



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2017 – 08:27 PM EDT

PDB ID : 3CCQ
Title : Structure of Anisomycin resistant 50S Ribosomal Subunit: 23S rRNA mutation A2488U
Authors : Blaha, G.; Gurel, G.
Deposited on : unknown
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

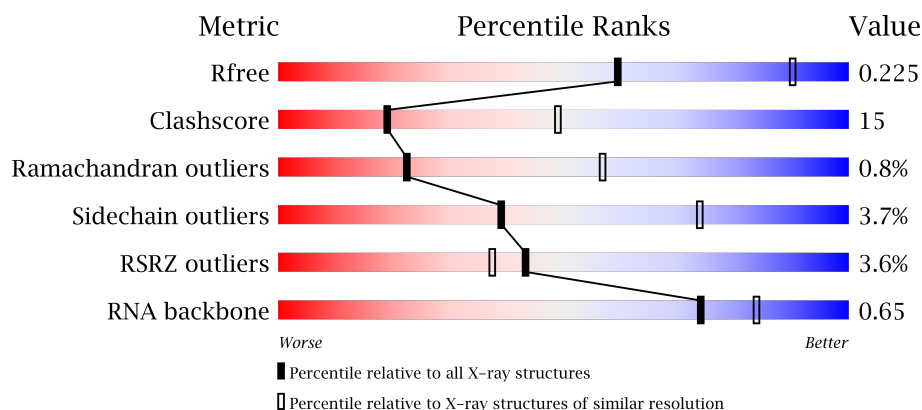
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)
RNA backbone	2435	1004 (3.20-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	240	<div> <div>3%</div> <div>71%</div> <div>25%</div> <div>..</div> </div>
2	B	338	<div> <div>0%</div> <div>68%</div> <div>29%</div> <div>.</div> </div>
3	C	246	<div> <div>2%</div> <div>72%</div> <div>26%</div> <div>.</div> </div>
4	D	177	<div> <div>28%</div> <div>40%</div> <div>37%</div> <div>21%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
5	E	178	
6	F	120	
7	G	348	
8	H	177	
9	I	162	
10	J	145	
11	K	132	
12	L	165	
13	M	196	
14	N	187	
15	O	116	
16	P	149	
17	Q	96	
18	R	155	
19	S	85	
20	T	120	
21	U	67	
22	V	71	
23	W	154	
24	X	92	
25	Y	241	
26	Z	116	
27	1	57	
28	2	50	
29	3	92	

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Mol	Chain	Length	Quality of chain
30	0	2923	
31	9	122	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	MG	0	8009	-	-	-	X
32	MG	0	8014	-	-	-	X
32	MG	0	8028	-	-	-	X
32	MG	0	8041	-	-	-	X
32	MG	0	8047	-	-	-	X
32	MG	0	8084	-	-	-	X
32	MG	0	8085	-	-	-	X
32	MG	A	8051	-	-	-	X
34	SR	0	8903	-	-	-	X
34	SR	0	8904	-	-	-	X
34	SR	0	8949	-	-	-	X
34	SR	B	8987	-	-	-	X
35	NA	0	8521	-	-	-	X
35	NA	0	8527	-	-	-	X
35	NA	0	8528	-	-	-	X
35	NA	0	8530	-	-	-	X
35	NA	0	8542	-	-	-	X
35	NA	0	8546	-	-	-	X
35	NA	0	8547	-	-	-	X
35	NA	0	8553	-	-	-	X
35	NA	0	8555	-	-	-	X
35	NA	0	8556	-	-	-	X
35	NA	0	8559	-	-	-	X
35	NA	0	8560	-	-	-	X
35	NA	0	8562	-	-	-	X
35	NA	0	8563	-	-	-	X
35	NA	0	8564	-	-	-	X
35	NA	0	8565	-	-	-	X
35	NA	0	8567	-	-	-	X
35	NA	9	8572	-	-	-	X
35	NA	R	8575	-	-	-	X
37	K	0	8401	-	-	-	X
37	K	0	8402	-	-	-	X

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99120 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L2P.

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

- Molecule 2 is a protein called 50S ribosomal protein L3P.

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

- Molecule 3 is a protein called 50S ribosomal protein L4P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	246	Total	C	N	O	S	0	0	0
			1860	1130	345	384	1			

- Molecule 4 is a protein called 50S ribosomal protein L5P.

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

- Molecule 5 is a protein called 50S ribosomal protein L6P.

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

- Molecule 6 is a protein called 50S ribosomal protein L7Ae.

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

- Molecule 7 is a protein called 50S ribosomal protein L10E.

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

- Molecule 8 is a protein called 50S ribosomal protein L10e.

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

- Molecule 9 is a protein called 50S ribosomal protein L11P.

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

- Molecule 10 is a protein called 50S ribosomal protein L13P.

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

- Molecule 11 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	132	Total	C	N	O	S	0	0	0
			994	609	189	192	4			

- Molecule 12 is a protein called 50S ribosomal protein L15P.

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

- Molecule 13 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	194	Total	C	N	O	S	0	0	0
			1558	943	333	281	1			

- Molecule 14 is a protein called 50S ribosomal protein L18P.

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

- Molecule 15 is a protein called 50S ribosomal protein L18e.

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

- Molecule 16 is a protein called 50S ribosomal protein L19e.

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

- Molecule 17 is a protein called 50S ribosomal protein L21e.

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

- Molecule 18 is a protein called 50S ribosomal protein L22P.

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

- Molecule 19 is a protein called 50S ribosomal protein L23P.

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

- Molecule 20 is a protein called 50S ribosomal protein L24P.

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

- Molecule 21 is a protein called 50S ribosomal protein L24e.

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

- Molecule 22 is a protein called 50S ribosomal protein L29P.

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

- Molecule 23 is a protein called 50S ribosomal protein L30P.

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

- Molecule 24 is a protein called 50S ribosomal protein L31e.

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

- Molecule 25 is a protein called 50S ribosomal protein L32e.

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

- Molecule 26 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	73	Total	C	N	O	S	0	0	0
			573	343	113	112	5			

- Molecule 27 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 28 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 29 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 30 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	0	2754	Total	C	N	O	P	0	0	0
			59018	26348	10870	19055	2745			

- Molecule 31 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	9	122	Total	C	N	O	P	0	0	0
			2599	1160	471	847	121			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	87	Total	Mg	0	0
			87	87		
32	9	1	Total	Mg	0	0
			1	1		
32	K	1	Total	Mg	0	0
			1	1		
32	B	1	Total	Mg	0	0
			1	1		
32	A	1	Total	Mg	0	0
			1	1		
32	T	1	Total	Mg	0	0
			1	1		
32	Y	1	Total	Mg	0	0
			1	1		

- Molecule 33 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	0	9	Total Cl 9 9	0	0
33	J	3	Total Cl 3 3	0	0
33	Q	1	Total Cl 1 1	0	0
33	B	1	Total Cl 1 1	0	0
33	A	1	Total Cl 1 1	0	0
33	N	1	Total Cl 1 1	0	0
33	O	1	Total Cl 1 1	0	0
33	R	1	Total Cl 1 1	0	0
33	Y	1	Total Cl 1 1	0	0
33	L	1	Total Cl 1 1	0	0
33	3	1	Total Cl 1 1	0	0
33	M	1	Total Cl 1 1	0	0

- Molecule 34 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	0	93	Total Sr 93 93	0	0
34	1	2	Total Sr 2 2	0	0
34	B	2	Total Sr 2 2	0	0
34	3	2	Total Sr 2 2	0	0
34	A	3	Total Sr 3 3	0	0
34	R	1	Total Sr 1 1	0	0
34	9	3	Total Sr 3 3	0	0
34	S	1	Total Sr 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	F	1	Total	Sr	0	0
			1	1		

- Molecule 35 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	65	Total	Na	0	0
			65	65		
35	J	1	Total	Na	0	0
			1	1		
35	Q	1	Total	Na	0	0
			1	1		
35	B	1	Total	Na	0	0
			1	1		
35	C	1	Total	Na	0	0
			1	1		
35	R	2	Total	Na	0	0
			2	2		
35	9	2	Total	Na	0	0
			2	2		
35	S	1	Total	Na	0	0
			1	1		
35	M	1	Total	Na	0	0
			1	1		

- Molecule 36 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	O	1	Total	Cd	0	0
			1	1		
36	Z	1	Total	Cd	0	0
			1	1		
36	1	1	Total	Cd	0	0
			1	1		
36	3	1	Total	Cd	0	0
			1	1		
36	U	1	Total	Cd	0	0
			1	1		

- Molecule 37 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	0	2	Total K 2 2	0	0

- Molecule 38 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	A	112	Total O 112 112	0	0
38	B	142	Total O 142 142	0	0
38	C	168	Total O 168 168	0	0
38	D	45	Total O 45 45	0	0
38	E	42	Total O 42 42	0	0
38	F	26	Total O 26 26	0	0
38	G	17	Total O 17 17	0	0
38	H	65	Total O 65 65	0	0
38	I	5	Total O 5 5	0	0
38	J	56	Total O 56 56	0	0
38	K	60	Total O 60 60	0	0
38	L	82	Total O 82 82	0	0
38	M	123	Total O 123 123	0	0
38	N	59	Total O 59 59	0	0
38	O	47	Total O 47 47	0	0
38	P	59	Total O 59 59	0	0
38	Q	47	Total O 47 47	0	0
38	R	76	Total O 76 76	0	0
38	S	33	Total O 33 33	0	0

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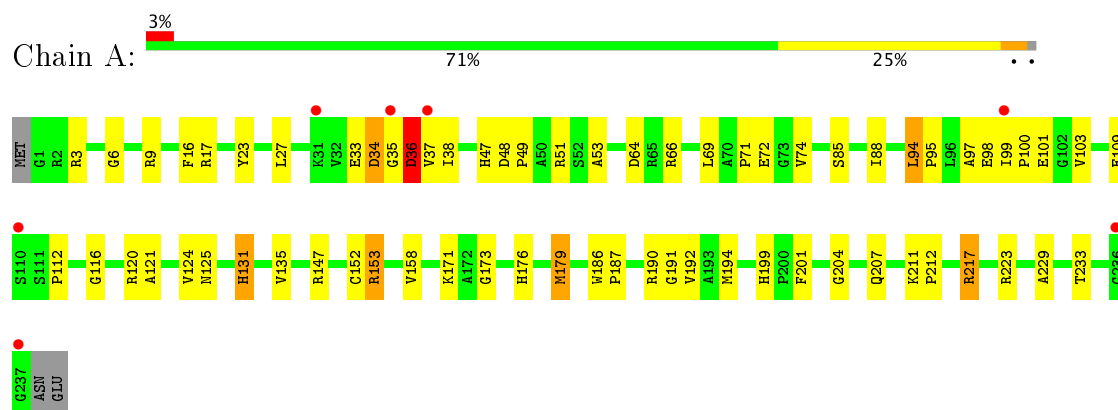
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	T	36	Total 36	O 36	0	0
38	U	26	Total 26	O 26	0	0
38	V	12	Total 12	O 12	0	0
38	W	66	Total 66	O 66	0	0
38	X	28	Total 28	O 28	0	0
38	Y	97	Total 97	O 97	0	0
38	Z	31	Total 31	O 31	0	0
38	1	54	Total 54	O 54	0	0
38	2	43	Total 43	O 43	0	0
38	3	68	Total 68	O 68	0	0
38	0	5950	Total 5950	O 5950	0	0
38	9	148	Total 148	O 148	0	0

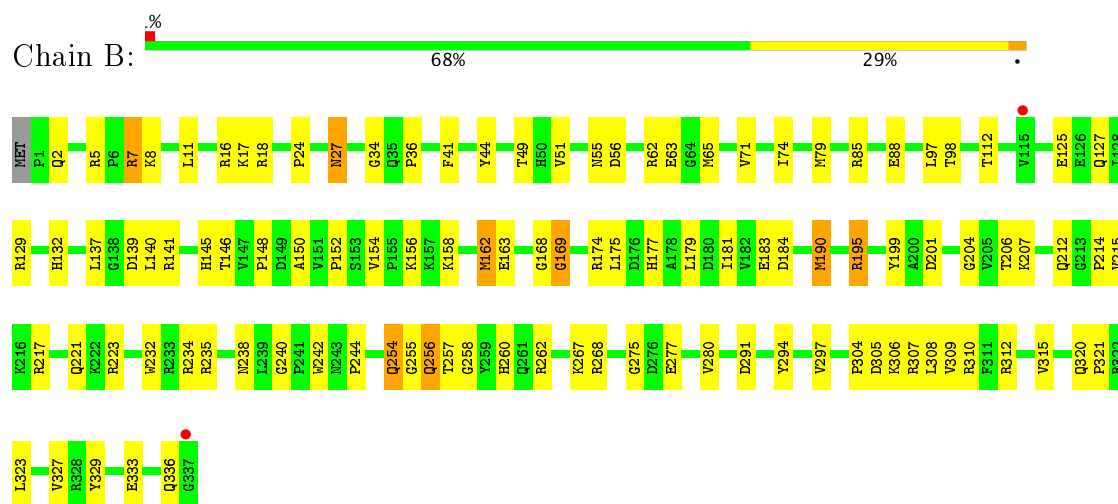
3 Residue-property plots [i](#)

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

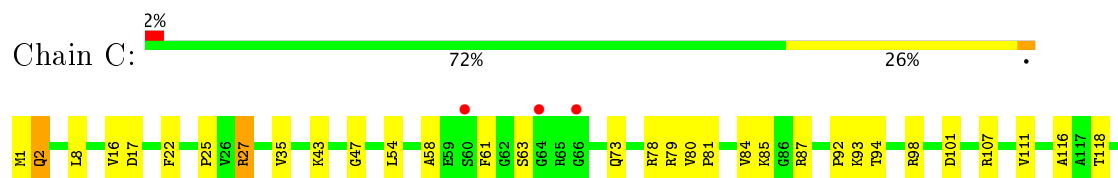
• Molecule 1: 50S ribosomal protein L2P

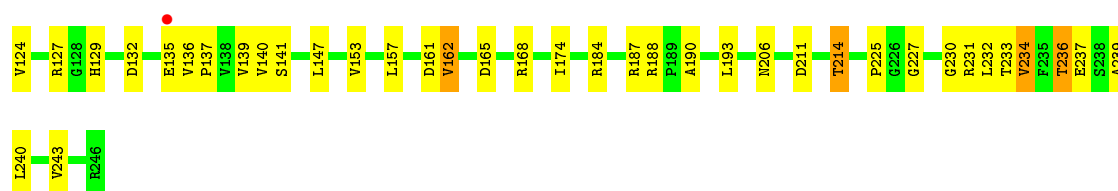


• Molecule 2: 50S ribosomal protein L3P

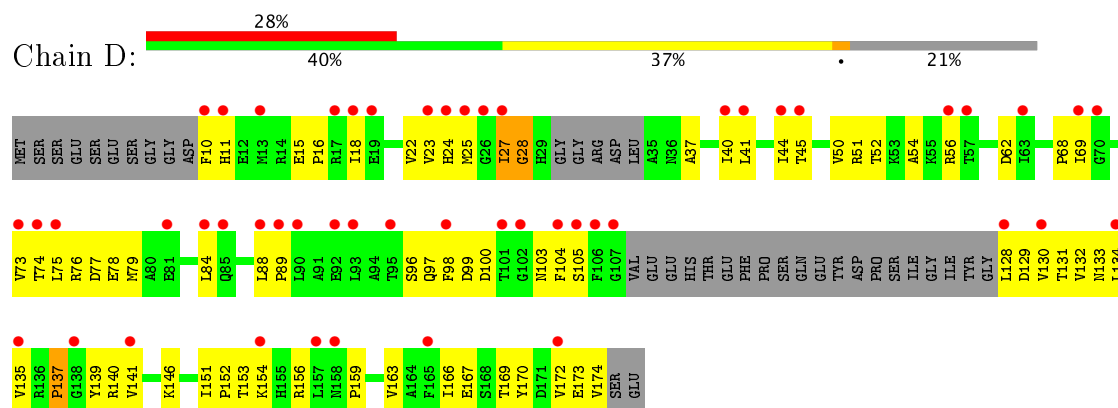


• Molecule 3: 50S ribosomal protein L4P

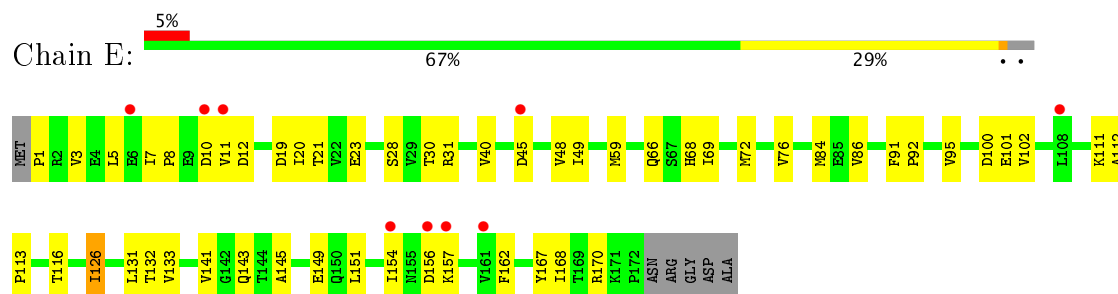




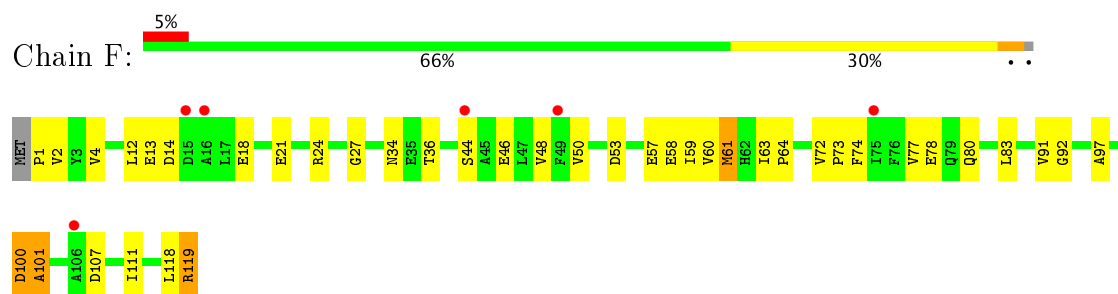
• Molecule 4: 50S ribosomal protein L5P



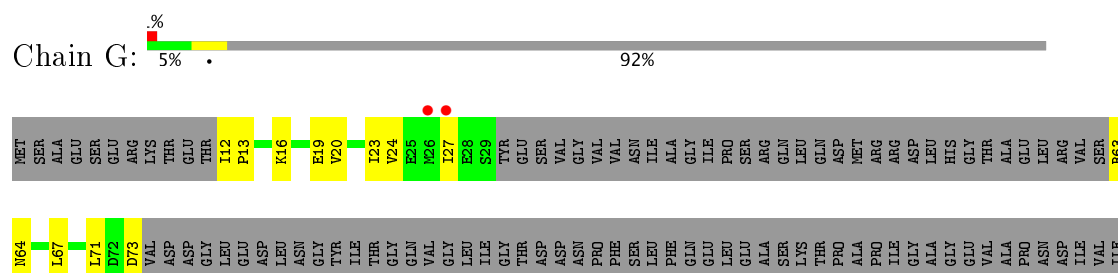
• Molecule 5: 50S ribosomal protein L6P



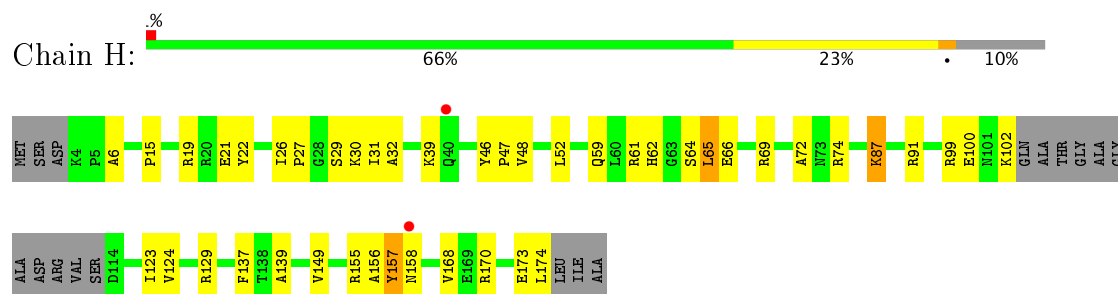
• Molecule 6: 50S ribosomal protein L7Ae



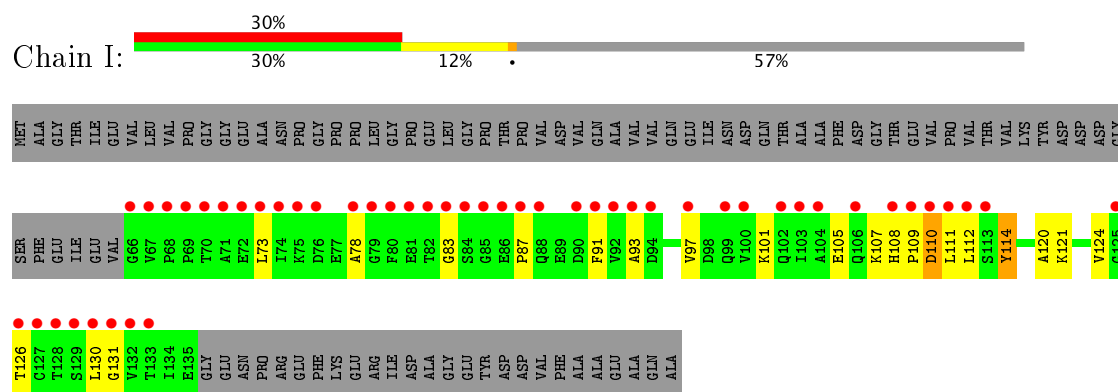
• Molecule 7: 50S ribosomal protein L10E



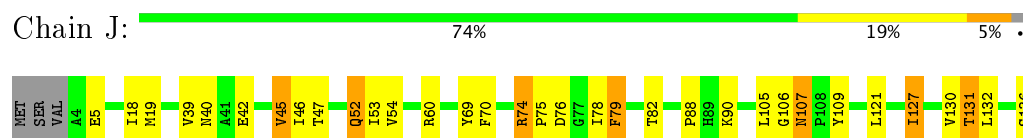
- Molecule 8: 50S ribosomal protein L10e



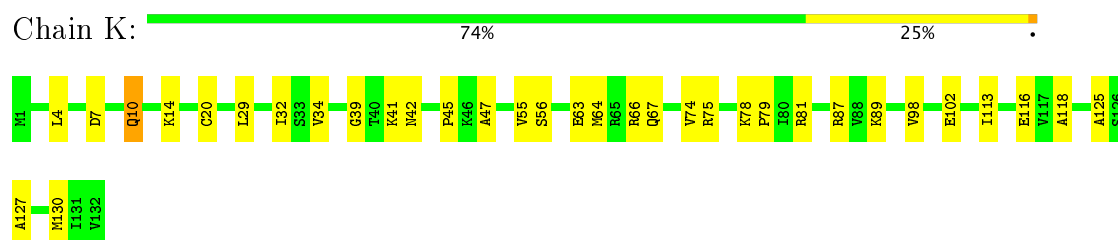
- Molecule 9: 50S ribosomal protein L11P



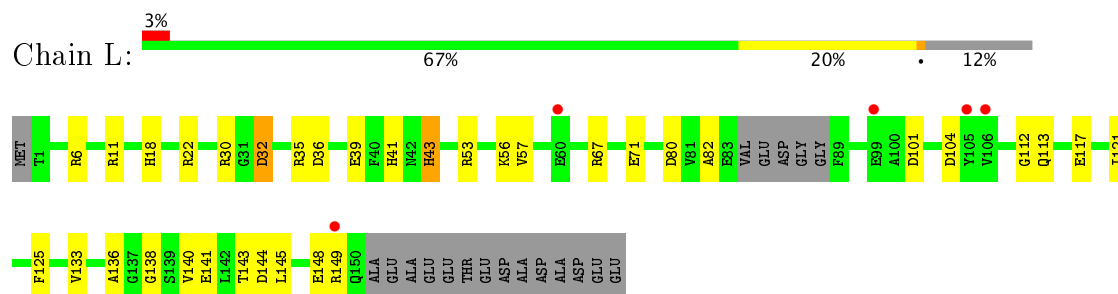
- Molecule 10: 50S ribosomal protein L13P



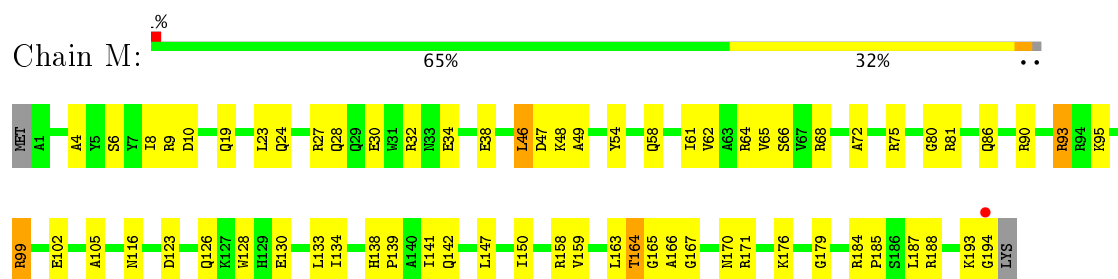
- Molecule 11: 50S ribosomal protein L14P



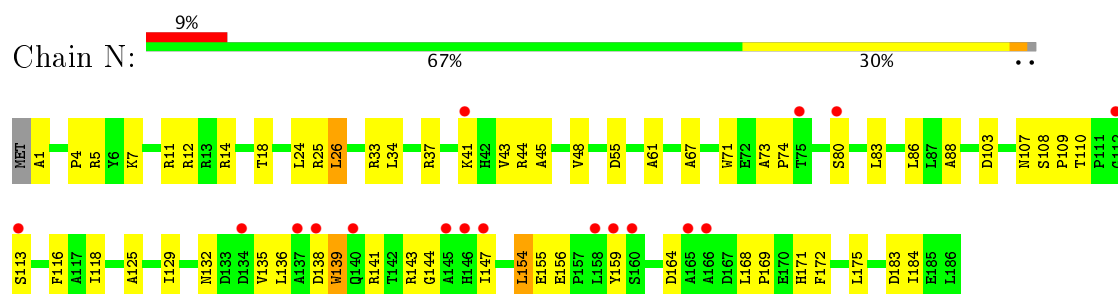
- Molecule 12: 50S ribosomal protein L15P



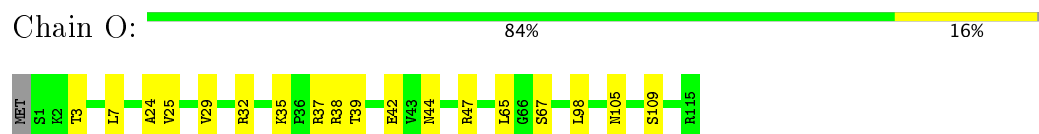
- Molecule 13: 50S ribosomal protein L15e



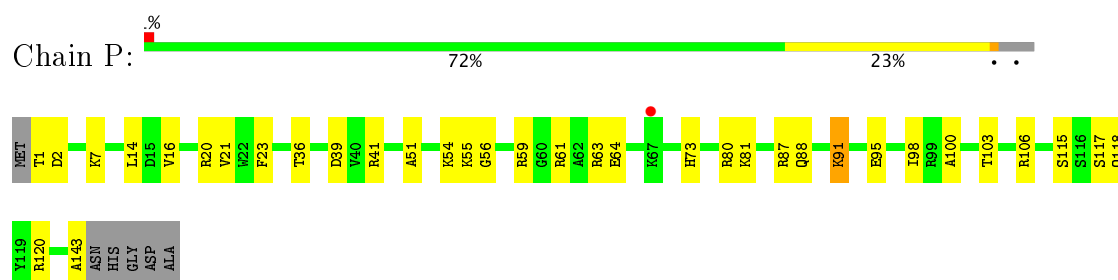
- Molecule 14: 50S ribosomal protein L18P



- Molecule 15: 50S ribosomal protein L18e



- Molecule 16: 50S ribosomal protein L19e



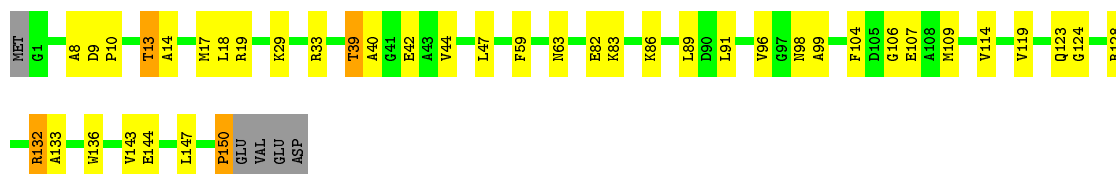
- Molecule 17: 50S ribosomal protein L21e

Chain Q:  72% 25% ..




- Molecule 18: 50S ribosomal protein L22P

Chain R:  70% 24% . .




- Molecule 19: 50S ribosomal protein L23P

Chain S:  2% 75% 20% 5%



- Molecule 20: 50S ribosomal protein L24P

Chain T:  3% 80% 18% ..



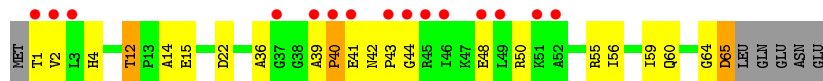
- Molecule 21: 50S ribosomal protein L24e

Chain U:  0% 51% 27% 21%



- Molecule 22: 50S ribosomal protein L29P

Chain V:  21% 61% 27% 8%



- Molecule 23: 50S ribosomal protein L30P

Chain W:  57% 42% .

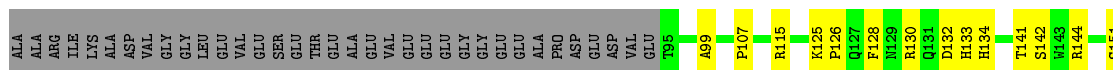




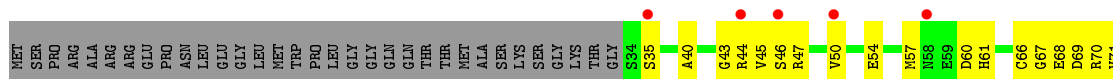
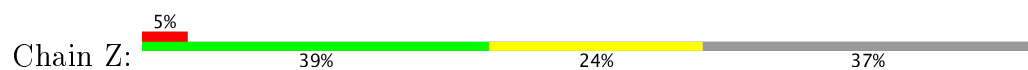
- Molecule 24: 50S ribosomal protein L31e



- Molecule 25: 50S ribosomal protein L32e



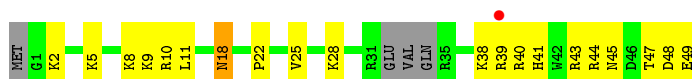
- Molecule 26: 50S ribosomal protein L37Ae



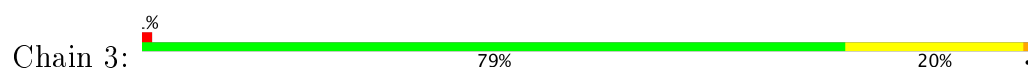
- Molecule 27: 50S ribosomal protein L37e



- Molecule 28: 50S ribosomal protein L39e

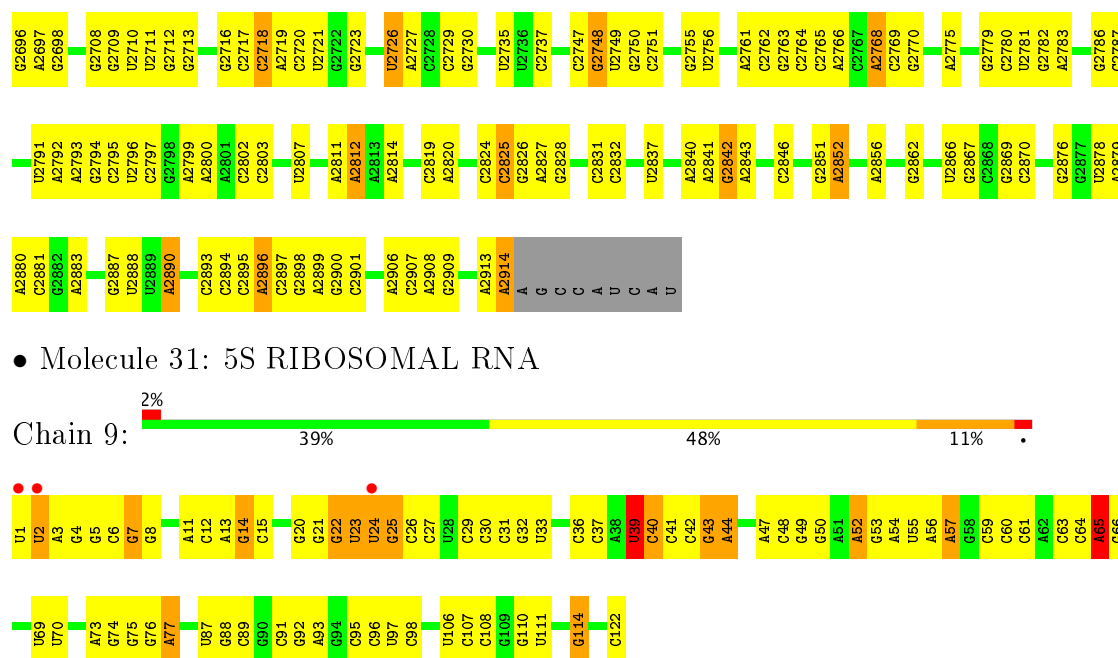


- Molecule 29: 50S ribosomal protein L44E





C2503	C2502	G2412	A2321	G	C2105	G2000	A1909	U1825	C1731	G1555	C1456	U1359	C1267
C2504	A2503	G2413	C2326	C	C2106	G2001	A1915	C1826	A1732	A1559	C1457	C1360	C1268
C2505	A2414	A2413	A2238	G	G2110	C2002	U1915	C1827	A1733	U	U1457	C1366	G1269
C2506	C2329	G2415	C2239	G	G2111	U2003	C1916	A1829	C1735	C1561	C1474	C1372	C1273
C2507	G2507	G2416	U2240	G	A2112	U2004	C1919	C1834	A1736	U1562	C1477	A1372	A1278
C2508	C2331	U2419	C2241	U	C2113	G2005	A1920	U1835	U1741	C1563	U1478	C1377	U1279
C2509	A2332	G2420	U2242	A	C2114	C2006	C1921	U1836	A1742	C1564	C1479	C1378	C1289
C2510	G2333	G2421	C2243	C	U2115	A2007	A1922	U1837	U1743	C1565	U1480	U1379	C1290
C2511	U2338	G2422	C2244	C	U2116	G2008	A1923	U1838	U1744	C1566	C1482	C1380	A1291
C2512	G2338	C2423	C2245	C	C2119	U2009	G1925	U1839	U1748	A1573	A1483	U1381	A1294
C2513	A	G2424	U2246	G	U2120	A2010	G1926	A1840	U1749	C1574	C1486	G1382	A1295
C2514	C	G2425	C2247	G	C2121	U2011	A1927	A1841	C1751	C1575	A1487	U1383	A1296
U2607	A	U2435	C2248	G	C2122	G2013	A1930	A1842	G1752	G1576	U1488	C1384	G1295
C2608	G	U2436	U2249	U	G2128	A2022	A1931	A1845	A1755	U1577	G1489	C1385	G1296
C2609	A	U2437	G2250	C	U2133	C2026	A1939	G1849	A1756	A1581	A1492	G1386	U1297
U2610	G2344	C2443	G2251	G	G2134	U2027	U1939	C1853	A1759	C1582	C1495	U1387	G1298
C2613	A2345	U2444	A2252	C	C2135	U2032	A1942	C1854	U1761	G1586	C1496	A1393	U1304
C2614	C2346	U2445	G2253	G	A2136	U2033	C1943	G1855	C1762	U1587	G1497	C1394	C1305
C2615	G2347	G2446	C2254	G	C	U2034	G1947	A1857	C1763	G1588	U1500	C1395	U1306
U2616	C2348	C2450	A2255	C	A	U2063	G1948	A1858	U1766	C1589	U1503	C1396	A1307
U2617	G2349	G2451	G2256	C	G	U2064	G1949	C1861	A1767	C1592	U1504	C1397	A1308
U2618	A2353	G2452	A2258	A	U	G2044	G1950	C1862	U1768	C1593	A1505	U1407	U1314
C2632	A2354	G2453	U2265	C	C	A2054	G1951	C1863	C1773	C1594	U1506	U1408	G1315
C2633	G2355	G2454	A2266	C	G	U2065	U	G1864	C1772	C1595	C1507	G1409	G1316
C2634	A2356	U2456	C2269	C	U	G2066	C	G1865	G1774	C1602	U1511	C1437	A1317
C2635	G2357	U2457	G2270	C	G	U2067	A	C1866	C1775	A1603	G1512	A1413	A1318
C2636	C2358	G2462	C2271	A	U	G2068	U	U1871	U1776	G1604	U1516	A1414	G1319
C2637	A2361	C2463	G2272	G	C	U2069	G	G1872	A1778	G1605	G1416	C1320	C1320
C2638	C2362	U2464	C2273	C	C	C2071	A	G1873	C1779	A1606	G1417	G1322	G1322
U2643	G2363	G2465	G2274	A	C	G2072	C	U1877	C1787	A1607	C1520	U1418	G1325
C2644	C2364	A2467	C2275	A	G	U2073	C	U1878	U1788	U1625	C1521	U1419	C1326
U2649	G2365	U2468	G2276	C	A	A2074	U1964	C1880	G1789	A1615	G1523	U1422	G1327
C2651	C2366	A2469	U2277	G	U	U2075	C1965	A1881	C1790	G1622	U1524	C1423	A1328
U2652	A2367	C2472	U2277	C	C	U2076	U1966	U1882	C1792	C1623	A1526	A1427	G1331
U2653	G2368	U2473	U2281	A	A	A2081	G1971	G1884	G1795	A1624	A1527	C1428	G1339
U2654	A2369	C2476	C2282	C	U	G2082	U1972	A1885	U1796	U1625	A1528	G1433	G1340
C2658	C2370	U2477	U2282	U	A	A2083	A1973	U1886	A1797	A1626	G1529	A1434	C1341
C2659	G2371	C2478	A2291	A	G	C2087	G1974	C1887	C1798	G1627	U1535	C1342	C1342
A2664	U2373	A2479	U2297	U	C	U2088	G1975	U1889	G1799	A1630	C1538	G1441	G1344
U	C2374	U2480	U2298	C	A	A2089	U1976	U1890	C1803	A1631	U1539	G1442	C1345
C2667	A2375	G2482	C2299	C	U	G2090	A1977	C1894	A1804	A1632	C1543	U1350	U1350
C2670	C2376	U2483	A2300	U	A	G2091	G1978	A1895	G1805	C1633	G1544	G1445	G1351
C2671	U2377	A2484	A2301	C	G	A2096	C1979	U1897	G1805	G1634	U1545	U1446	A1352
C2672	G2379	C2485	A2302	C	U	C	U1992	U1897	A1815	U1722	G1546	U1447	C1353
U2681	A2382	U2488	C2309	C	A	U2096	C1993	U1897	C1803	A1631	C1538	C1450	A1357
C2682	G2385	G2489	C2310	G	G	A2100	U1994	C1894	A1804	A1632	U1539	C1451	A1358
C2683	U2386	A2490	A2311	C	A	A2101	G1995	A1895	G1805	C1633	G1543	G1444	U1350
C2684	C2387	U2491	G2312	G	G	C2102	U1996	C1896	C1805	G1634	U1544	U1445	G1351
C2685	U2388	C2492	C2313	C	A	A2103	U1997	U1897	G1805	G1635	U1545	U1446	A1352
C2686	C2389	C2493	C2314	G	U	C2104	U1998	U1897	A1815	A1637	G1546	U1447	C1353
C2687	U2390	U2494	C2315	U	C		U1999	U1897	C1803	A1641	C1553	C1450	A1357
C2688	G2391	G2495	C2316	C	A		U1999	U1897	A1804	A1642	C1554	C1451	A1358
C2689	U2392	U2496	C2317	G	U		U1999	U1897	G1805	A1642	C1554	C1451	A1358
C2690	C2393	C2497	C2318	U	C		U1999	U1897	C1803	A1642	C1554	C1451	A1358
C2691	U2394	U2498	C2319	A	U		U1999	U1897	A1804	A1642	C1554	C1451	A1358
C2692	C2395	C2499	C2320	C	U		U1999	U1897	G1805	A1642	C1554	C1451	A1358
C2693	U2396	U2500	C2321	U	A		U1999	U1897	C1803	A1642	C1554	C1451	A1358
C2694	C2397	C2501	C2322	C	U		U1999	U1897	A1804	A1642	C1554	C1451	A1358
C2695	U2398	U2502	C2323	G	U		U1999	U1897	G1805	A1642	C1554	C1451	A1358
C2696	C2399	C2503	C2324	C	A		U1999	U1897	C1803	A1642	C1554	C1451	A1358
C2697	U2400	U2504	C2325	U	U		U1999	U1897	A1804	A1642	C1554	C1451	A1358
C2698	A2401	C2505	C2326	C	C		U1999	U1897	G1805	A1642	C1554	C1451	A1358
C2699	C2402	G2506	C2327	G	U		U1999	U1897	C1803	A1642	C1554	C1451	A1358
U2610	U2403	U2507	C2328	U	A		U1999	U1897	A1804	A1642	C1554	C1451	A1358
C2613	C2404	C2508	C2329	C	C		U1999	U1897	G1805	A1642	C1554	C1451	A1358
C2614	A2405	U2509	C2330	G	U		U1999	U1897	C1803	A1642	C1554	C1451	A1358
U2615	G2406	C2510	U2331	C	U		U1999	U1897	A1804	A1642	C1554	C1451	A1358
U2616	C2407	C2511	C2332	G	A		U1999	U1897	G1805	A1642	C1554	C1451	A1358
U2617	U2408	U2512	C2333	C	C		U1999	U1897	C1803	A1642	C1554	C1451	A1358
U2618	A2409	G2513	C2334	U	U		U1999	U1897	A1804	A1642	C1554	C1451	A1358
U2619	C2410	C2514	C2335	C	C		U1999	U1897	G1805	A1642	C1554	C1451	A1358
U2620	U2411	U2515	C2336	G	U		U1999	U1897	C1803	A1642	C1554	C1451	A1358
U2621	C2412	C2516	C2337	C	A		U1999	U1897	A1804	A1642	C1554	C1451	A1358
U2622	U2413	U2517	C2338	G	C		U1999	U1897	G1805	A1642	C1554	C1451	A1358
U2623	A2414	C2518	C2339	U	U		U1999	U1897	C1803	A1642	C1554	C1451	A1358
U2624	G2415	C2519	U2331	C	C		U1999	U1897	A1804	A1642	C1554	C1451	A1358
U2625	U2416	U2520	C2332	G	A		U1999	U1897	G1805	A1642	C1554	C1451	A1358
U2626	C2417	U2521	C2333	C	C		U1999	U1897	C1803	A1642	C1554	C1451	A1358
U2627	A2418	C2522	C2334	U	U		U1999	U1897	A1804	A1642	C1554	C1451	A1358
U2628	U2419	U2523	C2335	C	C		U1999	U1897	G1805	A1642	C1554	C1451	A1358
U2629	C2420	C2524	C2336	G	U		U1999	U1897	C1803	A1642	C1554	C1451	A1358
U2630	G2421	U2525	C2337	C	A		U1999	U1897	A1804	A1642	C1554	C1451	A1358
U2631	U2422	C2526	C2338	G	C		U1999	U1897	G1805	A1642	C1554	C1451	A1358
U2632	C2423	U2527	C2339	U	U		U1999	U1897	C1803	A1642	C1554	C1451	A1358
U2633	A2424	C2528	C2340	C	C		U1999	U1897	A1804	A1642	C1554	C1451	A1358
U2634	U2425	U2529	C2341	G	A		U1999	U1897	G1805	A1642	C1554	C1451	A1358
U2635	C2426	C2530	C2342	C	C		U1999	U1897	C1803	A1642	C1554	C1451	A1358
U2636	U2427	U2531	C2343	U	U		U1999	U1897	A1804	A1642	C1554	C1451	A1358
U2637	G2428	C2532	C2344	C	C		U1999	U1897	G1805	A1642	C1554	C1451	A1358
U2638	A2429	U2533	C2345	G	U		U1999	U1897	C1803	A1642	C1554	C1451	A1358
U2639	C2430	C2534	C2346	C	A		U1999	U1897	A1804	A1642	C1554	C1451	A1358
U2640	U2431	U2535	C2347	G	C		U1999	U1897	G1805	A1642	C1554	C1451	A1358
U2641	C2432	C2536	C2348	U	U		U1999	U1897	C1803	A1642	C1554	C1451	A1358
U2642	G2433	U2537	C2349	C	C		U1999	U1897	A1804	A1642	C1554	C1451	A1358
U2643	U2434	C2538	C2350	G	A		U1999	U1897	G1805	A1642	C1554	C1451	A1358
U2644	C2435	U2539	C2351	C	C		U1999	U1897	C1803	A1642	C1554	C1451	A1358
U2645	A2436	C2540	C2352	U	U		U1999	U1897	A1804	A1642	C1554	C1451	A1358
U2646	U2437	U2541	C2353	C	C		U1999	U1897	G1805	A1642	C1554	C1451	A1358
U2647	C2438	C2542	C2354	G	U		U1999	U1897	C1803	A1642	C1554	C1451	A1358
U2648	A2439	U2543	C2355										



• Molecule 31: 5S RIBOSOMAL RNA

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	212.33Å 299.62Å 575.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 85.65 – 2.41	Depositor EDS
% Data completeness (in resolution range)	98.1 (30.00-2.90) 98.2 (85.65-2.41)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.186 , 0.233 0.182 , 0.225	Depositor DCC
R_{free} test set	3843 reflections (0.99%)	DCC
Wilson B-factor (Å ²)	61.2	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 82.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	99120	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% 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: MG, OMG, CL, SR, NA, K, CD, OMU, UR3, 1MA, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.33	0/1786	0.64	0/2408
2	B	0.34	0/2690	0.65	0/3652
3	C	0.36	0/1885	0.62	0/2552
4	D	0.32	0/1111	0.56	1/1498 (0.1%)
5	E	0.33	0/1382	0.57	0/1880
6	F	0.35	0/901	0.57	0/1224
7	G	0.33	0/241	0.51	0/324
8	H	0.33	0/1302	0.63	0/1743
9	I	0.30	0/526	0.50	0/716
10	J	0.36	0/1136	0.61	0/1530
11	K	0.34	0/1004	0.66	0/1351
12	L	0.35	0/1130	0.64	0/1509
13	M	0.36	0/1582	0.61	0/2116
14	N	0.30	0/1474	0.61	0/1999
15	O	0.35	0/874	0.59	0/1181
16	P	0.33	0/1147	0.53	0/1528
17	Q	0.34	0/749	0.65	0/1005
18	R	1.26	7/1172 (0.6%)	1.09	6/1578 (0.4%)
19	S	0.33	0/648	0.54	0/875
20	T	0.32	0/958	0.64	0/1289
21	U	0.32	0/417	0.57	0/562
22	V	0.32	0/502	0.54	0/675
23	W	0.36	0/1219	0.63	0/1655
24	X	0.35	0/664	0.60	0/895
25	Y	0.37	0/1146	0.62	0/1536
26	Z	0.36	0/584	0.63	0/781
27	1	0.39	0/438	0.62	0/578
28	2	0.34	0/401	0.58	0/529
29	3	0.37	0/771	0.57	0/1024
30	0	0.39	0/65954	0.68	9/102862 (0.0%)
31	9	0.33	0/2904	0.68	1/4526 (0.0%)
All	All	0.40	7/98698 (0.0%)	0.67	17/147581 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
18	R	1	0
23	W	0	1
30	0	0	32
31	9	0	3
All	All	1	36

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	150	PRO	CB-CG	27.45	2.87	1.50
18	R	150	PRO	CA-C	-18.11	1.16	1.52
18	R	150	PRO	CG-CD	13.90	1.96	1.50
18	R	150	PRO	C-O	11.92	1.47	1.23
18	R	150	PRO	N-CA	11.35	1.66	1.47
18	R	150	PRO	N-CD	10.74	1.62	1.47
18	R	150	PRO	CA-CB	7.56	1.68	1.53

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	150	PRO	CB-CA-C	-22.47	55.81	112.00
18	R	150	PRO	N-CA-C	-19.38	61.71	112.10
18	R	150	PRO	CA-N-CD	12.28	128.89	111.70
18	R	150	PRO	N-CA-CB	10.98	116.47	103.30
18	R	150	PRO	CA-C-O	-8.52	99.75	120.20
31	9	39	U	N1-C1'-C2'	6.32	122.22	114.00
18	R	150	PRO	CA-CB-CG	-6.13	92.34	104.00
30	0	1592	G	N9-C1'-C2'	6.12	121.95	114.00
30	0	1504	A	C1'-O4'-C4'	-5.86	105.21	109.90
30	0	1504	A	N9-C1'-C2'	5.70	121.41	114.00
30	0	871	G	C5'-C4'-O4'	-5.36	102.67	109.10
30	0	1120	U	C5'-C4'-C3'	-5.35	107.45	116.00
30	0	841	A	C1'-O4'-C4'	-5.30	105.66	109.90
30	0	2726	U	N1-C1'-C2'	5.24	120.81	114.00
30	0	1819	G	C5'-C4'-C3'	5.05	124.07	116.00
30	0	2301	A	N9-C1'-C2'	5.01	120.52	114.00
4	D	170	TYR	N-CA-C	5.01	124.53	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	R	150	PRO	CA

All (36) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	1078	A	Sidechain
30	0	1080	C	Sidechain
30	0	1309	U	Sidechain
30	0	1327	G	Sidechain
30	0	1417	G	Sidechain
30	0	1592	G	Sidechain
30	0	1684	A	Sidechain
30	0	1829	A	Sidechain
30	0	1863	G	Sidechain
30	0	1877	G	Sidechain
30	0	1878	G	Sidechain
30	0	1979	G	Sidechain
30	0	202	U	Sidechain
30	0	205	U	Sidechain
30	0	221	G	Sidechain
30	0	2492	U	Sidechain
30	0	2493	C	Sidechain
30	0	2503	A	Sidechain
30	0	2506	A	Sidechain
30	0	2543	G	Sidechain
30	0	2607	U	Sidechain
30	0	2632	G	Sidechain
30	0	2673	U	Sidechain
30	0	2842	G	Sidechain
30	0	396	U	Sidechain
30	0	470	U	Sidechain
30	0	48	A	Sidechain
30	0	482	G	Sidechain
30	0	518	G	Sidechain
30	0	619	U	Sidechain
30	0	817	G	Sidechain
30	0	818	A	Sidechain
31	9	39	U	Sidechain
31	9	65	A	Sidechain
31	9	87	U	Sidechain
23	W	90	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1753	0	1766	66	0
2	B	2625	0	2533	94	0
3	C	1860	0	1813	53	0
4	D	1094	0	1085	52	0
5	E	1357	0	1266	36	0
6	F	890	0	843	30	0
7	G	240	0	231	11	0
8	H	1282	0	1292	41	0
9	I	519	0	500	21	0
10	J	1120	0	1098	38	0
11	K	994	0	1027	39	0
12	L	1118	0	1076	33	0
13	M	1558	0	1573	59	0
14	N	1445	0	1401	54	0
15	O	865	0	873	18	0
16	P	1136	0	1123	30	0
17	Q	735	0	729	26	0
18	R	1149	0	1122	32	0
19	S	641	0	605	10	0
20	T	950	0	924	22	0
21	U	410	0	364	17	0
22	V	499	0	511	17	0
23	W	1196	0	1137	66	0
24	X	654	0	653	22	0
25	Y	1130	0	1133	33	0
26	Z	573	0	531	21	0
27	1	431	0	426	21	0
28	2	396	0	413	21	0
29	3	755	0	728	17	0
30	0	59018	0	29809	1329	0
31	9	2599	0	1325	97	0
32	0	87	0	0	0	0
32	9	1	0	0	0	0
32	A	1	0	0	0	0
32	B	1	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	Y	1	0	0	0	0
33	0	9	0	0	3	0
33	3	1	0	0	0	0
33	A	1	0	0	0	0
33	B	1	0	0	0	0
33	J	3	0	0	2	0
33	L	1	0	0	0	0
33	M	1	0	0	1	0
33	N	1	0	0	1	0
33	O	1	0	0	0	0
33	Q	1	0	0	0	0
33	R	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	93	0	0	0	0
34	1	2	0	0	0	0
34	3	2	0	0	0	0
34	9	3	0	0	0	0
34	A	3	0	0	0	0
34	B	2	0	0	0	0
34	F	1	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
35	0	65	0	0	0	0
35	9	2	0	0	0	0
35	B	1	0	0	0	0
35	C	1	0	0	0	0
35	J	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	2	0	0	0	0
35	S	1	0	0	0	0
36	1	1	0	0	0	0
36	3	1	0	0	0	0
36	O	1	0	0	0	0
36	U	1	0	0	0	0
36	Z	1	0	0	0	0
37	0	2	0	0	0	0
38	0	5950	0	0	203	0
38	1	54	0	0	3	0
38	2	43	0	0	1	0
38	3	68	0	0	6	0
38	9	148	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	A	112	0	0	5	0
38	B	142	0	0	14	0
38	C	168	0	0	13	0
38	D	45	0	0	4	0
38	E	42	0	0	4	0
38	F	26	0	0	1	0
38	G	17	0	0	1	0
38	H	65	0	0	5	0
38	I	5	0	0	0	0
38	J	56	0	0	2	0
38	K	60	0	0	5	0
38	L	82	0	0	8	0
38	M	123	0	0	2	0
38	N	59	0	0	3	0
38	O	47	0	0	4	0
38	P	59	0	0	2	0
38	Q	47	0	0	2	0
38	R	76	0	0	1	0
38	S	33	0	0	0	0
38	T	36	0	0	4	0
38	U	26	0	0	2	0
38	V	12	0	0	1	0
38	W	66	0	0	6	0
38	X	28	0	0	3	0
38	Y	97	0	0	7	0
38	Z	31	0	0	4	0
All	All	99120	0	59910	2191	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 15.

All (2191) 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)
18:R:150:PRO:CG	18:R:150:PRO:CD	1.96	1.44
30:0:871:G:C8	30:0:871:G:H5'	1.75	1.21
14:N:37:ARG:NH1	31:9:6:C:H5''	1.62	1.12
31:9:56:A:H2'	31:9:57:A:H5''	1.21	1.11
30:0:1160:G:C5'	30:0:1161:A:H5'	1.79	1.11
30:0:1160:G:H5'	30:0:1161:A:C5'	1.83	1.09
30:0:871:G:H8	30:0:871:G:H5'	1.00	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:545:G:H8	30:0:545:G:H5'	1.12	1.08
18:R:150:PRO:CG	18:R:150:PRO:C	2.22	1.07
30:0:1474:C:H6	30:0:1474:C:H5'	1.19	1.07
30:0:1559:A:H1'	38:0:5888:HOH:O	1.54	1.07
13:M:171:ARG:HD3	30:0:156:C:H5''	1.38	1.04
30:0:69:A:H5'	30:0:69:A:C8	1.93	1.03
10:J:82:THR:HG23	30:0:1242:A:H5'	1.38	1.02
30:0:1474:C:C6	30:0:1474:C:H5'	1.96	1.01
4:D:154:LYS:HD2	4:D:154:LYS:H	1.26	1.01
30:0:1666:C:O2'	30:0:1667:A:H5''	1.62	0.99
30:0:2717:C:C2'	30:0:2718:C:H5''	1.93	0.99
31:9:76:G:H3'	31:9:77:A:H5''	1.41	0.98
30:0:69:A:H5'	30:0:69:A:H8	1.28	0.97
30:0:871:G:H8	30:0:871:G:C5'	1.78	0.96
30:0:1116:U:O2'	30:0:1118:A:H2	1.47	0.96
30:0:1205:U:H2'	30:0:1206:U:C5'	1.96	0.96
30:0:2717:C:H2'	30:0:2718:C:H5''	1.45	0.96
30:0:2812:A:H2	30:0:2814:A:H62	1.02	0.95
30:0:1603:A:H5'	30:0:1605:G:O4'	1.66	0.95
30:0:545:G:C8	30:0:545:G:H5'	2.00	0.95
30:0:1165:G:H21	30:0:1173:A:H5''	1.30	0.95
30:0:870:G:H2'	30:0:871:G:H5''	1.47	0.95
15:O:3:THR:HG22	30:0:656:G:H5'	1.45	0.95
30:0:2291:A:C8	30:0:2309:C:H5'	2.03	0.94
30:0:877:G:H5'	30:0:878:G:OP1	1.67	0.94
30:0:2316:G:H5''	38:0:6122:HOH:O	1.66	0.94
30:0:1666:C:C2'	30:0:1667:A:H5''	1.97	0.93
30:0:542:A:H5'	30:0:542:A:H8	1.30	0.93
3:C:236:THR:HG22	3:C:239:ALA:H	1.31	0.92
30:0:1206:U:H6	30:0:1206:U:H5'	1.34	0.92
30:0:2506:A:HO2'	30:0:2507:G:H8	1.10	0.92
30:0:381:G:H5''	38:0:4327:HOH:O	1.68	0.92
30:0:2502:C:C2'	30:0:2503:A:H5'	2.00	0.92
11:K:10:GLN:H	11:K:10:GLN:HE21	0.97	0.92
30:0:182:G:H5'	38:0:5177:HOH:O	1.68	0.92
16:P:115:SER:H	16:P:118:GLN:HE21	0.99	0.92
30:0:2502:C:H2'	30:0:2503:A:H5'	1.50	0.91
31:9:56:A:C2'	31:9:57:A:H5''	2.00	0.91
30:0:1160:G:H5'	30:0:1161:A:H5'	0.94	0.91
13:M:99:ARG:HD2	13:M:167:GLY:HA2	1.51	0.91
30:0:1187:U:HO2'	30:0:1189:A:H2	1.11	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2908:A:H2'	30:0:2909:G:O4'	1.69	0.90
30:0:2526:C:H5'	30:0:2526:C:H6	1.36	0.90
10:J:52:GLN:NE2	30:0:1119:G:H2'	1.85	0.90
30:0:1835:U:H5	30:0:1840:A:N7	1.70	0.90
2:B:221:GLN:HE22	11:K:42:ASN:HD22	1.17	0.90
30:0:2004:U:H4'	38:0:5326:HOH:O	1.70	0.90
30:0:1701:A:H4'	30:0:1702:U:H5''	1.51	0.89
30:0:1184:C:H1'	38:0:7505:HOH:O	1.70	0.89
6:F:91:VAL:HG12	6:F:92:GLY:H	1.34	0.89
30:0:2526:C:H5'	30:0:2526:C:C6	2.07	0.89
31:9:29:C:H2'	31:9:30:C:H5'	1.55	0.89
30:0:282:C:H1'	30:0:368:C:N4	1.86	0.89
30:0:506:G:H22	30:0:509:A:C5'	1.86	0.89
26:Z:70:ARG:HD2	26:Z:83:TYR:HB2	1.55	0.88
30:0:1189:A:H1'	30:0:1209:C:O4'	1.74	0.88
38:B:9099:HOH:O	30:0:2672:C:H1'	1.72	0.88
30:0:541:C:H2'	30:0:542:A:H5''	1.56	0.88
30:0:31:C:H2'	38:0:7724:HOH:O	1.73	0.87
30:0:541:C:C2'	30:0:542:A:H5''	2.05	0.87
2:B:238:ASN:HD22	2:B:240:GLY:H	1.20	0.87
30:0:1372:A:H3'	38:0:7228:HOH:O	1.74	0.87
30:0:2769:C:C2'	30:0:2770:G:H5'	2.05	0.87
30:0:2111:G:H1'	38:0:9054:HOH:O	1.75	0.87
30:0:214:U:H5'	38:0:6171:HOH:O	1.74	0.86
30:0:1205:U:H2'	30:0:1206:U:H5''	1.57	0.86
30:0:1183:C:H2'	38:0:6275:HOH:O	1.76	0.86
30:0:1165:G:N2	30:0:1173:A:H5''	1.89	0.86
31:9:14:G:H5'	31:9:14:G:H8	1.41	0.86
2:B:162:MET:HE3	2:B:308:LEU:HD21	1.56	0.86
30:0:2586:U:H3	30:0:2592:G:H22	1.16	0.85
2:B:36:PRO:HA	2:B:168:GLY:HA3	1.59	0.85
24:X:37:LEU:HD13	24:X:85:VAL:HG21	1.57	0.85
30:0:1165:G:H1'	30:0:1174:A:H1'	1.58	0.84
30:0:506:G:H22	30:0:509:A:H5'	1.42	0.84
30:0:2010:A:H2'	38:0:5984:HOH:O	1.77	0.84
15:O:3:THR:CG2	30:0:656:G:H5'	2.07	0.84
14:N:83:LEU:HD13	14:N:175:LEU:HD23	1.58	0.83
13:M:95:LYS:HE2	30:0:157:G:H4'	1.59	0.83
3:C:127:ARG:NH2	3:C:225:PRO:HG2	1.94	0.83
11:K:39:GLY:HA2	38:0:5241:HOH:O	1.79	0.83
30:0:1118:A:H3'	30:0:1118:A:C8	2.13	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1667:A:H8	30:0:1667:A:H5'	1.44	0.82
23:W:137:GLN:HE21	23:W:141:HIS:HE1	1.24	0.82
30:0:2073:G:H5''	38:0:3833:HOH:O	1.80	0.81
9:I:111:LEU:HD23	30:0:1163:G:H4'	1.60	0.81
30:0:1205:U:H2'	30:0:1206:U:H5'	1.62	0.81
8:H:59:GLN:NE2	8:H:129:ARG:HE	1.78	0.81
30:0:1118:A:H3'	30:0:1118:A:H8	1.46	0.80
10:J:52:GLN:HE22	30:0:1119:G:H2'	1.46	0.80
30:0:559:U:H5'	30:0:559:U:H6	1.46	0.80
30:0:1666:C:H2'	30:0:1667:A:C5'	2.12	0.80
30:0:1201:C:H2'	30:0:1202:A:H5'	1.65	0.79
30:0:871:G:C8	30:0:871:G:C5'	2.57	0.79
30:0:282:C:O2'	30:0:283:U:H5'	1.81	0.79
30:0:2766:A:H5'	38:0:9567:HOH:O	1.81	0.79
30:0:2769:C:H2'	30:0:2770:G:H5'	1.62	0.79
2:B:212:GLN:HB2	2:B:257:THR:HG21	1.63	0.79
30:0:1377:C:H6	30:0:1377:C:H5'	1.48	0.79
30:0:1300:G:H1'	38:0:4692:HOH:O	1.81	0.78
30:0:1119:G:N2	30:0:1246:A:C2	2.51	0.78
3:C:139:VAL:HG13	38:C:8646:HOH:O	1.83	0.78
2:B:74:ILE:HD13	2:B:309:VAL:HG21	1.64	0.78
30:0:2748:G:H5'	38:0:7581:HOH:O	1.83	0.78
30:0:10:U:H6	30:0:10:U:H3'	1.49	0.78
30:0:1942:A:H5'	38:0:7387:HOH:O	1.82	0.78
11:K:10:GLN:H	11:K:10:GLN:NE2	1.79	0.78
20:T:9:LYS:HE3	20:T:13:ARG:NH1	1.99	0.78
23:W:4:LEU:HD23	23:W:54:PHE:HB3	1.65	0.78
30:0:2103:A:H62	30:0:2538:A:H8	1.32	0.77
30:0:308:U:H5'	30:0:309:C:OP1	1.84	0.77
30:0:396:U:H1'	38:0:7666:HOH:O	1.83	0.77
30:0:541:C:H2'	30:0:542:A:C5'	2.14	0.77
23:W:88:THR:HB	38:W:6679:HOH:O	1.84	0.77
16:P:115:SER:H	16:P:118:GLN:NE2	1.81	0.77
30:0:2491:G:H1'	38:0:6907:HOH:O	1.86	0.76
26:Z:60:ASP:HB3	26:Z:69:ASP:HB3	1.68	0.76
30:0:1474:C:C5'	30:0:1474:C:H6	1.98	0.76
30:0:2533:C:H5'	30:0:2533:C:H6	1.50	0.76
30:0:870:G:C2'	30:0:871:G:H5''	2.13	0.76
28:2:43:ARG:HH22	30:0:1684:A:H1'	1.48	0.76
30:0:2420:G:O2'	30:0:2421:G:H5'	1.86	0.76
30:0:1205:U:C2'	30:0:1206:U:H5''	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:2:U:OP2	31:9:3:A:H5'	1.85	0.76
31:9:92:G:H2'	31:9:93:A:C8	2.21	0.76
30:0:2256:G:O2'	30:0:2257:G:H5'	1.85	0.75
30:0:558:C:C2'	30:0:559:U:H5''	2.16	0.75
22:V:1:THR:HG23	22:V:2:VAL:H	1.51	0.75
26:Z:61:HIS:HB2	26:Z:71:VAL:HB	1.66	0.75
30:0:1451:C:H5'	30:0:1505:U:C5	2.21	0.75
30:0:1632:A:H2'	30:0:1633:C:H5'	1.69	0.75
30:0:2256:G:C2'	30:0:2257:G:H5'	2.16	0.75
30:0:2717:C:O2'	30:0:2718:C:H5''	1.86	0.75
1:A:199:HIS:HD2	1:A:201:PHE:H	1.33	0.75
30:0:2787:C:H5	38:0:4643:HOH:O	1.69	0.75
30:0:558:C:O2'	30:0:559:U:H5''	1.87	0.75
5:E:116:THR:HG22	5:E:151:LEU:HD22	1.69	0.75
30:0:681:G:N3	30:0:681:G:H5'	2.02	0.75
30:0:1603:A:H5''	30:0:1605:G:H5'	1.68	0.74
5:E:143:GLN:HE21	30:0:2780:C:H1'	1.52	0.74
14:N:113:SER:HB2	38:N:8852:HOH:O	1.87	0.74
30:0:1878:G:H1'	38:0:6151:HOH:O	1.87	0.74
14:N:144:GLY:O	14:N:147:ILE:HG22	1.87	0.74
2:B:179:LEU:O	2:B:183:GLU:HG2	1.86	0.74
30:0:2135:A:O2'	30:0:2136:G:H5'	1.86	0.74
30:0:821:U:H3'	38:0:3779:HOH:O	1.87	0.74
6:F:58:GLU:HB3	13:M:8:ILE:HG23	1.69	0.74
30:0:1187:U:O2'	30:0:1189:A:H2	1.71	0.74
30:0:1116:U:H3	30:0:1246:A:H62	1.36	0.74
30:0:2103:A:HO2'	30:0:2104:C:H6	1.36	0.74
2:B:98:THR:HG22	30:0:2820:A:OP1	1.88	0.74
5:E:100:ASP:HB2	38:E:2789:HOH:O	1.86	0.74
30:0:107:U:H2'	30:0:108:U:H5'	1.70	0.73
38:C:8660:HOH:O	30:0:2100:A:H5'	1.87	0.73
30:0:283:U:H5	30:0:284:C:N3	1.86	0.73
19:S:51:GLN:HE21	19:S:53:ASN:HD21	1.33	0.73
30:0:2426:G:H1'	38:0:6122:HOH:O	1.88	0.73
30:0:2768:A:O2'	30:0:2769:C:H5'	1.88	0.73
30:0:12:U:H2'	30:0:13:G:H5'	1.69	0.73
30:0:1183:C:N4	30:0:1184:C:H41	1.85	0.73
13:M:171:ARG:CD	30:0:156:C:H5''	2.16	0.73
30:0:1835:U:C5	30:0:1840:A:N7	2.55	0.73
2:B:336:GLN:O	30:0:2862:G:H4'	1.88	0.73
24:X:61:ARG:HH12	24:X:67:PRO:HD3	1.54	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1166:A:H61	30:0:1180:U:H3	1.37	0.72
30:0:1182:C:H1'	30:0:1192:A:H8	1.54	0.72
30:0:1666:C:C2'	30:0:1667:A:C5'	2.67	0.72
30:0:1701:A:H5'	38:0:6316:HOH:O	1.89	0.72
30:0:1741:U:H5'	30:0:1742:A:OP1	1.89	0.72
29:3:70:ARG:HG2	29:3:77:ALA:HB2	1.70	0.72
30:0:2506:A:O2'	30:0:2507:G:H8	1.72	0.72
1:A:35:GLY:O	1:A:36:ASP:HB3	1.87	0.72
30:0:1189:A:H3'	38:0:7717:HOH:O	1.89	0.72
22:V:12:THR:HG22	22:V:15:GLU:HG3	1.72	0.72
30:0:2637:A:H5'	38:0:9282:HOH:O	1.88	0.72
6:F:63:ILE:HB	6:F:64:PRO:HD3	1.70	0.72
22:V:1:THR:HB	30:0:93:C:H5''	1.72	0.72
10:J:70:PHE:CE1	30:0:2676:C:H4'	2.25	0.72
30:0:2896:A:H5''	38:0:6129:HOH:O	1.90	0.72
11:K:10:GLN:N	11:K:10:GLN:HE21	1.81	0.71
31:9:14:G:H5'	31:9:14:G:C8	2.24	0.71
11:K:14:LYS:HB2	11:K:45:PRO:HG2	1.71	0.71
14:N:11:ARG:HD3	31:9:114:G:O6	1.90	0.71
24:X:71:ARG:HD3	38:X:2171:HOH:O	1.89	0.71
30:0:1973:A:H5'	30:0:1973:A:H8	1.54	0.71
30:0:2102:G:H5'	30:0:2538:A:C2	2.24	0.71
31:9:54:A:O2'	31:9:55:U:H5'	1.91	0.71
30:0:542:A:H5'	30:0:542:A:C8	2.20	0.71
30:0:564:G:H1'	38:0:6343:HOH:O	1.91	0.71
1:A:211:LYS:HB2	38:A:9077:HOH:O	1.90	0.71
4:D:25:MET:HE3	4:D:37:ALA:HB1	1.72	0.71
30:0:10:U:C6	30:0:10:U:H3'	2.26	0.71
20:T:61:GLU:HG2	38:T:3851:HOH:O	1.90	0.71
30:0:1187:U:H2'	38:0:6936:HOH:O	1.91	0.70
5:E:143:GLN:NE2	30:0:2779:G:H21	1.89	0.70
4:D:105:SER:OG	30:0:2338:G:H1'	1.89	0.70
30:0:2578:G:H5'	30:0:2578:G:H8	1.57	0.70
38:Y:8860:HOH:O	33:0:8817:CL:CL	2.46	0.70
31:9:23:U:O2'	31:9:24:U:H4'	1.91	0.70
23:W:88:THR:HG22	23:W:89:ASP:H	1.56	0.70
30:0:2256:G:H2'	30:0:2257:G:H5'	1.73	0.70
3:C:1:MET:HG2	3:C:2:GLN:H	1.55	0.70
23:W:88:THR:HG23	23:W:110:GLN:HB3	1.73	0.70
30:0:1205:U:C2'	30:0:1206:U:C5'	2.69	0.70
30:0:2781:U:C2'	30:0:2782:G:H5'	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2756:U:H3	30:0:2896:A:H2	1.37	0.70
31:9:64:C:H2'	31:9:65:A:H5'	1.74	0.70
11:K:98:VAL:CG1	11:K:102:GLU:HA	2.21	0.70
6:F:91:VAL:HG12	6:F:92:GLY:N	2.07	0.70
30:0:567:U:H5''	38:0:6437:HOH:O	1.90	0.70
4:D:103:ASN:HD22	4:D:134:LEU:H	1.39	0.70
30:0:545:G:H8	30:0:545:G:C5'	2.00	0.69
3:C:162:VAL:HG22	3:C:232:LEU:HD21	1.73	0.69
30:0:1058:A:H2'	30:0:1060:C:H5''	1.74	0.69
17:Q:11:ARG:HD3	38:0:6291:HOH:O	1.92	0.69
30:0:1174:A:C5	30:0:1201:C:H4'	2.27	0.69
30:0:794:U:H3	30:0:819:A:H61	1.40	0.69
30:0:1666:C:H2'	30:0:1667:A:H5'	1.75	0.69
30:0:1377:C:H1'	38:0:9044:HOH:O	1.91	0.69
1:A:223:ARG:HH22	30:0:2271:G:P	2.16	0.69
30:0:960:G:H3'	30:0:960:G:N3	2.07	0.69
30:0:1525:G:H5'	30:0:1526:A:OP2	1.93	0.69
30:0:847:C:H4'	38:0:3762:HOH:O	1.92	0.69
11:K:74:VAL:HG12	11:K:75:ARG:HG3	1.75	0.69
14:N:37:ARG:HH12	31:9:6:C:H5''	1.51	0.69
2:B:206:THR:HG21	30:0:2716:G:H5''	1.74	0.69
13:M:164:THR:HG22	13:M:167:GLY:H	1.58	0.69
30:0:821:U:H5''	38:0:3057:HOH:O	1.93	0.68
30:0:1118:A:H62	30:0:1244:U:H3	1.39	0.68
30:0:2852:A:H5''	38:0:5254:HOH:O	1.93	0.68
30:0:271:C:H41	30:0:378:A:H2	1.40	0.68
30:0:2769:C:H2'	30:0:2770:G:C5'	2.23	0.68
13:M:102:GLU:OE1	13:M:164:THR:HG21	1.94	0.68
22:V:50:ARG:HH12	30:0:56:G:H5''	1.59	0.68
30:0:1701:A:H4'	30:0:1702:U:C5'	2.20	0.68
30:0:2851:G:O2'	30:0:2852:A:H5'	1.92	0.68
11:K:98:VAL:HG13	11:K:102:GLU:HA	1.74	0.68
23:W:21:LEU:HD21	23:W:48:VAL:HG11	1.75	0.68
25:Y:169:ARG:HD2	30:0:1328:A:OP1	1.93	0.68
30:0:1595:G:O2'	30:0:1596:U:H5'	1.92	0.68
30:0:2635:A:O2'	30:0:2636:C:H5'	1.94	0.68
10:J:19:MET:HE3	10:J:132:LEU:HD21	1.75	0.68
23:W:137:GLN:HE21	23:W:141:HIS:CE1	2.11	0.68
2:B:97:LEU:HD22	2:B:127:GLN:HE21	1.57	0.68
18:R:150:PRO:O	18:R:150:PRO:CG	2.41	0.68
30:0:1132:A:N6	30:0:1229:C:H2'	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:0:8813:CL:CL	38:0:4692:HOH:O	2.48	0.68
1:A:135:VAL:HG11	1:A:147:ARG:NH2	2.09	0.68
18:R:96:VAL:HG13	18:R:106:GLY:HA3	1.76	0.68
11:K:81:ARG:HB2	11:K:87:ARG:HH11	1.59	0.67
30:0:559:U:H5'	30:0:559:U:C6	2.29	0.67
30:0:69:A:H8	30:0:69:A:C5'	2.06	0.67
30:0:506:G:H22	30:0:509:A:H5''	1.58	0.67
1:A:153:ARG:HH11	1:A:153:ARG:HB2	1.58	0.67
23:W:84:VAL:HG12	38:W:6679:HOH:O	1.95	0.67
25:Y:212:ARG:HD2	38:Y:8904:HOH:O	1.94	0.67
30:0:2812:A:C2	30:0:2814:A:N6	2.58	0.67
8:H:155:ARG:NH1	30:0:2503:A:H5''	2.09	0.67
8:H:30:LYS:H	8:H:62:HIS:HD2	1.39	0.67
30:0:380:A:H2'	38:0:7265:HOH:O	1.93	0.67
31:9:22:G:H5'	31:9:23:U:OP1	1.95	0.67
30:0:2317:C:C6	38:0:6122:HOH:O	2.46	0.67
14:N:80:SER:HB2	38:N:8833:HOH:O	1.94	0.67
30:0:1279:U:O2	30:0:1279:U:H2'	1.95	0.67
16:P:117:SER:HB3	30:0:1593:C:OP1	1.94	0.67
30:0:671:A:O2'	30:0:672:G:H2'	1.94	0.67
30:0:1183:C:O2	30:0:1183:C:H2'	1.93	0.67
5:E:133:VAL:HG12	5:E:141:VAL:HG13	1.76	0.67
8:H:59:GLN:HE21	8:H:129:ARG:HE	1.41	0.67
1:A:211:LYS:HB3	1:A:212:PRO:HD2	1.77	0.66
1:A:199:HIS:CD2	1:A:201:PHE:H	2.12	0.66
3:C:236:THR:HG22	3:C:239:ALA:N	2.08	0.66
23:W:4:LEU:HD22	23:W:52:VAL:HG21	1.76	0.66
30:0:1159:G:H21	30:0:1189:A:H8	1.43	0.66
30:0:2781:U:O2'	30:0:2782:G:H5'	1.96	0.66
28:2:41:HIS:HD2	28:2:44:ARG:H	1.42	0.66
2:B:5:ARG:HH11	2:B:8:LYS:HE2	1.61	0.66
12:L:39:GLU:HG2	30:0:926:A:H4'	1.76	0.66
23:W:137:GLN:NE2	23:W:141:HIS:HE1	1.94	0.66
30:0:2256:G:H2'	30:0:2257:G:C5'	2.25	0.66
31:9:64:C:C2'	31:9:65:A:H5'	2.26	0.66
10:J:82:THR:CG2	30:0:1242:A:H5'	2.21	0.66
11:K:74:VAL:HG11	11:K:113:ILE:HG12	1.76	0.66
30:0:2781:U:H2'	30:0:2782:G:H5'	1.76	0.66
28:2:18:ASN:HD21	28:2:40:ARG:H	1.41	0.66
31:9:7:G:H5'	38:9:9100:HOH:O	1.96	0.66
21:U:46:ALA:HB1	21:U:52:THR:HG21	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:204:ARG:HH22	30:0:553:G:P	2.18	0.66
30:0:1189:A:H1'	30:0:1209:C:C1'	2.25	0.66
30:0:1377:C:H5'	30:0:1377:C:C6	2.31	0.66
30:0:2001:G:O2'	30:0:2002:C:H5'	1.96	0.66
4:D:103:ASN:ND2	4:D:134:LEU:H	1.92	0.66
18:R:99:ALA:HB1	18:R:109:MET:HE1	1.76	0.66
30:0:2251:G:H2'	30:0:2252:A:C8	2.30	0.66
30:0:2769:C:O2'	30:0:2770:G:H5'	1.96	0.65
30:0:558:C:H2'	30:0:559:U:C5'	2.26	0.65
30:0:1118:A:C8	30:0:1118:A:C3'	2.77	0.65
30:0:1524:U:OP1	30:0:1524:U:H4'	1.96	0.65
8:H:72:ALA:HB2	8:H:156:ALA:HB2	1.78	0.65
30:0:1634:G:H3'	38:0:3903:HOH:O	1.96	0.65
30:0:2768:A:H2'	30:0:2769:C:O4'	1.96	0.65
30:0:603:A:H5''	30:0:604:G:OP1	1.97	0.65
3:C:174:ILE:HD11	30:0:338:C:H4'	1.78	0.65
30:0:1441:G:O2'	30:0:1442:A:H5'	1.97	0.65
30:0:2827:A:H2'	30:0:2828:G:O4'	1.97	0.65
30:0:1972:U:H2'	30:0:1973:A:C5'	2.26	0.65
30:0:2507:G:H2'	30:0:2510:C:H42	1.62	0.65
30:0:2613:G:O2'	30:0:2614:C:H5'	1.97	0.65
30:0:635:A:H2'	30:0:636:G:H5''	1.78	0.65
6:F:21:GLU:O	6:F:24:ARG:HG2	1.97	0.65
15:O:42:GLU:HB2	38:O:2176:HOH:O	1.96	0.65
10:J:88:PRO:HD3	30:0:1104:C:H4'	1.77	0.65
16:P:55:LYS:HG2	16:P:56:GLY:N	2.12	0.65
27:1:20:ARG:HG2	30:0:111:C:O2'	1.97	0.65
14:N:37:ARG:NH1	31:9:6:C:C5'	2.51	0.65
30:0:1632:A:C2'	30:0:1633:C:H5'	2.27	0.64
30:0:2005:G:H3'	30:0:2005:G:OP2	1.97	0.64
30:0:2281:C:H2'	30:0:2282:U:H5'	1.80	0.64
30:0:485:A:N3	30:0:487:G:H5''	2.12	0.64
30:0:1834:C:H2'	30:0:1840:A:N6	2.11	0.64
30:0:283:U:C5	30:0:284:C:N3	2.65	0.64
12:L:39:GLU:HG2	30:0:926:A:C4'	2.27	0.64
38:T:2217:HOH:O	30:0:317:A:H5'	1.97	0.64
30:0:1185:U:H2'	30:0:1186:C:C6	2.33	0.64
30:0:1667:A:C8	30:0:1667:A:H5'	2.29	0.64
30:0:2717:C:H2'	30:0:2718:C:C5'	2.22	0.64
30:0:283:U:H5	30:0:284:C:C2	2.15	0.64
30:0:363:C:O2'	30:0:364:U:H5'	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:30:LYS:H	8:H:62:HIS:CD2	2.14	0.64
30:0:272:A:H5'	30:0:273:G:OP2	1.97	0.64
30:0:613:C:H2'	30:0:614:U:H6	1.62	0.64
14:N:12:ARG:HD3	14:N:18:THR:OG1	1.97	0.64
21:U:17:THR:HG22	21:U:18:GLY:N	2.13	0.64
30:0:2563:U:H2'	30:0:2565:C:O5'	1.98	0.64
8:H:168:VAL:HG13	38:H:213:HOH:O	1.98	0.64
30:0:2371:G:H5'	38:0:5029:HOH:O	1.98	0.64
30:0:2638:G:H5'	38:0:4946:HOH:O	1.98	0.64
3:C:184:ARG:NH2	30:0:450:C:OP1	2.31	0.64
30:0:644:G:N3	30:0:644:G:H5'	2.13	0.64
21:U:17:THR:HG22	21:U:18:GLY:H	1.62	0.64
30:0:333:G:O2'	30:0:334:G:H5'	1.97	0.63
30:0:952:G:H4'	38:0:4042:HOH:O	1.97	0.63
30:0:1596:U:H2'	30:0:1598:A:OP2	1.99	0.63
30:0:1603:A:C5'	30:0:1605:G:H5'	2.27	0.63
30:0:2404:G:H5''	38:0:5231:HOH:O	1.97	0.63
30:0:2748:G:H2'	38:0:7581:HOH:O	1.98	0.63
2:B:162:MET:HG3	2:B:310:ARG:HD3	1.80	0.63
18:R:128:ARG:NH2	30:0:2054:A:N3	2.46	0.63
23:W:72:PRO:HG2	23:W:77:ALA:HB3	1.80	0.63
30:0:2718:C:H6	30:0:2718:C:H5'	1.63	0.63
30:0:2344:G:N3	30:0:2344:G:H2'	2.14	0.63
30:0:2610:U:H4'	38:0:9484:HOH:O	1.99	0.63
30:0:420:U:H2'	30:0:421:C:C6	2.33	0.63
30:0:1166:A:P	30:0:1174:A:H4'	2.38	0.63
30:0:544:G:H2'	30:0:545:G:H5''	1.81	0.63
2:B:238:ASN:HD22	2:B:240:GLY:N	1.93	0.63
30:0:1189:A:O2'	30:0:1208:C:H2'	1.98	0.63
5:E:143:GLN:NE2	30:0:2780:C:H1'	2.13	0.63
11:K:81:ARG:HB2	11:K:87:ARG:NH1	2.14	0.63
14:N:7:LYS:HE3	17:Q:21:ARG:O	1.99	0.63
16:P:115:SER:N	16:P:118:GLN:HE21	1.84	0.63
30:0:10:U:C3'	30:0:10:U:C6	2.82	0.63
30:0:1200:A:H3'	38:0:5774:HOH:O	1.99	0.63
30:0:1206:U:C5'	30:0:1206:U:H6	2.10	0.63
30:0:2281:C:C2'	30:0:2282:U:H5'	2.29	0.63
2:B:307:ARG:HH11	2:B:307:ARG:HG3	1.64	0.63
3:C:140:VAL:HB	38:C:8649:HOH:O	1.98	0.63
12:L:133:VAL:HA	38:L:8871:HOH:O	1.99	0.63
22:V:50:ARG:NH1	30:0:56:G:H5''	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1942:A:H3'	38:0:7387:HOH:O	1.98	0.62
27:1:16:HIS:HD2	30:0:470:U:O2'	1.81	0.62
30:0:1182:C:H1'	30:0:1192:A:C8	2.34	0.62
30:0:2781:U:H2'	30:0:2782:G:C5'	2.29	0.62
1:A:121:ALA:O	1:A:124:VAL:HG22	1.98	0.62
30:0:138:U:OP2	30:0:139:C:H5	1.82	0.62
30:0:2502:C:H2'	30:0:2503:A:C5'	2.28	0.62
30:0:2472:C:O2'	30:0:2634:G:H4'	1.99	0.62
10:J:127:ILE:HG22	33:J:8801:CL:CL	2.36	0.62
30:0:420:U:H2'	30:0:421:C:H6	1.64	0.62
30:0:559:U:C5	30:0:560:U:C5	2.88	0.62
3:C:236:THR:HG21	38:C:8573:HOH:O	2.00	0.62
3:C:27:ARG:NH2	30:0:657:G:OP1	2.32	0.62
30:0:2241:C:O2'	30:0:2242:U:H5'	2.00	0.62
30:0:1351:G:H1'	38:0:4064:HOH:O	1.98	0.62
4:D:22:VAL:HG22	4:D:74:THR:HG22	1.81	0.62
23:W:6:GLN:HB2	23:W:26:ILE:HD11	1.81	0.62
24:X:43:VAL:HG12	24:X:44:ASP:H	1.63	0.62
30:0:1477:C:H5'	30:0:1868:G:C5'	2.30	0.62
28:2:41:HIS:H	28:2:45:ASN:HD22	1.46	0.62
1:A:191:GLY:HA2	1:A:194:MET:CE	2.30	0.62
2:B:320:GLN:HE21	2:B:321:PRO:HD2	1.65	0.62
28:2:2:LYS:HG3	30:0:1486:A:C5	2.34	0.62
20:T:26:THR:HG23	20:T:97:ARG:HG3	1.82	0.62
30:0:107:U:C2'	30:0:108:U:H5'	2.29	0.62
30:0:2372:A:H2'	30:0:2373:U:H6	1.65	0.62
29:3:25:VAL:HG22	29:3:68:LYS:HG3	1.80	0.62
30:0:2643:G:H5''	38:0:3937:HOH:O	1.99	0.61
2:B:18:ARG:HG3	2:B:256:GLN:HG3	1.82	0.61
25:Y:189:ASN:HA	25:Y:217:ILE:HD11	1.82	0.61
30:0:958:G:O2'	30:0:959:C:H5'	2.01	0.61
3:C:129:HIS:CE1	3:C:231:ARG:HA	2.35	0.61
21:U:56:ARG:HD2	38:0:6278:HOH:O	1.98	0.61
30:0:196:G:H2'	38:0:6690:HOH:O	2.00	0.61
30:0:2802:C:H2'	30:0:2803:C:C6	2.35	0.61
30:0:1015:C:H2'	30:0:1016:U:H6	1.65	0.61
30:0:1972:U:H2'	30:0:1973:A:H5''	1.80	0.61
30:0:2509:A:OP2	30:0:2510:C:H5	1.82	0.61
30:0:407:A:H3'	38:0:4471:HOH:O	2.00	0.61
30:0:308:U:C4	30:0:342:C:H1'	2.36	0.61
31:9:29:C:C2'	31:9:30:C:H5'	2.27	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:63:GLU:HG2	38:K:6344:HOH:O	2.00	0.61
12:L:136:ALA:HB3	38:L:8871:HOH:O	2.00	0.61
23:W:80:ASP:O	23:W:84:VAL:HG23	1.99	0.61
30:0:705:C:H2'	30:0:705:C:O2	2.01	0.61
30:0:1183:C:H42	30:0:1184:C:H41	1.47	0.61
18:R:99:ALA:HB1	18:R:109:MET:CE	2.31	0.61
30:0:1174:A:C6	30:0:1201:C:H4'	2.36	0.61
27:1:1:THR:HA	38:1:435:HOH:O	2.00	0.61
2:B:201:ASP:HB2	2:B:312:ARG:HD2	1.82	0.61
2:B:7:ARG:HG2	2:B:7:ARG:HH11	1.66	0.61
12:L:30:ARG:HD3	30:0:164:G:H4'	1.82	0.61
31:9:39:U:H3'	31:9:40:C:H5''	1.83	0.61
14:N:11:ARG:HG3	14:N:14:ARG:NH1	2.15	0.61
16:P:91:LYS:O	16:P:95:GLU:HG3	2.00	0.61
30:0:1165:G:N2	30:0:1173:A:C5'	2.63	0.61
30:0:1972:U:C2'	30:0:1973:A:H5''	2.31	0.61
27:1:28:HIS:HE1	30:0:776:A:OP1	1.84	0.61
29:3:15:ASN:O	30:0:2408:A:H4'	2.01	0.60
30:0:510:U:H6	38:0:7477:HOH:O	1.83	0.60
31:9:39:U:H1'	31:9:44:A:H61	1.65	0.60
22:V:39:ALA:N	22:V:40:PRO:HD2	2.14	0.60
30:0:544:G:C2'	30:0:545:G:H5''	2.31	0.60
4:D:135:VAL:HG21	4:D:139:TYR:CD1	2.36	0.60
8:H:6:ALA:HA	8:H:61:ARG:HH12	1.67	0.60
30:0:1379:A:H1'	38:0:9696:HOH:O	2.01	0.60
30:0:1819:G:H5'	38:0:5835:HOH:O	2.01	0.60
30:0:2768:A:H5''	38:0:4438:HOH:O	2.00	0.60
30:0:1116:U:C2'	30:0:1118:A:H2	2.14	0.60
30:0:31:C:H4'	38:0:7464:HOH:O	2.00	0.60
30:0:407:A:H5'	38:0:6054:HOH:O	2.00	0.60
30:0:69:A:C8	30:0:69:A:C5'	2.78	0.60
19:S:55:GLN:NE2	30:0:1446:U:H2'	2.17	0.60
30:0:2787:C:C5	38:0:4643:HOH:O	2.49	0.60
30:0:2581:U:H1'	38:0:4486:HOH:O	2.01	0.60
30:0:285:A:H2'	30:0:286:U:O4'	2.01	0.60
1:A:47:HIS:HD2	30:0:1654:U:H2'	1.66	0.60
30:0:363:C:H1'	38:0:5301:HOH:O	2.01	0.60
2:B:258:GLY:H	2:B:260:HIS:CE1	2.19	0.60
18:R:8:ALA:HB1	18:R:13:THR:HG21	1.82	0.60
25:Y:187:VAL:HG22	25:Y:192:ASP:HB3	1.84	0.60
30:0:2893:C:O2'	30:0:2894:C:H5'	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:960:G:N3	30:0:960:G:C2'	2.65	0.60
11:K:74:VAL:CG1	11:K:113:ILE:HG12	2.32	0.60
20:T:9:LYS:HE3	20:T:13:ARG:CZ	2.32	0.60
30:0:164:G:H3'	38:0:3650:HOH:O	2.02	0.60
30:0:853:C:H3'	38:0:4563:HOH:O	2.01	0.60
30:0:2103:A:O2'	30:0:2104:C:H6	1.85	0.59
30:0:2453:G:H3'	38:0:5945:HOH:O	2.01	0.59
10:J:75:PRO:HG2	10:J:105:LEU:HD21	1.83	0.59
25:Y:216:ARG:HD2	38:Y:8873:HOH:O	2.02	0.59
30:0:2134:G:N2	30:0:2242:U:C2	2.70	0.59
30:0:2637:A:H4'	38:0:4946:HOH:O	2.02	0.59
30:0:941:G:C5	30:0:942:U:C4	2.91	0.59
3:C:233:THR:HG22	3:C:234:VAL:H	1.67	0.59
12:L:56:LYS:HE3	30:0:2443:C:H1'	1.84	0.59
13:M:86:GLN:NE2	30:0:2274:A:H1'	2.17	0.59
19:S:17:ASP:HB3	19:S:23:LYS:HB2	1.83	0.59
24:X:76:ARG:HH11	24:X:76:ARG:HG3	1.66	0.59
30:0:2361:A:H8	30:0:2361:A:H5'	1.68	0.59
30:0:2795:C:O2'	30:0:2796:U:H5'	2.02	0.59
2:B:162:MET:CE	2:B:308:LEU:HD21	2.32	0.59
10:J:18:ILE:HD13	30:0:1244:U:OP1	2.01	0.59
17:Q:25:PRO:HB2	38:9:9079:HOH:O	2.01	0.59
30:0:1249:U:H2'	30:0:1250:C:C6	2.36	0.59
30:0:1527:A:H1'	30:0:1528:A:C8	2.37	0.59
30:0:1819:G:H2'	30:0:1820:G:C5'	2.32	0.59
30:0:2372:A:H2'	30:0:2373:U:C6	2.37	0.59
30:0:821:U:H2'	30:0:822:C:H6	1.67	0.59
5:E:49:ILE:HD11	5:E:69:ILE:HD12	1.85	0.59
6:F:58:GLU:CD	13:M:27:ARG:HH22	2.05	0.59
15:O:24:ALA:HB3	30:0:710:G:OP1	2.02	0.59
30:0:1625:U:H4'	38:0:4676:HOH:O	2.03	0.59
2:B:234:ARG:HG3	30:0:1735:C:OP2	2.02	0.59
11:K:45:PRO:HB2	38:K:7169:HOH:O	2.01	0.59
13:M:99:ARG:HE	13:M:170:ASN:HD22	1.49	0.59
30:0:1202:A:H2'	30:0:1203:G:O4'	2.03	0.59
8:H:174:LEU:HD21	30:0:1220:U:H4'	1.83	0.59
30:0:2073:G:OP2	30:0:2490:A:H5'	2.01	0.59
21:U:6:CYS:HB2	21:U:32:CYS:HB3	1.85	0.59
30:0:1603:A:H5'	30:0:1605:G:C4'	2.33	0.59
30:0:2756:U:N3	30:0:2896:A:H2	2.01	0.59
30:0:905:C:H3'	38:0:5207:HOH:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2265:U:H2'	30:0:2266:A:C8	2.37	0.59
30:0:2846:C:H4'	38:0:5100:HOH:O	2.03	0.59
30:0:513:A:N3	38:0:3665:HOH:O	2.32	0.59
4:D:54:ALA:HB2	4:D:69:ILE:HD12	1.84	0.59
30:0:1116:U:HO2'	30:0:1118:A:H2	0.68	0.59
11:K:87:ARG:HG3	30:0:2721:U:H4'	1.85	0.59
30:0:2756:U:N3	30:0:2896:A:C2	2.67	0.59
29:3:60:LYS:HG3	29:3:61:PRO:HD2	1.83	0.59
30:0:1120:U:H5'	30:0:1121:G:OP2	2.03	0.59
2:B:141:ARG:HD2	2:B:163:GLU:OE2	2.03	0.59
30:0:137:U:H2'	30:0:139:C:C5	2.38	0.58
30:0:2539:U:H1'	38:0:7825:HOH:O	2.02	0.58
30:0:737:A:H2'	30:0:738:G:O4'	2.02	0.58
1:A:191:GLY:HA2	1:A:194:MET:HE3	1.84	0.58
30:0:2526:C:C6	30:0:2526:C:C5'	2.85	0.58
30:0:2607:U:H4'	38:0:9447:HOH:O	2.03	0.58
29:3:73:GLU:HB3	38:3:9052:HOH:O	2.02	0.58
14:N:37:ARG:HH11	31:9:6:C:H5"	1.61	0.58
2:B:215:VAL:HB	38:B:9087:HOH:O	2.02	0.58
30:0:1641:A:H2'	30:0:1642:A:H5'	1.85	0.58
5:E:143:GLN:HE22	30:0:2779:G:H21	1.48	0.58
1:A:23:TYR:HB2	30:0:1872:C:C5	2.38	0.58
2:B:145:HIS:HD2	2:B:146:THR:O	1.87	0.58
3:C:236:THR:CG2	3:C:239:ALA:H	2.10	0.58
10:J:76:ASP:HA	38:J:5907:HOH:O	2.03	0.58
26:Z:81:CYS:SG	26:Z:83:TYR:HB3	2.43	0.58
30:0:282:C:O2'	30:0:283:U:C5'	2.52	0.58
30:0:304:G:H1'	30:0:347:A:N6	2.18	0.58
30:0:368:C:H2'	30:0:369:G:H5'	1.85	0.58
29:3:70:ARG:HB3	38:3:9064:HOH:O	2.03	0.58
8:H:48:VAL:HA	8:H:170:ARG:O	2.02	0.58
10:J:107:ASN:HD22	10:J:109:TYR:H	1.50	0.58
30:0:1919:A:H4'	38:0:4867:HOH:O	2.03	0.58
2:B:212:GLN:HB2	2:B:257:THR:CG2	2.32	0.58
30:0:1291:A:H2	38:0:5311:HOH:O	1.86	0.58
30:0:185:G:H4'	30:0:186:A:OP1	2.02	0.58
30:0:638:C:H2'	30:0:639:A:C8	2.39	0.58
30:0:899:C:H5'	38:0:3211:HOH:O	2.03	0.58
30:0:960:G:H4'	38:0:7470:HOH:O	2.03	0.58
12:L:67:ARG:HB2	12:L:112:GLY:HA3	1.85	0.58
28:2:2:LYS:HG3	30:0:1486:A:C4	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1701:A:H5''	30:0:1702:U:H3'	1.85	0.58
26:Z:40:ALA:HA	30:0:1773:G:C8	2.38	0.58
20:T:52:ARG:HD2	30:0:317:A:H5''	1.85	0.58
28:2:11:LEU:HD22	30:0:1417:G:O2'	2.04	0.58
2:B:36:PRO:HG3	2:B:169:GLY:H	1.69	0.58
3:C:101:ASP:HB2	30:0:750:A:O3'	2.04	0.58
3:C:2:GLN:HB3	38:C:8583:HOH:O	2.03	0.58
3:C:58:ALA:HA	3:C:73:GLN:HE21	1.69	0.58
13:M:30:GLU:O	13:M:34:GLU:HG3	2.04	0.58
30:0:1206:U:C6	30:0:1206:U:H5'	2.26	0.58
30:0:1507:C:H4'	38:0:3609:HOH:O	2.03	0.58
30:0:2670:G:O2'	30:0:2671:U:H5'	2.03	0.58
9:I:107:LYS:HB3	9:I:110:ASP:HB2	1.85	0.58
14:N:141:ARG:NH2	31:9:48:C:H4'	2.19	0.58
30:0:17:G:H2'	30:0:18:C:H6	1.68	0.58
30:0:2802:C:H2'	30:0:2803:C:H6	1.66	0.58
30:0:2842:G:H2'	30:0:2843:A:H5'	1.85	0.58
30:0:877:G:C5'	30:0:878:G:OP1	2.48	0.58
1:A:100:PRO:HG2	1:A:103:VAL:HG21	1.84	0.58
2:B:112:THR:HG23	2:B:158:LYS:NZ	2.18	0.58
5:E:84:MET:HG2	5:E:168:ILE:HA	1.86	0.58
9:I:73:LEU:HD12	9:I:107:LYS:NZ	2.19	0.58
27:1:25:LYS:HD2	28:2:49:GLU:H	1.68	0.58
2:B:207:LYS:HG3	30:0:2717:C:OP1	2.04	0.58
17:Q:19:ARG:HH21	31:9:11:A:P	2.27	0.58
12:L:6:ARG:HD3	30:0:1299:G:O6	2.03	0.57
30:0:2356:A:H5'	38:0:5655:HOH:O	2.03	0.57
30:0:2445:U:H2'	30:0:2446:G:C8	2.39	0.57
30:0:2510:C:H5'	30:0:2511:A:OP2	2.04	0.57
30:0:2755:G:H1'	38:0:4691:HOH:O	2.03	0.57
2:B:256:GLN:HG2	38:B:9121:HOH:O	2.04	0.57
7:G:16:LYS:O	7:G:20:VAL:HG23	2.03	0.57
7:G:64:ASN:N	7:G:64:ASN:HD22	2.02	0.57
14:N:61:ALA:HB3	14:N:88:ALA:HB2	1.85	0.57
30:0:2238:A:O2'	30:0:2239:C:H5'	2.03	0.57
30:0:297:U:H1'	38:0:3945:HOH:O	2.04	0.57
30:0:441:A:H1'	30:0:442:A:N7	2.20	0.57
30:0:812:A:H1'	38:0:3967:HOH:O	2.03	0.57
31:9:39:U:H1'	31:9:44:A:N6	2.18	0.57
2:B:5:ARG:NH1	2:B:8:LYS:HE2	2.19	0.57
30:0:1741:U:O2'	30:0:2723:G:H4'	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2004:U:H2'	30:0:2004:U:O2	2.04	0.57
29:3:48:ASN:HD21	30:0:2468:A:H61	1.50	0.57
30:0:1795:G:H2'	30:0:1796:A:O4'	2.04	0.57
23:W:44:MET:CE	30:0:944:G:H21	2.17	0.57
30:0:1278:A:H4'	30:0:1279:U:C4	2.40	0.57
30:0:232:A:H4'	38:0:6113:HOH:O	2.05	0.57
30:0:2505:G:O2'	30:0:2506:A:H5'	2.05	0.57
30:0:1167:G:H2'	30:0:1168:C:O4'	2.04	0.57
30:0:558:C:H2'	30:0:559:U:H5''	1.84	0.57
30:0:820:G:O2'	30:0:856:G:H4'	2.03	0.57
19:S:77:VAL:O	19:S:80:ARG:HG2	2.05	0.57
31:9:39:U:HO2'	31:9:42:C:H5	1.53	0.57
23:W:52:VAL:HG22	23:W:53:ALA:H	1.68	0.57
30:0:1538:C:O2'	30:0:1539:U:H5'	2.05	0.57
30:0:168:C:O5'	30:0:168:C:H6	1.88	0.57
30:0:2589:U:H2'	30:0:2590:U:C6	2.40	0.57
30:0:2597:U:H2'	30:0:2598:U:H5'	1.87	0.57
30:0:558:C:C2'	30:0:559:U:C5'	2.83	0.57
30:0:945:U:H2'	30:0:946:C:H6	1.70	0.57
12:L:41:HIS:CD2	30:0:926:A:O2'	2.58	0.57
10:J:70:PHE:HE1	30:0:2676:C:H4'	1.68	0.57
30:0:2291:A:N9	30:0:2309:C:H5'	2.19	0.57
30:0:292:G:H2'	30:0:358:G:N2	2.20	0.57
30:0:483:C:C4	30:0:484:A:C6	2.93	0.57
1:A:51:ARG:NH1	1:A:120:ARG:O	2.38	0.57
14:N:24:LEU:HD13	17:Q:26:PRO:HB3	1.86	0.57
30:0:1205:U:O2'	30:0:1206:U:H5''	2.05	0.56
30:0:287:C:H42	30:0:365:G:H1	1.53	0.56
38:C:8559:HOH:O	30:0:338:C:H5''	2.04	0.56
30:0:1214:G:H4'	38:0:4759:HOH:O	2.03	0.56
30:0:125:U:H2'	38:0:3775:HOH:O	2.04	0.56
23:W:125:HIS:HD2	23:W:127:GLY:H	1.53	0.56
30:0:119:A:H2'	30:0:120:A:H5''	1.87	0.56
30:0:1528:A:H2'	30:0:1529:G:O4'	2.05	0.56
30:0:17:G:H2'	30:0:18:C:C6	2.40	0.56
30:0:2720:C:H3'	38:0:6454:HOH:O	2.05	0.56
30:0:334:G:C5	30:0:335:U:C5	2.94	0.56
31:9:55:U:H4'	31:9:56:A:C8	2.40	0.56
14:N:147:ILE:HD12	38:9:9089:HOH:O	2.04	0.56
25:Y:126:PRO:HG2	25:Y:128:PHE:CE1	2.40	0.56
30:0:945:U:H2'	30:0:946:C:C6	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:69:TYR:CE1	30:0:2081:A:H4'	2.40	0.56
16:P:64:GLU:HG2	38:P:2495:HOH:O	2.05	0.56
30:0:1342:C:C2'	30:0:1343:C:H5'	2.35	0.56
8:H:15:PRO:HG3	30:0:1053:G:OP1	2.06	0.56
23:W:139:GLY:O	23:W:141:HIS:HD2	1.87	0.56
25:Y:115:ARG:HH21	30:0:1266:U:H4'	1.71	0.56
25:Y:235:GLU:H	25:Y:235:GLU:CD	2.08	0.56
30:0:1181:A:C2	30:0:1192:A:C8	2.94	0.56
30:0:136:C:H2'	30:0:137:U:O4'	2.05	0.56
1:A:47:HIS:CD2	30:0:1654:U:H2'	2.41	0.56
30:0:2252:A:C5	30:0:2253:G:H1'	2.40	0.56
2:B:297:VAL:HB	38:B:9075:HOH:O	2.05	0.56
8:H:69:ARG:HD3	38:H:232:HOH:O	2.06	0.56
18:R:39:THR:HG23	18:R:107:GLU:O	2.04	0.56
30:0:1679:C:H5'	38:0:9330:HOH:O	2.05	0.56
13:M:64:ARG:HD2	38:M:8878:HOH:O	2.04	0.56
30:0:1903:U:O2'	30:0:1904:A:N7	2.39	0.56
11:K:130:MET:SD	21:U:25:ASP:O	2.64	0.56
12:L:143:THR:HG22	12:L:144:ASP:N	2.21	0.56
31:9:49:G:H2'	31:9:50:G:O4'	2.06	0.56
5:E:149:GLU:HG3	5:E:167:TYR:HA	1.86	0.56
6:F:50:VAL:HG13	6:F:60:VAL:HG11	1.87	0.56
11:K:118:ALA:HA	11:K:125:ALA:HB2	1.88	0.56
31:9:63:C:O2'	31:9:64:C:H5'	2.06	0.56
2:B:294:TYR:HE2	38:B:9114:HOH:O	1.89	0.56
21:U:9:CYS:HA	21:U:52:THR:CG2	2.36	0.56
31:9:36:C:C5	31:9:37:C:C5	2.94	0.56
7:G:20:VAL:O	7:G:24:VAL:HG23	2.06	0.56
30:0:2253:G:O2'	30:0:2254:G:H5'	2.06	0.55
30:0:396:U:O2'	30:0:418:C:H4'	2.05	0.55
4:D:172:VAL:HG12	4:D:173:GLU:H	1.70	0.55
7:G:12:ILE:HG23	38:0:5477:HOH:O	2.07	0.55
23:W:48:VAL:HG12	23:W:52:VAL:HB	1.87	0.55
30:0:1183:C:N3	30:0:1184:C:C5	2.74	0.55
30:0:1198:U:H1'	30:0:1201:C:H5	1.71	0.55
30:0:1664:A:H8	30:0:1664:A:OP1	1.89	0.55
30:0:1768:C:H2'	30:0:1769:C:O4'	2.06	0.55
30:0:283:U:C5	30:0:284:C:C2	2.93	0.55
30:0:960:G:C3'	30:0:960:G:N3	2.70	0.55
30:0:2419:U:H5''	30:0:2420:G:H5'	1.89	0.55
30:0:2608:C:H2'	38:0:3579:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:141:ARG:HH21	31:9:48:C:H4'	1.72	0.55
3:C:236:THR:HA	38:C:8649:HOH:O	2.05	0.55
3:C:47:GLY:HA2	3:C:92:PRO:HB2	1.87	0.55
10:J:19:MET:HE1	10:J:79:PHE:HA	1.89	0.55
30:0:628:1MA:H4'	38:0:3149:HOH:O	2.06	0.55
30:0:65:C:O2'	30:0:66:G:H5'	2.06	0.55
6:F:77:VAL:HG21	6:F:83:LEU:HD13	1.88	0.55
8:H:22:TYR:CZ	30:0:1007:A:H2'	2.41	0.55
9:I:111:LEU:CD2	30:0:1163:G:H4'	2.35	0.55
11:K:32:ILE:HD11	11:K:56:SER:HB3	1.88	0.55
14:N:11:ARG:HG3	14:N:14:ARG:HH12	1.71	0.55
30:0:2478:U:O2'	30:0:2479:A:H5'	2.06	0.55
30:0:2509:A:C2	30:0:2510:C:H1'	2.42	0.55
30:0:558:C:H2'	30:0:559:U:H5'	1.89	0.55
12:L:22:ARG:HG2	38:0:3241:HOH:O	2.05	0.55
30:0:1666:C:H2'	30:0:1667:A:H5''	1.71	0.55
30:0:1787:C:H4'	30:0:2883:A:O4'	2.07	0.55
30:0:2353:A:H4'	30:0:2354:A:O5'	2.06	0.55
30:0:2908:A:O5'	30:0:2908:A:H8	1.89	0.55
38:O:1484:HOH:O	30:0:710:G:H1'	2.06	0.55
2:B:62:ARG:HA	2:B:65:MET:CE	2.36	0.55
30:0:1127:C:C5	30:0:1128:U:C4	2.95	0.55
30:0:1159:G:H1	30:0:1208:C:H42	1.54	0.55
30:0:2320:U:H4'	30:0:2321:A:O4'	2.07	0.55
30:0:2565:C:H4'	38:0:4851:HOH:O	2.06	0.55
30:0:567:U:C5'	38:0:6437:HOH:O	2.50	0.55
30:0:960:G:H2'	30:0:960:G:N3	2.22	0.55
8:H:6:ALA:HA	8:H:61:ARG:NH1	2.21	0.55
12:L:36:ASP:HB2	38:L:8836:HOH:O	2.07	0.55
23:W:154:ARG:NH1	30:0:588:G:O6	2.40	0.55
25:Y:130:ARG:HB2	25:Y:142:SER:O	2.07	0.55
30:0:1120:U:H5''	30:0:1120:U:C6	2.42	0.55
30:0:2896:A:N3	30:0:2896:A:H2'	2.22	0.55
30:0:89:G:H4'	38:0:4779:HOH:O	2.05	0.55
30:0:1819:G:H2'	30:0:1820:G:H4'	1.89	0.55
30:0:1838:U:H3'	38:0:5544:HOH:O	2.07	0.55
30:0:2249:G:C2	30:0:2253:G:C6	2.95	0.55
16:P:87:ARG:HG2	38:0:5970:HOH:O	2.07	0.55
30:0:1066:U:H2'	30:0:1067:A:C8	2.41	0.54
30:0:1118:A:H8	30:0:1119:G:H5''	1.73	0.54
30:0:1474:C:C5'	30:0:1474:C:C6	2.79	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:76:G:C3'	31:9:77:A:H5''	2.27	0.54
1:A:109:GLU:HG2	1:A:116:GLY:H	1.72	0.54
9:I:112:LEU:CD1	30:0:1162:G:H1'	2.37	0.54
27:1:9:GLY:HA2	30:0:1687:C:O2	2.07	0.54
30:0:1750:C:H5''	38:0:3673:HOH:O	2.07	0.54
3:C:174:ILE:CD1	30:0:338:C:H4'	2.36	0.54
22:V:64:GLY:O	22:V:65:ASP:HB2	2.06	0.54
23:W:142:ASP:HB3	23:W:145:GLY:H	1.71	0.54
24:X:43:VAL:HG11	24:X:82:GLU:HA	1.88	0.54
38:Z:8707:HOH:O	30:0:1886:A:H4'	2.06	0.54
27:1:16:HIS:HE1	30:0:775:G:OP1	1.91	0.54
30:0:876:A:N3	30:0:876:A:H2'	2.23	0.54
2:B:221:GLN:HE22	11:K:42:ASN:ND2	1.98	0.54
16:P:80:ARG:HG2	16:P:87:ARG:CZ	2.37	0.54
23:W:64:THR:O	23:W:68:THR:HG22	2.06	0.54
30:0:1016:U:H1'	38:0:3664:HOH:O	2.06	0.54
30:0:2387:U:H2'	30:0:2388:C:C6	2.42	0.54
29:3:11:CYS:HB2	29:3:20:HIS:CE1	2.42	0.54
2:B:275:GLY:O	2:B:291:ASP:HA	2.07	0.54
2:B:305:ASP:O	2:B:306:LYS:HB2	2.08	0.54
4:D:141:VAL:HG21	31:9:57:A:H8	1.72	0.54
8:H:59:GLN:HE21	8:H:129:ARG:NE	2.05	0.54
30:0:138:U:OP1	30:0:259:G:H5'	2.07	0.54
31:9:12:C:H5'	31:9:70:U:O4'	2.06	0.54
13:M:66:SER:HB3	13:M:128:TRP:CD1	2.42	0.54
24:X:23:HIS:HE1	30:0:2044:G:OP1	1.89	0.54
30:0:711:G:C2	30:0:718:C:C2	2.96	0.54
30:0:962:C:H2'	30:0:963:C:H5'	1.89	0.54
15:O:105:ASN:HD21	15:O:109:SER:N	2.05	0.54
20:T:68:ASP:HB2	38:0:5678:HOH:O	2.08	0.54
30:0:2271:G:N3	30:0:2271:G:H2'	2.22	0.54
31:9:1:U:O3'	31:9:3:A:H5''	2.07	0.54
13:M:159:VAL:HG12	33:M:8818:CL:CL	2.45	0.54
23:W:88:THR:HG22	23:W:90:TYR:HD1	1.72	0.54
26:Z:75:GLY:HA3	38:Z:8717:HOH:O	2.06	0.54
30:0:2414:A:H2'	30:0:2415:A:C8	2.43	0.54
31:9:3:A:N6	31:9:22:G:H1'	2.22	0.54
8:H:87:LYS:NZ	8:H:87:LYS:HB2	2.23	0.54
23:W:13:MET:HE1	23:W:18:GLN:HA	1.88	0.54
30:0:1205:U:H5	38:0:4451:HOH:O	1.91	0.54
30:0:1342:C:O2'	30:0:1343:C:H5'	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2880:A:H2'	30:0:2881:C:H5'	1.89	0.54
4:D:18:ILE:HD13	4:D:84:LEU:HD12	1.89	0.54
9:I:97:VAL:HG12	9:I:101:LYS:HE3	1.90	0.54
13:M:24:GLN:NE2	13:M:27:ARG:HH11	2.06	0.54
30:0:1450:C:H5''	38:0:9624:HOH:O	2.08	0.54
30:0:1624:A:H5'	30:0:1626:A:O4'	2.07	0.54
30:0:1926:G:H2'	30:0:1927:A:C8	2.42	0.54
30:0:567:U:H5''	38:0:5308:HOH:O	2.08	0.54
19:S:11:THR:H	19:S:14:ALA:HB3	1.73	0.54
30:0:1137:G:H1'	38:0:3888:HOH:O	2.07	0.53
2:B:254:GLN:HG2	2:B:255:GLY:N	2.23	0.53
16:P:7:LYS:HD3	16:P:21:VAL:HG22	1.90	0.53
24:X:30:MET:HE1	24:X:58:ALA:HB3	1.90	0.53
24:X:72:VAL:HG22	24:X:85:VAL:HG12	1.90	0.53
30:0:1201:C:C2'	30:0:1202:A:H5'	2.37	0.53
30:0:1766:U:O2	30:0:1778:A:H5'	2.08	0.53
30:0:1973:A:H5'	30:0:1973:A:C8	2.41	0.53
17:Q:15:LYS:HD3	30:0:2364:A:H5''	1.89	0.53
30:0:2697:A:H2'	30:0:2698:G:O4'	2.08	0.53
1:A:17:ARG:HD2	38:A:9005:HOH:O	2.07	0.53
30:0:121:U:H2'	38:0:9854:HOH:O	2.08	0.53
30:0:1304:U:H2'	30:0:1305:C:C6	2.43	0.53
30:0:644:G:H1'	38:0:6440:HOH:O	2.08	0.53
30:0:682:A:H2'	30:0:683:G:O4'	2.08	0.53
31:9:1:U:O3'	31:9:3:A:C5'	2.57	0.53
30:0:2102:G:C5'	30:0:2538:A:C2	2.91	0.53
30:0:2311:A:H3'	38:0:7716:HOH:O	2.07	0.53
30:0:2445:U:H2'	30:0:2446:G:H8	1.72	0.53
30:0:280:C:H2'	30:0:281:U:O4'	2.07	0.53
30:0:700:A:H5''	30:0:701:U:H5'	1.91	0.53
2:B:154:VAL:HG12	2:B:156:LYS:HG2	1.89	0.53
4:D:141:VAL:HG21	31:9:57:A:C8	2.43	0.53
19:S:37:VAL:O	19:S:41:VAL:HG23	2.08	0.53
30:0:2354:A:C2	30:0:2367:A:C8	2.97	0.53
30:0:2002:C:H2'	30:0:2003:U:H5'	1.90	0.53
30:0:482:G:H4'	30:0:508:A:N1	2.24	0.53
28:2:22:PRO:HG2	28:2:25:VAL:HG23	1.90	0.53
14:N:139:TRP:HA	14:N:139:TRP:CE3	2.44	0.53
23:W:5:VAL:HG11	23:W:153:MET:CE	2.39	0.53
30:0:1562:C:N4	38:0:5888:HOH:O	2.41	0.53
30:0:1714:C:O2'	30:0:1715:C:H5'	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:407:A:H2'	30:0:408:A:C8	2.44	0.53
27:1:42:SER:HB2	38:1:354:HOH:O	2.08	0.53
8:H:6:ALA:HB3	30:0:2521:A:OP2	2.09	0.53
30:0:559:U:C5'	30:0:559:U:H6	2.20	0.53
3:C:127:ARG:HD3	3:C:129:HIS:HE1	1.73	0.53
4:D:23:VAL:HG21	4:D:45:THR:HG21	1.90	0.53
17:Q:42:LYS:HE2	30:0:952:G:OP1	2.09	0.53
26:Z:66:CYS:SG	26:Z:67:GLY:N	2.82	0.53
30:0:1495:C:H1'	30:0:1573:A:H1'	1.91	0.53
30:0:2256:G:C2'	30:0:2257:G:C5'	2.86	0.53
30:0:2764:C:O2'	30:0:2765:C:H5'	2.08	0.53
1:A:190:ARG:NH1	30:0:1845:A:OP2	2.42	0.53
1:A:192:VAL:CG1	1:A:207:GLN:HB3	2.39	0.53
8:H:26:ILE:HA	8:H:123:ILE:HG21	1.91	0.53
13:M:188:ARG:NH1	30:0:154:C:H3'	2.23	0.53
14:N:86:LEU:HD12	14:N:125:ALA:HB2	1.91	0.53
25:Y:132:ASP:OD2	30:0:621:C:H5'	2.08	0.53
25:Y:141:THR:HG23	38:Y:8892:HOH:O	2.08	0.53
30:0:1060:C:H6	30:0:1060:C:H5'	1.72	0.53
10:J:107:ASN:C	10:J:107:ASN:HD22	2.13	0.53
30:0:603:A:H1'	30:0:605:C:C2	2.43	0.52
14:N:48:VAL:CG1	14:N:55:ASP:HB3	2.39	0.52
16:P:115:SER:OG	16:P:118:GLN:HG3	2.09	0.52
30:0:1183:C:C2	30:0:1184:C:C5	2.97	0.52
30:0:138:U:C5	30:0:140:G:O6	2.62	0.52
30:0:704:C:H2'	30:0:705:C:H6	1.74	0.52
31:9:13:A:O2'	31:9:14:G:H5''	2.10	0.52
1:A:36:ASP:O	1:A:38:ILE:N	2.41	0.52
1:A:99:ILE:O	1:A:131:HIS:HE1	1.92	0.52
30:0:1014:A:H2'	30:0:1015:C:H5'	1.92	0.52
30:0:2359:G:H3'	38:0:5709:HOH:O	2.09	0.52
30:0:2509:A:H2'	30:0:2510:C:O4'	2.09	0.52
30:0:282:C:O2'	30:0:283:U:H4'	2.09	0.52
30:0:304:G:H1'	30:0:347:A:H61	1.73	0.52
4:D:134:LEU:HD11	4:D:166:ILE:HD11	1.91	0.52
13:M:134:ILE:HG23	13:M:141:ILE:HD13	1.92	0.52
18:R:18:LEU:HB2	18:R:143:VAL:CG1	2.40	0.52
18:R:114:VAL:HA	18:R:144:GLU:O	2.09	0.52
30:0:2265:U:H2'	30:0:2266:A:H8	1.75	0.52
31:9:42:C:H5'	31:9:43:G:OP2	2.09	0.52
3:C:25:PRO:HG2	38:C:8521:HOH:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:3:VAL:HG22	5:E:49:ILE:HB	1.91	0.52
7:G:19:GLU:O	7:G:23:ILE:HG13	2.09	0.52
17:Q:21:ARG:HH12	30:0:2353:A:H1'	1.74	0.52
20:T:28:SER:O	20:T:32:ARG:HG3	2.08	0.52
23:W:88:THR:HG22	23:W:89:ASP:N	2.23	0.52
30:0:1180:U:O2'	30:0:1181:A:H5'	2.10	0.52
30:0:1289:C:O2'	30:0:1290:G:H5'	2.09	0.52
30:0:138:U:OP2	30:0:139:C:C5	2.62	0.52
30:0:1724:U:H5''	38:0:3739:HOH:O	2.09	0.52
6:F:13:GLU:OE2	6:F:78:GLU:HG2	2.09	0.52
14:N:33:ARG:NH2	31:9:6:C:O2'	2.43	0.52
18:R:150:PRO:CG	18:R:150:PRO:CB	2.87	0.52
30:0:1185:U:H5'	38:0:7505:HOH:O	2.08	0.52
30:0:1249:U:H2'	30:0:1250:C:H6	1.75	0.52
2:B:267:LYS:HD3	38:0:9567:HOH:O	2.09	0.52
4:D:154:LYS:HD2	4:D:154:LYS:N	2.10	0.52
4:D:28:GLY:HA2	4:D:69:ILE:HG23	1.92	0.52
5:E:5:LEU:HD21	5:E:66:GLN:HG3	1.91	0.52
30:0:1175:G:O2'	30:0:1193:A:H2'	2.09	0.52
30:0:1477:C:H5'	30:0:1868:G:H5'	1.91	0.52
30:0:204:A:H2'	30:0:205:U:H5'	1.92	0.52
30:0:2072:G:C6	30:0:2533:C:H1'	2.45	0.52
30:0:2840:A:H3'	38:0:7686:HOH:O	2.09	0.52
30:0:298:C:H1'	38:0:3853:HOH:O	2.09	0.52
30:0:661:G:C5	30:0:686:A:C2	2.98	0.52
4:D:25:MET:CE	4:D:37:ALA:HB1	2.39	0.52
30:0:1878:G:O2'	30:0:1879:U:C6	2.59	0.52
30:0:1972:U:H2'	30:0:1973:A:H5'	1.91	0.52
30:0:2498:C:O2'	30:0:2499:U:H5'	2.09	0.52
30:0:2604:A:H4'	38:0:7644:HOH:O	2.09	0.52
1:A:217:ARG:HG2	1:A:229:ALA:HB2	1.91	0.52
6:F:2:VAL:HG22	6:F:57:GLU:OE1	2.09	0.52
12:L:121:ILE:HG12	12:L:141:GLU:HB2	1.92	0.52
13:M:188:ARG:HD3	30:0:155:C:OP2	2.09	0.52
30:0:2526:C:O2'	30:0:2527:U:H5'	2.10	0.52
3:C:16:VAL:HG12	3:C:17:ASP:H	1.73	0.52
5:E:154:ILE:HD11	5:E:157:LYS:HE2	1.92	0.52
7:G:23:ILE:O	7:G:27:ILE:HG13	2.09	0.52
18:R:18:LEU:HB2	18:R:143:VAL:HG12	1.92	0.52
30:0:999:C:O2'	30:0:1000:C:H5'	2.10	0.52
30:0:545:G:C8	30:0:545:G:C5'	2.83	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:734:U:O2'	30:0:736:A:N7	2.37	0.52
30:0:821:U:H2'	30:0:822:C:C6	2.45	0.52
17:Q:95:GLU:HA	30:0:949:U:H4'	1.92	0.52
4:D:128:LEU:HB2	38:D:6007:HOH:O	2.08	0.52
30:0:1419:U:H2'	30:0:1685:A:C2	2.45	0.51
30:0:1675:C:H3'	38:0:7847:HOH:O	2.10	0.51
1:A:33:GLU:O	1:A:34:ASP:HB2	2.09	0.51
30:0:2083:A:H3'	38:0:7617:HOH:O	2.10	0.51
30:0:137:U:OP1	30:0:259:G:O2'	2.28	0.51
30:0:334:G:C6	30:0:335:U:C4	2.98	0.51
15:O:37:ARG:HD2	30:0:656:G:OP2	2.09	0.51
2:B:212:GLN:HA	30:0:1733:A:H4'	1.92	0.51
15:O:7:LEU:HD22	38:O:5650:HOH:O	2.10	0.51
30:0:1393:A:H2'	30:0:1394:C:C6	2.46	0.51
30:0:2637:A:OP1	30:0:2637:A:H3'	2.10	0.51
30:0:432:G:O2'	30:0:433:C:H5'	2.10	0.51
30:0:652:G:H8	38:0:3020:HOH:O	1.93	0.51
13:M:34:GLU:HB3	13:M:38:GLU:HG3	1.91	0.51
18:R:14:ALA:HB3	18:R:147:LEU:HB2	1.93	0.51
30:0:1307:A:H2'	30:0:1308:A:C8	2.46	0.51
26:Z:76:THR:HG21	30:0:1652:C:H4'	1.91	0.51
30:0:2493:C:O2	30:0:2493:C:H2'	2.10	0.51
30:0:346:U:H4'	38:0:6881:HOH:O	2.10	0.51
27:1:16:HIS:CD2	30:0:470:U:O2'	2.63	0.51
8:H:27:PRO:HD3	8:H:123:ILE:HG22	1.91	0.51
26:Z:57:MET:SD	26:Z:73:ARG:HD2	2.51	0.51
30:0:1181:A:H2'	30:0:1182:C:H5'	1.93	0.51
30:0:1422:U:H2'	30:0:1423:C:C6	2.46	0.51
30:0:466:A:H2'	30:0:467:G:O4'	2.10	0.51
27:1:8:GLN:HE22	27:1:11:LYS:NZ	2.07	0.51
31:9:95:C:O2'	31:9:96:C:H5'	2.11	0.51
4:D:62:ASP:HA	38:D:4233:HOH:O	2.10	0.51
2:B:221:GLN:NE2	11:K:42:ASN:HD22	1.96	0.51
24:X:85:VAL:HG12	24:X:86:GLU:N	2.26	0.51
30:0:120:A:H2'	30:0:120:A:N3	2.26	0.51
30:0:1477:C:O2'	30:0:1478:U:H5'	2.10	0.51
30:0:2105:C:H2'	30:0:2106:C:C6	2.45	0.51
30:0:2329:C:O2'	30:0:2330:U:H5'	2.10	0.51
30:0:553:G:H5'	38:0:3506:HOH:O	2.11	0.51
31:9:3:A:OP2	31:9:25:G:N2	2.43	0.51
5:E:21:THR:HG23	5:E:30:THR:OG1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:7:LYS:HG2	16:P:23:PHE:CE2	2.46	0.51
20:T:24:ARG:HH21	20:T:39:ASN:HD22	1.59	0.51
30:0:1056:U:H2'	30:0:1057:A:O4'	2.11	0.51
28:2:10:ARG:NH2	30:0:121:U:OP2	2.42	0.51
30:0:281:U:H2'	30:0:282:C:O4'	2.10	0.51
30:0:282:C:H2'	30:0:283:U:O4'	2.10	0.51
30:0:2826:G:C6	30:0:2913:A:N6	2.78	0.51
28:2:38:LYS:HE3	38:0:4239:HOH:O	2.10	0.51
10:J:42:GLU:O	10:J:131:THR:HG23	2.11	0.51
18:R:40:ALA:O	18:R:44:VAL:HG23	2.11	0.51
23:W:81:ASP:OD1	23:W:92:ASP:HB2	2.11	0.51
30:0:1166:A:C6	30:0:1181:A:C2	2.99	0.51
30:0:1181:A:C2'	30:0:1182:C:H5'	2.40	0.51
30:0:694:A:H2'	30:0:695:C:H5'	1.91	0.51
30:0:764:C:H2'	30:0:765:G:O4'	2.11	0.51
2:B:223:ARG:HG3	2:B:232:TRP:O	2.10	0.51
23:W:13:MET:CE	23:W:17:ILE:HG22	2.41	0.51
30:0:1183:C:O2	30:0:1183:C:C2'	2.59	0.51
30:0:1209:C:H2'	30:0:1210:G:H8	1.76	0.51
30:0:2786:G:H5''	38:0:4643:HOH:O	2.10	0.51
30:0:2894:C:O2'	30:0:2895:C:H5'	2.11	0.51
30:0:951:A:C2'	30:0:952:G:H5'	2.40	0.51
18:R:39:THR:HG22	18:R:42:GLU:H	1.75	0.51
23:W:80:ASP:HB2	38:W:3312:HOH:O	2.11	0.51
30:0:1131:G:C6	30:0:1230:A:C4	2.99	0.51
30:0:172:U:H5'	38:0:4171:HOH:O	2.11	0.51
3:C:63:SER:OG	30:0:2101:A:H2'	2.11	0.51
30:0:255:A:C5	30:0:256:C:C5	2.98	0.51
30:0:255:A:H2'	30:0:256:C:H6	1.76	0.51
30:0:90:A:H2'	30:0:91:G:O4'	2.11	0.51
28:2:41:HIS:CD2	28:2:44:ARG:H	2.26	0.51
31:9:55:U:H4'	31:9:56:A:H8	1.76	0.51
38:C:8567:HOH:O	20:T:2:LYS:HE2	2.10	0.51
25:Y:174:VAL:HG23	25:Y:177:LYS:HD2	1.93	0.51
30:0:2553:A:H2'	30:0:2553:A:N3	2.25	0.50
30:0:305:A:C5	30:0:329:A:C2	2.99	0.50
27:1:10:LYS:HG3	38:1:2979:HOH:O	2.10	0.50
1:A:173:GLY:O	1:A:176:HIS:HB3	2.10	0.50
9:I:114:TYR:N	9:I:114:TYR:CD1	2.80	0.50
23:W:5:VAL:HG11	23:W:153:MET:HE1	1.92	0.50
30:0:1657:A:H2'	30:0:1658:A:C8	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2269:C:C2'	30:0:2270:G:H5'	2.40	0.50
30:0:282:C:O2'	30:0:283:U:C4'	2.59	0.50
30:0:512:G:O3'	30:0:513:A:H8	1.93	0.50
31:9:29:C:H2'	31:9:30:C:C5'	2.36	0.50
1:A:192:VAL:HG12	1:A:207:GLN:HB3	1.93	0.50
6:F:61:MET:HB3	13:M:19:GLN:OE1	2.11	0.50
30:0:1594:C:O2'	30:0:1607:A:H4'	2.11	0.50
30:0:398:U:H2'	30:0:399:C:C6	2.47	0.50
1:A:33:GLU:CD	1:A:33:GLU:H	2.14	0.50
2:B:41:PHE:CZ	2:B:79:MET:HG3	2.46	0.50
30:0:1515:A:H2'	30:0:1516:U:C6	2.46	0.50
30:0:23:G:H1'	30:0:520:A:N6	2.26	0.50
31:9:75:G:H1	31:9:106:U:H3	1.59	0.50
6:F:91:VAL:CG1	6:F:92:GLY:H	2.16	0.50
10:J:19:MET:HE3	10:J:132:LEU:HD11	1.92	0.50
14:N:37:ARG:NH1	31:9:6:C:OP1	2.44	0.50
21:U:6:CYS:HA	21:U:13:ILE:HD11	1.94	0.50
30:0:1903:U:O2'	30:0:1904:A:C8	2.63	0.50
30:0:2589:U:H2'	30:0:2590:U:H6	1.76	0.50
31:9:54:A:C2	31:9:55:U:N3	2.80	0.50
31:9:59:C:H6	31:9:59:C:O5'	1.94	0.50
4:D:159:PRO:O	4:D:163:VAL:HG23	2.12	0.50
5:E:7:ILE:HG22	5:E:45:ASP:O	2.10	0.50
13:M:9:ARG:HD2	30:0:380:A:OP2	2.11	0.50
8:H:19:ARG:HH12	30:0:1008:C:H5''	1.76	0.50
30:0:1015:C:H2'	30:0:1016:U:C6	2.47	0.50
30:0:10:U:O4	30:0:532:A:OP2	2.30	0.50
30:0:602:A:O2'	30:0:605:C:H4'	2.11	0.50
30:0:814:G:H4'	38:0:3140:HOH:O	2.11	0.50
7:G:63:ARG:NH1	30:0:1151:G:OP1	2.45	0.50
26:Z:50:VAL:O	26:Z:54:GLU:HG3	2.11	0.50
30:0:11:A:N3	30:0:11:A:H2'	2.26	0.50
30:0:1883:U:C2'	30:0:1884:G:H5'	2.42	0.50
30:0:2878:U:H2'	30:0:2879:A:O4'	2.12	0.50
11:K:20:CYS:HB2	11:K:29:LEU:HG	1.94	0.50
16:P:14:LEU:HD13	16:P:51:ALA:HB2	1.93	0.50
20:T:38:ARG:NH1	38:0:6719:HOH:O	2.45	0.50
30:0:1588:G:C6	30:0:1589:G:N1	2.80	0.50
30:0:2842:G:C2'	30:0:2843:A:H5'	2.41	0.50
31:9:1:U:H4'	31:9:3:A:OP1	2.12	0.50
30:0:1170:U:H2'	30:0:1172:G:OP2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1186:C:N4	30:0:1187:U:C4	2.80	0.50
30:0:1520:G:H2'	30:0:1521:C:C6	2.46	0.50
30:0:1759:A:N3	30:0:1818:C:H2'	2.27	0.50
30:0:1840:A:H4'	30:0:1841:C:O5'	2.12	0.50
30:0:1947:G:N2	30:0:1966:U:C2	2.80	0.50
30:0:2898:G:O2'	30:0:2899:A:H5'	2.11	0.50
30:0:319:A:H4'	30:0:338:C:C4	2.47	0.50
14:N:67:ALA:HA	14:N:71:TRP:HB3	1.93	0.50
30:0:1377:C:C5'	30:0:1377:C:H6	2.19	0.49
30:0:1896:G:C6	30:0:1897:U:C4	3.00	0.49
2:B:307:ARG:NH1	2:B:307:ARG:HG3	2.26	0.49
10:J:74:ARG:HH11	10:J:74:ARG:HB3	1.76	0.49
11:K:4:LEU:HD22	11:K:116:GLU:HB3	1.93	0.49
23:W:125:HIS:CE1	30:0:1097:A:H5''	2.47	0.49
30:0:1350:U:H5''	38:0:5143:HOH:O	2.11	0.49
30:0:711:G:O2'	30:0:712:C:H5'	2.12	0.49
30:0:923:A:H2'	38:0:5697:HOH:O	2.12	0.49
12:L:143:THR:HG22	12:L:144:ASP:H	1.78	0.49
14:N:5:ARG:HG3	14:N:5:ARG:HH11	1.77	0.49
24:X:43:VAL:HG12	24:X:44:ASP:N	2.26	0.49
1:A:217:ARG:NH2	30:0:1853:C:O2'	2.46	0.49
13:M:75:ARG:HH11	30:0:1864:C:H5	1.59	0.49
30:0:1947:G:H2'	30:0:1948:G:H8	1.77	0.49
30:0:2415:A:H2'	30:0:2416:G:H5'	1.94	0.49
31:9:107:C:O2'	31:9:108:C:H5'	2.11	0.49
23:W:119:HIS:HE1	38:0:9559:HOH:O	1.95	0.49
30:0:861:A:H4'	30:0:1697:G:H4'	1.94	0.49
30:0:735:C:C5	30:0:736:A:C4	2.99	0.49
30:0:920:C:H5''	30:0:921:G:O5'	2.13	0.49
9:I:73:LEU:HD12	9:I:107:LYS:HZ1	1.77	0.49
30:0:1221:G:C8	38:0:6014:HOH:O	2.55	0.49
30:0:1947:G:H2'	30:0:1948:G:C8	2.47	0.49
30:0:2134:G:C6	30:0:2258:A:C8	3.01	0.49
30:0:2276:U:H2'	30:0:2277:U:C6	2.47	0.49
30:0:2638:G:H1'	38:0:7796:HOH:O	2.11	0.49
30:0:2651:C:H2'	30:0:2652:U:O4'	2.12	0.49
16:P:61:ARG:NH2	30:0:2737:C:OP2	2.37	0.49
30:0:939:A:C2	30:0:1027:G:N3	2.81	0.49
27:1:21:ARG:HD2	27:1:37:CYS:SG	2.53	0.49
1:A:51:ARG:HB2	38:A:9061:HOH:O	2.11	0.49
24:X:21:PRO:HG2	24:X:24:LYS:HD3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1878:G:O2'	30:0:1879:U:P	2.71	0.49
30:0:2345:A:H3'	30:0:2346:C:C6	2.46	0.49
31:9:2:U:P	31:9:3:A:H5'	2.52	0.49
10:J:75:PRO:HG2	10:J:105:LEU:CD2	2.42	0.49
23:W:125:HIS:CD2	23:W:127:GLY:H	2.31	0.49
30:0:1119:G:H22	30:0:1246:A:H2	1.51	0.49
16:P:54:LYS:HB2	30:0:1717:A:H5''	1.94	0.49
30:0:2385:G:H2'	30:0:2386:U:C6	2.47	0.49
30:0:291:C:H2'	30:0:292:G:O4'	2.12	0.49
30:0:370:G:O2'	30:0:371:U:H5'	2.12	0.49
30:0:711:G:C2'	30:0:712:C:H5'	2.42	0.49
27:1:20:ARG:HH21	30:0:120:A:H5'	1.77	0.49
2:B:17:LYS:O	2:B:260:HIS:HD2	1.94	0.49
3:C:233:THR:HG22	3:C:234:VAL:N	2.26	0.49
9:I:114:TYR:N	9:I:114:TYR:HD1	2.10	0.49
14:N:159:TYR:HE1	31:9:50:G:H5''	1.78	0.49
15:O:32:ARG:HD3	15:O:32:ARG:O	2.12	0.49
25:Y:186:ARG:HG2	25:Y:186:ARG:HH11	1.77	0.49
30:0:1298:U:H2'	30:0:1299:G:C8	2.48	0.49
30:0:185:G:H4'	30:0:186:A:H4'	1.93	0.49
30:0:256:C:H2'	30:0:257:G:O4'	2.12	0.49
30:0:699:C:C2	30:0:743:G:N2	2.81	0.49
30:0:806:A:H2'	30:0:807:A:O4'	2.13	0.49
30:0:941:G:C6	30:0:942:U:C4	3.01	0.49
30:0:958:G:H2'	30:0:959:C:C6	2.48	0.49
8:H:32:ALA:HB3	8:H:69:ARG:HH12	1.78	0.49
9:I:130:LEU:HD22	30:0:1167:G:H4'	1.95	0.49
17:Q:18:PRO:O	17:Q:21:ARG:HB2	2.12	0.49
17:Q:53:HIS:CD2	30:0:2389:U:H4'	2.47	0.49
24:X:66:THR:HG23	24:X:67:PRO:HD2	1.95	0.49
30:0:1118:A:C8	30:0:1119:G:H5''	2.48	0.49
30:0:1268:C:H2'	30:0:1269:G:H8	1.77	0.49
30:0:1755:A:H2'	30:0:1756:G:O4'	2.12	0.49
30:0:1849:G:H1'	30:0:2011:A:N1	2.28	0.49
12:L:41:HIS:HD2	30:0:926:A:O2'	1.95	0.49
29:3:3:MET:O	29:3:90:PHE:HA	2.12	0.49
31:9:49:G:O2'	31:9:50:G:H5'	2.13	0.49
1:A:135:VAL:HG21	1:A:147:ARG:HB3	1.94	0.49
8:H:100:GLU:HB3	8:H:124:VAL:HG11	1.94	0.49
13:M:99:ARG:HD2	13:M:167:GLY:CA	2.35	0.49
30:0:1667:A:H2'	30:0:1668:U:C6	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:182:G:H5''	38:0:3730:HOH:O	2.13	0.49
30:0:2103:A:N7	30:0:2538:A:N7	2.60	0.49
30:0:2064:U:H5'	30:0:2652:U:H4'	1.95	0.49
21:U:56:ARG:NH2	30:0:2890:A:H1'	2.28	0.49
30:0:522:U:O2'	30:0:1366:C:H5'	2.13	0.49
30:0:699:C:H6	30:0:744:G:O4'	1.96	0.49
30:0:1158:G:O2'	30:0:1159:G:H5'	2.13	0.48
30:0:1909:A:N1	30:0:2128:G:H1'	2.27	0.48
30:0:299:U:H5'	38:0:7377:HOH:O	2.12	0.48
30:0:876:A:N3	30:0:876:A:C2'	2.76	0.48
28:2:39:ARG:HG2	38:2:3143:HOH:O	2.13	0.48
2:B:41:PHE:HA	2:B:79:MET:HE2	1.94	0.48
9:I:101:LYS:O	9:I:105:GLU:HG3	2.12	0.48
14:N:132:ASN:O	14:N:135:VAL:HG12	2.13	0.48
24:X:74:ALA:HB2	24:X:85:VAL:HG13	1.95	0.48
16:P:1:THR:O	30:0:1396:C:H1'	2.13	0.48
12:L:18:HIS:HD2	30:0:902:G:N7	2.12	0.48
31:9:91:C:H2'	31:9:92:G:O4'	2.13	0.48
1:A:94:LEU:N	1:A:94:LEU:HD23	2.28	0.48
8:H:64:SER:OG	30:0:2520:G:H5'	2.13	0.48
10:J:5:GLU:HA	38:J:1652:HOH:O	2.11	0.48
11:K:34:VAL:HG22	11:K:47:ALA:HB2	1.94	0.48
12:L:138:GLY:HA3	38:L:8853:HOH:O	2.13	0.48
13:M:23:LEU:HD13	13:M:27:ARG:NH2	2.28	0.48
30:0:2534:C:H1'	38:0:3502:HOH:O	2.12	0.48
30:0:369:G:O2'	30:0:370:G:H5'	2.13	0.48
30:0:1634:G:H2'	30:0:1635:U:C6	2.48	0.48
30:0:1778:A:H2'	30:0:1779:A:H5'	1.94	0.48
2:B:262:ARG:HG3	30:0:2716:G:H5'	1.95	0.48
30:0:2768:A:N3	30:0:2768:A:H3'	2.27	0.48
30:0:652:G:H5''	38:0:3020:HOH:O	2.12	0.48
30:0:958:G:H2'	30:0:959:C:H6	1.77	0.48
22:V:56:ILE:O	22:V:60:GLN:HG3	2.14	0.48
30:0:1592:G:O2'	30:0:1593:C:O5'	2.30	0.48
30:0:2032:U:H2'	30:0:2033:G:C5'	2.43	0.48
30:0:2851:G:C2'	30:0:2852:A:H5'	2.44	0.48
13:M:99:ARG:CD	13:M:167:GLY:HA2	2.34	0.48
22:V:55:ARG:O	22:V:59:ILE:HG12	2.13	0.48
23:W:125:HIS:HE1	38:W:3071:HOH:O	1.95	0.48
30:0:1615:A:H5'	38:0:4195:HOH:O	2.13	0.48
30:0:1625:U:H3'	30:0:1625:U:H6	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1972:U:C2'	30:0:1973:A:C5'	2.91	0.48
30:0:2315:C:O2'	30:0:2316:G:H5'	2.13	0.48
30:0:2899:A:O2'	30:0:2900:G:H5'	2.13	0.48
30:0:2900:G:H2'	30:0:2901:C:O4'	2.13	0.48
30:0:2906:A:H5'	30:0:2907:C:O4'	2.14	0.48
31:9:31:C:H2'	31:9:32:G:O4'	2.14	0.48
31:9:54:A:C2'	31:9:55:U:H5'	2.43	0.48
2:B:217:ARG:HG3	2:B:257:THR:HG22	1.95	0.48
4:D:99:ASP:HB3	4:D:103:ASN:H	1.79	0.48
4:D:25:MET:SD	4:D:40:ILE:HD11	2.53	0.48
9:I:126:THR:O	9:I:130:LEU:HG	2.14	0.48
18:R:47:LEU:HB2	18:R:89:LEU:HD21	1.95	0.48
30:0:1183:C:H42	30:0:1184:C:N4	2.11	0.48
25:Y:142:SER:OG	30:0:1331:G:OP2	2.31	0.48
30:0:368:C:C2'	30:0:369:G:H5'	2.43	0.48
30:0:736:A:H2'	30:0:737:A:O4'	2.14	0.48
4:D:10:PHE:CG	4:D:11:HIS:N	2.81	0.48
30:0:241:A:C2	30:0:378:A:H4'	2.49	0.48
30:0:2488:U:O2'	30:0:2489:G:H5'	2.14	0.48
30:0:318:U:H5'	30:0:339:A:C2	2.49	0.48
3:C:132:ASP:HB2	3:C:161:ASP:HB3	1.95	0.48
8:H:30:LYS:N	8:H:62:HIS:HD2	2.10	0.48
11:K:87:ARG:NH1	38:K:4066:HOH:O	2.46	0.48
13:M:99:ARG:HE	13:M:170:ASN:ND2	2.10	0.48
14:N:154:LEU:C	14:N:156:GLU:H	2.16	0.48
19:S:33:SER:O	19:S:37:VAL:HG23	2.12	0.48
23:W:130:HIS:O	23:W:136:GLY:HA3	2.13	0.48
23:W:125:HIS:HB2	23:W:137:GLN:HG2	1.94	0.48
25:Y:170:SER:OG	25:Y:175:ARG:HG3	2.13	0.48
30:0:1173:A:C2	30:0:1177:A:C8	3.02	0.48
30:0:1221:G:H8	38:0:6014:HOH:O	1.94	0.48
30:0:1592:G:H2'	30:0:1593:C:H6	1.78	0.48
30:0:1692:C:H2'	38:0:9867:HOH:O	2.12	0.48
30:0:2133:U:H4'	30:0:2134:G:C5'	2.44	0.48
30:0:2505:G:C2'	30:0:2506:A:H5'	2.44	0.48
30:0:2672:C:O2'	30:0:2673:U:H5'	2.14	0.48
30:0:559:U:C3'	30:0:559:U:C6	2.97	0.48
30:0:633:C:O2'	30:0:634:G:H5'	2.14	0.48
30:0:843:A:C2	30:0:846:A:C8	3.02	0.48
2:B:44:TYR:OH	2:B:148:PRO:HG3	2.13	0.48
2:B:310:ARG:HD2	38:B:9112:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1198:U:C6	30:0:1200:A:OP2	2.67	0.48
30:0:128:A:O2'	30:0:129:A:H5'	2.14	0.48
30:0:1790:C:H2'	30:0:1791:U:H6	1.78	0.48
38:K:992:HOH:O	30:0:2583:A:H5'	2.13	0.48
30:0:2649:A:H5'	30:0:2649:A:H8	1.79	0.48
30:0:2718:C:H5'	30:0:2718:C:C6	2.46	0.48
30:0:2781:U:C2'	30:0:2782:G:C5'	2.91	0.48
30:0:281:U:O2'	30:0:282:C:H5'	2.14	0.48
30:0:334:G:C4	30:0:335:U:C6	3.02	0.48
30:0:484:A:N1	30:0:506:G:H4'	2.29	0.48
30:0:660:A:H4'	30:0:661:G:O5'	2.14	0.48
2:B:79:MET:HE1	38:B:9092:HOH:O	2.12	0.48
3:C:188:ARG:HD3	38:C:8563:HOH:O	2.13	0.48
22:V:4:HIS:HB3	38:V:6622:HOH:O	2.13	0.48
23:W:122:ARG:NH2	38:0:6437:HOH:O	2.46	0.48
30:0:1206:U:H2'	30:0:1207:A:O4'	2.14	0.47
30:0:861:A:C4'	30:0:1697:G:H4'	2.44	0.47
30:0:2526:C:H6	30:0:2526:C:C5'	2.18	0.47
15:O:25:VAL:HG12	30:0:709:G:O2'	2.14	0.47
30:0:727:G:H3'	30:0:728:C:H6	1.79	0.47
4:D:173:GLU:HG3	4:D:174:VAL:HG23	1.96	0.47
30:0:1634:G:H2'	30:0:1635:U:H6	1.79	0.47
30:0:1855:G:H4'	30:0:1856:C:O5'	2.13	0.47
30:0:559:U:H2'	30:0:560:U:O4'	2.15	0.47
30:0:571:C:H6	30:0:571:C:O5'	1.97	0.47
30:0:699:C:C2	30:0:744:G:C2	3.02	0.47
31:9:7:G:C5'	38:9:9100:HOH:O	2.58	0.47
1:A:36:ASP:HB2	1:A:85:SER:H	1.79	0.47
2:B:41:PHE:HB3	2:B:190:MET:HE3	1.95	0.47
2:B:280:VAL:HG13	2:B:333:GLU:O	2.13	0.47
4:D:23:VAL:HG21	4:D:45:THR:CG2	2.44	0.47
10:J:107:ASN:ND2	10:J:109:TYR:H	2.11	0.47
20:T:82:THR:HA	38:0:3998:HOH:O	2.12	0.47
30:0:1497:G:H4'	30:0:1627:G:O2'	2.14	0.47
30:0:619:U:H3'	38:0:3287:HOH:O	2.13	0.47
30:0:816:G:C6	30:0:817:G:N1	2.83	0.47
2:B:85:ARG:NH1	38:B:9099:HOH:O	2.47	0.47
10:J:70:PHE:CD1	30:0:2676:C:H4'	2.49	0.47
15:O:39:THR:HB	38:0:4627:HOH:O	2.14	0.47
25:Y:107:PRO:HB3	25:Y:182:PHE:CD2	2.50	0.47
30:0:1154:A:H2'	30:0:1155:G:C8	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1172:G:H1'	38:0:4992:HOH:O	2.14	0.47
30:0:1217:G:C2	30:0:1218:U:C2	3.03	0.47
30:0:12:U:C2'	30:0:13:G:H5'	2.40	0.47
30:0:2467:A:H8	38:0:7512:HOH:O	1.97	0.47
30:0:350:G:O2'	30:0:351:A:H5'	2.13	0.47
30:0:638:C:H2'	30:0:639:A:H8	1.78	0.47
30:0:724:G:O2'	30:0:725:C:H5'	2.14	0.47
30:0:963:C:O2	30:0:1005:A:N1	2.47	0.47
27:1:22:CYS:HB3	27:1:37:CYS:SG	2.55	0.47
31:9:76:G:H3'	31:9:77:A:C5'	2.30	0.47
2:B:27:ASN:H	2:B:27:ASN:HD22	1.63	0.47
2:B:312:ARG:HD3	2:B:315:VAL:HG13	1.95	0.47
16:P:103:THR:HA	16:P:106:ARG:NH2	2.29	0.47
23:W:21:LEU:HD21	23:W:48:VAL:CG1	2.43	0.47
30:0:968:G:C2	30:0:1001:U:O2	2.67	0.47
30:0:1636:G:O2'	30:0:1637:A:H5'	2.13	0.47
30:0:1856:C:H5'	30:0:1858:A:O4'	2.15	0.47
30:0:1878:G:C1'	38:0:6151:HOH:O	2.51	0.47
30:0:2121:G:O2'	30:0:2122:C:H5'	2.14	0.47
30:0:255:A:H2'	30:0:256:C:O4'	2.14	0.47
30:0:2577:A:H5'	38:0:7788:HOH:O	2.14	0.47
30:0:2614:C:O2'	30:0:2615:U:H5'	2.14	0.47
30:0:297:U:H2'	30:0:298:C:C6	2.49	0.47
30:0:541:C:C2'	30:0:542:A:C5'	2.81	0.47
30:0:74:G:H2'	30:0:75:U:C6	2.49	0.47
31:9:1:U:H5''	31:9:3:A:OP1	2.15	0.47
1:A:64:ASP:OD2	1:A:66:ARG:HD2	2.15	0.47
2:B:307:ARG:HB3	38:B:9117:HOH:O	2.15	0.47
6:F:34:ASN:HA	13:M:4:ALA:HB2	1.95	0.47
30:0:1587:U:H2'	30:0:1588:G:O4'	2.14	0.47
30:0:2524:G:H21	30:0:2526:C:N4	2.12	0.47
30:0:2769:C:H2'	30:0:2770:G:O4'	2.15	0.47
30:0:2842:G:H2'	30:0:2843:A:C5'	2.44	0.47
13:M:28:GLN:O	13:M:32:ARG:HG3	2.15	0.47
16:P:16:VAL:CG1	16:P:20:ARG:HB2	2.45	0.47
16:P:59:ARG:O	16:P:63:ARG:HG3	2.15	0.47
30:0:1339:G:C6	30:0:1340:G:N1	2.83	0.47
1:A:223:ARG:NH2	30:0:2271:G:OP1	2.45	0.47
30:0:2587:OMU:O3'	30:0:2587:OMU:HM22	2.15	0.47
30:0:27:U:H5	38:0:5910:HOH:O	1.96	0.47
30:0:736:A:H5''	38:0:4282:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:41:PHE:HB3	2:B:190:MET:CE	2.44	0.47
3:C:153:VAL:O	3:C:157:LEU:HG	2.15	0.47
6:F:36:THR:HG23	6:F:97:ALA:HB2	1.97	0.47
10:J:90:LYS:HB2	33:J:8802:CL:CL	2.51	0.47
11:K:66:ARG:HH22	30:0:1994:A:P	2.37	0.47
30:0:1268:C:O2'	30:0:1269:G:H5'	2.15	0.47
30:0:1803:C:H2'	30:0:1804:A:C8	2.50	0.47
30:0:1925:G:O2'	30:0:1926:G:H5'	2.15	0.47
2:B:242:TRP:CZ2	30:0:2607:U:C4	3.02	0.47
30:0:2649:A:H5'	30:0:2649:A:C8	2.50	0.47
30:0:758:A:H2'	30:0:759:C:O4'	2.15	0.47
30:0:772:G:H2'	30:0:773:A:O4'	2.15	0.47
2:B:244:PRO:HB3	30:0:1234:U:N3	2.29	0.47
5:E:145:ALA:HB1	5:E:168:ILE:CD1	2.45	0.47
20:T:62:VAL:N	38:T:3851:HOH:O	2.47	0.47
23:W:122:ARG:NH2	38:0:5308:HOH:O	2.48	0.47
24:X:78:GLU:HB3	38:X:5564:HOH:O	2.15	0.47
30:0:1183:C:N3	30:0:1184:C:N4	2.62	0.47
30:0:2326:C:H4'	30:0:2412:G:C4'	2.45	0.47
30:0:24:G:N2	30:0:518:G:H1'	2.30	0.47
30:0:70:A:H4'	30:0:71:G:O5'	2.15	0.47
3:C:87:ARG:NH2	30:0:894:A:C2	2.83	0.47
27:1:28:HIS:O	27:1:32:LYS:N	2.47	0.47
31:9:52:A:O2'	31:9:53:G:H5'	2.15	0.47
31:9:5:G:O2'	31:9:6:C:H5'	2.15	0.47
5:E:11:VAL:HG12	5:E:12:ASP:N	2.30	0.47
30:0:1204:C:H2'	30:0:1205:U:O4'	2.15	0.47
30:0:2133:U:H4'	30:0:2134:G:H5'	1.96	0.47
30:0:625:U:H5''	30:0:1044:C:N4	2.30	0.47
30:0:834:G:H3'	30:0:835:U:H4'	1.97	0.47
30:0:862:U:H2'	30:0:863:G:H8	1.80	0.47
31:9:33:U:H2'	38:9:9066:HOH:O	2.15	0.47
1:A:112:PRO:HD3	1:A:152:CYS:SG	2.55	0.47
2:B:139:ASP:HB2	38:B:8997:HOH:O	2.14	0.47
6:F:46:GLU:OE1	6:F:100:ASP:HA	2.15	0.47
18:R:18:LEU:HG	18:R:91:LEU:HD13	1.97	0.47
18:R:29:LYS:HE2	30:0:524:A:C5'	2.45	0.47
22:V:44:GLY:O	22:V:48:GLU:HG2	2.15	0.47
30:0:1181:A:N1	30:0:1192:A:O2'	2.42	0.47
30:0:1622:G:H2'	30:0:1623:C:H5'	1.97	0.47
30:0:1641:A:C2'	30:0:1642:A:H5'	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:790:A:H1'	30:0:1710:A:H2'	1.97	0.47
30:0:383:A:H2'	30:0:384:G:O4'	2.15	0.47
30:0:595:U:H2'	30:0:596:C:H6	1.80	0.47
2:B:62:ARG:HA	2:B:65:MET:HE2	1.97	0.47
13:M:123:ASP:OD1	13:M:126:GLN:HG2	2.15	0.47
13:M:184:ARG:HG3	13:M:185:PRO:HA	1.97	0.47
14:N:4:PRO:HG3	31:9:69:U:OP1	2.15	0.47
23:W:4:LEU:O	23:W:32:CYS:HA	2.15	0.47
30:0:1116:U:C2'	30:0:1118:A:C2	2.92	0.46
30:0:153:C:O2	30:0:439:A:H2	1.98	0.46
30:0:1589:G:N2	30:0:1605:G:H1'	2.29	0.46
30:0:2533:C:C6	30:0:2533:C:H5'	2.39	0.46
30:0:737:A:O5'	30:0:737:A:H8	1.98	0.46
1:A:186:TRP:CG	1:A:187:PRO:HA	2.50	0.46
3:C:236:THR:HG22	3:C:239:ALA:CB	2.45	0.46
15:O:29:VAL:HG11	15:O:98:LEU:HD21	1.96	0.46
30:0:1196:C:C2	30:0:1197:G:C8	3.03	0.46
16:P:120:ARG:HD2	30:0:1594:C:OP2	2.16	0.46
30:0:1819:G:H2'	30:0:1820:G:C4'	2.45	0.46
30:0:2511:A:H2'	30:0:2512:U:O4'	2.15	0.46
30:0:2587:OMU:H2'	30:0:2589:U:H5''	1.96	0.46
30:0:2791:U:H1'	30:0:2792:A:H5''	1.96	0.46
30:0:284:C:H6	30:0:284:C:OP2	1.98	0.46
30:0:541:C:O2'	30:0:542:A:H5''	2.15	0.46
30:0:920:C:H4'	30:0:921:G:C2	2.49	0.46
31:9:110:G:C6	31:9:111:U:C5	3.03	0.46
4:D:77:ASP:HB3	4:D:78:GLU:H	1.55	0.46
10:J:130:VAL:HG12	10:J:131:THR:N	2.30	0.46
23:W:13:MET:HE3	23:W:17:ILE:HG22	1.95	0.46
30:0:1666:C:HO2'	30:0:1667:A:H5''	1.72	0.46
30:0:1706:G:C6	30:0:1707:G:C6	3.04	0.46
30:0:2089:A:O2'	30:0:2090:G:H5'	2.15	0.46
30:0:2269:C:H2'	30:0:2270:G:H5'	1.96	0.46
30:0:2361:A:H2'	30:0:2362:A:O4'	2.15	0.46
30:0:264:G:H1'	30:0:265:U:H5	1.80	0.46
30:0:515:C:H5''	38:0:5665:HOH:O	2.13	0.46
1:A:101:GLU:OE2	1:A:131:HIS:HB2	2.15	0.46
2:B:62:ARG:HA	2:B:65:MET:HE3	1.97	0.46
23:W:35:VAL:HA	23:W:36:PRO:HD3	1.80	0.46
25:Y:99:ALA:HB2	25:Y:233:TYR:CZ	2.50	0.46
30:0:105:G:O2'	30:0:106:A:H5'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:128:A:H3'	30:0:128:A:C8	2.50	0.46
30:0:1948:G:H1	30:0:1964:U:H3	1.63	0.46
30:0:1966:U:O5'	30:0:1966:U:H6	1.99	0.46
30:0:2000:G:O2'	30:0:2001:G:H5'	2.15	0.46
30:0:204:A:C2'	30:0:205:U:H5'	2.45	0.46
30:0:254:C:O2	30:0:254:C:H2'	2.14	0.46
30:0:506:G:N2	30:0:509:A:H5'	2.21	0.46
30:0:890:C:O2'	30:0:891:G:H5'	2.16	0.46
2:B:112:THR:HG23	2:B:158:LYS:HZ2	1.80	0.46
2:B:125:GLU:O	2:B:129:ARG:HG3	2.15	0.46
4:D:129:ASP:OD1	30:0:2338:G:H2'	2.16	0.46
10:J:19:MET:CE	10:J:132:LEU:HD11	2.45	0.46
11:K:87:ARG:NH2	30:0:2720:C:O2	2.49	0.46
30:0:1581:A:C5	30:0:1582:C:C5	3.03	0.46
16:P:88:GLN:HE22	30:0:1799:G:H21	1.63	0.46
30:0:2326:C:H4'	30:0:2412:G:H4'	1.97	0.46
30:0:2506:A:N6	30:0:2511:A:O2'	2.49	0.46
30:0:300:U:C4	30:0:301:C:C5	3.03	0.46
30:0:419:A:H1'	30:0:1921:A:C2	2.51	0.46
1:A:71:PRO:HD2	1:A:74:VAL:HG21	1.98	0.46
2:B:177:HIS:O	2:B:181:ILE:HG13	2.15	0.46
6:F:101:ALA:HA	38:F:5413:HOH:O	2.15	0.46
12:L:148:GLU:HA	38:L:8870:HOH:O	2.14	0.46
13:M:72:ALA:HB2	13:M:93:ARG:HG2	1.97	0.46
23:W:43:GLY:HA3	30:0:945:U:O2'	2.15	0.46
30:0:129:A:O2'	30:0:131:A:OP1	2.33	0.46
30:0:1543:G:N1	30:0:1641:A:OP2	2.35	0.46
30:0:2775:A:C6	30:0:2799:A:C8	3.04	0.46
30:0:441:A:H8	30:0:441:A:O5'	1.97	0.46
11:K:118:ALA:CA	11:K:125:ALA:HB2	2.45	0.46
23:W:139:GLY:O	23:W:141:HIS:CD2	2.66	0.46
23:W:73:LEU:HA	23:W:73:LEU:HD12	1.85	0.46
30:0:1156:C:O5'	30:0:1156:C:H6	1.99	0.46
30:0:1321:A:H2'	30:0:1322:G:C8	2.51	0.46
30:0:1393:A:N1	30:0:1725:C:O2'	2.39	0.46
30:0:1588:G:C6	30:0:1589:G:C6	3.04	0.46
30:0:2115:U:H2'	30:0:2116:U:C6	2.51	0.46
13:M:86:GLN:HE22	30:0:2274:A:H1'	1.79	0.46
30:0:2658:G:H4'	30:0:2842:G:C8	2.51	0.46
2:B:214:PRO:HD2	38:0:9083:HOH:O	2.14	0.46
3:C:214:THR:HG23	38:C:8635:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:35:LYS:HD3	38:O:4627:HOH:O	2.15	0.46
15:O:38:ARG:NH1	38:O:7674:HOH:O	2.49	0.46
30:0:1115:U:O2'	30:0:1116:U:H5'	2.15	0.46
30:0:1130:U:H2'	30:0:1131:G:O4'	2.16	0.46
30:0:1586:G:O2'	30:0:1587:U:H5'	2.16	0.46
1:A:6:GLY:O	30:0:1861:C:H4'	2.15	0.46
30:0:1973:A:H2'	30:0:1974:G:O4'	2.15	0.46
30:0:2252:A:C6	30:0:2253:G:H1'	2.51	0.46
30:0:2366:C:O5'	30:0:2366:C:H6	1.99	0.46
9:I:78:ALA:HB1	9:I:93:ALA:HB1	1.96	0.46
30:0:2112:A:H2'	30:0:2113:G:C8	2.50	0.46
30:0:2301:A:H5''	30:0:2302:A:H5'	1.97	0.46
30:0:2385:G:H2'	30:0:2386:U:H6	1.81	0.46
30:0:2710:U:H2'	30:0:2711:U:C6	2.50	0.46
31:9:20:G:O2'	31:9:21:G:H5'	2.16	0.46
23:W:119:HIS:CD2	23:W:120:PRO:HD2	2.50	0.46
25:Y:133:HIS:HD2	38:Y:8884:HOH:O	1.98	0.46
30:0:1598:A:N6	33:0:8815:CL:CL	2.86	0.46
30:0:1445:G:N2	30:0:1678:A:H1'	2.31	0.46
30:0:1930:A:H2'	30:0:1931:A:C8	2.51	0.46
4:D:131:THR:HG21	30:0:2348:C:H1'	1.96	0.46
30:0:2831:C:C2'	30:0:2832:C:H5'	2.46	0.46
30:0:417:G:P	38:0:7458:HOH:O	2.73	0.46
30:0:440:C:H2'	30:0:441:A:C8	2.51	0.46
30:0:567:U:O2'	30:0:568:G:H5'	2.15	0.46
30:0:999:C:H2'	30:0:1000:C:O4'	2.16	0.46
2:B:140:LEU:HD12	2:B:174:ARG:HG3	1.97	0.46
4:D:75:LEU:HD22	4:D:79:MET:HB3	1.98	0.46
10:J:54:VAL:HG11	10:J:138:THR:HG21	1.98	0.46
14:N:110:THR:HB	14:N:113:SER:OG	2.16	0.46
16:P:73:HIS:HE1	30:0:1789:G:O6	1.98	0.46
18:R:82:GLU:HG3	18:R:83:LYS:N	2.30	0.46
22:V:39:ALA:C	22:V:41:GLU:H	2.20	0.46
23:W:26:ILE:HB	38:W:5420:HOH:O	2.15	0.46
30:0:1169:U:C5	30:0:1170:U:C4	3.03	0.45
30:0:1456:C:H2'	30:0:1457:U:C6	2.50	0.45
30:0:2299:G:C6	30:0:2300:A:C6	3.05	0.45
30:0:253:U:H1'	30:0:256:C:H41	1.80	0.45
28:2:28:LYS:O	30:0:87:C:H2'	2.16	0.45
1:A:95:PRO:HA	1:A:153:ARG:HA	1.97	0.45
6:F:53:ASP:OD1	6:F:80:GLN:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:112:LEU:HG	30:0:1162:G:O2'	2.15	0.45
26:Z:46:SER:O	26:Z:50:VAL:HG23	2.16	0.45
30:0:123:U:O2'	30:0:124:C:H5'	2.16	0.45
30:0:1669:G:O2'	30:0:1670:A:H5'	2.16	0.45
30:0:861:A:H4'	30:0:1697:G:C4'	2.47	0.45
30:0:1896:G:C5	30:0:1897:U:C5	3.04	0.45
30:0:851:C:O2	30:0:2022:A:H2	1.99	0.45
30:0:2604:A:H5'	38:0:5810:HOH:O	2.16	0.45
30:0:282:C:H1'	30:0:368:C:H41	1.74	0.45
30:0:2869:G:H2'	30:0:2870:C:C6	2.51	0.45
13:M:90:ARG:NH2	30:0:2266:A:OP2	2.49	0.45
16:P:36:THR:O	16:P:39:ASP:HB2	2.16	0.45
23:W:56:GLU:O	23:W:143:THR:HG23	2.16	0.45
23:W:88:THR:HG21	23:W:96:LEU:HD13	1.98	0.45
25:Y:177:LYS:HD3	25:Y:181:GLY:O	2.17	0.45
30:0:1188:A:C5	30:0:1189:A:C2	3.03	0.45
30:0:1309:U:O2'	30:0:1310:U:H5'	2.16	0.45
30:0:1314:U:H5''	30:0:1316:G:O4'	2.16	0.45
30:0:1506:U:H5'	30:0:1506:U:H6	1.82	0.45
30:0:1788:U:C2	30:0:1805:G:N2	2.84	0.45
30:0:2421:G:H4'	38:0:4797:HOH:O	2.16	0.45
30:0:2664:A:H8	30:0:2664:A:OP1	1.99	0.45
30:0:2712:G:O2'	30:0:2713:G:H5'	2.16	0.45
31:9:39:U:C2'	31:9:40:C:OP1	2.65	0.45
1:A:109:GLU:HG2	1:A:116:GLY:N	2.30	0.45
1:A:217:ARG:HH11	1:A:217:ARG:HG3	1.79	0.45
3:C:206:ASN:HB2	30:0:329:A:OP2	2.16	0.45
3:C:93:LYS:O	3:C:98:ARG:NH2	2.49	0.45
4:D:76:ARG:NE	31:9:44:A:O4'	2.49	0.45
8:H:52:LEU:HB3	8:H:137:PHE:HB2	1.99	0.45
14:N:44:ARG:HG3	14:N:45:ALA:N	2.32	0.45
14:N:37:ARG:HD3	33:N:8807:CL:CL	2.54	0.45
15:O:32:ARG:HE	15:O:35:LYS:HD2	1.81	0.45
20:T:26:THR:HA	20:T:39:ASN:HB3	1.98	0.45
22:V:39:ALA:N	22:V:40:PRO:CD	2.80	0.45
30:0:1189:A:C3'	38:0:7717:HOH:O	2.59	0.45
30:0:1790:C:H2'	30:0:1791:U:C6	2.51	0.45
30:0:228:C:H2'	30:0:229:G:H5'	1.98	0.45
30:0:2594:C:O2'	30:0:2595:U:H5'	2.16	0.45
30:0:397:A:O2'	30:0:417:G:N3	2.39	0.45
31:9:110:G:C5	31:9:111:U:C5	3.04	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:40:HIS:HE1	30:0:949:U:O2'	1.99	0.45
30:0:1002:G:H2'	30:0:1003:U:O5'	2.17	0.45
30:0:1116:U:H2'	30:0:1118:A:C2	2.52	0.45
30:0:1398:G:O2'	30:0:1399:A:H5'	2.16	0.45
30:0:1563:G:H4'	38:0:4241:HOH:O	2.16	0.45
30:0:158:A:C2'	30:0:159:G:H5'	2.47	0.45
28:2:8:LYS:NZ	30:0:1677:U:OP2	2.43	0.45
16:P:55:LYS:HD3	30:0:1716:A:H4'	1.97	0.45
30:0:2332:A:H5'	30:0:2333:G:OP2	2.17	0.45
30:0:482:G:O4'	30:0:511:A:C2	2.70	0.45
18:R:128:ARG:HH12	30:0:840:U:H2'	1.80	0.45
30:0:955:A:C2	30:0:1013:A:C4	3.05	0.45
3:C:129:HIS:HE1	3:C:231:ARG:HA	1.78	0.45
4:D:23:VAL:HG12	4:D:130:VAL:HG22	1.98	0.45
9:I:121:LYS:HB3	30:0:1184:C:H4'	1.97	0.45
11:K:81:ARG:HD3	11:K:87:ARG:NH1	2.31	0.45
23:W:6:GLN:CB	23:W:26:ILE:HD11	2.45	0.45
30:0:1023:C:H2'	30:0:1024:G:O4'	2.16	0.45
30:0:1503:U:H2'	30:0:1504:A:O4'	2.16	0.45
30:0:1964:U:C2	30:0:1965:C:C5	3.05	0.45
30:0:228:C:C2'	30:0:229:G:H5'	2.46	0.45
3:C:35:VAL:HG21	3:C:227:GLY:HA2	1.98	0.45
3:C:236:THR:H	3:C:239:ALA:HB3	1.80	0.45
6:F:72:VAL:HA	6:F:73:PRO:HD3	1.87	0.45
9:I:87:PRO:HG3	38:0:7157:HOH:O	2.17	0.45
13:M:179:GLY:O	30:0:399:C:H5'	2.17	0.45
17:Q:11:ARG:HG3	30:0:2363:G:O2'	2.16	0.45
24:X:30:MET:HG2	30:0:1384:C:H5'	1.98	0.45
30:0:1921:A:O2'	30:0:1922:A:H5'	2.17	0.45
30:0:685:C:O2	30:0:748:C:H4'	2.17	0.45
31:9:60:C:H2'	31:9:61:C:H6	1.81	0.45
2:B:162:MET:HE2	2:B:310:ARG:HD3	1.99	0.45
12:L:30:ARG:HD2	30:0:164:G:H5"	1.99	0.45
23:W:29:VAL:O	23:W:30:ASN:HB2	2.16	0.45
25:Y:99:ALA:HB2	25:Y:233:TYR:CE2	2.51	0.45
30:0:1573:A:N7	30:0:1574:C:C2	2.85	0.45
30:0:2251:G:H2'	30:0:2252:A:H8	1.79	0.45
38:3:9030:HOH:O	30:0:2382:A:H5'	2.16	0.45
30:0:2793:A:H2'	30:0:2794:G:H5'	1.98	0.45
30:0:559:U:H3'	30:0:559:U:C6	2.52	0.45
4:D:15:GLU:HA	4:D:16:PRO:HD3	1.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:41:LYS:HD3	38:9:9060:HOH:O	2.17	0.45
19:S:6:LYS:HB2	19:S:27:ALA:O	2.17	0.45
30:0:2316:G:OP1	30:0:2317:C:H1'	2.16	0.45
30:0:2419:U:H5''	30:0:2420:G:C5'	2.46	0.45
30:0:2897:C:O2'	30:0:2898:G:H5'	2.17	0.45
30:0:962:C:C2'	30:0:963:C:H5'	2.47	0.45
28:2:22:PRO:HG2	28:2:25:VAL:CG2	2.47	0.45
2:B:199:TYR:HE2	2:B:268:ARG:HB2	1.82	0.45
3:C:127:ARG:HD3	3:C:129:HIS:CE1	2.52	0.45
5:E:10:ASP:HA	38:E:6017:HOH:O	2.17	0.45
14:N:169:PRO:O	14:N:172:PHE:HB3	2.17	0.45
17:Q:3:SER:HB3	38:Q:5998:HOH:O	2.16	0.45
23:W:69:ARG:HD2	23:W:117:ARG:O	2.16	0.45
26:Z:45:VAL:HG12	38:Z:8714:HOH:O	2.17	0.45
30:0:1120:U:H6	30:0:1120:U:H5''	1.81	0.45
30:0:1268:C:H2'	30:0:1269:G:C8	2.51	0.45
30:0:1700:C:H5''	30:0:1701:A:OP2	2.16	0.45
30:0:2002:C:C2'	30:0:2003:U:H5'	2.46	0.45
30:0:249:G:O2'	30:0:250:C:H5'	2.17	0.45
29:3:11:CYS:HB2	29:3:20:HIS:HE1	1.81	0.45
5:E:23:GLU:HG2	5:E:28:SER:HB3	1.98	0.45
9:I:108:HIS:H	9:I:109:PRO:HD2	1.82	0.45
10:J:52:GLN:HE22	30:0:1119:G:H8	1.65	0.45
23:W:119:HIS:CG	38:0:5308:HOH:O	2.69	0.45
30:0:1209:C:O2'	30:0:1210:G:H5'	2.16	0.44
30:0:1904:A:H2'	30:0:1905:U:O4'	2.17	0.44
30:0:2831:C:H2'	30:0:2832:C:H5'	1.98	0.44
30:0:62:C:C4	30:0:63:U:C4	3.05	0.44
30:0:81:G:N3	30:0:98:A:C2	2.85	0.44
4:D:140:ARG:HG3	4:D:140:ARG:HH11	1.82	0.44
8:H:61:ARG:HH11	8:H:61:ARG:HG3	1.83	0.44
12:L:53:ARG:NH2	12:L:57:VAL:HG12	2.31	0.44
13:M:6:SER:O	13:M:10:ASP:HB2	2.17	0.44
14:N:43:VAL:HG13	14:N:118:ILE:HD11	1.98	0.44
23:W:68:THR:HG23	23:W:69:ARG:HG2	1.99	0.44
23:W:88:THR:HG22	23:W:90:TYR:CD1	2.50	0.44
30:0:1524:U:H5''	30:0:1524:U:C6	2.52	0.44
30:0:177:A:H2'	30:0:178:U:O4'	2.16	0.44
30:0:2070:G:H2'	30:0:2072:G:OP1	2.17	0.44
30:0:2103:A:N6	30:0:2538:A:H8	2.09	0.44
30:0:812:A:H2'	30:0:813:C:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:920:C:H4'	30:0:921:G:N2	2.32	0.44
27:1:28:HIS:CD2	27:1:31:LYS:HG3	2.52	0.44
3:C:54:LEU:HD23	3:C:79:ARG:HG3	1.99	0.44
30:0:1626:A:H2'	30:0:1627:G:C5'	2.48	0.44
28:2:43:ARG:NH2	30:0:1684:A:H1'	2.25	0.44
30:0:2072:G:H3'	30:0:2073:G:C5'	2.47	0.44
30:0:2297:U:H1'	38:0:5197:HOH:O	2.17	0.44
30:0:2329:C:H2'	30:0:2330:U:C6	2.52	0.44
14:N:25:ARG:HG2	30:0:2416:G:O2'	2.17	0.44
31:9:59:C:C4	31:9:60:C:N4	2.86	0.44
31:9:97:U:O2'	31:9:98:C:H5'	2.18	0.44
5:E:72:MET:O	5:E:76:VAL:HG22	2.18	0.44
11:K:89:LYS:HE2	21:U:19:THR:HG21	2.00	0.44
21:U:37:GLU:HB3	38:U:408:HOH:O	2.18	0.44
26:Z:61:HIS:O	26:Z:69:ASP:HA	2.18	0.44
30:0:1190:G:H2'	38:0:4068:HOH:O	2.15	0.44
30:0:130:C:H2'	38:0:3168:HOH:O	2.17	0.44
30:0:1712:A:H2'	30:0:1713:G:O4'	2.18	0.44
1:A:204:GLY:N	30:0:2634:G:OP2	2.51	0.44
1:A:212:PRO:HA	30:0:1943:C:O4'	2.18	0.44
1:A:88:ILE:HD13	1:A:100:PRO:HD3	1.99	0.44
3:C:168:ARG:NH2	3:C:190:ALA:O	2.51	0.44
5:E:19:ASP:HA	5:E:31:ARG:O	2.17	0.44
7:G:67:LEU:O	7:G:71:LEU:HG	2.18	0.44
24:X:47:ALA:HB1	24:X:82:GLU:HB3	2.00	0.44
30:0:1447:U:H3'	30:0:1506:U:O2	2.18	0.44
30:0:1523:G:H2'	30:0:1524:U:O4'	2.17	0.44
30:0:1592:G:H2'	30:0:1593:C:C6	2.52	0.44
30:0:1902:G:O2'	30:0:1903:U:H5'	2.17	0.44
30:0:1947:G:N2	30:0:1965:C:O2	2.50	0.44
30:0:2135:A:C2'	30:0:2136:G:H5'	2.47	0.44
30:0:2104:C:O2	30:0:2485:A:N1	2.50	0.44
30:0:506:G:N2	30:0:509:A:H5''	2.30	0.44
30:0:559:U:C4	30:0:560:U:C4	3.06	0.44
30:0:677:C:O2'	30:0:678:G:H5'	2.17	0.44
1:A:171:LYS:HB2	30:0:820:G:C5	2.53	0.44
30:0:858:U:H2'	30:0:859:C:C6	2.52	0.44
5:E:20:ILE:HD11	5:E:40:VAL:HG11	1.99	0.44
7:G:64:ASN:N	7:G:64:ASN:ND2	2.66	0.44
10:J:39:VAL:HG13	10:J:106:GLY:O	2.17	0.44
12:L:43:HIS:HD2	38:L:8827:HOH:O	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:167:GLY:O	13:M:171:ARG:HG3	2.17	0.44
23:W:90:TYR:N	23:W:90:TYR:CD1	2.85	0.44
26:Z:78:ILE:HD12	38:Z:8717:HOH:O	2.18	0.44
30:0:1052:G:H2'	30:0:1052:G:N3	2.31	0.44
30:0:113:A:OP2	30:0:114:A:H2'	2.17	0.44
30:0:1173:A:H3'	38:0:4358:HOH:O	2.16	0.44
30:0:1166:A:OP1	30:0:1174:A:H4'	2.17	0.44
30:0:1182:C:C1'	30:0:1192:A:C8	3.01	0.44
30:0:128:A:C8	30:0:128:A:C3'	3.01	0.44
30:0:1825:U:O2'	30:0:1826:C:H5'	2.18	0.44
30:0:255:A:C4	30:0:256:C:C6	3.06	0.44
30:0:295:C:H2'	30:0:296:G:O4'	2.18	0.44
30:0:39:G:N2	30:0:444:C:C2	2.86	0.44
30:0:594:C:C4	30:0:595:U:C4	3.06	0.44
30:0:645:U:O2	30:0:761:A:H2	2.00	0.44
30:0:735:C:H5	30:0:736:A:C4	2.36	0.44
29:3:48:ASN:ND2	30:0:169:A:H1'	2.33	0.44
4:D:41:LEU:HA	4:D:44:ILE:HG22	1.99	0.44
5:E:170:ARG:NH2	38:E:4761:HOH:O	2.50	0.44
11:K:125:ALA:C	11:K:127:ALA:H	2.21	0.44
14:N:139:TRP:HA	14:N:139:TRP:HE3	1.81	0.44
30:0:1226:G:H5'	38:0:4543:HOH:O	2.18	0.44
30:0:1318:A:H4'	30:0:1343:C:H4'	2.00	0.44
30:0:1503:U:C2'	30:0:1504:A:H5'	2.48	0.44
30:0:2087:C:O2'	30:0:2088:C:H5'	2.18	0.44
1:A:179:MET:HG2	1:A:186:TRP:CB	2.48	0.44
1:A:199:HIS:HE1	30:0:1881:A:OP1	2.01	0.44
1:A:94:LEU:HD12	1:A:98:GLU:HB2	2.00	0.44
13:M:80:GLY:O	13:M:81:ARG:HD2	2.17	0.44
20:T:28:SER:HA	20:T:97:ARG:HD3	2.00	0.44
24:X:25:ARG:HD2	38:X:5356:HOH:O	2.16	0.44
30:0:1135:G:H5'	38:0:5953:HOH:O	2.17	0.44
30:0:1180:U:H2'	30:0:1181:A:O4'	2.18	0.44
30:0:1553:C:O5'	30:0:1553:C:H6	2.00	0.44
30:0:1882:C:H2'	30:0:1883:U:H6	1.83	0.44
30:0:307:G:H3'	38:0:6719:HOH:O	2.18	0.44
30:0:696:C:O2'	30:0:697:G:H5'	2.17	0.44
30:0:729:C:C2	30:0:743:G:C2	3.06	0.44
30:0:734:U:H2'	30:0:736:A:OP2	2.18	0.44
31:9:2:U:H4'	38:9:9103:HOH:O	2.18	0.44
2:B:304:PRO:HD2	2:B:307:ARG:NE	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:112:ALA:HA	5:E:113:PRO:HD3	1.85	0.44
6:F:1:PRO:H3	6:F:4:VAL:HG23	1.83	0.44
8:H:39:LYS:HD2	30:0:969:G:H5'	1.98	0.44
11:K:98:VAL:HG11	11:K:102:GLU:HA	1.98	0.44
12:L:113:GLN:O	30:0:700:A:N6	2.47	0.44
15:O:105:ASN:HD21	15:O:109:SER:H	1.65	0.44
18:R:104:PHE:HB3	18:R:109:MET:HE1	2.00	0.44
30:0:1279:U:C2'	30:0:1279:U:O2	2.64	0.44
30:0:2256:G:C6	30:0:2257:G:C4	3.05	0.44
4:D:52:THR:HG21	30:0:2346:C:O2'	2.17	0.44
30:0:2533:C:O2'	30:0:2534:C:H5'	2.18	0.44
6:F:59:ILE:HD13	30:0:263:U:O4'	2.17	0.44
30:0:2914:A:H5''	30:0:2914:A:H8	1.83	0.44
30:0:812:A:H2'	30:0:813:C:O4'	2.17	0.44
30:0:935:G:O2'	30:0:936:C:H5'	2.18	0.44
4:D:167:GLU:C	4:D:169:THR:H	2.21	0.44
8:H:29:SER:HA	8:H:62:HIS:HD2	1.82	0.44
26:Z:66:CYS:SG	26:Z:68:GLU:HB2	2.58	0.44
30:0:1342:C:H2'	30:0:1343:C:H5'	2.00	0.43
30:0:1386:G:O2'	30:0:1387:G:H5'	2.18	0.43
30:0:1444:G:O2'	30:0:1445:G:H5'	2.18	0.43
30:0:2796:U:H2'	30:0:2797:C:O5'	2.18	0.43
30:0:553:G:O4'	30:0:1325:G:H5'	2.18	0.43
30:0:629:A:H2'	30:0:630:A:O4'	2.18	0.43
1:A:191:GLY:HA2	1:A:194:MET:HE2	1.99	0.43
8:H:139:ALA:HB3	8:H:149:VAL:HG21	2.00	0.43
13:M:47:ASP:CG	13:M:48:LYS:N	2.71	0.43
14:N:143:ARG:HG2	14:N:172:PHE:CD2	2.52	0.43
15:O:47:ARG:HG3	15:O:47:ARG:HH11	1.82	0.43
24:X:23:HIS:CD2	24:X:24:LYS:HG3	2.53	0.43
30:0:1705:C:O2	30:0:2735:U:H5''	2.18	0.43
30:0:2332:A:H3'	30:0:2333:G:H8	1.83	0.43
30:0:2717:C:C2'	30:0:2718:C:C5'	2.81	0.43
30:0:2761:A:C4	30:0:2763:G:C8	3.06	0.43
30:0:282:C:C2'	30:0:283:U:H5'	2.47	0.43
30:0:238:C:H4'	30:0:287:C:OP1	2.18	0.43
30:0:544:G:C3'	30:0:545:G:H5''	2.46	0.43
30:0:696:C:O2'	30:0:731:U:OP1	2.35	0.43
1:A:48:ASP:HB3	38:A:9061:HOH:O	2.18	0.43
5:E:8:PRO:HB2	5:E:11:VAL:HG23	1.99	0.43
12:L:71:GLU:HG2	30:0:700:A:C2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:44:ASN:OD1	15:O:65:LEU:HB2	2.18	0.43
16:P:100:ALA:HA	38:O:5526:HOH:O	2.17	0.43
17:Q:26:PRO:O	17:Q:30:VAL:HG23	2.17	0.43
17:Q:28:ARG:HG2	38:9:9079:HOH:O	2.17	0.43
30:0:1098:A:H2'	30:0:1099:G:O4'	2.18	0.43
30:0:1181:A:H2'	30:0:1182:C:C5'	2.49	0.43
30:0:312:U:C2	30:0:320:G:N2	2.87	0.43
2:B:232:TRP:CD1	2:B:235:ARG:HD2	2.52	0.43
9:I:120:ALA:O	9:I:124:VAL:HG23	2.18	0.43
16:P:7:LYS:HD3	16:P:21:VAL:CG2	2.47	0.43
20:T:52:ARG:O	30:0:317:A:OP1	2.36	0.43
20:T:53:GLY:HA3	38:T:6384:HOH:O	2.19	0.43
24:X:34:ARG:NH1	24:X:48:VAL:O	2.51	0.43
25:Y:126:PRO:HG2	25:Y:128:PHE:CZ	2.53	0.43
30:0:912:A:C4	30:0:1294:A:C2	3.05	0.43
13:M:188:ARG:HH11	30:0:154:C:H3'	1.82	0.43
30:0:815:U:O2'	30:0:1598:A:H4'	2.19	0.43
30:0:1622:G:C2'	30:0:1623:C:H5'	2.48	0.43
30:0:1889:C:O2'	30:0:1890:U:H5'	2.18	0.43
17:Q:45:PRO:O	30:0:2365:G:H4'	2.18	0.43
30:0:2491:G:H5'	38:0:9387:HOH:O	2.19	0.43
30:0:300:U:C2	30:0:301:C:C6	3.06	0.43
30:0:483:C:N4	30:0:484:A:C6	2.87	0.43
1:A:187:PRO:HB2	30:0:1845:A:O3'	2.19	0.43
1:A:36:ASP:CB	1:A:85:SER:H	2.31	0.43
2:B:329:TYR:CE2	21:U:15:PRO:HG2	2.53	0.43
6:F:57:GLU:O	6:F:61:MET:HG3	2.18	0.43
23:W:44:MET:HE2	30:0:944:G:H21	1.83	0.43
24:X:15:ARG:HH22	30:0:2856:A:P	2.41	0.43
10:J:60:ARG:NH2	30:0:1242:A:OP2	2.45	0.43
30:0:2247:C:O2'	30:0:2248:C:H5'	2.18	0.43
30:0:2421:G:H3'	30:0:2422:U:C5'	2.48	0.43
30:0:2819:C:H2'	30:0:2820:A:C8	2.53	0.43
30:0:844:A:C6	30:0:882:A:C5	3.06	0.43
30:0:962:C:H5''	38:0:4933:HOH:O	2.19	0.43
29:3:70:ARG:HD3	38:3:9064:HOH:O	2.18	0.43
2:B:162:MET:CE	2:B:310:ARG:HD3	2.48	0.43
4:D:103:ASN:ND2	4:D:133:ASN:HA	2.33	0.43
13:M:147:LEU:O	13:M:150:ILE:HG22	2.18	0.43
13:M:158:ARG:HB2	13:M:163:LEU:HB2	2.01	0.43
14:N:7:LYS:HB3	17:Q:21:ARG:NH2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:104:PHE:CB	18:R:109:MET:HE1	2.48	0.43
25:Y:144:ARG:NE	38:Y:8914:HOH:O	2.52	0.43
30:0:1482:A:H1'	38:0:9428:HOH:O	2.18	0.43
30:0:1735:C:O2'	30:0:1736:A:H5'	2.18	0.43
30:0:1842:A:C4	30:0:1979:G:C6	3.06	0.43
30:0:213:G:N2	30:0:225:G:H2'	2.34	0.43
30:0:2566:A:C2	30:0:2696:G:O4'	2.71	0.43
30:0:2727:A:N1	30:0:2756:U:C2	2.87	0.43
30:0:2869:G:H5'	38:0:5515:HOH:O	2.18	0.43
30:0:451:C:O2'	30:0:452:G:H5'	2.18	0.43
30:0:653:U:H2'	30:0:654:A:C8	2.53	0.43
27:1:25:LYS:O	27:1:25:LYS:HG2	2.19	0.43
1:A:9:ARG:HG2	1:A:16:PHE:CD2	2.54	0.43
12:L:6:ARG:NH1	30:0:1299:G:N7	2.67	0.43
17:Q:25:PRO:HA	17:Q:26:PRO:HD3	1.79	0.43
23:W:134:GLU:OE2	31:9:97:U:H1'	2.19	0.43
23:W:88:THR:CG2	23:W:90:TYR:HD1	2.32	0.43
30:0:1165:G:H1'	30:0:1174:A:O2'	2.19	0.43
30:0:1184:C:O2'	30:0:1185:U:OP2	2.33	0.43
30:0:1248:A:H3'	38:0:7547:HOH:O	2.17	0.43
30:0:1477:C:C5'	30:0:1868:G:H5''	2.48	0.43
30:0:1524:U:H5''	30:0:1524:U:H6	1.84	0.43
30:0:1684:A:O2'	30:0:1685:A:H5''	2.18	0.43
30:0:191:A:C4	30:0:237:G:N7	2.87	0.43
30:0:2075:G:C6	30:0:2076:U:C4	3.07	0.43
29:3:28:GLY:HA3	30:0:2435:U:OP1	2.18	0.43
30:0:2664:A:C8	30:0:2664:A:OP1	2.72	0.43
30:0:2812:A:H2	30:0:2814:A:N6	1.86	0.43
13:M:193:LYS:HB3	30:0:392:U:H4'	2.00	0.43
30:0:629:A:C2	30:0:2074:A:C2	3.07	0.43
28:2:40:ARG:HD2	28:2:47:THR:HG22	1.99	0.43
31:9:1:U:C4'	31:9:3:A:OP1	2.67	0.43
31:9:88:G:N2	31:9:89:C:C2	2.87	0.43
5:E:101:GLU:HB2	5:E:116:THR:O	2.18	0.43
11:K:74:VAL:HG13	11:K:113:ILE:HG23	2.01	0.43
18:R:124:GLY:HA3	18:R:136:TRP:O	2.18	0.43
30:0:111:C:H2'	30:0:112:G:O4'	2.18	0.43
30:0:1482:A:O2'	30:0:1483:C:H5'	2.18	0.43
30:0:1545:C:H2'	30:0:1546:G:O4'	2.18	0.43
30:0:1882:C:H2'	30:0:1883:U:C6	2.53	0.43
8:H:46:TYR:HA	8:H:47:PRO:HD3	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:75:PRO:HD3	10:J:136:SER:OG	2.19	0.43
12:L:143:THR:HG21	38:L:8839:HOH:O	2.17	0.43
30:0:1157:C:O2'	30:0:1158:G:H5'	2.18	0.43
30:0:1176:C:N4	38:0:9957:HOH:O	2.52	0.43
30:0:1132:A:H61	30:0:1229:C:H2'	1.83	0.43
30:0:1029:U:O2'	30:0:1273:C:OP1	2.33	0.43
30:0:1815:A:H4'	30:0:2751:C:O4'	2.19	0.43
30:0:1819:G:H2'	30:0:1820:G:H5'	2.01	0.43
30:0:1883:U:H5'	30:0:2012:U:OP2	2.18	0.43
30:0:2096:A:H2'	30:0:2539:U:O4'	2.19	0.43
30:0:212:A:O3'	30:0:213:G:H4'	2.19	0.43
30:0:2255:A:O2'	30:0:2256:G:H5'	2.18	0.43
30:0:2456:A:H2'	30:0:2457:U:C6	2.54	0.43
30:0:2482:G:H4'	30:0:2483:A:C5'	2.48	0.43
11:K:41:LYS:HA	30:0:2582:G:O3'	2.19	0.43
30:0:47:G:N3	30:0:114:A:C2	2.87	0.43
30:0:722:G:H22	30:0:938:G:P	2.42	0.43
5:E:40:VAL:HA	5:E:48:VAL:O	2.19	0.43
6:F:48:VAL:CG2	6:F:74:PHE:HB3	2.48	0.43
13:M:24:GLN:NE2	13:M:27:ARG:NH1	2.67	0.43
25:Y:125:LYS:HB2	25:Y:126:PRO:HD2	2.00	0.43
26:Z:43:GLY:O	26:Z:47:ARG:HG2	2.19	0.43
30:0:1520:G:C6	30:0:1521:C:N4	2.87	0.43
30:0:169:A:H5''	38:0:9693:HOH:O	2.18	0.43
30:0:1787:C:O2'	30:0:1788:U:H5'	2.19	0.43
30:0:2729:C:O2'	30:0:2730:G:H5'	2.19	0.43
30:0:790:A:H2'	30:0:791:A:O4'	2.19	0.43
31:9:2:U:H4'	31:9:2:U:OP2	2.19	0.43
2:B:148:PRO:HD2	38:B:9048:HOH:O	2.19	0.43
6:F:27:GLY:HA3	6:F:101:ALA:O	2.18	0.43
8:H:65:LEU:HD12	8:H:65:LEU:HA	1.84	0.43
6:F:57:GLU:HB2	13:M:23:LEU:HD11	1.99	0.43
14:N:116:PHE:HB3	14:N:136:LEU:HD23	2.00	0.43
14:N:11:ARG:NH1	31:9:8:G:O6	2.52	0.43
14:N:164:ASP:OD2	14:N:168:LEU:HG	2.19	0.43
21:U:17:THR:CG2	21:U:18:GLY:N	2.82	0.43
30:0:1044:C:H5''	38:0:9030:HOH:O	2.18	0.42
30:0:1315:G:H4'	30:0:1316:G:OP2	2.19	0.42
30:0:1521:C:H2'	30:0:1522:A:H8	1.84	0.42
30:0:162:C:H2'	30:0:163:U:H5'	2.01	0.42
30:0:1706:G:C5	30:0:1707:G:C6	3.06	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1894:C:N4	30:0:1939:U:H2'	2.33	0.42
30:0:2026:C:O2'	30:0:2027:U:H5'	2.19	0.42
30:0:2756:U:H1'	38:0:5024:HOH:O	2.19	0.42
30:0:2866:U:H4'	30:0:2867:G:H5'	2.01	0.42
30:0:1787:C:C4'	30:0:2883:A:O4'	2.67	0.42
30:0:365:G:C6	30:0:366:U:C4	3.07	0.42
30:0:85:C:H3'	30:0:86:A:H2'	2.01	0.42
31:9:14:G:O2'	31:9:15:C:H5'	2.19	0.42
1:A:6:GLY:HA3	38:0:4633:HOH:O	2.19	0.42
18:R:82:GLU:O	18:R:86:LYS:HG3	2.19	0.42
30:0:1189:A:H1'	30:0:1209:C:H1'	2.01	0.42
30:0:1741:U:C4	30:0:2033:G:C8	3.06	0.42
30:0:1976:G:O2'	30:0:1977:U:H5'	2.19	0.42
30:0:2783:A:H5''	38:0:5252:HOH:O	2.19	0.42
30:0:366:U:H2'	30:0:367:G:O4'	2.19	0.42
30:0:907:A:H2'	30:0:908:A:C8	2.53	0.42
2:B:112:THR:HG23	2:B:158:LYS:HZ1	1.84	0.42
2:B:232:TRP:HD1	2:B:235:ARG:HD2	1.83	0.42
3:C:107:ARG:O	3:C:111:VAL:HG23	2.19	0.42
7:G:12:ILE:N	7:G:13:PRO:HD3	2.35	0.42
19:S:10:VAL:HG11	22:V:36:ALA:HA	2.00	0.42
30:0:1381:A:N3	30:0:1382:G:H1'	2.34	0.42
30:0:1603:A:C8	30:0:1605:G:C2	3.07	0.42
30:0:255:A:H2'	30:0:256:C:C6	2.54	0.42
30:0:844:A:C6	30:0:882:A:C6	3.07	0.42
29:3:71:CYS:SG	38:3:9052:HOH:O	2.61	0.42
4:D:76:ARG:NH1	31:9:42:C:O2	2.49	0.42
3:C:22:PHE:HA	3:C:116:ALA:HA	2.00	0.42
4:D:104:PHE:CE2	4:D:132:VAL:HB	2.54	0.42
5:E:68:HIS:CE1	38:0:6506:HOH:O	2.72	0.42
10:J:74:ARG:O	10:J:78:ILE:HG13	2.19	0.42
14:N:108:SER:HA	14:N:109:PRO:HD3	1.82	0.42
15:O:65:LEU:HD13	30:0:746:A:C6	2.54	0.42
26:Z:84:CYS:O	26:Z:85:ASP:HB2	2.19	0.42
30:0:1681:G:H4'	30:0:1682:A:N3	2.34	0.42
30:0:2244:A:C4	30:0:2258:A:C2	3.08	0.42
30:0:2414:A:N1	30:0:2415:A:C6	2.87	0.42
8:H:158:ASN:ND2	30:0:2502:C:H4'	2.35	0.42
30:0:2506:A:O2'	30:0:2507:G:P	2.78	0.42
30:0:26:U:H3'	38:0:5910:HOH:O	2.18	0.42
30:0:2780:C:C4	30:0:2781:U:C4	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:29:LYS:HE2	30:0:524:A:H5'	2.01	0.42
30:0:590:A:H2'	30:0:591:A:H5'	2.01	0.42
1:A:97:ALA:HA	1:A:131:HIS:NE2	2.33	0.42
2:B:51:VAL:HG23	2:B:329:TYR:O	2.20	0.42
4:D:156:ARG:NH1	38:D:5234:HOH:O	2.51	0.42
8:H:157:TYR:C	8:H:157:TYR:CD1	2.93	0.42
4:D:146:LYS:NZ	14:N:107:ASN:ND2	2.67	0.42
14:N:73:ALA:HB1	14:N:74:PRO:CD	2.49	0.42
16:P:143:ALA:HA	38:P:5521:HOH:O	2.18	0.42
17:Q:94:GLN:O	17:Q:95:GLU:HB2	2.19	0.42
18:R:98:ASN:HD21	30:0:500:G:H21	1.66	0.42
20:T:64:ASN:HB3	20:T:73:HIS:HB2	2.01	0.42
30:0:1964:U:O2	30:0:1964:U:H2'	2.18	0.42
30:0:255:A:C5	30:0:256:C:C4	3.08	0.42
30:0:2708:G:H2'	30:0:2709:G:O4'	2.19	0.42
30:0:2727:A:C5	30:0:2756:U:C4	3.07	0.42
30:0:583:C:H2'	30:0:584:U:H6	1.85	0.42
30:0:858:U:H2'	30:0:859:C:H6	1.84	0.42
31:9:1:U:O3'	31:9:3:A:OP1	2.37	0.42
31:9:74:G:C6	31:9:75:G:N7	2.87	0.42
1:A:53:ALA:HB3	38:A:9061:HOH:O	2.18	0.42
3:C:193:LEU:HA	3:C:211:ASP:O	2.20	0.42
5:E:162:PHE:CD1	5:E:162:PHE:N	2.88	0.42
11:K:14:LYS:CB	11:K:45:PRO:HG2	2.43	0.42
13:M:164:THR:CG2	13:M:165:GLY:N	2.82	0.42
14:N:37:ARG:HH11	31:9:6:C:C5'	2.28	0.42
23:W:115:THR:HG23	38:W:5420:HOH:O	2.18	0.42
30:0:1748:U:C5	30:0:1749:U:C5	3.08	0.42
30:0:1791:U:O2'	30:0:1792:C:H5'	2.20	0.42
30:0:445:U:O2'	30:0:446:G:H5'	2.19	0.42
30:0:595:U:O2'	30:0:596:C:H5'	2.20	0.42
30:0:960:G:C8	38:0:5997:HOH:O	2.57	0.42
29:3:91:GLN:O	29:3:92:GLU:HB2	2.19	0.42
31:9:106:U:O2'	31:9:107:C:H5'	2.20	0.42
4:D:137:PRO:O	31:9:30:C:OP1	2.37	0.42
13:M:187:LEU:CD2	13:M:194:GLY:HA3	2.49	0.42
17:Q:19:ARG:HH22	31:9:11:A:H3'	1.84	0.42
21:U:50:GLU:HB2	30:0:2866:U:C5	2.55	0.42
22:V:12:THR:HG23	22:V:14:ALA:H	1.85	0.42
30:0:1063:G:H8	38:0:9865:HOH:O	2.02	0.42
30:0:1185:U:C5'	38:0:7505:HOH:O	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1555:G:H4'	30:0:1630:A:H2	1.85	0.42
30:0:1878:G:H5'	38:0:4379:HOH:O	2.19	0.42
30:0:2450:C:C2'	30:0:2451:G:O5'	2.67	0.42
30:0:2637:A:C5'	38:0:9282:HOH:O	2.57	0.42
30:0:699:C:H2'	30:0:744:G:N3	2.34	0.42
30:0:800:G:H2'	30:0:801:U:C6	2.55	0.42
2:B:217:ARG:CD	2:B:257:THR:HG22	2.50	0.42
2:B:55:ASN:HB3	2:B:63:GLU:HA	2.00	0.42
4:D:151:ILE:HB	4:D:156:ARG:HE	1.85	0.42
4:D:23:VAL:CG2	4:D:73:VAL:HB	2.50	0.42
4:D:40:ILE:HG23	38:D:5583:HOH:O	2.20	0.42
4:D:27:ILE:HB	4:D:69:ILE:O	2.20	0.42
20:T:32:ARG:NH1	20:T:38:ARG:HH12	2.18	0.42
30:0:1119:G:N2	30:0:1246:A:H2	2.10	0.42
16:P:41:ARG:NH2	30:0:1500:U:OP2	2.51	0.42
30:0:1878:G:O2'	30:0:1879:U:OP2	2.37	0.42
30:0:2135:A:O4'	30:0:2243:C:N4	2.53	0.42
30:0:336:G:H5'	38:0:7404:HOH:O	2.20	0.42
30:0:907:A:H2'	30:0:908:A:H8	1.85	0.42
31:9:3:A:H2	31:9:21:G:N3	2.18	0.42
1:A:153:ARG:CB	1:A:153:ARG:HH11	2.28	0.42
1:A:217:ARG:CG	1:A:217:ARG:HH11	2.32	0.42
6:F:107:ASP:O	6:F:111:ILE:HG13	2.19	0.42
7:G:63:ARG:N	38:G:2569:HOH:O	2.53	0.42
8:H:31:ILE:HG23	38:H:232:HOH:O	2.19	0.42
13:M:171:ARG:NH2	30:0:189:A:OP1	2.52	0.42
14:N:33:ARG:NH1	14:N:103:ASP:OD2	2.51	0.42
17:Q:55:ARG:HD2	38:Q:2875:HOH:O	2.19	0.42
25:Y:134:HIS:HE1	30:0:538:C:OP2	2.02	0.42
30:0:939:A:H2	30:0:1027:G:N3	2.16	0.42
30:0:1167:G:O2'	30:0:1168:C:H5'	2.20	0.42
30:0:1178:G:C6	30:0:1179:C:N4	2.87	0.42
30:0:1343:C:H2'	30:0:1344:G:O5'	2.20	0.42
30:0:1477:C:H5'	30:0:1868:G:H5''	1.99	0.42
30:0:1515:A:H2'	30:0:1516:U:H6	1.83	0.42
30:0:1762:C:H2'	30:0:1763:C:H6	1.84	0.42
30:0:2007:A:N3	30:0:2627:G:O2'	2.48	0.42
30:0:2113:G:C6	30:0:2114:C:C4	3.08	0.42
30:0:807:A:C6	30:0:808:A:C6	3.07	0.42
30:0:907:A:H4'	30:0:1328:A:C2	2.54	0.42
30:0:947:U:O2'	30:0:948:G:H5'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:1:8:GLN:HE22	27:1:11:LYS:HZ2	1.68	0.42
13:M:61:ILE:HG22	13:M:62:VAL:N	2.35	0.42
14:N:171:HIS:CE1	38:N:8858:HOH:O	2.71	0.42
21:U:33:SER:O	21:U:37:GLU:HG3	2.18	0.42
30:0:1433:G:O2'	30:0:1434:A:H5'	2.20	0.42
30:0:1992:U:H2'	30:0:1994:A:OP2	2.19	0.42
30:0:2765:C:H2'	30:0:2766:A:C8	2.54	0.42
30:0:382:U:O2'	30:0:430:A:H1'	2.19	0.42
30:0:470:U:H2'	30:0:471:G:O4'	2.20	0.42
30:0:536:A:H4'	38:0:5552:HOH:O	2.18	0.42
30:0:920:C:H5'	30:0:921:G:C4	2.55	0.42
27:1:12:ASN:O	30:0:1415:G:H5'	2.19	0.42
31:9:26:C:H2'	31:9:27:C:C6	2.55	0.42
3:C:129:HIS:HD2	3:C:165:ASP:OD2	2.03	0.42
4:D:88:LEU:N	4:D:89:PRO:CD	2.83	0.42
5:E:95:VAL:HG11	5:E:131:LEU:HD11	2.02	0.42
8:H:123:ILE:HD12	8:H:123:ILE:N	2.35	0.42
18:R:17:MET:HE3	18:R:19:ARG:NH2	2.35	0.42
8:H:99:ARG:NH1	30:0:1055:G:OP2	2.53	0.41
30:0:1950:G:H2'	30:0:1951:G:C8	2.55	0.41
30:0:2112:A:H2'	30:0:2113:G:H8	1.85	0.41
30:0:213:G:O2'	30:0:214:U:OP2	2.38	0.41
30:0:2502:C:O2'	30:0:2503:A:H5'	2.17	0.41
2:B:27:ASN:HD21	30:0:2807:U:P	2.43	0.41
30:0:152:A:H1'	30:0:440:C:O2'	2.21	0.41
1:A:72:GLU:HG3	26:Z:90:GLY:HA2	2.01	0.41
1:A:94:LEU:HG	1:A:99:ILE:CD1	2.50	0.41
2:B:162:MET:HG3	2:B:310:ARG:NH1	2.35	0.41
3:C:8:LEU:HD13	3:C:147:LEU:HD21	2.01	0.41
4:D:146:LYS:NZ	14:N:107:ASN:HD21	2.18	0.41
4:D:51:ARG:HH11	4:D:68:PRO:HB3	1.84	0.41
6:F:118:LEU:O	6:F:119:ARG:HB3	2.20	0.41
6:F:14:ASP:O	6:F:18:GLU:HG3	2.20	0.41
11:K:78:LYS:HA	11:K:79:PRO:HD3	1.94	0.41
12:L:57:VAL:HG21	30:0:2443:C:H5'	2.02	0.41
13:M:58:GLN:NE2	30:0:259:G:H21	2.17	0.41
14:N:26:LEU:HA	14:N:26:LEU:HD12	1.93	0.41
30:0:1409:G:H5'	38:0:3732:HOH:O	2.20	0.41
30:0:1414:A:H2	38:0:4921:HOH:O	2.03	0.41
30:0:1524:U:C5'	30:0:1524:U:H6	2.33	0.41
30:0:158:A:H2'	30:0:159:G:H5'	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1667:A:C2	30:0:1668:U:C2	3.07	0.41
30:0:1871:U:O4'	30:0:1873:G:C8	2.73	0.41
30:0:1883:U:H2'	30:0:1884:G:H5'	2.02	0.41
30:0:1890:U:H4'	30:0:2010:A:C6	2.55	0.41
30:0:2245:C:H6	30:0:2245:C:O5'	2.02	0.41
30:0:526:U:H2'	30:0:527:U:C6	2.55	0.41
30:0:51:G:O2'	30:0:52:A:H5'	2.20	0.41
30:0:539:G:H2'	30:0:540:A:C8	2.55	0.41
25:Y:144:ARG:NH1	30:0:905:C:OP1	2.54	0.41
30:0:969:G:H1	30:0:999:C:N4	2.18	0.41
31:9:24:U:H3'	31:9:25:G:C5'	2.51	0.41
2:B:88:GLU:HB3	2:B:97:LEU:HG	2.01	0.41
3:C:118:THR:HG22	3:C:137:PRO:HB3	2.00	0.41
3:C:61:PHE:HB3	38:C:8643:HOH:O	2.20	0.41
6:F:58:GLU:HA	6:F:61:MET:HG3	2.01	0.41
10:J:45:VAL:HG11	10:J:121:LEU:HD22	2.02	0.41
10:J:39:VAL:HG12	10:J:40:ASN:ND2	2.35	0.41
12:L:57:VAL:O	12:L:57:VAL:HG12	2.20	0.41
12:L:67:ARG:O	12:L:71:GLU:HG3	2.20	0.41
13:M:46:LEU:HG	38:M:8913:HOH:O	2.20	0.41
13:M:49:ALA:C	13:M:54:TYR:HB3	2.40	0.41
18:R:9:ASP:HA	18:R:10:PRO:HD2	1.91	0.41
23:W:11:VAL:O	23:W:12:ASN:HB2	2.19	0.41
30:0:1015:C:O5'	30:0:1015:C:H6	2.02	0.41
30:0:1119:G:C5	30:0:1243:C:C4	3.08	0.41
30:0:2330:U:H4'	30:0:2331:C:OP1	2.20	0.41
30:0:2344:G:N7	38:0:4937:HOH:O	2.49	0.41
30:0:2379:G:N7	30:0:2408:A:N1	2.67	0.41
30:0:2500:C:H1'	38:0:4674:HOH:O	2.20	0.41
30:0:2506:A:O2'	30:0:2507:G:O5'	2.38	0.41
30:0:2508:C:H2'	38:0:6793:HOH:O	2.19	0.41
30:0:2598:U:O2	30:0:2600:A:H8	2.03	0.41
30:0:372:A:H2'	30:0:373:G:C8	2.55	0.41
30:0:708:A:H2'	30:0:709:G:O4'	2.20	0.41
5:E:95:VAL:O	5:E:126:ILE:HD12	2.20	0.41
8:H:66:GLU:HA	38:H:232:HOH:O	2.19	0.41
12:L:125:PHE:CE1	12:L:140:VAL:HG13	2.55	0.41
13:M:24:GLN:HE22	13:M:27:ARG:HH11	1.67	0.41
18:R:59:PHE:O	18:R:63:ASN:HB3	2.20	0.41
20:T:21:LYS:HA	20:T:24:ARG:HG3	2.03	0.41
25:Y:151:SER:HB3	25:Y:154:ARG:CB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:189:ASN:HD22	25:Y:189:ASN:C	2.23	0.41
25:Y:212:ARG:HB2	30:0:1315:G:C4	2.55	0.41
30:0:1058:A:H2'	30:0:1060:C:C5'	2.48	0.41
30:0:1213:C:O2'	30:0:1214:G:H5'	2.21	0.41
30:0:1427:A:O2'	30:0:1428:C:H5'	2.20	0.41
30:0:2011:A:H4'	30:0:2012:U:O5'	2.20	0.41
30:0:2237:G:H1'	38:0:4871:HOH:O	2.20	0.41
30:0:2269:C:H2'	30:0:2270:G:C5'	2.50	0.41
30:0:2375:A:H2'	30:0:2376:C:C6	2.56	0.41
30:0:2512:U:H4'	30:0:2514:U:O4	2.20	0.41
30:0:2791:U:H4'	30:0:2792:A:OP1	2.20	0.41
30:0:393:G:C6	30:0:394:G:C6	3.08	0.41
30:0:485:A:O2'	30:0:487:G:H5'	2.19	0.41
30:0:735:C:C5	30:0:736:A:N3	2.89	0.41
2:B:24:PRO:CG	2:B:204:GLY:HA2	2.50	0.41
11:K:34:VAL:HB	38:K:7169:HOH:O	2.20	0.41
11:K:41:LYS:O	11:K:42:ASN:HB2	2.20	0.41
30:0:1132:A:H2'	30:0:1133:A:C8	2.56	0.41
30:0:1388:U:H2'	30:0:1389:G:O4'	2.20	0.41
30:0:1488:U:H4'	30:0:1489:G:OP1	2.21	0.41
30:0:1522:A:C2	30:0:1665:G:C6	3.09	0.41
30:0:1603:A:C5'	30:0:1605:G:O4'	2.53	0.41
30:0:1748:U:C4	30:0:1749:U:C4	3.09	0.41
30:0:1883:U:O2'	30:0:1884:G:H5'	2.20	0.41
30:0:1976:G:H1'	30:0:2005:G:N2	2.36	0.41
30:0:2067:A:H2'	30:0:2068:G:O4'	2.20	0.41
30:0:284:C:OP2	30:0:284:C:C6	2.73	0.41
30:0:491:C:O2'	30:0:492:C:H5'	2.21	0.41
30:0:699:C:C6	30:0:744:G:O4'	2.73	0.41
31:9:73:A:N1	31:9:108:C:O2	2.54	0.41
1:A:125:ASN:HB3	1:A:158:VAL:HG12	2.02	0.41
2:B:51:VAL:CG2	2:B:327:VAL:HG13	2.50	0.41
2:B:74:ILE:HG13	38:B:9075:HOH:O	2.20	0.41
4:D:96:SER:C	4:D:98:PHE:H	2.24	0.41
13:M:133:LEU:O	13:M:134:ILE:HD13	2.21	0.41
23:W:108:ARG:HE	23:W:114:PRO:HG3	1.85	0.41
25:Y:182:PHE:HD2	25:Y:200:THR:O	2.03	0.41
30:0:1319:G:H1'	38:0:4701:HOH:O	2.19	0.41
30:0:1761:U:H2'	30:0:1762:C:C6	2.55	0.41
30:0:1926:G:H2'	30:0:1927:A:H8	1.84	0.41
30:0:240:C:O2	30:0:240:C:H2'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2478:U:H2'	30:0:2479:A:C8	2.55	0.41
30:0:259:G:O2'	30:0:260:C:H5'	2.20	0.41
30:0:284:C:H4'	30:0:285:A:H8	1.85	0.41
30:0:300:U:N3	30:0:301:C:C5	2.88	0.41
30:0:523:C:H2'	30:0:524:A:C8	2.56	0.41
29:3:30:GLN:NE2	38:3:9046:HOH:O	2.51	0.41
31:9:2:U:C4'	38:9:9103:HOH:O	2.67	0.41
2:B:7:ARG:CG	2:B:7:ARG:HH11	2.31	0.41
3:C:140:VAL:HG12	3:C:141:SER:N	2.35	0.41
3:C:184:ARG:HD2	30:0:1306:U:H5''	2.01	0.41
9:I:91:PHE:HD2	9:I:131:GLY:HA2	1.85	0.41
12:L:117:GLU:HG2	38:L:8860:HOH:O	2.20	0.41
13:M:139:PRO:HA	13:M:142:GLN:HB2	2.03	0.41
25:Y:216:ARG:NH1	38:Y:8834:HOH:O	2.53	0.41
30:0:1206:U:C3'	30:0:1206:U:C6	3.04	0.41
30:0:1417:G:N3	30:0:1417:G:H2'	2.35	0.41
30:0:1523:G:C6	30:0:1524:U:C4	3.09	0.41
30:0:1662:C:H2'	30:0:1663:G:O4'	2.21	0.41
30:0:2421:G:H3'	30:0:2422:U:H5''	2.02	0.41
30:0:2597:U:C2'	30:0:2598:U:H5'	2.50	0.41
5:E:111:LYS:HE3	30:0:2690:U:H4'	2.02	0.41
30:0:2878:U:OP1	30:0:2878:U:H6	2.03	0.41
30:0:64:G:H2'	30:0:65:C:O4'	2.21	0.41
30:0:853:C:H2'	30:0:854:G:O4'	2.21	0.41
31:9:5:G:C2'	31:9:6:C:H5'	2.50	0.41
2:B:137:LEU:HD21	2:B:140:LEU:HD21	2.03	0.41
4:D:154:LYS:H	4:D:154:LYS:CD	2.09	0.41
10:J:127:ILE:O	10:J:127:ILE:HG12	2.21	0.41
10:J:47:THR:O	10:J:53:ILE:HD11	2.21	0.41
24:X:78:GLU:HG2	24:X:79:GLU:H	1.86	0.41
30:0:123:U:H5'	38:0:6689:HOH:O	2.20	0.41
30:0:1265:G:H1'	38:0:5020:HOH:O	2.21	0.41
30:0:1576:G:H2'	30:0:1577:U:O4'	2.21	0.41
30:0:1762:C:H2'	30:0:1763:C:C6	2.56	0.41
30:0:2090:G:H2'	30:0:2091:G:C8	2.55	0.41
30:0:466:A:C2	30:0:476:A:C4	3.09	0.41
30:0:541:C:H2'	30:0:542:A:H5'	1.95	0.41
30:0:60:A:C2	30:0:61:G:C8	3.09	0.41
30:0:862:U:H2'	30:0:863:G:C8	2.56	0.41
1:A:212:PRO:HB2	38:0:4373:HOH:O	2.20	0.41
3:C:84:VAL:HG12	3:C:85:LYS:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:91:PHE:HA	5:E:92:PRO:HD3	1.87	0.41
6:F:91:VAL:CG1	6:F:92:GLY:N	2.78	0.41
9:I:108:HIS:N	9:I:109:PRO:HD2	2.35	0.41
9:I:114:TYR:HE1	30:0:1186:C:H4'	1.85	0.41
17:Q:66:LYS:HB2	17:Q:70:ALA:O	2.21	0.41
23:W:59:GLN:NE2	23:W:97:ALA:HB3	2.36	0.41
26:Z:35:SER:HB3	26:Z:47:ARG:HB2	2.03	0.41
26:Z:70:ARG:CD	26:Z:83:TYR:HB2	2.36	0.41
30:0:1589:G:H22	30:0:1605:G:H1'	1.85	0.41
30:0:2063:U:O4	30:0:2083:A:H2	2.03	0.41
30:0:711:G:N2	30:0:718:C:C2	2.89	0.41
28:2:5:LYS:O	28:2:9:LYS:HG3	2.21	0.41
29:3:3:MET:HG3	29:3:4:PRO:HD2	2.03	0.41
2:B:195:ARG:HG2	2:B:323:LEU:HD22	2.03	0.41
5:E:132:THR:HB	38:E:2227:HOH:O	2.21	0.41
10:J:75:PRO:HB3	10:J:132:LEU:HB3	2.02	0.41
12:L:11:ARG:O	30:0:903:U:C2	2.73	0.41
13:M:65:VAL:HG21	13:M:105:ALA:HB2	2.03	0.41
22:V:12:THR:HB	22:V:15:GLU:OE2	2.20	0.41
23:W:11:VAL:HG11	30:0:1086:A:C6	2.56	0.41
30:0:1250:C:O2'	30:0:1251:C:H5'	2.20	0.41
30:0:1486:A:H4'	30:0:1487:A:OP2	2.20	0.41
30:0:1592:G:O2'	30:0:1593:C:O4'	2.32	0.41
30:0:1632:A:C3'	30:0:1633:C:H5'	2.51	0.41
30:0:1878:G:C4'	38:0:6151:HOH:O	2.69	0.41
30:0:2511:A:H4'	38:0:5487:HOH:O	2.21	0.41
30:0:2543:G:H2'	30:0:2544:G:O4'	2.21	0.41
2:B:307:ARG:HG3	30:0:2837:U:O2	2.21	0.41
20:T:2:LYS:HG2	30:0:447:A:OP1	2.21	0.41
1:A:211:LYS:HB3	1:A:212:PRO:CD	2.49	0.41
2:B:150:ALA:O	2:B:152:PRO:HD3	2.21	0.41
10:J:132:LEU:HA	10:J:132:LEU:HD23	1.92	0.41
13:M:61:ILE:N	13:M:61:ILE:HD12	2.36	0.41
19:S:57:THR:HG22	19:S:58:MET:N	2.35	0.41
21:U:44:ARG:HB3	38:U:3805:HOH:O	2.21	0.41
23:W:122:ARG:HH11	23:W:122:ARG:HG3	1.85	0.41
23:W:61:THR:HG23	23:W:151:GLU:HG3	2.03	0.41
30:0:1119:G:N2	30:0:1246:A:N1	2.68	0.41
30:0:1167:G:H1	30:0:1179:C:H42	1.69	0.41
30:0:1525:G:OP1	30:0:1525:G:H4'	2.21	0.41
30:0:1771:U:O2'	30:0:1773:G:N7	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2088:C:H1'	30:0:2841:A:C2	2.56	0.41
12:L:32:ASP:HB3	30:0:222:A:H5''	2.03	0.41
30:0:2318:C:H2'	30:0:2319:C:H6	1.86	0.41
30:0:2361:A:H2'	30:0:2362:A:C8	2.55	0.41
30:0:2680:A:O2'	30:0:2681:A:C4	2.72	0.41
30:0:2712:G:H5'	38:0:5241:HOH:O	2.19	0.41
30:0:2824:C:H5''	30:0:2825:C:H5'	2.02	0.41
30:0:2887:G:H2'	30:0:2888:U:O4'	2.20	0.41
31:9:76:G:O5'	31:9:76:G:H8	2.04	0.41
31:9:93:A:H8	31:9:93:A:O5'	2.04	0.41
1:A:233:THR:HB	30:0:1942:A:H5''	2.03	0.41
1:A:48:ASP:HA	1:A:49:PRO:HD3	1.89	0.41
12:L:145:LEU:O	12:L:148:GLU:HG3	2.21	0.41
14:N:154:LEU:O	14:N:155:GLU:HB3	2.21	0.41
17:Q:34:ASP:O	17:Q:37:GLU:HB2	2.21	0.41
18:R:33:ARG:NH2	38:R:8935:HOH:O	2.54	0.41
30:0:1265:G:C5	30:0:1266:U:C5	3.09	0.40
30:0:1635:U:O2'	30:0:1636:G:H5'	2.19	0.40
30:0:2531:U:O2'	30:0:2532:A:H5'	2.21	0.40
30:0:371:U:H2'	30:0:372:A:H8	1.85	0.40
30:0:488:U:H2'	38:0:4016:HOH:O	2.21	0.40
30:0:613:C:C2	30:0:614:U:C5	3.09	0.40
30:0:932:U:O2'	30:0:1296:A:H1'	2.21	0.40
27:1:21:ARG:HD2	27:1:39:PHE:HB2	2.03	0.40
28:2:11:LEU:HA	28:2:11:LEU:HD23	1.91	0.40
3:C:80:VAL:HA	3:C:81:PRO:HD3	1.88	0.40
13:M:138:HIS:O	13:M:142:GLN:HG3	2.21	0.40
14:N:34:LEU:HD22	14:N:129:ILE:HD13	2.02	0.40
17:Q:64:GLU:HG3	17:Q:74:ASP:OD2	2.21	0.40
22:V:42:ASN:O	22:V:44:GLY:N	2.55	0.40
30:0:1252:A:H2'	30:0:1253:C:O4'	2.21	0.40
30:0:634:G:O2'	30:0:1358:A:OP1	2.36	0.40
30:0:1413:A:H2'	30:0:1414:A:O4'	2.20	0.40
30:0:1505:U:H4'	38:0:5200:HOH:O	2.22	0.40
30:0:154:C:H2'	30:0:155:C:H6	1.86	0.40
30:0:1573:A:H2'	30:0:1574:C:O4'	2.21	0.40
30:0:1632:A:H2'	30:0:1633:C:C5'	2.46	0.40
30:0:2010:A:C2'	38:0:5984:HOH:O	2.51	0.40
30:0:2119:C:O2'	30:0:2120:U:H5'	2.22	0.40
30:0:2348:C:O2'	30:0:2349:G:H5'	2.21	0.40
30:0:1838:U:O2'	30:0:2644:C:H5'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2716:G:H1'	38:0:3037:HOH:O	2.21	0.40
30:0:625:U:H5'	38:0:3194:HOH:O	2.20	0.40
14:N:1:ALA:HB2	31:9:14:G:O2'	2.21	0.40
3:C:124:VAL:HA	3:C:230:GLY:O	2.21	0.40
8:H:100:GLU:HG2	8:H:102:LYS:HB3	2.03	0.40
13:M:164:THR:HG22	13:M:166:ALA:N	2.36	0.40
25:Y:219:GLU:HG3	25:Y:220:GLU:N	2.36	0.40
30:0:1202:A:C2'	30:0:1203:G:H5'	2.52	0.40
30:0:1511:U:O2'	30:0:1512:G:H5'	2.22	0.40
30:0:2467:A:H3'	38:0:5475:HOH:O	2.22	0.40
30:0:2765:C:H2'	30:0:2766:A:H8	1.86	0.40
3:C:43:LYS:HG2	30:0:449:A:N7	2.36	0.40
30:0:613:C:H2'	30:0:614:U:C6	2.49	0.40
30:0:622:G:O2'	30:0:623:U:H5'	2.21	0.40
27:1:25:LYS:HD2	28:2:48:ASP:HA	2.03	0.40
31:9:47:A:C2	31:9:48:C:C2	3.09	0.40
2:B:16:ARG:NH2	38:B:9021:HOH:O	2.49	0.40
5:E:1:PRO:HG2	5:E:59:MET:SD	2.61	0.40
13:M:176:LYS:HB3	13:M:176:LYS:HE2	1.95	0.40
18:R:132:ARG:HG2	18:R:133:ALA:N	2.36	0.40
21:U:20:MET:CG	21:U:28:THR:HG23	2.51	0.40
23:W:22:GLU:HG2	23:W:27:HIS:CD2	2.56	0.40
25:Y:182:PHE:CG	25:Y:202:ALA:HB2	2.57	0.40
16:P:2:ASP:OD1	30:0:1396:C:H4'	2.21	0.40
30:0:1565:C:H2'	30:0:1566:C:H6	1.86	0.40
30:0:1576:G:H2'	30:0:1577:U:C6	2.56	0.40
30:0:1588:G:C5	30:0:1589:G:C6	3.09	0.40
30:0:1603:A:C5'	30:0:1605:G:C5'	2.98	0.40
16:P:81:LYS:HB3	30:0:1707:G:O3'	2.21	0.40
30:0:1915:U:O2'	30:0:1916:C:H5'	2.22	0.40
30:0:1996:U:O2'	30:0:1997:A:H5'	2.21	0.40
30:0:222:A:H2'	30:0:223:G:O4'	2.21	0.40
8:H:6:ALA:HB3	30:0:2521:A:P	2.61	0.40
30:0:2598:U:O2	30:0:2600:A:C8	2.74	0.40
30:0:37:A:H2'	30:0:38:G:C8	2.57	0.40
30:0:596:C:H2'	30:0:597:A:C8	2.56	0.40
30:0:645:U:H2'	30:0:646:G:C8	2.56	0.40
2:B:141:ARG:N	38:B:9047:HOH:O	2.54	0.40
4:D:151:ILE:HA	4:D:152:PRO:HD3	1.95	0.40
5:E:116:THR:CG2	5:E:151:LEU:HD22	2.43	0.40
17:Q:16:ASN:HD22	17:Q:16:ASN:HA	1.71	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:97:ARG:NH2	30:0:309:C:OP1	2.54	0.40
30:0:1188:A:C6	30:0:1189:A:C6	3.09	0.40
26:Z:70:ARG:NH2	30:0:1602:C:OP2	2.53	0.40
8:H:74:ARG:NH1	30:0:2504:A:H4'	2.36	0.40
30:0:535:G:C5	30:0:2063:U:C4	3.09	0.40
14:N:44:ARG:NH1	31:9:4:G:H21	2.20	0.40
3:C:135:GLU:HB3	38:C:8576:HOH:O	2.22	0.40
6:F:59:ILE:CD1	30:0:263:U:C2	3.04	0.40
8:H:155:ARG:NE	38:H:198:HOH:O	2.54	0.40
11:K:64:MET:HA	11:K:67:GLN:HE21	1.87	0.40
20:T:16:LEU:HB2	30:0:100:C:H4'	2.03	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	
1	A	235/240 (98%)	213 (91%)	18 (8%)	4 (2%)	11	36
2	B	335/338 (99%)	309 (92%)	22 (7%)	4 (1%)	15	46
3	C	244/246 (99%)	222 (91%)	22 (9%)	0	100	100
4	D	134/177 (76%)	107 (80%)	22 (16%)	5 (4%)	4	16
5	E	170/178 (96%)	156 (92%)	14 (8%)	0	100	100
6	F	117/120 (98%)	104 (89%)	9 (8%)	4 (3%)	4	18
7	G	25/348 (7%)	23 (92%)	2 (8%)	0	100	100
8	H	156/177 (88%)	145 (93%)	11 (7%)	0	100	100
9	I	68/162 (42%)	54 (79%)	13 (19%)	1 (2%)	12	39
10	J	140/145 (97%)	132 (94%)	8 (6%)	0	100	100
11	K	130/132 (98%)	124 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	L	141/165 (86%)	124 (88%)	14 (10%)	3 (2%)	8	30
13	M	192/196 (98%)	182 (95%)	10 (5%)	0	100	100
14	N	184/187 (98%)	169 (92%)	11 (6%)	4 (2%)	8	29
15	O	113/116 (97%)	108 (96%)	5 (4%)	0	100	100
16	P	141/149 (95%)	138 (98%)	3 (2%)	0	100	100
17	Q	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
18	R	148/155 (96%)	137 (93%)	11 (7%)	0	100	100
19	S	79/85 (93%)	72 (91%)	7 (9%)	0	100	100
20	T	117/120 (98%)	107 (92%)	9 (8%)	1 (1%)	20	54
21	U	51/67 (76%)	48 (94%)	3 (6%)	0	100	100
22	V	63/71 (89%)	58 (92%)	3 (5%)	2 (3%)	5	19
23	W	152/154 (99%)	145 (95%)	6 (4%)	1 (1%)	25	60
24	X	80/92 (87%)	71 (89%)	8 (10%)	1 (1%)	14	43
25	Y	140/241 (58%)	140 (100%)	0	0	100	100
26	Z	71/116 (61%)	62 (87%)	8 (11%)	1 (1%)	13	41
27	1	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
28	2	42/50 (84%)	37 (88%)	5 (12%)	0	100	100
29	3	90/92 (98%)	89 (99%)	1 (1%)	0	100	100
All	All	3705/4472 (83%)	3416 (92%)	258 (7%)	31 (1%)	22	57

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	36	ASP
1	A	37	VAL
6	F	101	ALA
14	N	154	LEU
14	N	183	ASP
14	N	184	ILE
1	A	34	ASP
4	D	27	ILE
6	F	44	SER
24	X	70	ILE
4	D	97	GLN
12	L	149	ARG

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Mol	Chain	Res	Type
14	N	139	TRP
26	Z	44	ARG
2	B	2	GLN
2	B	184	ASP
4	D	56	ARG
6	F	100	ASP
12	L	80	ASP
22	V	43	PRO
6	F	61	MET
9	I	83	GLY
20	T	53	GLY
23	W	49	ASN
12	L	82	ALA
2	B	34	GLY
2	B	169	GLY
4	D	28	GLY
4	D	137	PRO
22	V	40	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	179/182 (98%)	171 (96%)	8 (4%)	32	66
2	B	282/283 (100%)	268 (95%)	14 (5%)	28	62
3	C	193/193 (100%)	180 (93%)	13 (7%)	19	48
4	D	117/148 (79%)	113 (97%)	4 (3%)	42	76
5	E	152/156 (97%)	148 (97%)	4 (3%)	51	83
6	F	93/94 (99%)	91 (98%)	2 (2%)	57	86
7	G	27/282 (10%)	26 (96%)	1 (4%)	39	74
8	H	134/145 (92%)	128 (96%)	6 (4%)	32	66
9	I	58/130 (45%)	56 (97%)	2 (3%)	42	76
10	J	118/121 (98%)	110 (93%)	8 (7%)	18	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	106/106 (100%)	103 (97%)	3 (3%)	49	82
12	L	113/127 (89%)	108 (96%)	5 (4%)	33	67
13	M	158/160 (99%)	151 (96%)	7 (4%)	33	67
14	N	149/150 (99%)	147 (99%)	2 (1%)	73	93
15	O	93/94 (99%)	92 (99%)	1 (1%)	78	94
16	P	113/117 (97%)	111 (98%)	2 (2%)	64	89
17	Q	79/80 (99%)	75 (95%)	4 (5%)	28	62
18	R	117/122 (96%)	112 (96%)	5 (4%)	33	68
19	S	71/74 (96%)	71 (100%)	0	100	100
20	T	105/106 (99%)	101 (96%)	4 (4%)	38	73
21	U	44/53 (83%)	42 (96%)	2 (4%)	32	66
22	V	51/57 (90%)	48 (94%)	3 (6%)	23	55
23	W	130/130 (100%)	127 (98%)	3 (2%)	56	85
24	X	66/74 (89%)	63 (96%)	3 (4%)	32	66
25	Y	120/196 (61%)	116 (97%)	4 (3%)	43	77
26	Z	60/94 (64%)	59 (98%)	1 (2%)	66	89
27	1	46/47 (98%)	46 (100%)	0	100	100
28	2	42/46 (91%)	41 (98%)	1 (2%)	54	84
29	3	79/79 (100%)	78 (99%)	1 (1%)	73	93
All	All	3095/3646 (85%)	2982 (96%)	113 (4%)	39	74

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	36	ASP
1	A	69	LEU
1	A	94	LEU
1	A	131	HIS
1	A	153	ARG
1	A	179	MET
1	A	217	ARG
2	B	7	ARG
2	B	11	LEU
2	B	27	ASN

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Mol	Chain	Res	Type
2	B	49	THR
2	B	56	ASP
2	B	71	VAL
2	B	132	HIS
2	B	162	MET
2	B	175	LEU
2	B	190	MET
2	B	195	ARG
2	B	254	GLN
2	B	256	GLN
2	B	277	GLU
3	C	2	GLN
3	C	27	ARG
3	C	78	ARG
3	C	94	THR
3	C	136	VAL
3	C	162	VAL
3	C	187	ARG
3	C	214	THR
3	C	234	VAL
3	C	236	THR
3	C	237	GLU
3	C	240	LEU
3	C	243	VAL
4	D	24	HIS
4	D	50	VAL
4	D	100	ASP
4	D	153	THR
5	E	86	VAL
5	E	102	VAL
5	E	126	ILE
5	E	156	ASP
6	F	12	LEU
6	F	119	ARG
7	G	73	ASP
8	H	21	GLU
8	H	65	LEU
8	H	87	LYS
8	H	91	ARG
8	H	157	TYR
8	H	173	GLU
9	I	110	ASP

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Mol	Chain	Res	Type
9	I	114	TYR
10	J	45	VAL
10	J	46	ILE
10	J	52	GLN
10	J	74	ARG
10	J	79	PHE
10	J	107	ASN
10	J	127	ILE
10	J	131	THR
11	K	7	ASP
11	K	10	GLN
11	K	55	VAL
12	L	32	ASP
12	L	35	ARG
12	L	43	HIS
12	L	101	ASP
12	L	104	ASP
13	M	46	LEU
13	M	68	ARG
13	M	93	ARG
13	M	99	ARG
13	M	116	ASN
13	M	130	GLU
13	M	164	THR
14	N	26	LEU
14	N	138	ASP
15	O	67	SER
16	P	91	LYS
16	P	98	ILE
17	Q	16	ASN
17	Q	18	PRO
17	Q	20	ASP
17	Q	57	ASP
18	R	13	THR
18	R	39	THR
18	R	119	VAL
18	R	123	GLN
18	R	132	ARG
20	T	39	ASN
20	T	48	VAL
20	T	89	ARG
20	T	117	ASP

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Mol	Chain	Res	Type
21	U	52	THR
21	U	53	ASP
22	V	12	THR
22	V	22	ASP
22	V	65	ASP
23	W	35	VAL
23	W	76	ASP
23	W	146	ILE
24	X	27	ASP
24	X	46	ASP
24	X	88	GLU
25	Y	163	THR
25	Y	186	ARG
25	Y	189	ASN
25	Y	203	VAL
26	Z	106	SER
28	2	18	ASN
29	3	3	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	199	HIS
2	B	27	ASN
2	B	127	GLN
2	B	145	HIS
2	B	221	GLN
2	B	238	ASN
2	B	260	HIS
2	B	320	GLN
3	C	2	GLN
3	C	39	GLN
3	C	73	GLN
3	C	129	HIS
3	C	151	GLN
4	D	103	ASN
5	E	74	HIS
5	E	119	HIS
5	E	143	GLN
7	G	17	GLN
7	G	64	ASN
8	H	34	HIS

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Mol	Chain	Res	Type
8	H	59	GLN
8	H	62	HIS
8	H	158	ASN
9	I	106	GLN
10	J	52	GLN
10	J	107	ASN
10	J	126	ASN
11	K	10	GLN
11	K	44	HIS
11	K	67	GLN
12	L	18	HIS
12	L	41	HIS
12	L	116	HIS
13	M	24	GLN
13	M	58	GLN
13	M	137	ASN
13	M	170	ASN
14	N	53	ASN
14	N	93	GLN
14	N	107	ASN
16	P	50	GLN
16	P	66	GLN
16	P	73	HIS
16	P	88	GLN
16	P	118	GLN
17	Q	40	HIS
18	R	94	ASN
18	R	98	ASN
18	R	113	HIS
18	R	117	HIS
19	S	9	HIS
19	S	44	GLN
19	S	53	ASN
20	T	39	ASN
21	U	39	ASN
21	U	48	ASN
22	V	4	HIS
22	V	34	GLN
22	V	60	GLN
23	W	2	HIS
23	W	27	HIS
23	W	110	GLN

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Mol	Chain	Res	Type
23	W	119	HIS
23	W	125	HIS
23	W	141	HIS
24	X	23	HIS
25	Y	134	HIS
25	Y	149	GLN
25	Y	189	ASN
27	1	8	GLN
27	1	16	HIS
27	1	28	HIS
28	2	18	ASN
28	2	37	HIS
28	2	41	HIS
28	2	45	ASN
29	3	48	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	242 (8%)	22 (0%)
31	9	121/122 (99%)	18 (14%)	1 (0%)
All	All	2866/3045 (94%)	260 (9%)	23 (0%)

All (260) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	0	31	C
30	0	67	A
30	0	69	A
30	0	70	A
30	0	71	G
30	0	86	A
30	0	87	C
30	0	88	G
30	0	114	A
30	0	115	U
30	0	130	C
30	0	131	A
30	0	138	U
30	0	139	C
30	0	141	C

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Mol	Chain	Res	Type
30	0	151	A
30	0	166	A
30	0	186	A
30	0	191	A
30	0	192	A
30	0	198	A
30	0	204	A
30	0	219	G
30	0	237	G
30	0	271	C
30	0	272	A
30	0	273	G
30	0	283	U
30	0	284	C
30	0	308	U
30	0	309	C
30	0	318	U
30	0	337	A
30	0	358	G
30	0	368	C
30	0	381	G
30	0	417	G
30	0	461	C
30	0	487	G
30	0	510	U
30	0	511	A
30	0	514	G
30	0	537	G
30	0	538	C
30	0	539	G
30	0	542	A
30	0	545	G
30	0	553	G
30	0	559	U
30	0	581	G
30	0	588	G
30	0	604	G
30	0	620	A
30	0	632	A
30	0	644	G
30	0	660	A
30	0	688	A

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Mol	Chain	Res	Type
30	0	701	U
30	0	702	G
30	0	759	C
30	0	777	U
30	0	809	G
30	0	821	U
30	0	835	U
30	0	840	U
30	0	857	A
30	0	858	U
30	0	868	G
30	0	869	G
30	0	871	G
30	0	872	U
30	0	875	A
30	0	877	G
30	0	878	G
30	0	882	A
30	0	885	G
30	0	898	G
30	0	905	C
30	0	920	C
30	0	921	G
30	0	953	G
30	0	960	G
30	0	961	A
30	0	1006	A
30	0	1008	C
30	0	1015	C
30	0	1029	U
30	0	1045	G
30	0	1059	G
30	0	1060	C
30	0	1072	G
30	0	1081	A
30	0	1088	A
30	0	1109	U
30	0	1110	G
30	0	1119	G
30	0	1130	U
30	0	1137	G
30	0	1151	G

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Mol	Chain	Res	Type
30	0	1164	U
30	0	1165	G
30	0	1166	A
30	0	1174	A
30	0	1175	G
30	0	1185	U
30	0	1192	A
30	0	1193	A
30	0	1206	U
30	0	1208	C
30	0	1216	G
30	0	1237	U
30	0	1238	C
30	0	1239	G
30	0	1242	A
30	0	1279	U
30	0	1289	C
30	0	1331	G
30	0	1342	C
30	0	1353	C
30	0	1357	A
30	0	1360	C
30	0	1377	C
30	0	1378	G
30	0	1407	A
30	0	1409	G
30	0	1474	C
30	0	1492	A
30	0	1505	U
30	0	1506	U
30	0	1524	U
30	0	1525	G
30	0	1526	A
30	0	1528	A
30	0	1535	G
30	0	1559	A
30	0	1592	G
30	0	1625	U
30	0	1626	A
30	0	1634	G
30	0	1656	A
30	0	1667	A

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Mol	Chain	Res	Type
30	0	1682	A
30	0	1684	A
30	0	1685	A
30	0	1692	C
30	0	1701	A
30	0	1722	U
30	0	1723	G
30	0	1725	C
30	0	1730	G
30	0	1731	C
30	0	1752	G
30	0	1774	G
30	0	1778	A
30	0	1779	A
30	0	1798	C
30	0	1819	G
30	0	1820	G
30	0	1829	A
30	0	1856	C
30	0	1879	U
30	0	1919	A
30	0	1942	A
30	0	1965	C
30	0	1971	G
30	0	1973	A
30	0	1979	G
30	0	1996	U
30	0	2004	U
30	0	2008	U
30	0	2011	A
30	0	2012	U
30	0	2013	G
30	0	2033	G
30	0	2034	U
30	0	2064	U
30	0	2072	G
30	0	2073	G
30	0	2074	A
30	0	2096	A
30	0	2101	A
30	0	2102	G
30	0	2110	G

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Mol	Chain	Res	Type
30	0	2243	C
30	0	2258	A
30	0	2271	G
30	0	2272	G
30	0	2291	A
30	0	2317	C
30	0	2321	A
30	0	2345	A
30	0	2354	A
30	0	2361	A
30	0	2369	A
30	0	2379	G
30	0	2422	U
30	0	2462	G
30	0	2465	A
30	0	2467	A
30	0	2469	A
30	0	2476	C
30	0	2483	A
30	0	2507	G
30	0	2509	A
30	0	2511	A
30	0	2526	C
30	0	2527	U
30	0	2533	C
30	0	2537	G
30	0	2541	U
30	0	2553	A
30	0	2564	G
30	0	2570	G
30	0	2589	U
30	0	2601	A
30	0	2602	G
30	0	2608	C
30	0	2613	G
30	0	2638	G
30	0	2649	A
30	0	2664	A
30	0	2676	C
30	0	2681	A
30	0	2682	C
30	0	2718	C

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Mol	Chain	Res	Type
30	0	2719	A
30	0	2726	U
30	0	2747	C
30	0	2748	G
30	0	2749	U
30	0	2750	G
30	0	2762	C
30	0	2768	A
30	0	2800	A
30	0	2811	A
30	0	2812	A
30	0	2825	C
30	0	2852	A
30	0	2876	G
30	0	2890	A
30	0	2896	A
30	0	2914	A
31	9	2	U
31	9	7	G
31	9	14	G
31	9	22	G
31	9	23	U
31	9	24	U
31	9	25	G
31	9	39	U
31	9	40	C
31	9	41	C
31	9	43	G
31	9	44	A
31	9	52	A
31	9	57	A
31	9	66	G
31	9	77	A
31	9	114	G
31	9	122	C

All (23) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	69	A
30	0	129	A
30	0	603	A

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Mol	Chain	Res	Type
30	0	644	G
30	0	699	C
30	0	834	G
30	0	857	A
30	0	871	G
30	0	877	G
30	0	1237	U
30	0	1246	A
30	0	1352	A
30	0	1377	C
30	0	1474	C
30	0	1506	U
30	0	1692	C
30	0	2467	A
30	0	2526	C
30	0	2536	C
30	0	2649	A
30	0	2681	A
30	0	2718	C
31	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$
30	OMU	0	2587	30	14,22,23	0.98	1 (7%)	18,31,34	3.69	2 (11%)
30	OMG	0	2588	30	18,26,27	1.05	1 (5%)	22,38,41	2.46	5 (22%)
30	UR3	0	2619	30	14,22,23	0.73	0	16,32,35	0.75	0
30	PSU	0	2621	30	16,21,22	1.58	3 (18%)	20,30,33	6.13	5 (25%)
30	1MA	0	628	30,35	16,25,26	1.06	1 (6%)	13,37,40	1.25	1 (7%)

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
30	OMU	0	2587	30	-	0/5/27/28	0/2/2/2
30	OMG	0	2588	30	-	0/5/27/28	0/3/3/3
30	UR3	0	2619	30	-	0/3/25/26	0/2/2/2
30	PSU	0	2621	30	-	0/7/25/26	0/2/2/2
30	1MA	0	628	30,35	-	0/3/25/26	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C5-C1'	-4.88	1.48	1.52
30	0	2621	PSU	C2-N1	2.26	1.42	1.38
30	0	2621	PSU	C4-N3	2.61	1.37	1.33
30	0	2587	OMU	C4-N3	2.64	1.37	1.33
30	0	628	1MA	C6-N6	2.71	1.33	1.27
30	0	2588	OMG	C6-N1	3.32	1.39	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2621	PSU	N1-C2-N3	-19.11	114.66	128.40
30	0	2621	PSU	C5-C4-N3	-13.03	114.74	125.43
30	0	2588	OMG	C5-C6-N1	-8.30	111.66	123.48
30	0	628	1MA	C2-N3-C4	-3.78	110.61	116.41
30	0	2587	OMU	C5-C4-N3	-3.56	114.63	123.12
30	0	2588	OMG	C2-N3-C4	-2.76	111.94	115.16
30	0	2588	OMG	N3-C2-N1	-2.50	123.81	127.46
30	0	2621	PSU	C5-C1'-C2'	-2.11	111.90	115.55
30	0	2588	OMG	C6-C5-C4	-2.00	118.85	120.84
30	0	2621	PSU	C6-N1-C2	2.81	119.86	115.36
30	0	2588	OMG	C6-N1-C2	6.36	125.21	116.06
30	0	2621	PSU	C4-N3-C2	13.89	127.31	115.16
30	0	2587	OMU	C4-N3-C2	15.12	127.12	114.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	2587	OMU	2	0
30	0	628	1MA	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 305 ligands modelled in this entry, 305 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	A	237/240 (98%)	-0.22	7 (2%) 51 44	34, 56, 94, 116	0
2	B	337/338 (99%)	-0.42	2 (0%) 89 88	34, 58, 89, 99	0
3	C	246/246 (100%)	-0.24	4 (1%) 72 70	32, 51, 75, 87	0
4	D	140/177 (79%)	1.64	50 (35%) 0 0	69, 106, 134, 144	0
5	E	172/178 (96%)	-0.10	9 (5%) 28 23	49, 73, 97, 102	0
6	F	119/120 (99%)	-0.01	6 (5%) 30 25	52, 76, 109, 124	0
7	G	29/348 (8%)	0.52	2 (6%) 18 13	79, 103, 110, 113	0
8	H	160/177 (90%)	-0.34	2 (1%) 77 76	53, 73, 107, 111	0
9	I	70/162 (43%)	3.81	49 (70%) 0 0	137, 155, 173, 175	0
10	J	142/145 (97%)	-0.65	0 100 100	43, 57, 77, 99	0
11	K	132/132 (100%)	-0.62	0 100 100	39, 54, 79, 83	0
12	L	145/165 (87%)	0.33	5 (3%) 46 39	32, 71, 123, 134	0
13	M	194/196 (98%)	-0.48	1 (0%) 90 90	35, 49, 64, 71	0
14	N	186/187 (99%)	0.24	17 (9%) 10 7	51, 74, 121, 131	0
15	O	115/116 (99%)	-0.49	0 100 100	44, 61, 78, 85	0
16	P	143/149 (95%)	-0.42	1 (0%) 87 86	47, 61, 74, 83	0
17	Q	95/96 (98%)	-0.49	0 100 100	44, 55, 72, 85	0
18	R	150/155 (96%)	-0.50	0 100 100	37, 51, 73, 84	0
19	S	81/85 (95%)	-0.05	2 (2%) 58 53	49, 64, 87, 97	0
20	T	119/120 (99%)	-0.17	3 (2%) 58 53	42, 62, 92, 121	0
21	U	53/67 (79%)	0.01	1 (1%) 67 64	51, 64, 83, 91	0
22	V	65/71 (91%)	1.07	15 (23%) 1 0	53, 76, 130, 134	0
23	W	154/154 (100%)	-0.69	0 100 100	41, 56, 74, 88	0
24	X	82/92 (89%)	-0.31	0 100 100	49, 66, 91, 108	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	142/241 (58%)	-0.51	1 (0%) 87 86	34, 48, 72, 94	0
26	Z	73/116 (62%)	0.19	6 (8%) 12 9	59, 77, 92, 101	0
27	1	56/57 (98%)	-0.24	0 100 100	33, 39, 48, 56	0
28	2	46/50 (92%)	-0.14	1 (2%) 62 59	41, 69, 102, 114	0
29	3	92/92 (100%)	-0.13	1 (1%) 80 79	43, 65, 78, 91	0
30	0	2749/2923 (94%)	-0.32	51 (1%) 67 64	28, 51, 95, 171	0
31	9	122/122 (100%)	-0.23	3 (2%) 58 53	45, 72, 95, 154	0
All	All	6646/7517 (88%)	-0.20	239 (3%) 43 37	28, 57, 106, 175	0

All (239) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	I	71	ALA	15.4
9	I	74	ILE	13.1
31	9	1	U	12.2
22	V	1	THR	11.9
9	I	72	GLU	11.1
22	V	43	PRO	10.7
9	I	70	THR	9.9
9	I	80	PHE	8.8
9	I	82	THR	8.6
9	I	83	GLY	8.3
14	N	166	ALA	7.9
9	I	88	GLN	7.8
9	I	132	VAL	7.1
9	I	112	LEU	6.8
9	I	79	GLY	6.8
9	I	81	GLU	6.8
9	I	128	THR	6.3
30	0	1169	U	6.1
9	I	69	PRO	5.9
22	V	40	PRO	5.8
4	D	18	ILE	5.6
9	I	84	SER	5.6
22	V	39	ALA	5.5
9	I	92	VAL	5.4
4	D	10	PHE	5.3
4	D	63	ILE	5.3
30	0	1170	U	5.3
14	N	147	ILE	5.3

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Mol	Chain	Res	Type	RSRZ
9	I	75	LYS	5.2
9	I	111	LEU	5.2
30	0	1172	G	5.2
4	D	69	ILE	5.1
12	L	60	GLU	5.1
22	V	46	ILE	5.1
30	0	735	C	5.1
9	I	86	GLU	5.1
9	I	66	GLY	4.9
4	D	57	THR	4.9
20	T	119	ALA	4.8
26	Z	35	SER	4.8
4	D	26	GLY	4.7
30	0	1175	G	4.7
9	I	93	ALA	4.6
9	I	130	LEU	4.6
9	I	131	GLY	4.6
30	0	1171	A	4.5
4	D	134	LEU	4.5
1	A	37	VAL	4.4
26	Z	46	SER	4.4
14	N	138	ASP	4.3
14	N	75	THR	4.3
30	0	1168	C	4.3
4	D	75	LEU	4.2
30	0	1173	A	4.2
1	A	237	GLY	4.1
30	0	1166	A	4.1
30	0	1174	A	4.1
30	0	1177	A	4.1
9	I	91	PHE	4.1
9	I	126	THR	4.1
9	I	109	PRO	4.0
9	I	127	CYS	4.0
9	I	113	SER	4.0
30	0	1195	G	3.9
30	0	1198	U	3.9
30	0	1176	C	3.9
4	D	101	THR	3.9
4	D	27	ILE	3.9
30	0	1192	A	3.9
4	D	104	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
9	I	129	SER	3.8
30	0	1181	A	3.8
30	0	1193	A	3.8
4	D	85	GLN	3.7
4	D	44	ILE	3.7
9	I	76	ASP	3.7
30	0	1164	U	3.7
1	A	35	GLY	3.7
26	Z	58	ASN	3.7
4	D	23	VAL	3.7
30	0	1199	A	3.7
6	F	106	ALA	3.7
14	N	165	ALA	3.7
1	A	236	GLY	3.6
4	D	90	LEU	3.6
4	D	17	ARG	3.6
4	D	135	VAL	3.6
4	D	25	MET	3.6
30	0	1207	A	3.6
7	G	27	ILE	3.6
4	D	102	GLY	3.6
4	D	128	LEU	3.6
4	D	107	GLY	3.6
14	N	113	SER	3.5
12	L	106	VAL	3.5
30	0	1202	A	3.5
9	I	97	VAL	3.5
4	D	154	LYS	3.4
30	0	1167	G	3.4
22	V	51	LYS	3.4
4	D	70	GLY	3.4
4	D	73	VAL	3.4
30	0	1190	G	3.4
30	0	1165	G	3.4
30	0	1178	G	3.4
22	V	44	GLY	3.4
4	D	93	LEU	3.3
9	I	106	GLN	3.3
14	N	158	LEU	3.3
9	I	73	LEU	3.3
30	0	970	U	3.3
20	T	118	SER	3.3

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Mol	Chain	Res	Type	RSRZ
8	H	158	ASN	3.3
9	I	67	VAL	3.3
30	0	1947	G	3.3
9	I	104	ALA	3.2
9	I	103	ILE	3.2
22	V	52	ALA	3.2
5	E	157	LYS	3.1
30	0	1163	G	3.1
30	0	2237	G	3.1
9	I	85	GLY	3.1
9	I	125	GLY	3.1
4	D	92	GLU	3.1
5	E	108	LEU	3.1
4	D	130	VAL	3.1
4	D	165	PHE	3.1
31	9	2	U	3.1
4	D	106	PHE	3.0
9	I	100	VAL	3.0
16	P	67	LYS	3.0
4	D	98	PHE	3.0
30	0	1200	A	3.0
22	V	2	VAL	3.0
9	I	87	PRO	2.9
4	D	19	GLU	2.9
30	0	1951	G	2.9
9	I	108	HIS	2.9
30	0	1206	U	2.9
4	D	89	PRO	2.9
4	D	40	ILE	2.9
28	2	39	ARG	2.9
5	E	10	ASP	2.9
4	D	56	ARG	2.8
5	E	154	ILE	2.8
14	N	80	SER	2.8
19	S	81	ILE	2.8
5	E	45	ASP	2.8
30	0	1191	A	2.7
12	L	99	GLU	2.7
22	V	48	GLU	2.7
31	9	24	U	2.7
30	0	282	C	2.7
6	F	49	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
20	T	82	THR	2.6
19	S	76	GLU	2.6
9	I	110	ASP	2.6
2	B	337	GLY	2.6
9	I	133	THR	2.6
1	A	99	ILE	2.6
4	D	24	HIS	2.6
4	D	41	LEU	2.6
30	0	1162	G	2.6
30	0	1180	U	2.6
12	L	105	TYR	2.6
9	I	99	GLN	2.5
4	D	81	GLU	2.5
4	D	74	THR	2.5
4	D	11	HIS	2.5
5	E	11	VAL	2.5
13	M	194	GLY	2.5
7	G	26	MET	2.5
6	F	44	SER	2.5
30	0	1194	A	2.5
9	I	94	ASP	2.5
14	N	134	ASP	2.5
14	N	159	TYR	2.5
3	C	60	SER	2.4
30	0	1203	G	2.4
30	0	1179	C	2.4
3	C	64	GLY	2.4
2	B	115	VAL	2.4
9	I	90	ASP	2.4
4	D	157	LEU	2.4
4	D	158	ASN	2.4
30	0	1208	C	2.4
1	A	31	LYS	2.4
14	N	160	SER	2.4
4	D	45	THR	2.4
14	N	41	LYS	2.4
5	E	6	GLU	2.3
30	0	1201	C	2.3
5	E	156	ASP	2.3
6	F	15	ASP	2.3
30	0	1204	C	2.3
9	I	78	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
4	D	172	VAL	2.3
4	D	95	THR	2.3
9	I	68	PRO	2.3
22	V	37	GLY	2.3
30	0	280	C	2.3
9	I	102	GLN	2.3
4	D	88	LEU	2.2
22	V	3	LEU	2.2
30	0	1161	A	2.2
22	V	41	GLU	2.2
1	A	110	SER	2.2
30	0	10	U	2.2
30	0	2004	U	2.2
6	F	16	ALA	2.2
26	Z	50	VAL	2.2
4	D	84	LEU	2.2
29	3	13	HIS	2.2
26	Z	44	ARG	2.2
30	0	1182	C	2.2
6	F	75	ILE	2.2
12	L	149	ARG	2.2
14	N	145	ALA	2.2
25	Y	235	GLU	2.2
4	D	138	GLY	2.1
8	H	40	GLN	2.1
3	C	135	GLU	2.1
14	N	112	GLY	2.1
14	N	146	HIS	2.1
4	D	13	MET	2.1
21	U	51	TRP	2.1
30	0	1196	C	2.1
30	0	138	U	2.1
5	E	161	VAL	2.1
14	N	140	GLN	2.1
14	N	137	ALA	2.1
4	D	105	SER	2.1
30	0	1965	C	2.1
30	0	1948	G	2.1
3	C	66	GLY	2.0
26	Z	83	TYR	2.0
4	D	141	VAL	2.0
22	V	45	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
22	V	49	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
30	1MA	0	628	23/24	0.98	0.18	-	33,37,38,39	0
30	OMG	0	2588	24/25	0.99	0.14	-	36,39,42,43	0
30	OMU	0	2587	21/22	0.99	0.13	-	38,40,44,45	0
30	PSU	0	2621	20/21	0.98	0.18	-	34,35,47,48	0
30	UR3	0	2619	21/22	0.98	0.15	-	42,44,47,47	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
35	NA	0	8565	1/1	0.87	1.24	97.52	79,79,79,79	0
35	NA	0	8547	1/1	0.91	0.70	73.51	80,80,80,80	0
35	NA	0	8562	1/1	0.69	1.31	72.93	78,78,78,78	0
35	NA	0	8560	1/1	0.19	0.89	36.93	101,101,101,101	0
37	K	0	8401	1/1	0.41	0.78	30.06	128,128,128,128	0
35	NA	0	8564	1/1	0.93	0.39	27.90	68,68,68,68	0
35	NA	0	8555	1/1	0.96	0.81	25.22	75,75,75,75	0
35	NA	9	8572	1/1	0.96	0.89	21.13	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	0	8559	1/1	0.92	0.29	16.79	91,91,91,91	0
35	NA	0	8528	1/1	0.65	0.55	13.46	66,66,66,66	0
35	NA	0	8553	1/1	0.98	0.46	12.64	65,65,65,65	0
32	MG	0	8085	1/1	0.98	0.53	12.56	97,97,97,97	0
34	SR	B	8987	1/1	0.80	0.56	10.79	200,200,200,200	0
35	NA	0	8521	1/1	0.91	0.39	9.53	61,61,61,61	0
35	NA	0	8542	1/1	0.96	0.45	9.03	49,49,49,49	0
35	NA	0	8567	1/1	0.88	0.36	8.01	76,76,76,76	0
35	NA	0	8556	1/1	0.96	0.82	7.68	64,64,64,64	0
34	SR	0	8903	1/1	1.00	0.19	7.63	59,59,59,59	0
32	MG	A	8051	1/1	0.93	0.65	7.37	70,70,70,70	0
35	NA	0	8546	1/1	0.84	0.40	7.31	65,65,65,65	0
32	MG	0	8047	1/1	0.96	0.32	6.31	51,51,51,51	0
35	NA	0	8527	1/1	0.81	0.27	5.82	71,71,71,71	0
35	NA	0	8563	1/1	0.69	0.28	4.99	88,88,88,88	0
34	SR	0	8949	1/1	0.98	0.16	4.90	122,122,122,122	0
35	NA	R	8575	1/1	0.93	0.25	4.29	99,99,99,99	0
32	MG	0	8014	1/1	0.95	0.20	3.99	33,33,33,33	0
32	MG	0	8009	1/1	0.98	0.25	3.75	36,36,36,36	0
35	NA	0	8530	1/1	0.74	0.32	3.55	59,59,59,59	0
37	K	0	8402	1/1	0.98	0.25	3.53	76,76,76,76	0
32	MG	0	8041	1/1	0.96	0.21	3.23	29,29,29,29	0
34	SR	0	8904	1/1	0.99	0.18	3.08	65,65,65,65	0
32	MG	0	8028	1/1	0.98	0.16	2.27	26,26,26,26	0
32	MG	0	8084	1/1	0.99	0.15	2.17	33,33,33,33	0
35	NA	M	8539	1/1	0.99	0.18	1.97	34,34,34,34	0
34	SR	A	8929	1/1	0.92	0.23	1.84	144,144,144,144	0
35	NA	0	8537	1/1	0.95	0.18	1.65	38,38,38,38	0
34	SR	0	8918	1/1	0.99	0.15	1.59	80,80,80,80	0
32	MG	0	8003	1/1	0.96	0.19	1.54	45,45,45,45	0
32	MG	0	8004	1/1	1.00	0.19	1.41	32,32,32,32	0
34	SR	0	8944	1/1	0.79	0.14	1.21	169,169,169,169	0
35	NA	0	8558	1/1	0.97	0.23	1.14	49,49,49,49	0
32	MG	0	8088	1/1	0.98	0.21	1.12	52,52,52,52	0
34	SR	R	8912	1/1	0.99	0.17	0.80	92,92,92,92	0
34	SR	0	8985	1/1	0.90	0.13	0.72	134,134,134,134	0
32	MG	0	8044	1/1	0.92	0.16	0.60	50,50,50,50	0
32	MG	K	8054	1/1	0.99	0.16	0.39	46,46,46,46	0
35	NA	C	8503	1/1	0.97	0.21	0.28	36,36,36,36	0
35	NA	0	8519	1/1	0.96	0.20	0.28	43,43,43,43	0
35	NA	0	8515	1/1	0.94	0.20	0.26	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	0	8504	1/1	0.88	0.18	0.22	44,44,44,44	0
32	MG	0	8053	1/1	0.95	0.20	0.15	47,47,47,47	0
32	MG	0	8011	1/1	0.92	0.23	0.08	25,25,25,25	0
35	NA	0	8568	1/1	0.79	0.21	0.02	52,52,52,52	0
35	NA	J	8538	1/1	0.83	0.18	-0.02	56,56,56,56	0
32	MG	0	8034	1/1	0.98	0.16	-0.07	46,46,46,46	0
32	MG	0	8010	1/1	0.99	0.22	-0.15	45,45,45,45	0
32	MG	0	8015	1/1	0.99	0.13	-0.20	30,30,30,30	0
34	SR	0	8992	1/1	0.88	0.15	-0.21	136,136,136,136	0
36	CD	Z	8703	1/1	0.99	0.13	-0.35	75,75,75,75	0
34	SR	0	8972	1/1	0.90	0.14	-0.54	146,146,146,146	0
33	CL	J	8821	1/1	0.95	0.14	-0.63	67,67,67,67	0
36	CD	1	8702	1/1	0.99	0.13	-0.66	67,67,67,67	0
32	MG	0	8002	1/1	0.97	0.15	-0.67	36,36,36,36	0
32	MG	0	8067	1/1	0.83	0.16	-0.75	40,40,40,40	0
34	SR	0	8975	1/1	0.91	0.14	-0.77	130,130,130,130	0
35	NA	0	8517	1/1	0.99	0.15	-0.93	31,31,31,31	0
32	MG	0	8062	1/1	0.91	0.15	-1.12	59,59,59,59	0
35	NA	Q	8540	1/1	0.78	0.11	-1.14	64,64,64,64	0
35	NA	0	8569	1/1	0.93	0.15	-1.15	48,48,48,48	0
36	CD	3	8704	1/1	1.00	0.10	-1.17	74,74,74,74	0
35	NA	0	8520	1/1	0.95	0.07	-1.19	49,49,49,49	0
32	MG	T	8057	1/1	0.94	0.12	-1.22	60,60,60,60	0
32	MG	0	8058	1/1	1.00	0.10	-1.22	22,22,22,22	0
32	MG	0	8043	1/1	0.99	0.06	-1.23	52,52,52,52	0
34	SR	1	8913	1/1	0.97	0.14	-1.41	95,95,95,95	0
32	MG	0	8025	1/1	0.98	0.12	-1.42	37,37,37,37	0
34	SR	0	8936	1/1	0.91	0.11	-1.42	94,94,94,94	0
34	SR	F	9005	1/1	0.99	0.08	-1.45	133,133,133,133	0
34	SR	0	8902	1/1	0.99	0.17	-1.55	66,66,66,66	0
36	CD	U	8701	1/1	0.99	0.10	-1.57	63,63,63,63	0
34	SR	0	8935	1/1	0.99	0.09	-1.62	79,79,79,79	0
35	NA	0	8534	1/1	0.97	0.14	-1.65	44,44,44,44	0
35	NA	0	8533	1/1	0.95	0.10	-1.68	55,55,55,55	0
33	CL	L	8810	1/1	0.94	0.09	-1.84	68,68,68,68	0
32	MG	0	8045	1/1	0.92	0.09	-1.92	44,44,44,44	0
33	CL	O	8808	1/1	0.91	0.08	-1.93	70,70,70,70	0
32	MG	0	8012	1/1	0.98	0.14	-2.02	18,18,18,18	0
35	NA	0	8557	1/1	0.82	0.06	-2.02	53,53,53,53	0
34	SR	0	8969	1/1	0.94	0.12	-2.02	159,159,159,159	0
33	CL	M	8818	1/1	0.96	0.09	-2.03	40,40,40,40	0
32	MG	0	8008	1/1	1.00	0.09	-2.10	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	0	8050	1/1	0.97	0.09	-2.13	32,32,32,32	0
32	MG	0	8016	1/1	0.96	0.14	-2.26	48,48,48,48	0
33	CL	0	8813	1/1	0.93	0.09	-2.26	66,66,66,66	0
35	NA	0	8523	1/1	0.96	0.09	-2.51	50,50,50,50	0
33	CL	0	8816	1/1	0.99	0.08	-2.53	79,79,79,79	0
33	CL	3	8804	1/1	0.98	0.06	-2.60	63,63,63,63	0
35	NA	0	8512	1/1	0.94	0.15	-2.69	52,52,52,52	0
32	MG	0	8056	1/1	0.93	0.11	-2.89	47,47,47,47	0
34	SR	A	8930	1/1	0.99	0.06	-2.98	97,97,97,97	0
32	MG	0	8079	1/1	0.97	0.11	-2.98	51,51,51,51	0
34	SR	0	8948	1/1	0.99	0.10	-3.14	92,92,92,92	0
33	CL	0	8812	1/1	0.98	0.06	-3.18	58,58,58,58	0
35	NA	0	8507	1/1	0.98	0.11	-3.20	37,37,37,37	0
34	SR	0	8943	1/1	0.96	0.04	-3.33	124,124,124,124	0
33	CL	0	8805	1/1	0.98	0.06	-3.47	67,67,67,67	0
32	MG	0	8006	1/1	0.93	0.10	-3.62	32,32,32,32	0
32	MG	0	8021	1/1	0.97	0.05	-3.62	40,40,40,40	0
32	MG	Y	8086	1/1	0.99	0.08	-3.72	44,44,44,44	0
32	MG	0	8001	1/1	0.96	0.11	-3.88	33,33,33,33	0
32	MG	0	8052	1/1	0.98	0.07	-3.98	56,56,56,56	0
32	MG	0	8013	1/1	0.97	0.06	-4.46	25,25,25,25	0
32	MG	0	8065	1/1	0.98	0.06	-4.68	57,57,57,57	0
35	NA	B	8552	1/1	0.98	0.10	-5.15	83,83,83,83	0
34	SR	0	8970	1/1	0.99	0.01	-6.07	123,123,123,123	0
32	MG	0	8075	1/1	0.93	0.03	-6.54	42,42,42,42	0
34	SR	0	8945	1/1	0.97	0.07	-6.57	106,106,106,106	0
34	SR	0	8910	1/1	0.98	0.04	-7.09	100,100,100,100	0
34	SR	0	8984	1/1	0.98	0.03	-9.15	121,121,121,121	0
33	CL	B	8819	1/1	0.98	0.09	-9.73	58,58,58,58	0
32	MG	0	8029	1/1	0.99	0.15	-	49,49,49,49	0
32	MG	0	8089	1/1	0.93	0.17	-	72,72,72,72	0
34	SR	0	8955	1/1	0.68	0.21	-	199,199,199,199	0
34	SR	9	8978	1/1	0.99	0.08	-	135,135,135,135	0
34	SR	0	8967	1/1	0.99	0.06	-	133,133,133,133	0
35	NA	0	8536	1/1	0.91	0.24	-	61,61,61,61	0
33	CL	0	8815	1/1	0.91	0.12	-	77,77,77,77	0
32	MG	0	8035	1/1	0.96	0.10	-	54,54,54,54	0
35	NA	0	8561	1/1	0.94	0.22	-	68,68,68,68	0
34	SR	0	8927	1/1	0.90	0.09	-	153,153,153,153	0
32	MG	0	8092	1/1	0.89	0.18	-	53,53,53,53	0
33	CL	0	8822	1/1	0.97	0.45	-	81,81,81,81	0
34	SR	0	8954	1/1	0.97	0.10	-	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	SR	0	9002	1/1	0.92	0.29	-	177,177,177,177	0
35	NA	0	8531	1/1	0.97	0.06	-	40,40,40,40	0
32	MG	0	8033	1/1	0.94	0.09	-	55,55,55,55	0
34	SR	0	8966	1/1	0.95	0.10	-	107,107,107,107	0
32	MG	0	8063	1/1	0.98	0.14	-	80,80,80,80	0
32	MG	0	8020	1/1	0.97	0.07	-	40,40,40,40	0
34	SR	0	8923	1/1	0.98	0.11	-	101,101,101,101	0
32	MG	0	8078	1/1	0.98	0.27	-	69,69,69,69	0
32	MG	0	8024	1/1	0.97	0.12	-	49,49,49,49	0
35	NA	0	8550	1/1	0.86	0.96	-	57,57,57,57	0
34	SR	0	8941	1/1	0.98	0.14	-	108,108,108,108	0
32	MG	0	8080	1/1	0.99	0.12	-	75,75,75,75	0
35	NA	0	8549	1/1	0.91	0.51	-	52,52,52,52	0
35	NA	0	8509	1/1	0.70	0.92	-	85,85,85,85	0
32	MG	0	8073	1/1	0.99	0.34	-	73,73,73,73	0
32	MG	0	8083	1/1	0.91	0.10	-	60,60,60,60	0
34	SR	0	8997	1/1	0.84	0.84	-	200,200,200,200	0
34	SR	0	8914	1/1	0.98	0.32	-	120,120,120,120	0
34	SR	0	8920	1/1	0.97	0.08	-	135,135,135,135	0
33	CL	0	8814	1/1	0.94	0.21	-	72,72,72,72	0
32	MG	0	8023	1/1	0.98	0.10	-	37,37,37,37	0
34	SR	0	8905	1/1	1.00	0.27	-	61,61,61,61	0
32	MG	0	8018	1/1	1.00	0.24	-	40,40,40,40	0
32	MG	B	8042	1/1	0.99	0.07	-	44,44,44,44	0
34	SR	0	8938	1/1	0.98	0.02	-	147,147,147,147	0
32	MG	0	8072	1/1	0.81	0.18	-	63,63,63,63	0
33	CL	0	8803	1/1	0.95	0.10	-	58,58,58,58	0
32	MG	0	8036	1/1	0.94	0.12	-	56,56,56,56	0
35	NA	0	8501	1/1	0.87	0.08	-	40,40,40,40	0
34	SR	0	8991	1/1	0.64	0.07	-	199,199,199,199	0
33	CL	Y	8820	1/1	0.97	0.04	-	48,48,48,48	0
32	MG	0	8069	1/1	0.98	0.30	-	73,73,73,73	0
35	NA	0	8524	1/1	0.97	0.25	-	58,58,58,58	0
34	SR	0	8981	1/1	0.98	0.34	-	178,178,178,178	0
34	SR	0	8982	1/1	0.73	2.26	-	200,200,200,200	0
34	SR	0	8933	1/1	0.98	0.16	-	139,139,139,139	0
34	SR	0	8921	1/1	0.96	0.15	-	96,96,96,96	0
32	MG	9	8074	1/1	0.84	0.09	-	86,86,86,86	0
34	SR	0	8989	1/1	0.92	0.16	-	168,168,168,168	0
33	CL	A	8809	1/1	0.91	0.11	-	80,80,80,80	0
32	MG	0	8066	1/1	0.92	0.18	-	70,70,70,70	0
32	MG	0	8059	1/1	0.99	0.07	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	SR	0	9006	1/1	-0.20	2.27	-	200,200,200,200	0
35	NA	0	8571	1/1	0.82	0.16	-	76,76,76,76	0
32	MG	0	8060	1/1	0.94	0.08	-	53,53,53,53	0
34	SR	0	8947	1/1	0.54	0.51	-	200,200,200,200	0
34	SR	0	8906	1/1	0.99	0.23	-	64,64,64,64	0
35	NA	0	8573	1/1	0.88	0.35	-	73,73,73,73	0
33	CL	N	8807	1/1	0.93	0.17	-	69,69,69,69	0
35	NA	0	8514	1/1	0.98	0.50	-	56,56,56,56	0
32	MG	0	8070	1/1	0.95	0.12	-	46,46,46,46	0
34	SR	0	8998	1/1	0.82	0.19	-	173,173,173,173	0
32	MG	0	8064	1/1	0.99	0.18	-	44,44,44,44	0
32	MG	0	8082	1/1	0.95	0.78	-	89,89,89,89	0
32	MG	0	8077	1/1	0.93	0.06	-	45,45,45,45	0
32	MG	0	8037	1/1	0.93	0.14	-	88,88,88,88	0
34	SR	3	8999	1/1	0.98	0.10	-	110,110,110,110	0
34	SR	0	8963	1/1	0.96	0.17	-	112,112,112,112	0
34	SR	0	8926	1/1	0.98	0.17	-	108,108,108,108	0
34	SR	0	8916	1/1	1.00	0.03	-	120,120,120,120	0
34	SR	0	8958	1/1	0.96	0.06	-	122,122,122,122	0
34	SR	0	8901	1/1	0.94	0.08	-	91,91,91,91	0
34	SR	0	8951	1/1	0.90	0.04	-	148,148,148,148	0
32	MG	0	8039	1/1	0.92	0.27	-	76,76,76,76	0
34	SR	0	9001	1/1	0.81	0.08	-	173,173,173,173	0
34	SR	S	8961	1/1	0.94	0.06	-	121,121,121,121	0
32	MG	0	8022	1/1	0.97	0.21	-	44,44,44,44	0
34	SR	0	8931	1/1	0.99	0.07	-	113,113,113,113	0
34	SR	0	8957	1/1	0.97	0.14	-	195,195,195,195	0
34	SR	0	9000	1/1	0.94	0.07	-	176,176,176,176	0
34	SR	0	8973	1/1	0.94	0.05	-	130,130,130,130	0
35	NA	0	8544	1/1	0.86	0.17	-	67,67,67,67	0
33	CL	0	8817	1/1	0.99	0.15	-	67,67,67,67	0
32	MG	0	8040	1/1	0.96	0.21	-	96,96,96,96	0
32	MG	0	8055	1/1	0.94	0.16	-	53,53,53,53	0
34	SR	0	8939	1/1	0.97	0.09	-	149,149,149,149	0
32	MG	0	8076	1/1	0.99	0.08	-	40,40,40,40	0
32	MG	0	8049	1/1	0.88	0.30	-	69,69,69,69	0
35	NA	0	8506	1/1	0.69	0.16	-	64,64,64,64	0
32	MG	0	8091	1/1	0.93	0.07	-	57,57,57,57	0
34	SR	0	8956	1/1	0.99	0.06	-	155,155,155,155	0
35	NA	0	8522	1/1	0.90	1.14	-	79,79,79,79	0
32	MG	0	8019	1/1	0.99	0.20	-	28,28,28,28	0
34	SR	0	8907	1/1	1.00	0.15	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	SR	0	8911	1/1	0.99	0.08	-	85,85,85,85	0
32	MG	0	8026	1/1	0.97	0.08	-	35,35,35,35	0
33	CL	J	8802	1/1	0.95	0.21	-	75,75,75,75	0
34	SR	0	8908	1/1	0.96	0.08	-	116,116,116,116	0
34	SR	0	8990	1/1	0.99	0.10	-	139,139,139,139	0
35	NA	0	8570	1/1	0.91	0.09	-	52,52,52,52	0
32	MG	0	8017	1/1	0.98	0.19	-	52,52,52,52	0
35	NA	0	8535	1/1	0.83	0.53	-	61,61,61,61	0
35	NA	0	8526	1/1	0.93	0.08	-	47,47,47,47	0
34	SR	0	8942	1/1	0.93	0.08	-	122,122,122,122	0
34	SR	0	9004	1/1	0.96	0.30	-	200,200,200,200	0
34	SR	0	8962	1/1	0.53	0.19	-	169,169,169,169	0
33	CL	Q	8811	1/1	0.93	0.15	-	82,82,82,82	0
34	SR	0	8994	1/1	0.75	0.43	-	200,200,200,200	0
34	SR	0	8940	1/1	0.98	0.07	-	97,97,97,97	0
34	SR	3	8932	1/1	0.99	0.14	-	76,76,76,76	0
35	NA	0	8525	1/1	0.29	0.25	-	92,92,92,92	0
34	SR	0	9008	1/1	0.95	0.17	-	95,95,95,95	0
34	SR	9	9003	1/1	0.94	0.09	-	171,171,171,171	0
34	SR	0	8934	1/1	0.98	0.25	-	134,134,134,134	0
34	SR	0	8993	1/1	0.74	0.10	-	176,176,176,176	0
32	MG	0	8046	1/1	0.96	0.14	-	43,43,43,43	0
34	SR	0	8928	1/1	0.93	0.06	-	135,135,135,135	0
32	MG	0	8038	1/1	0.90	0.15	-	70,70,70,70	0
32	MG	0	8081	1/1	0.90	0.23	-	73,73,73,73	0
35	NA	0	8518	1/1	0.85	0.59	-	88,88,88,88	0
35	NA	0	8566	1/1	0.98	0.12	-	64,64,64,64	0
32	MG	0	8048	1/1	0.98	0.24	-	33,33,33,33	0
34	SR	0	8971	1/1	0.96	0.07	-	171,171,171,171	0
35	NA	0	8513	1/1	0.98	0.21	-	54,54,54,54	0
32	MG	0	8068	1/1	0.98	0.08	-	51,51,51,51	0
32	MG	0	8005	1/1	0.99	0.23	-	35,35,35,35	0
34	SR	0	8995	1/1	0.94	0.15	-	136,136,136,136	0
32	MG	0	8087	1/1	0.92	0.12	-	51,51,51,51	0
34	SR	0	8960	1/1	0.83	0.10	-	141,141,141,141	0
35	NA	0	8541	1/1	0.98	0.18	-	75,75,75,75	0
34	SR	0	8968	1/1	0.94	0.03	-	160,160,160,160	0
32	MG	0	8090	1/1	0.99	0.10	-	65,65,65,65	0
33	CL	J	8801	1/1	0.99	0.07	-	79,79,79,79	0
34	SR	A	8977	1/1	0.83	0.06	-	160,160,160,160	0
34	SR	0	8917	1/1	0.96	0.10	-	107,107,107,107	0
34	SR	0	9007	1/1	0.97	0.67	-	200,200,200,200	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	0	8508	1/1	0.98	0.20	-	35,35,35,35	0
34	SR	9	8980	1/1	0.93	0.15	-	175,175,175,175	0
35	NA	0	8529	1/1	0.92	0.15	-	39,39,39,39	0
34	SR	0	8988	1/1	0.93	0.05	-	158,158,158,158	0
32	MG	0	8030	1/1	0.98	0.30	-	68,68,68,68	0
35	NA	0	8574	1/1	0.89	0.26	-	59,59,59,59	0
32	MG	0	8093	1/1	0.95	0.08	-	42,42,42,42	0
34	SR	0	8925	1/1	1.00	0.08	-	86,86,86,86	0
34	SR	B	8950	1/1	0.98	0.14	-	116,116,116,116	0
35	NA	0	8516	1/1	0.96	0.11	-	45,45,45,45	0
36	CD	O	8705	1/1	0.99	0.06	-	118,118,118,118	0
32	MG	0	8061	1/1	0.99	0.23	-	37,37,37,37	0
32	MG	0	8031	1/1	0.91	0.11	-	62,62,62,62	0
35	NA	0	8505	1/1	0.93	0.86	-	48,48,48,48	0
34	SR	0	8959	1/1	0.91	0.37	-	163,163,163,163	0
34	SR	1	8952	1/1	0.98	0.15	-	89,89,89,89	0
32	MG	0	8027	1/1	0.99	0.11	-	51,51,51,51	0
35	NA	0	8551	1/1	0.94	0.38	-	52,52,52,52	0
32	MG	0	8032	1/1	0.99	0.05	-	44,44,44,44	0
34	SR	0	8996	1/1	0.78	1.20	-	200,200,200,200	0
32	MG	0	8007	1/1	0.99	0.15	-	32,32,32,32	0
35	NA	0	8548	1/1	0.74	0.26	-	58,58,58,58	0
35	NA	R	8532	1/1	0.96	0.11	-	58,58,58,58	0
34	SR	0	8909	1/1	0.99	0.15	-	88,88,88,88	0
35	NA	S	8510	1/1	0.81	0.48	-	64,64,64,64	0
34	SR	0	8924	1/1	0.34	0.09	-	154,154,154,154	0
32	MG	0	8071	1/1	0.97	0.10	-	72,72,72,72	0
35	NA	0	8545	1/1	0.88	0.26	-	47,47,47,47	0
35	NA	0	8502	1/1	0.72	0.15	-	66,66,66,66	0
34	SR	0	8983	1/1	0.98	0.24	-	170,170,170,170	0
34	SR	0	8915	1/1	0.92	0.08	-	121,121,121,121	0
35	NA	0	8511	1/1	0.75	0.29	-	69,69,69,69	0
34	SR	0	8986	1/1	0.78	0.42	-	200,200,200,200	0
34	SR	0	8979	1/1	0.76	0.13	-	200,200,200,200	0
34	SR	0	8919	1/1	0.97	0.07	-	170,170,170,170	0
35	NA	0	8554	1/1	0.90	1.00	-	65,65,65,65	0
34	SR	0	8964	1/1	0.99	0.09	-	131,131,131,131	0
34	SR	0	8937	1/1	0.98	0.27	-	112,112,112,112	0
34	SR	0	8976	1/1	0.88	0.28	-	194,194,194,194	0
34	SR	0	8922	1/1	0.88	0.47	-	161,161,161,161	0
34	SR	0	8953	1/1	0.96	0.13	-	144,144,144,144	0
34	SR	0	8946	1/1	0.91	0.22	-	123,123,123,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	CL	R	8806	1/1	0.99	0.17	-	57,57,57,57	0
35	NA	9	8543	1/1	0.77	0.11	-	74,74,74,74	0
34	SR	0	8974	1/1	0.87	0.24	-	165,165,165,165	0
34	SR	0	8965	1/1	0.93	0.09	-	132,132,132,132	0

6.5 Other polymers [i](#)

There are no such residues in this entry.