1120	0	1098	58	0
13	K	992	0	1031	54	0
14	L	1118	0	1076	65	0
15	M	1558	0	1566	58	0
16	N	1445	0	1401	114	0
17	O	865	0	873	29	0
18	P	1136	0	1123	42	0
19	Q	735	0	729	22	0
20	R	1149	0	1122	52	0
21	S	641	0	605	28	0
22	T	950	0	923	47	0
23	U	410	0	364	31	0
24	V	499	0	511	36	0
25	W	1196	0	1137	102	0
26	X	654	0	653	48	0
27	Y	1130	0	1133	65	0
28	Z	578	0	539	28	0
29	1	431	0	426	33	0
30	2	396	0	413	32	0
31	3	755	0	728	30	0
32	0	51	0	67	0	0
33	0	108	0	0	0	0
33	2	1	0	0	0	0
33	3	1	0	0	0	0
33	9	1	0	0	0	0
33	A	1	0	0	0	0
33	B	1	0	0	0	0
33	K	1	0	0	0	0
33	T	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	0	71	0	0	0	0
35	9	2	0	0	0	0
35	A	1	0	0	0	0
35	C	1	0	0	0	0
35	H	2	0	0	0	0
35	J	1	0	0	0	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	3	0	0	0	0
35	S	1	0	0	0	0
35	T	1	0	0	0	0
36	0	10	0	0	0	0
36	3	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	J	3	0	0	1	0
36	L	1	0	0	0	0
36	M	1	0	0	0	0
36	N	1	0	0	1	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
36	Y	1	0	0	0	0
37	1	1	0	0	0	0
37	3	1	0	0	0	0
37	O	1	0	0	0	0
37	U	1	0	0	0	0
37	Z	1	0	0	0	0
38	0	5869	0	0	163	0
38	1	54	0	0	3	0
38	2	45	0	0	6	0
38	3	78	0	0	10	0
38	9	138	0	0	9	0
38	A	121	0	0	16	0
38	B	151	0	0	20	0
38	C	168	0	0	27	0
38	D	50	0	0	17	0
38	E	42	0	0	11	0
38	F	28	0	0	8	0
38	G	19	0	0	1	0
38	H	71	0	0	17	0
38	I	9	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	J	55	0	0	4	0
38	K	61	0	0	11	0
38	L	81	0	0	23	0
38	M	124	0	0	11	0
38	N	67	0	0	13	0
38	O	43	0	0	6	0
38	P	66	0	0	2	0
38	Q	49	0	0	6	0
38	R	80	0	0	6	0
38	S	37	0	0	5	0
38	T	37	0	0	7	0
38	U	27	0	0	4	0
38	V	14	0	0	3	0
38	W	73	0	0	12	0
38	X	27	0	0	9	0
38	Y	94	0	0	14	0
38	Z	30	0	0	1	0
All	All	99086	0	59985	2416	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 16.

All (2416) 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)
10:H:172:GLU:HB2	38:H:8591:HOH:O	1.34	1.21
1:O:1160:G:H5'	1:O:1161:A:H5'	1.24	1.17
5:C:236:THR:HG22	5:C:239:ALA:H	1.04	1.16
10:H:174:LEU:HA	38:H:8571:HOH:O	1.50	1.11
2:9:6:C:H5''	16:N:37:ARG:NH1	1.66	1.10
6:D:154:LYS:H	6:D:154:LYS:HD2	1.21	1.03
1:O:1242:A:H5'	12:J:82:THR:HG23	1.35	1.03
6:D:25:MET:HE2	6:D:41:LEU:HG	1.41	1.03
1:O:156:C:H5''	15:M:171:ARG:HD3	1.38	1.02
26:X:37:LEU:HD13	26:X:85:VAL:HG21	1.40	1.01
13:K:10:GLN:NE2	13:K:10:GLN:H	1.59	0.99
5:C:78:ARG:HH11	5:C:78:ARG:HG3	1.23	0.99
22:T:71:VAL:HG11	22:T:90:PRO:HB3	1.44	0.99
28:Z:46:ARG:HD2	28:Z:59:TYR:HB2	1.43	0.99
1:O:2717:C:H2'	1:O:2718:C:H5''	1.46	0.98
3:A:211:LYS:HB3	3:A:212:PRO:HD2	1.46	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:871:G:C8	1:0:871:G:H5'	1.98	0.97
2:9:56:A:H2'	2:9:57:A:H5''	1.44	0.97
1:0:1559:A:H1'	38:0:5823:HOH:O	1.64	0.96
1:0:871:G:H5'	1:0:871:G:H8	1.29	0.96
10:H:59:GLN:HE21	10:H:129:ARG:HE	1.10	0.96
6:D:134:LEU:HD11	6:D:166:ILE:HD11	1.47	0.95
5:C:127:ARG:NH2	5:C:225:PRO:HG2	1.81	0.95
12:J:76:ASP:HA	38:J:5907:HOH:O	1.67	0.95
25:W:149:LEU:HG	25:W:153:MET:HE2	1.46	0.94
2:9:6:C:H5''	16:N:37:ARG:HH12	1.24	0.94
2:9:76:G:H3'	2:9:77:A:H5''	1.47	0.94
18:P:115:SER:H	18:P:118:GLN:HE21	0.96	0.93
3:A:191:GLY:HA2	3:A:194:MET:HE2	1.47	0.93
15:M:164:THR:HG22	15:M:167:GLY:H	1.33	0.93
16:N:83:LEU:HD13	16:N:175:LEU:HD23	1.51	0.93
16:N:144:GLY:O	16:N:147:ILE:HG22	1.67	0.93
3:A:35:GLY:O	3:A:36:ASP:HB3	1.68	0.93
13:K:10:GLN:HE21	13:K:10:GLN:N	1.65	0.92
1:0:870:G:H2'	1:0:871:G:H5''	1.48	0.92
30:2:41:HIS:H	30:2:45:ASN:HD22	1.13	0.92
1:0:1751:G:H2'	1:0:1752:G:H5''	1.50	0.92
13:K:39:GLY:HA2	38:K:4183:HOH:O	1.70	0.92
4:B:264:GLU:HG2	4:B:267:LYS:HE2	1.50	0.91
1:0:2717:C:C2'	1:0:2718:C:H5''	2.00	0.91
1:0:381:G:H5''	38:0:4294:HOH:O	1.70	0.91
1:0:545:G:H5'	1:0:545:G:H8	1.36	0.90
5:C:236:THR:HG22	5:C:239:ALA:N	1.84	0.90
13:K:74:VAL:HG11	13:K:113:ILE:HG12	1.53	0.90
4:B:212:GLN:HB2	4:B:257:THR:HG21	1.52	0.90
10:H:170:ARG:HD2	38:H:8540:HOH:O	1.72	0.90
15:M:102:GLU:OE1	15:M:164:THR:HG21	1.71	0.90
1:0:21:G:H5'	20:R:2:ILE:HA	1.54	0.90
24:V:12:THR:HG22	24:V:15:GLU:HG3	1.50	0.90
20:R:99:ALA:HB1	20:R:109:MET:HE1	1.52	0.89
1:0:1474:C:H6	1:0:1474:C:H5'	1.37	0.89
25:W:88:THR:HB	38:W:6679:HOH:O	1.73	0.89
1:0:2506:A:HO2'	1:0:2507:G:H8	0.89	0.88
4:B:238:ASN:HD22	4:B:240:GLY:H	1.22	0.88
13:K:29:LEU:HB3	13:K:55:VAL:HG11	1.56	0.88
25:W:5:VAL:HG11	25:W:153:MET:HE1	1.54	0.88
1:0:541:C:H2'	1:0:542:A:H5''	1.55	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:97:VAL:HG12	38:E:4191:HOH:O	1.75	0.87
8:F:58:GLU:HA	8:F:61:MET:HE2	1.54	0.87
1:0:1835:U:H5	1:0:1840:A:N7	1.72	0.87
25:W:137:GLN:HE21	25:W:141:HIS:HE1	1.20	0.86
28:Z:10:ARG:HA	38:Z:8714:HOH:O	1.75	0.86
1:0:1160:G:C5'	1:0:1161:A:H5'	2.06	0.86
6:D:28:GLY:HA2	6:D:69:ILE:HG23	1.56	0.86
1:0:962:C:H1'	16:N:5:ARG:NH1	1.90	0.86
1:0:542:A:H5'	1:0:542:A:H8	1.40	0.86
7:E:100:ASP:HB2	38:E:2789:HOH:O	1.74	0.86
11:I:127:CYS:HB3	11:I:132:VAL:HB	1.56	0.85
1:0:1116:U:HO2'	1:0:1118:A:H2	0.89	0.85
1:0:2812:A:H2	1:0:2814:A:H62	1.25	0.85
4:B:320:GLN:HE21	4:B:321:PRO:HD2	1.41	0.85
27:Y:187:VAL:HG23	27:Y:192:ASP:HB2	1.58	0.85
1:0:2890:A:H1'	23:U:56:ARG:NH2	1.92	0.85
1:0:2716:G:H5''	4:B:206:THR:HG21	1.59	0.84
5:C:236:THR:H	5:C:239:ALA:HB3	1.43	0.84
1:0:1667:A:H8	1:0:1667:A:H5'	1.39	0.84
4:B:190:MET:HE2	4:B:194:PHE:CD1	2.13	0.84
25:W:13:MET:HE2	25:W:18:GLN:HA	1.59	0.84
17:O:42:GLU:HB2	38:O:2176:HOH:O	1.76	0.84
20:R:17:MET:HE1	20:R:19:ARG:NH2	1.93	0.84
1:0:214:U:H5'	38:0:6098:HOH:O	1.78	0.83
4:B:86:ALA:HA	38:B:8879:HOH:O	1.78	0.83
25:W:72:PRO:HG2	25:W:77:ALA:HB3	1.60	0.83
13:K:98:VAL:CG1	13:K:102:GLU:HA	2.09	0.83
18:P:115:SER:OG	18:P:118:GLN:HG3	1.77	0.83
1:0:282:C:H1'	1:0:368:C:N4	1.92	0.83
5:C:5:ILE:HD11	5:C:16:VAL:HG23	1.58	0.83
1:0:1184:C:H1'	38:0:7413:HOH:O	1.77	0.83
2:9:73:A:H61	2:9:108:C:H42	1.23	0.83
11:I:97:VAL:HG12	11:I:101:LYS:HE3	1.60	0.83
4:B:321:PRO:HA	38:B:8961:HOH:O	1.79	0.82
1:0:1160:G:H5'	1:0:1161:A:C5'	2.07	0.82
22:T:9:LYS:HE3	22:T:13:ARG:NH1	1.93	0.82
3:A:191:GLY:HA2	3:A:194:MET:CE	2.10	0.81
4:B:62:ARG:HA	4:B:65:MET:HE3	1.61	0.81
8:F:91:VAL:HG12	8:F:92:GLY:H	1.45	0.81
1:0:2586:U:H3	1:0:2592:G:H22	1.26	0.81
14:L:133:VAL:HA	38:L:8871:HOH:O	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:21:G:C5'	20:R:2:ILE:HA	2.10	0.81
20:R:8:ALA:HB1	20:R:13:THR:HG21	1.61	0.81
4:B:162:MET:HE1	4:B:308:LEU:HD21	1.61	0.81
10:H:59:GLN:NE2	10:H:129:ARG:HE	1.79	0.81
24:V:1:THR:HG23	24:V:2:VAL:H	1.46	0.81
1:0:1116:U:O2'	1:0:1118:A:H2	1.64	0.80
1:0:1119:G:H2'	12:J:52:GLN:NE2	1.95	0.80
1:0:1162:G:H1'	11:I:112:LEU:HD11	1.62	0.80
25:W:21:LEU:HD22	25:W:26:ILE:CD1	2.12	0.80
1:0:962:C:H1'	16:N:5:ARG:HH12	1.43	0.80
23:U:20:MET:HE2	23:U:30:HIS:NE2	1.97	0.80
25:W:6:GLN:HB2	25:W:26:ILE:HD12	1.64	0.80
5:C:132:ASP:HB3	38:C:8564:HOH:O	1.82	0.80
25:W:68:THR:HG23	25:W:69:ARG:HG2	1.63	0.80
6:D:57:THR:HG23	6:D:63:ILE:HA	1.62	0.80
10:H:49:GLN:HE21	10:H:140:TYR:HE2	1.26	0.80
25:W:21:LEU:HD22	25:W:26:ILE:HD11	1.64	0.80
2:9:14:G:H5'	2:9:14:G:H8	1.47	0.79
7:E:84:MET:HE1	7:E:148:ILE:HD12	1.64	0.79
1:0:1684:A:H1'	30:2:43:ARG:HH22	1.45	0.79
26:X:72:VAL:HG22	26:X:85:VAL:HG12	1.63	0.79
4:B:179:LEU:O	4:B:183:GLU:HG2	1.83	0.79
18:P:115:SER:N	18:P:118:GLN:HE21	1.79	0.79
13:K:10:GLN:H	13:K:10:GLN:HE21	0.85	0.79
1:0:2291:A:C8	1:0:2309:C:H5'	2.18	0.78
12:J:74:ARG:HB3	12:J:74:ARG:HH11	1.48	0.78
1:0:2270:G:H4'	3:A:223:ARG:HH12	1.48	0.78
3:A:36:ASP:OD2	3:A:85:SER:HB2	1.82	0.78
1:0:871:G:H8	1:0:871:G:C5'	1.97	0.78
1:0:2756:U:H3	1:0:2896:A:H2	1.30	0.78
4:B:201:ASP:HB2	4:B:312:ARG:HD2	1.64	0.78
20:R:99:ALA:HB1	20:R:109:MET:CE	2.14	0.78
26:X:76:ARG:HH11	26:X:76:ARG:HG3	1.49	0.78
1:0:541:C:C2'	1:0:542:A:H5''	2.14	0.77
4:B:140:LEU:HD23	38:B:8879:HOH:O	1.82	0.77
1:0:960:G:H4'	38:0:7379:HOH:O	1.83	0.77
13:K:14:LYS:HB2	13:K:45:PRO:HG2	1.66	0.77
1:0:1701:A:H4'	1:0:1702:U:H5''	1.64	0.77
5:C:242:GLU:HG3	38:C:8583:HOH:O	1.83	0.77
10:H:30:LYS:H	10:H:62:HIS:HD2	1.31	0.77
25:W:21:LEU:HD21	25:W:48:VAL:HG11	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:162:MET:HE2	4:B:310:ARG:HD3	1.66	0.77
1:0:2506:A:O2'	1:0:2507:G:H8	1.64	0.77
1:0:182:G:H5'	38:0:5115:HOH:O	1.83	0.77
1:0:236:A:H4'	1:0:237:G:H5'	1.67	0.77
38:0:6824:HOH:O	15:M:178:LYS:HB2	1.84	0.77
7:E:84:MET:HE2	7:E:133:VAL:CG2	2.15	0.76
14:L:148:GLU:HA	38:L:8870:HOH:O	1.85	0.76
38:9:8673:HOH:O	16:N:23:ARG:HD3	1.83	0.76
1:0:1450:C:H4'	1:0:1451:C:OP2	1.86	0.76
27:Y:174:VAL:HG13	27:Y:177:LYS:HD2	1.65	0.76
13:K:62:PRO:HG3	13:K:65:ARG:HH21	1.50	0.76
12:J:93:ARG:HB3	12:J:93:ARG:HH11	1.48	0.76
1:0:870:G:C2'	1:0:871:G:H5''	2.15	0.76
1:0:1116:U:H3	1:0:1246:A:H62	1.33	0.76
1:0:1118:A:H8	1:0:1118:A:H3'	1.51	0.76
25:W:13:MET:HE2	25:W:18:GLN:CA	2.16	0.76
1:0:200:C:H2'	38:0:3429:HOH:O	1.85	0.75
8:F:96:ALA:HA	38:F:3111:HOH:O	1.84	0.75
1:0:877:G:H5'	1:0:878:G:OP1	1.87	0.75
1:0:1183:C:H2'	38:0:6204:HOH:O	1.86	0.75
26:X:30:MET:HE1	26:X:58:ALA:HB3	1.66	0.75
30:2:39:ARG:HG2	38:2:3143:HOH:O	1.85	0.75
12:J:45:VAL:HG23	12:J:130:VAL:O	1.85	0.75
16:N:113:SER:HB2	38:N:8860:HOH:O	1.85	0.75
1:0:272:A:H3'	38:0:7476:HOH:O	1.87	0.75
1:0:2908:A:H2'	1:0:2909:G:O4'	1.87	0.75
1:0:2637:A:H5'	38:0:9265:HOH:O	1.85	0.75
8:F:63:ILE:HB	8:F:64:PRO:HD3	1.69	0.75
18:P:59:ARG:NH2	18:P:66:GLN:HE22	1.83	0.75
2:9:56:A:C2'	2:9:57:A:H5''	2.16	0.75
25:W:65:VAL:HA	25:W:68:THR:HG22	1.69	0.75
25:W:4:LEU:HD23	25:W:54:PHE:HB3	1.69	0.75
8:F:91:VAL:HG12	8:F:92:GLY:N	2.01	0.74
25:W:13:MET:HE3	25:W:17:ILE:HG22	1.68	0.74
1:0:1234:U:N3	4:B:244:PRO:HB3	2.02	0.74
1:0:1603:A:H5'	1:0:1605:G:O4'	1.87	0.74
1:0:2426:G:H1'	38:0:6048:HOH:O	1.86	0.74
38:0:5416:HOH:O	9:G:12:ILE:HA	1.88	0.74
6:D:146:LYS:NZ	16:N:107:ASN:HD21	1.84	0.74
13:K:74:VAL:CG1	13:K:113:ILE:HG12	2.15	0.74
1:0:544:G:H2'	1:0:545:G:H5''	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:O:7172:HOH:O	3:A:11:ARG:HA	1.88	0.74
1:O:506:G:H22	1:O:509:A:C5'	2.00	0.74
1:O:2533:C:H5'	1:O:2533:C:H6	1.51	0.74
16:N:48:VAL:CG1	16:N:55:ASP:HB3	2.18	0.74
20:R:39:THR:HG22	20:R:42:GLU:H	1.52	0.74
5:C:78:ARG:HG3	5:C:78:ARG:NH1	2.00	0.74
5:C:236:THR:HA	38:C:8650:HOH:O	1.87	0.74
25:W:137:GLN:HE21	25:W:141:HIS:CE1	2.05	0.74
1:O:657:G:OP1	5:C:27:ARG:NH2	2.20	0.74
5:C:1:MET:HG2	5:C:2:GLN:H	1.52	0.74
1:O:1118:A:H3'	1:O:1118:A:C8	2.22	0.74
1:O:2508:C:H2'	38:O:6705:HOH:O	1.88	0.73
16:N:7:LYS:HE3	19:Q:21:ARG:O	1.87	0.73
3:A:88:ILE:HD13	3:A:100:PRO:HD3	1.70	0.73
11:I:94:ASP:OD1	11:I:133:THR:HB	1.88	0.73
16:N:164:ASP:CG	16:N:167:ASP:HA	2.13	0.73
1:O:396:U:H1'	38:O:7576:HOH:O	1.87	0.73
1:O:1474:C:H5'	1:O:1474:C:C6	2.23	0.73
27:Y:187:VAL:HG23	27:Y:192:ASP:CB	2.19	0.73
3:A:105:VAL:HG11	3:A:154:ALA:HB1	1.70	0.73
20:R:39:THR:HG23	20:R:107:GLU:O	1.89	0.73
1:O:450:C:OP1	5:C:184:ARG:NH2	2.21	0.73
1:O:1206:U:H5'	1:O:1206:U:H6	1.54	0.73
8:F:2:VAL:HG22	8:F:57:GLU:OE1	1.89	0.73
25:W:88:THR:HG22	25:W:89:ASP:H	1.52	0.73
1:O:2768:A:H2'	1:O:2769:C:O4'	1.87	0.73
6:D:54:ALA:HB2	6:D:69:ILE:HD12	1.70	0.73
24:V:12:THR:HG22	24:V:15:GLU:CG	2.18	0.73
14:L:77:ALA:HB3	38:L:8830:HOH:O	1.89	0.72
24:V:42:ASN:HB3	38:V:7247:HOH:O	1.87	0.72
1:O:2768:A:H5''	38:O:4399:HOH:O	1.89	0.72
1:O:559:U:H6	1:O:559:U:H5'	1.54	0.72
25:W:88:THR:HG23	25:W:110:GLN:HE21	1.54	0.72
2:9:6:C:C5'	16:N:37:ARG:NH1	2.51	0.72
23:U:9:CYS:HA	23:U:52:THR:HG23	1.71	0.72
28:Z:11:SER:HB3	28:Z:23:ARG:HB2	1.70	0.72
1:O:1165:G:H4'	1:O:1174:A:O2'	1.89	0.71
10:H:12:ILE:HD12	10:H:57:THR:HG22	1.70	0.71
1:O:2694:A:H4'	7:E:91:PHE:HE1	1.55	0.71
15:M:58:GLN:HG3	38:M:8907:HOH:O	1.88	0.71
1:O:545:G:H5'	1:O:545:G:C8	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:711:G:H1'	38:0:7045:HOH:O	1.88	0.71
2:9:75:G:H1	2:9:106:U:H3	1.38	0.71
1:0:1666:C:O2'	1:0:1667:A:H5''	1.91	0.71
1:0:281:U:H2'	1:0:282:C:O4'	1.91	0.71
10:H:102:LYS:HD3	10:H:122:LYS:HD3	1.71	0.71
20:R:14:ALA:HB3	20:R:147:LEU:HB2	1.72	0.71
1:0:2054:A:N3	20:R:128:ARG:NH2	2.39	0.70
4:B:36:PRO:HA	4:B:168:GLY:HA3	1.72	0.70
18:P:64:GLU:HG2	38:P:170:HOH:O	1.90	0.70
29:1:8:GLN:HE22	29:1:11:LYS:NZ	1.89	0.70
1:0:1119:G:H2'	12:J:52:GLN:HE22	1.52	0.70
1:0:2364:A:H5''	19:Q:15:LYS:HD3	1.71	0.70
1:0:1819:G:H2'	1:0:1820:G:H4'	1.73	0.70
4:B:18:ARG:HG3	4:B:256:GLN:HG3	1.71	0.70
8:F:50:VAL:HG13	8:F:60:VAL:HG11	1.74	0.70
1:0:2783:A:H3'	38:0:5190:HOH:O	1.91	0.70
1:0:1641:A:H2'	1:0:1642:A:H5'	1.72	0.70
5:C:139:VAL:HG13	38:C:8647:HOH:O	1.91	0.70
1:0:2851:G:O2'	1:0:2852:A:H5'	1.90	0.70
16:N:132:ASN:O	16:N:135:VAL:HG12	1.91	0.70
2:9:69:U:OP1	16:N:4:PRO:HG3	1.92	0.70
3:A:179:MET:HA	3:A:179:MET:HE3	1.74	0.70
5:C:2:GLN:HB3	38:C:8536:HOH:O	1.91	0.70
5:C:236:THR:HG21	38:C:8575:HOH:O	1.92	0.70
7:E:84:MET:HE1	7:E:148:ILE:CD1	2.22	0.70
1:0:645:U:OP2	14:L:4:LYS:HE2	1.91	0.70
1:0:1701:A:H5'	38:0:6242:HOH:O	1.90	0.70
5:C:236:THR:CG2	5:C:239:ALA:H	1.95	0.70
10:H:12:ILE:O	10:H:12:ILE:HG22	1.90	0.70
13:K:98:VAL:HG13	13:K:102:GLU:HA	1.72	0.70
27:Y:141:THR:HG23	38:Y:8887:HOH:O	1.91	0.69
1:0:56:G:H5''	24:V:50:ARG:NH1	2.07	0.69
16:N:80:SER:HB2	38:N:8837:HOH:O	1.92	0.69
18:P:13:VAL:HG21	18:P:41:ARG:HG2	1.73	0.69
1:0:56:G:H5''	24:V:50:ARG:HH12	1.57	0.69
1:0:1328:A:OP1	27:Y:169:ARG:HD2	1.92	0.69
25:W:21:LEU:HD21	25:W:48:VAL:CG1	2.23	0.69
1:0:1189:A:H1'	1:0:1209:C:C1'	2.22	0.69
1:0:1666:C:H2'	1:0:1667:A:H5'	1.74	0.69
1:0:2533:C:H5'	1:0:2533:C:C6	2.26	0.69
11:I:73:LEU:HD12	11:I:107:LYS:HZ2	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2629:C:N4	3:A:206:ARG:HH21	1.91	0.69
2:9:114:G:O6	16:N:11:ARG:HD3	1.91	0.69
14:L:143:THR:HG22	14:L:144:ASP:N	2.07	0.69
12:J:74:ARG:HH11	12:J:74:ARG:CB	2.06	0.69
7:E:20:ILE:HD11	7:E:40:VAL:HG11	1.75	0.69
7:E:166:VAL:HG12	38:E:3134:HOH:O	1.92	0.69
10:H:32:ALA:HB3	10:H:69:ARG:HH12	1.56	0.68
11:I:120:ALA:O	11:I:124:VAL:HG23	1.92	0.68
14:L:79:ASP:HB3	38:L:8857:HOH:O	1.91	0.68
10:H:6:ALA:HA	10:H:61:ARG:NH1	2.09	0.68
11:I:73:LEU:HD12	11:I:107:LYS:NZ	2.09	0.68
12:J:19:MET:CE	12:J:132:LEU:HD11	2.24	0.68
1:0:447:A:OP2	22:T:1:SER:HB2	1.93	0.68
1:0:1119:G:N2	1:0:1246:A:C2	2.62	0.68
1:0:1751:G:C2'	1:0:1752:G:H5''	2.23	0.68
1:0:2755:G:H1'	38:0:4650:HOH:O	1.94	0.68
2:9:39:U:H1'	2:9:44:A:H61	1.57	0.68
27:Y:144:ARG:CZ	38:Y:8910:HOH:O	2.41	0.68
26:X:78:GLU:HG2	26:X:79:GLU:H	1.58	0.68
1:0:2548:C:OP2	4:B:5:ARG:NH2	2.26	0.68
20:R:106:GLY:HA2	20:R:109:MET:HE3	1.75	0.68
16:N:164:ASP:OD1	16:N:167:ASP:HA	1.94	0.68
25:W:22:GLU:HG2	25:W:27:HIS:CD2	2.28	0.68
25:W:81:ASP:OD1	25:W:92:ASP:HB2	1.93	0.68
16:N:47:LEU:HD11	16:N:127:LEU:HD21	1.76	0.68
8:F:53:ASP:OD1	8:F:80:GLN:HB2	1.94	0.68
14:L:143:THR:HG21	38:L:8838:HOH:O	1.92	0.68
31:3:25:VAL:HG22	31:3:68:LYS:HG3	1.75	0.68
1:0:541:C:H2'	1:0:542:A:C5'	2.23	0.67
1:0:2004:U:H4'	38:0:5268:HOH:O	1.93	0.67
1:0:1372:A:H3'	38:0:7141:HOH:O	1.94	0.67
4:B:55:ASN:HB3	4:B:63:GLU:HA	1.76	0.67
4:B:162:MET:CE	4:B:308:LEU:HD21	2.24	0.67
25:W:88:THR:HG23	25:W:110:GLN:HB3	1.76	0.67
4:B:320:GLN:NE2	4:B:321:PRO:HD2	2.10	0.67
1:0:544:G:C2'	1:0:545:G:H5''	2.24	0.67
3:A:94:LEU:HG	3:A:99:ILE:HD11	1.76	0.67
7:E:81:GLU:HG2	7:E:134:SER:HB3	1.76	0.67
10:H:114:ASP:HB2	38:H:8547:HOH:O	1.94	0.67
10:H:165:ARG:HD3	38:H:8583:HOH:O	1.94	0.67
1:0:1130:U:H5'	38:0:7620:HOH:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:506:G:H22	1:0:509:A:H5'	1.58	0.67
3:A:105:VAL:CG1	3:A:154:ALA:HB1	2.25	0.67
3:A:200:PRO:HG2	3:A:225:VAL:HG21	1.77	0.67
5:C:140:VAL:HB	38:C:8650:HOH:O	1.94	0.67
15:M:164:THR:HG22	15:M:167:GLY:N	2.07	0.67
17:O:32:ARG:O	17:O:32:ARG:HD3	1.94	0.67
3:A:192:VAL:CG1	3:A:207:GLN:HB3	2.25	0.67
3:A:223:ARG:HG3	38:A:8900:HOH:O	1.94	0.67
11:I:87:PRO:C	11:I:89:GLU:H	2.02	0.67
14:L:121:ILE:HG12	14:L:141:GLU:HB2	1.77	0.67
1:0:1667:A:H5'	1:0:1667:A:C8	2.28	0.67
15:M:24:GLN:NE2	15:M:27:ARG:HH11	1.92	0.67
24:V:39:ALA:N	24:V:40:PRO:HD2	2.09	0.67
30:2:41:HIS:HD2	30:2:44:ARG:H	1.41	0.67
11:I:88:GLN:HA	11:I:91:PHE:CE2	2.30	0.66
15:M:60:VAL:C	15:M:61:ILE:HD12	2.20	0.66
20:R:39:THR:HB	20:R:42:GLU:HG3	1.76	0.66
2:9:35:C:H5''	38:9:8653:HOH:O	1.96	0.66
24:V:4:HIS:HB3	38:V:6622:HOH:O	1.94	0.66
1:0:2840:A:OP1	4:B:211:THR:HG23	1.95	0.66
31:3:60:LYS:HG3	31:3:61:PRO:HD2	1.77	0.66
12:J:99:GLU:HA	38:J:7377:HOH:O	1.95	0.66
2:9:14:G:H5'	2:9:14:G:C8	2.29	0.66
13:K:81:ARG:HB2	13:K:87:ARG:NH1	2.11	0.66
15:M:169:ARG:HD2	38:M:8892:HOH:O	1.94	0.66
7:E:11:VAL:HG12	7:E:12:ASP:N	2.10	0.66
8:F:58:GLU:CD	15:M:27:ARG:HH22	2.02	0.66
1:0:1244:U:OP1	12:J:18:ILE:HD13	1.96	0.66
38:0:3826:HOH:O	10:H:14:LYS:HE2	1.96	0.66
3:A:100:PRO:HG2	3:A:103:VAL:HG21	1.78	0.66
7:E:6:GLU:HA	7:E:46:THR:HG22	1.76	0.66
7:E:31:ARG:HH12	7:E:68:HIS:CG	2.14	0.66
13:K:62:PRO:HG3	13:K:65:ARG:NH2	2.09	0.66
1:0:1189:A:H1'	1:0:1209:C:H1'	1.78	0.66
1:0:1835:U:C5	1:0:1840:A:N7	2.60	0.66
4:B:140:LEU:HA	38:B:8879:HOH:O	1.96	0.65
9:G:64:ASN:HD22	9:G:64:ASN:N	1.93	0.65
17:O:21:SER:OG	17:O:106:PRO:HB2	1.96	0.65
22:T:71:VAL:HG11	22:T:90:PRO:CB	2.24	0.65
25:W:84:VAL:HG12	38:W:6679:HOH:O	1.96	0.65
6:D:136:ARG:HD2	6:D:155:HIS:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:97:VAL:CG1	11:I:101:LYS:HE3	2.27	0.65
1:0:272:A:H5'	1:0:273:G:OP2	1.96	0.65
15:M:31:TRP:HA	15:M:34:GLU:HG3	1.79	0.65
16:N:169:PRO:O	16:N:172:PHE:HB3	1.96	0.65
4:B:41:PHE:CD1	4:B:79:MET:HE2	2.31	0.65
1:0:338:C:H4'	5:C:174:ILE:CD1	2.27	0.65
1:0:2780:C:H1'	7:E:143:GLN:HE21	1.61	0.65
1:0:2850:C:H6	1:0:2850:C:H5'	1.59	0.65
6:D:99:ASP:HB3	6:D:103:ASN:H	1.61	0.65
1:0:814:G:H4'	38:0:3121:HOH:O	1.96	0.65
2:9:39:U:H1'	2:9:44:A:N6	2.10	0.65
2:9:54:A:O2'	2:9:55:U:H5'	1.96	0.65
5:C:233:THR:HG22	5:C:234:VAL:H	1.62	0.65
21:S:37:VAL:O	21:S:41:VAL:HG23	1.96	0.65
1:0:871:G:C8	1:0:871:G:C5'	2.73	0.65
1:0:1741:U:H5'	1:0:1742:A:OP1	1.97	0.65
27:Y:133:HIS:HD2	38:Y:8880:HOH:O	1.79	0.65
38:C:8559:HOH:O	17:O:3:THR:HG21	1.96	0.65
10:H:61:ARG:HH11	10:H:61:ARG:HG3	1.62	0.65
18:P:115:SER:H	18:P:118:GLN:NE2	1.81	0.65
21:S:43:GLU:HB3	38:S:8545:HOH:O	1.97	0.65
24:V:64:GLY:O	24:V:65:ASP:HB2	1.95	0.65
28:Z:37:HIS:HB2	28:Z:47:VAL:HB	1.77	0.65
25:W:38:THR:HG22	25:W:39:ASP:H	1.61	0.64
1:0:2488:A:H61	1:0:2534:C:H42	1.43	0.64
3:A:95:PRO:HG2	3:A:98:GLU:HG2	1.78	0.64
3:A:121:ALA:O	3:A:124:VAL:HG22	1.97	0.64
6:D:99:ASP:HA	38:D:5675:HOH:O	1.97	0.64
1:0:1634:G:H3'	38:0:3873:HOH:O	1.96	0.64
6:D:163:VAL:HA	38:D:6326:HOH:O	1.96	0.64
11:I:124:VAL:HG13	11:I:134:ILE:HD11	1.79	0.64
14:L:143:THR:HG22	14:L:144:ASP:H	1.62	0.64
3:A:192:VAL:HG12	3:A:207:GLN:HB3	1.79	0.64
4:B:314:ALA:HB3	4:B:317:PRO:HG3	1.79	0.64
16:N:47:LEU:HD13	16:N:97:VAL:HG11	1.79	0.64
3:A:81:GLN:HB2	3:A:92:ASN:ND2	2.13	0.64
11:I:108:HIS:HE1	11:I:116:LEU:HD22	1.62	0.64
20:R:18:LEU:HD12	20:R:143:VAL:HG11	1.80	0.64
24:V:44:GLY:O	24:V:48:GLU:HG2	1.97	0.64
28:Z:57:CYS:SG	28:Z:59:TYR:HB3	2.38	0.64
1:0:1086:A:C6	25:W:11:VAL:HG11	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:46:GLU:OE1	8:F:100:ASP:HA	1.97	0.64
1:0:2827:A:H2'	1:0:2828:G:O4'	1.98	0.64
1:0:2243:C:H5''	38:0:3732:HOH:O	1.98	0.64
38:0:6723:HOH:O	16:N:4:PRO:HD2	1.97	0.64
6:D:154:LYS:H	6:D:154:LYS:CD	2.00	0.64
2:9:73:A:N6	2:9:108:C:H42	1.96	0.64
2:9:92:G:H2'	2:9:93:A:C8	2.33	0.64
4:B:7:ARG:HG2	4:B:7:ARG:HH11	1.63	0.64
13:K:74:VAL:HG12	13:K:75:ARG:HG3	1.80	0.64
38:0:9348:HOH:O	29:1:1:THR:HA	1.98	0.63
3:A:164:ARG:NE	38:A:8886:HOH:O	2.31	0.63
13:K:98:VAL:HG11	13:K:102:GLU:HA	1.79	0.63
1:0:1679:C:H5'	38:0:9314:HOH:O	1.99	0.63
4:B:56:ASP:OD1	4:B:322:ARG:HB3	1.98	0.63
5:C:115:LEU:HD13	5:C:223:LEU:HD21	1.79	0.63
1:0:777:U:O2'	29:1:11:LYS:HG2	1.98	0.63
1:0:797:A:C4'	28:Z:10:ARG:N	2.61	0.63
2:9:49:G:H5''	38:9:8665:HOH:O	1.97	0.63
18:P:91:LYS:O	18:P:95:GLU:HG3	1.98	0.63
1:0:1189:A:H1'	1:0:1209:C:O4'	1.99	0.63
4:B:154:VAL:HG12	4:B:156:LYS:HG2	1.79	0.63
6:D:88:LEU:HB2	6:D:89:PRO:HD3	1.81	0.63
27:Y:189:ASN:HA	27:Y:217:ILE:HD11	1.80	0.63
1:0:603:A:H5''	1:0:604:G:OP1	1.99	0.63
1:0:1377:C:H5'	1:0:1377:C:H6	1.64	0.63
5:C:142:ASP:OD1	5:C:237:GLU:HB3	1.99	0.63
38:E:2512:HOH:O	12:J:127:ILE:HD11	1.98	0.63
31:3:73:GLU:HB3	38:3:8865:HOH:O	1.97	0.63
20:R:9:ASP:O	20:R:13:THR:HB	1.98	0.63
26:X:74:ALA:HB2	26:X:85:VAL:HG13	1.79	0.63
1:0:558:C:C2'	1:0:559:U:H5''	2.29	0.63
3:A:199:HIS:HD2	3:A:201:PHE:H	1.46	0.63
23:U:14:GLU:OE1	23:U:15:PRO:HD2	1.98	0.63
24:V:57:LYS:HA	24:V:60:GLN:HE21	1.62	0.63
25:W:4:LEU:HD22	25:W:52:VAL:HG21	1.80	0.63
25:W:88:THR:HG23	25:W:110:GLN:NE2	2.13	0.63
4:B:217:ARG:HG3	4:B:257:THR:HG22	1.80	0.63
10:H:12:ILE:HG23	10:H:129:ARG:CZ	2.29	0.63
13:K:34:VAL:HG22	13:K:47:ALA:HB2	1.81	0.63
14:L:22:ARG:HG2	38:L:8823:HOH:O	1.98	0.63
24:V:13:PRO:O	24:V:17:GLU:HG3	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1165:G:H4'	1:0:1174:A:HO2'	1.63	0.63
1:0:2505:G:O2'	1:0:2506:A:H5'	1.99	0.63
5:C:16:VAL:HG12	5:C:17:ASP:H	1.64	0.63
27:Y:186:ARG:HG2	27:Y:186:ARG:HH11	1.64	0.63
1:0:777:U:HO2'	29:1:11:LYS:HG2	1.62	0.62
1:0:2320:U:H4'	1:0:2321:A:O4'	1.98	0.62
1:0:2491:G:H1'	38:0:6818:HOH:O	1.98	0.62
1:0:2630:G:O6	3:A:206:ARG:NH2	2.32	0.62
6:D:25:MET:CE	6:D:37:ALA:HB1	2.29	0.62
3:A:211:LYS:HB3	3:A:212:PRO:CD	2.26	0.62
4:B:74:ILE:HD13	4:B:309:VAL:HG21	1.81	0.62
23:U:17:THR:HG22	23:U:18:GLY:N	2.14	0.62
27:Y:200:THR:HG22	27:Y:201:GLU:HG3	1.81	0.62
1:0:111:C:O2'	29:1:20:ARG:HG2	1.99	0.62
16:N:154:LEU:O	16:N:155:GLU:HB3	1.97	0.62
24:V:38:GLY:C	24:V:40:PRO:HD2	2.24	0.62
24:V:56:ILE:O	24:V:60:GLN:HG3	2.00	0.62
1:0:2694:A:H4'	7:E:91:PHE:CE1	2.34	0.62
12:J:107:ASN:ND2	12:J:109:TYR:H	1.97	0.62
3:A:153:ARG:HB2	3:A:153:ARG:HH11	1.64	0.62
16:N:151:ASP:O	16:N:154:LEU:HB2	2.00	0.62
27:Y:187:VAL:CG2	27:Y:192:ASP:HB2	2.29	0.62
30:2:22:PRO:HG2	30:2:25:VAL:HG23	1.82	0.62
38:0:4202:HOH:O	30:2:38:LYS:HE3	1.99	0.62
14:L:136:ALA:HB3	38:L:8871:HOH:O	1.98	0.62
30:2:35:ARG:HB2	38:2:2691:HOH:O	1.99	0.62
1:0:2420:G:O2'	1:0:2421:G:H5'	2.00	0.62
5:C:16:VAL:HG12	5:C:17:ASP:N	2.14	0.62
7:E:84:MET:HE2	7:E:133:VAL:HG23	1.80	0.62
2:9:29:C:H2'	2:9:30:C:H5'	1.82	0.62
4:B:329:TYR:CE2	23:U:15:PRO:HG2	2.35	0.62
16:N:11:ARG:HG3	16:N:14:ARG:NH1	2.15	0.62
2:9:73:A:H61	2:9:108:C:N4	1.97	0.62
1:0:21:G:H4'	20:R:2:ILE:HG22	1.81	0.62
1:0:282:C:O2'	1:0:283:U:H5'	2.00	0.62
4:B:190:MET:HE2	4:B:194:PHE:HD1	1.65	0.62
20:R:25:PHE:CE2	20:R:29:LYS:HE2	2.35	0.62
23:U:39:ASN:ND2	23:U:44:ARG:HH11	1.97	0.62
1:0:2502:C:C2'	1:0:2503:A:H5'	2.30	0.61
1:0:2710:U:H1'	38:0:7568:HOH:O	2.00	0.61
4:B:162:MET:HG3	4:B:310:ARG:HD3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:115:LEU:HD21	5:C:243:VAL:HG13	1.80	0.61
6:D:146:LYS:HZ3	16:N:107:ASN:HD21	1.46	0.61
10:H:31:ILE:HA	10:H:66:GLU:OE1	2.00	0.61
12:J:45:VAL:HG21	12:J:129:PHE:CD1	2.35	0.61
12:J:74:ARG:NH1	12:J:76:ASP:HB2	2.14	0.61
1:O:558:C:O2'	1:O:559:U:H5''	2.00	0.61
16:N:139:TRP:HA	16:N:139:TRP:CE3	2.35	0.61
1:O:870:G:OP2	3:A:3:ARG:HD3	2.00	0.61
1:O:2578:G:H5'	1:O:2578:G:H8	1.65	0.61
3:A:33:GLU:O	3:A:34:ASP:HB2	2.01	0.61
11:I:101:LYS:O	11:I:105:GLU:HG3	2.00	0.61
25:W:6:GLN:HB2	25:W:26:ILE:CD1	2.30	0.61
29:1:10:LYS:HG3	38:1:8732:HOH:O	1.99	0.61
1:O:31:C:H2'	38:O:7636:HOH:O	2.00	0.61
3:A:94:LEU:HG	3:A:99:ILE:CD1	2.30	0.61
4:B:275:GLY:O	4:B:291:ASP:HA	2.01	0.61
4:B:304:PRO:HD2	4:B:307:ARG:HD2	1.82	0.61
1:O:709:G:O2'	17:O:25:VAL:HG12	2.01	0.61
20:R:33:ARG:NH1	38:R:8840:HOH:O	2.33	0.61
26:X:31:ILE:O	26:X:35:GLU:HG3	1.99	0.61
1:O:1185:U:H5'	38:O:7413:HOH:O	2.01	0.61
1:O:1477:C:H5'	1:O:1868:G:C5'	2.31	0.61
1:O:1701:A:H4'	1:O:1702:U:C5'	2.29	0.61
4:B:51:VAL:HG13	4:B:53:LEU:HD13	1.82	0.61
12:J:75:PRO:HG2	12:J:105:LEU:HD21	1.83	0.61
18:P:80:ARG:HG2	18:P:87:ARG:CZ	2.31	0.61
30:2:41:HIS:N	30:2:45:ASN:HD22	1.93	0.61
1:O:447:A:P	22:T:1:SER:HB2	2.41	0.61
5:C:12:THR:HB	38:C:8640:HOH:O	2.00	0.61
24:V:39:ALA:C	24:V:41:GLU:H	2.09	0.61
6:D:41:LEU:HA	6:D:44:ILE:HG22	1.82	0.61
15:M:134:ILE:HG23	15:M:141:ILE:HD13	1.83	0.61
16:N:49:THR:HG22	16:N:56:ASP:HB2	1.82	0.61
5:C:77:ALA:O	5:C:78:ARG:HG3	2.00	0.61
6:D:22:VAL:HG22	6:D:74:THR:HG22	1.83	0.61
8:F:61:MET:HB3	15:M:19:GLN:OE1	2.01	0.61
3:A:96:LEU:HD22	3:A:128:LEU:HD13	1.82	0.60
4:B:108:GLU:HB3	4:B:111:ARG:HD2	1.83	0.60
6:D:84:LEU:HA	6:D:87:ALA:HB3	1.82	0.60
1:O:1008:C:H5''	10:H:19:ARG:HH12	1.66	0.60
12:J:19:MET:HE2	12:J:79:PHE:HA	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:114:VAL:HG11	38:L:8871:HOH:O	1.99	0.60
26:X:37:LEU:CD1	26:X:85:VAL:HG21	2.23	0.60
1:O:31:C:H4'	38:O:7373:HOH:O	2.01	0.60
1:O:1505:U:H6	1:O:1505:U:H5'	1.65	0.60
38:O:6657:HOH:O	27:Y:165:GLU:HB3	2.00	0.60
7:E:93:MET:HE1	7:E:165:GLY:N	2.16	0.60
9:G:16:LYS:O	9:G:20:VAL:HG23	2.01	0.60
11:I:108:HIS:N	11:I:109:PRO:HD2	2.17	0.60
21:S:57:THR:HG22	21:S:59:ASP:H	1.65	0.60
25:W:13:MET:HE3	25:W:17:ILE:CG2	2.31	0.60
1:O:1080:C:H4'	1:O:1081:A:OP1	2.00	0.60
1:O:470:U:O2'	29:1:16:HIS:HD2	1.85	0.60
1:O:558:C:H2'	1:O:559:U:C5'	2.31	0.60
1:O:797:A:H4'	28:Z:10:ARG:N	2.16	0.60
3:A:36:ASP:HA	3:A:83:GLY:HA3	1.83	0.60
3:A:53:ALA:HB3	38:A:8905:HOH:O	2.02	0.60
6:D:166:ILE:HB	38:D:6326:HOH:O	2.00	0.60
1:O:584:U:H3'	38:O:6051:HOH:O	2.00	0.60
1:O:2081:A:H4'	12:J:69:TYR:CE1	2.36	0.60
1:O:2717:C:H2'	1:O:2718:C:C5'	2.28	0.60
3:A:164:ARG:CZ	38:A:8886:HOH:O	2.48	0.60
4:B:66:GLU:OE1	4:B:328:ARG:HD2	2.01	0.60
8:F:99:THR:HA	38:F:3461:HOH:O	2.01	0.60
16:N:12:ARG:HD3	16:N:18:THR:OG1	2.02	0.60
27:Y:189:ASN:C	27:Y:189:ASN:HD22	2.09	0.60
1:O:136:C:H2'	1:O:137:U:O4'	2.02	0.60
4:B:16:ARG:NH1	38:B:8918:HOH:O	2.34	0.60
5:C:145:GLU:HG3	38:C:8575:HOH:O	2.01	0.60
6:D:50:VAL:O	6:D:71:ALA:HA	2.02	0.60
12:J:131:THR:HB	12:J:134:GLU:HG3	1.82	0.60
14:L:133:VAL:HB	38:L:8856:HOH:O	2.00	0.60
17:O:38:ARG:NH1	38:O:7674:HOH:O	2.33	0.60
17:O:73:ASP:HA	17:O:92:VAL:O	2.00	0.60
1:O:1593:C:H5'	18:P:116:SER:O	2.01	0.60
11:I:129:SER:O	11:I:130:LEU:HD23	2.01	0.60
12:J:93:ARG:HB3	12:J:93:ARG:NH1	2.15	0.60
16:N:71:TRP:HE3	16:N:175:LEU:HD22	1.67	0.60
1:O:396:U:O2'	1:O:418:C:H4'	2.02	0.60
3:A:65:ARG:C	3:A:66:ARG:HG3	2.26	0.60
3:A:88:ILE:O	3:A:88:ILE:HG22	2.00	0.60
38:O:9208:HOH:O	3:A:11:ARG:HD3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:26:TRP:HB2	38:O:3062:HOH:O	2.02	0.60
25:W:38:THR:HG22	38:W:3580:HOH:O	2.01	0.60
1:O:818:A:O2'	28:Z:13:ARG:HD3	2.02	0.59
1:O:1058:A:H2'	1:O:1060:C:H5''	1.82	0.59
1:O:1187:U:O2'	1:O:1189:A:H2	1.84	0.59
38:O:6978:HOH:O	3:A:211:LYS:HG2	2.01	0.59
3:A:109:GLU:HG2	3:A:116:GLY:N	2.17	0.59
4:B:312:ARG:HD3	4:B:315:VAL:HG13	1.83	0.59
13:K:55:VAL:HG12	13:K:56:SER:N	2.16	0.59
1:O:1168:C:H4'	38:I:5128:HOH:O	2.01	0.59
1:O:2064:U:H5'	1:O:2652:U:H4'	1.84	0.59
1:O:2721:U:H4'	13:K:87:ARG:HG3	1.84	0.59
5:C:246:ARG:NH2	38:C:8627:HOH:O	2.33	0.59
12:J:131:THR:HG22	12:J:134:GLU:H	1.65	0.59
25:W:126:ASP:HB3	25:W:135:GLY:O	2.02	0.59
3:A:194:MET:HE3	3:A:199:HIS:HB2	1.83	0.59
12:J:103:VAL:HG12	38:J:5907:HOH:O	2.00	0.59
1:O:621:C:H5'	27:Y:132:ASP:OD2	2.02	0.59
1:O:2036:C:O4'	13:K:44:LEU:HG	2.02	0.59
3:A:66:ARG:HH11	3:A:66:ARG:HB2	1.67	0.59
3:A:94:LEU:HD23	3:A:94:LEU:N	2.18	0.59
7:E:31:ARG:NH1	7:E:68:HIS:CG	2.71	0.59
1:O:2414:A:H2'	1:O:2415:A:C8	2.36	0.59
4:B:221:GLN:HE22	13:K:42:ASN:HD22	1.49	0.59
1:O:506:G:H22	1:O:509:A:H5''	1.68	0.59
1:O:1596:U:H2'	1:O:1598:A:OP2	2.02	0.59
4:B:51:VAL:HG23	4:B:330:VAL:HG22	1.83	0.59
5:C:246:ARG:NE	38:C:8627:HOH:O	2.35	0.59
12:J:19:MET:HE3	12:J:132:LEU:HD11	1.84	0.59
16:N:47:LEU:CD1	16:N:97:VAL:HG11	2.32	0.59
29:1:25:LYS:O	29:1:25:LYS:HG2	2.02	0.59
3:A:192:VAL:HG13	38:A:8855:HOH:O	2.03	0.59
7:E:20:ILE:HD11	7:E:40:VAL:CG1	2.33	0.59
7:E:23:GLU:HG2	7:E:28:SER:HB3	1.84	0.59
16:N:71:TRP:CE3	16:N:175:LEU:HD22	2.37	0.59
20:R:132:ARG:CZ	38:R:8878:HOH:O	2.51	0.59
25:W:13:MET:CE	25:W:17:ILE:HG22	2.32	0.59
26:X:43:VAL:HG12	26:X:44:ASP:N	2.17	0.59
1:O:188:C:H5''	15:M:163:LEU:HD21	1.84	0.59
1:O:542:A:H5'	1:O:542:A:C8	2.29	0.59
1:O:1053:G:OP1	10:H:15:PRO:HG3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:3:VAL:HG22	7:E:49:ILE:HB	1.84	0.59
18:P:103:THR:O	18:P:107:GLU:HG3	2.03	0.59
23:U:14:GLU:O	23:U:17:THR:HB	2.02	0.59
1:0:1973:A:H5'	1:0:1973:A:H8	1.67	0.59
1:0:2635:A:O2'	1:0:2636:C:H5'	2.03	0.59
2:9:13:A:O2'	2:9:14:G:H5''	2.03	0.59
1:0:681:G:N3	1:0:681:G:H5'	2.18	0.58
38:9:8665:HOH:O	16:N:147:ILE:HB	2.00	0.58
20:R:111:ILE:HG23	20:R:145:LEU:HD11	1.84	0.58
1:0:1278:A:H4'	1:0:1279:U:C4	2.37	0.58
1:0:1787:C:OP1	18:P:68:LYS:HE2	2.03	0.58
38:0:3737:HOH:O	22:T:9:LYS:HD3	2.03	0.58
4:B:162:MET:HE2	4:B:310:ARG:CD	2.33	0.58
10:H:49:GLN:HG3	10:H:140:TYR:CE2	2.38	0.58
18:P:134:VAL:O	18:P:137:LEU:HB3	2.03	0.58
27:Y:189:ASN:ND2	27:Y:192:ASP:H	2.01	0.58
1:0:285:A:H2'	1:0:286:U:O4'	2.04	0.58
11:I:87:PRO:O	11:I:89:GLU:HG3	2.03	0.58
18:P:115:SER:C	18:P:117:SER:H	2.12	0.58
1:0:1159:G:H21	1:0:1189:A:H8	1.52	0.58
1:0:2769:C:C2'	1:0:2770:G:H5'	2.34	0.58
5:C:104:ASP:HA	5:C:107:ARG:HH12	1.68	0.58
1:0:1120:U:H5'	1:0:1121:G:OP2	2.02	0.58
1:0:1183:C:N4	1:0:1184:C:H41	2.01	0.58
1:0:2717:C:O2'	1:0:2718:C:H5''	2.03	0.58
4:B:185:GLY:HA2	38:B:8934:HOH:O	2.04	0.58
16:N:139:TRP:HA	16:N:139:TRP:HE3	1.69	0.58
1:0:2748:G:H5'	38:0:7487:HOH:O	2.02	0.58
1:0:2769:C:H2'	1:0:2770:G:O4'	2.03	0.58
4:B:139:ASP:HB2	4:B:165:ARG:HE	1.68	0.58
11:I:70:THR:HA	11:I:107:LYS:NZ	2.17	0.58
13:K:22:ASP:HB2	38:K:5264:HOH:O	2.04	0.58
5:C:162:VAL:HG13	5:C:192:ILE:HD11	1.83	0.58
13:K:109:LEU:HD13	13:K:113:ILE:HD11	1.85	0.58
18:P:143:ALA:HA	38:P:192:HOH:O	2.02	0.58
4:B:51:VAL:CG2	4:B:327:VAL:HG13	2.34	0.58
29:1:8:GLN:HE22	29:1:11:LYS:HZ2	1.48	0.58
1:0:1299:G:O6	14:L:6:ARG:HD3	2.04	0.58
14:L:104:ASP:HB2	38:L:8874:HOH:O	2.03	0.58
1:0:793:A:H5''	18:P:83:LYS:HG2	1.86	0.58
1:0:2265:U:H2'	1:0:2266:A:C8	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:30:LYS:H	10:H:62:HIS:CD2	2.16	0.58
1:O:20:G:H21	20:R:117:HIS:HD2	1.52	0.57
8:F:16:ALA:HA	8:F:111:ILE:HD13	1.86	0.57
8:F:39:SER:HB3	8:F:45:ALA:HB2	1.86	0.57
20:R:18:LEU:HB2	20:R:143:VAL:CG1	2.33	0.57
27:Y:144:ARG:NH2	38:Y:8910:HOH:O	2.37	0.57
20:R:99:ALA:CB	20:R:109:MET:HE1	2.31	0.57
21:S:52:VAL:C	21:S:53:ASN:HD22	2.11	0.57
25:W:4:LEU:HD22	25:W:52:VAL:CG2	2.33	0.57
1:O:485:A:N3	1:O:487:G:H5''	2.19	0.57
1:O:1667:A:H2'	1:O:1668:U:C6	2.39	0.57
1:O:1741:U:O2'	1:O:2723:G:H4'	2.05	0.57
1:O:1878:G:H1'	38:O:6077:HOH:O	2.04	0.57
1:O:2241:C:O2'	1:O:2242:U:H5'	2.04	0.57
6:D:64:ARG:HB3	6:D:67:ASP:OD2	2.04	0.57
6:D:149:ARG:NH1	38:D:3066:HOH:O	2.37	0.57
7:E:137:ASP:OD1	7:E:139:GLU:HB2	2.04	0.57
28:Z:11:SER:CB	28:Z:23:ARG:HB2	2.34	0.57
31:3:62:THR:HB	38:3:8854:HOH:O	2.04	0.57
1:O:263:U:O4'	8:F:59:ILE:HD13	2.04	0.57
1:O:1187:U:H2'	38:O:6847:HOH:O	2.04	0.57
6:D:65:GLU:HG3	38:D:6752:HOH:O	2.03	0.57
1:O:1477:C:H5'	1:O:1868:G:H5''	1.86	0.57
4:B:63:GLU:HG3	4:B:63:GLU:O	2.05	0.57
8:F:117:GLU:C	8:F:119:ARG:H	2.11	0.57
15:M:61:ILE:HG13	38:M:8922:HOH:O	2.03	0.57
25:W:38:THR:HG22	25:W:39:ASP:N	2.20	0.57
27:Y:155:ARG:NH1	38:Y:8856:HOH:O	2.36	0.57
1:O:1163:G:H5'	11:I:110:ASP:O	2.05	0.57
7:E:68:HIS:O	7:E:72:MET:HG3	2.05	0.57
11:I:70:THR:HA	11:I:107:LYS:HZ3	1.70	0.57
11:I:100:VAL:HG11	11:I:124:VAL:HG22	1.87	0.57
1:O:121:U:OP2	30:2:10:ARG:NH2	2.35	0.57
4:B:195:ARG:HG2	4:B:323:LEU:HD22	1.86	0.57
7:E:31:ARG:NH1	38:E:5919:HOH:O	2.37	0.57
11:I:113:SER:HB2	11:I:118:ASN:HB2	1.85	0.57
13:K:32:ILE:HD11	13:K:56:SER:HB3	1.86	0.57
13:K:74:VAL:HG13	13:K:113:ILE:HG23	1.85	0.57
15:M:64:ARG:HD2	38:M:8887:HOH:O	2.04	0.57
22:T:71:VAL:CG1	22:T:90:PRO:HB3	2.29	0.57
1:O:1242:A:H5'	12:J:82:THR:CG2	2.23	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1926:G:H2'	1:0:1927:A:C8	2.40	0.57
5:C:214:THR:HG23	38:C:8636:HOH:O	2.04	0.57
12:J:107:ASN:C	12:J:107:ASN:HD22	2.12	0.57
12:J:107:ASN:HD21	12:J:109:TYR:HB2	1.69	0.57
15:M:66:SER:HB3	15:M:128:TRP:CD1	2.39	0.57
16:N:152:GLU:C	16:N:154:LEU:H	2.10	0.57
20:R:39:THR:HB	20:R:42:GLU:CG	2.34	0.57
21:S:33:SER:O	21:S:37:VAL:HG23	2.04	0.57
23:U:52:THR:HG22	23:U:54:THR:N	2.20	0.57
26:X:25:ARG:HD3	26:X:64:ALA:O	2.05	0.57
1:0:1654:U:H2'	3:A:47:HIS:HD2	1.68	0.57
1:0:1766:U:O2	1:0:1778:A:H5'	2.04	0.57
1:0:1834:C:H2'	1:0:1840:A:N6	2.20	0.57
1:0:2748:G:H2'	38:0:7487:HOH:O	2.04	0.57
3:A:105:VAL:HG12	3:A:106:CYS:N	2.20	0.57
6:D:58:VAL:CG1	6:D:60:GLU:HG2	2.35	0.57
25:W:88:THR:HG22	25:W:89:ASP:N	2.19	0.57
31:3:56:PRO:N	38:3:8853:HOH:O	2.38	0.57
1:0:558:C:H2'	1:0:559:U:H5'	1.87	0.57
1:0:2346:C:O2'	6:D:52:THR:HG21	2.04	0.57
5:C:235:PHE:HE2	5:C:243:VAL:HG21	1.69	0.57
9:G:12:ILE:HG22	9:G:17:GLN:NE2	2.19	0.57
10:H:172:GLU:CD	38:H:8591:HOH:O	2.48	0.57
22:T:106:GLU:HG3	38:T:4913:HOH:O	2.05	0.57
26:X:9:VAL:HG22	26:X:88:GLU:OE2	2.04	0.57
27:Y:115:ARG:NE	38:Y:8854:HOH:O	2.37	0.57
1:0:69:A:H5'	1:0:69:A:C8	2.40	0.56
1:0:2502:C:H2'	1:0:2503:A:H5'	1.87	0.56
1:0:2756:U:N3	1:0:2896:A:H2	2.03	0.56
38:0:9071:HOH:O	4:B:214:PRO:HD2	2.05	0.56
3:A:199:HIS:CD2	3:A:201:PHE:H	2.22	0.56
7:E:69:ILE:HA	7:E:72:MET:CE	2.35	0.56
10:H:41:LYS:HE2	10:H:45:ASP:HB2	1.86	0.56
23:U:52:THR:CG2	23:U:54:THR:HB	2.35	0.56
27:Y:200:THR:HG22	27:Y:201:GLU:CG	2.35	0.56
1:0:2094:G:H4'	4:B:245:SER:HB3	1.86	0.56
1:0:2323:G:H5'	38:0:6971:HOH:O	2.05	0.56
6:D:54:ALA:CB	6:D:69:ILE:HD12	2.33	0.56
16:N:37:ARG:NE	38:N:8834:HOH:O	2.38	0.56
28:Z:36:ASP:HB3	28:Z:45:ASP:HB3	1.87	0.56
29:1:21:ARG:HD2	29:1:39:PHE:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:244:C:OP2	8:F:38:LYS:HE3	2.04	0.56
1:0:1060:C:H6	1:0:1060:C:H5'	1.70	0.56
1:0:1205:U:H2'	1:0:1206:U:C5'	2.34	0.56
1:0:2676:C:H4'	12:J:70:PHE:CE1	2.40	0.56
38:0:7404:HOH:O	5:C:188:ARG:HD2	2.05	0.56
4:B:212:GLN:HB2	4:B:257:THR:CG2	2.31	0.56
5:C:5:ILE:HD11	5:C:16:VAL:CG2	2.32	0.56
5:C:25:PRO:HG2	38:C:8523:HOH:O	2.05	0.56
10:H:6:ALA:HA	10:H:61:ARG:HH12	1.71	0.56
14:L:144:ASP:HA	14:L:147:GLU:HG3	1.87	0.56
25:W:6:GLN:HG2	25:W:29:VAL:HA	1.87	0.56
25:W:130:HIS:O	25:W:136:GLY:HA3	2.05	0.56
27:Y:107:PRO:HB3	27:Y:182:PHE:CE2	2.40	0.56
1:0:2781:U:H1'	7:E:139:GLU:OE2	2.05	0.56
1:0:2896:A:H5''	38:0:6055:HOH:O	2.04	0.56
4:B:85:ARG:NH1	38:B:8935:HOH:O	2.39	0.56
4:B:132:HIS:HB2	4:B:137:LEU:HD22	1.87	0.56
6:D:135:VAL:HG22	6:D:136:ARG:N	2.20	0.56
8:F:50:VAL:CG1	8:F:60:VAL:HG11	2.35	0.56
16:N:143:ARG:HA	16:N:172:PHE:CD2	2.40	0.56
1:0:280:C:H2'	1:0:281:U:O4'	2.06	0.56
1:0:1132:A:N6	1:0:1229:C:H2'	2.21	0.56
5:C:115:LEU:O	5:C:118:THR:HB	2.06	0.56
1:0:125:U:H2'	38:0:3747:HOH:O	2.05	0.56
1:0:1118:A:H62	1:0:1244:U:H3	1.52	0.56
2:9:1:U:H5''	2:9:3:A:OP1	2.06	0.56
2:9:44:A:O4'	6:D:76:ARG:NE	2.39	0.56
4:B:137:LEU:HD21	4:B:140:LEU:HD21	1.88	0.56
4:B:248:ARG:O	4:B:251:VAL:HG13	2.05	0.56
4:B:280:VAL:HG13	4:B:333:GLU:O	2.06	0.56
4:B:297:VAL:HB	38:B:8907:HOH:O	2.06	0.56
5:C:233:THR:HG22	5:C:234:VAL:N	2.19	0.56
16:N:154:LEU:HD11	16:N:157:PRO:HA	1.86	0.56
18:P:7:LYS:HD3	18:P:21:VAL:CG2	2.36	0.56
3:A:109:GLU:HG2	3:A:116:GLY:H	1.71	0.56
24:V:39:ALA:N	24:V:40:PRO:CD	2.68	0.56
31:3:17:HIS:O	31:3:18:GLN:HG3	2.06	0.56
1:0:1377:C:H5'	1:0:1377:C:C6	2.41	0.56
4:B:145:HIS:HD2	4:B:146:THR:O	1.87	0.56
1:0:447:A:O2'	1:0:448:G:H5'	2.06	0.56
1:0:902:G:N7	14:L:18:HIS:HD2	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:141:ARG:HD2	4:B:163:GLU:OE2	2.06	0.56
10:H:62:HIS:HA	10:H:65:LEU:HD23	1.87	0.56
12:J:52:GLN:HG3	12:J:53:ILE:N	2.21	0.56
29:1:25:LYS:HD2	30:2:48:ASP:HA	1.88	0.56
1:0:2587:OMU:H2'	1:0:2589:U:H5''	1.88	0.56
3:A:39:ALA:HB3	3:A:61:GLU:OE2	2.06	0.56
5:C:1:MET:HG2	5:C:2:GLN:N	2.20	0.56
6:D:135:VAL:HG21	6:D:139:TYR:CD1	2.41	0.56
11:I:129:SER:N	38:I:7330:HOH:O	2.37	0.56
22:T:16:LEU:HA	22:T:19:ARG:HG3	1.88	0.56
28:Z:26:VAL:O	28:Z:30:GLU:HG3	2.06	0.56
1:0:1166:A:H1'	1:0:1192:A:C2	2.41	0.55
1:0:1441:G:O2'	1:0:1442:A:H5'	2.05	0.55
1:0:2559:C:H4'	38:0:7209:HOH:O	2.04	0.55
4:B:238:ASN:HD22	4:B:240:GLY:N	1.97	0.55
6:D:135:VAL:HG22	6:D:136:ARG:H	1.71	0.55
8:F:28:ALA:CB	8:F:99:THR:HG23	2.36	0.55
14:L:145:LEU:O	14:L:148:GLU:HG3	2.06	0.55
15:M:99:ARG:HH21	15:M:170:ASN:HD22	1.54	0.55
26:X:10:VAL:HG11	26:X:36:HIS:HE1	1.70	0.55
1:0:90:A:H2'	1:0:91:G:O4'	2.05	0.55
1:0:2629:C:H41	3:A:206:ARG:HH21	1.54	0.55
1:0:2712:G:H5'	38:K:4183:HOH:O	2.06	0.55
3:A:211:LYS:NZ	38:A:8919:HOH:O	2.37	0.55
27:Y:184:GLU:OE1	27:Y:204:ARG:NH1	2.40	0.55
1:0:926:A:O2'	14:L:41:HIS:HD2	1.89	0.55
1:0:1819:G:H5'	38:0:4679:HOH:O	2.06	0.55
1:0:1878:G:O2'	1:0:1879:U:C6	2.55	0.55
1:0:2064:U:H5'	1:0:2652:U:O3'	2.07	0.55
38:0:7093:HOH:O	29:1:1:THR:HB	2.05	0.55
4:B:305:ASP:O	4:B:306:LYS:HB2	2.07	0.55
6:D:92:GLU:HB2	38:D:3862:HOH:O	2.07	0.55
7:E:137:ASP:O	7:E:141:VAL:HG23	2.05	0.55
11:I:130:LEU:HA	38:I:7210:HOH:O	2.06	0.55
13:K:14:LYS:CB	13:K:45:PRO:HG2	2.34	0.55
17:O:14:LEU:HD23	17:O:102:ILE:HD11	1.87	0.55
22:T:26:THR:HA	22:T:39:ASN:HB3	1.88	0.55
28:Z:81:ARG:O	28:Z:82:SER:C	2.50	0.55
4:B:154:VAL:CG1	4:B:156:LYS:HG2	2.37	0.55
6:D:25:MET:HE3	6:D:37:ALA:HB1	1.88	0.55
7:E:107:PHE:CE2	7:E:108:LEU:HD13	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:81:ARG:HB2	13:K:87:ARG:HH11	1.71	0.55
27:Y:235:GLU:CD	27:Y:235:GLU:H	2.13	0.55
1:0:417:G:P	38:0:7367:HOH:O	2.64	0.55
9:G:23:ILE:O	9:G:27:ILE:HG13	2.06	0.55
11:I:71:ALA:O	11:I:75:LYS:HG3	2.07	0.55
13:K:34:VAL:CG2	13:K:47:ALA:HB2	2.36	0.55
13:K:87:ARG:NH1	38:K:4066:HOH:O	2.39	0.55
16:N:37:ARG:NH2	38:N:8834:HOH:O	2.39	0.55
25:W:139:GLY:O	25:W:141:HIS:CD2	2.60	0.55
26:X:25:ARG:NH1	38:X:3861:HOH:O	2.40	0.55
1:0:318:U:O2'	1:0:338:C:H2'	2.06	0.55
1:0:625:U:H5''	1:0:1044:C:N4	2.21	0.55
1:0:656:G:H5'	17:O:3:THR:HB	1.88	0.55
1:0:1182:C:H1'	1:0:1192:A:H8	1.70	0.55
2:9:6:C:OP1	16:N:37:ARG:NH1	2.40	0.55
8:F:37:THR:O	8:F:41:GLU:HG3	2.05	0.55
20:R:18:LEU:HD12	20:R:143:VAL:CG1	2.36	0.55
23:U:13:ILE:HG12	23:U:32:CYS:HB3	1.89	0.55
27:Y:99:ALA:HB2	27:Y:233:TYR:CZ	2.42	0.55
1:0:282:C:H1'	1:0:368:C:H42	1.71	0.55
1:0:1594:C:OP2	18:P:120:ARG:HD2	2.06	0.55
1:0:2365:G:H4'	19:Q:45:PRO:O	2.07	0.55
11:I:118:ASN:HA	11:I:121:LYS:HD2	1.88	0.55
22:T:47:THR:HB	22:T:100:ASP:HB3	1.88	0.55
1:0:119:A:H2'	1:0:120:A:H5''	1.88	0.55
1:0:536:A:H3'	38:0:5012:HOH:O	2.06	0.55
1:0:1118:A:C8	1:0:1118:A:C3'	2.86	0.55
5:C:236:THR:O	5:C:237:GLU:C	2.49	0.55
1:0:1926:G:H2'	1:0:1927:A:H8	1.72	0.55
1:0:2878:U:H2'	1:0:2879:A:O4'	2.07	0.55
4:B:119:HIS:O	4:B:121:PRO:HD3	2.07	0.55
5:C:78:ARG:HH11	5:C:78:ARG:CG	2.06	0.55
16:N:61:ALA:HB3	16:N:88:ALA:HB2	1.88	0.55
25:W:139:GLY:O	25:W:141:HIS:HD2	1.90	0.55
26:X:30:MET:CE	26:X:58:ALA:HB3	2.35	0.55
1:0:1130:U:H2'	1:0:1131:G:O4'	2.07	0.54
2:9:48:C:H4'	16:N:141:ARG:HH21	1.72	0.54
8:F:46:GLU:O	8:F:73:PRO:HD2	2.07	0.54
8:F:48:VAL:HG12	8:F:97:ALA:CB	2.37	0.54
11:I:134:ILE:C	11:I:135:GLU:HG3	2.32	0.54
1:0:1044:C:H5''	38:0:9020:HOH:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1118:A:H8	1:0:1119:G:H5''	1.71	0.54
1:0:2837:U:H1'	4:B:307:ARG:HH12	1.72	0.54
38:0:9689:HOH:O	4:B:254:GLN:HG3	2.06	0.54
2:9:30:C:OP1	6:D:137:PRO:O	2.25	0.54
3:A:217:ARG:HH11	3:A:217:ARG:CG	2.19	0.54
8:F:21:GLU:O	8:F:24:ARG:HG3	2.07	0.54
20:R:23:MET:HE3	20:R:28:SER:OG	2.07	0.54
21:S:42:GLU:HG2	21:S:49:VAL:HG23	1.89	0.54
22:T:53:GLY:HA3	38:T:6384:HOH:O	2.05	0.54
25:W:21:LEU:HD13	25:W:26:ILE:HD11	1.88	0.54
27:Y:107:PRO:HB3	27:Y:182:PHE:CD2	2.42	0.54
1:0:1342:C:O2'	1:0:1343:C:H5'	2.08	0.54
1:0:1701:A:H5''	1:0:1702:U:H3'	1.89	0.54
11:I:67:VAL:HG13	11:I:68:PRO:HD2	1.90	0.54
12:J:19:MET:HE1	12:J:78:ILE:HG22	1.89	0.54
15:M:34:GLU:HB3	15:M:38:GLU:HG3	1.90	0.54
17:O:14:LEU:CD2	17:O:102:ILE:HD11	2.37	0.54
21:S:57:THR:HG22	21:S:59:ASP:N	2.22	0.54
25:W:108:ARG:HG3	25:W:114:PRO:HG3	1.89	0.54
1:0:204:A:H2'	1:0:205:U:H5'	1.88	0.54
38:0:4042:HOH:O	4:B:27:ASN:HB2	2.07	0.54
11:I:124:VAL:O	11:I:124:VAL:HG12	2.07	0.54
1:0:299:U:H5'	38:0:7287:HOH:O	2.07	0.54
1:0:2769:C:O2'	1:0:2770:G:H5'	2.07	0.54
2:9:55:U:H4'	2:9:56:A:H8	1.71	0.54
13:K:75:ARG:CZ	38:K:4172:HOH:O	2.55	0.54
23:U:9:CYS:CA	23:U:52:THR:HG23	2.38	0.54
27:Y:144:ARG:NH1	38:Y:8874:HOH:O	2.39	0.54
31:3:70:ARG:HB3	38:3:8877:HOH:O	2.07	0.54
10:H:48:VAL:HA	10:H:170:ARG:O	2.07	0.54
1:0:553:G:P	27:Y:204:ARG:HH22	2.30	0.54
1:0:2301:A:H5''	1:0:2302:A:H5'	1.90	0.54
20:R:132:ARG:HG2	20:R:133:ALA:N	2.21	0.54
1:0:69:A:H5'	1:0:69:A:H8	1.73	0.54
1:0:500:G:H21	20:R:98:ASN:HD21	1.54	0.54
1:0:1119:G:H8	12:J:52:GLN:HE22	1.54	0.54
1:0:1351:G:OP1	5:C:96:LYS:NZ	2.31	0.54
1:0:1778:A:H2'	1:0:1779:A:H5'	1.89	0.54
38:0:6243:HOH:O	27:Y:158:LYS:HD3	2.07	0.54
6:D:36:ASN:HA	38:D:7500:HOH:O	2.07	0.54
22:T:9:LYS:CE	22:T:13:ARG:NH1	2.68	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:138:U:H5''	1:0:139:C:OP2	2.08	0.54
1:0:517:U:H1'	38:0:7523:HOH:O	2.08	0.54
1:0:1010:C:H4'	16:N:4:PRO:HB2	1.89	0.54
1:0:1506:U:H6	1:0:1506:U:H5'	1.72	0.54
2:9:31:C:H1'	38:9:8593:HOH:O	2.08	0.54
3:A:194:MET:HE3	3:A:199:HIS:CB	2.38	0.54
3:A:217:ARG:HH11	3:A:217:ARG:HG3	1.73	0.54
5:C:219:ASN:O	5:C:222:ASP:OD1	2.25	0.54
13:K:87:ARG:NE	38:K:4854:HOH:O	2.41	0.54
21:S:10:VAL:HG11	24:V:36:ALA:HA	1.89	0.54
1:0:67:A:H5''	1:0:69:A:C8	2.43	0.54
1:0:88:G:H8	1:0:88:G:H5'	1.72	0.54
1:0:1641:A:C2'	1:0:1642:A:H5'	2.38	0.54
2:9:91:C:H2'	2:9:92:G:O4'	2.08	0.54
8:F:101:ALA:HA	38:F:5413:HOH:O	2.08	0.54
11:I:88:GLN:HA	11:I:91:PHE:HE2	1.72	0.54
21:S:33:SER:OG	21:S:36:GLU:HG3	2.08	0.54
23:U:46:ALA:HB1	23:U:52:THR:HG21	1.88	0.54
27:Y:216:ARG:HD3	38:Y:8868:HOH:O	2.08	0.54
1:0:2256:G:H2'	1:0:2257:G:C5'	2.38	0.53
1:0:2604:A:H5'	38:0:5748:HOH:O	2.08	0.53
8:F:28:ALA:HB3	8:F:99:THR:O	2.08	0.53
20:R:119:VAL:HG21	20:R:142:ASP:CG	2.33	0.53
22:T:52:ARG:HB2	22:T:95:ASN:HB3	1.90	0.53
25:W:80:ASP:O	25:W:84:VAL:HG23	2.07	0.53
27:Y:112:GLU:OE2	27:Y:115:ARG:NH1	2.41	0.53
27:Y:117:LEU:HD12	27:Y:174:VAL:HG11	1.90	0.53
31:3:48:ASN:ND2	31:3:50:GLY:H	2.05	0.53
1:0:559:U:H5'	1:0:559:U:C6	2.41	0.53
4:B:71:VAL:HG11	4:B:296:LEU:HB3	1.89	0.53
6:D:44:ILE:HG12	6:D:83:PHE:HE1	1.73	0.53
7:E:24:GLY:HA3	7:E:76:VAL:HB	1.91	0.53
7:E:84:MET:HB2	7:E:131:LEU:HB2	1.89	0.53
8:F:91:VAL:CG1	8:F:92:GLY:H	2.17	0.53
18:P:115:SER:O	18:P:117:SER:N	2.41	0.53
1:0:204:A:C2'	1:0:205:U:H5'	2.37	0.53
1:0:407:A:H5'	38:0:5983:HOH:O	2.07	0.53
1:0:1086:A:N6	25:W:11:VAL:HG11	2.23	0.53
1:0:1116:U:O2'	1:0:1118:A:C2	2.48	0.53
1:0:1525:G:H5'	1:0:1526:A:OP2	2.08	0.53
1:0:2256:G:H2'	1:0:2257:G:H5'	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:41:PHE:HB3	4:B:190:MET:HE1	1.90	0.53
5:C:118:THR:O	5:C:136:VAL:HG13	2.08	0.53
7:E:172:PRO:HB3	38:E:6931:HOH:O	2.07	0.53
16:N:37:ARG:CZ	38:N:8834:HOH:O	2.56	0.53
16:N:110:THR:HB	16:N:113:SER:OG	2.08	0.53
1:O:328:U:O4'	5:C:202:THR:HG22	2.08	0.53
1:O:602:A:O2'	1:O:605:C:H4'	2.07	0.53
1:O:775:G:OP1	29:1:16:HIS:HE1	1.92	0.53
1:O:1527:A:H1'	1:O:1528:A:C8	2.43	0.53
1:O:2346:C:H6	1:O:2346:C:O5'	1.92	0.53
2:9:64:C:H2'	2:9:65:A:H5'	1.90	0.53
19:Q:53:HIS:ND1	19:Q:55:ARG:HB2	2.23	0.53
14:L:21:ARG:N	38:L:8831:HOH:O	2.41	0.53
25:W:125:HIS:HE1	38:W:3071:HOH:O	1.90	0.53
29:1:28:HIS:CE1	29:1:31:LYS:HE2	2.44	0.53
1:O:2256:G:C2'	1:O:2257:G:H5'	2.39	0.53
6:D:95:THR:OG1	6:D:174:VAL:HG22	2.08	0.53
17:O:87:THR:O	17:O:91:GLN:HG3	2.08	0.53
25:W:41:TYR:HA	25:W:44:MET:HE3	1.90	0.53
26:X:76:ARG:O	26:X:77:PHE:HB3	2.08	0.53
27:Y:151:SER:HB3	27:Y:154:ARG:HB3	1.91	0.53
1:O:285:A:C2	1:O:368:C:H4'	2.43	0.53
1:O:399:C:H5'	15:M:179:GLY:O	2.09	0.53
1:O:776:A:OP1	29:1:28:HIS:HE1	1.92	0.53
1:O:1185:U:H2'	1:O:1186:C:C6	2.43	0.53
1:O:1266:U:H4'	27:Y:115:ARG:HH21	1.73	0.53
1:O:1289:C:O2'	1:O:1290:G:H5'	2.09	0.53
1:O:1333:U:H2'	1:O:1334:C:C6	2.44	0.53
5:C:39:GLN:O	5:C:43:LYS:HD3	2.09	0.53
10:H:43:ALA:HB1	10:H:140:TYR:CE2	2.44	0.53
1:O:2526:C:O2'	1:O:2527:U:H5'	2.09	0.53
1:O:2904:U:H4'	26:X:8:ARG:NH1	2.24	0.53
4:B:264:GLU:HG2	4:B:267:LYS:CE	2.33	0.53
9:G:20:VAL:O	9:G:24:VAL:HG23	2.09	0.53
13:K:125:ALA:C	13:K:127:ALA:H	2.17	0.53
21:S:77:VAL:O	21:S:80:ARG:HG2	2.08	0.53
23:U:52:THR:HG22	23:U:54:THR:H	1.74	0.53
25:W:6:GLN:CB	25:W:26:ILE:HD12	2.37	0.53
27:Y:178:HIS:CG	27:Y:179:PRO:HD2	2.44	0.53
1:O:316:A:H5'	22:T:54:ASP:OD2	2.08	0.53
1:O:2649:A:H5'	1:O:2649:A:H8	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:86:THR:C	6:D:89:PRO:HD2	2.34	0.53
1:O:1205:U:H2'	1:O:1206:U:H5''	1.90	0.53
1:O:2300:A:H4'	1:O:2301:A:O5'	2.09	0.53
5:C:61:PHE:HB3	38:C:8643:HOH:O	2.09	0.53
10:H:157:TYR:CD1	10:H:157:TYR:C	2.86	0.53
21:S:81:ILE:HG12	38:S:8538:HOH:O	2.08	0.53
4:B:62:ARG:CA	4:B:65:MET:HE3	2.34	0.52
12:J:130:VAL:HG12	12:J:131:THR:N	2.24	0.52
14:L:61:ALA:HA	38:L:8862:HOH:O	2.08	0.52
21:S:11:THR:H	21:S:14:ALA:HB3	1.74	0.52
22:T:18:GLU:O	22:T:21:LYS:HG2	2.09	0.52
27:Y:103:THR:HG22	27:Y:104:GLU:OE2	2.09	0.52
27:Y:112:GLU:CD	27:Y:115:ARG:NH1	2.67	0.52
1:O:2064:U:H4'	1:O:2653:A:OP1	2.09	0.52
1:O:2401:A:H5'	38:O:9483:HOH:O	2.10	0.52
38:O:9529:HOH:O	18:P:81:LYS:HG2	2.09	0.52
9:G:64:ASN:N	9:G:64:ASN:ND2	2.55	0.52
10:H:50:ILE:HG12	10:H:168:VAL:HG22	1.92	0.52
12:J:74:ARG:O	12:J:78:ILE:HG12	2.09	0.52
18:P:103:THR:HA	18:P:106:ARG:NH1	2.24	0.52
19:Q:25:PRO:HB2	38:Q:4350:HOH:O	2.08	0.52
22:T:80:GLU:HA	38:T:6653:HOH:O	2.08	0.52
1:O:654:A:OP2	17:O:38:ARG:HD3	2.09	0.52
1:O:794:U:H3	1:O:819:A:H61	1.57	0.52
1:O:1135:G:H5'	38:O:5887:HOH:O	2.08	0.52
1:O:1236:A:H2'	1:O:1237:U:O4'	2.09	0.52
1:O:1636:G:O2'	1:O:1637:A:H5'	2.09	0.52
2:9:34:A:H2'	2:9:35:C:O4'	2.08	0.52
3:A:105:VAL:HG11	3:A:154:ALA:CB	2.38	0.52
3:A:192:VAL:HB	38:A:8892:HOH:O	2.10	0.52
4:B:125:GLU:O	4:B:129:ARG:HG3	2.09	0.52
7:E:7:ILE:HD11	7:E:11:VAL:C	2.34	0.52
10:H:146:ALA:O	10:H:149:VAL:HG12	2.09	0.52
24:V:11:MET:HE1	24:V:19:GLU:HG2	1.92	0.52
26:X:71:ARG:HB3	26:X:88:GLU:OE1	2.09	0.52
1:O:1544:U:H2'	1:O:1545:C:H6	1.75	0.52
1:O:1942:A:O2'	1:O:1943:C:H5'	2.10	0.52
7:E:77:THR:OG1	7:E:78:GLU:N	2.43	0.52
7:E:80:TRP:O	7:E:134:SER:HA	2.09	0.52
11:I:87:PRO:C	11:I:89:GLU:N	2.66	0.52
16:N:67:ALA:C	16:N:69:TYR:H	2.16	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:V:64:GLY:O	24:V:65:ASP:CB	2.57	0.52
1:0:1173:A:H2	38:0:6239:HOH:O	1.92	0.52
1:0:1535:G:H2'	1:0:1536:C:C6	2.44	0.52
4:B:30:PRO:HB2	4:B:39:GLN:NE2	2.24	0.52
5:C:104:ASP:HA	5:C:107:ARG:NH1	2.23	0.52
5:C:127:ARG:HD2	5:C:229:PRO:O	2.09	0.52
6:D:64:ARG:CD	6:D:67:ASP:HB3	2.39	0.52
24:V:5:VAL:HG23	38:V:2271:HOH:O	2.09	0.52
1:0:447:A:OP1	22:T:2:LYS:HG2	2.09	0.52
1:0:474:C:O3'	5:C:73:LEU:HD21	2.09	0.52
1:0:2237:G:H1'	38:0:4818:HOH:O	2.10	0.52
1:0:2862:G:H4'	4:B:336:GLN:O	2.09	0.52
38:0:9545:HOH:O	25:W:119:HIS:HE1	1.92	0.52
2:9:55:U:H4'	2:9:56:A:C8	2.45	0.52
4:B:254:GLN:HG2	4:B:255:GLY:N	2.24	0.52
6:D:146:LYS:NZ	16:N:107:ASN:ND2	2.55	0.52
8:F:19:ALA:O	8:F:22:VAL:HG22	2.10	0.52
24:V:55:ARG:O	24:V:59:ILE:HG12	2.10	0.52
31:3:65:THR:HG23	31:3:67:LEU:HG	1.90	0.52
31:3:70:ARG:HG2	31:3:77:ALA:HB2	1.92	0.52
1:0:343:C:O2'	1:0:344:C:H5'	2.09	0.52
1:0:588:G:O6	25:W:154:ARG:NH1	2.42	0.52
1:0:820:G:OP2	3:A:171:LYS:NZ	2.42	0.52
1:0:2668:G:H2'	1:0:2669:U:C6	2.45	0.52
2:9:49:G:O2'	2:9:50:G:H5'	2.09	0.52
4:B:62:ARG:HA	4:B:65:MET:CE	2.35	0.52
4:B:294:TYR:HE2	38:B:8954:HOH:O	1.93	0.52
6:D:44:ILE:HG23	6:D:45:THR:HG23	1.92	0.52
23:U:52:THR:HG22	23:U:54:THR:HB	1.92	0.52
1:0:638:C:H2'	1:0:639:A:C8	2.45	0.52
1:0:926:A:O2'	14:L:41:HIS:CD2	2.63	0.52
1:0:2715:G:N2	4:B:264:GLU:OE1	2.41	0.52
1:0:407:A:H2'	1:0:408:A:C8	2.45	0.52
1:0:2506:A:H1'	38:0:3728:HOH:O	2.09	0.52
1:0:2524:G:H21	1:0:2526:C:N4	2.08	0.52
3:A:179:MET:HG2	3:A:186:TRP:CG	2.45	0.52
7:E:145:ALA:HB1	7:E:168:ILE:HD11	1.92	0.52
13:K:34:VAL:HB	38:K:7169:HOH:O	2.10	0.52
27:Y:187:VAL:HB	38:Y:8869:HOH:O	2.10	0.52
28:Z:56:GLN:HA	28:Z:62:TYR:O	2.09	0.52
1:0:960:G:N3	1:0:960:G:H2'	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:76:VAL:HG23	28:Z:63:LYS:HB3	1.91	0.52
4:B:24:PRO:CG	4:B:204:GLY:HA2	2.40	0.52
4:B:43:GLY:O	4:B:308:LEU:HD12	2.10	0.52
5:C:47:GLY:HA2	5:C:92:PRO:HB2	1.91	0.52
10:H:39:LYS:HD3	38:H:8578:HOH:O	2.09	0.52
1:O:1681:G:H5''	1:O:1682:A:H5'	1.91	0.51
1:O:2718:C:H6	1:O:2718:C:H5'	1.76	0.51
4:B:103:ASP:HB2	38:B:8894:HOH:O	2.10	0.51
22:T:41:ARG:HG2	22:T:41:ARG:HH11	1.75	0.51
29:1:28:HIS:CD2	29:1:31:LYS:HG3	2.45	0.51
1:O:1730:G:H5''	1:O:1731:C:H6	1.76	0.51
3:A:211:LYS:HB2	38:A:8918:HOH:O	2.09	0.51
5:C:111:VAL:HB	38:C:8522:HOH:O	2.10	0.51
5:C:168:ARG:NH2	5:C:190:ALA:O	2.43	0.51
10:H:157:TYR:C	10:H:157:TYR:HD1	2.18	0.51
20:R:111:ILE:HG23	20:R:145:LEU:CD1	2.39	0.51
23:U:17:THR:CG2	23:U:18:GLY:N	2.73	0.51
25:W:125:HIS:CD2	25:W:127:GLY:H	2.28	0.51
1:O:474:C:O3'	5:C:73:LEU:CD2	2.58	0.51
1:O:1044:C:H5	38:O:6557:HOH:O	1.92	0.51
1:O:1717:A:H5''	18:P:54:LYS:HB2	1.91	0.51
1:O:2073:G:OP2	1:O:2490:A:H5'	2.09	0.51
1:O:2815:G:N7	12:J:80:LYS:NZ	2.58	0.51
2:9:76:G:C3'	2:9:77:A:H5''	2.31	0.51
4:B:195:ARG:CG	4:B:323:LEU:HD22	2.40	0.51
5:C:133:ARG:NE	5:C:135:GLU:O	2.43	0.51
6:D:167:GLU:C	6:D:169:THR:H	2.19	0.51
21:S:57:THR:CG2	21:S:58:MET:N	2.73	0.51
25:W:21:LEU:HD22	25:W:26:ILE:HD13	1.90	0.51
25:W:76:ASP:O	25:W:77:ALA:C	2.53	0.51
27:Y:117:LEU:CD1	27:Y:174:VAL:HG11	2.40	0.51
1:O:2468:A:H61	31:3:48:ASN:HD21	1.57	0.51
4:B:202:VAL:HG11	4:B:301:VAL:HG13	1.93	0.51
5:C:13:ASP:OD1	5:C:13:ASP:O	2.27	0.51
7:E:11:VAL:HG12	7:E:12:ASP:H	1.72	0.51
38:O:6815:HOH:O	3:A:211:LYS:HD3	2.11	0.51
38:O:7373:HOH:O	22:T:9:LYS:HB2	2.10	0.51
4:B:75:GLU:C	4:B:77:PRO:HD3	2.36	0.51
9:G:67:LEU:O	9:G:71:LEU:HG	2.10	0.51
13:K:115:ARG:HG3	13:K:116:GLU:N	2.25	0.51
25:W:65:VAL:HA	25:W:68:THR:CG2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:X:71:ARG:HD3	38:X:2171:HOH:O	2.10	0.51
1:0:558:C:H5'	38:0:5218:HOH:O	2.11	0.51
1:0:1979:G:H2'	38:0:3283:HOH:O	2.10	0.51
22:T:38:ARG:NH1	38:T:6217:HOH:O	2.42	0.51
29:1:45:ARG:NH2	38:1:8728:HOH:O	2.32	0.51
4:B:82:VAL:O	4:B:82:VAL:HG12	2.09	0.51
4:B:141:ARG:HG2	4:B:165:ARG:HA	1.93	0.51
6:D:23:VAL:HG23	6:D:23:VAL:O	2.11	0.51
8:F:78:GLU:HG3	38:F:5966:HOH:O	2.10	0.51
16:N:179:LEU:HD23	16:N:184:ILE:HD12	1.93	0.51
22:T:9:LYS:HE3	22:T:13:ARG:CZ	2.41	0.51
26:X:45:GLU:HG3	38:X:6178:HOH:O	2.09	0.51
1:0:482:G:H4'	1:0:508:A:N1	2.26	0.51
1:0:1189:A:H3'	38:0:7628:HOH:O	2.10	0.51
1:0:1682:A:H5''	38:0:9445:HOH:O	2.11	0.51
16:N:86:LEU:HD21	16:N:180:LEU:CD1	2.40	0.51
21:S:51:GLN:HB3	21:S:67:ARG:NH1	2.24	0.51
1:0:2533:C:H6	1:0:2533:C:C5'	2.22	0.51
8:F:91:VAL:CG1	8:F:92:GLY:N	2.71	0.51
21:S:23:LYS:HE2	38:S:8532:HOH:O	2.10	0.51
25:W:21:LEU:HB3	25:W:26:ILE:HG12	1.93	0.51
26:X:78:GLU:HG2	26:X:79:GLU:N	2.26	0.51
29:1:21:ARG:HD2	29:1:37:CYS:SG	2.51	0.51
30:2:40:ARG:HD2	30:2:47:THR:HG22	1.92	0.51
1:0:958:G:H2'	1:0:959:C:C6	2.46	0.51
1:0:2256:G:O2'	1:0:2257:G:H5'	2.11	0.51
1:0:2521:A:OP2	10:H:6:ALA:HB3	2.10	0.51
1:0:2781:U:H2'	1:0:2782:G:H5'	1.92	0.51
1:0:2795:C:O2'	1:0:2796:U:H5'	2.09	0.51
38:0:6240:HOH:O	28:Z:49:ARG:HD2	2.11	0.51
38:0:7309:HOH:O	3:A:177:HIS:HE1	1.94	0.51
3:A:51:ARG:NH1	3:A:120:ARG:O	2.44	0.51
4:B:314:ALA:CB	4:B:317:PRO:HG3	2.41	0.51
7:E:99:GLY:N	38:E:4191:HOH:O	2.44	0.51
9:G:12:ILE:N	9:G:13:PRO:HD3	2.26	0.51
1:0:559:U:H2'	1:0:560:U:O4'	2.11	0.50
1:0:944:G:H21	25:W:44:MET:CE	2.24	0.50
1:0:1176:C:H1'	38:0:3909:HOH:O	2.10	0.50
1:0:1625:U:H4'	38:0:4635:HOH:O	2.11	0.50
38:0:6167:HOH:O	4:B:2:GLN:HA	2.10	0.50
3:A:1:GLY:HA2	3:A:197:VAL:HG23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:47:LEU:HD12	16:N:92:ALA:HB1	1.92	0.50
1:0:644:G:H5'	1:0:644:G:N3	2.25	0.50
1:0:1014:A:H2'	1:0:1015:C:H5'	1.93	0.50
1:0:2270:G:H4'	3:A:223:ARG:NH1	2.23	0.50
17:O:47:ARG:HH11	17:O:47:ARG:HG3	1.76	0.50
22:T:50:VAL:HG12	22:T:56:ALA:HA	1.94	0.50
26:X:75:ALA:O	26:X:83:ALA:HA	2.10	0.50
5:C:79:ARG:O	5:C:87:ARG:HG2	2.11	0.50
5:C:95:GLU:HG3	38:C:8671:HOH:O	2.11	0.50
13:K:29:LEU:HB3	13:K:55:VAL:CG1	2.37	0.50
15:M:61:ILE:HA	38:M:8922:HOH:O	2.11	0.50
20:R:39:THR:HB	20:R:42:GLU:CD	2.36	0.50
1:0:42:C:H1'	38:0:4644:HOH:O	2.10	0.50
1:0:259:G:H21	15:M:58:GLN:NE2	2.09	0.50
1:0:1687:C:O2	29:1:9:GLY:HA2	2.11	0.50
1:0:1825:U:O2'	1:0:1826:C:H5'	2.11	0.50
1:0:2679:G:H2'	1:0:2681:A:OP2	2.12	0.50
4:B:48:MET:HG2	4:B:72:THR:HA	1.93	0.50
4:B:139:ASP:CB	4:B:165:ARG:HE	2.23	0.50
5:C:165:ASP:O	5:C:168:ARG:HB3	2.11	0.50
5:C:180:SER:HB2	38:C:8644:HOH:O	2.12	0.50
7:E:32:ARG:O	7:E:33:LEU:HD23	2.12	0.50
11:I:67:VAL:CG1	11:I:68:PRO:HD2	2.42	0.50
12:J:133:GLY:O	12:J:137:GLU:HG3	2.10	0.50
16:N:48:VAL:HG11	16:N:55:ASP:HB3	1.92	0.50
1:0:558:C:C2'	1:0:559:U:C5'	2.89	0.50
1:0:1201:C:H2'	1:0:1202:A:H5'	1.93	0.50
1:0:1434:A:H2'	1:0:1436:C:C5	2.46	0.50
1:0:1603:A:H5''	1:0:1605:G:H5'	1.93	0.50
1:0:1790:C:H2'	1:0:1791:U:H6	1.75	0.50
4:B:329:TYR:HE2	23:U:15:PRO:HG2	1.77	0.50
8:F:46:GLU:N	38:F:3461:HOH:O	2.43	0.50
12:J:75:PRO:HG2	12:J:105:LEU:CD2	2.41	0.50
26:X:43:VAL:HG12	26:X:47:ALA:HB3	1.93	0.50
28:Z:60:CYS:O	28:Z:61:ASP:HB2	2.10	0.50
1:0:660:A:H4'	1:0:661:G:O5'	2.12	0.50
1:0:2506:A:O2'	1:0:2507:G:O5'	2.29	0.50
1:0:2781:U:C2'	1:0:2782:G:H5'	2.42	0.50
11:I:133:THR:HG22	11:I:134:ILE:N	2.26	0.50
11:I:134:ILE:HG22	11:I:135:GLU:N	2.26	0.50
27:Y:234:VAL:HG12	27:Y:235:GLU:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2563:U:H2'	1:0:2565:C:O5'	2.11	0.50
1:0:2601:A:N1	13:K:38:SER:HB2	2.27	0.50
4:B:7:ARG:HD3	4:B:9:GLY:O	2.11	0.50
14:L:104:ASP:HB3	38:L:8862:HOH:O	2.10	0.50
16:N:154:LEU:C	16:N:156:GLU:H	2.19	0.50
25:W:38:THR:HB	38:W:5390:HOH:O	2.12	0.50
27:Y:106:THR:HG23	27:Y:107:PRO:HD2	1.92	0.50
30:2:22:PRO:HG2	30:2:25:VAL:CG2	2.40	0.50
1:0:1180:U:H4'	11:I:86:GLU:HG2	1.94	0.50
1:0:1537:C:H1'	38:0:6542:HOH:O	2.11	0.50
1:0:1862:C:H1'	38:0:7172:HOH:O	2.12	0.50
4:B:162:MET:HE2	4:B:310:ARG:CG	2.42	0.50
5:C:127:ARG:HG2	5:C:127:ARG:HH11	1.76	0.50
5:C:133:ARG:NH2	38:C:8629:HOH:O	2.44	0.50
6:D:35:ALA:N	38:D:5576:HOH:O	2.45	0.50
6:D:154:LYS:HD2	6:D:154:LYS:N	2.06	0.50
8:F:58:GLU:OE1	15:M:27:ARG:NH2	2.40	0.50
25:W:65:VAL:HG12	25:W:116:LEU:HD13	1.92	0.50
31:3:3:MET:O	31:3:90:PHE:HA	2.12	0.50
1:0:1029:U:O2'	1:0:1273:C:OP1	2.29	0.50
1:0:2676:C:H4'	12:J:70:PHE:HE1	1.76	0.50
6:D:23:VAL:HG21	6:D:45:THR:CG2	2.42	0.50
6:D:94:ALA:HA	6:D:174:VAL:O	2.11	0.50
15:M:164:THR:HG23	15:M:165:GLY:N	2.26	0.50
17:O:25:VAL:HG23	17:O:26:TRP:N	2.27	0.50
22:T:64:ASN:HB3	22:T:73:HIS:HB2	1.93	0.50
31:3:69:TYR:HB2	31:3:78:HIS:CE1	2.46	0.50
1:0:2570:G:H5''	38:0:4876:HOH:O	2.12	0.49
2:9:2:U:OP2	2:9:3:A:H5'	2.12	0.49
3:A:210:GLY:HA3	38:A:8883:HOH:O	2.12	0.49
5:C:140:VAL:HG12	5:C:141:SER:N	2.25	0.49
6:D:51:ARG:HD3	38:D:7636:HOH:O	2.10	0.49
14:L:42:ASN:HB2	38:L:8873:HOH:O	2.12	0.49
15:M:24:GLN:HE22	15:M:27:ARG:HH11	1.59	0.49
16:N:11:ARG:NH2	38:N:8819:HOH:O	2.45	0.49
20:R:132:ARG:NH2	38:R:8878:HOH:O	2.45	0.49
25:W:19:ASP:O	25:W:23:MET:HG3	2.12	0.49
1:0:21:G:H5''	20:R:1:GLY:O	2.13	0.49
1:0:694:A:H2'	1:0:695:C:H5'	1.94	0.49
1:0:1342:C:C2'	1:0:1343:C:H5'	2.42	0.49
8:F:48:VAL:HG12	8:F:97:ALA:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:101:ASP:C	14:L:103:ALA:H	2.19	0.49
25:W:110:GLN:NE2	25:W:110:GLN:HA	2.27	0.49
27:Y:126:PRO:HG2	27:Y:128:PHE:CE1	2.46	0.49
1:O:316:A:N3	1:O:336:G:O2'	2.44	0.49
1:O:1528:A:H2'	1:O:1529:G:O4'	2.12	0.49
1:O:2445:U:H2'	1:O:2446:G:C8	2.47	0.49
1:O:2507:G:H2'	1:O:2510:C:H42	1.77	0.49
3:A:190:ARG:NH2	3:A:207:GLN:OE1	2.44	0.49
4:B:258:GLY:H	4:B:260:HIS:CE1	2.29	0.49
4:B:279:THR:OG1	4:B:290:VAL:HB	2.12	0.49
5:C:246:ARG:NH1	38:C:8571:HOH:O	2.45	0.49
6:D:28:GLY:CA	6:D:69:ILE:HG23	2.36	0.49
7:E:5:LEU:HD21	7:E:66:GLN:HG3	1.94	0.49
15:M:184:ARG:HG3	15:M:185:PRO:HA	1.94	0.49
16:N:67:ALA:C	16:N:69:TYR:N	2.70	0.49
16:N:176:ARG:O	16:N:180:LEU:HD13	2.13	0.49
1:O:669:G:O2'	1:O:670:G:H5'	2.12	0.49
1:O:894:A:C2	5:C:87:ARG:NH2	2.81	0.49
1:O:1615:A:H5'	38:O:4158:HOH:O	2.11	0.49
6:D:128:LEU:N	38:D:6007:HOH:O	2.46	0.49
7:E:101:GLU:HB2	7:E:116:THR:O	2.12	0.49
21:S:57:THR:HG22	21:S:58:MET:N	2.27	0.49
1:O:64:G:H2'	1:O:65:C:O4'	2.13	0.49
1:O:284:C:H4'	1:O:285:A:O5'	2.12	0.49
4:B:217:ARG:CG	4:B:257:THR:HG22	2.42	0.49
11:I:108:HIS:N	11:I:109:PRO:CD	2.76	0.49
1:O:281:U:H3'	38:O:7159:HOH:O	2.11	0.49
1:O:1666:C:H2'	1:O:1667:A:C5'	2.42	0.49
1:O:1878:G:O2'	1:O:1879:U:P	2.71	0.49
1:O:2649:A:H5'	1:O:2649:A:C8	2.48	0.49
38:O:4337:HOH:O	3:A:212:PRO:HB2	2.12	0.49
4:B:280:VAL:CG1	4:B:334:SER:HA	2.43	0.49
5:C:200:PRO:HB3	5:C:212:VAL:HG23	1.95	0.49
10:H:49:GLN:HG3	10:H:140:TYR:CD2	2.48	0.49
10:H:151:GLU:OE1	10:H:151:GLU:HA	2.13	0.49
13:K:24:THR:HB	13:K:64:MET:HE2	1.95	0.49
20:R:18:LEU:HB2	20:R:143:VAL:HG13	1.93	0.49
25:W:26:ILE:O	25:W:26:ILE:HG13	2.12	0.49
26:X:21:PRO:HG2	26:X:24:LYS:HD3	1.92	0.49
29:1:25:LYS:HD2	30:2:49:GLU:H	1.77	0.49
1:O:1175:G:H1'	1:O:1193:A:H2'	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:41:LYS:HE2	10:H:45:ASP:CB	2.43	0.49
14:L:53:ARG:NH2	14:L:57:VAL:HG12	2.27	0.49
22:T:69:LYS:O	22:T:71:VAL:HG23	2.13	0.49
1:O:1733:A:H4'	4:B:212:GLN:HA	1.93	0.49
7:E:139:GLU:CD	38:E:5919:HOH:O	2.54	0.49
10:H:61:ARG:NH1	10:H:61:ARG:HG3	2.28	0.49
14:L:30:ARG:NH2	38:L:8820:HOH:O	2.42	0.49
16:N:65:ASP:HB3	38:N:8824:HOH:O	2.11	0.49
16:N:78:MET:HB2	16:N:79:PRO:HD3	1.94	0.49
16:N:151:ASP:OD1	16:N:154:LEU:HD13	2.13	0.49
16:N:154:LEU:O	16:N:155:GLU:CB	2.61	0.49
16:N:171:HIS:CE1	38:N:8868:HOH:O	2.66	0.49
18:P:10:ALA:HA	18:P:13:VAL:HG12	1.94	0.49
29:1:37:CYS:SG	29:1:39:PHE:HB2	2.53	0.49
1:O:380:A:OP2	15:M:9:ARG:HD2	2.12	0.49
1:O:1544:U:H2'	1:O:1545:C:C6	2.48	0.49
1:O:2403:C:H3'	38:O:5171:HOH:O	2.11	0.49
1:O:2825:C:H4'	1:O:2826:G:O5'	2.13	0.49
7:E:132:THR:HB	38:E:2227:HOH:O	2.13	0.49
14:L:67:ARG:O	14:L:71:GLU:HG3	2.12	0.49
18:P:131:PHE:CD1	18:P:137:LEU:HD13	2.47	0.49
28:Z:80:ARG:O	28:Z:81:ARG:O	2.30	0.49
1:O:714:U:H3'	38:O:6893:HOH:O	2.13	0.49
1:O:757:C:OP1	14:L:27:ARG:HD2	2.12	0.49
1:O:1191:A:H2'	1:O:1193:A:H5'	1.95	0.49
1:O:1450:C:O2'	1:O:1494:A:H5'	2.12	0.49
1:O:2453:G:H4'	14:L:50:GLY:C	2.38	0.49
5:C:27:ARG:HG3	5:C:29:ASP:OD1	2.13	0.49
6:D:35:ALA:C	6:D:37:ALA:H	2.21	0.49
20:R:113:HIS:HE1	20:R:144:GLU:CD	2.20	0.49
20:R:119:VAL:HG12	20:R:119:VAL:O	2.12	0.49
25:W:5:VAL:O	25:W:52:VAL:HG22	2.13	0.49
1:O:558:C:H2'	1:O:559:U:H5''	1.94	0.48
1:O:1666:C:C2'	1:O:1667:A:C5'	2.91	0.48
1:O:2894:C:O2'	1:O:2895:C:H5'	2.12	0.48
4:B:5:ARG:NH1	4:B:8:LYS:HE2	2.27	0.48
6:D:56:ARG:N	38:D:6752:HOH:O	2.45	0.48
14:L:67:ARG:HB2	14:L:112:GLY:HA3	1.95	0.48
22:T:40:VAL:HG22	22:T:41:ARG:N	2.27	0.48
1:O:820:G:O2'	1:O:856:G:H4'	2.13	0.48
4:B:17:LYS:O	4:B:260:HIS:HD2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:95:GLU:H	5:C:95:GLU:CD	2.21	0.48
5:C:127:ARG:HG2	5:C:127:ARG:NH1	2.28	0.48
11:I:108:HIS:CE1	11:I:116:LEU:HD22	2.44	0.48
14:L:125:PHE:CZ	14:L:140:VAL:HG13	2.48	0.48
18:P:115:SER:C	18:P:117:SER:N	2.71	0.48
1:0:475:G:H5'	5:C:73:LEU:HD23	1.95	0.48
1:0:2251:G:H2'	1:0:2252:A:C8	2.47	0.48
3:A:55:VAL:HG22	3:A:68:ILE:O	2.13	0.48
15:M:46:LEU:HG	38:M:8921:HOH:O	2.13	0.48
15:M:61:ILE:CG2	15:M:62:VAL:N	2.75	0.48
22:T:61:GLU:HG3	38:T:3851:HOH:O	2.13	0.48
27:Y:186:ARG:HG2	27:Y:186:ARG:NH1	2.27	0.48
1:0:538:C:OP2	27:Y:134:HIS:HE1	1.96	0.48
1:0:1589:G:N2	1:0:1605:G:H1'	2.28	0.48
1:0:2004:U:H2'	1:0:2004:U:O2	2.12	0.48
1:0:2670:G:O2'	1:0:2671:U:H5'	2.14	0.48
38:O:5903:HOH:O	18:P:87:ARG:HG2	2.14	0.48
3:A:88:ILE:HD13	3:A:100:PRO:CD	2.41	0.48
4:B:102:THR:HG21	4:B:182:VAL:O	2.13	0.48
5:C:157:LEU:HD22	5:C:162:VAL:CG1	2.43	0.48
19:Q:32:GLU:HA	19:Q:71:TYR:OH	2.13	0.48
26:X:43:VAL:HG12	26:X:44:ASP:H	1.78	0.48
1:0:790:A:H2'	1:0:791:A:O4'	2.13	0.48
1:0:1183:C:H42	1:0:1184:C:H41	1.62	0.48
1:0:1675:C:H5''	30:2:5:LYS:HD2	1.95	0.48
1:0:1972:U:H2'	1:0:1973:A:H5'	1.96	0.48
38:9:8638:HOH:O	16:N:41:LYS:HD3	2.13	0.48
5:C:78:ARG:NH1	5:C:78:ARG:CG	2.70	0.48
5:C:246:ARG:CZ	38:C:8627:HOH:O	2.62	0.48
6:D:91:ALA:HB1	38:D:5198:HOH:O	2.12	0.48
10:H:23:ILE:HG23	10:H:123:ILE:HD11	1.95	0.48
11:I:105:GLU:HA	11:I:108:HIS:NE2	2.28	0.48
12:J:6:PHE:HB3	12:J:109:TYR:OH	2.13	0.48
13:K:30:LYS:O	13:K:55:VAL:HG13	2.13	0.48
16:N:73:ALA:HB1	16:N:74:PRO:CD	2.43	0.48
22:T:87:VAL:HB	38:T:5545:HOH:O	2.13	0.48
25:W:149:LEU:CG	25:W:153:MET:HE2	2.31	0.48
27:Y:144:ARG:NE	38:Y:8910:HOH:O	2.46	0.48
1:0:120:A:H2'	1:0:120:A:N3	2.29	0.48
1:0:1118:A:C8	1:0:1119:G:H5''	2.48	0.48
1:0:1787:C:H4'	1:0:2883:A:O4'	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2314:G:C2'	1:0:2315:C:H5'	2.44	0.48
1:0:2800:A:H5'	1:0:2801:A:OP2	2.13	0.48
38:0:6088:HOH:O	30:2:20:ARG:HB3	2.13	0.48
4:B:315:VAL:HG23	4:B:316:ARG:HG2	1.96	0.48
5:C:7:ASP:C	5:C:9:ASP:H	2.21	0.48
9:G:71:LEU:C	9:G:73:ASP:H	2.21	0.48
11:I:100:VAL:HG11	11:I:124:VAL:CG2	2.43	0.48
14:L:73:VAL:HG11	14:L:118:LEU:HD21	1.95	0.48
14:L:149:ARG:O	14:L:150:GLN:HB2	2.14	0.48
23:U:44:ARG:HB3	38:U:3805:HOH:O	2.13	0.48
30:2:48:ASP:O	30:2:49:GLU:HB2	2.14	0.48
1:0:821:U:H2'	1:0:822:C:H6	1.78	0.48
4:B:171:VAL:O	4:B:175:LEU:HB2	2.14	0.48
5:C:2:GLN:HB3	38:C:8586:HOH:O	2.12	0.48
6:D:21:VAL:HG23	6:D:80:ALA:HB1	1.95	0.48
7:E:69:ILE:HA	7:E:72:MET:HE3	1.95	0.48
22:T:37:GLN:OE1	22:T:118:SER:HA	2.12	0.48
25:W:151:GLU:O	25:W:154:ARG:HB3	2.13	0.48
31:3:18:GLN:OE1	31:3:73:GLU:HB3	2.14	0.48
1:0:377:C:H5	38:0:3296:HOH:O	1.97	0.48
1:0:484:A:N1	1:0:506:G:H4'	2.29	0.48
1:0:952:G:N3	1:0:2302:A:H2'	2.28	0.48
7:E:81:GLU:HG2	7:E:134:SER:CB	2.43	0.48
7:E:126:ILE:HB	7:E:131:LEU:CD2	2.44	0.48
22:T:71:VAL:HG13	22:T:91:LEU:O	2.13	0.48
1:0:564:G:H1'	38:0:6268:HOH:O	2.12	0.48
1:0:1120:U:H5''	1:0:1120:U:C6	2.49	0.48
1:0:1641:A:H2'	1:0:1642:A:C5'	2.42	0.48
1:0:1972:U:H2'	1:0:1973:A:C5'	2.44	0.48
1:0:2050:G:H5''	20:R:80:TYR:O	2.13	0.48
10:H:12:ILE:HD12	10:H:57:THR:CG2	2.41	0.48
18:P:94:TRP:CZ2	18:P:98:ILE:HG13	2.48	0.48
23:U:47:ARG:HG3	38:U:4381:HOH:O	2.13	0.48
26:X:66:THR:HG23	26:X:67:PRO:HD2	1.95	0.48
1:0:170:U:H2'	1:0:171:C:H5'	1.94	0.48
1:0:1020:A:H1'	38:Q:6976:HOH:O	2.12	0.48
1:0:2362:A:H2'	1:0:2363:G:C8	2.49	0.48
1:0:2787:C:H2'	1:0:2788:A:O4'	2.13	0.48
1:0:2815:G:OP2	12:J:99:GLU:HG2	2.14	0.48
4:B:243:ASN:HA	4:B:244:PRO:C	2.39	0.48
7:E:69:ILE:HA	7:E:72:MET:HE2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:28:ALA:HB3	8:F:99:THR:HG23	1.94	0.48
8:F:50:VAL:CG2	8:F:63:ILE:HG21	2.44	0.48
10:H:30:LYS:N	10:H:62:HIS:HD2	2.07	0.48
25:W:88:THR:CG2	25:W:110:GLN:NE2	2.76	0.48
1:0:245:C:H2'	38:0:5530:HOH:O	2.14	0.47
1:0:1881:A:OP1	3:A:199:HIS:HE1	1.97	0.47
1:0:2597:U:H2'	1:0:2598:U:H5'	1.96	0.47
1:0:2909:G:H2'	1:0:2910:A:H8	1.79	0.47
38:0:7373:HOH:O	22:T:9:LYS:HD2	2.13	0.47
2:9:20:G:O2'	2:9:21:G:H5'	2.14	0.47
3:A:8:ARG:HG2	38:A:8850:HOH:O	2.13	0.47
7:E:7:ILE:HG22	7:E:45:ASP:O	2.14	0.47
15:M:47:ASP:CG	15:M:48:LYS:N	2.72	0.47
18:P:20:ARG:NH1	18:P:54:LYS:HD3	2.28	0.47
20:R:61:GLN:CD	38:R:8837:HOH:O	2.56	0.47
25:W:13:MET:HE2	25:W:18:GLN:N	2.29	0.47
28:Z:46:ARG:CD	28:Z:59:TYR:HB2	2.29	0.47
1:0:281:U:O2'	1:0:282:C:H5'	2.14	0.47
1:0:1353:C:P	38:0:4647:HOH:O	2.72	0.47
1:0:2421:G:H3'	1:0:2422:U:H5''	1.95	0.47
1:0:2768:A:H3'	38:0:4399:HOH:O	2.14	0.47
1:0:2897:C:H2'	1:0:2898:G:H8	1.78	0.47
38:0:6278:HOH:O	6:D:55:LYS:HB2	2.13	0.47
2:9:29:C:C2'	2:9:30:C:H5'	2.44	0.47
5:C:246:ARG:NH1	5:C:246:ARG:HB3	2.29	0.47
11:I:127:CYS:C	11:I:129:SER:H	2.21	0.47
16:N:116:PHE:HB3	16:N:136:LEU:HD23	1.96	0.47
20:R:47:LEU:O	20:R:51:ILE:HG13	2.14	0.47
24:V:1:THR:O	24:V:4:HIS:CE1	2.67	0.47
26:X:41:PHE:O	26:X:43:VAL:HG23	2.14	0.47
1:0:338:C:H4'	5:C:174:ILE:HD11	1.94	0.47
1:0:1427:A:H61	1:0:1440:U:H1'	1.79	0.47
1:0:2135:A:O2'	1:0:2136:G:H5'	2.14	0.47
1:0:2779:G:H21	7:E:143:GLN:NE2	2.11	0.47
3:A:33:GLU:OE1	3:A:33:GLU:N	2.43	0.47
15:M:48:LYS:HE3	15:M:52:GLN:NE2	2.28	0.47
16:N:170:GLU:O	16:N:174:GLU:HG3	2.14	0.47
16:N:181:ASP:O	16:N:184:ILE:HG22	2.15	0.47
24:V:7:GLU:O	24:V:11:MET:HG3	2.13	0.47
1:0:820:G:C6	3:A:171:LYS:HB2	2.48	0.47
6:D:10:PHE:N	38:D:7345:HOH:O	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:20:ILE:CD1	7:E:40:VAL:HG11	2.42	0.47
15:M:9:ARG:HG3	38:M:8846:HOH:O	2.14	0.47
21:S:73:ASP:OD1	21:S:76:GLU:HG3	2.14	0.47
1:O:907:A:H4'	1:O:1328:A:C2	2.49	0.47
1:O:1252:A:H2'	1:O:1253:C:O4'	2.15	0.47
1:O:1299:G:H5'	38:O:4049:HOH:O	2.13	0.47
1:O:2001:G:O2'	1:O:2002:C:H5'	2.14	0.47
38:O:3224:HOH:O	11:I:87:PRO:HD2	2.15	0.47
5:C:19:PRO:HG2	5:C:22:PHE:CE1	2.50	0.47
8:F:31:LYS:HE3	38:F:2623:HOH:O	2.14	0.47
25:W:69:ARG:NH2	38:W:4276:HOH:O	2.24	0.47
25:W:129:LYS:HG2	38:W:1990:HOH:O	2.14	0.47
1:O:371:U:H2'	1:O:372:A:H8	1.79	0.47
1:O:949:U:O2'	19:Q:40:HIS:HE1	1.97	0.47
1:O:1205:U:H2'	1:O:1206:U:H5'	1.97	0.47
1:O:1847:A:OP1	3:A:175:LYS:HG3	2.14	0.47
1:O:2851:G:C2'	1:O:2852:A:H5'	2.45	0.47
38:O:4165:HOH:O	27:Y:186:ARG:HD2	2.14	0.47
3:A:37:VAL:HG13	38:A:8909:HOH:O	2.13	0.47
4:B:24:PRO:HG2	4:B:204:GLY:HA2	1.95	0.47
5:C:22:PHE:HA	5:C:116:ALA:HA	1.96	0.47
8:F:57:GLU:O	8:F:61:MET:HG3	2.14	0.47
13:K:99:ASP:OD1	13:K:101:ASN:N	2.46	0.47
16:N:42:HIS:CG	16:N:62:HIS:HE1	2.32	0.47
27:Y:95:THR:N	27:Y:236:VAL:O	2.46	0.47
1:O:1044:C:H3'	1:O:1045:G:H5''	1.97	0.47
1:O:1163:G:N2	38:O:4693:HOH:O	2.45	0.47
1:O:1287:A:O4'	25:W:117:ARG:HD3	2.15	0.47
1:O:1853:C:O2'	3:A:217:ARG:NH2	2.47	0.47
38:O:7404:HOH:O	5:C:188:ARG:CD	2.61	0.47
3:A:94:LEU:HD12	3:A:98:GLU:HB2	1.96	0.47
3:A:153:ARG:HH11	3:A:153:ARG:CB	2.27	0.47
4:B:62:ARG:HG2	4:B:65:MET:HE3	1.96	0.47
4:B:205:VAL:O	4:B:307:ARG:NE	2.47	0.47
4:B:270:ILE:O	4:B:271:ASP:HB2	2.15	0.47
5:C:133:ARG:NE	5:C:138:VAL:HG22	2.30	0.47
8:F:111:ILE:O	8:F:115:VAL:HG23	2.15	0.47
10:H:65:LEU:H	10:H:65:LEU:HD22	1.79	0.47
11:I:133:THR:HG22	11:I:134:ILE:H	1.78	0.47
13:K:34:VAL:HG21	13:K:46:LYS:O	2.15	0.47
13:K:65:ARG:HD3	38:K:5358:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:118:ALA:HA	13:K:125:ALA:HB2	1.97	0.47
16:N:115:VAL:HG23	38:N:8860:HOH:O	2.15	0.47
18:P:98:ILE:HD12	18:P:102:ARG:NE	2.30	0.47
20:R:17:MET:HE1	20:R:19:ARG:CZ	2.44	0.47
22:T:41:ARG:NH1	22:T:42:VAL:O	2.48	0.47
26:X:8:ARG:NH1	38:X:2479:HOH:O	2.41	0.47
26:X:76:ARG:HG3	26:X:76:ARG:NH1	2.21	0.47
1:O:449:A:N7	5:C:43:LYS:HG2	2.30	0.47
1:O:475:G:OP1	5:C:73:LEU:HD22	2.15	0.47
1:O:783:C:OP1	3:A:180:LYS:HE3	2.14	0.47
1:O:1497:G:H4'	1:O:1627:G:O2'	2.14	0.47
13:K:55:VAL:CG1	13:K:56:SER:N	2.77	0.47
14:L:65:ASP:CG	14:L:111:ALA:HB3	2.40	0.47
14:L:89:PHE:N	38:L:8869:HOH:O	2.48	0.47
22:T:32:ARG:NH1	22:T:38:ARG:HH12	2.13	0.47
1:O:290:C:O2'	1:O:291:C:H5'	2.14	0.47
1:O:920:C:H5'	1:O:921:G:C4	2.50	0.47
16:N:82:TYR:C	16:N:82:TYR:CD2	2.93	0.47
24:V:58:THR:O	24:V:62:GLU:HG3	2.15	0.47
1:O:2252:A:C5	1:O:2253:G:H1'	2.50	0.47
1:O:2392:C:H4'	38:O:4243:HOH:O	2.14	0.47
1:O:2456:A:H5'	38:O:5653:HOH:O	2.15	0.47
6:D:23:VAL:HG12	6:D:130:VAL:HG22	1.97	0.47
10:H:66:GLU:HA	38:H:8580:HOH:O	2.15	0.47
10:H:91:ARG:NH1	10:H:138:THR:OG1	2.43	0.47
14:L:121:ILE:HA	14:L:141:GLU:O	2.14	0.47
28:Z:22:SER:O	28:Z:26:VAL:HG23	2.15	0.47
1:O:157:G:H4'	15:M:95:LYS:HE3	1.97	0.46
1:O:612:U:H2'	1:O:613:C:C6	2.50	0.46
3:A:131:HIS:O	3:A:132:ASP:HB2	2.14	0.46
3:A:217:ARG:HG2	3:A:229:ALA:HB2	1.97	0.46
8:F:60:VAL:O	8:F:60:VAL:HG12	2.15	0.46
16:N:163:PHE:O	16:N:164:ASP:O	2.32	0.46
25:W:4:LEU:O	25:W:32:CYS:HA	2.15	0.46
1:O:292:G:H2'	1:O:358:G:N2	2.29	0.46
2:9:28:U:H5''	16:N:40:ASN:ND2	2.30	0.46
7:E:154:ILE:HD11	7:E:157:LYS:HE2	1.97	0.46
15:M:99:ARG:CD	15:M:167:GLY:HA2	2.44	0.46
17:O:23:GLY:C	38:O:3062:HOH:O	2.59	0.46
17:O:78:ALA:C	17:O:98:LEU:HD13	2.40	0.46
22:T:71:VAL:HG12	22:T:72:ILE:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:951:A:C2'	1:0:952:G:H5'	2.45	0.46
1:0:1477:C:C5'	1:0:1868:G:H5''	2.45	0.46
38:0:4936:HOH:O	10:H:61:ARG:HG3	2.15	0.46
3:A:66:ARG:HH11	3:A:66:ARG:CB	2.28	0.46
3:A:105:VAL:HG13	3:A:155:THR:O	2.15	0.46
4:B:41:PHE:HA	4:B:79:MET:HE2	1.97	0.46
4:B:84:LEU:HD23	4:B:142:LEU:HD23	1.97	0.46
5:C:4:THR:HG21	5:C:12:THR:HG22	1.96	0.46
7:E:43:ASP:HA	38:E:5864:HOH:O	2.15	0.46
10:H:69:ARG:HB3	38:H:8580:HOH:O	2.15	0.46
26:X:70:ILE:HG23	26:X:70:ILE:O	2.15	0.46
1:0:303:C:H2'	1:0:304:G:O4'	2.16	0.46
1:0:542:A:H2'	1:0:543:G:O4'	2.15	0.46
1:0:1189:A:O2'	1:0:1208:C:H2'	2.15	0.46
2:9:31:C:H2'	2:9:32:G:O4'	2.16	0.46
2:9:49:G:H2'	2:9:50:G:O4'	2.16	0.46
4:B:42:ALA:HB1	4:B:308:LEU:HD11	1.97	0.46
8:F:110:ASP:O	8:F:114:LYS:HG3	2.15	0.46
11:I:95:LEU:O	11:I:134:ILE:HG23	2.15	0.46
11:I:126:THR:HG22	11:I:126:THR:O	2.14	0.46
1:0:392:U:C5'	15:M:193:LYS:HB3	2.46	0.46
1:0:1234:U:C4	4:B:244:PRO:HB3	2.51	0.46
1:0:2638:G:H5'	38:0:4893:HOH:O	2.16	0.46
1:0:2768:A:O2'	1:0:2769:C:H5'	2.15	0.46
2:9:107:C:H5	38:9:8634:HOH:O	1.99	0.46
3:A:153:ARG:HD3	38:A:8828:HOH:O	2.14	0.46
5:C:237:GLU:HB2	38:C:8633:HOH:O	2.15	0.46
6:D:57:THR:HG23	6:D:63:ILE:CA	2.41	0.46
6:D:62:ASP:HA	38:D:4233:HOH:O	2.16	0.46
14:L:104:ASP:O	14:L:105:TYR:HB3	2.15	0.46
15:M:99:ARG:HD2	15:M:167:GLY:HA2	1.96	0.46
16:N:89:GLY:O	16:N:92:ALA:HB3	2.15	0.46
1:0:1209:C:H2'	1:0:1210:G:H8	1.81	0.46
1:0:1503:U:H2'	1:0:1504:A:O4'	2.16	0.46
1:0:2044:G:OP1	26:X:23:HIS:HE1	1.98	0.46
1:0:2434:A:O3'	31:3:28:GLY:HA3	2.15	0.46
38:0:9615:HOH:O	8:F:38:LYS:HE2	2.15	0.46
3:A:132:ASP:OD1	3:A:133:ARG:N	2.45	0.46
4:B:238:ASN:ND2	4:B:240:GLY:H	2.02	0.46
6:D:41:LEU:HA	6:D:44:ILE:CG2	2.44	0.46
13:K:66:ARG:HG2	13:K:66:ARG:HH11	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:72:ASN:HB2	38:L:8880:HOH:O	2.16	0.46
19:Q:64:GLU:HG3	19:Q:74:ASP:OD2	2.16	0.46
20:R:114:VAL:HG13	20:R:114:VAL:O	2.15	0.46
28:Z:32:GLU:HA	28:Z:35:GLU:HG3	1.96	0.46
31:3:3:MET:HG3	31:3:4:PRO:HD2	1.98	0.46
31:3:18:GLN:HG2	38:3:8816:HOH:O	2.14	0.46
1:0:256:C:H2'	1:0:257:G:O4'	2.16	0.46
1:0:308:U:C4	1:0:342:C:H1'	2.50	0.46
1:0:1151:G:OP1	9:G:63:ARG:NH1	2.48	0.46
1:0:1819:G:H2'	1:0:1820:G:C4'	2.41	0.46
8:F:50:VAL:HG21	8:F:63:ILE:HG21	1.98	0.46
10:H:88:MET:HA	10:H:139:ALA:HA	1.98	0.46
15:M:169:ARG:NH1	38:M:8872:HOH:O	2.48	0.46
18:P:7:LYS:HD3	18:P:21:VAL:HG21	1.98	0.46
25:W:54:PHE:CZ	25:W:140:LYS:HB2	2.50	0.46
1:0:816:G:H5'	1:0:1598:A:H4'	1.97	0.46
1:0:1268:C:O2'	27:Y:169:ARG:HB2	2.16	0.46
1:0:1494:A:O2'	1:0:1505:U:O2	2.28	0.46
1:0:1555:G:H4'	1:0:1630:A:H2	1.79	0.46
1:0:2005:G:H3'	1:0:2005:G:OP2	2.16	0.46
1:0:2385:G:H2'	1:0:2386:U:C6	2.51	0.46
1:0:2421:G:H3'	1:0:2422:U:C5'	2.46	0.46
1:0:2837:U:H2'	38:0:6789:HOH:O	2.16	0.46
3:A:93:THR:HG23	3:A:154:ALA:O	2.16	0.46
5:C:54:LEU:HD23	5:C:79:ARG:HG3	1.98	0.46
7:E:126:ILE:HB	7:E:131:LEU:HD23	1.97	0.46
8:F:99:THR:HG23	8:F:99:THR:O	2.15	0.46
9:G:71:LEU:C	9:G:73:ASP:N	2.73	0.46
13:K:27:ARG:HD2	38:K:4747:HOH:O	2.16	0.46
21:S:53:ASN:HD22	21:S:53:ASN:N	2.14	0.46
24:V:49:LEU:O	24:V:53:ILE:HG13	2.16	0.46
31:3:15:ASN:ND2	38:3:8851:HOH:O	2.48	0.46
1:0:1123:A:C6	1:0:1238:C:H5'	2.51	0.46
1:0:1427:A:H61	1:0:1440:U:C1'	2.29	0.46
1:0:1595:G:O2'	1:0:1596:U:H5'	2.16	0.46
1:0:2906:A:H5'	1:0:2907:C:O4'	2.16	0.46
38:0:9889:HOH:O	12:J:46:ILE:HA	2.16	0.46
4:B:16:ARG:NE	38:B:8853:HOH:O	2.30	0.46
12:J:107:ASN:ND2	12:J:107:ASN:C	2.73	0.46
12:J:131:THR:HG22	12:J:133:GLY:N	2.31	0.46
14:L:10:SER:O	14:L:11:ARG:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:216:ARG:CD	38:Y:8868:HOH:O	2.64	0.46
30:2:10:ARG:HH11	30:2:49:GLU:CD	2.24	0.46
1:0:166:A:N7	14:L:25:GLY:HA2	2.31	0.46
1:0:1119:G:H8	12:J:52:GLN:NE2	2.14	0.46
1:0:1206:U:H2'	1:0:1207:A:O4'	2.16	0.46
1:0:1398:G:O2'	1:0:1399:A:H5'	2.16	0.46
2:9:64:C:C2'	2:9:65:A:H5'	2.46	0.46
4:B:54:VAL:HB	38:B:8914:HOH:O	2.15	0.46
4:B:313:PRO:O	4:B:314:ALA:C	2.58	0.46
5:C:136:VAL:HA	5:C:137:PRO:C	2.41	0.46
11:I:94:ASP:HA	11:I:133:THR:O	2.15	0.46
15:M:12:TRP:O	15:M:15:PRO:HD3	2.16	0.46
16:N:163:PHE:O	16:N:164:ASP:OD1	2.34	0.46
19:Q:30:VAL:HG12	19:Q:30:VAL:O	2.16	0.46
25:W:122:ARG:HG3	25:W:122:ARG:HH11	1.81	0.46
26:X:9:VAL:HG13	26:X:88:GLU:OE2	2.16	0.46
27:Y:106:THR:CG2	27:Y:107:PRO:HD2	2.45	0.46
31:3:30:GLN:NE2	38:3:8857:HOH:O	2.47	0.46
1:0:445:U:H2'	1:0:446:G:H8	1.81	0.45
1:0:1007:A:H2'	10:H:22:TYR:CZ	2.51	0.45
2:9:88:G:OP1	25:W:130:HIS:NE2	2.46	0.45
3:A:220:PRO:HD2	3:A:223:ARG:HD3	1.97	0.45
6:D:23:VAL:HG21	6:D:45:THR:HG21	1.99	0.45
7:E:11:VAL:CG1	7:E:12:ASP:N	2.77	0.45
17:O:44:ASN:OD1	17:O:65:LEU:HB2	2.16	0.45
19:Q:11:ARG:NH1	38:Q:5620:HOH:O	2.49	0.45
20:R:4:TYR:N	38:R:8844:HOH:O	2.49	0.45
20:R:47:LEU:HB2	20:R:89:LEU:HD21	1.98	0.45
1:0:702:G:O2'	1:0:703:G:H5'	2.16	0.45
1:0:1768:C:H2'	1:0:1769:C:O4'	2.16	0.45
1:0:1850:U:H2'	1:0:1851:G:H8	1.81	0.45
1:0:1996:U:O2'	1:0:1997:A:H5'	2.16	0.45
1:0:2793:A:H2'	1:0:2794:G:H5'	1.98	0.45
2:9:34:A:O5'	2:9:34:A:H8	1.99	0.45
4:B:62:ARG:NH2	4:B:66:GLU:O	2.48	0.45
6:D:40:ILE:HG23	38:D:5583:HOH:O	2.16	0.45
10:H:41:LYS:HD3	10:H:46:TYR:OH	2.16	0.45
10:H:86:TYR:CD1	10:H:86:TYR:C	2.94	0.45
10:H:149:VAL:HG13	38:H:8577:HOH:O	2.16	0.45
14:L:143:THR:CG2	14:L:144:ASP:N	2.76	0.45
20:R:39:THR:O	20:R:40:ALA:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:4:LEU:HD21	25:W:52:VAL:HG11	1.99	0.45
1:0:65:C:O2'	1:0:66:G:H5'	2.16	0.45
1:0:920:C:H5''	1:0:921:G:O5'	2.17	0.45
1:0:1333:U:H2'	1:0:1334:C:H6	1.82	0.45
1:0:1617:C:C4	1:0:1643:C:H4'	2.51	0.45
1:0:1790:C:H2'	1:0:1791:U:C6	2.50	0.45
1:0:2361:A:H5''	38:0:9001:HOH:O	2.17	0.45
1:0:2419:U:H5''	1:0:2420:G:H5'	1.99	0.45
1:0:2769:C:H2'	1:0:2770:G:H5'	1.99	0.45
1:0:2769:C:H2'	1:0:2770:G:C5'	2.45	0.45
1:0:2900:G:H2'	1:0:2901:C:O4'	2.16	0.45
5:C:72:LYS:HG2	5:C:77:ALA:HA	1.97	0.45
7:E:37:ASP:OD1	12:J:125:SER:HB3	2.16	0.45
12:J:93:ARG:HH11	12:J:93:ARG:CB	2.23	0.45
13:K:82:ARG:NH2	13:K:115:ARG:HG2	2.31	0.45
25:W:4:LEU:CD2	25:W:54:PHE:HB3	2.44	0.45
1:0:24:G:N2	1:0:518:G:H1'	2.32	0.45
1:0:249:G:O2'	1:0:250:C:H5'	2.17	0.45
1:0:944:G:C8	25:W:23:MET:HE1	2.52	0.45
1:0:1352:A:N1	5:C:48:SER:HB3	2.31	0.45
1:0:1419:U:H2'	1:0:1685:A:C2	2.52	0.45
1:0:1559:A:OP2	1:0:1559:A:H8	2.00	0.45
1:0:1845:A:O3'	3:A:187:PRO:HB2	2.16	0.45
2:9:20:G:H3'	38:9:8633:HOH:O	2.16	0.45
5:C:150:THR:HA	5:C:203:ALA:O	2.15	0.45
11:I:84:SER:HB3	11:I:92:VAL:CG2	2.47	0.45
15:M:49:ALA:C	15:M:54:TYR:HB3	2.42	0.45
16:N:143:ARG:NH1	16:N:173:ASP:OD2	2.49	0.45
16:N:183:ASP:O	16:N:184:ILE:O	2.34	0.45
1:0:278:A:H2'	1:0:279:C:O4'	2.16	0.45
1:0:289:G:O2'	1:0:290:C:H5'	2.16	0.45
1:0:709:G:O2'	17:O:25:VAL:CG1	2.64	0.45
4:B:248:ARG:NH2	38:B:8824:HOH:O	2.49	0.45
6:D:18:ILE:HD13	6:D:84:LEU:CD1	2.47	0.45
7:E:22:VAL:O	7:E:28:SER:HA	2.17	0.45
11:I:111:LEU:HD22	11:I:122:GLU:OE1	2.16	0.45
12:J:39:VAL:HG12	12:J:40:ASN:ND2	2.31	0.45
16:N:43:VAL:HG11	16:N:81:ALA:HA	1.97	0.45
17:O:39:THR:O	17:O:115:ARG:NH2	2.49	0.45
23:U:13:ILE:HG12	23:U:32:CYS:CB	2.46	0.45
25:W:108:ARG:NH2	38:W:2359:HOH:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:97:LEU:C	27:Y:98:GLN:HG2	2.42	0.45
1:O:100:C:H4'	22:T:16:LEU:HB2	1.98	0.45
1:O:138:U:OP2	1:O:139:C:H5	2.00	0.45
1:O:2498:C:O2'	1:O:2499:U:H5'	2.15	0.45
1:O:2714:U:H4'	4:B:10:SER:HB2	1.98	0.45
4:B:148:PRO:HD2	38:B:8880:HOH:O	2.16	0.45
6:D:41:LEU:CA	6:D:44:ILE:HG22	2.46	0.45
9:G:19:GLU:HG2	9:G:66:LEU:HD13	1.99	0.45
16:N:100:ALA:O	16:N:129:ILE:HG23	2.16	0.45
17:O:41:ALA:HA	38:O:5104:HOH:O	2.17	0.45
1:O:106:A:H2'	1:O:107:U:O4'	2.17	0.45
1:O:426:G:H2'	1:O:427:C:O4'	2.17	0.45
1:O:1853:C:OP1	3:A:231:LYS:HG3	2.16	0.45
3:A:135:VAL:HG21	3:A:147:ARG:HG2	1.98	0.45
4:B:41:PHE:HB3	4:B:190:MET:CE	2.46	0.45
4:B:268:ARG:NE	38:B:8909:HOH:O	2.50	0.45
5:C:7:ASP:OD1	5:C:11:ASN:O	2.34	0.45
7:E:31:ARG:HH12	7:E:68:HIS:CE1	2.35	0.45
10:H:172:GLU:CB	38:H:8591:HOH:O	2.20	0.45
14:L:143:THR:CG2	14:L:144:ASP:H	2.28	0.45
15:M:61:ILE:HG22	15:M:62:VAL:N	2.31	0.45
16:N:34:LEU:HA	16:N:47:LEU:HD23	1.99	0.45
16:N:73:ALA:HB1	16:N:74:PRO:HD2	1.97	0.45
16:N:147:ILE:HG23	16:N:148:ALA:N	2.31	0.45
16:N:183:ASP:O	16:N:184:ILE:C	2.60	0.45
29:1:28:HIS:HD2	29:1:30:LYS:H	1.64	0.45
1:O:86:A:C2	30:2:25:VAL:HG13	2.52	0.45
1:O:932:U:H2'	1:O:933:C:C6	2.52	0.45
1:O:1023:C:H2'	1:O:1024:G:O4'	2.16	0.45
1:O:2115:U:H2'	1:O:2116:U:C6	2.52	0.45
6:D:99:ASP:CB	6:D:103:ASN:H	2.30	0.45
6:D:173:GLU:O	6:D:174:VAL:C	2.60	0.45
7:E:112:ALA:HA	7:E:113:PRO:HD3	1.83	0.45
11:I:94:ASP:HB3	11:I:135:GLU:OE1	2.17	0.45
12:J:42:GLU:O	12:J:131:THR:HG23	2.17	0.45
13:K:98:VAL:CG1	13:K:99:ASP:N	2.80	0.45
14:L:35:ARG:C	14:L:35:ARG:HD3	2.41	0.45
24:V:39:ALA:O	24:V:41:GLU:N	2.50	0.45
25:W:38:THR:O	25:W:42:ARG:HB2	2.16	0.45
26:X:30:MET:CE	26:X:55:ASN:HA	2.46	0.45
27:Y:185:VAL:HG12	38:Y:8869:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:407:A:H8	38:0:4433:HOH:O	2.00	0.45
1:0:512:G:O3'	1:0:513:A:H8	2.00	0.45
1:0:1422:U:H2'	1:0:1423:C:C6	2.52	0.45
1:0:1450:C:C4'	1:0:1451:C:OP2	2.60	0.45
1:0:1482:A:O2'	1:0:1483:C:H5'	2.17	0.45
6:D:58:VAL:HG12	6:D:60:GLU:HG2	1.98	0.45
6:D:64:ARG:HG2	6:D:67:ASP:HB3	1.99	0.45
8:F:117:GLU:C	8:F:119:ARG:N	2.74	0.45
11:I:87:PRO:CB	11:I:129:SER:C	2.90	0.45
14:L:6:ARG:NH2	38:L:8849:HOH:O	2.50	0.45
15:M:134:ILE:CG2	15:M:141:ILE:HD13	2.45	0.45
24:V:1:THR:HG23	24:V:2:VAL:N	2.24	0.45
25:W:39:ASP:HB2	38:W:3580:HOH:O	2.17	0.45
25:W:90:TYR:CE2	25:W:99:ALA:HB2	2.51	0.45
1:0:68:U:O2'	1:0:69:A:H5''	2.17	0.45
1:0:1279:U:O2	1:0:1279:U:H2'	2.16	0.45
1:0:1730:G:C5'	1:0:1731:C:C6	3.00	0.45
10:H:72:ALA:HB2	10:H:156:ALA:HB2	1.99	0.45
16:N:37:ARG:HD3	36:N:8807:CL:CL	2.54	0.45
16:N:61:ALA:CB	16:N:88:ALA:HB2	2.47	0.45
17:O:53:GLN:HG2	17:O:56:GLU:OE1	2.17	0.45
17:O:96:VAL:CG1	17:O:100:GLN:HB2	2.47	0.45
20:R:12:THR:HG22	20:R:149:GLU:OE1	2.16	0.45
20:R:29:LYS:HD3	38:R:8830:HOH:O	2.16	0.45
22:T:32:ARG:CZ	22:T:38:ARG:NH1	2.80	0.45
23:U:11:THR:HG22	23:U:53:ASP:OD2	2.16	0.45
25:W:90:TYR:CD1	25:W:90:TYR:N	2.85	0.45
31:3:55:VAL:HB	31:3:56:PRO:HD2	1.98	0.45
1:0:319:A:H4'	1:0:338:C:C4	2.51	0.44
1:0:432:G:O2'	1:0:433:C:H5'	2.16	0.44
1:0:1250:C:O2'	1:0:1251:C:H5'	2.17	0.44
1:0:2002:C:H2'	1:0:2003:U:H5'	1.99	0.44
1:0:2036:C:C1'	13:K:44:LEU:HG	2.47	0.44
4:B:175:LEU:C	4:B:175:LEU:HD23	2.42	0.44
4:B:268:ARG:NH2	4:B:325:PRO:HG3	2.32	0.44
8:F:20:LEU:HD13	8:F:49:PHE:CE1	2.52	0.44
8:F:32:GLY:N	38:F:3111:HOH:O	2.50	0.44
8:F:34:ASN:HA	15:M:4:ALA:HB2	2.00	0.44
14:L:91:VAL:HB	38:L:8857:HOH:O	2.17	0.44
17:O:26:TRP:HA	17:O:26:TRP:CE3	2.52	0.44
18:P:141:ILE:C	18:P:143:ALA:H	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:816:G:C6	1:0:817:G:N1	2.85	0.44
1:0:1940:C:H4'	38:0:7297:HOH:O	2.15	0.44
1:0:2846:C:OP1	4:B:158:LYS:HD3	2.17	0.44
2:9:23:U:O2'	2:9:24:U:H4'	2.17	0.44
6:D:159:PRO:O	6:D:163:VAL:HG23	2.17	0.44
10:H:6:ALA:CA	10:H:61:ARG:HH12	2.29	0.44
10:H:167:LYS:HE2	10:H:169:GLU:OE1	2.18	0.44
13:K:20:CYS:HB2	13:K:29:LEU:HG	2.00	0.44
19:Q:11:ARG:HD3	38:Q:5620:HOH:O	2.16	0.44
21:S:57:THR:C	21:S:59:ASP:H	2.25	0.44
25:W:122:ARG:HG3	25:W:152:ALA:O	2.18	0.44
1:0:671:A:O2'	1:0:672:G:H2'	2.17	0.44
1:0:2104:C:O2	1:0:2485:A:N1	2.51	0.44
2:9:47:A:C2	2:9:48:C:C2	3.05	0.44
6:D:35:ALA:C	6:D:37:ALA:N	2.73	0.44
6:D:170:TYR:O	6:D:171:ASP:HB3	2.17	0.44
27:Y:154:ARG:NH1	27:Y:155:ARG:HG3	2.33	0.44
31:3:74:CYS:N	38:3:8865:HOH:O	2.50	0.44
1:0:656:G:OP2	17:O:37:ARG:HD2	2.18	0.44
1:0:960:G:N3	1:0:960:G:C2'	2.80	0.44
1:0:1882:C:O2'	1:0:2012:U:OP2	2.32	0.44
3:A:129:LEU:CD1	3:A:145:MET:HE1	2.48	0.44
3:A:135:VAL:HG11	3:A:147:ARG:NH1	2.33	0.44
4:B:36:PRO:CA	4:B:168:GLY:HA3	2.45	0.44
4:B:175:LEU:HD23	4:B:175:LEU:O	2.18	0.44
16:N:15:GLU:HB3	16:N:17:ARG:HG3	2.00	0.44
19:Q:4:ASN:ND2	38:Q:7115:HOH:O	2.51	0.44
22:T:49:GLU:HB3	22:T:59:GLU:HG2	1.99	0.44
22:T:73:HIS:CD2	22:T:88:PRO:HG3	2.52	0.44
24:V:12:THR:O	24:V:13:PRO:C	2.60	0.44
25:W:11:VAL:O	25:W:12:ASN:HB2	2.17	0.44
25:W:21:LEU:HB3	25:W:26:ILE:CG1	2.48	0.44
25:W:107:LEU:O	25:W:112:LEU:HB2	2.17	0.44
30:2:31:ARG:NH1	38:2:7177:HOH:O	2.50	0.44
1:0:587:A:H5''	38:0:7237:HOH:O	2.17	0.44
1:0:1783:A:O2'	1:0:1784:U:H5'	2.17	0.44
1:0:2667:G:H1'	1:0:2914:A:N3	2.32	0.44
1:0:2754:G:C2'	1:0:2755:G:H5'	2.48	0.44
2:9:14:G:O2'	16:N:1:ALA:HB2	2.17	0.44
3:A:173:GLY:O	3:A:176:HIS:HB3	2.17	0.44
5:C:127:ARG:CZ	5:C:225:PRO:HG2	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:49:PHE:HE1	8:F:98:VAL:HG23	1.82	0.44
14:L:57:VAL:HG12	14:L:57:VAL:O	2.17	0.44
20:R:122:GLN:HB3	20:R:138:SER:HB2	2.00	0.44
23:U:6:CYS:HB2	23:U:32:CYS:HB3	1.99	0.44
23:U:37:GLU:HB3	38:U:408:HOH:O	2.17	0.44
1:O:241:A:C2	1:O:378:A:H4'	2.53	0.44
1:O:1562:C:N4	38:O:5823:HOH:O	2.49	0.44
1:O:1613:C:H2'	1:O:1614:G:O4'	2.17	0.44
1:O:1942:A:H3'	38:O:7297:HOH:O	2.18	0.44
1:O:2515:C:H2'	1:O:2516:G:O4'	2.17	0.44
1:O:2724:U:H2'	1:O:2725:G:O4'	2.17	0.44
3:A:135:VAL:HG21	3:A:147:ARG:NH1	2.33	0.44
6:D:38:GLU:HB3	6:D:49:PRO:HG3	1.99	0.44
10:H:12:ILE:HG23	10:H:129:ARG:NE	2.32	0.44
15:M:78:LYS:HD3	38:M:8940:HOH:O	2.17	0.44
16:N:147:ILE:CG2	16:N:148:ALA:N	2.81	0.44
19:Q:64:GLU:OE1	19:Q:64:GLU:HA	2.17	0.44
1:O:1213:C:O2'	1:O:1214:G:H5'	2.17	0.44
1:O:1268:C:O2'	1:O:1269:G:H5'	2.17	0.44
1:O:1393:A:H2'	1:O:1394:C:C6	2.53	0.44
1:O:1441:G:H1'	38:O:7711:HOH:O	2.18	0.44
1:O:1552:G:H2'	1:O:1553:C:C6	2.53	0.44
1:O:1593:C:OP1	18:P:117:SER:HB3	2.18	0.44
1:O:2359:G:H3'	38:O:5649:HOH:O	2.17	0.44
3:A:186:TRP:CG	3:A:187:PRO:HA	2.53	0.44
4:B:74:ILE:HG13	38:B:8907:HOH:O	2.17	0.44
4:B:81:ALA:O	4:B:186:GLY:HA3	2.17	0.44
4:B:307:ARG:HH11	4:B:307:ARG:HB2	1.83	0.44
7:E:22:VAL:HG12	7:E:76:VAL:HG11	2.00	0.44
7:E:23:GLU:HG2	7:E:28:SER:CB	2.47	0.44
8:F:79:GLN:HG3	8:F:82:ASP:OD2	2.18	0.44
16:N:119:GLN:O	16:N:123:ILE:HG13	2.18	0.44
17:O:63:LYS:HG3	17:O:80:ASP:O	2.18	0.44
21:S:81:ILE:HG23	38:S:8538:HOH:O	2.17	0.44
23:U:6:CYS:C	23:U:8:TYR:H	2.24	0.44
1:O:553:G:OP2	27:Y:204:ARG:NH2	2.48	0.44
1:O:738:G:H3'	38:O:6999:HOH:O	2.18	0.44
1:O:834:G:H3'	1:O:835:U:H4'	1.99	0.44
1:O:951:A:O2'	1:O:952:G:H5'	2.17	0.44
1:O:1184:C:O2'	1:O:1185:U:OP2	2.32	0.44
1:O:1754:A:H2'	1:O:1755:A:O4'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:O:9106:HOH:O	5:C:103:ASN:HB3	2.17	0.44
4:B:84:LEU:HD23	4:B:178:ALA:HB1	2.00	0.44
4:B:312:ARG:HG2	4:B:313:PRO:N	2.32	0.44
5:C:84:VAL:O	5:C:85:LYS:HB2	2.18	0.44
5:C:214:THR:HB	38:C:8525:HOH:O	2.17	0.44
5:C:222:ASP:OD1	5:C:222:ASP:N	2.48	0.44
7:E:133:VAL:HG12	7:E:141:VAL:HG13	2.00	0.44
15:M:61:ILE:HD12	15:M:61:ILE:N	2.32	0.44
19:Q:25:PRO:HA	19:Q:26:PRO:HD3	1.81	0.44
30:2:40:ARG:HG3	30:2:45:ASN:CB	2.48	0.44
31:3:70:ARG:HD3	38:3:8877:HOH:O	2.17	0.44
1:O:583:C:H2'	1:O:584:U:H6	1.83	0.44
1:O:1015:C:H2'	1:O:1016:U:C6	2.52	0.44
1:O:1391:G:H2'	1:O:1392:A:H5'	1.99	0.44
1:O:2846:C:H4'	4:B:156:LYS:HB3	2.00	0.44
3:A:217:ARG:CG	3:A:217:ARG:NH1	2.77	0.44
4:B:7:ARG:HH11	4:B:7:ARG:CG	2.26	0.44
9:G:23:ILE:HD13	9:G:67:LEU:HD23	1.99	0.44
11:I:127:CYS:C	11:I:129:SER:N	2.76	0.44
12:J:90:LYS:HB2	36:J:8802:CL:CL	2.55	0.44
13:K:63:GLU:CG	38:K:6344:HOH:O	2.64	0.44
14:L:125:PHE:CE1	14:L:140:VAL:HG13	2.53	0.44
18:P:38:GLU:HA	18:P:41:ARG:NH1	2.33	0.44
22:T:92:ASP:OD1	22:T:94:SER:HB3	2.18	0.44
26:X:80:GLU:HB3	38:X:5564:HOH:O	2.16	0.44
1:O:585:C:H6	38:O:6051:HOH:O	2.00	0.43
1:O:2720:C:O2	13:K:87:ARG:NH2	2.50	0.43
1:O:2781:U:H2'	1:O:2782:G:C5'	2.48	0.43
2:9:3:A:H2	2:9:21:G:N3	2.16	0.43
2:9:114:G:H2'	2:9:115:C:C6	2.53	0.43
3:A:57:ALA:HA	3:A:67:LEU:HD23	2.00	0.43
5:C:157:LEU:HD22	5:C:162:VAL:HG12	2.00	0.43
6:D:58:VAL:HB	6:D:62:ASP:HB3	1.99	0.43
7:E:93:MET:HE1	7:E:165:GLY:H	1.81	0.43
7:E:125:GLU:HB2	7:E:132:THR:CG2	2.48	0.43
8:F:36:THR:HG23	8:F:97:ALA:HB2	2.00	0.43
11:I:87:PRO:HD3	38:I:6825:HOH:O	2.18	0.43
12:J:74:ARG:HH12	12:J:76:ASP:HB2	1.78	0.43
12:J:107:ASN:HD22	12:J:109:TYR:H	1.63	0.43
15:M:59:GLY:C	15:M:141:ILE:HD11	2.43	0.43
17:O:25:VAL:O	17:O:29:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Q:18:PRO:O	19:Q:21:ARG:HB2	2.18	0.43
30:2:49:GLU:HB2	38:2:719:HOH:O	2.17	0.43
31:3:91:GLN:O	31:3:92:GLU:HB2	2.18	0.43
1:0:23:G:H1'	1:0:520:A:N6	2.33	0.43
1:0:93:C:H5''	24:V:1:THR:HG21	1.99	0.43
1:0:321:A:H1'	38:0:6985:HOH:O	2.18	0.43
1:0:441:A:H1'	1:0:442:A:N7	2.33	0.43
1:0:2356:A:H2'	1:0:2357:G:O4'	2.18	0.43
1:0:2850:C:H5'	1:0:2850:C:C6	2.47	0.43
3:A:192:VAL:CG1	3:A:192:VAL:O	2.65	0.43
6:D:99:ASP:HB2	6:D:103:ASN:O	2.18	0.43
7:E:11:VAL:HG11	7:E:22:VAL:HG13	2.00	0.43
7:E:154:ILE:HG23	7:E:154:ILE:O	2.18	0.43
8:F:60:VAL:HG13	8:F:63:ILE:HG13	2.00	0.43
16:N:24:LEU:HD13	19:Q:26:PRO:HB3	2.00	0.43
16:N:114:LYS:O	16:N:117:ALA:HB3	2.18	0.43
21:S:10:VAL:HG11	24:V:36:ALA:CA	2.48	0.43
26:X:74:ALA:CB	26:X:85:VAL:HG22	2.48	0.43
1:0:162:C:H2'	1:0:163:U:H5'	2.00	0.43
1:0:812:A:H2'	1:0:813:C:O4'	2.17	0.43
1:0:1209:C:H4'	38:0:5241:HOH:O	2.19	0.43
1:0:1363:G:OP1	5:C:76:ARG:NH2	2.45	0.43
4:B:177:HIS:O	4:B:181:ILE:HG13	2.18	0.43
5:C:7:ASP:OD2	5:C:9:ASP:HB2	2.18	0.43
10:H:70:LEU:O	10:H:74:ARG:HB2	2.18	0.43
17:O:26:TRP:HA	17:O:26:TRP:HE3	1.82	0.43
25:W:3:ALA:O	25:W:54:PHE:HA	2.19	0.43
25:W:48:VAL:HG12	25:W:52:VAL:HB	1.99	0.43
26:X:74:ALA:HB2	26:X:85:VAL:CG1	2.48	0.43
28:Z:46:ARG:O	28:Z:57:CYS:HA	2.17	0.43
29:1:2:GLY:O	29:1:6:PRO:HG2	2.18	0.43
30:2:40:ARG:HA	30:2:45:ASN:ND2	2.34	0.43
1:0:661:G:C5	1:0:686:A:C2	3.06	0.43
1:0:2326:C:H4'	1:0:2412:G:H4'	2.01	0.43
1:0:2379:G:H5'	1:0:2381:C:O4'	2.18	0.43
38:0:4693:HOH:O	11:I:125:GLY:C	2.61	0.43
38:0:4697:HOH:O	16:N:21:HIS:HD2	2.01	0.43
2:9:57:A:C8	6:D:141:VAL:HG21	2.53	0.43
3:A:211:LYS:CB	38:A:8918:HOH:O	2.67	0.43
4:B:69:VAL:HA	4:B:70:PRO:HD3	1.87	0.43
6:D:35:ALA:HB3	38:D:3279:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:132:THR:HG23	7:E:132:THR:O	2.18	0.43
12:J:80:LYS:NZ	38:J:7377:HOH:O	2.50	0.43
16:N:38:LYS:HD2	16:N:114:LYS:HE3	2.01	0.43
24:V:39:ALA:C	24:V:41:GLU:N	2.76	0.43
30:2:20:ARG:CG	30:2:21:VAL:N	2.82	0.43
1:0:47:G:N3	1:0:114:A:C2	2.87	0.43
1:0:503:G:H2'	1:0:504:G:H8	1.84	0.43
1:0:581:G:H5'	38:0:7630:HOH:O	2.18	0.43
1:0:1242:A:OP2	12:J:60:ARG:NH2	2.45	0.43
1:0:1878:G:O2'	1:0:1879:U:OP2	2.37	0.43
3:A:37:VAL:HG22	38:A:8895:HOH:O	2.18	0.43
3:A:211:LYS:CB	3:A:212:PRO:HD2	2.33	0.43
4:B:16:ARG:NH2	38:B:8853:HOH:O	2.40	0.43
5:C:129:HIS:CE1	5:C:231:ARG:HA	2.54	0.43
10:H:149:VAL:HG22	38:H:8577:HOH:O	2.19	0.43
11:I:130:LEU:HB2	11:I:132:VAL:HG23	1.99	0.43
14:L:134:GLU:HG3	38:L:8856:HOH:O	2.18	0.43
15:M:95:LYS:HG2	15:M:99:ARG:HB3	1.99	0.43
16:N:73:ALA:N	38:N:8868:HOH:O	2.51	0.43
25:W:6:GLN:HA	25:W:52:VAL:HG23	2.00	0.43
26:X:9:VAL:HG13	26:X:88:GLU:OE1	2.19	0.43
28:Z:13:ARG:NH1	28:Z:14:PHE:CZ	2.86	0.43
30:2:5:LYS:O	30:2:9:LYS:HG3	2.18	0.43
1:0:291:C:H2'	1:0:292:G:O4'	2.19	0.43
1:0:949:U:H4'	19:Q:95:GLU:HA	1.99	0.43
2:9:28:U:H2'	2:9:29:C:C6	2.54	0.43
3:A:113:GLY:HA2	3:A:153:ARG:NH2	2.34	0.43
6:D:76:ARG:O	6:D:77:ASP:HB2	2.19	0.43
15:M:115:LEU:HD23	15:M:150:ILE:HD12	2.00	0.43
21:S:50:GLU:OE2	21:S:69:SER:HB3	2.19	0.43
25:W:48:VAL:HG12	25:W:48:VAL:O	2.18	0.43
26:X:18:ARG:NH1	38:X:4132:HOH:O	2.48	0.43
28:Z:42:CYS:SG	28:Z:44:GLU:HB2	2.58	0.43
1:0:1087:G:H4'	1:0:1088:A:OP1	2.19	0.43
1:0:1589:G:H4'	38:0:6807:HOH:O	2.18	0.43
1:0:1878:G:O2'	1:0:1879:U:H6	2.01	0.43
1:0:2132:C:H1'	15:M:124:GLY:HA3	2.01	0.43
1:0:2265:U:H2'	1:0:2266:A:H8	1.81	0.43
2:9:42:C:H5'	2:9:43:G:OP2	2.18	0.43
4:B:41:PHE:HA	4:B:79:MET:CE	2.47	0.43
8:F:14:ASP:O	8:F:18:GLU:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:120:ARG:NH2	18:P:123:TYR:CD2	2.87	0.43
21:S:39:ASP:O	21:S:40:ALA:C	2.61	0.43
23:U:9:CYS:HA	23:U:52:THR:CG2	2.45	0.43
1:0:226:A:H1'	1:0:393:G:C5	2.54	0.43
1:0:1299:G:N7	14:L:6:ARG:NH1	2.67	0.43
1:0:1380:U:H5'	38:0:9209:HOH:O	2.19	0.43
1:0:2456:A:H2'	1:0:2457:U:C6	2.53	0.43
38:0:5479:HOH:O	4:B:298:LYS:HD3	2.18	0.43
4:B:14:GLY:HA2	4:B:15:PRO:C	2.43	0.43
5:C:118:THR:HG22	5:C:137:PRO:HB3	2.00	0.43
5:C:142:ASP:OD1	5:C:236:THR:HG23	2.18	0.43
6:D:67:ASP:O	6:D:69:ILE:HG13	2.18	0.43
8:F:43:GLY:C	8:F:45:ALA:H	2.26	0.43
38:K:7438:HOH:O	23:U:20:MET:HE1	2.19	0.43
19:Q:28:ARG:HG2	38:Q:4350:HOH:O	2.18	0.43
29:1:22:CYS:SG	29:1:24:GLU:HB2	2.58	0.43
1:0:87:C:H2'	30:2:28:LYS:O	2.19	0.43
1:0:195:C:H2'	1:0:196:G:H5'	2.01	0.43
1:0:451:C:O2'	1:0:452:G:H5'	2.19	0.43
1:0:1131:G:C6	1:0:1230:A:C4	3.07	0.43
1:0:1167:G:O2'	1:0:1168:C:H5'	2.18	0.43
1:0:1172:G:H5''	38:0:7212:HOH:O	2.19	0.43
1:0:1925:G:O2'	1:0:1926:G:H5'	2.19	0.43
1:0:2896:A:OP1	26:X:15:ARG:NH1	2.51	0.43
38:9:8665:HOH:O	16:N:147:ILE:HD12	2.18	0.43
7:E:10:ASP:HA	38:E:3707:HOH:O	2.19	0.43
8:F:22:VAL:CG2	8:F:104:ALA:HB2	2.49	0.43
10:H:66:GLU:O	10:H:70:LEU:HB2	2.19	0.43
10:H:87:LYS:HB2	10:H:87:LYS:NZ	2.33	0.43
29:1:8:GLN:HE22	29:1:11:LYS:HZ1	1.63	0.43
31:3:34:LYS:HD2	31:3:34:LYS:N	2.33	0.43
1:0:920:C:H4'	1:0:921:G:C2	2.53	0.43
1:0:1021:G:O2'	1:0:1022:A:H5'	2.19	0.43
1:0:1470:A:OP1	15:M:93:ARG:HD2	2.18	0.43
1:0:1943:C:O4'	3:A:212:PRO:HA	2.19	0.43
1:0:2387:U:H2'	1:0:2388:C:C6	2.54	0.43
2:9:92:G:C6	2:9:93:A:C6	3.07	0.43
8:F:60:VAL:O	8:F:60:VAL:CG1	2.67	0.43
16:N:49:THR:HB	16:N:58:LEU:CD1	2.49	0.43
23:U:34:SER:HA	23:U:37:GLU:OE1	2.19	0.43
25:W:65:VAL:CA	25:W:68:THR:HG22	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:105:LYS:HE2	27:Y:198:GLY:O	2.19	0.43
29:1:25:LYS:HD2	30:2:48:ASP:CA	2.48	0.43
1:0:703:G:O2'	1:0:704:C:H5'	2.19	0.42
1:0:827:A:H2'	1:0:828:G:O4'	2.19	0.42
1:0:1109:U:O4	12:J:21:ARG:HA	2.19	0.42
1:0:1163:G:N2	38:0:6005:HOH:O	2.51	0.42
1:0:2831:C:H2'	1:0:2832:C:H5'	2.01	0.42
4:B:217:ARG:CD	4:B:257:THR:HG22	2.49	0.42
5:C:107:ARG:NH1	5:C:107:ARG:HB3	2.34	0.42
16:N:120:GLU:HG3	16:N:136:LEU:HD13	2.01	0.42
20:R:18:LEU:HG	20:R:91:LEU:HD13	2.00	0.42
1:0:324:G:O2'	1:0:325:U:H5'	2.20	0.42
1:0:488:U:H2'	38:0:3984:HOH:O	2.18	0.42
1:0:612:U:H2'	1:0:613:C:H6	1.84	0.42
1:0:969:G:H1	1:0:999:C:H42	1.67	0.42
1:0:1684:A:O2'	1:0:1685:A:H5''	2.18	0.42
1:0:1702:U:H5'	38:0:3411:HOH:O	2.19	0.42
1:0:1771:U:O2'	1:0:1773:G:N7	2.49	0.42
1:0:2415:A:O2'	16:N:29:SER:HB3	2.19	0.42
1:0:2504:A:H4'	10:H:74:ARG:HH11	1.84	0.42
38:0:3737:HOH:O	22:T:9:LYS:CD	2.65	0.42
38:0:6207:HOH:O	23:U:56:ARG:HD3	2.19	0.42
3:A:51:ARG:HB2	38:A:8905:HOH:O	2.18	0.42
3:A:101:GLU:OE2	3:A:131:HIS:HB2	2.18	0.42
4:B:54:VAL:O	4:B:55:ASN:C	2.62	0.42
5:C:27:ARG:HG2	5:C:30:LEU:HD12	2.01	0.42
6:D:86:THR:O	6:D:90:LEU:HG	2.19	0.42
10:H:81:GLY:C	10:H:83:GLU:H	2.27	0.42
14:L:73:VAL:HG23	14:L:74:THR:N	2.34	0.42
15:M:98:GLN:O	15:M:102:GLU:HG3	2.19	0.42
18:P:94:TRP:CH2	18:P:98:ILE:HG13	2.54	0.42
22:T:24:ARG:HH21	22:T:39:ASN:HD22	1.67	0.42
25:W:13:MET:HE1	25:W:21:LEU:HD12	2.01	0.42
1:0:1174:A:C5	1:0:1201:C:H4'	2.54	0.42
1:0:2784:A:H1'	7:E:60:SER:OG	2.19	0.42
1:0:2883:A:H2'	1:0:2884:G:O4'	2.20	0.42
2:9:56:A:C3'	2:9:57:A:H5''	2.48	0.42
2:9:57:A:O2'	6:D:152:PRO:HD2	2.19	0.42
3:A:128:LEU:HD21	3:A:131:HIS:HE1	1.85	0.42
4:B:102:THR:CG2	4:B:182:VAL:HG12	2.50	0.42
5:C:133:ARG:HD2	38:C:8613:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:20:LYS:HA	6:D:75:LEU:O	2.20	0.42
7:E:15:GLN:HG3	7:E:20:ILE:HG12	2.00	0.42
7:E:81:GLU:HA	7:E:133:VAL:O	2.20	0.42
16:N:44:ARG:HG3	16:N:45:ALA:N	2.34	0.42
21:S:29:ASP:OD1	21:S:31:ARG:NH1	2.52	0.42
25:W:125:HIS:HD2	25:W:127:GLY:H	1.67	0.42
27:Y:122:ARG:NH2	38:Y:8834:HOH:O	2.51	0.42
1:0:682:A:H2'	1:0:683:G:O4'	2.19	0.42
1:0:1406:A:H4'	1:0:1407:A:H5''	2.01	0.42
1:0:2092:G:H2'	1:0:2613:G:OP1	2.20	0.42
3:A:17:ARG:HD2	38:A:8838:HOH:O	2.20	0.42
4:B:23:THR:HG23	4:B:162:MET:HE3	2.01	0.42
4:B:72:THR:HB	38:B:8907:HOH:O	2.19	0.42
6:D:104:PHE:CE2	6:D:132:VAL:HB	2.55	0.42
10:H:50:ILE:HG21	38:H:8577:HOH:O	2.19	0.42
22:T:38:ARG:HG3	22:T:38:ARG:HH11	1.84	0.42
1:0:10:U:O4	1:0:532:A:OP2	2.38	0.42
1:0:419:A:H1'	1:0:1921:A:C2	2.54	0.42
1:0:1495:C:H1'	1:0:1573:A:H1'	2.02	0.42
1:0:1624:A:H5'	1:0:1626:A:O4'	2.19	0.42
1:0:1730:G:H5''	1:0:1731:C:C6	2.52	0.42
1:0:1761:U:H5'	18:P:81:LYS:O	2.20	0.42
1:0:2719:A:C2	4:B:70:PRO:HG3	2.54	0.42
7:E:31:ARG:HH12	7:E:68:HIS:CD2	2.37	0.42
8:F:20:LEU:O	8:F:23:ALA:HB3	2.19	0.42
8:F:56:PRO:CG	15:M:44:THR:HA	2.50	0.42
17:O:35:LYS:HD3	38:O:3360:HOH:O	2.18	0.42
21:S:17:ASP:HB3	21:S:23:LYS:HB2	2.01	0.42
26:X:25:ARG:O	26:X:26:ALA:C	2.63	0.42
27:Y:184:GLU:CD	27:Y:204:ARG:HH11	2.27	0.42
28:Z:19:GLY:O	28:Z:23:ARG:HG2	2.19	0.42
1:0:255:A:H2'	1:0:256:C:O4'	2.19	0.42
1:0:1201:C:H5''	38:O:6193:HOH:O	2.19	0.42
1:0:1423:C:O2'	1:0:1424:A:H5'	2.19	0.42
1:0:1657:A:H2'	1:0:1658:A:C8	2.55	0.42
1:0:1762:C:H2'	1:0:1763:C:H6	1.84	0.42
1:0:2326:C:H4'	1:0:2412:G:C4'	2.49	0.42
1:0:2453:G:H5''	38:L:8842:HOH:O	2.19	0.42
1:0:2503:A:OP1	10:H:154:ARG:NH2	2.45	0.42
38:O:6240:HOH:O	28:Z:33:MET:HE3	2.19	0.42
4:B:55:ASN:HB3	4:B:64:GLY:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:117:ARG:O	10:H:118:ALA:C	2.63	0.42
16:N:38:LYS:HE3	16:N:38:LYS:HB2	1.77	0.42
16:N:163:PHE:HZ	16:N:171:HIS:HD1	1.65	0.42
1:0:212:A:O4'	1:0:214:U:C6	2.73	0.42
1:0:812:A:H1'	38:0:3936:HOH:O	2.18	0.42
1:0:1167:G:H4'	11:I:130:LEU:HD22	2.02	0.42
1:0:1334:C:H2'	1:0:1335:C:H6	1.85	0.42
1:0:1377:C:H1'	38:0:9033:HOH:O	2.19	0.42
1:0:1461:U:H2'	1:0:1462:C:C6	2.54	0.42
1:0:1730:G:H5'	1:0:1731:C:C5	2.54	0.42
1:0:2072:G:C6	1:0:2533:C:H1'	2.54	0.42
1:0:2694:A:C4'	7:E:91:PHE:HE1	2.26	0.42
1:0:2821:C:H4'	4:B:116:PRO:HB3	2.01	0.42
1:0:2866:U:H4'	1:0:2867:G:H5'	2.01	0.42
38:0:4592:HOH:O	3:A:6:GLY:HA3	2.20	0.42
38:0:7503:HOH:O	31:3:60:LYS:HG3	2.18	0.42
3:A:114:ASP:C	3:A:114:ASP:OD1	2.62	0.42
5:C:154:VAL:O	5:C:158:GLU:HG3	2.20	0.42
6:D:170:TYR:CD1	6:D:170:TYR:N	2.88	0.42
7:E:11:VAL:CG1	7:E:12:ASP:H	2.33	0.42
7:E:16:ASP:O	7:E:17:HIS:HB2	2.19	0.42
9:G:63:ARG:N	38:G:2569:HOH:O	2.53	0.42
10:H:80:LEU:HD12	10:H:86:TYR:CD2	2.55	0.42
10:H:83:GLU:HA	38:H:8584:HOH:O	2.20	0.42
11:I:66:GLY:O	11:I:67:VAL:C	2.62	0.42
15:M:28:GLN:HA	15:M:31:TRP:HB2	2.01	0.42
16:N:24:LEU:O	16:N:28:LYS:HG3	2.20	0.42
16:N:62:HIS:O	16:N:65:ASP:OD1	2.37	0.42
25:W:88:THR:HG22	25:W:90:TYR:HD1	1.85	0.42
30:2:18:ASN:O	30:2:18:ASN:ND2	2.53	0.42
31:3:70:ARG:CB	38:3:8877:HOH:O	2.67	0.42
1:0:222:A:H2'	1:0:223:G:O4'	2.19	0.42
1:0:327:A:H4'	1:0:329:A:C8	2.55	0.42
1:0:371:U:H2'	1:0:372:A:C8	2.55	0.42
1:0:470:U:O2'	29:1:16:HIS:CD2	2.68	0.42
1:0:1119:G:H22	1:0:1246:A:H2	1.58	0.42
1:0:2547:C:OP2	4:B:5:ARG:NH1	2.53	0.42
1:0:2716:G:C5'	4:B:206:THR:HG21	2.42	0.42
4:B:60:SER:C	4:B:62:ARG:H	2.28	0.42
5:C:129:HIS:HD2	5:C:165:ASP:OD2	2.01	0.42
5:C:138:VAL:O	5:C:234:VAL:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:91:ALA:HB2	6:D:106:PHE:CD2	2.54	0.42
14:L:36:ASP:HB2	38:L:8836:HOH:O	2.19	0.42
16:N:179:LEU:HD23	16:N:184:ILE:CD1	2.50	0.42
26:X:25:ARG:HD2	38:X:3861:HOH:O	2.19	0.42
26:X:43:VAL:HG11	26:X:82:GLU:HA	2.02	0.42
1:O:130:C:H5'	38:O:5173:HOH:O	2.19	0.42
1:O:189:A:OP1	15:M:171:ARG:NH2	2.52	0.42
1:O:366:U:H2'	1:O:367:G:O4'	2.19	0.42
1:O:485:A:O2'	1:O:487:G:H5'	2.20	0.42
1:O:544:G:H2'	1:O:545:G:C5'	2.46	0.42
1:O:1298:U:H2'	1:O:1299:G:C8	2.54	0.42
1:O:1375:A:C2'	1:O:1376:G:H5'	2.50	0.42
1:O:1702:U:H1'	38:O:5732:HOH:O	2.20	0.42
1:O:2472:C:O2'	1:O:2634:G:H4'	2.20	0.42
9:G:64:ASN:O	9:G:68:GLU:HG3	2.20	0.42
10:H:46:TYR:HA	10:H:47:PRO:HD3	1.78	0.42
11:I:96:SER:H	11:I:99:GLN:NE2	2.18	0.42
14:L:126:SER:O	14:L:127:GLU:C	2.61	0.42
15:M:72:ALA:HB2	15:M:93:ARG:HG2	2.00	0.42
21:S:57:THR:HG23	38:S:8530:HOH:O	2.19	0.42
22:T:113:GLU:O	22:T:114:SER:C	2.62	0.42
23:U:33:SER:O	23:U:37:GLU:HG3	2.20	0.42
25:W:4:LEU:HD23	25:W:4:LEU:HA	1.85	0.42
25:W:48:VAL:CG1	25:W:48:VAL:O	2.67	0.42
27:Y:189:ASN:CA	27:Y:217:ILE:HD11	2.47	0.42
1:O:247:A:H2'	38:O:3902:HOH:O	2.19	0.42
1:O:567:U:H5''	38:W:5817:HOH:O	2.19	0.42
1:O:922:A:N7	1:O:2281:C:H5'	2.35	0.42
1:O:1415:G:H5'	29:1:12:ASN:O	2.19	0.42
1:O:1829:A:H2'	1:O:1830:C:H5'	2.02	0.42
2:9:3:A:OP2	2:9:25:G:N2	2.53	0.42
3:A:192:VAL:HG12	3:A:192:VAL:O	2.19	0.42
4:B:271:ASP:HB3	4:B:296:LEU:HD12	2.01	0.42
4:B:320:GLN:NE2	4:B:321:PRO:CD	2.80	0.42
5:C:185:LYS:HD3	5:C:186:TYR:CE1	2.55	0.42
7:E:24:GLY:CA	7:E:76:VAL:HB	2.50	0.42
7:E:108:LEU:HD11	7:E:164:ASP:HB2	2.02	0.42
10:H:139:ALA:HB3	10:H:149:VAL:HG21	2.02	0.42
10:H:141:CYS:HB2	38:H:8545:HOH:O	2.20	0.42
16:N:21:HIS:HB2	38:N:8833:HOH:O	2.19	0.42
16:N:58:LEU:N	16:N:58:LEU:HD12	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:47:ARG:CG	38:U:4381:HOH:O	2.67	0.42
25:W:21:LEU:CD2	25:W:48:VAL:HG11	2.42	0.42
26:X:76:ARG:NH1	26:X:76:ARG:CG	2.81	0.42
27:Y:126:PRO:HG2	27:Y:128:PHE:CZ	2.55	0.42
27:Y:220:GLU:HG2	38:Y:8847:HOH:O	2.19	0.42
1:0:172:U:H5'	38:0:4135:HOH:O	2.18	0.41
1:0:177:A:H2'	1:0:178:U:O4'	2.19	0.41
1:0:317:A:OP1	22:T:52:ARG:O	2.38	0.41
1:0:1181:A:H2'	1:0:1182:C:O4'	2.20	0.41
1:0:1887:U:OP1	28:Z:21:VAL:HG23	2.20	0.41
1:0:2324:G:H4'	1:0:2418:G:O2'	2.20	0.41
1:0:2681:A:H4'	1:0:2682:C:H5'	2.02	0.41
1:0:2880:A:H2'	1:0:2881:C:H5'	2.02	0.41
4:B:55:ASN:CB	4:B:63:GLU:HA	2.46	0.41
4:B:146:THR:O	4:B:159:PRO:HB3	2.19	0.41
5:C:49:ASP:HB3	5:C:52:ALA:HB2	2.02	0.41
7:E:145:ALA:HB1	7:E:168:ILE:CD1	2.49	0.41
16:N:86:LEU:HD21	16:N:180:LEU:HD11	2.02	0.41
21:S:8:PRO:HD2	24:V:32:ALA:HA	2.02	0.41
22:T:38:ARG:NH1	22:T:38:ARG:HG3	2.35	0.41
29:1:8:GLN:NE2	29:1:11:LYS:NZ	2.64	0.41
30:2:11:LEU:HD23	30:2:11:LEU:HA	1.85	0.41
1:0:74:G:H2'	1:0:75:U:C6	2.54	0.41
1:0:1460:G:OP1	3:A:17:ARG:NH1	2.52	0.41
1:0:1789:G:H2'	1:0:1790:C:O5'	2.20	0.41
38:0:3224:HOH:O	11:I:87:PRO:CD	2.68	0.41
4:B:153:SER:HB2	4:B:287:TYR:CZ	2.54	0.41
5:C:102:LEU:HD12	38:C:8515:HOH:O	2.20	0.41
5:C:188:ARG:NH2	38:C:8524:HOH:O	2.53	0.41
11:I:88:GLN:NE2	11:I:128:THR:HG21	2.35	0.41
14:L:35:ARG:O	14:L:40:PHE:HA	2.20	0.41
15:M:122:GLN:OE1	15:M:127:LYS:HE2	2.19	0.41
27:Y:108:ASP:OD1	27:Y:108:ASP:N	2.52	0.41
31:3:31:THR:HB	31:3:33:MET:HE3	2.03	0.41
1:0:130:C:H2'	38:0:3149:HOH:O	2.19	0.41
1:0:677:C:O2'	1:0:678:G:H5'	2.20	0.41
1:0:1515:A:H2'	1:0:1516:U:C6	2.55	0.41
1:0:1625:U:H6	1:0:1625:U:H3'	1.85	0.41
1:0:1654:U:H2'	3:A:47:HIS:CD2	2.54	0.41
1:0:1819:G:H2'	1:0:1820:G:C5'	2.50	0.41
1:0:2036:C:C4'	13:K:44:LEU:HG	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2353:A:H4'	1:0:2354:A:O5'	2.19	0.41
1:0:2445:U:H2'	1:0:2446:G:H8	1.84	0.41
2:9:11:A:O2'	2:9:12:C:H3'	2.19	0.41
4:B:30:PRO:HB2	4:B:39:GLN:HE21	1.85	0.41
4:B:149:ASP:HB2	38:B:8880:HOH:O	2.21	0.41
4:B:175:LEU:C	4:B:175:LEU:CD2	2.94	0.41
4:B:180:ASP:O	4:B:181:ILE:C	2.64	0.41
6:D:81:GLU:C	6:D:83:PHE:N	2.78	0.41
9:G:12:ILE:HG22	9:G:17:GLN:HE21	1.83	0.41
16:N:151:ASP:OD2	16:N:165:ALA:O	2.38	0.41
22:T:45:GLY:C	38:T:3851:HOH:O	2.63	0.41
25:W:26:ILE:O	25:W:26:ILE:CG1	2.67	0.41
25:W:69:ARG:NE	38:W:4276:HOH:O	2.48	0.41
25:W:73:LEU:HD12	25:W:73:LEU:HA	1.67	0.41
29:1:28:HIS:O	29:1:32:LYS:N	2.52	0.41
1:0:113:A:H2'	1:0:115:U:O4	2.20	0.41
1:0:137:U:OP1	1:0:259:G:O2'	2.38	0.41
1:0:538:C:H5''	1:0:539:G:C8	2.55	0.41
1:0:664:U:O4	1:0:681:G:H5''	2.20	0.41
1:0:1711:A:O2'	1:0:1712:A:H5'	2.20	0.41
1:0:1850:U:H2'	1:0:1851:G:C8	2.55	0.41
1:0:1973:A:H2'	1:0:1974:G:O4'	2.21	0.41
4:B:109:LEU:HG	4:B:113:LEU:HD12	2.02	0.41
4:B:224:LYS:HA	4:B:224:LYS:HD3	1.95	0.41
5:C:170:ASP:C	5:C:171:GLU:HG3	2.45	0.41
6:D:57:THR:HG23	6:D:63:ILE:HG22	2.03	0.41
10:H:115:GLY:N	38:H:8589:HOH:O	2.54	0.41
15:M:39:ARG:NH2	38:M:8922:HOH:O	2.53	0.41
24:V:12:THR:H	24:V:15:GLU:HB2	1.85	0.41
1:0:645:U:OP2	14:L:4:LYS:CE	2.63	0.41
1:0:821:U:H2'	1:0:822:C:C6	2.56	0.41
1:0:1314:U:H2'	38:0:5832:HOH:O	2.20	0.41
1:0:1398:G:H2'	1:0:1399:A:C8	2.55	0.41
1:0:1904:A:H2'	1:0:1905:U:O4'	2.20	0.41
1:0:1973:A:H5'	1:0:1973:A:C8	2.52	0.41
1:0:2588:OMG:H3'	1:0:2589:U:H5''	2.02	0.41
4:B:195:ARG:HD2	4:B:324:ASP:OD1	2.21	0.41
4:B:255:GLY:O	4:B:257:THR:HG23	2.20	0.41
5:C:7:ASP:O	5:C:9:ASP:N	2.53	0.41
12:J:45:VAL:HG22	12:J:46:ILE:N	2.34	0.41
16:N:93:GLN:HG2	38:N:8858:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:108:SER:HA	16:N:109:PRO:HD3	1.85	0.41
16:N:152:GLU:C	16:N:154:LEU:N	2.78	0.41
16:N:163:PHE:O	16:N:164:ASP:CG	2.63	0.41
18:P:98:ILE:O	18:P:98:ILE:HD13	2.20	0.41
20:R:145:LEU:HD12	20:R:146:ILE:N	2.36	0.41
24:V:12:THR:CG2	24:V:15:GLU:HG3	2.35	0.41
24:V:60:GLN:O	24:V:65:ASP:N	2.52	0.41
25:W:59:GLN:NE2	25:W:97:ALA:HB3	2.35	0.41
25:W:146:ILE:HD13	25:W:146:ILE:HA	1.85	0.41
27:Y:107:PRO:HD3	27:Y:182:PHE:CE1	2.55	0.41
1:O:947:U:O2'	1:O:948:G:H5'	2.20	0.41
1:O:1500:U:P	18:P:41:ARG:HH22	2.43	0.41
1:O:2000:G:O2'	1:O:2001:G:H5'	2.20	0.41
1:O:2832:C:H5	38:O:7166:HOH:O	2.04	0.41
5:C:107:ARG:HB3	5:C:107:ARG:CZ	2.50	0.41
6:D:16:PRO:HB2	6:D:165:PHE:CG	2.56	0.41
6:D:23:VAL:HG11	6:D:83:PHE:CZ	2.55	0.41
12:J:6:PHE:O	12:J:8:ALA:N	2.53	0.41
15:M:42:ARG:HA	15:M:43:PRO:HD3	1.91	0.41
16:N:157:PRO:HA	38:N:8826:HOH:O	2.21	0.41
19:Q:66:LYS:HB2	19:Q:70:ALA:O	2.21	0.41
26:X:72:VAL:HG22	26:X:85:VAL:CG1	2.43	0.41
27:Y:219:GLU:HG3	27:Y:220:GLU:N	2.35	0.41
1:O:245:C:H2'	1:O:246:G:H5'	2.03	0.41
1:O:705:C:O2	1:O:705:C:H2'	2.21	0.41
1:O:737:A:H2'	1:O:738:G:O4'	2.20	0.41
1:O:764:C:H2'	1:O:765:G:O4'	2.20	0.41
1:O:1773:G:N2	1:O:1774:G:C8	2.88	0.41
1:O:2764:C:O2'	1:O:2765:C:H5'	2.20	0.41
5:C:140:VAL:CG1	5:C:141:SER:N	2.84	0.41
6:D:65:GLU:HA	38:D:6752:HOH:O	2.20	0.41
12:J:54:VAL:HG11	12:J:138:THR:HG21	2.02	0.41
15:M:125:ARG:HD3	38:M:8897:HOH:O	2.20	0.41
26:X:25:ARG:HG2	38:X:5356:HOH:O	2.20	0.41
29:1:25:LYS:HE2	38:2:7213:HOH:O	2.20	0.41
1:O:153:C:P	38:O:6803:HOH:O	2.79	0.41
1:O:164:G:O3'	14:L:30:ARG:HB2	2.21	0.41
1:O:317:A:H5'	38:O:3753:HOH:O	2.19	0.41
1:O:1015:C:H2'	1:O:1016:U:H6	1.85	0.41
1:O:1594:C:O2'	1:O:1607:A:H4'	2.21	0.41
1:O:2840:A:H3'	38:O:7595:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:O:7401:HOH:O	4:B:211:THR:HG21	2.20	0.41
2:9:57:A:H8	6:D:141:VAL:HG21	1.86	0.41
4:B:24:PRO:HG3	4:B:204:GLY:HA2	2.03	0.41
4:B:102:THR:HG23	4:B:182:VAL:HG12	2.03	0.41
8:F:13:GLU:OE2	8:F:78:GLU:HG2	2.21	0.41
8:F:100:ASP:HB3	38:F:5691:HOH:O	2.19	0.41
10:H:69:ARG:CZ	38:H:8580:HOH:O	2.69	0.41
14:L:24:ALA:HB2	14:L:30:ARG:HD2	2.03	0.41
14:L:34:GLY:HA3	14:L:38:HIS:CE1	2.56	0.41
14:L:54:PRO:HG2	14:L:57:VAL:CG2	2.51	0.41
19:Q:94:GLN:O	19:Q:95:GLU:HB2	2.20	0.41
22:T:49:GLU:OE2	22:T:97:ARG:HD2	2.20	0.41
26:X:27:ASP:OD2	26:X:27:ASP:N	2.52	0.41
31:3:69:TYR:CZ	31:3:80:ARG:HD2	2.56	0.41
1:0:383:A:H2'	1:0:384:G:O4'	2.21	0.41
1:0:401:C:H2'	1:0:402:U:C6	2.56	0.41
1:0:498:A:H2'	1:0:499:G:O4'	2.21	0.41
1:0:711:G:C2	1:0:718:C:C2	3.09	0.41
1:0:806:A:H2'	1:0:807:A:O4'	2.21	0.41
1:0:820:G:C5	3:A:171:LYS:HB2	2.55	0.41
1:0:940:G:C5	1:0:1027:G:C2	3.09	0.41
1:0:958:G:H2'	1:0:959:C:H6	1.86	0.41
1:0:1167:G:H2'	1:0:1168:C:O4'	2.21	0.41
1:0:2270:G:C4'	3:A:223:ARG:HH12	2.25	0.41
1:0:2372:A:H2'	1:0:2373:U:C6	2.56	0.41
1:0:2783:A:H2'	1:0:2784:A:C8	2.56	0.41
38:O:6229:HOH:O	18:P:63:ARG:NH2	2.51	0.41
2:9:106:U:O2'	2:9:107:C:H5'	2.21	0.41
4:B:7:ARG:CG	4:B:7:ARG:NH1	2.84	0.41
4:B:13:PHE:CD1	4:B:13:PHE:N	2.89	0.41
4:B:144:THR:HG21	38:B:8926:HOH:O	2.21	0.41
5:C:21:VAL:HG23	5:C:22:PHE:CD1	2.56	0.41
5:C:151:GLN:O	5:C:154:VAL:HB	2.21	0.41
7:E:137:ASP:OD1	7:E:137:ASP:C	2.64	0.41
8:F:58:GLU:HG3	8:F:61:MET:HE2	2.02	0.41
11:I:92:VAL:O	11:I:92:VAL:HG12	2.20	0.41
16:N:32:PRO:HD2	16:N:99:GLU:O	2.21	0.41
19:Q:26:PRO:O	19:Q:30:VAL:HG23	2.21	0.41
25:W:63:GLU:HG2	25:W:93:ILE:HG22	2.02	0.41
25:W:154:ARG:C	38:W:4276:HOH:O	2.64	0.41
26:X:78:GLU:CG	26:X:79:GLU:H	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:1:44:LYS:NZ	38:1:8755:HOH:O	2.53	0.41
1:0:92:G:H4'	24:V:44:GLY:HA3	2.02	0.41
1:0:1592:G:O2'	1:0:1593:C:O4'	2.37	0.41
1:0:1675:C:O2'	1:0:1676:G:H5'	2.21	0.41
1:0:1684:A:H1'	30:2:43:ARG:NH2	2.25	0.41
1:0:2443:C:H1'	14:L:56:LYS:HE3	2.03	0.41
1:0:2505:G:C2'	1:0:2506:A:H5'	2.50	0.41
1:0:2791:U:H1'	1:0:2792:A:H5''	2.02	0.41
3:A:99:ILE:O	3:A:131:HIS:CE1	2.74	0.41
4:B:84:LEU:HD23	4:B:142:LEU:CD2	2.51	0.41
4:B:150:ALA:O	4:B:152:PRO:HD3	2.21	0.41
5:C:16:VAL:CG1	5:C:17:ASP:N	2.82	0.41
7:E:20:ILE:O	7:E:30:THR:HA	2.21	0.41
9:G:27:ILE:HD12	9:G:70:ALA:HB1	2.02	0.41
11:I:87:PRO:HB3	11:I:130:LEU:N	2.37	0.41
11:I:105:GLU:HA	11:I:108:HIS:CE1	2.56	0.41
12:J:77:GLY:O	12:J:78:ILE:C	2.64	0.41
13:K:78:LYS:HA	13:K:79:PRO:HD3	1.92	0.41
14:L:145:LEU:C	14:L:147:GLU:N	2.80	0.41
18:P:141:ILE:O	18:P:143:ALA:N	2.47	0.41
27:Y:189:ASN:HD22	27:Y:192:ASP:H	1.66	0.41
1:0:338:C:H5''	38:0:3781:HOH:O	2.21	0.40
1:0:396:U:P	31:3:38:ARG:HH11	2.43	0.40
1:0:539:G:H2'	1:0:540:A:C8	2.55	0.40
1:0:545:G:H2'	1:0:546:C:O4'	2.21	0.40
1:0:685:C:O2	1:0:748:C:H4'	2.20	0.40
1:0:1066:U:H2'	1:0:1067:A:C8	2.56	0.40
1:0:1505:U:H5'	1:0:1505:U:C6	2.50	0.40
1:0:2361:A:H2'	1:0:2362:A:C8	2.55	0.40
4:B:307:ARG:HH11	4:B:307:ARG:CG	2.34	0.40
7:E:156:ASP:OD1	7:E:156:ASP:N	2.51	0.40
9:G:19:GLU:HG2	9:G:66:LEU:CD1	2.51	0.40
11:I:70:THR:OG1	11:I:107:LYS:HE2	2.22	0.40
16:N:103:ASP:OD1	16:N:103:ASP:C	2.65	0.40
18:P:131:PHE:CE1	18:P:137:LEU:HD13	2.56	0.40
20:R:18:LEU:HB2	20:R:143:VAL:HG12	2.01	0.40
20:R:104:PHE:HB2	20:R:109:MET:HE2	2.03	0.40
26:X:73:ARG:HB2	26:X:88:GLU:OE2	2.21	0.40
29:1:28:HIS:CD2	29:1:30:LYS:HB2	2.55	0.40
30:2:35:ARG:HG2	38:2:6391:HOH:O	2.21	0.40
1:0:213:G:O2'	1:0:214:U:OP2	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:330:C:H5	5:C:170:ASP:OD2	2.04	0.40
1:0:2316:G:H4'	38:0:6048:HOH:O	2.21	0.40
1:0:2415:A:H2'	1:0:2416:G:H5'	2.02	0.40
1:0:2766:A:O2'	1:0:2767:C:H5'	2.20	0.40
5:C:219:ASN:OD1	5:C:222:ASP:OD1	2.40	0.40
14:L:130:ARG:HA	38:L:8856:HOH:O	2.21	0.40
16:N:164:ASP:OD2	16:N:167:ASP:HA	2.21	0.40
19:Q:75:ILE:HD13	19:Q:84:ILE:HD11	2.03	0.40
20:R:113:HIS:O	20:R:145:LEU:HD12	2.21	0.40
23:U:6:CYS:C	23:U:8:TYR:N	2.80	0.40
26:X:80:GLU:N	38:X:5564:HOH:O	2.54	0.40
27:Y:187:VAL:HG23	27:Y:192:ASP:HB3	2.01	0.40
27:Y:197:ASP:C	27:Y:197:ASP:OD1	2.64	0.40
28:Z:20:ARG:O	28:Z:21:VAL:C	2.64	0.40
1:0:466:A:H2'	1:0:467:G:O4'	2.21	0.40
1:0:525:G:H2'	1:0:526:U:O4'	2.20	0.40
1:0:848:C:H5'	38:0:7224:HOH:O	2.22	0.40
1:0:1234:U:C2	4:B:244:PRO:HB3	2.56	0.40
1:0:1755:A:H2'	1:0:1756:G:O4'	2.21	0.40
1:0:1930:A:H2'	1:0:1931:A:C8	2.56	0.40
1:0:1947:G:N2	1:0:1966:U:C2	2.89	0.40
1:0:2269:C:H2'	1:0:2270:G:H5'	2.03	0.40
1:0:2807:U:P	4:B:27:ASN:HD21	2.45	0.40
4:B:174:ARG:HA	4:B:177:HIS:HB3	2.02	0.40
4:B:207:LYS:HG2	4:B:304:PRO:HB3	2.02	0.40
14:L:120:LEU:HD12	14:L:133:VAL:HG21	2.03	0.40
18:P:59:ARG:NH2	18:P:66:GLN:NE2	2.60	0.40
20:R:25:PHE:CE2	20:R:29:LYS:CE	3.05	0.40
25:W:21:LEU:CD2	25:W:26:ILE:HD11	2.44	0.40
28:Z:79:VAL:O	28:Z:80:ARG:C	2.64	0.40
31:3:65:THR:HB	31:3:83:TRP:H	1.87	0.40
1:0:215:A:OP1	14:L:52:LYS:NZ	2.52	0.40
1:0:1735:C:O2'	1:0:1736:A:H5'	2.20	0.40
1:0:2089:A:O2'	1:0:2090:G:H5'	2.22	0.40
1:0:2577:A:H5'	38:0:7697:HOH:O	2.21	0.40
3:A:32:VAL:O	3:A:33:GLU:C	2.65	0.40
4:B:77:PRO:HG2	4:B:151:VAL:CG2	2.51	0.40
4:B:305:ASP:O	4:B:306:LYS:CB	2.68	0.40
5:C:14:GLY:O	5:C:15:GLU:HB3	2.21	0.40
5:C:145:GLU:OE1	5:C:198:ASP:HB2	2.21	0.40
6:D:11:HIS:CG	6:D:12:GLU:N	2.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:37:ALA:O	6:D:40:ILE:HG12	2.22	0.40
12:J:19:MET:HE1	12:J:132:LEU:HD11	2.02	0.40
13:K:65:ARG:O	13:K:66:ARG:HB2	2.21	0.40
14:L:146:GLY:C	14:L:148:GLU:H	2.30	0.40
21:S:69:SER:C	21:S:71:ASP:N	2.78	0.40
27:Y:189:ASN:ND2	27:Y:192:ASP:N	2.70	0.40
30:2:41:HIS:H	30:2:45:ASN:ND2	1.97	0.40
30:2:41:HIS:CD2	30:2:44:ARG:H	2.29	0.40
1:0:470:U:H3	1:0:775:G:HO2'	1.70	0.40
1:0:968:G:O2'	1:0:969:G:H5'	2.21	0.40
1:0:1041:U:H4'	1:0:1295:G:H5'	2.04	0.40
1:0:1205:U:C2'	1:0:1206:U:H5''	2.51	0.40
1:0:2564:G:OP2	1:0:2565:C:H5''	2.22	0.40
1:0:2708:G:H2'	1:0:2709:G:O4'	2.22	0.40
1:0:2812:A:N7	38:0:7464:HOH:O	2.37	0.40
38:0:7370:HOH:O	3:A:22:ARG:HD2	2.21	0.40
2:9:28:U:H5''	16:N:40:ASN:HD21	1.85	0.40
2:9:39:U:H3'	2:9:40:C:H5''	2.04	0.40
7:E:35:TYR:HA	12:J:127:ILE:HD12	2.02	0.40
8:F:48:VAL:CG2	8:F:74:PHE:HB3	2.51	0.40
8:F:63:ILE:HB	8:F:64:PRO:CD	2.47	0.40
13:K:62:PRO:CG	13:K:65:ARG:HH21	2.29	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	235/240 (98%)	213 (91%)	20 (8%)	2 (1%)	14	24
4	B	335/338 (99%)	300 (90%)	30 (9%)	5 (2%)	8	13
5	C	244/246 (99%)	222 (91%)	21 (9%)	1 (0%)	30	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	D	134/177 (76%)	98 (73%)	27 (20%)	9 (7%)	1	0
7	E	170/178 (96%)	160 (94%)	10 (6%)	0	100	100
8	F	117/120 (98%)	101 (86%)	12 (10%)	4 (3%)	3	4
9	G	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
10	H	156/177 (88%)	144 (92%)	10 (6%)	2 (1%)	9	16
11	I	68/162 (42%)	53 (78%)	15 (22%)	0	100	100
12	J	140/145 (97%)	130 (93%)	5 (4%)	5 (4%)	2	4
13	K	130/132 (98%)	119 (92%)	10 (8%)	1 (1%)	16	27
14	L	141/165 (86%)	121 (86%)	19 (14%)	1 (1%)	18	30
15	M	192/195 (98%)	178 (93%)	14 (7%)	0	100	100
16	N	184/187 (98%)	166 (90%)	13 (7%)	5 (3%)	4	6
17	O	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
18	P	141/149 (95%)	133 (94%)	7 (5%)	1 (1%)	18	30
19	Q	93/96 (97%)	86 (92%)	7 (8%)	0	100	100
20	R	148/155 (96%)	140 (95%)	8 (5%)	0	100	100
21	S	79/85 (93%)	72 (91%)	7 (9%)	0	100	100
22	T	117/120 (98%)	109 (93%)	7 (6%)	1 (1%)	14	24
23	U	51/66 (77%)	47 (92%)	4 (8%)	0	100	100
24	V	63/71 (89%)	56 (89%)	5 (8%)	2 (3%)	3	4
25	W	152/154 (99%)	147 (97%)	3 (2%)	2 (1%)	9	16
26	X	80/92 (87%)	71 (89%)	9 (11%)	0	100	100
27	Y	140/241 (58%)	137 (98%)	3 (2%)	0	100	100
28	Z	71/83 (86%)	60 (84%)	7 (10%)	4 (6%)	1	1
29	1	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
30	2	42/50 (84%)	40 (95%)	2 (5%)	0	100	100
31	3	90/92 (98%)	85 (94%)	4 (4%)	1 (1%)	11	19
All	All	3705/4437 (84%)	3374 (91%)	285 (8%)	46 (1%)	10	17

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	34	ASP
6	D	173	GLU

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Mol	Chain	Res	Type
8	F	101	ALA
14	L	80	ASP
16	N	154	LEU
16	N	164	ASP
16	N	184	ILE
28	Z	81	ARG
4	B	34	GLY
4	B	139	ASP
4	B	169	GLY
5	C	8	LEU
8	F	44	SER
10	H	172	GLU
12	J	5	GLU
18	P	116	SER
31	3	57	GLY
4	B	185	GLY
6	D	56	ARG
6	D	171	ASP
22	T	53	GLY
24	V	43	PRO
25	W	49	ASN
25	W	77	ALA
6	D	27	ILE
6	D	65	GLU
6	D	137	PRO
12	J	89	HIS
16	N	139	TRP
28	Z	20	ARG
28	Z	41	ASN
28	Z	42	CYS
6	D	61	PHE
8	F	100	ASP
12	J	7	ASP
12	J	65	ASN
12	J	143	LYS
13	K	126	SER
16	N	155	GLU
4	B	2	GLN
6	D	16	PRO
10	H	143	VAL
6	D	69	ILE
8	F	64	PRO

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Mol	Chain	Res	Type
24	V	40	PRO
3	A	37	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	179/182 (98%)	168 (94%)	11 (6%)	17	30
4	B	282/283 (100%)	264 (94%)	18 (6%)	16	28
5	C	193/193 (100%)	174 (90%)	19 (10%)	7	11
6	D	117/148 (79%)	113 (97%)	4 (3%)	32	53
7	E	152/156 (97%)	147 (97%)	5 (3%)	33	55
8	F	93/94 (99%)	91 (98%)	2 (2%)	45	67
9	G	27/283 (10%)	26 (96%)	1 (4%)	30	50
10	H	134/145 (92%)	127 (95%)	7 (5%)	21	36
11	I	58/130 (45%)	58 (100%)	0	100	100
12	J	118/121 (98%)	108 (92%)	10 (8%)	10	17
13	K	106/106 (100%)	103 (97%)	3 (3%)	38	60
14	L	113/127 (89%)	111 (98%)	2 (2%)	51	72
15	M	158/159 (99%)	154 (98%)	4 (2%)	42	64
16	N	149/150 (99%)	142 (95%)	7 (5%)	23	40
17	O	93/94 (99%)	90 (97%)	3 (3%)	34	55
18	P	113/117 (97%)	109 (96%)	4 (4%)	32	52
19	Q	79/80 (99%)	75 (95%)	4 (5%)	21	36
20	R	117/122 (96%)	113 (97%)	4 (3%)	32	53
21	S	71/74 (96%)	68 (96%)	3 (4%)	26	45
22	T	105/106 (99%)	101 (96%)	4 (4%)	29	49
23	U	44/52 (85%)	44 (100%)	0	100	100
24	V	51/57 (90%)	49 (96%)	2 (4%)	28	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	W	130/130 (100%)	121 (93%)	9 (7%)	14	24
26	X	66/74 (89%)	63 (96%)	3 (4%)	24	42
27	Y	120/196 (61%)	112 (93%)	8 (7%)	15	25
28	Z	60/68 (88%)	60 (100%)	0	100	100
29	1	46/47 (98%)	46 (100%)	0	100	100
30	2	42/46 (91%)	42 (100%)	0	100	100
31	3	79/79 (100%)	78 (99%)	1 (1%)	61	77
All	All	3095/3619 (86%)	2957 (96%)	138 (4%)	24	42

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	3	ARG
3	A	33	GLU
3	A	36	ASP
3	A	55	VAL
3	A	69	LEU
3	A	94	LEU
3	A	131	HIS
3	A	153	ARG
3	A	175	LYS
3	A	179	MET
3	A	217	ARG
4	B	7	ARG
4	B	11	LEU
4	B	27	ASN
4	B	33	ASP
4	B	97	LEU
4	B	98	THR
4	B	175	LEU
4	B	190	MET
4	B	195	ARG
4	B	245	SER
4	B	251	VAL
4	B	254	GLN
4	B	256	GLN
4	B	264	GLU
4	B	277	GLU
4	B	304	PRO
4	B	307	ARG

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Mol	Chain	Res	Type
4	B	312	ARG
5	C	2	GLN
5	C	27	ARG
5	C	67	GLN
5	C	76	ARG
5	C	78	ARG
5	C	91	PRO
5	C	94	THR
5	C	101	ASP
5	C	115	LEU
5	C	136	VAL
5	C	162	VAL
5	C	187	ARG
5	C	214	THR
5	C	222	ASP
5	C	223	LEU
5	C	234	VAL
5	C	236	THR
5	C	240	LEU
5	C	243	VAL
6	D	24	HIS
6	D	136	ARG
6	D	137	PRO
6	D	149	ARG
7	E	7	ILE
7	E	12	ASP
7	E	16	ASP
7	E	86	VAL
7	E	102	VAL
8	F	12	LEU
8	F	78	GLU
9	G	64	ASN
10	H	21	GLU
10	H	33	GLN
10	H	87	LYS
10	H	91	ARG
10	H	114	ASP
10	H	157	TYR
10	H	172	GLU
12	J	46	ILE
12	J	47	THR
12	J	52	GLN

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Mol	Chain	Res	Type
12	J	74	ARG
12	J	76	ASP
12	J	93	ARG
12	J	120	SER
12	J	127	ILE
12	J	131	THR
12	J	132	LEU
13	K	7	ASP
13	K	10	GLN
13	K	49	LEU
14	L	99	GLU
14	L	140	VAL
15	M	46	LEU
15	M	93	ARG
15	M	99	ARG
15	M	164	THR
16	N	26	LEU
16	N	43	VAL
16	N	47	LEU
16	N	49	THR
16	N	138	ASP
16	N	139	TRP
16	N	152	GLU
17	O	3	THR
17	O	28	ASP
17	O	111	VAL
18	P	21	VAL
18	P	52	LYS
18	P	91	LYS
18	P	98	ILE
19	Q	11	ARG
19	Q	16	ASN
19	Q	57	ASP
19	Q	95	GLU
20	R	13	THR
20	R	39	THR
20	R	82	GLU
20	R	143	VAL
21	S	53	ASN
21	S	71	ASP
21	S	80	ARG
22	T	26	THR

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Mol	Chain	Res	Type
22	T	39	ASN
22	T	48	VAL
22	T	96	VAL
24	V	13	PRO
24	V	43	PRO
25	W	4	LEU
25	W	13	MET
25	W	26	ILE
25	W	35	VAL
25	W	45	VAL
25	W	52	VAL
25	W	73	LEU
25	W	146	ILE
25	W	154	ARG
26	X	15	ARG
26	X	72	VAL
26	X	85	VAL
27	Y	103	THR
27	Y	163	THR
27	Y	172	THR
27	Y	189	ASN
27	Y	200	THR
27	Y	203	VAL
27	Y	220	GLU
27	Y	235	GLU
31	3	34	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (107) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	47	HIS
3	A	92	ASN
3	A	199	HIS
3	A	218	ASN
4	B	27	ASN
4	B	106	HIS
4	B	145	HIS
4	B	221	GLN
4	B	238	ASN
4	B	256	GLN
4	B	260	HIS
4	B	320	GLN

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Mol	Chain	Res	Type
4	B	332	ASN
5	C	2	GLN
5	C	39	GLN
5	C	67	GLN
5	C	129	HIS
5	C	151	GLN
5	C	163	HIS
6	D	97	GLN
6	D	103	ASN
6	D	133	ASN
7	E	66	GLN
7	E	71	ASN
7	E	106	ASN
7	E	119	HIS
7	E	143	GLN
8	F	80	GLN
9	G	17	GLN
9	G	64	ASN
10	H	34	HIS
10	H	59	GLN
10	H	62	HIS
10	H	75	HIS
10	H	131	GLN
10	H	148	HIS
11	I	88	GLN
11	I	106	GLN
11	I	108	HIS
12	J	25	GLN
12	J	29	GLN
12	J	52	GLN
12	J	107	ASN
13	K	10	GLN
14	L	18	HIS
14	L	41	HIS
14	L	42	ASN
14	L	58	GLN
14	L	116	HIS
15	M	24	GLN
15	M	26	GLN
15	M	58	GLN
15	M	137	ASN
15	M	170	ASN

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Mol	Chain	Res	Type
16	N	22	GLN
16	N	40	ASN
16	N	107	ASN
16	N	140	GLN
18	P	50	GLN
18	P	66	GLN
18	P	73	HIS
18	P	118	GLN
19	Q	16	ASN
19	Q	40	HIS
20	R	22	GLN
20	R	61	GLN
20	R	94	ASN
20	R	98	ASN
20	R	113	HIS
20	R	117	HIS
20	R	122	GLN
21	S	9	HIS
21	S	21	GLN
21	S	53	ASN
21	S	55	GLN
21	S	56	ASN
22	T	39	ASN
22	T	43	ASN
22	T	73	HIS
23	U	39	ASN
24	V	4	HIS
24	V	6	GLN
24	V	60	GLN
25	W	28	HIS
25	W	110	GLN
25	W	119	HIS
25	W	125	HIS
25	W	141	HIS
26	X	23	HIS
26	X	36	HIS
27	Y	133	HIS
27	Y	134	HIS
27	Y	149	GLN
27	Y	189	ASN
28	Z	37	HIS
29	1	8	GLN

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Mol	Chain	Res	Type
29	1	16	HIS
29	1	28	HIS
30	2	16	ASN
30	2	18	ASN
30	2	37	HIS
30	2	41	HIS
30	2	45	ASN
31	3	2	GLN
31	3	15	ASN
31	3	30	GLN
31	3	48	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2746/2922 (93%)	249 (9%)	35 (1%)
2	9	121/122 (99%)	16 (13%)	1 (0%)
All	All	2867/3044 (94%)	265 (9%)	36 (1%)

All (265) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	11	A
1	0	31	C
1	0	60	A
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G
1	0	87	C
1	0	88	G
1	0	114	A
1	0	115	U
1	0	120	A
1	0	130	C
1	0	139	C
1	0	141	C
1	0	151	A
1	0	166	A
1	0	169	A
1	0	170	U

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Mol	Chain	Res	Type
1	0	185	G
1	0	186	A
1	0	191	A
1	0	192	A
1	0	200	C
1	0	219	G
1	0	237	G
1	0	271	C
1	0	272	A
1	0	273	G
1	0	283	U
1	0	284	C
1	0	285	A
1	0	308	U
1	0	309	C
1	0	317	A
1	0	319	A
1	0	336	G
1	0	337	A
1	0	358	G
1	0	381	G
1	0	397	A
1	0	417	G
1	0	461	C
1	0	487	G
1	0	498	A
1	0	510	U
1	0	511	A
1	0	514	G
1	0	537	G
1	0	538	C
1	0	539	G
1	0	542	A
1	0	545	G
1	0	553	G
1	0	559	U
1	0	581	G
1	0	588	G
1	0	604	G
1	0	620	A
1	0	632	A
1	0	644	G

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Mol	Chain	Res	Type
1	0	660	A
1	0	688	A
1	0	701	U
1	0	759	C
1	0	777	U
1	0	809	G
1	0	821	U
1	0	835	U
1	0	840	U
1	0	857	A
1	0	858	U
1	0	868	G
1	0	869	G
1	0	871	G
1	0	872	U
1	0	875	A
1	0	877	G
1	0	878	G
1	0	884	C
1	0	885	G
1	0	898	G
1	0	905	C
1	0	920	C
1	0	921	G
1	0	923	A
1	0	953	G
1	0	960	G
1	0	961	A
1	0	1006	A
1	0	1008	C
1	0	1029	U
1	0	1045	G
1	0	1059	G
1	0	1060	C
1	0	1072	G
1	0	1081	A
1	0	1088	A
1	0	1109	U
1	0	1110	G
1	0	1119	G
1	0	1130	U
1	0	1137	G

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Mol	Chain	Res	Type
1	0	1162	G
1	0	1164	U
1	0	1165	G
1	0	1166	A
1	0	1174	A
1	0	1175	G
1	0	1185	U
1	0	1192	A
1	0	1193	A
1	0	1206	U
1	0	1208	C
1	0	1216	G
1	0	1237	U
1	0	1238	C
1	0	1239	G
1	0	1279	U
1	0	1289	C
1	0	1342	C
1	0	1353	C
1	0	1360	C
1	0	1377	C
1	0	1407	A
1	0	1451	C
1	0	1474	C
1	0	1488	U
1	0	1505	U
1	0	1506	U
1	0	1524	U
1	0	1525	G
1	0	1526	A
1	0	1559	A
1	0	1564	C
1	0	1580	A
1	0	1592	G
1	0	1625	U
1	0	1626	A
1	0	1633	C
1	0	1634	G
1	0	1656	A
1	0	1667	A
1	0	1682	A
1	0	1684	A

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Mol	Chain	Res	Type
1	0	1685	A
1	0	1692	C
1	0	1701	A
1	0	1722	U
1	0	1723	G
1	0	1725	C
1	0	1730	G
1	0	1731	C
1	0	1752	G
1	0	1778	A
1	0	1798	C
1	0	1819	G
1	0	1820	G
1	0	1829	A
1	0	1856	C
1	0	1857	A
1	0	1879	U
1	0	1919	A
1	0	1942	A
1	0	1943	C
1	0	1971	G
1	0	1973	A
1	0	1974	G
1	0	1978	A
1	0	1979	G
1	0	1980	U
1	0	1996	U
1	0	2004	U
1	0	2008	U
1	0	2011	A
1	0	2012	U
1	0	2013	G
1	0	2033	G
1	0	2034	U
1	0	2064	U
1	0	2072	G
1	0	2073	G
1	0	2074	A
1	0	2096	A
1	0	2101	A
1	0	2102	G
1	0	2103	A

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Mol	Chain	Res	Type
1	0	2110	G
1	0	2243	C
1	0	2258	A
1	0	2271	G
1	0	2272	G
1	0	2291	A
1	0	2317	C
1	0	2321	A
1	0	2354	A
1	0	2361	A
1	0	2369	A
1	0	2379	G
1	0	2422	U
1	0	2462	G
1	0	2467	A
1	0	2469	A
1	0	2476	C
1	0	2480	G
1	0	2483	A
1	0	2507	G
1	0	2511	A
1	0	2526	C
1	0	2527	U
1	0	2533	C
1	0	2537	G
1	0	2541	U
1	0	2553	A
1	0	2564	G
1	0	2589	U
1	0	2601	A
1	0	2602	G
1	0	2608	C
1	0	2613	G
1	0	2634	G
1	0	2638	G
1	0	2649	A
1	0	2650	U
1	0	2664	A
1	0	2681	A
1	0	2682	C
1	0	2718	C
1	0	2719	A

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Mol	Chain	Res	Type
1	0	2726	U
1	0	2727	A
1	0	2747	C
1	0	2748	G
1	0	2749	U
1	0	2750	G
1	0	2762	C
1	0	2768	A
1	0	2786	G
1	0	2792	A
1	0	2800	A
1	0	2811	A
1	0	2825	C
1	0	2840	A
1	0	2850	C
1	0	2876	G
1	0	2890	A
1	0	2896	A
1	0	2903	C
1	0	2914	A
2	9	2	U
2	9	7	G
2	9	14	G
2	9	22	G
2	9	23	U
2	9	24	U
2	9	25	G
2	9	40	C
2	9	41	C
2	9	43	G
2	9	52	A
2	9	57	A
2	9	66	G
2	9	77	A
2	9	114	G
2	9	122	C

All (36) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	10	U
1	0	69	A

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Mol	Chain	Res	Type
1	0	129	A
1	0	169	A
1	0	318	U
1	0	338	C
1	0	603	A
1	0	699	C
1	0	834	G
1	0	857	A
1	0	871	G
1	0	877	G
1	0	898	G
1	0	1080	C
1	0	1237	U
1	0	1246	A
1	0	1352	A
1	0	1377	C
1	0	1450	C
1	0	1506	U
1	0	1563	G
1	0	1692	C
1	0	1856	C
1	0	1942	A
1	0	1979	G
1	0	2011	A
1	0	2313	C
1	0	2467	A
1	0	2526	C
1	0	2536	C
1	0	2649	A
1	0	2718	C
1	0	2726	U
1	0	2761	A
1	0	2791	U
2	9	65	A

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

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	0	2621	1	18,21,22	1.49	2 (11%)	21,30,33	1.26	3 (14%)
1	1MA	0	628	1	21,25,26	0.69	1 (4%)	30,37,40	0.79	1 (3%)
1	OMU	0	2587	1	19,22,23	0.31	0	25,31,34	0.38	0
1	OMG	0	2588	1	23,26,27	0.29	0	32,38,41	0.34	0
1	UR3	0	2619	1	19,22,23	0.46	0	26,32,35	0.71	1 (3%)

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

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C2-N1	4.98	1.43	1.36
1	0	2621	PSU	C6-C5	3.04	1.38	1.35
1	0	628	1MA	C6-N6	2.39	1.33	1.28

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	C6-C5-C4	2.88	120.12	118.17
1	0	2621	PSU	C6-N1-C2	-2.88	120.02	122.69
1	0	2621	PSU	O2-C2-N1	2.85	125.72	122.79
1	0	628	1MA	N1-C2-N3	2.82	129.34	126.00
1	0	2619	UR3	C4-N3-C2	2.73	126.77	124.58

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	1	0
1	0	2588	OMG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 232 ligands modelled in this entry, 231 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
32	ERY	0	9000	-	53,53,53	1.26	5 (9%)	82,82,82	0.99	5 (6%)

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	ERY	0	9000	-	-	4/72/107/107	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	0	9000	ERY	C6-C5	3.44	1.61	1.55
32	0	9000	ERY	C7-C6	2.56	1.58	1.54
32	0	9000	ERY	O2-C13	2.25	1.50	1.46
32	0	9000	ERY	C2-C3	2.22	1.60	1.54
32	0	9000	ERY	O4-C18	2.07	1.49	1.44

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	0	9000	ERY	C3-C2-C1	-2.58	104.71	109.93
32	0	9000	ERY	C25-C24-C23	-2.45	106.50	110.02
32	0	9000	ERY	O5-C16-C17	2.09	106.88	103.86
32	0	9000	ERY	O13-C12-C35	-2.05	103.65	107.84
32	0	9000	ERY	C6-C5-C4	-2.04	110.94	113.89

There are no chirality outliers.

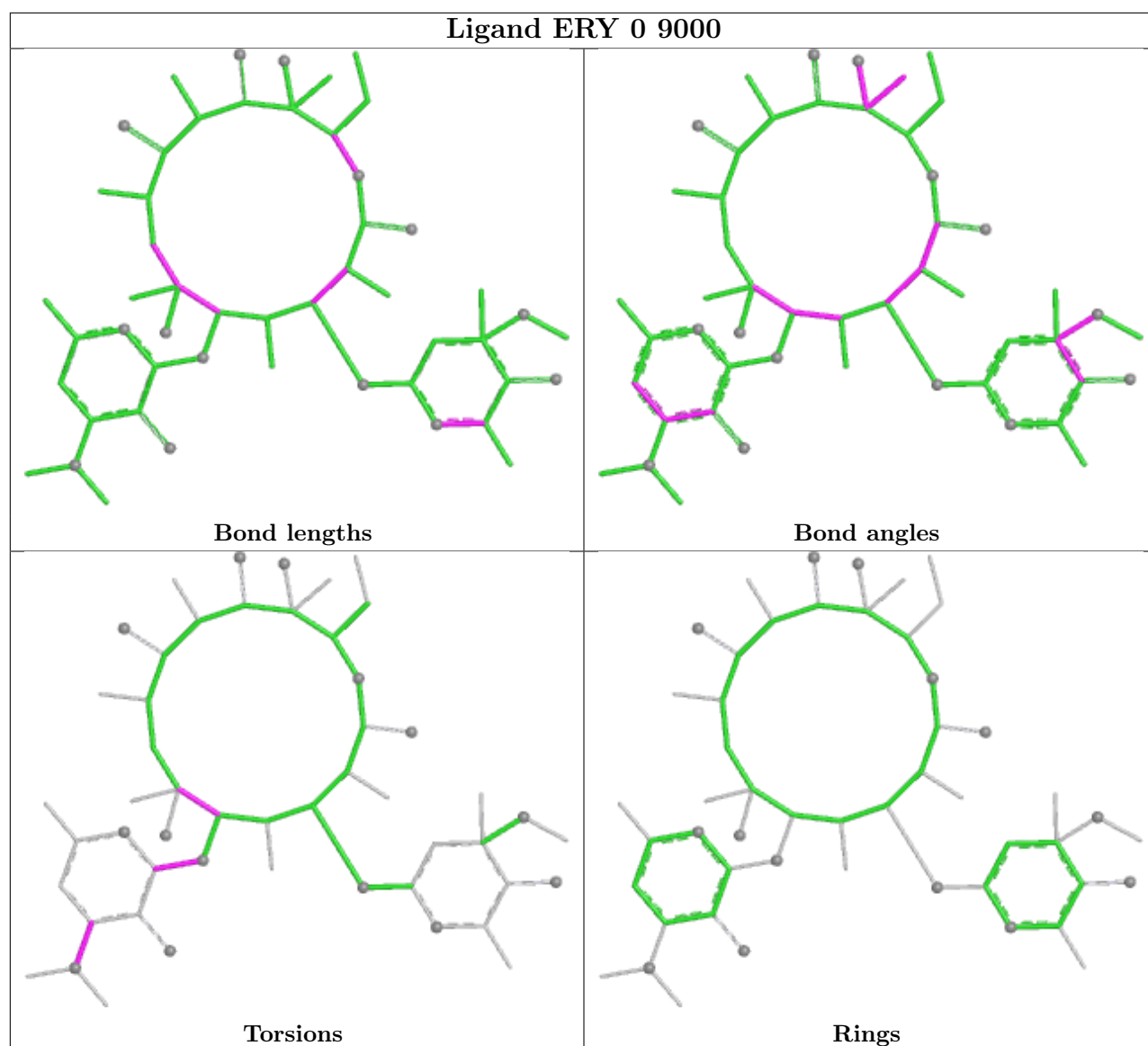
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	0	9000	ERY	O9-C22-O7-C5
32	0	9000	ERY	O7-C5-C6-C7
32	0	9000	ERY	C23-C22-O7-C5
32	0	9000	ERY	C25-C24-N1-C29

There are no ring outliers.

No monomer is involved in short contacts.

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	2749/2922 (94%)	-0.65	30 (1%) 78 75	26, 49, 94, 152	0
2	9	122/122 (100%)	-0.20	4 (3%) 49 40	40, 65, 90, 154	0
3	A	237/240 (98%)	-0.08	6 (2%) 58 52	31, 54, 88, 109	0
4	B	337/338 (99%)	-0.05	1 (0%) 90 89	30, 58, 83, 92	0
5	C	246/246 (100%)	-0.17	0 100 100	26, 48, 73, 82	0
6	D	140/177 (79%)	1.07	19 (13%) 7 5	56, 101, 125, 132	0
7	E	172/178 (96%)	0.24	6 (3%) 47 38	49, 71, 90, 94	0
8	F	119/120 (99%)	0.39	2 (1%) 69 64	51, 76, 95, 111	0
9	G	29/348 (8%)	1.01	7 (24%) 2 1	77, 93, 102, 104	0
10	H	160/177 (90%)	0.01	6 (3%) 44 36	39, 59, 92, 99	0
11	I	70/162 (43%)	1.88	27 (38%) 1 0	109, 122, 139, 141	0
12	J	142/145 (97%)	-0.12	2 (1%) 73 69	38, 53, 75, 95	0
13	K	132/132 (100%)	-0.03	2 (1%) 72 67	34, 55, 75, 86	0
14	L	145/165 (87%)	0.35	10 (6%) 23 17	27, 68, 109, 122	0
15	M	194/195 (99%)	-0.36	1 (0%) 87 85	34, 46, 61, 70	0
16	N	186/187 (99%)	0.29	5 (2%) 56 49	41, 64, 108, 119	0
17	O	115/116 (99%)	0.07	0 100 100	39, 57, 74, 78	0
18	P	143/149 (95%)	0.03	2 (1%) 73 69	41, 58, 71, 80	0
19	Q	95/96 (98%)	-0.36	1 (1%) 78 75	38, 46, 62, 76	0
20	R	150/155 (96%)	-0.46	0 100 100	35, 48, 67, 77	0
21	S	81/85 (95%)	-0.11	0 100 100	47, 63, 83, 88	0
22	T	119/120 (99%)	0.05	0 100 100	40, 61, 85, 97	0
23	U	53/66 (80%)	0.07	0 100 100	46, 59, 76, 86	0
24	V	65/71 (91%)	0.63	6 (9%) 14 11	58, 77, 114, 118	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	154/154 (100%)	-0.30	0 100 100	35, 50, 67, 78	0
26	X	82/92 (89%)	0.16	4 (4%) 35 27	48, 61, 85, 101	0
27	Y	142/241 (58%)	-0.26	2 (1%) 73 69	28, 47, 71, 89	0
28	Z	73/83 (87%)	0.35	3 (4%) 41 33	52, 64, 80, 95	0
29	1	56/57 (98%)	-0.70	0 100 100	29, 36, 42, 52	0
30	2	46/50 (92%)	0.21	1 (2%) 62 56	37, 61, 87, 102	0
31	3	92/92 (100%)	-0.05	0 100 100	37, 56, 70, 83	0
All	All	6646/7481 (88%)	-0.24	147 (2%) 62 56	26, 55, 99, 154	0

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	9	1	U	7.0
6	D	10	PHE	6.9
11	I	128	THR	6.4
24	V	1	THR	6.3
24	V	2	VAL	5.5
1	0	10	U	5.0
3	A	37	VAL	4.7
6	D	55	LYS	4.5
11	I	71	ALA	4.5
10	H	174	LEU	4.4
16	N	168	LEU	4.4
26	X	88	GLU	4.3
2	9	2	U	4.2
1	0	2345	A	4.2
6	D	63	ILE	4.0
14	L	82	ALA	4.0
28	Z	82	SER	4.0
1	0	1165	G	3.9
1	0	138	U	3.9
4	B	1	PRO	3.8
1	0	1176	C	3.7
6	D	174	VAL	3.7
1	0	1175	G	3.6
11	I	91	PHE	3.6
1	0	1173	A	3.6
10	H	43	ALA	3.5
11	I	74	ILE	3.5
11	I	112	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
16	N	154	LEU	3.4
3	A	36	ASP	3.4
11	I	88	GLN	3.3
11	I	80	PHE	3.3
6	D	69	ILE	3.3
11	I	133	THR	3.3
24	V	40	PRO	3.3
24	V	39	ALA	3.3
11	I	116	LEU	3.2
11	I	82	THR	3.2
12	J	4	ALA	3.2
1	O	960	G	3.1
28	Z	11	SER	3.1
27	Y	235	GLU	3.1
24	V	43	PRO	3.0
1	O	1161	A	3.0
11	I	85	GLY	3.0
15	M	194	GLY	3.0
6	D	172	VAL	3.0
8	F	91	VAL	3.0
7	E	10	ASP	3.0
26	X	85	VAL	2.9
16	N	165	ALA	2.9
11	I	108	HIS	2.9
6	D	107	GLY	2.9
10	H	169	GLU	2.8
1	O	1524	U	2.8
11	I	100	VAL	2.8
11	I	83	GLY	2.8
24	V	44	GLY	2.8
10	H	171	GLY	2.8
11	I	114	TYR	2.8
3	A	211	LYS	2.7
7	E	154	ILE	2.7
11	I	73	LEU	2.7
28	Z	10	ARG	2.7
14	L	99	GLU	2.7
14	L	148	GLU	2.7
26	X	87	ALA	2.7
27	Y	236	VAL	2.7
14	L	81	VAL	2.7
1	O	1171	A	2.6

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Mol	Chain	Res	Type	RSRZ
3	A	237	GLY	2.6
18	P	143	ALA	2.6
6	D	53	LYS	2.6
14	L	105	TYR	2.6
14	L	83	GLU	2.6
11	I	97	VAL	2.6
11	I	132	VAL	2.6
11	I	113	SER	2.6
1	0	1193	A	2.6
7	E	45	ASP	2.6
1	0	1174	A	2.5
9	G	63	ARG	2.5
6	D	59	GLY	2.5
11	I	67	VAL	2.5
11	I	130	LEU	2.5
2	9	23	U	2.5
2	9	24	U	2.5
10	H	172	GLU	2.5
1	0	1192	A	2.4
7	E	156	ASP	2.4
1	0	128	A	2.4
30	2	49	GLU	2.4
1	0	2344	G	2.4
1	0	1204	C	2.4
1	0	1279	U	2.4
26	X	83	ALA	2.4
9	G	27	ILE	2.4
16	N	158	LEU	2.4
9	G	73	ASP	2.4
6	D	68	PRO	2.4
14	L	78	ALA	2.4
11	I	134	ILE	2.3
6	D	11	HIS	2.3
6	D	171	ASP	2.3
12	J	62	ASP	2.3
16	N	169	PRO	2.3
6	D	56	ARG	2.3
1	0	1166	A	2.3
6	D	61	PHE	2.3
11	I	101	LYS	2.3
9	G	71	LEU	2.3
9	G	12	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
7	E	53	GLU	2.2
6	D	62	ASP	2.2
11	I	129	SER	2.2
14	L	146	GLY	2.2
6	D	17	ARG	2.2
14	L	150	GLN	2.2
9	G	24	VAL	2.2
6	D	35	ALA	2.2
11	I	104	ALA	2.2
19	Q	92	ARG	2.2
6	D	105	SER	2.2
1	0	1162	G	2.2
13	K	119	GLN	2.2
11	I	107	LYS	2.2
18	P	116	SER	2.2
1	0	1525	G	2.1
9	G	26	MET	2.1
3	A	210	GLY	2.1
1	0	970	U	2.1
1	0	1190	G	2.1
1	0	1130	U	2.1
14	L	102	ASP	2.1
13	K	63	GLU	2.1
1	0	288	A	2.1
1	0	1191	A	2.1
6	D	106	PHE	2.1
8	F	90	GLU	2.0
7	E	172	PRO	2.0
1	0	1929	G	2.0
3	A	32	VAL	2.0
11	I	95	LEU	2.0
1	0	1169	U	2.0
1	0	1561	U	2.0
1	0	1177	A	2.0
10	H	170	ARG	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	1MA	0	628	23/24	0.98	0.06	30,33,34,36	0
1	OMU	0	2587	21/22	0.98	0.06	35,37,40,43	0
1	OMG	0	2588	24/25	0.98	0.06	34,36,38,40	0
1	PSU	0	2621	20/21	0.98	0.05	28,31,35,36	0
1	UR3	0	2619	21/22	0.99	0.05	35,37,41,45	0

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
35	NA	0	8529	1/1	0.56	0.18	76,76,76,76	0
35	NA	R	8586	1/1	0.68	0.58	87,87,87,87	0
35	NA	0	8571	1/1	0.75	0.20	58,58,58,58	0
35	NA	0	8582	1/1	0.77	0.17	80,80,80,80	0
33	MG	0	8087	1/1	0.79	0.21	63,63,63,63	0
33	MG	0	8049	1/1	0.80	0.16	74,74,74,74	0
33	MG	0	8092	1/1	0.81	0.15	83,83,83,83	0
35	NA	0	8584	1/1	0.82	0.14	54,54,54,54	0
35	NA	0	8524	1/1	0.83	0.31	62,62,62,62	0
35	NA	9	8551	1/1	0.85	0.29	39,39,39,39	0
35	NA	0	8541	1/1	0.86	0.15	53,53,53,53	0
33	MG	0	8050	1/1	0.86	0.08	71,71,71,71	0
33	MG	0	8088	1/1	0.87	0.07	38,38,38,38	0
35	NA	0	8564	1/1	0.87	0.15	49,49,49,49	0
35	NA	0	8568	1/1	0.87	0.24	76,76,76,76	0
35	NA	0	8540	1/1	0.87	0.14	52,52,52,52	0
35	NA	0	8566	1/1	0.88	0.12	59,59,59,59	0
33	MG	2	8076	1/1	0.88	0.08	53,53,53,53	0
35	NA	0	8570	1/1	0.88	0.27	63,63,63,63	0
35	NA	9	8583	1/1	0.88	0.13	58,58,58,58	0
33	MG	9	8095	1/1	0.88	0.15	72,72,72,72	0
35	NA	0	8562	1/1	0.89	0.19	63,63,63,63	0
35	NA	0	8563	1/1	0.89	0.21	63,63,63,63	0
35	NA	0	8533	1/1	0.89	0.11	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	0	8526	1/1	0.89	0.13	55,55,55,55	0
33	MG	0	8112	1/1	0.89	0.09	47,47,47,47	0
35	NA	0	8557	1/1	0.89	0.16	60,60,60,60	0
35	NA	0	8514	1/1	0.90	0.14	40,40,40,40	0
35	NA	0	8569	1/1	0.90	0.16	57,57,57,57	0
35	NA	0	8585	1/1	0.90	0.27	53,53,53,53	0
32	ERY	0	9000	51/51	0.91	0.16	69,75,79,80	0
35	NA	0	8581	1/1	0.91	0.08	51,51,51,51	0
35	NA	0	8508	1/1	0.92	0.14	68,68,68,68	0
33	MG	0	8102	1/1	0.92	0.07	55,55,55,55	0
33	MG	0	8094	1/1	0.92	0.15	72,72,72,72	0
35	NA	0	8559	1/1	0.92	0.16	64,64,64,64	0
35	NA	0	8560	1/1	0.92	0.26	50,50,50,50	0
35	NA	0	8567	1/1	0.93	0.10	50,50,50,50	0
35	NA	0	8511	1/1	0.93	0.10	58,58,58,58	0
35	NA	0	8542	1/1	0.93	0.17	52,52,52,52	0
35	NA	0	8552	1/1	0.93	0.21	57,57,57,57	0
35	NA	0	8555	1/1	0.93	0.11	72,72,72,72	0
35	NA	0	8579	1/1	0.93	0.11	58,58,58,58	0
33	MG	0	8082	1/1	0.93	0.13	64,64,64,64	0
33	MG	0	8045	1/1	0.93	0.10	60,60,60,60	0
33	MG	0	8101	1/1	0.93	0.10	58,58,58,58	0
35	NA	0	8502	1/1	0.93	0.09	56,56,56,56	0
35	NA	0	8532	1/1	0.93	0.10	40,40,40,40	0
35	NA	0	8507	1/1	0.93	0.11	54,54,54,54	0
35	NA	L	8580	1/1	0.93	0.30	60,60,60,60	0
33	MG	0	8070	1/1	0.93	0.06	50,50,50,50	0
35	NA	0	8572	1/1	0.94	0.13	64,64,64,64	0
35	NA	0	8573	1/1	0.94	0.06	58,58,58,58	0
35	NA	0	8577	1/1	0.94	0.20	62,62,62,62	0
35	NA	0	8518	1/1	0.94	0.08	39,39,39,39	0
33	MG	0	8053	1/1	0.94	0.07	45,45,45,45	0
35	NA	0	8565	1/1	0.94	0.20	46,46,46,46	0
33	MG	0	8062	1/1	0.94	0.07	66,66,66,66	0
35	NA	0	8527	1/1	0.94	0.07	45,45,45,45	0
33	MG	0	8066	1/1	0.94	0.08	96,96,96,96	0
33	MG	0	8114	1/1	0.94	0.06	55,55,55,55	0
33	MG	0	8099	1/1	0.94	0.09	55,55,55,55	0
35	NA	R	8537	1/1	0.94	0.06	42,42,42,42	0
33	MG	T	8073	1/1	0.94	0.05	61,61,61,61	0
36	CL	0	8815	1/1	0.94	0.18	81,81,81,81	0
36	CL	3	8804	1/1	0.94	0.08	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	0	8574	1/1	0.95	0.16	65,65,65,65	0
33	MG	0	8051	1/1	0.95	0.06	71,71,71,71	0
35	NA	0	8510	1/1	0.95	0.09	45,45,45,45	0
33	MG	0	8047	1/1	0.95	0.10	77,77,77,77	0
35	NA	0	8513	1/1	0.95	0.06	54,54,54,54	0
33	MG	0	8085	1/1	0.95	0.06	50,50,50,50	0
35	NA	0	8516	1/1	0.95	0.09	51,51,51,51	0
35	NA	0	8549	1/1	0.95	0.06	46,46,46,46	0
35	NA	0	8550	1/1	0.95	0.09	47,47,47,47	0
35	NA	H	8522	1/1	0.95	0.22	56,56,56,56	0
33	MG	0	8100	1/1	0.95	0.13	69,69,69,69	0
35	NA	Q	8548	1/1	0.95	0.05	47,47,47,47	0
33	MG	0	8041	1/1	0.95	0.07	69,69,69,69	0
33	MG	0	8046	1/1	0.95	0.04	43,43,43,43	0
35	NA	S	8512	1/1	0.95	0.11	22,22,22,22	0
36	CL	0	8805	1/1	0.95	0.09	63,63,63,63	0
35	NA	0	8558	1/1	0.95	0.26	102,102,102,102	0
36	CL	0	8822	1/1	0.95	0.27	83,83,83,83	0
36	CL	L	8810	1/1	0.95	0.07	60,60,60,60	0
33	MG	0	8105	1/1	0.95	0.05	54,54,54,54	0
33	MG	0	8063	1/1	0.96	0.04	68,68,68,68	0
35	NA	0	8535	1/1	0.96	0.08	49,49,49,49	0
35	NA	A	8545	1/1	0.96	0.07	50,50,50,50	0
35	NA	C	8504	1/1	0.96	0.08	46,46,46,46	0
33	MG	0	8064	1/1	0.96	0.07	34,34,34,34	0
33	MG	0	8103	1/1	0.96	0.08	67,67,67,67	0
35	NA	0	8520	1/1	0.96	0.08	37,37,37,37	0
35	NA	0	8575	1/1	0.96	0.18	50,50,50,50	0
35	NA	0	8576	1/1	0.96	0.09	52,52,52,52	0
33	MG	0	8104	1/1	0.96	0.06	53,53,53,53	0
33	MG	0	8096	1/1	0.96	0.05	45,45,45,45	0
36	CL	0	8813	1/1	0.96	0.09	57,57,57,57	0
33	MG	0	8098	1/1	0.96	0.08	34,34,34,34	0
36	CL	0	8816	1/1	0.96	0.09	60,60,60,60	0
33	MG	0	8048	1/1	0.96	0.06	71,71,71,71	0
36	CL	A	8809	1/1	0.96	0.08	66,66,66,66	0
35	NA	0	8556	1/1	0.96	0.17	44,44,44,44	0
33	MG	0	8043	1/1	0.96	0.05	49,49,49,49	0
35	NA	0	8530	1/1	0.97	0.07	49,49,49,49	0
35	NA	0	8561	1/1	0.97	0.07	58,58,58,58	0
33	MG	0	8113	1/1	0.97	0.07	51,51,51,51	0
34	K	0	8402	1/1	0.97	0.15	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	0	8534	1/1	0.97	0.14	44,44,44,44	0
35	NA	0	8515	1/1	0.97	0.10	48,48,48,48	0
35	NA	0	8539	1/1	0.97	0.04	28,28,28,28	0
35	NA	H	8509	1/1	0.97	0.04	34,34,34,34	0
33	MG	0	8057	1/1	0.97	0.06	49,49,49,49	0
35	NA	0	8517	1/1	0.97	0.06	46,46,46,46	0
35	NA	M	8547	1/1	0.97	0.05	33,33,33,33	0
35	NA	0	8505	1/1	0.97	0.05	33,33,33,33	0
35	NA	0	8544	1/1	0.97	0.04	32,32,32,32	0
35	NA	0	8506	1/1	0.97	0.19	42,42,42,42	0
35	NA	0	8521	1/1	0.97	0.11	57,57,57,57	0
35	NA	0	8523	1/1	0.97	0.10	38,38,38,38	0
35	NA	0	8554	1/1	0.97	0.11	41,41,41,41	0
33	MG	0	8115	1/1	0.97	0.04	55,55,55,55	0
35	NA	0	8525	1/1	0.97	0.07	59,59,59,59	0
36	CL	0	8817	1/1	0.97	0.05	63,63,63,63	0
33	MG	0	8042	1/1	0.97	0.07	40,40,40,40	0
35	NA	0	8578	1/1	0.97	0.14	52,52,52,52	0
36	CL	J	8801	1/1	0.97	0.13	65,65,65,65	0
36	CL	J	8802	1/1	0.97	0.05	63,63,63,63	0
33	MG	K	8069	1/1	0.97	0.03	57,57,57,57	0
36	CL	N	8807	1/1	0.97	0.07	63,63,63,63	0
36	CL	O	8808	1/1	0.97	0.07	72,72,72,72	0
36	CL	Y	8820	1/1	0.97	0.06	46,46,46,46	0
33	MG	0	8090	1/1	0.97	0.09	60,60,60,60	0
33	MG	0	8107	1/1	0.98	0.07	68,68,68,68	0
33	MG	0	8111	1/1	0.98	0.10	34,34,34,34	0
33	MG	0	8075	1/1	0.98	0.03	44,44,44,44	0
35	NA	R	8538	1/1	0.98	0.04	57,57,57,57	0
33	MG	0	8097	1/1	0.98	0.05	36,36,36,36	0
35	NA	0	8531	1/1	0.98	0.05	40,40,40,40	0
35	NA	T	8543	1/1	0.98	0.07	39,39,39,39	0
36	CL	0	8803	1/1	0.98	0.07	59,59,59,59	0
33	MG	0	8039	1/1	0.98	0.04	50,50,50,50	0
33	MG	0	8044	1/1	0.98	0.06	49,49,49,49	0
36	CL	0	8814	1/1	0.98	0.07	48,48,48,48	0
33	MG	0	8116	1/1	0.98	0.04	37,37,37,37	0
33	MG	0	8040	1/1	0.98	0.03	61,61,61,61	0
33	MG	B	8055	1/1	0.98	0.04	52,52,52,52	0
33	MG	0	8014	1/1	0.98	0.07	34,34,34,34	0
33	MG	0	8052	1/1	0.98	0.04	58,58,58,58	0
36	CL	B	8819	1/1	0.98	0.08	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	0	8067	1/1	0.98	0.06	49,49,49,49	0
33	MG	3	8078	1/1	0.98	0.09	47,47,47,47	0
36	CL	J	8821	1/1	0.98	0.05	55,55,55,55	0
34	K	0	8401	1/1	0.98	0.17	75,75,75,75	0
33	MG	0	8093	1/1	0.98	0.06	48,48,48,48	0
35	NA	0	8501	1/1	0.98	0.10	35,35,35,35	0
36	CL	R	8806	1/1	0.98	0.06	50,50,50,50	0
35	NA	J	8546	1/1	0.98	0.06	55,55,55,55	0
33	MG	0	8024	1/1	0.98	0.03	23,23,23,23	0
33	MG	A	8065	1/1	0.99	0.04	42,42,42,42	0
33	MG	0	8091	1/1	0.99	0.03	59,59,59,59	0
33	MG	0	8004	1/1	0.99	0.03	27,27,27,27	0
33	MG	0	8016	1/1	0.99	0.03	35,35,35,35	0
33	MG	Y	8108	1/1	0.99	0.04	40,40,40,40	0
35	NA	0	8528	1/1	0.99	0.15	49,49,49,49	0
33	MG	0	8019	1/1	0.99	0.02	37,37,37,37	0
33	MG	0	8022	1/1	0.99	0.02	41,41,41,41	0
33	MG	0	8012	1/1	0.99	0.03	34,34,34,34	0
33	MG	0	8068	1/1	0.99	0.02	68,68,68,68	0
33	MG	0	8025	1/1	0.99	0.02	46,46,46,46	0
33	MG	0	8071	1/1	0.99	0.03	72,72,72,72	0
36	CL	0	8811	1/1	0.99	0.05	54,54,54,54	0
36	CL	0	8812	1/1	0.99	0.05	54,54,54,54	0
35	NA	0	8503	1/1	0.99	0.05	39,39,39,39	0
35	NA	0	8536	1/1	0.99	0.02	47,47,47,47	0
33	MG	0	8072	1/1	0.99	0.03	56,56,56,56	0
33	MG	0	8027	1/1	0.99	0.04	49,49,49,49	0
33	MG	0	8080	1/1	0.99	0.03	46,46,46,46	0
33	MG	0	8081	1/1	0.99	0.03	53,53,53,53	0
33	MG	0	8028	1/1	0.99	0.02	37,37,37,37	0
33	MG	0	8083	1/1	0.99	0.05	41,41,41,41	0
33	MG	0	8110	1/1	0.99	0.02	41,41,41,41	0
33	MG	0	8084	1/1	0.99	0.06	48,48,48,48	0
35	NA	0	8553	1/1	0.99	0.05	30,30,30,30	0
33	MG	0	8058	1/1	0.99	0.05	44,44,44,44	0
36	CL	M	8818	1/1	0.99	0.03	48,48,48,48	0
33	MG	0	8086	1/1	0.99	0.05	48,48,48,48	0
33	MG	0	8059	1/1	0.99	0.04	33,33,33,33	0
33	MG	0	8060	1/1	0.99	0.05	42,42,42,42	0
33	MG	0	8089	1/1	0.99	0.10	56,56,56,56	0
33	MG	0	8061	1/1	0.99	0.03	40,40,40,40	0
37	CD	O	8705	1/1	0.99	0.02	74,74,74,74	0

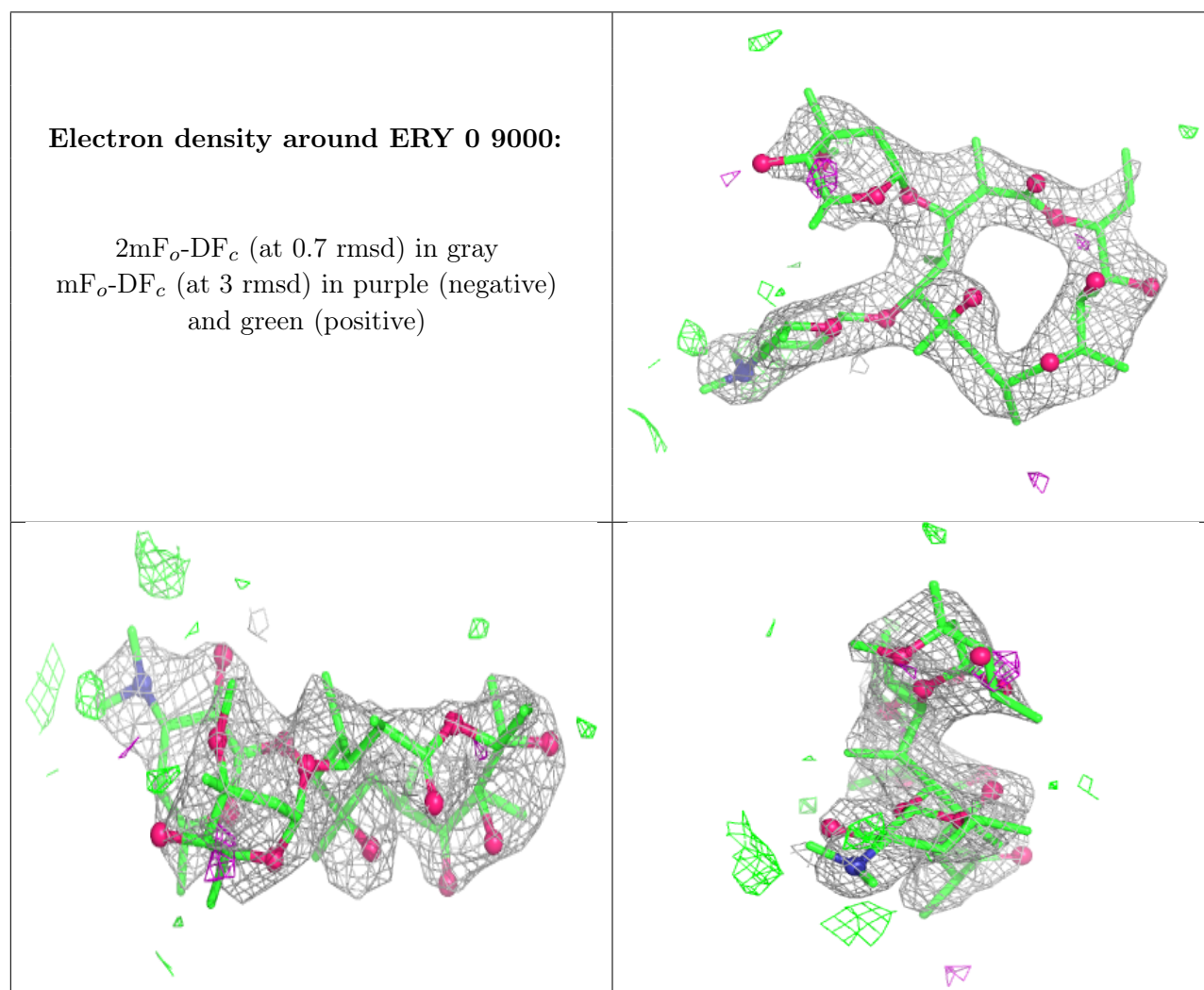
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
37	CD	1	8702	1/1	0.99	0.03	63,63,63,63	0
33	MG	0	8008	1/1	1.00	0.02	33,33,33,33	0
33	MG	0	8054	1/1	1.00	0.02	32,32,32,32	0
33	MG	0	8056	1/1	1.00	0.02	53,53,53,53	0
33	MG	0	8026	1/1	1.00	0.01	29,29,29,29	0
33	MG	0	8009	1/1	1.00	0.02	33,33,33,33	0
33	MG	0	8010	1/1	1.00	0.02	37,37,37,37	0
33	MG	0	8029	1/1	1.00	0.01	49,49,49,49	0
33	MG	0	8030	1/1	1.00	0.01	29,29,29,29	0
33	MG	0	8031	1/1	1.00	0.01	34,34,34,34	0
33	MG	0	8032	1/1	1.00	0.07	39,39,39,39	0
33	MG	0	8033	1/1	1.00	0.02	32,32,32,32	0
33	MG	0	8034	1/1	1.00	0.02	34,34,34,34	0
33	MG	0	8035	1/1	1.00	0.01	49,49,49,49	0
35	NA	0	8519	1/1	1.00	0.04	36,36,36,36	0
33	MG	0	8106	1/1	1.00	0.01	42,42,42,42	0
33	MG	0	8036	1/1	1.00	0.03	35,35,35,35	0
33	MG	0	8109	1/1	1.00	0.02	23,23,23,23	0
33	MG	0	8037	1/1	1.00	0.02	45,45,45,45	0
33	MG	0	8038	1/1	1.00	0.01	32,32,32,32	0
33	MG	0	8011	1/1	1.00	0.05	25,25,25,25	0
33	MG	0	8074	1/1	1.00	0.01	38,38,38,38	0
33	MG	0	8002	1/1	1.00	0.06	33,33,33,33	0
33	MG	0	8077	1/1	1.00	0.02	30,30,30,30	0
33	MG	0	8079	1/1	1.00	0.02	30,30,30,30	0
33	MG	0	8013	1/1	1.00	0.02	45,45,45,45	0
33	MG	0	8003	1/1	1.00	0.01	32,32,32,32	0
33	MG	0	8015	1/1	1.00	0.02	35,35,35,35	0
33	MG	0	8001	1/1	1.00	0.03	33,33,33,33	0
33	MG	0	8017	1/1	1.00	0.04	25,25,25,25	0
33	MG	0	8018	1/1	1.00	0.02	45,45,45,45	0
33	MG	0	8005	1/1	1.00	0.01	30,30,30,30	0
33	MG	0	8020	1/1	1.00	0.01	36,36,36,36	0
33	MG	0	8021	1/1	1.00	0.01	35,35,35,35	0
33	MG	0	8006	1/1	1.00	0.02	38,38,38,38	0
33	MG	0	8023	1/1	1.00	0.02	39,39,39,39	0
37	CD	U	8701	1/1	1.00	0.01	67,67,67,67	0
37	CD	Z	8703	1/1	1.00	0.01	63,63,63,63	0
33	MG	0	8007	1/1	1.00	0.03	27,27,27,27	0
37	CD	3	8704	1/1	1.00	0.02	62,62,62,62	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers ⓘ

There are no such residues in this entry.