



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2020 – 07:12 PM BST

PDB ID : 3CCL
Title : Structure of Anisomycin resistant 50S Ribosomal Subunit: 23S rRNA mutation U2535C. Density for Anisomycin is visible but not included in model.
Authors : Blaha, G.; Gurel, G.
Deposited on : 2008-02-26
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13

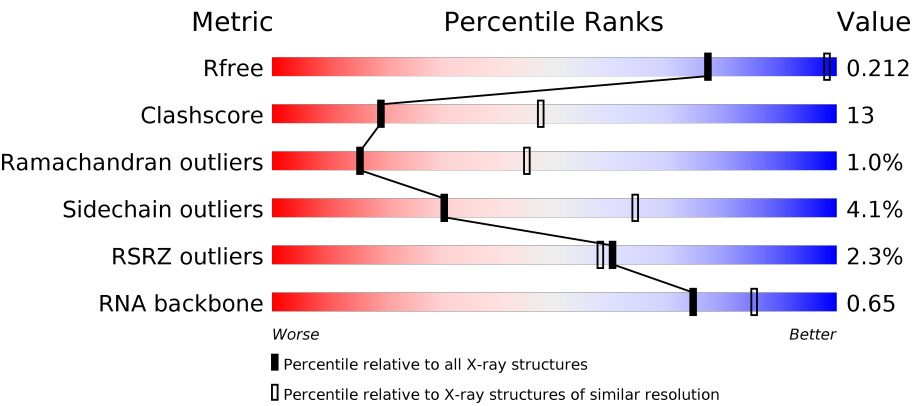
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



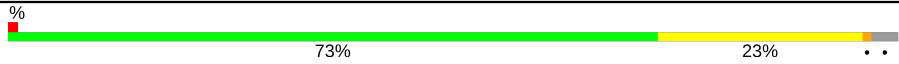

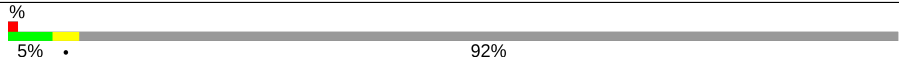
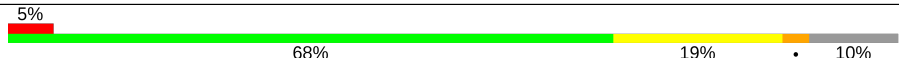

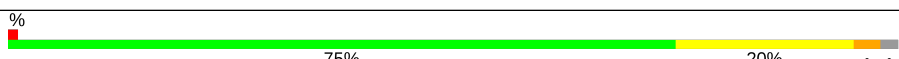
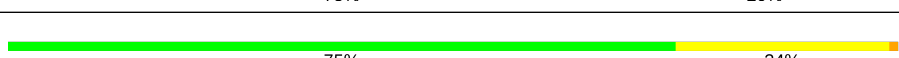
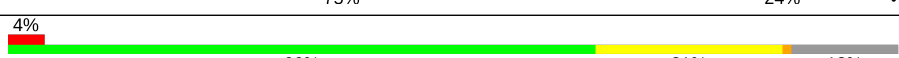
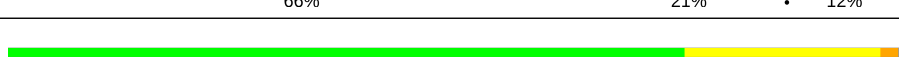

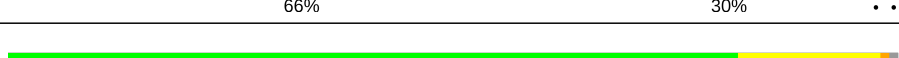







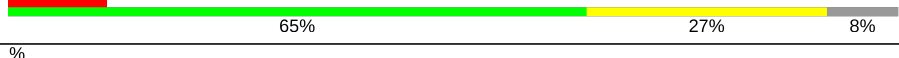
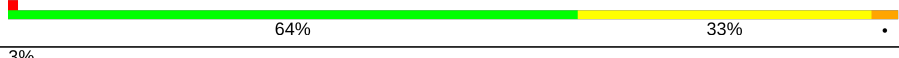

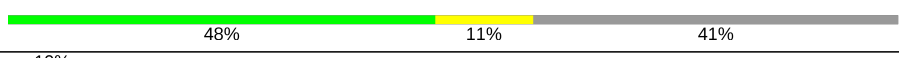
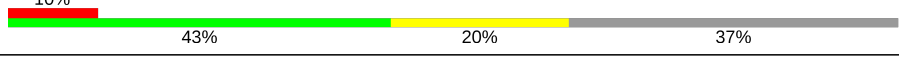


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	240	<div><div>2%</div><div><div></div><div></div><div></div><div></div></div><div>72%23% . .</div></div>
2	B	338	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>66%31% .</div></div>
3	C	246	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>72%24% .</div></div>
4	D	177	<div><div>16%</div><div><div></div><div></div><div></div><div></div></div><div>45%32%.21%</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
34	SR	0	8982	-	-	-	X
34	SR	0	8994	-	-	-	X
34	SR	0	8997	-	-	-	X
34	SR	0	9006	-	-	-	X
34	SR	B	8987	-	-	-	X
35	NA	0	8505	-	-	-	X
35	NA	0	8518	-	-	-	X
35	NA	0	8546	-	-	-	X
35	NA	0	8555	-	-	-	X
35	NA	0	8562	-	-	-	X

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99122 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
			59020	26349	10874	19052	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	10	Total Cl 10 10	0	0
33	J	3	Total Cl 3 3	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
34	F	1	Total Sr 1 1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	67	Total	Na	0	0
			67	67		
35	J	1	Total	Na	0	0
			1	1		
35	Q	1	Total	Na	0	0
			1	1		
35	C	1	Total	Na	0	0
			1	1		
35	R	1	Total	Na	0	0
			1	1		
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	0	0
			2	2		

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	A	116	Total	O	0	0
			116	116		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	B	141	Total 141	O 141	0	0
38	C	170	Total 170	O 170	0	0
38	D	44	Total 44	O 44	0	0
38	E	45	Total 45	O 45	0	0
38	F	27	Total 27	O 27	0	0
38	G	19	Total 19	O 19	0	0
38	H	63	Total 63	O 63	0	0
38	I	8	Total 8	O 8	0	0
38	J	53	Total 53	O 53	0	0
38	K	56	Total 56	O 56	0	0
38	L	85	Total 85	O 85	0	0
38	M	123	Total 123	O 123	0	0
38	N	55	Total 55	O 55	0	0
38	O	43	Total 43	O 43	0	0
38	P	67	Total 67	O 67	0	0
38	Q	50	Total 50	O 50	0	0
38	R	85	Total 85	O 85	0	0
38	S	33	Total 33	O 33	0	0
38	T	34	Total 34	O 34	0	0
38	U	27	Total 27	O 27	0	0
38	V	13	Total 13	O 13	0	0

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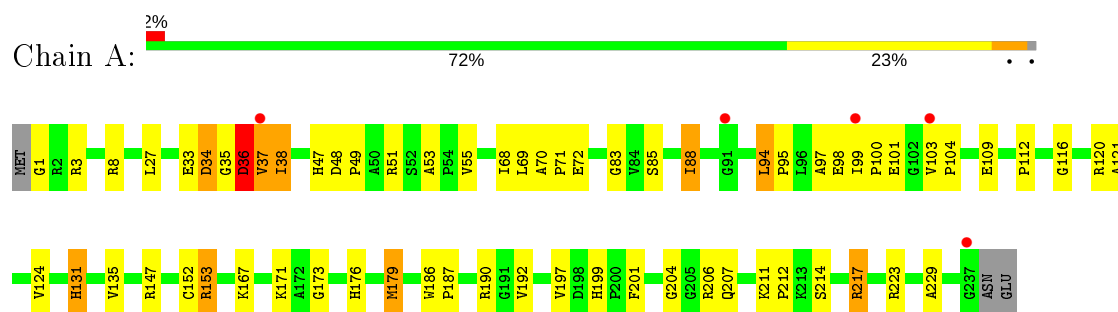
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	W	69	Total 69	O 69	0	0
38	X	25	Total 25	O 25	0	0
38	Y	95	Total 95	O 95	0	0
38	Z	26	Total 26	O 26	0	0
38	1	63	Total 63	O 63	0	0
38	2	50	Total 50	O 50	0	0
38	3	62	Total 62	O 62	0	0
38	0	5929	Total 5929	O 5929	0	0
38	9	147	Total 147	O 147	0	0

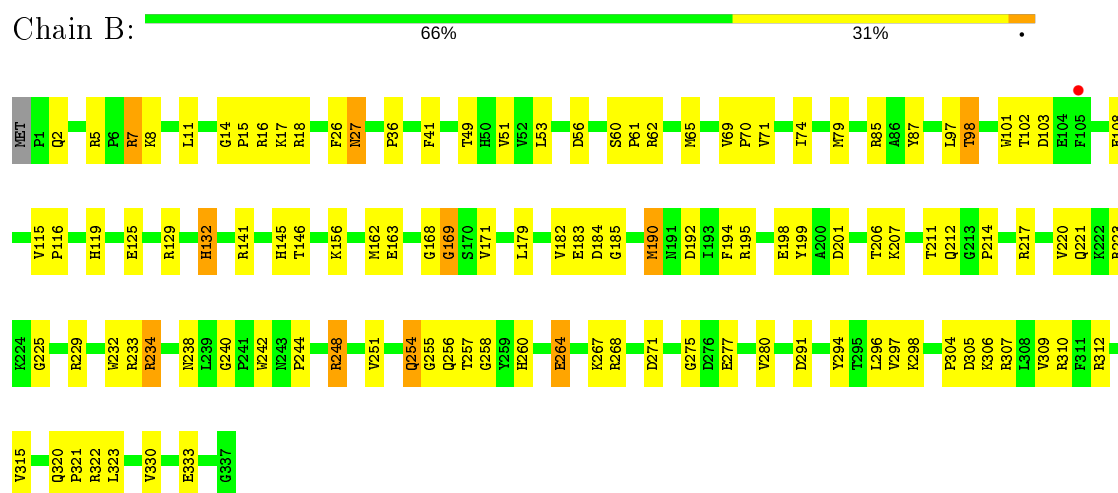
3 Residue-property plots

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

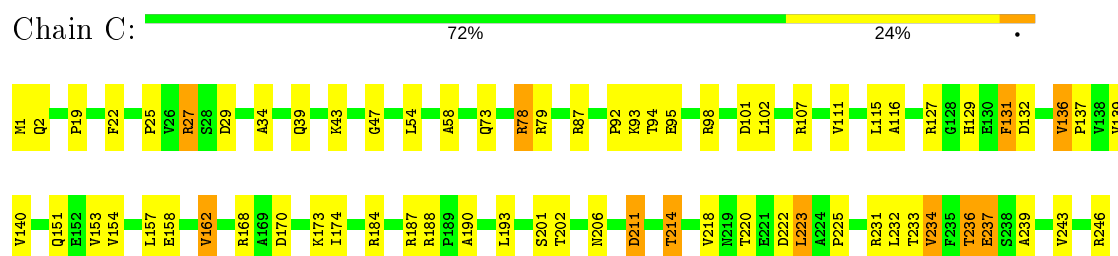
- Molecule 1: 50S ribosomal protein L2P



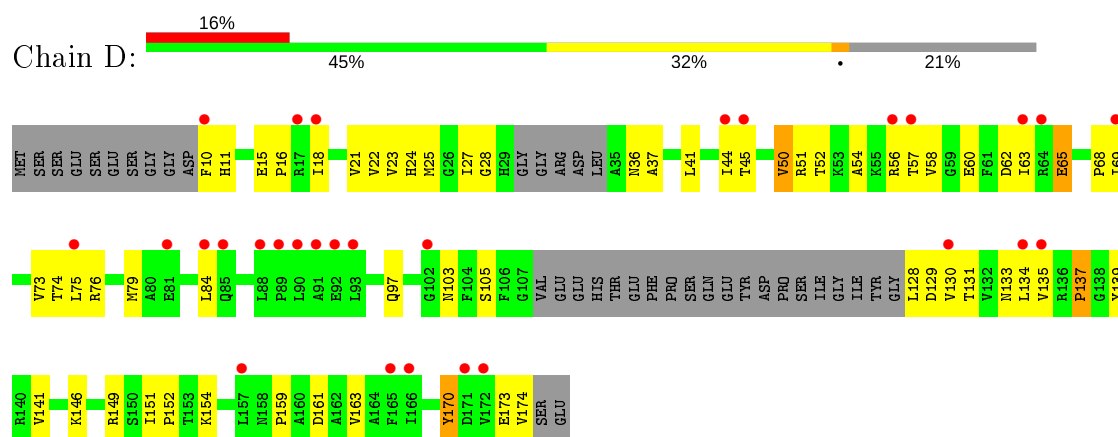
- Molecule 2: 50S ribosomal protein L3P



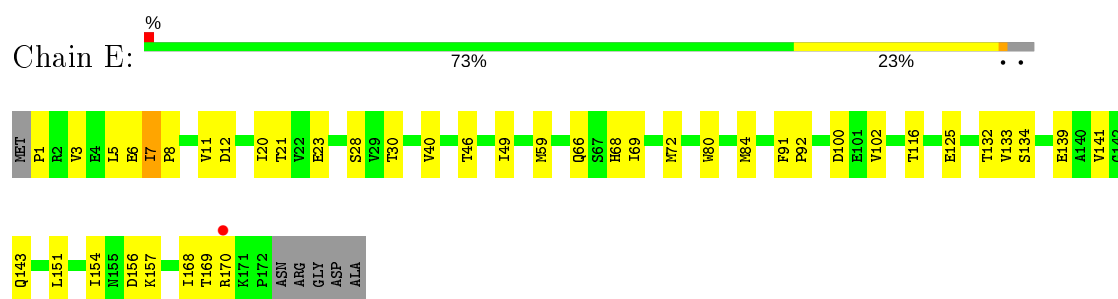
- Molecule 3: 50S ribosomal protein L4P



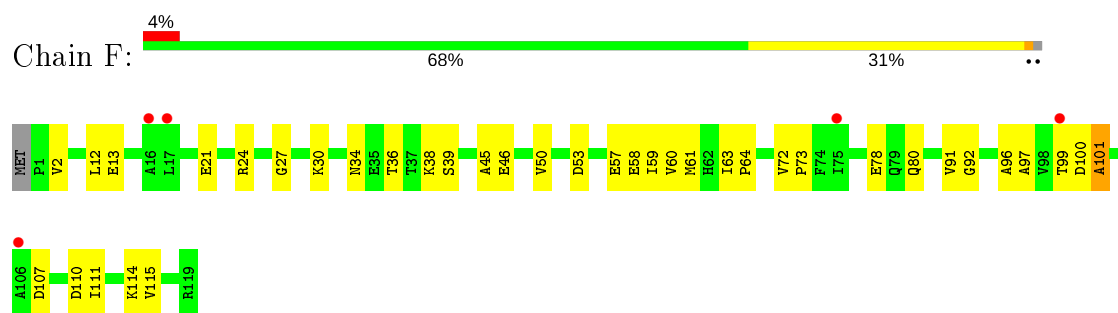
- Molecule 4: 50S ribosomal protein L5P



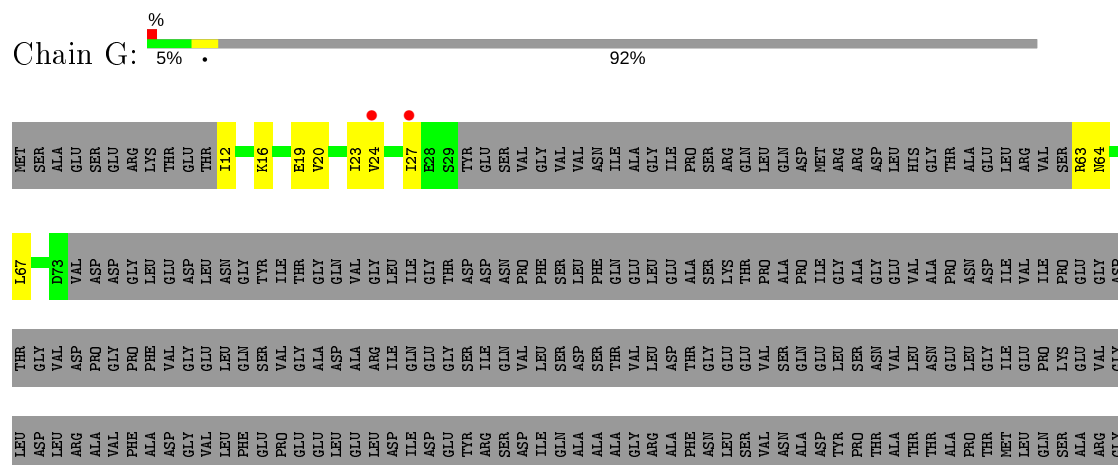
- Molecule 5: 50S ribosomal protein L6P

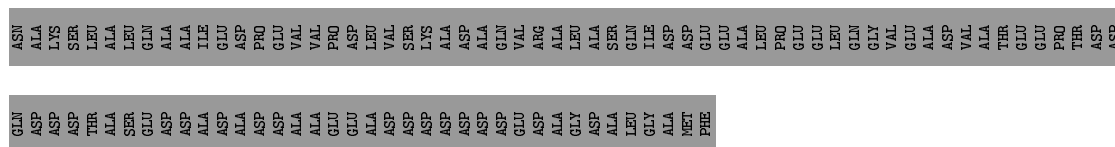


- Molecule 6: 50S ribosomal protein L7Ae

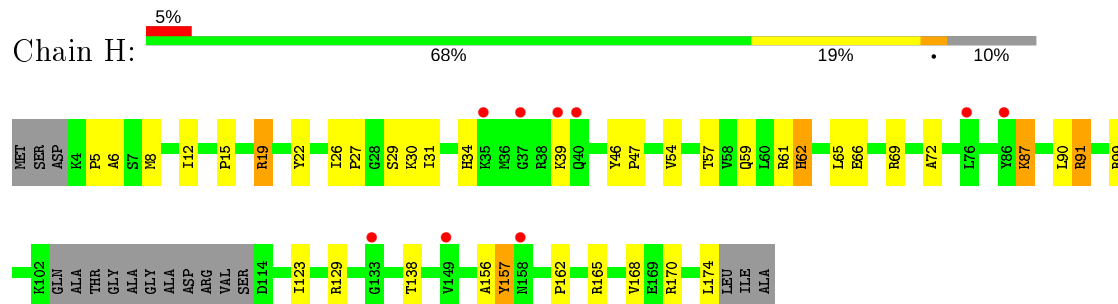


- Molecule 7: 50S ribosomal protein L10E

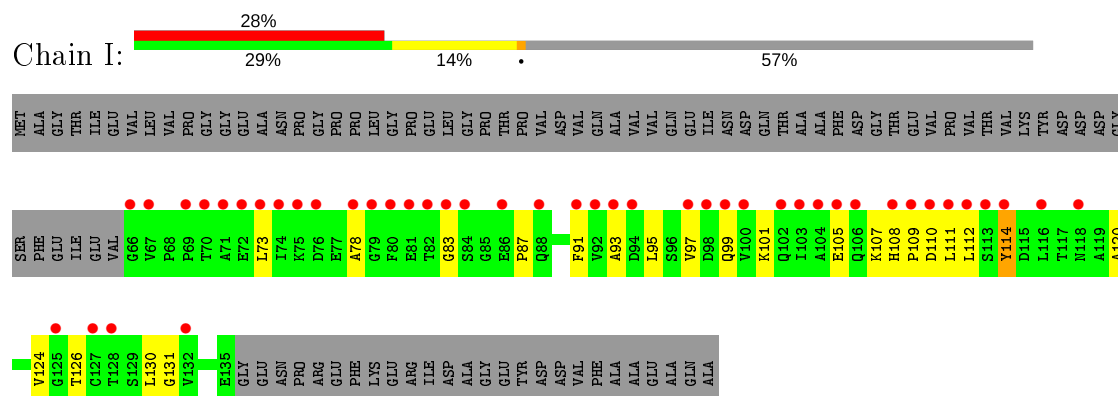




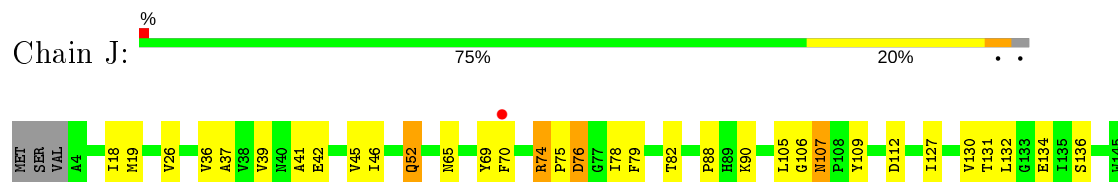
- Molecule 8: 50S ribosomal protein L10e



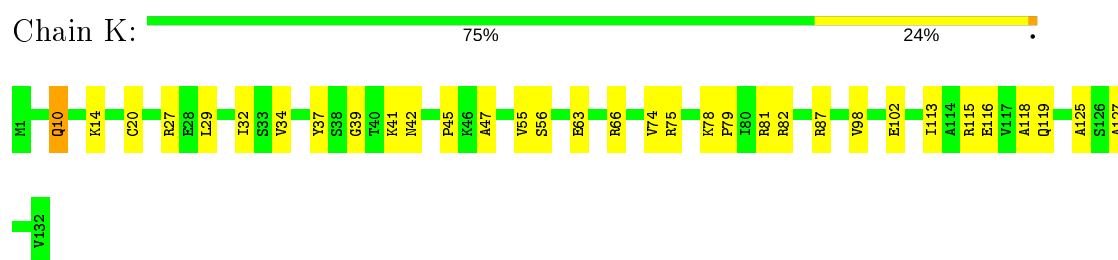
- Molecule 9: 50S ribosomal protein L11P



- Molecule 10: 50S ribosomal protein L13P

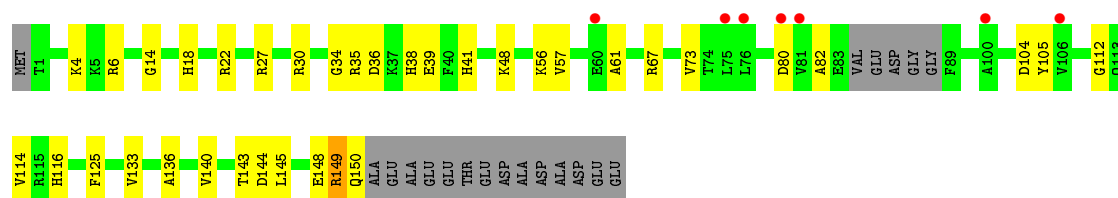


- Molecule 11: 50S ribosomal protein L14P



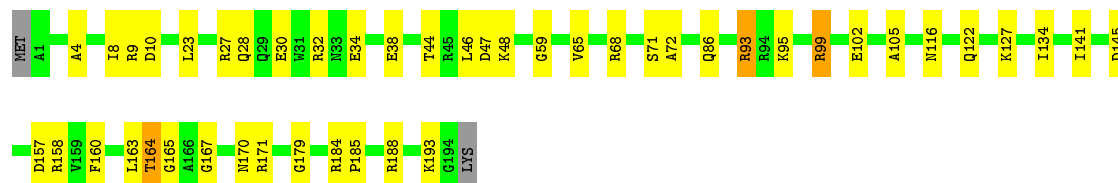
- Molecule 12: 50S ribosomal protein L15P





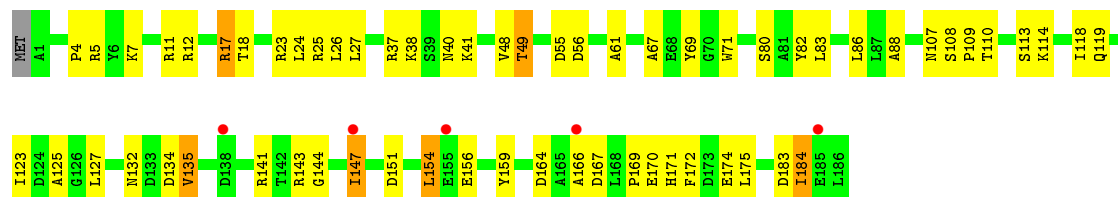
- Molecule 13: 50S ribosomal protein L15e

Chain M: 76% 22%



- Molecule 14: 50S ribosomal protein L18P

Chain N: 3% 66% 30%



- Molecule 15: 50S ribosomal protein L18e

Chain O: 82% 16%



- Molecule 16: 50S ribosomal protein L19e

Chain P: 77% 17%




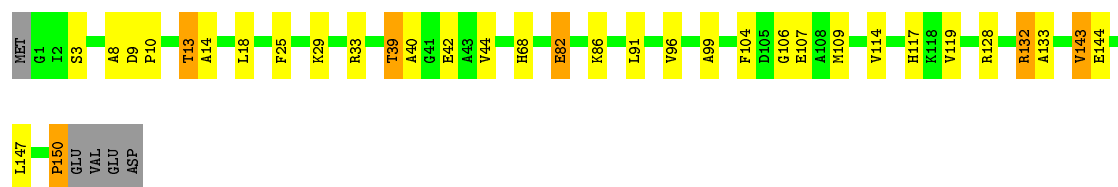
- Molecule 17: 50S ribosomal protein L21e

Chain Q: 78% 20%




- Molecule 18: 50S ribosomal protein L22P

Chain R:  75% 18%



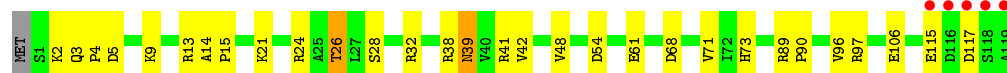
- Molecule 19: 50S ribosomal protein L23P

Chain S:  78% 18% 5%



- Molecule 20: 50S ribosomal protein L24P

Chain T:  4% 74% 23%



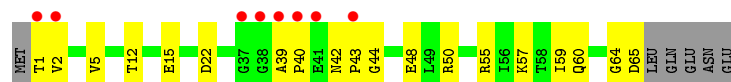
- Molecule 21: 50S ribosomal protein L24e

Chain U:  61% 18% 21%



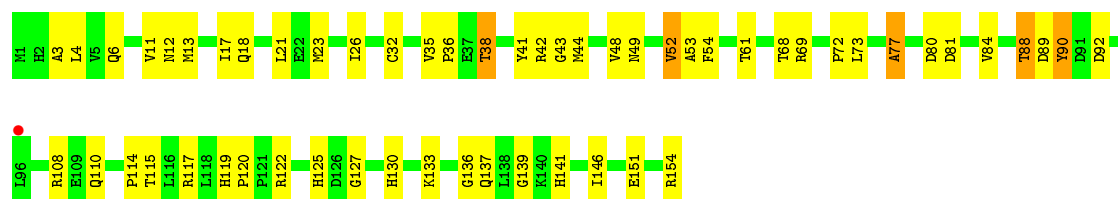
- Molecule 22: 50S ribosomal protein L29P

Chain V:  11% 65% 27% 8%



- Molecule 23: 50S ribosomal protein L30P

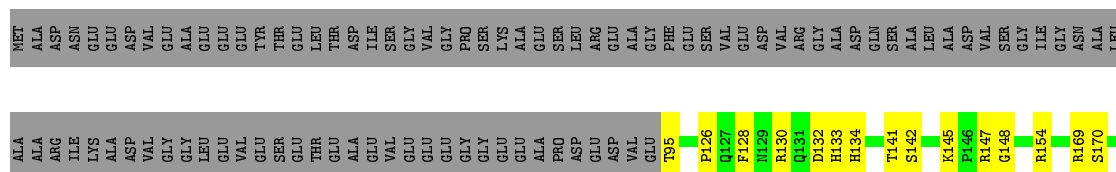
Chain W:  64% 33%



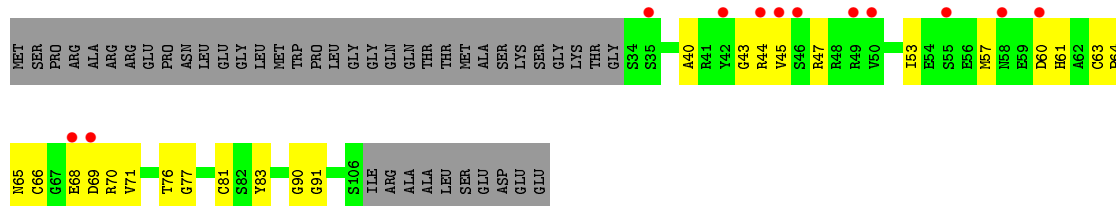
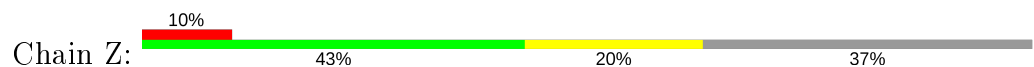
- Molecule 24: 50S ribosomal protein L31e



- Molecule 25: 50S ribosomal protein L32e



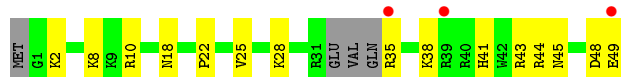
- Molecule 26: 50S ribosomal protein L37Ae



- Molecule 27: 50S ribosomal protein L37e



- Molecule 28: 50S ribosomal protein L39e

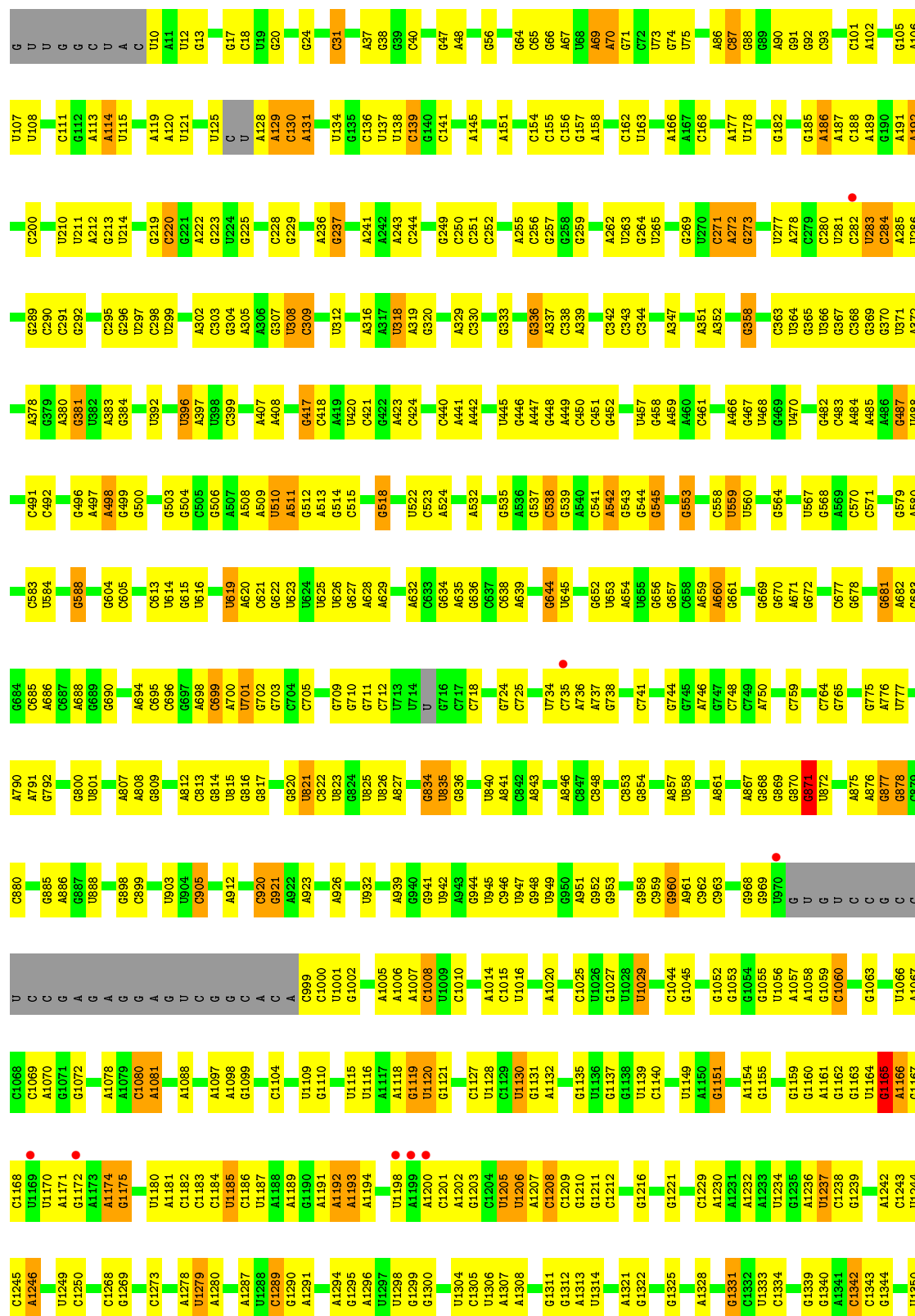


- Molecule 29: 50S ribosomal protein L44E

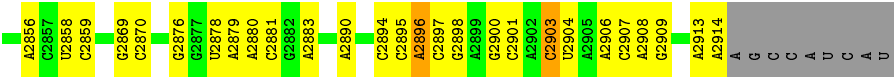


• Molecule 30: 23S RIBOSOMAL RNA

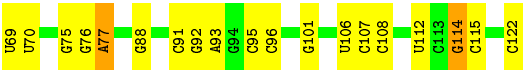
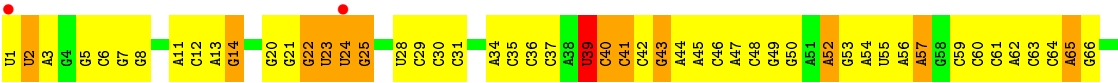
Chain 0: 



G2670	A2483	G2385	C2309	C	U	G2082	C	C1856	G1752	G1655	C1554	G1351
U2671	U2484	U2387	C2313	C	A	A2083	U1964	A1857	A1759	A1656	G1555	A1352
C2672	C2388	C2388	G2314	U	A	C2088	C1965	A1858	U1760	A1657	G	C1353
U2673	U2389	C2315	G2316	C	A	C2089	H1967	G1863	U1761	U	A1559	
C2676	A2480	A2401	C2317	C	G	G2090	A1968	G1868	C1762	U1561	U1446	A1358
	U2482	C2403	U2320	U	U	G2091	A1969	G1871	C1763	C1666	U1447	U1359
A2680	C2493	G2404	U2321	A	C	A2096	G1970	U1871	U1766	U1667	C1450	C1360
C2682	C2498	U2408	C2326	C	U	A2096	U1972	G1872	U1767	U1668	A1573	C1366
A2689	U2499			U	A	A2101	A1973	G1873	C1768	U1677	G1586	A1372
U2690	C2502	G2412	C2329	G	C	G2102	G1974	U1877	C1769	A1678	U1587	C1373
A2691	A2413	U2595	U2330	C	A	A2103	A1978	U1878	U1770	G1679	C1462	G1374
C2692	A2504	A2414	C2331	C	A	C2104	G1979	U1879	C1771	A1682	C1474	A1375
U2693	G2505	A2415	A2332	C2238	A	C2105	U1980	U1883	G1773	G1683	G1593	G1376
A2694	A2506	G2416	G2333	U2240	G	C2106	U1992	G1894	G1774	A1685	C1594	G1378
C2695	C2507	U2419	C2334	C2241	U	G2110	A1993	A1895	A1778	C1686	G1595	U1390
G2696	U2420	A2402	C2335	U2242	A	G2111	U1994	A1896	A1779	C1687	U1596	C1483
A2697	C2493	C2403	G2336	C2243	C	A2112	G1995	G1484	U1770	A1597	G1484	G1382
G2698	G2421	U2422	C2337	C	C	G2113	U1996	U1896	C1787	C1692	A1598	G1383
	U2422		G2338	C2248	C	C2114	U1996	U1897	U1783	G1697	A1486	C1384
G2709	U2512	G2426	A	C2248	G	U2115	G2000	U1903	G1789	C1790	A1603	G1386
U2710	C2513		C	G2250	C	U2116	G2001	A1904	U1791	C1700	G1604	G1387
U2711	U2514	A2433	A	G2251	C	G2121	U2002	U1905	U1791	A1701	G1605	
G2713	A2521	U2434	A2252	C2253	U	C2122	U2004	A1909	G1795	U1702	A1607	C1495
	G2522	U2434	G2253	G2254	A		G2005	A1909	A1796	G1706	C1613	U1503
G2716	U2523	U2435	G2344	G2254	G	G2128	A2007	A1919	U1797	C1707	G1614	A1504
C2717	G2524	U2436	A2345	A2255	C		C2006	C1920	C1798	U1715	U1505	C1394
U2718	G2525	A2437	C2346	G2256	G	G2134	U2008	G1819	G1805	A1710	U1506	C1395
C2719	C2526	G2438	C2347	G2257	C	A2135	G2009	A1921	G1806	A1616	C1396	C1396
A2719	U2527		C2348	A2258	G	G2136	G2009	A1922		C1617	G1513	G1397
C2720	U2528	C2443	A2353	G2263	C	A	A2010	A1922		C1714	C1514	G1398
U2721	G2529	U2444	A2354	A2264	C	C	U2011	A1922	U1825	C1715	A1515	A1399
G2722	C2533	U2445	A2354	A2264	A	G	G2012	G1925	C1818	C1622	U1516	
C2723	G2534	G2446	A2355	U2265	C	A	U2013	G1926	G1819	C1623	C1400	
	C2535		A2356	A2266	C	U	U2032	A1927	G1820	A1717	G1520	G1401
U2726	C2536	G2453	C2359	C2269	C	C	U2032	C1940	U1825	U1625	G1520	
A2727	G2537	A2456	G2350	G2270	A	U	G2033	A1941	C1826	A1626	C1521	
G2734	U2541	U2461	A2361	G2271	G	C	U2034	A1942		G1627	A1522	H1408
U2735	C2542	U2462	G2362	C2272	A	C	A	A1943		U1724	G1523	G1409
C2736	G2543	G2462	G2363	C2273	C	C	G2039	C1943		C1725	U1630	
U2737	G2544		A2364	A2274	C	C	G2044	G1947	C1830	A1631	G1524	A1413
	A2465	A2466	A2367	G2275	A	A	C	G1948	G1834	C1730	A1632	A1414
C2747	C2547	A2467	A2368	G2276	C	A	A2054	G1949	U1835	C1731	C1633	G1415
U2748	C2548		U2277	U2276	A	U	A2055	G1950		A1732	A1527	
A2749	A2468	A2469	A2369	U2277	C	A	G		U1838	C1733	G1635	U1528
G2750	C2552		A2371	C2281	G	G	G2058	G1951		G1734	U1635	G1529
	A2553		A2372	U2282	U	U	U	U		C1735	G1636	
G2751	C2559	C2472	G2373	U2282	C	A	U2064	A	A1840	A1736	A1637	U1422
C2752	C2560		G2374	U2280	A	C		C	A1845	G1739	A1641	C1536
U2753	A2375	C2476	A2375	A2291	A	G	G2070	U	U1846	U1740	A1642	C1423
U2756	C2376	C2477	U2376	C2071	U	C	C2071	A	G1847	U1741	C1644	A1424
A2757	U2563	G2478	G2299	G2072	A	A	G2072	U	A1742	U1742	U1645	C1425
C2758	G2564	A2479	G2300	G2073	C	U	A	G		G1743	C1545	C1426
C2759	A	U	A2301	A2074	U	C	A2074	A			G1546	G1430
	A2566	G2480	G2380	A2301	C	U		G				
G2762	C2567	G2481	A2302	A2302	A	C		C			C1652	A1434
					C	G		C			G1552	A1435
C2765	C2570				A	C		C			G1554	C1436



● 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	213.16Å 300.03Å 576.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.98 – 2.90 85.91 – 2.41	Depositor EDS
% Data completeness (in resolution range)	92.2 (49.98-2.90) 92.3 (85.91-2.41)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.171 , 0.220 0.165 , 0.212	Depositor DCC
R_{free} test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	57.0	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 81.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	99122	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% of the height of the origin peak. No significant pseudotranslation is detected.*

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	0.32	0/1786	0.64	0/2408
2	B	0.32	0/2690	0.64	0/3652
3	C	0.36	0/1885	0.63	0/2552
4	D	0.32	0/1111	0.56	0/1498
5	E	0.33	0/1382	0.56	0/1880
6	F	0.34	0/901	0.58	0/1224
7	G	0.31	0/241	0.49	0/324
8	H	0.33	0/1302	0.63	0/1743
9	I	0.29	0/526	0.51	0/716
10	J	0.36	0/1136	0.60	0/1530
11	K	0.35	0/1004	0.67	0/1351
12	L	0.33	0/1130	0.63	0/1509
13	M	0.35	0/1582	0.61	0/2116
14	N	0.30	0/1474	0.62	0/1999
15	O	0.34	0/874	0.59	0/1181
16	P	0.32	0/1147	0.51	0/1528
17	Q	0.33	0/749	0.65	0/1005
18	R	1.26	7/1172 (0.6%)	1.10	6/1578 (0.4%)
19	S	0.32	0/648	0.55	0/875
20	T	0.33	0/958	0.64	0/1289
21	U	0.33	0/417	0.59	0/562
22	V	0.33	0/502	0.52	0/675
23	W	0.34	0/1219	0.63	0/1655
24	X	0.35	0/664	0.60	0/895
25	Y	0.36	0/1146	0.62	0/1536
26	Z	0.37	0/584	0.60	0/781
27	1	0.39	0/438	0.59	0/578
28	2	0.34	0/401	0.60	0/529
29	3	0.36	0/771	0.55	0/1024
30	0	0.37	0/65957	0.68	13/102867 (0.0%)
31	9	0.32	0/2904	0.68	1/4526 (0.0%)
All	All	0.38	7/98701 (0.0%)	0.67	20/147586 (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	28
31	9	0	1
All	All	1	30

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	150	PRO	CB-CG	27.29	2.86	1.50
18	R	150	PRO	CA-C	-18.25	1.16	1.52
18	R	150	PRO	CG-CD	13.93	1.96	1.50
18	R	150	PRO	C-O	11.88	1.47	1.23
18	R	150	PRO	N-CA	11.37	1.66	1.47
18	R	150	PRO	N-CD	10.73	1.62	1.47
18	R	150	PRO	CA-CB	7.62	1.68	1.53

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	150	PRO	CB-CA-C	-22.47	55.83	112.00
18	R	150	PRO	N-CA-C	-19.40	61.65	112.10
18	R	150	PRO	CA-N-CD	12.30	128.92	111.70
18	R	150	PRO	N-CA-CB	10.97	116.46	103.30
18	R	150	PRO	CA-C-O	-8.51	99.79	120.20
30	0	1120	U	C5'-C4'-C3'	-6.39	105.78	116.00
30	0	1942	A	C5'-C4'-C3'	6.16	125.85	116.00
18	R	150	PRO	CA-CB-CG	-6.09	92.42	104.00
30	0	1592	G	N9-C1'-C2'	5.90	121.67	114.00
30	0	1504	A	C1'-O4'-C4'	-5.90	105.18	109.90
31	9	39	U	N1-C1'-C2'	5.83	121.57	114.00
30	0	871	G	C5'-C4'-O4'	-5.67	102.30	109.10
30	0	2316	G	C5'-C4'-C3'	-5.59	107.06	116.00
30	0	1504	A	N9-C1'-C2'	5.50	121.15	114.00
30	0	841	A	C1'-O4'-C4'	-5.46	105.53	109.90
30	0	2313	C	C5'-C4'-O4'	5.29	115.45	109.10
30	0	2726	U	N1-C1'-C2'	5.25	120.83	114.00
30	0	1165	G	C1'-O4'-C4'	-5.21	105.73	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2291	A	N9-C1'-C2'	5.20	120.75	114.00
30	0	2301	A	N9-C1'-C2'	5.11	120.65	114.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	R	150	PRO	CA

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	1078	A	Sidechain
30	0	131	A	Sidechain
30	0	1430	G	Sidechain
30	0	1592	G	Sidechain
30	0	1829	A	Sidechain
30	0	1848	G	Sidechain
30	0	1863	G	Sidechain
30	0	1877	G	Sidechain
30	0	1878	G	Sidechain
30	0	1970	G	Sidechain
30	0	220	C	Sidechain
30	0	2301	A	Sidechain
30	0	2412	G	Sidechain
30	0	2465	A	Sidechain
30	0	2493	C	Sidechain
30	0	2503	A	Sidechain
30	0	2524	G	Sidechain
30	0	2552	C	Sidechain
30	0	2607	U	Sidechain
30	0	2673	U	Sidechain
30	0	2842	G	Sidechain
30	0	333	G	Sidechain
30	0	396	U	Sidechain
30	0	458	G	Sidechain
30	0	48	A	Sidechain
30	0	518	G	Sidechain
30	0	619	U	Sidechain
30	0	888	U	Sidechain
31	9	39	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	63	0
2	B	2625	0	2533	89	0
3	C	1860	0	1813	59	0
4	D	1094	0	1085	45	0
5	E	1357	0	1266	29	0
6	F	890	0	843	26	0
7	G	240	0	231	8	0
8	H	1282	0	1292	33	0
9	I	519	0	500	23	0
10	J	1120	0	1098	32	0
11	K	994	0	1027	32	0
12	L	1118	0	1076	29	0
13	M	1558	0	1573	42	0
14	N	1445	0	1401	51	0
15	O	865	0	873	18	0
16	P	1136	0	1123	24	0
17	Q	735	0	729	21	0
18	R	1149	0	1122	37	0
19	S	641	0	605	10	0
20	T	950	0	924	21	0
21	U	410	0	364	8	0
22	V	499	0	511	17	0
23	W	1196	0	1137	56	0
24	X	654	0	653	18	0
25	Y	1130	0	1133	23	0
26	Z	573	0	532	15	0
27	1	431	0	426	23	0
28	2	396	0	413	15	0
29	3	755	0	728	18	0
30	0	59020	0	29811	1159	0
31	9	2599	0	1325	100	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	10	0	0	4	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	0	0
33	N	1	0	0	1	0
33	O	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	67	0	0	0	0
35	9	2	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	1	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	5929	0	0	185	0
38	1	63	0	0	4	0
38	2	50	0	0	1	0
38	3	62	0	0	3	0
38	9	147	0	0	7	0
38	A	116	0	0	5	0
38	B	141	0	0	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	C	170	0	0	13	0
38	D	44	0	0	3	0
38	E	45	0	0	2	0
38	F	27	0	0	2	0
38	G	19	0	0	1	0
38	H	63	0	0	7	0
38	I	8	0	0	3	0
38	J	53	0	0	1	0
38	K	56	0	0	5	0
38	L	85	0	0	6	0
38	M	123	0	0	2	0
38	N	55	0	0	5	0
38	O	43	0	0	3	0
38	P	67	0	0	2	0
38	Q	50	0	0	3	0
38	R	85	0	0	1	0
38	S	33	0	0	2	0
38	T	34	0	0	2	0
38	U	27	0	0	2	0
38	V	13	0	0	2	0
38	W	69	0	0	4	0
38	X	25	0	0	2	0
38	Y	95	0	0	5	0
38	Z	26	0	0	3	0
All	All	99122	0	59913	1941	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 13.

All (1941) 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	1.43
30:0:1160:G:C5'	30:0:1161:A:H5'	1.77	1.12
30:0:871:G:C8	30:0:871:G:H5'	1.84	1.11
30:0:871:G:H8	30:0:871:G:H5'	1.09	1.10
31:9:56:A:H2'	31:9:57:A:H5''	1.31	1.10
14:N:37:ARG:NH1	31:9:6:C:H5''	1.63	1.09
30:0:1160:G:H5'	30:0:1161:A:C5'	1.82	1.09
13:M:171:ARG:HD3	30:0:156:C:H5''	1.33	1.09
18:R:150:PRO:CG	18:R:150:PRO:C	2.22	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:76:G:H3'	31:9:77:A:H5''	1.36	1.06
30:0:545:G:H8	30:0:545:G:H5'	1.19	1.06
30:0:1205:U:H2'	30:0:1206:U:H5''	1.32	1.04
30:0:1160:G:H5'	30:0:1161:A:H5'	1.03	1.02
30:0:1701:A:H4'	30:0:1702:U:H5''	1.42	1.01
10:J:82:THR:HG23	30:0:1242:A:H5'	1.39	1.01
15:O:3:THR:HG22	30:0:656:G:H5'	1.41	1.01
30:0:2717:C:C2'	30:0:2718:C:H5''	1.92	0.99
30:0:1979:G:H2'	38:0:3301:HOH:O	1.61	0.98
31:9:29:C:H2'	31:9:30:C:H5'	1.44	0.98
20:T:71:VAL:HG11	20:T:90:PRO:HB3	1.46	0.97
11:K:10:GLN:H	11:K:10:GLN:HE21	0.95	0.95
30:0:182:G:H5'	38:0:5168:HOH:O	1.67	0.95
30:0:1666:C:O2'	30:0:1667:A:H5''	1.67	0.94
30:0:1118:A:H3'	30:0:1118:A:H8	1.30	0.94
30:0:2717:C:H2'	30:0:2718:C:H5''	1.50	0.94
30:0:381:G:H5''	38:0:4330:HOH:O	1.67	0.93
30:0:1187:U:HO2'	30:0:1189:A:H2	1.01	0.93
30:0:1205:U:H2'	30:0:1206:U:C5'	1.99	0.93
30:0:1118:A:H3'	30:0:1118:A:C8	2.03	0.93
30:0:1603:A:H5'	30:0:1605:G:O4'	1.67	0.92
30:0:1634:G:H3'	38:0:3907:HOH:O	1.70	0.91
30:0:282:C:H1'	30:0:368:C:N4	1.84	0.91
16:P:115:SER:H	16:P:118:GLN:HE21	1.03	0.91
10:J:52:GLN:NE2	30:0:1119:G:H2'	1.85	0.91
30:0:271:C:H41	30:0:378:A:H2	1.17	0.90
2:B:162:MET:SD	2:B:310:ARG:HD3	2.11	0.90
30:0:559:U:H5'	30:0:559:U:H6	1.35	0.90
30:0:545:G:C8	30:0:545:G:H5'	2.05	0.90
30:0:871:G:H8	30:0:871:G:C5'	1.85	0.90
23:W:137:GLN:HE21	23:W:141:HIS:HE1	1.20	0.90
30:0:542:A:H5'	30:0:542:A:H8	1.36	0.90
31:9:14:G:H5'	31:9:14:G:H8	1.37	0.90
31:9:56:A:C2'	31:9:57:A:H5''	2.03	0.89
26:Z:70:ARG:HD3	26:Z:83:TYR:HB2	1.55	0.89
30:0:1119:G:H22	30:0:1246:A:H2	1.20	0.89
30:0:870:G:H2'	30:0:871:G:H5''	1.53	0.89
8:H:59:GLN:HE21	8:H:129:ARG:HE	1.17	0.88
30:0:1632:A:H2'	30:0:1633:C:H5'	1.56	0.88
30:0:2508:C:H2'	38:0:6764:HOH:O	1.73	0.87
30:0:1835:U:H5	30:0:1840:A:N7	1.72	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:558:C:C2'	30:0:559:U:H5''	2.05	0.86
30:0:1205:U:C2'	30:0:1206:U:H5''	2.05	0.86
30:0:506:G:H22	30:0:509:A:H5'	1.40	0.86
30:0:1184:C:H1'	38:0:7480:HOH:O	1.74	0.86
30:0:2507:G:H2'	30:0:2510:C:H42	1.41	0.86
8:H:59:GLN:NE2	8:H:129:ARG:HE	1.73	0.86
30:0:2908:A:H2'	30:0:2909:G:O4'	1.76	0.86
30:0:541:C:C2'	30:0:542:A:H5''	2.06	0.86
30:0:1189:A:H1'	30:0:1209:C:O4'	1.76	0.85
4:D:25:MET:HE3	4:D:37:ALA:HB1	1.58	0.85
30:0:1183:C:H2'	38:0:6249:HOH:O	1.76	0.85
24:X:37:LEU:HD13	24:X:85:VAL:HG21	1.58	0.85
30:0:1667:A:H8	30:0:1667:A:H5'	1.41	0.85
16:P:117:SER:HB3	30:0:1593:C:OP1	1.75	0.85
30:0:2717:C:O2'	30:0:2718:C:H5''	1.77	0.85
30:0:541:C:H2'	30:0:542:A:H5''	1.58	0.85
30:0:2586:U:H3	30:0:2592:G:H22	1.22	0.84
30:0:2291:A:C8	30:0:2309:C:H5'	2.12	0.84
2:B:238:ASN:HD22	2:B:240:GLY:H	1.24	0.84
38:O:7674:HOH:O	30:0:653:U:H5''	1.77	0.84
30:0:1206:U:H6	30:0:1206:U:H5'	1.41	0.84
30:0:2710:U:H1'	38:0:7632:HOH:O	1.77	0.84
30:0:2506:A:HO2'	30:0:2507:G:H8	1.21	0.84
31:9:2:U:OP2	31:9:3:A:H5'	1.78	0.84
30:0:1474:C:H5'	30:0:1474:C:H6	1.43	0.83
30:0:1474:C:H5'	30:0:1474:C:C6	2.13	0.83
18:R:29:LYS:HE2	30:0:524:A:C5'	2.08	0.83
30:0:558:C:O2'	30:0:559:U:H5''	1.78	0.83
4:D:154:LYS:HD2	4:D:154:LYS:H	1.43	0.83
30:0:506:G:H22	30:0:509:A:C5'	1.92	0.83
30:0:877:G:H5'	30:0:878:G:OP1	1.79	0.83
30:0:1119:G:N2	30:0:1246:A:C2	2.46	0.82
30:0:1116:U:O2'	30:0:1118:A:H2	1.62	0.82
14:N:37:ARG:HH12	31:9:6:C:H5''	1.43	0.82
18:R:29:LYS:HE2	30:0:524:A:H5''	1.59	0.82
30:0:1116:U:H3	30:0:1246:A:H62	1.24	0.82
30:0:283:U:H5	30:0:284:C:N3	1.78	0.81
2:B:221:GLN:HE22	11:K:42:ASN:HD22	1.27	0.81
30:0:69:A:H5'	30:0:69:A:C8	2.15	0.81
23:W:4:LEU:HD23	23:W:54:PHE:HB3	1.62	0.81
30:0:1878:G:H1'	38:0:6126:HOH:O	1.77	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2852:A:H5'	38:0:5244:HOH:O	1.80	0.81
15:O:3:THR:CG2	30:0:656:G:H5'	2.10	0.81
2:B:74:ILE:HD13	2:B:309:VAL:HG21	1.63	0.81
30:0:541:C:H2'	30:0:542:A:C5'	2.11	0.81
30:0:2529:G:H3'	38:0:7197:HOH:O	1.80	0.80
30:0:2506:A:O2'	30:0:2507:G:H8	1.64	0.79
22:V:12:THR:HG22	22:V:15:GLU:HG3	1.62	0.79
10:J:75:PRO:HG2	10:J:105:LEU:HD21	1.63	0.79
11:K:10:GLN:H	11:K:10:GLN:NE2	1.79	0.79
30:0:2502:C:C2'	30:0:2503:A:H5'	2.13	0.78
2:B:217:ARG:HG3	2:B:257:THR:HG22	1.65	0.78
14:N:83:LEU:HD13	14:N:175:LEU:HD23	1.64	0.78
11:K:39:GLY:HA2	38:0:5232:HOH:O	1.83	0.78
30:0:2578:G:H5'	30:0:2578:G:H8	1.48	0.78
30:0:1632:A:C2'	30:0:1633:C:H5'	2.13	0.78
30:0:2256:G:O2'	30:0:2257:G:H5'	1.82	0.78
3:C:236:THR:HG22	3:C:239:ALA:H	1.46	0.78
18:R:8:ALA:HB1	18:R:13:THR:HG21	1.66	0.78
30:0:282:C:O2'	30:0:283:U:H5'	1.84	0.78
14:N:113:SER:HB2	38:N:8849:HOH:O	1.84	0.77
23:W:6:GLN:HB2	23:W:26:ILE:HD11	1.67	0.77
30:0:2526:C:H5'	30:0:2526:C:C6	2.19	0.77
2:B:195:ARG:HG2	2:B:323:LEU:HD22	1.65	0.77
30:0:1300:G:H1'	38:0:4694:HOH:O	1.83	0.77
30:0:2635:A:O2'	30:0:2636:C:H5'	1.84	0.77
30:0:272:A:H3'	38:0:7542:HOH:O	1.84	0.77
13:M:164:THR:HG22	13:M:167:GLY:H	1.50	0.77
30:0:2502:C:H2'	30:0:2503:A:H5'	1.65	0.77
30:0:2608:C:H3'	38:0:7824:HOH:O	1.85	0.77
30:0:396:U:H1'	38:0:7640:HOH:O	1.85	0.77
31:9:14:G:H5'	31:9:14:G:C8	2.19	0.77
30:0:69:A:H5'	30:0:69:A:H8	1.50	0.76
2:B:179:LEU:O	2:B:183:GLU:HG2	1.84	0.76
2:B:36:PRO:HA	2:B:168:GLY:HA3	1.67	0.76
30:0:1118:A:H62	30:0:1244:U:H3	1.31	0.76
30:0:1701:A:H5'	38:0:6290:HOH:O	1.83	0.76
30:0:2783:A:H3'	38:0:5242:HOH:O	1.83	0.76
30:0:2812:A:H2	30:0:2814:A:H62	1.31	0.76
30:0:2679:G:H2'	30:0:2681:A:OP2	1.86	0.76
31:9:54:A:O2'	31:9:55:U:H5'	1.85	0.76
30:0:1372:A:H3'	38:0:7202:HOH:O	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2403:C:H5'	38:0:6033:HOH:O	1.84	0.76
22:V:1:THR:HB	30:0:93:C:H5''	1.68	0.76
30:0:192:A:H5'	38:0:7655:HOH:O	1.85	0.76
30:0:1603:A:H5''	30:0:1605:G:H5'	1.68	0.75
26:Z:61:HIS:HB2	26:Z:71:VAL:HB	1.69	0.75
6:F:91:VAL:HG12	6:F:92:GLY:H	1.52	0.75
30:0:1172:G:H5''	38:0:7271:HOH:O	1.85	0.75
10:J:74:ARG:HB3	10:J:74:ARG:HH11	1.51	0.75
30:0:1116:U:HO2'	30:0:1118:A:H2	0.79	0.74
30:0:558:C:H2'	30:0:559:U:C5'	2.17	0.74
30:0:1701:A:H4'	30:0:1702:U:C5'	2.15	0.74
3:C:1:MET:HG2	3:C:2:GLN:H	1.51	0.74
30:0:2748:G:H5'	38:0:7554:HOH:O	1.87	0.74
30:0:2768:A:O2'	30:0:2769:C:H5'	1.87	0.74
30:0:2420:G:O2'	30:0:2421:G:H5'	1.86	0.74
6:F:63:ILE:HB	6:F:64:PRO:HD3	1.69	0.74
30:0:2717:C:H2'	30:0:2718:C:C5'	2.18	0.74
13:M:99:ARG:HD2	13:M:167:GLY:HA2	1.70	0.74
30:0:2404:G:H5''	38:0:5222:HOH:O	1.88	0.74
3:C:127:ARG:NH2	3:C:225:PRO:HG2	2.03	0.74
18:R:25:PHE:CE2	18:R:29:LYS:HE3	2.23	0.73
33:0:8812:CL:CL	38:0:5135:HOH:O	2.41	0.73
11:K:10:GLN:N	11:K:10:GLN:HE21	1.79	0.73
30:0:1666:C:H2'	30:0:1667:A:H5'	1.70	0.73
22:V:1:THR:HG23	22:V:2:VAL:H	1.53	0.73
30:0:2004:U:H4'	38:0:5316:HOH:O	1.88	0.73
5:E:143:GLN:HE21	30:0:2780:C:H1'	1.54	0.73
29:3:65:THR:HG22	29:3:67:LEU:HG	1.69	0.73
1:A:211:LYS:HB2	38:A:9082:HOH:O	1.87	0.73
30:0:138:U:H5''	30:0:139:C:OP2	1.88	0.73
15:O:42:GLU:HB2	38:O:2176:HOH:O	1.87	0.73
30:0:2896:A:H5''	38:0:6105:HOH:O	1.87	0.73
15:O:47:ARG:HG3	15:O:47:ARG:HH11	1.53	0.73
38:Z:8707:HOH:O	30:0:1886:A:H4'	1.89	0.73
3:C:139:VAL:HG13	38:C:8644:HOH:O	1.88	0.73
18:R:99:ALA:HB1	18:R:109:MET:HE1	1.71	0.73
30:0:1666:C:C2'	30:0:1667:A:H5''	2.19	0.72
30:0:1641:A:H2'	30:0:1642:A:H5'	1.71	0.72
30:0:2765:C:H4'	38:0:5531:HOH:O	1.88	0.72
5:E:100:ASP:HB2	38:E:2789:HOH:O	1.88	0.72
30:0:870:G:C2'	30:0:871:G:H5''	2.18	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:50:ARG:NH1	30:0:56:G:H5''	2.04	0.72
30:0:1118:A:C8	30:0:1118:A:C3'	2.69	0.72
30:0:2256:G:C2'	30:0:2257:G:H5'	2.18	0.72
28:2:41:HIS:H	28:2:45:ASN:HD22	1.35	0.72
30:0:468:U:H3'	38:0:7580:HOH:O	1.89	0.72
30:0:827:A:H1'	38:0:6220:HOH:O	1.88	0.72
30:0:871:G:C8	30:0:871:G:C5'	2.64	0.72
30:0:1187:U:O2'	30:0:1189:A:H2	1.71	0.72
30:0:1201:C:H5''	38:0:6238:HOH:O	1.89	0.72
10:J:70:PHE:CE1	30:0:2676:C:H4'	2.24	0.72
30:0:2769:C:C2'	30:0:2770:G:H5'	2.20	0.72
20:T:9:LYS:HE2	20:T:13:ARG:NH1	2.04	0.72
22:V:50:ARG:HH12	30:0:56:G:H5''	1.55	0.72
1:A:135:VAL:HG11	1:A:147:ARG:NH2	2.04	0.71
33:0:8813:CL:CL	38:0:4694:HOH:O	2.45	0.71
30:0:1183:C:N4	30:0:1184:C:H41	1.87	0.71
10:J:52:GLN:HE22	30:0:1119:G:H2'	1.55	0.71
30:0:1525:G:H5'	30:0:1526:A:OP2	1.91	0.71
30:0:2491:G:H1'	38:0:6878:HOH:O	1.89	0.71
31:9:29:C:C2'	31:9:30:C:H5'	2.18	0.71
30:0:1189:A:H3'	38:0:7693:HOH:O	1.90	0.71
30:0:1741:U:H5'	30:0:1742:A:OP1	1.90	0.71
30:0:2372:A:H2'	30:0:2373:U:H6	1.56	0.70
25:Y:187:VAL:HG23	25:Y:192:ASP:CB	2.21	0.70
25:Y:169:ARG:HD2	30:0:1328:A:OP1	1.92	0.70
2:B:206:THR:HG21	30:0:2716:G:H5''	1.73	0.70
2:B:307:ARG:HH11	2:B:307:ARG:HG3	1.57	0.70
30:0:2659:U:H5''	38:0:4138:HOH:O	1.92	0.70
28:2:43:ARG:HH22	30:0:1684:A:H1'	1.57	0.70
31:9:20:G:O2'	31:9:21:G:H5'	1.91	0.70
30:0:2637:A:H5'	38:0:9281:HOH:O	1.92	0.70
31:9:92:G:H2'	31:9:93:A:C8	2.27	0.70
30:0:567:U:H5''	38:0:5297:HOH:O	1.92	0.70
30:0:1973:A:H5'	30:0:1973:A:H8	1.57	0.69
30:0:1835:U:C5	30:0:1840:A:N7	2.59	0.69
30:0:1750:C:H5''	38:0:3676:HOH:O	1.91	0.69
30:0:2010:A:H2'	38:0:5965:HOH:O	1.91	0.69
30:0:380:A:H2'	38:0:7240:HOH:O	1.92	0.69
30:0:544:G:H2'	30:0:545:G:H5''	1.74	0.69
10:J:19:MET:HE3	10:J:132:LEU:HD21	1.75	0.69
24:X:71:ARG:HD3	38:X:2171:HOH:O	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:12:ILE:HG23	38:0:5468:HOH:O	1.93	0.69
30:0:281:U:O2'	30:0:282:C:H5'	1.93	0.69
11:K:98:VAL:CG1	11:K:102:GLU:HA	2.23	0.69
16:P:115:SER:H	16:P:118:GLN:NE2	1.85	0.69
30:0:1441:G:O2'	30:0:1442:A:H5'	1.91	0.69
1:A:51:ARG:HB2	38:A:9066:HOH:O	1.91	0.69
11:K:14:LYS:HB2	11:K:45:PRO:HG2	1.75	0.69
23:W:72:PRO:HG2	23:W:77:ALA:HB3	1.73	0.69
30:0:1377:C:H6	30:0:1377:C:H5'	1.58	0.69
30:0:2251:G:H2'	30:0:2252:A:C8	2.28	0.69
27:1:25:LYS:HD2	28:2:49:GLU:H	1.58	0.68
30:0:1666:C:H2'	30:0:1667:A:C5'	2.22	0.68
30:0:2111:G:H1'	38:0:9053:HOH:O	1.92	0.68
8:H:59:GLN:HE21	8:H:129:ARG:NE	1.91	0.68
30:0:2768:A:H2'	30:0:2769:C:O4'	1.93	0.68
30:0:2563:U:H2'	30:0:2565:C:O5'	1.94	0.68
30:0:1183:C:H42	30:0:1184:C:H41	1.42	0.68
3:C:174:ILE:HD11	30:0:338:C:H4'	1.75	0.68
13:M:23:LEU:HD13	13:M:27:ARG:HH21	1.57	0.68
23:W:88:THR:HG23	23:W:110:GLN:HB3	1.75	0.68
12:L:133:VAL:HA	38:L:8874:HOH:O	1.92	0.68
30:0:1603:A:C5'	30:0:1605:G:H5'	2.23	0.68
30:0:2453:G:H3'	38:0:5927:HOH:O	1.94	0.68
14:N:141:ARG:HH21	31:9:48:C:H4'	1.58	0.68
6:F:91:VAL:HG12	6:F:92:GLY:N	2.09	0.68
14:N:80:SER:HB2	38:N:8830:HOH:O	1.93	0.68
30:0:2256:G:H2'	30:0:2257:G:C5'	2.23	0.67
30:0:558:C:H2'	30:0:559:U:H5''	1.72	0.67
18:R:106:GLY:HA2	18:R:109:MET:HE3	1.76	0.67
31:9:39:U:H1'	31:9:44:A:H61	1.59	0.67
29:3:25:VAL:HG22	29:3:68:LYS:HG3	1.75	0.67
31:9:23:U:O2'	31:9:24:U:H4'	1.94	0.67
22:V:57:LYS:HA	22:V:60:GLN:HE21	1.60	0.67
1:A:36:ASP:HB2	1:A:85:SER:H	1.60	0.67
18:R:150:PRO:CG	18:R:150:PRO:O	2.41	0.67
3:C:27:ARG:NH2	30:0:657:G:OP1	2.28	0.67
30:0:1730:G:H5'	30:0:1731:C:C5	2.30	0.67
30:0:285:A:H2'	30:0:286:U:O4'	1.95	0.67
30:0:1834:C:H2'	30:0:1840:A:N6	2.09	0.66
23:W:4:LEU:HD22	23:W:52:VAL:HG21	1.77	0.66
23:W:88:THR:HG22	23:W:89:ASP:H	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:125:U:H2'	38:0:3776:HOH:O	1.94	0.66
30:0:2237:G:H1'	38:0:4866:HOH:O	1.94	0.66
30:0:2509:A:OP2	30:0:2510:C:H5	1.78	0.66
30:0:853:C:H3'	38:0:4563:HOH:O	1.95	0.66
9:I:111:LEU:HD23	30:0:1163:G:H4'	1.76	0.66
30:0:1524:U:OP1	30:0:1524:U:H4'	1.95	0.66
30:0:2256:G:H2'	30:0:2257:G:H5'	1.77	0.66
30:0:2372:A:H2'	30:0:2373:U:C6	2.30	0.66
30:0:1120:U:H5'	30:0:1121:G:OP2	1.95	0.66
14:N:67:ALA:HA	14:N:71:TRP:HB3	1.76	0.66
21:U:14:GLU:O	21:U:17:THR:HB	1.95	0.66
30:0:1159:G:H21	30:0:1189:A:H8	1.42	0.66
31:9:22:G:H5'	31:9:23:U:OP1	1.94	0.66
30:0:1667:A:C8	30:0:1667:A:H5'	2.29	0.66
30:0:2498:C:O2'	30:0:2499:U:H5'	1.94	0.66
30:0:2836:G:H1'	38:0:6850:HOH:O	1.95	0.66
30:0:31:C:H2'	38:0:7702:HOH:O	1.95	0.66
23:W:21:LEU:HD21	23:W:48:VAL:HG11	1.76	0.66
10:J:82:THR:CG2	30:0:1242:A:H5'	2.21	0.66
30:0:2320:U:H4'	30:0:2321:A:O4'	1.95	0.66
8:H:29:SER:HA	8:H:62:HIS:HD2	1.60	0.66
10:J:69:TYR:CE1	30:0:2081:A:H4'	2.31	0.66
23:W:26:ILE:HB	38:W:5420:HOH:O	1.95	0.66
30:0:1562:C:O2	30:0:1562:C:H2'	1.95	0.66
30:0:1819:G:H2'	30:0:1820:G:H4'	1.76	0.66
30:0:2505:G:C2'	30:0:2506:A:H5'	2.25	0.66
30:0:2505:G:O2'	30:0:2506:A:H5'	1.95	0.66
30:0:283:U:C5	30:0:284:C:N3	2.63	0.66
30:0:544:G:C2'	30:0:545:G:H5''	2.26	0.66
30:0:2748:G:H1'	38:0:7914:HOH:O	1.95	0.65
30:0:485:A:N3	30:0:487:G:H5''	2.10	0.65
30:0:2795:C:O2'	30:0:2796:U:H5'	1.96	0.65
13:M:171:ARG:CD	30:0:156:C:H5''	2.18	0.65
29:3:70:ARG:HG2	29:3:77:ALA:HB2	1.78	0.65
1:A:35:GLY:O	1:A:36:ASP:HB3	1.96	0.65
2:B:320:GLN:HE21	2:B:321:PRO:HD2	1.62	0.65
30:0:1477:C:H5'	30:0:1868:G:C5'	2.26	0.65
13:M:102:GLU:OE1	13:M:164:THR:HG21	1.96	0.65
30:0:1666:C:C2'	30:0:1667:A:C5'	2.74	0.65
30:0:2766:A:H5'	38:0:9565:HOH:O	1.97	0.65
30:0:836:G:H5''	38:0:9288:HOH:O	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:3:48:ASN:HD21	30:0:2468:A:H61	1.43	0.65
10:J:74:ARG:O	10:J:78:ILE:HG12	1.97	0.65
30:0:558:C:C2'	30:0:559:U:C5'	2.75	0.64
30:0:960:G:H3'	30:0:960:G:N3	2.12	0.64
30:0:1741:U:O2'	30:0:2723:G:H4'	1.97	0.64
30:0:1183:C:O2	30:0:1183:C:H2'	1.95	0.64
30:0:1279:U:O2	30:0:1279:U:H2'	1.95	0.64
30:0:281:U:H2'	30:0:282:C:O4'	1.96	0.64
31:9:31:C:H1'	38:9:9014:HOH:O	1.96	0.64
18:R:29:LYS:HE2	30:0:524:A:H5'	1.79	0.64
19:S:43:GLU:HB3	38:S:8991:HOH:O	1.97	0.64
2:B:51:VAL:HG13	2:B:53:LEU:HD13	1.80	0.64
10:J:107:ASN:ND2	10:J:109:TYR:H	1.96	0.64
23:W:137:GLN:HE21	23:W:141:HIS:CE1	2.10	0.64
30:0:814:G:H4'	38:0:3141:HOH:O	1.98	0.64
23:W:108:ARG:HH21	23:W:114:PRO:HG2	1.63	0.64
30:0:564:G:H1'	38:0:6317:HOH:O	1.97	0.64
29:3:73:GLU:HB3	38:3:9049:HOH:O	1.97	0.64
11:K:98:VAL:HG13	11:K:102:GLU:HA	1.79	0.64
30:0:2481:G:H5''	38:0:4558:HOH:O	1.97	0.64
2:B:212:GLN:HB2	2:B:257:THR:HG21	1.80	0.64
30:0:1701:A:H5''	30:0:1702:U:H3'	1.80	0.64
30:0:2827:A:H2'	30:0:2828:G:O4'	1.98	0.64
14:N:37:ARG:NH1	31:9:6:C:C5'	2.52	0.63
18:R:9:ASP:O	18:R:13:THR:HB	1.98	0.63
20:T:71:VAL:CG1	20:T:90:PRO:HB3	2.27	0.63
30:0:1058:A:H2'	30:0:1060:C:H5''	1.78	0.63
30:0:12:U:H2'	30:0:13:G:H5'	1.80	0.63
3:C:184:ARG:NH2	30:0:450:C:OP1	2.32	0.63
14:N:11:ARG:HD3	31:9:114:G:O6	1.99	0.63
12:L:41:HIS:HD2	30:0:926:A:O2'	1.80	0.63
38:I:1549:HOH:O	30:0:1180:U:H1'	1.97	0.63
18:R:117:HIS:HD2	30:0:20:G:H21	1.45	0.63
3:C:140:VAL:HB	38:C:8647:HOH:O	1.99	0.63
23:W:6:GLN:CB	23:W:26:ILE:HD11	2.28	0.63
30:0:2768:A:H5''	38:0:4438:HOH:O	1.98	0.63
30:0:1243:C:H3'	38:0:4848:HOH:O	1.99	0.63
30:0:1166:A:OP1	30:0:1174:A:H4'	1.99	0.62
30:0:2509:A:H2'	30:0:2510:C:O4'	1.99	0.62
30:0:671:A:O2'	30:0:672:G:H2'	1.99	0.62
30:0:1185:U:H5'	38:0:7480:HOH:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2426:G:H1'	38:0:6098:HOH:O	1.99	0.62
30:0:2781:U:H2'	30:0:2782:G:H5'	1.79	0.62
30:0:1527:A:H1'	30:0:1528:A:C8	2.34	0.62
30:0:371:U:H2'	30:0:372:A:H8	1.65	0.62
30:0:848:C:H5'	38:0:7283:HOH:O	1.99	0.62
27:1:8:GLN:HE22	27:1:11:LYS:NZ	1.97	0.62
31:9:114:G:H2'	31:9:115:C:C6	2.35	0.62
31:9:49:G:O2'	31:9:50:G:H5'	1.99	0.62
25:Y:187:VAL:HG23	25:Y:192:ASP:HB2	1.80	0.62
30:0:559:U:H5'	30:0:559:U:C6	2.26	0.62
31:9:39:U:H3'	31:9:40:C:H5'	1.82	0.62
11:K:32:ILE:HD11	11:K:56:SER:HB3	1.82	0.62
12:L:136:ALA:HB3	38:L:8874:HOH:O	2.00	0.62
30:0:2316:G:H4'	38:0:6098:HOH:O	2.00	0.62
26:Z:66:CYS:SG	26:Z:68:GLU:HB2	2.39	0.62
30:0:1398:G:O2'	30:0:1399:A:H5'	2.00	0.62
27:1:28:HIS:HE1	30:0:776:A:OP1	1.83	0.62
2:B:156:LYS:HB3	30:0:2846:C:H4'	1.81	0.62
30:0:1278:A:H4'	30:0:1279:U:C4	2.34	0.62
30:0:2748:G:H2'	38:0:7554:HOH:O	1.98	0.62
30:0:378:A:H1'	38:0:3510:HOH:O	1.98	0.62
30:0:542:A:H5'	30:0:542:A:C8	2.25	0.62
30:0:681:G:N3	30:0:681:G:H5'	2.15	0.62
30:0:1603:A:H5'	30:0:1605:G:C4'	2.30	0.61
30:0:2597:U:H2'	30:0:2598:U:H5'	1.81	0.61
38:B:9095:HOH:O	30:0:2672:C:H1'	2.00	0.61
11:K:87:ARG:HG3	30:0:2721:U:H4'	1.81	0.61
30:0:1185:U:H2'	30:0:1186:C:C6	2.35	0.61
30:0:2781:U:C2'	30:0:2782:G:H5'	2.30	0.61
30:0:128:A:O2'	30:0:129:A:H5'	2.00	0.61
30:0:2300:A:H4'	30:0:2301:A:O5'	2.01	0.61
30:0:1342:C:C2'	30:0:1343:C:H5'	2.30	0.61
30:0:2252:A:C5	30:0:2253:G:H1'	2.34	0.61
30:0:2769:C:H2'	30:0:2770:G:H5'	1.82	0.61
30:0:2851:G:O2'	30:0:2852:A:H5'	2.00	0.61
10:J:70:PHE:HE1	30:0:2676:C:H4'	1.65	0.61
30:0:1166:A:H61	30:0:1180:U:H3	1.46	0.61
30:0:138:U:OP2	30:0:139:C:H5	1.83	0.61
9:I:110:ASP:O	30:0:1163:G:H5'	2.01	0.61
23:W:81:ASP:OD1	23:W:92:ASP:HB2	1.99	0.61
30:0:308:U:H5'	30:0:309:C:OP1	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:558:C:H2'	30:0:559:U:H5'	1.82	0.61
21:U:39:ASN:ND2	21:U:44:ARG:HH11	1.98	0.61
30:0:2507:G:H2'	30:0:2510:C:N4	2.12	0.61
30:0:255:A:H2'	30:0:256:C:H6	1.64	0.61
5:E:116:THR:HG22	5:E:151:LEU:HD22	1.83	0.61
20:T:61:GLU:HG2	38:T:3851:HOH:O	2.00	0.61
30:0:2894:C:O2'	30:0:2895:C:H5'	2.01	0.61
23:W:61:THR:HG23	23:W:151:GLU:HG3	1.83	0.61
30:0:1171:A:H2'	30:0:1172:G:H5'	1.81	0.61
30:0:2419:U:H5''	30:0:2420:G:H5'	1.83	0.61
31:9:1:U:O3'	31:9:3:A:H5''	2.01	0.61
13:M:164:THR:HG22	13:M:167:GLY:N	2.15	0.61
30:0:1878:G:O2'	30:0:1879:U:C6	2.52	0.60
28:2:41:HIS:HD2	28:2:44:ARG:H	1.49	0.60
30:0:2344:G:N3	30:0:2344:G:H2'	2.16	0.60
30:0:2718:C:H6	30:0:2718:C:H5'	1.66	0.60
2:B:294:TYR:HE2	38:B:9111:HOH:O	1.84	0.60
5:E:8:PRO:HB2	5:E:11:VAL:HG23	1.81	0.60
13:M:145:ASP:HB2	38:M:8862:HOH:O	1.99	0.60
30:0:2616:G:H1'	38:0:9433:HOH:O	2.00	0.60
31:9:49:G:H2'	31:9:50:G:O4'	2.01	0.60
2:B:264:GLU:HG2	2:B:267:LYS:HE2	1.83	0.60
18:R:128:ARG:NH2	30:0:2054:A:N3	2.49	0.60
30:0:1080:C:H4'	30:0:1081:A:OP1	2.01	0.60
30:0:1192:A:H3'	30:0:1193:A:H5'	1.83	0.60
30:0:1174:A:C5	30:0:1201:C:H4'	2.36	0.60
30:0:1730:G:H5''	30:0:1731:C:H6	1.65	0.60
30:0:1766:U:O2	30:0:1778:A:H5'	2.01	0.60
30:0:1972:U:H2'	30:0:1973:A:C5'	2.31	0.60
1:A:199:HIS:CD2	1:A:201:PHE:H	2.19	0.60
4:D:103:ASN:ND2	4:D:134:LEU:H	1.99	0.60
4:D:58:VAL:HB	4:D:62:ASP:HB2	1.83	0.60
11:K:74:VAL:HG11	11:K:113:ILE:HG12	1.83	0.60
23:W:137:GLN:NE2	23:W:141:HIS:HE1	1.94	0.60
23:W:48:VAL:HG12	23:W:52:VAL:HB	1.83	0.60
27:1:10:LYS:HG3	38:1:8981:HOH:O	2.01	0.60
18:R:39:THR:HG22	18:R:42:GLU:H	1.67	0.60
30:0:2900:G:H2'	30:0:2901:C:O4'	2.01	0.60
2:B:62:ARG:HA	2:B:65:MET:CE	2.32	0.60
30:0:1182:C:H1'	30:0:1192:A:H8	1.67	0.60
8:H:6:ALA:HA	8:H:61:ARG:HH12	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:25:PRO:HB2	38:Q:4350:HOH:O	2.01	0.60
30:0:1119:G:N2	30:0:1246:A:H2	1.92	0.60
30:0:1730:G:H5''	30:0:1731:C:C6	2.37	0.60
1:A:48:ASP:HB3	38:A:9066:HOH:O	2.02	0.60
2:B:41:PHE:HB3	2:B:190:MET:HE1	1.83	0.60
26:Z:81:CYS:SG	26:Z:83:TYR:HB3	2.42	0.60
30:0:1116:U:O2'	30:0:1118:A:C2	2.46	0.59
30:0:1528:A:H2'	30:0:1529:G:O4'	2.02	0.59
30:0:515:C:H5''	38:0:5654:HOH:O	2.01	0.59
31:9:64:C:C2'	31:9:65:A:H5'	2.32	0.59
20:T:24:ARG:HH21	20:T:39:ASN:HD22	1.50	0.59
9:I:112:LEU:HD11	30:0:1162:G:H1'	1.83	0.59
30:0:2505:G:H2'	30:0:2506:A:H5'	1.84	0.59
5:E:139:GLU:OE2	30:0:2781:U:H1'	2.02	0.59
30:0:1641:A:C2'	30:0:1642:A:H5'	2.32	0.59
30:0:659:A:H5''	38:0:7111:HOH:O	2.03	0.59
30:0:2472:C:O2'	30:0:2634:G:H4'	2.03	0.59
30:0:2637:A:H4'	38:0:6071:HOH:O	2.02	0.59
30:0:1189:A:O2'	30:0:1208:C:H2'	2.03	0.59
31:9:49:G:H5''	38:9:9092:HOH:O	2.02	0.59
31:9:64:C:H2'	31:9:65:A:H5'	1.84	0.59
30:0:1189:A:H1'	30:0:1209:C:C1'	2.32	0.59
30:0:2613:G:O2'	30:0:2614:C:H5'	2.03	0.59
31:9:54:A:C2'	31:9:55:U:H5'	2.32	0.59
1:A:36:ASP:CB	1:A:85:SER:H	2.16	0.59
12:L:41:HIS:CD2	30:0:926:A:O2'	2.56	0.59
22:V:39:ALA:N	22:V:40:PRO:HD2	2.17	0.59
24:X:43:VAL:HG12	24:X:44:ASP:H	1.66	0.59
27:1:9:GLY:HA2	30:0:1687:C:O2	2.03	0.59
5:E:84:MET:HG2	5:E:168:ILE:HA	1.85	0.59
8:H:6:ALA:HA	8:H:61:ARG:NH1	2.18	0.59
30:0:2089:A:O2'	30:0:2090:G:H5'	2.03	0.59
5:E:143:GLN:NE2	30:0:2779:G:H21	2.00	0.59
30:0:960:G:N3	30:0:960:G:C2'	2.65	0.59
30:0:2802:C:H2'	30:0:2803:C:H6	1.68	0.59
30:0:583:C:H2'	30:0:584:U:H6	1.68	0.59
4:D:22:VAL:HG22	4:D:74:THR:HG22	1.84	0.59
25:Y:187:VAL:HG23	25:Y:192:ASP:HB3	1.84	0.59
30:0:1200:A:H3'	38:0:5763:HOH:O	2.03	0.58
31:9:76:G:C3'	31:9:77:A:H5''	2.24	0.58
23:W:139:GLY:O	23:W:141:HIS:HD2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:13:MET:HE1	23:W:18:GLN:HA	1.83	0.58
30:0:2526:C:H5'	30:0:2526:C:H6	1.64	0.58
30:0:807:A:O2'	30:0:808:A:H5'	2.03	0.58
31:9:1:U:H4'	31:9:3:A:OP1	2.03	0.58
4:D:135:VAL:HG21	4:D:139:TYR:CD1	2.38	0.58
30:0:1730:G:C5'	30:0:1731:C:C6	2.86	0.58
30:0:1942:A:O2'	30:0:1943:C:H5'	2.02	0.58
31:9:2:U:H4'	38:9:9104:HOH:O	2.02	0.58
30:0:1183:C:N3	30:0:1184:C:C5	2.72	0.58
30:0:2421:G:H1'	38:0:7033:HOH:O	2.03	0.58
1:A:192:VAL:HG12	1:A:207:GLN:HB3	1.85	0.58
2:B:304:PRO:HD2	2:B:307:ARG:NE	2.18	0.58
8:H:168:VAL:HG13	38:H:210:HOH:O	2.03	0.58
17:Q:21:ARG:HH12	30:0:2353:A:H1'	1.68	0.58
23:W:44:MET:CE	30:0:944:G:H21	2.16	0.58
30:0:90:A:H2'	30:0:91:G:O4'	2.02	0.58
1:A:100:PRO:HG2	1:A:103:VAL:HG21	1.84	0.58
13:M:134:ILE:HG23	13:M:141:ILE:HD13	1.84	0.58
30:0:1187:U:H2'	38:0:6907:HOH:O	2.04	0.58
30:0:1175:G:H1'	30:0:1193:A:H2'	1.84	0.58
30:0:644:G:N3	30:0:644:G:H5'	2.19	0.58
3:C:115:LEU:HD13	3:C:223:LEU:HD21	1.85	0.58
6:F:2:VAL:HG22	6:F:57:GLU:OE1	2.04	0.58
14:N:37:ARG:HH11	31:9:6:C:H5''	1.65	0.58
1:A:94:LEU:HD12	1:A:98:GLU:HB2	1.84	0.58
3:C:174:ILE:CD1	30:0:338:C:H4'	2.33	0.58
30:0:1174:A:C6	30:0:1201:C:H4'	2.39	0.58
8:H:174:LEU:HA	38:H:220:HOH:O	2.02	0.58
21:U:17:THR:HG22	21:U:18:GLY:N	2.19	0.58
2:B:258:GLY:H	2:B:260:HIS:CE1	2.21	0.58
9:I:126:THR:O	9:I:130:LEU:HG	2.03	0.58
31:9:107:C:O2'	31:9:108:C:H5'	2.04	0.57
21:U:6:CYS:HB2	21:U:32:CYS:HB3	1.85	0.57
30:0:2589:U:H2'	30:0:2590:U:C6	2.39	0.57
30:0:2712:G:H5'	38:0:5232:HOH:O	2.03	0.57
30:0:2769:C:O2'	30:0:2770:G:H5'	2.04	0.57
30:0:952:G:N3	30:0:2302:A:H2'	2.19	0.57
2:B:98:THR:HG22	30:0:2820:A:OP1	2.04	0.57
30:0:2756:U:H3	30:0:2896:A:H2	1.48	0.57
30:0:420:U:H2'	30:0:421:C:C6	2.39	0.57
31:9:29:C:H2'	31:9:30:C:C5'	2.28	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:73:LEU:HD12	9:I:107:LYS:NZ	2.20	0.57
30:0:185:G:H4'	30:0:186:A:OP1	2.05	0.57
4:D:52:THR:HG21	30:0:2346:C:O2'	2.04	0.57
30:0:272:A:H5'	30:0:273:G:OP2	2.03	0.57
30:0:541:C:H2'	30:0:542:A:H5'	1.86	0.57
9:I:112:LEU:CD1	30:0:1162:G:H1'	2.34	0.57
13:M:23:LEU:HD13	13:M:27:ARG:NH2	2.19	0.57
14:N:7:LYS:HE3	17:Q:21:ARG:O	2.04	0.57
24:X:76:ARG:HH11	24:X:76:ARG:HG3	1.68	0.57
30:0:2135:A:O2'	30:0:2136:G:H5'	2.04	0.57
14:N:25:ARG:HG2	30:0:2416:G:O2'	2.04	0.57
30:0:280:C:H2'	30:0:281:U:O4'	2.04	0.57
30:0:559:U:C5'	30:0:559:U:H6	2.12	0.57
17:Q:18:PRO:O	17:Q:21:ARG:HB2	2.03	0.57
17:Q:27:GLN:HE21	31:9:8:G:H4'	1.70	0.57
30:0:10:U:O4	30:0:532:A:OP2	2.23	0.57
30:0:2604:A:H5'	38:0:5798:HOH:O	2.04	0.57
30:0:2787:C:H5	38:0:4643:HOH:O	1.86	0.57
13:M:28:GLN:O	13:M:32:ARG:HG3	2.04	0.57
18:R:39:THR:HG23	18:R:107:GLU:O	2.04	0.57
30:0:1171:A:C2'	30:0:1172:G:H5'	2.35	0.57
30:0:1377:C:H5'	30:0:1377:C:C6	2.40	0.57
30:0:1942:A:H3'	38:0:7360:HOH:O	2.03	0.57
1:A:36:ASP:O	1:A:38:ILE:N	2.38	0.57
12:L:4:LYS:HE2	30:0:645:U:OP2	2.05	0.57
30:0:1016:U:H1'	38:0:3667:HOH:O	2.04	0.57
31:9:75:G:H1	31:9:106:U:H3	1.53	0.57
13:M:72:ALA:HB2	13:M:93:ARG:HG2	1.86	0.57
31:9:39:U:H1'	31:9:44:A:N6	2.19	0.57
2:B:201:ASP:HB2	2:B:312:ARG:HD2	1.87	0.57
3:C:188:ARG:HD3	38:C:8559:HOH:O	2.04	0.57
30:0:2005:G:OP2	30:0:2005:G:H3'	2.05	0.57
30:0:228:C:H2'	30:0:229:G:H5'	1.86	0.57
30:0:2488:A:H1'	38:0:9096:HOH:O	2.03	0.57
30:0:2559:C:H4'	38:0:7268:HOH:O	2.05	0.57
30:0:960:G:H2'	30:0:960:G:N3	2.20	0.57
2:B:264:GLU:HG2	2:B:267:LYS:CE	2.35	0.57
10:J:127:ILE:HG22	33:J:8801:CL:CL	2.42	0.57
30:0:1304:U:H2'	30:0:1305:C:C6	2.40	0.56
30:0:711:G:H1'	38:0:7108:HOH:O	2.04	0.56
30:0:941:G:C5	30:0:942:U:C4	2.93	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ILE:O	1:A:131:HIS:HE1	1.88	0.56
3:C:1:MET:HG2	3:C:2:GLN:N	2.19	0.56
14:N:48:VAL:CG1	14:N:55:ASP:HB3	2.35	0.56
30:0:1838:U:O2'	30:0:2644:C:H5'	2.05	0.56
30:0:2578:G:C8	30:0:2578:G:H5'	2.36	0.56
12:L:143:THR:HG22	12:L:144:ASP:N	2.20	0.56
30:0:1632:A:C3'	30:0:1633:C:H5'	2.35	0.56
30:0:734:U:O2'	30:0:736:A:N7	2.39	0.56
29:3:70:ARG:HB3	38:3:9059:HOH:O	2.04	0.56
30:0:1474:C:H6	30:0:1474:C:C5'	2.15	0.56
30:0:1947:G:N2	30:0:1966:U:C2	2.73	0.56
11:K:66:ARG:HH22	30:0:1994:A:P	2.29	0.56
1:A:88:ILE:HD13	1:A:100:PRO:HD3	1.86	0.56
10:J:18:ILE:HD13	30:0:1244:U:OP1	2.05	0.56
20:T:2:LYS:HG2	30:0:447:A:OP1	2.05	0.56
2:B:125:GLU:O	2:B:129:ARG:HG3	2.06	0.56
14:N:143:ARG:HH21	14:N:169:PRO:HB2	1.69	0.56
30:0:31:C:H4'	38:0:7437:HOH:O	2.06	0.56
30:0:506:G:N2	30:0:509:A:H5'	2.18	0.56
27:1:42:SER:HB2	38:1:8956:HOH:O	2.05	0.56
16:P:143:ALA:HA	38:P:192:HOH:O	2.04	0.56
30:0:1209:C:H2'	30:0:1210:G:H8	1.70	0.56
30:0:2032:U:H2'	30:0:2033:G:C5'	2.36	0.56
31:9:13:A:O2'	31:9:14:G:H5''	2.06	0.56
30:0:363:C:O2'	30:0:364:U:H5'	2.06	0.56
30:0:368:C:H2'	30:0:369:G:H5'	1.88	0.56
30:0:876:A:N3	30:0:876:A:H2'	2.21	0.56
27:1:16:HIS:HD2	30:0:470:U:O2'	1.88	0.56
1:A:199:HIS:HD2	1:A:201:PHE:H	1.54	0.56
10:J:107:ASN:HD21	10:J:109:TYR:HB2	1.71	0.56
30:0:119:A:H2'	30:0:120:A:H5''	1.87	0.55
30:0:1904:A:H2'	30:0:1905:U:O4'	2.05	0.55
30:0:1972:U:H2'	30:0:1973:A:H5''	1.87	0.55
1:A:153:ARG:HH11	1:A:153:ARG:HB2	1.70	0.55
9:I:120:ALA:O	9:I:124:VAL:HG23	2.06	0.55
30:0:2064:U:H5'	30:0:2652:U:H4'	1.88	0.55
3:C:58:ALA:HA	3:C:73:GLN:HE21	1.69	0.55
4:D:25:MET:CE	4:D:37:ALA:HB1	2.35	0.55
10:J:107:ASN:C	10:J:107:ASN:HD22	2.09	0.55
10:J:107:ASN:HD22	10:J:109:TYR:H	1.54	0.55
25:Y:212:ARG:HD2	38:Y:8900:HOH:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:15:PRO:HG3	30:0:1053:G:OP1	2.06	0.55
28:2:10:ARG:NH2	30:0:121:U:OP2	2.35	0.55
30:0:821:U:H3'	38:0:3780:HOH:O	2.07	0.55
6:F:50:VAL:HG13	6:F:60:VAL:HG11	1.89	0.55
30:0:2781:U:H2'	30:0:2782:G:C5'	2.36	0.55
4:D:159:PRO:O	4:D:163:VAL:HG23	2.05	0.55
30:0:168:C:O5'	30:0:168:C:H6	1.89	0.55
30:0:2254:G:H1'	38:0:5546:HOH:O	2.07	0.55
30:0:2840:A:H3'	38:0:7659:HOH:O	2.05	0.55
30:0:396:U:O2'	30:0:418:C:H4'	2.07	0.55
30:0:407:A:H5'	38:0:6032:HOH:O	2.06	0.55
14:N:132:ASN:HD22	30:0:2413:A:H4'	1.72	0.55
16:P:7:LYS:HD3	16:P:21:VAL:HG22	1.87	0.55
30:0:1060:C:H6	30:0:1060:C:H5'	1.72	0.55
8:H:6:ALA:HB3	30:0:2521:A:OP2	2.06	0.55
30:0:660:A:H4'	30:0:661:G:O5'	2.07	0.55
30:0:711:G:C2	30:0:718:C:C2	2.95	0.55
29:3:15:ASN:O	30:0:2408:A:H4'	2.06	0.55
2:B:51:VAL:HG23	2:B:330:VAL:HG22	1.88	0.55
4:D:54:ALA:HB2	4:D:69:ILE:HD12	1.88	0.55
9:I:130:LEU:HD22	30:0:1167:G:H4'	1.89	0.55
30:0:1132:A:N6	30:0:1229:C:H2'	2.22	0.55
30:0:1596:U:H2'	30:0:1598:A:OP2	2.07	0.55
3:C:132:ASP:HB3	38:C:8560:HOH:O	2.06	0.55
5:E:23:GLU:HG2	5:E:28:SER:HB3	1.89	0.55
30:0:2510:C:H5'	30:0:2511:A:OP2	2.07	0.55
27:1:1:THR:HA	38:1:8958:HOH:O	2.06	0.55
31:9:24:U:H3'	31:9:25:G:C5'	2.37	0.55
31:9:55:U:H4'	31:9:56:A:C8	2.42	0.55
4:D:173:GLU:HG3	4:D:174:VAL:HG23	1.89	0.55
4:D:65:GLU:HA	38:D:6752:HOH:O	2.05	0.55
7:G:64:ASN:N	7:G:64:ASN:HD22	2.04	0.55
23:W:68:THR:HG23	23:W:69:ARG:HG2	1.89	0.55
30:0:1538:C:O2'	30:0:1539:U:H5'	2.06	0.55
13:M:95:LYS:HE2	30:0:157:G:H4'	1.89	0.55
2:B:145:HIS:HD2	2:B:146:THR:O	1.90	0.55
7:G:23:ILE:O	7:G:27:ILE:HG13	2.06	0.55
30:0:2577:A:H8	38:0:9602:HOH:O	1.89	0.54
1:A:121:ALA:O	1:A:124:VAL:HG22	2.07	0.54
2:B:102:THR:HG23	2:B:182:VAL:HG12	1.90	0.54
12:L:150:GLN:HB3	38:L:8869:HOH:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2083:A:H3'	38:0:7590:HOH:O	2.07	0.54
1:A:192:VAL:CG1	1:A:207:GLN:HB3	2.38	0.54
30:0:1154:A:H2'	30:0:1155:G:C8	2.42	0.54
30:0:1291:A:H2	38:0:5300:HOH:O	1.89	0.54
30:0:1523:G:C5	30:0:1524:U:C4	2.96	0.54
30:0:2878:U:H2'	30:0:2879:A:O4'	2.06	0.54
31:9:59:C:H6	31:9:59:C:O5'	1.90	0.54
2:B:27:ASN:H	2:B:27:ASN:HD22	1.56	0.54
30:0:1202:A:H2'	30:0:1203:G:O4'	2.07	0.54
30:0:2256:G:C2'	30:0:2257:G:C5'	2.84	0.54
30:0:292:G:H2'	30:0:358:G:N2	2.23	0.54
30:0:812:A:H1'	38:0:3969:HOH:O	2.06	0.54
26:Z:40:ALA:HA	30:0:1773:G:C8	2.42	0.54
24:X:23:HIS:HE1	30:0:2044:G:OP1	1.89	0.54
31:9:52:A:O2'	31:9:53:G:H5'	2.08	0.54
11:K:74:VAL:CG1	11:K:113:ILE:HG12	2.38	0.54
30:0:1477:C:H5'	30:0:1868:G:H5'	1.89	0.54
5:E:143:GLN:NE2	30:0:2780:C:H1'	2.22	0.54
30:0:241:A:C2	30:0:378:A:H4'	2.42	0.54
3:C:154:VAL:O	3:C:158:GLU:HG3	2.07	0.54
30:0:1342:C:O2'	30:0:1343:C:H5'	2.07	0.54
30:0:282:C:H1'	30:0:368:C:H41	1.72	0.54
30:0:441:A:H1'	30:0:442:A:N7	2.23	0.54
17:Q:27:GLN:HE21	31:9:8:G:C5'	2.20	0.54
31:9:3:A:H2	31:9:21:G:N3	2.06	0.54
6:F:53:ASP:OD1	6:F:80:GLN:HB2	2.08	0.54
12:L:73:VAL:HG21	12:L:116:HIS:CE1	2.42	0.54
25:Y:204:ARG:HH22	30:0:553:G:P	2.31	0.54
18:R:68:HIS:O	30:0:2842:G:H5'	2.08	0.54
3:C:218:VAL:HG12	38:C:8620:HOH:O	2.07	0.54
7:G:16:LYS:O	7:G:20:VAL:HG23	2.08	0.54
1:A:112:PRO:HD3	1:A:152:CYS:SG	2.48	0.54
4:D:41:LEU:HA	4:D:44:ILE:HG22	1.88	0.54
5:E:49:ILE:HD11	5:E:69:ILE:HD12	1.90	0.54
12:L:143:THR:HG22	12:L:144:ASP:H	1.71	0.54
19:S:33:SER:O	19:S:37:VAL:HG23	2.07	0.54
4:D:105:SER:OG	30:0:2338:G:H1'	2.07	0.53
18:R:132:ARG:HG2	18:R:133:ALA:N	2.23	0.53
30:0:2670:G:O2'	30:0:2671:U:H5'	2.07	0.53
3:C:236:THR:HA	38:C:8647:HOH:O	2.08	0.53
8:H:26:ILE:HA	8:H:123:ILE:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:39:VAL:HG13	10:J:106:GLY:O	2.08	0.53
13:M:30:GLU:O	13:M:34:GLU:HG3	2.09	0.53
15:O:73:ASP:HA	15:O:92:VAL:O	2.08	0.53
18:R:150:PRO:CG	18:R:150:PRO:CB	2.86	0.53
30:0:1586:G:O2'	30:0:1587:U:H5'	2.08	0.53
30:0:1819:G:H2'	30:0:1820:G:C4'	2.39	0.53
6:F:34:ASN:HA	13:M:4:ALA:HB2	1.91	0.53
30:0:136:C:H2'	30:0:137:U:O4'	2.08	0.53
30:0:1373:G:H1'	38:0:6143:HOH:O	2.08	0.53
30:0:1919:A:H4'	38:0:4862:HOH:O	2.07	0.53
30:0:2064:U:H5'	30:0:2652:U:O3'	2.08	0.53
30:0:2842:G:H2'	30:0:2843:A:H5'	1.90	0.53
30:0:488:U:H2'	38:0:4019:HOH:O	2.08	0.53
2:B:307:ARG:NH1	2:B:307:ARG:HG3	2.23	0.53
30:0:1339:G:C6	30:0:1340:G:N1	2.77	0.53
30:0:1592:G:H2'	30:0:1593:C:H6	1.72	0.53
30:0:1205:U:C2'	30:0:1206:U:C5'	2.76	0.53
30:0:1451:C:H5'	30:0:1505:U:C5	2.43	0.53
14:N:144:GLY:O	14:N:147:ILE:HG23	2.08	0.53
23:W:125:HIS:HE1	38:W:3071:HOH:O	1.91	0.53
30:0:2502:C:H2'	30:0:2503:A:C5'	2.37	0.53
31:9:24:U:H3'	31:9:25:G:H5'	1.91	0.53
10:J:70:PHE:CD1	30:0:2676:C:H4'	2.43	0.53
18:R:99:ALA:HB1	18:R:109:MET:CE	2.37	0.53
30:0:1135:G:H5'	38:0:5935:HOH:O	2.07	0.53
30:0:2250:G:H2'	30:0:2251:G:O4'	2.09	0.53
30:0:2769:C:H2'	30:0:2770:G:C5'	2.39	0.53
30:0:544:G:C3'	30:0:545:G:H5''	2.39	0.53
30:0:920:C:H5''	30:0:921:G:O5'	2.09	0.53
1:A:135:VAL:HG21	1:A:147:ARG:HB3	1.91	0.53
3:C:129:HIS:CE1	3:C:231:ARG:HA	2.44	0.53
4:D:154:LYS:HD2	4:D:154:LYS:N	2.16	0.53
4:D:51:ARG:HH11	4:D:68:PRO:HB3	1.74	0.53
22:V:55:ARG:O	22:V:59:ILE:HG12	2.09	0.53
30:0:299:U:H5'	38:0:7349:HOH:O	2.08	0.53
30:0:510:U:H6	38:0:7450:HOH:O	1.92	0.53
30:0:635:A:H2'	30:0:636:G:H5''	1.90	0.53
3:C:47:GLY:HA2	3:C:92:PRO:HB2	1.91	0.53
9:I:91:PHE:HD2	9:I:131:GLY:HA2	1.74	0.53
30:0:1066:U:H2'	30:0:1067:A:C8	2.42	0.53
30:0:1166:A:P	30:0:1174:A:H4'	2.49	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:282:C:O2'	30:0:283:U:C5'	2.56	0.53
30:0:513:A:N3	38:0:3668:HOH:O	2.34	0.53
23:W:154:ARG:NH1	30:0:588:G:O6	2.42	0.53
30:0:820:G:H3'	38:0:3058:HOH:O	2.08	0.53
9:I:108:HIS:H	9:I:109:PRO:HD2	1.74	0.53
16:P:59:ARG:HH22	16:P:66:GLN:HE22	1.57	0.53
30:0:284:C:C6	30:0:284:C:OP2	2.62	0.52
27:1:16:HIS:HE1	30:0:775:G:OP1	1.92	0.52
30:0:958:G:H2'	30:0:959:C:C6	2.43	0.52
13:M:34:GLU:HB3	13:M:38:GLU:HG3	1.91	0.52
30:0:1819:G:H2'	30:0:1820:G:C5'	2.39	0.52
2:B:254:GLN:HG2	2:B:255:GLY:N	2.24	0.52
5:E:11:VAL:HG12	5:E:12:ASP:N	2.24	0.52
5:E:3:VAL:HG22	5:E:49:ILE:HB	1.90	0.52
30:0:2356:A:H5'	38:0:5644:HOH:O	2.09	0.52
30:0:1787:C:H4'	30:0:2883:A:O4'	2.09	0.52
31:9:91:C:H2'	31:9:92:G:O4'	2.09	0.52
2:B:312:ARG:HD3	2:B:315:VAL:HG13	1.91	0.52
10:J:41:ALA:HB3	38:J:5907:HOH:O	2.09	0.52
25:Y:216:ARG:HD2	38:Y:8870:HOH:O	2.08	0.52
14:N:5:ARG:NH1	30:0:1010:C:OP1	2.42	0.52
30:0:1268:C:O2'	30:0:1269:G:H5'	2.08	0.52
30:0:255:A:H2'	30:0:256:C:C6	2.45	0.52
30:0:920:C:H4'	30:0:921:G:C2	2.44	0.52
5:E:6:GLU:HG2	5:E:46:THR:HG22	1.92	0.52
14:N:12:ARG:HD3	14:N:18:THR:OG1	2.09	0.52
30:0:1181:A:N1	30:0:1192:A:O2'	2.43	0.52
30:0:1515:A:H2'	30:0:1516:U:C6	2.44	0.52
30:0:1624:A:H5'	30:0:1626:A:O4'	2.09	0.52
30:0:2263:G:H1'	38:0:6631:HOH:O	2.09	0.52
30:0:2291:A:N9	30:0:2309:C:H5'	2.25	0.52
30:0:2478:U:O2'	30:0:2479:A:H5'	2.09	0.52
2:B:36:PRO:HG3	2:B:169:GLY:H	1.75	0.52
13:M:158:ARG:HB2	13:M:163:LEU:HB2	1.91	0.52
15:O:32:ARG:HD3	15:O:32:ARG:O	2.09	0.52
25:Y:126:PRO:HG2	25:Y:128:PHE:CZ	2.44	0.52
30:0:120:A:H2'	30:0:120:A:N3	2.25	0.52
30:0:1314:U:H2'	38:0:5880:HOH:O	2.09	0.52
8:H:72:ALA:HB2	8:H:156:ALA:HB2	1.91	0.52
14:N:86:LEU:HD12	14:N:125:ALA:HB2	1.91	0.52
30:0:1342:C:H2'	30:0:1343:C:H5'	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2103:A:H2'	30:0:2104:C:H5'	1.92	0.52
12:L:56:LYS:HE3	30:0:2443:C:H1'	1.92	0.52
30:0:2445:U:H2'	30:0:2446:G:H8	1.75	0.52
25:Y:169:ARG:HD3	30:0:1328:A:C8	2.44	0.52
30:0:1679:C:H5'	38:0:9331:HOH:O	2.10	0.52
30:0:1972:U:C2'	30:0:1973:A:H5''	2.39	0.52
30:0:2359:G:H3'	38:0:5698:HOH:O	2.10	0.52
30:0:2756:U:N3	30:0:2896:A:H2	2.08	0.52
31:9:45:A:H2'	31:9:46:C:H6	1.75	0.52
2:B:141:ARG:HD2	2:B:163:GLU:OE2	2.10	0.52
30:0:1170:U:H2'	30:0:1172:G:OP2	2.09	0.52
30:0:1730:G:C5'	30:0:1731:C:C5	2.93	0.52
30:0:2326:C:H4'	30:0:2412:G:H4'	1.92	0.52
30:0:2769:C:H2'	30:0:2770:G:O4'	2.09	0.52
30:0:2756:U:N3	30:0:2896:A:C2	2.74	0.52
30:0:694:A:H2'	30:0:695:C:H5'	1.90	0.52
17:Q:19:ARG:HH21	31:9:11:A:P	2.33	0.52
6:F:21:GLU:O	6:F:24:ARG:HG2	2.09	0.52
22:V:64:GLY:O	22:V:65:ASP:HB2	2.09	0.52
30:0:2764:C:O2'	30:0:2765:C:H5'	2.09	0.52
3:C:43:LYS:HG2	30:0:449:A:N7	2.25	0.52
30:0:567:U:H5''	38:0:6408:HOH:O	2.08	0.52
1:A:217:ARG:HG2	1:A:229:ALA:HB2	1.91	0.52
1:A:72:GLU:HG3	26:Z:90:GLY:HA2	1.91	0.52
2:B:79:MET:HE1	38:B:9089:HOH:O	2.09	0.52
30:0:1477:C:O2'	30:0:1478:U:H5'	2.10	0.51
13:M:188:ARG:NH1	30:0:154:C:H3'	2.24	0.51
30:0:2105:C:H2'	30:0:2106:C:C6	2.45	0.51
30:0:2524:G:H21	30:0:2526:C:N4	2.08	0.51
30:0:497:A:H2'	30:0:498:A:C5'	2.40	0.51
30:0:541:C:O2'	30:0:542:A:H5''	2.10	0.51
30:0:613:C:H2'	30:0:614:U:H6	1.74	0.51
30:0:619:U:H3'	38:0:3289:HOH:O	2.09	0.51
2:B:207:LYS:HG3	30:0:2717:C:OP1	2.10	0.51
14:N:37:ARG:HD3	33:N:8807:CL:CL	2.47	0.51
18:R:18:LEU:HB2	18:R:143:VAL:CG1	2.40	0.51
30:0:2269:C:C2'	30:0:2270:G:H5'	2.40	0.51
30:0:2768:A:N3	30:0:2768:A:H3'	2.25	0.51
30:0:65:C:O2'	30:0:66:G:H5'	2.10	0.51
31:9:2:U:C4'	38:9:9104:HOH:O	2.57	0.51
13:M:188:ARG:HD3	30:0:155:C:OP2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:115:SER:OG	16:P:118:GLN:HG3	2.10	0.51
18:R:18:LEU:HD12	18:R:143:VAL:CG1	2.40	0.51
30:0:1131:G:C6	30:0:1230:A:C4	2.99	0.51
30:0:1592:G:H2'	30:0:1593:C:C6	2.45	0.51
30:0:1878:G:C1'	38:0:6126:HOH:O	2.44	0.51
13:M:179:GLY:O	30:0:399:C:H5'	2.10	0.51
30:0:506:G:H22	30:0:509:A:H5''	1.73	0.51
30:0:812:A:H2'	30:0:813:C:C6	2.45	0.51
12:L:61:ALA:HB2	12:L:105:TYR:CE2	2.45	0.51
14:N:61:ALA:HB3	14:N:88:ALA:HB2	1.91	0.51
26:Z:57:MET:HE3	38:0:6288:HOH:O	2.09	0.51
30:0:1029:U:O2'	30:0:1273:C:OP1	2.25	0.51
30:0:1447:U:H3'	30:0:1506:U:O2	2.11	0.51
30:0:447:A:O2'	30:0:448:G:H5'	2.11	0.51
3:C:153:VAL:O	3:C:157:LEU:HG	2.10	0.51
14:N:38:LYS:HE2	14:N:107:ASN:ND2	2.26	0.51
19:S:11:THR:H	19:S:14:ALA:HB3	1.75	0.51
30:0:1080:C:O5'	30:0:1080:C:H6	1.94	0.51
30:0:1730:G:H5'	30:0:1731:C:H5	1.74	0.51
30:0:2445:U:H2'	30:0:2446:G:C8	2.46	0.51
30:0:256:C:H2'	30:0:257:G:O4'	2.10	0.51
30:0:2717:C:C2'	30:0:2718:C:C5'	2.75	0.51
30:0:445:U:H2'	30:0:446:G:H8	1.75	0.51
30:0:512:G:O3'	30:0:513:A:H8	1.92	0.51
31:9:12:C:H5'	31:9:70:U:O4'	2.11	0.51
2:B:7:ARG:HG2	2:B:7:ARG:HH11	1.76	0.51
12:L:14:GLY:O	30:0:1295:G:H5''	2.10	0.51
30:0:1535:G:H2'	30:0:1536:C:C6	2.46	0.51
30:0:228:C:C2'	30:0:229:G:H5'	2.41	0.51
30:0:318:U:H5'	30:0:339:A:C2	2.46	0.51
30:0:690:G:H4'	30:0:741:C:O2	2.11	0.51
4:D:75:LEU:HD22	4:D:79:MET:HB3	1.93	0.51
12:L:149:ARG:O	12:L:150:GLN:HB2	2.10	0.51
23:W:125:HIS:CD2	23:W:127:GLY:H	2.29	0.51
30:0:1015:C:H2'	30:0:1016:U:H6	1.75	0.51
30:0:1422:U:H2'	30:0:1423:C:C6	2.45	0.51
30:0:1973:A:H2'	30:0:1974:G:O4'	2.10	0.51
30:0:2401:A:H2'	30:0:2402:A:C8	2.46	0.51
30:0:545:G:H8	30:0:545:G:C5'	2.06	0.51
4:D:25:MET:HE2	4:D:41:LEU:HG	1.92	0.51
18:R:18:LEU:HB2	18:R:143:VAL:HG13	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:139:GLY:O	23:W:141:HIS:CD2	2.64	0.51
2:B:234:ARG:HG3	30:0:1735:C:OP2	2.11	0.51
30:0:968:G:C2	30:0:1001:U:O2	2.63	0.51
28:2:35:ARG:HB2	38:2:2691:HOH:O	2.09	0.51
31:9:1:U:O3'	31:9:3:A:C5'	2.58	0.51
6:F:101:ALA:HA	38:F:5413:HOH:O	2.10	0.51
30:0:1160:G:H5''	30:0:1161:A:H5'	1.84	0.51
30:0:1183:C:C2	30:0:1184:C:C5	2.99	0.51
30:0:483:C:C4	30:0:484:A:C6	2.99	0.51
27:1:25:LYS:HD2	28:2:49:GLU:N	2.23	0.51
2:B:85:ARG:NH1	38:B:9095:HOH:O	2.44	0.51
16:P:1:THR:O	30:0:1396:C:H1'	2.11	0.51
19:S:17:ASP:HB3	19:S:23:LYS:HB2	1.93	0.51
30:0:2326:C:H4'	30:0:2412:G:C4'	2.41	0.51
2:B:41:PHE:CD1	2:B:79:MET:HE2	2.45	0.51
2:B:41:PHE:HA	2:B:79:MET:HE2	1.91	0.51
30:0:101:C:H2'	30:0:102:A:H8	1.76	0.50
30:0:1139:U:H2'	30:0:1140:C:C6	2.46	0.50
30:0:1268:C:H2'	30:0:1269:G:H8	1.76	0.50
30:0:2754:G:H2'	30:0:2755:G:O4'	2.11	0.50
30:0:407:A:H3'	38:0:4473:HOH:O	2.10	0.50
29:3:60:LYS:HG3	29:3:61:PRO:HD2	1.92	0.50
14:N:4:PRO:HG3	31:9:69:U:OP1	2.11	0.50
3:C:95:GLU:HG3	38:C:8672:HOH:O	2.12	0.50
30:0:1193:A:C2	30:0:1194:A:N6	2.79	0.50
30:0:1739:G:O2'	30:0:1740:U:H5'	2.11	0.50
30:0:951:A:C2'	30:0:952:G:H5'	2.41	0.50
27:1:8:GLN:HE22	27:1:11:LYS:HZ2	1.58	0.50
1:A:51:ARG:NH1	1:A:120:ARG:O	2.44	0.50
3:C:236:THR:HG22	3:C:239:ALA:N	2.20	0.50
8:H:69:ARG:HD3	38:H:229:HOH:O	2.11	0.50
9:I:95:LEU:HD22	9:I:99:GLN:HB3	1.93	0.50
30:0:1160:G:H5'	30:0:1161:A:C4'	2.40	0.50
30:0:1878:G:O2'	30:0:1879:U:H6	1.95	0.50
30:0:899:C:H5'	38:0:3209:HOH:O	2.12	0.50
27:1:2:GLY:O	27:1:6:PRO:HG2	2.11	0.50
31:9:76:G:H3'	31:9:77:A:C5'	2.24	0.50
2:B:214:PRO:HD2	38:B:8990:HOH:O	2.11	0.50
2:B:62:ARG:HA	2:B:65:MET:HE2	1.93	0.50
10:J:26:VAL:HG13	10:J:36:VAL:HG11	1.93	0.50
16:P:59:ARG:HH22	16:P:66:GLN:NE2	2.08	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1118:A:H8	30:0:1119:G:H5''	1.75	0.50
30:0:1183:C:O2	30:0:1183:C:C2'	2.60	0.50
30:0:185:G:H4'	30:0:186:A:H4'	1.93	0.50
30:0:1878:G:O2'	30:0:1879:U:P	2.70	0.50
29:3:29:ARG:NH2	30:0:1925:G:H5'	2.26	0.50
30:0:2269:C:H2'	30:0:2270:G:H5'	1.93	0.50
30:0:271:C:C2	30:0:273:G:O4'	2.64	0.50
30:0:700:A:H5''	30:0:701:U:H5'	1.93	0.50
30:0:737:A:H2'	30:0:738:G:O4'	2.10	0.50
30:0:960:G:C3'	30:0:960:G:N3	2.74	0.50
2:B:305:ASP:O	2:B:306:LYS:HB2	2.12	0.50
12:L:143:THR:HG21	38:L:8838:HOH:O	2.10	0.50
30:0:1289:C:O2'	30:0:1290:G:H5'	2.12	0.50
20:T:54:ASP:OD2	30:0:316:A:H5'	2.11	0.50
30:0:661:G:C5	30:0:686:A:C2	3.00	0.50
2:B:217:ARG:CG	2:B:257:THR:HG22	2.38	0.50
2:B:310:ARG:HB3	38:B:9109:HOH:O	2.11	0.50
3:C:214:THR:HG23	38:C:8633:HOH:O	2.11	0.50
8:H:170:ARG:HD2	38:H:190:HOH:O	2.11	0.50
12:L:27:ARG:HH21	12:L:30:ARG:HG2	1.77	0.50
14:N:37:ARG:NH1	31:9:6:C:OP1	2.44	0.50
30:0:1181:A:H2'	30:0:1182:C:H5'	1.94	0.50
30:0:1244:U:H4'	30:0:1246:A:O4'	2.11	0.50
30:0:2276:U:H2'	30:0:2277:U:C6	2.46	0.50
30:0:440:C:H2'	30:0:441:A:C8	2.47	0.50
30:0:947:U:H2'	30:0:948:G:C8	2.47	0.50
31:9:5:G:O2'	31:9:6:C:H5'	2.11	0.50
31:9:95:C:O2'	31:9:96:C:H5'	2.12	0.50
4:D:28:GLY:HA2	4:D:69:ILE:HG23	1.93	0.50
7:G:20:VAL:O	7:G:24:VAL:HG23	2.12	0.50
11:K:87:ARG:NH1	38:K:4066:HOH:O	2.45	0.50
19:S:77:VAL:O	19:S:80:ARG:HG2	2.12	0.50
30:0:1166:A:C6	30:0:1181:A:C2	2.99	0.50
30:0:137:U:OP1	30:0:259:G:O2'	2.30	0.50
4:D:58:VAL:CG1	4:D:60:GLU:HG2	2.42	0.50
18:R:33:ARG:NH1	38:R:8950:HOH:O	2.45	0.50
20:T:28:SER:O	20:T:32:ARG:HG3	2.11	0.50
30:0:1056:U:H2'	30:0:1057:A:O4'	2.12	0.50
30:0:2511:A:H4'	38:0:5478:HOH:O	2.12	0.50
1:A:171:LYS:HB2	30:0:820:G:C5	2.47	0.50
2:B:275:GLY:O	2:B:291:ASP:HA	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:97:VAL:HG12	9:I:101:LYS:HE3	1.92	0.50
30:0:1185:U:H2'	30:0:1186:C:H6	1.77	0.50
30:0:182:G:H5''	38:0:3733:HOH:O	2.12	0.50
30:0:2010:A:C2'	38:0:5965:HOH:O	2.55	0.50
30:0:541:C:C2'	30:0:542:A:C5'	2.78	0.50
15:O:37:ARG:HD2	30:0:656:G:OP2	2.12	0.50
30:0:816:G:C6	30:0:817:G:N1	2.80	0.50
30:0:877:G:C5'	30:0:878:G:OP1	2.57	0.50
23:W:80:ASP:O	23:W:84:VAL:HG23	2.10	0.50
24:X:61:ARG:HH12	24:X:67:PRO:HD3	1.77	0.50
30:0:1211:G:H2'	30:0:1212:C:H6	1.77	0.49
30:0:1743:G:N7	38:0:9265:HOH:O	2.35	0.49
14:N:110:THR:HB	14:N:113:SER:OG	2.12	0.49
30:0:1588:G:C6	30:0:1589:G:N1	2.81	0.49
30:0:1657:A:H2'	30:0:1658:A:C8	2.47	0.49
2:B:212:GLN:HA	30:0:1733:A:H4'	1.93	0.49
30:0:1972:U:H2'	30:0:1973:A:H5'	1.93	0.49
30:0:2414:A:H2'	30:0:2415:A:C8	2.47	0.49
30:0:364:U:H2'	30:0:365:G:O4'	2.12	0.49
30:0:509:A:H2'	38:0:7099:HOH:O	2.11	0.49
30:0:2851:G:C2'	30:0:2852:A:H5'	2.43	0.49
22:V:1:THR:CB	30:0:93:C:H5''	2.40	0.49
28:2:38:LYS:HE3	38:0:4239:HOH:O	2.12	0.49
31:9:59:C:H2'	31:9:60:C:C6	2.47	0.49
3:C:34:ALA:HB3	3:C:220:THR:HG21	1.93	0.49
22:V:42:ASN:HB3	38:V:7247:HOH:O	2.11	0.49
30:0:1625:U:H3'	30:0:1625:U:H6	1.75	0.49
30:0:1856:C:H5'	30:0:1858:A:O4'	2.12	0.49
30:0:1903:U:O2'	30:0:1904:A:N7	2.42	0.49
5:E:133:VAL:HG12	5:E:141:VAL:HG13	1.94	0.49
5:E:5:LEU:HD21	5:E:66:GLN:HG3	1.93	0.49
14:N:154:LEU:C	14:N:156:GLU:H	2.14	0.49
20:T:5:ASP:O	20:T:9:LYS:HB2	2.13	0.49
24:X:43:VAL:HG11	24:X:82:GLU:HA	1.93	0.49
28:2:8:LYS:NZ	30:0:1677:U:OP2	2.45	0.49
30:0:1762:C:H2'	30:0:1763:C:H6	1.77	0.49
30:0:1790:C:H2'	30:0:1791:U:H6	1.76	0.49
30:0:1838:U:H3'	38:0:5533:HOH:O	2.12	0.49
30:0:669:G:O2'	30:0:670:G:H5'	2.12	0.49
11:K:27:ARG:HD2	38:K:3442:HOH:O	2.11	0.49
11:K:63:GLU:HG2	38:K:6344:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:40:ALA:O	18:R:44:VAL:HG23	2.12	0.49
30:0:1503:U:H2'	30:0:1504:A:O4'	2.11	0.49
30:0:1545:C:H2'	30:0:1546:G:O4'	2.12	0.49
30:0:1940:C:H4'	38:0:7360:HOH:O	2.12	0.49
30:0:2493:C:O2	30:0:2493:C:H2'	2.11	0.49
30:0:2709:G:N2	38:0:7632:HOH:O	2.46	0.49
30:0:407:A:H2'	30:0:408:A:C8	2.48	0.49
6:F:58:GLU:HB3	13:M:8:ILE:HG23	1.95	0.49
30:0:2271:G:N3	30:0:2271:G:H2'	2.27	0.49
30:0:2345:A:H3'	30:0:2346:C:C6	2.47	0.49
30:0:2435:U:H1'	38:0:5440:HOH:O	2.13	0.49
30:0:876:A:N3	30:0:876:A:C2'	2.76	0.49
1:A:33:GLU:CD	1:A:33:GLU:H	2.15	0.49
2:B:238:ASN:HD22	2:B:240:GLY:N	2.02	0.49
14:N:169:PRO:O	14:N:172:PHE:HB3	2.13	0.49
30:0:1391:G:H2'	30:0:1392:A:H5'	1.95	0.49
30:0:702:G:O2'	30:0:703:G:H5'	2.13	0.49
31:9:3:A:N6	31:9:22:G:H1'	2.28	0.49
31:9:3:A:C2	31:9:21:G:N3	2.81	0.49
3:C:78:ARG:HH11	3:C:78:ARG:HG3	1.78	0.49
4:D:103:ASN:ND2	4:D:133:ASN:HA	2.27	0.49
30:0:1149:U:H5''	30:0:1151:G:O4'	2.13	0.49
2:B:244:PRO:HB3	30:0:1234:U:N3	2.27	0.49
24:X:30:MET:HG2	30:0:1384:C:H5'	1.94	0.49
30:0:2649:A:H5'	30:0:2649:A:H8	1.77	0.49
30:0:2880:A:H2'	30:0:2881:C:H5'	1.95	0.49
15:O:25:VAL:HG12	30:0:709:G:O2'	2.11	0.49
30:0:951:A:O2'	30:0:952:G:H5'	2.13	0.49
1:A:186:TRP:CG	1:A:187:PRO:HA	2.48	0.49
3:C:162:VAL:HG22	3:C:232:LEU:HD21	1.94	0.49
8:H:30:LYS:H	8:H:62:HIS:CD2	2.30	0.49
30:0:2387:U:H2'	30:0:2388:C:C6	2.48	0.49
30:0:2802:C:H2'	30:0:2803:C:C6	2.46	0.49
30:0:2908:A:O5'	30:0:2908:A:H8	1.94	0.49
30:0:297:U:H2'	30:0:298:C:C6	2.48	0.49
30:0:815:U:O2'	30:0:1598:A:H4'	2.12	0.49
2:B:41:PHE:HB3	2:B:190:MET:CE	2.43	0.49
2:B:8:LYS:HG3	2:B:220:VAL:HG12	1.94	0.49
8:H:27:PRO:HD3	8:H:123:ILE:HG22	1.95	0.49
15:O:47:ARG:HG3	15:O:47:ARG:NH1	2.23	0.49
17:Q:66:LYS:HB2	17:Q:70:ALA:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1118:A:C8	30:0:1119:G:H5''	2.47	0.48
30:0:2353:A:H4'	30:0:2354:A:O5'	2.13	0.48
31:9:56:A:C3'	31:9:57:A:H5''	2.43	0.48
31:9:63:C:O2'	31:9:64:C:H5'	2.13	0.48
24:X:85:VAL:HG12	24:X:86:GLU:N	2.28	0.48
30:0:1159:G:H1	30:0:1208:C:H42	1.61	0.48
30:0:2335:C:H2'	30:0:2336:G:C8	2.48	0.48
30:0:2420:G:H2'	30:0:2421:G:C8	2.48	0.48
30:0:2697:A:H2'	30:0:2698:G:O4'	2.13	0.48
31:9:2:U:P	31:9:3:A:H5'	2.53	0.48
4:D:62:ASP:HA	38:D:4233:HOH:O	2.14	0.48
6:F:39:SER:HB3	6:F:45:ALA:HB2	1.95	0.48
26:Z:60:ASP:HB3	26:Z:69:ASP:HB3	1.95	0.48
30:0:1181:A:C2'	30:0:1182:C:H5'	2.43	0.48
30:0:1477:C:H5'	30:0:1868:G:H5''	1.94	0.48
30:0:2781:U:O2'	30:0:2782:G:H5'	2.13	0.48
9:I:78:ALA:HB1	9:I:93:ALA:HB1	1.95	0.48
11:K:81:ARG:HB2	11:K:87:ARG:NH1	2.28	0.48
23:W:38:THR:O	23:W:42:ARG:HB2	2.13	0.48
30:0:1119:G:N2	30:0:1246:A:N1	2.61	0.48
30:0:1419:U:H2'	30:0:1685:A:C2	2.48	0.48
30:0:947:U:H2'	30:0:948:G:H8	1.78	0.48
17:Q:1:PRO:HA	30:0:2299:G:O6	2.13	0.48
17:Q:50:GLY:HA2	38:0:6033:HOH:O	2.12	0.48
22:V:12:THR:HG22	22:V:15:GLU:CG	2.39	0.48
30:0:1221:G:C8	38:0:5995:HOH:O	2.55	0.48
30:0:1523:G:H2'	30:0:1524:U:C6	2.48	0.48
30:0:2134:G:C6	30:0:2258:A:C8	3.02	0.48
30:0:2419:U:H5''	30:0:2420:G:C5'	2.42	0.48
30:0:2825:C:H4'	30:0:2826:G:O5'	2.13	0.48
30:0:2842:G:C2'	30:0:2843:A:H5'	2.43	0.48
2:B:18:ARG:HE	2:B:256:GLN:NE2	2.11	0.48
4:D:170:TYR:CD1	4:D:170:TYR:N	2.81	0.48
8:H:34:HIS:HD2	8:H:90:LEU:O	1.96	0.48
9:I:87:PRO:HB3	38:I:6825:HOH:O	2.13	0.48
10:J:130:VAL:HG12	10:J:131:THR:N	2.28	0.48
11:K:74:VAL:HG12	11:K:75:ARG:HG3	1.95	0.48
23:W:90:TYR:N	23:W:90:TYR:CD1	2.80	0.48
30:0:1206:U:C5'	30:0:1206:U:H6	2.18	0.48
30:0:1513:C:O2'	30:0:1514:C:H5'	2.13	0.48
30:0:482:G:H4'	30:0:508:A:N1	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:17:LYS:O	2:B:260:HIS:HD2	1.96	0.48
3:C:87:ARG:HD3	38:0:3517:HOH:O	2.14	0.48
10:J:75:PRO:HG2	10:J:105:LEU:CD2	2.39	0.48
17:Q:15:LYS:HD3	30:0:2364:A:H5''	1.95	0.48
30:0:2335:C:H2'	30:0:2336:G:H8	1.77	0.48
30:0:2896:A:N3	30:0:2896:A:H2'	2.29	0.48
17:Q:40:HIS:HE1	30:0:949:U:O2'	1.95	0.48
13:M:167:GLY:O	13:M:171:ARG:HG3	2.13	0.48
20:T:68:ASP:HB2	38:0:5667:HOH:O	2.12	0.48
30:0:2001:G:O2'	30:0:2002:C:H5'	2.13	0.48
30:0:2598:U:O2	30:0:2600:A:H8	1.97	0.48
30:0:535:G:C6	30:0:2064:U:C5	3.01	0.48
1:A:36:ASP:HA	1:A:83:GLY:HA3	1.96	0.48
7:G:19:GLU:O	7:G:23:ILE:HG13	2.14	0.48
8:H:61:ARG:HG3	8:H:61:ARG:HH11	1.78	0.48
10:J:74:ARG:CB	10:J:74:ARG:HH11	2.25	0.48
16:P:13:VAL:HG21	16:P:41:ARG:HG2	1.96	0.48
30:0:130:C:H2'	38:0:3167:HOH:O	2.14	0.48
30:0:2415:A:H2'	30:0:2416:G:H5'	1.96	0.48
30:0:2506:A:N6	30:0:2511:A:O2'	2.46	0.48
30:0:2587:OMU:H5	38:0:7497:HOH:O	2.12	0.48
30:0:2649:A:H5'	30:0:2649:A:C8	2.49	0.48
29:3:91:GLN:O	29:3:92:GLU:HB2	2.14	0.48
6:F:91:VAL:CG1	6:F:92:GLY:H	2.25	0.48
13:M:164:THR:HG23	13:M:165:GLY:N	2.29	0.48
8:H:19:ARG:HH12	30:0:1008:C:H5''	1.78	0.48
30:0:1562:C:O2	30:0:1562:C:C2'	2.62	0.48
13:M:163:LEU:HD21	30:0:188:C:H5''	1.96	0.48
30:0:834:G:H4'	30:0:835:U:OP2	2.13	0.48
28:2:22:PRO:HG2	28:2:25:VAL:HG23	1.95	0.48
4:D:15:GLU:HA	4:D:16:PRO:HD3	1.73	0.48
14:N:119:GLN:O	14:N:123:ILE:HG13	2.14	0.48
18:R:14:ALA:HB3	18:R:147:LEU:HB2	1.96	0.48
23:W:23:MET:O	30:0:1025:C:H5'	2.14	0.48
1:A:212:PRO:HA	30:0:1943:C:O4'	2.14	0.47
4:D:23:VAL:HG21	4:D:45:THR:HG21	1.95	0.47
11:K:118:ALA:HA	11:K:125:ALA:HB2	1.95	0.47
12:L:22:ARG:HG2	38:0:9996:HOH:O	2.14	0.47
14:N:11:ARG:NH1	31:9:8:G:O6	2.47	0.47
14:N:49:THR:HG22	14:N:56:ASP:HB2	1.95	0.47
30:0:1130:U:H2'	30:0:1131:G:O4'	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1209:C:O2'	30:0:1210:G:H5'	2.13	0.47
30:0:1947:G:N2	30:0:1966:U:N3	2.61	0.47
30:0:821:U:H2'	30:0:822:C:H6	1.79	0.47
11:K:20:CYS:HB2	11:K:29:LEU:HG	1.96	0.47
23:W:4:LEU:HD22	23:W:52:VAL:CG2	2.44	0.47
25:Y:210:GLY:N	30:0:1313:A:H5''	2.29	0.47
30:0:1161:A:O5'	30:0:1161:A:H8	1.96	0.47
30:0:2334:C:O2'	30:0:2335:C:H5'	2.14	0.47
30:0:407:A:H8	38:0:4473:HOH:O	1.98	0.47
30:0:523:C:H2'	30:0:524:A:C8	2.50	0.47
2:B:62:ARG:HA	2:B:65:MET:HE3	1.95	0.47
2:B:5:ARG:HD2	2:B:8:LYS:NZ	2.30	0.47
3:C:19:PRO:HG2	3:C:22:PHE:CE1	2.49	0.47
3:C:246:ARG:NE	38:C:8620:HOH:O	2.40	0.47
6:F:13:GLU:OE2	6:F:78:GLU:HG2	2.14	0.47
18:R:114:VAL:HA	18:R:144:GLU:O	2.14	0.47
23:W:119:HIS:HE1	38:0:9557:HOH:O	1.97	0.47
26:Z:43:GLY:O	26:Z:47:ARG:HG2	2.14	0.47
30:0:1762:C:H2'	30:0:1763:C:C6	2.50	0.47
30:0:1768:C:H2'	30:0:1769:C:O4'	2.14	0.47
30:0:2112:A:H2'	30:0:2113:G:C8	2.49	0.47
30:0:2589:U:H2'	30:0:2590:U:H6	1.77	0.47
30:0:567:U:C5'	38:0:6408:HOH:O	2.63	0.47
30:0:823:U:H3'	38:0:4459:HOH:O	2.14	0.47
30:0:920:C:H5'	30:0:921:G:C4	2.49	0.47
31:9:47:A:C2	31:9:48:C:C2	3.02	0.47
1:A:33:GLU:O	1:A:34:ASP:HB2	2.14	0.47
3:C:22:PHE:HA	3:C:116:ALA:HA	1.96	0.47
3:C:233:THR:HG22	3:C:234:VAL:N	2.29	0.47
5:E:21:THR:HG23	5:E:30:THR:OG1	2.14	0.47
4:D:146:LYS:NZ	14:N:107:ASN:HD21	2.11	0.47
23:W:4:LEU:CD2	23:W:54:PHE:HB3	2.39	0.47
30:0:1343:C:H2'	30:0:1344:G:O5'	2.15	0.47
30:0:2420:G:H2'	30:0:2421:G:H8	1.79	0.47
31:9:114:G:H2'	31:9:115:C:H6	1.78	0.47
3:C:136:VAL:HG22	3:C:137:PRO:HA	1.97	0.47
5:E:91:PHE:CE1	30:0:2694:A:H4'	2.48	0.47
30:0:1450:C:H5''	38:0:9621:HOH:O	2.15	0.47
30:0:1589:G:N2	30:0:1605:G:H1'	2.29	0.47
30:0:1615:A:H5'	38:0:4194:HOH:O	2.14	0.47
30:0:2587:OMU:H6	30:0:2587:OMU:O5'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:523:C:H2'	30:0:524:A:H8	1.80	0.47
27:1:16:HIS:CD2	30:0:470:U:O2'	2.67	0.47
1:A:171:LYS:HB2	30:0:820:G:C6	2.50	0.47
1:A:47:HIS:HD2	30:0:1654:U:H2'	1.80	0.47
8:H:66:GLU:HA	38:H:229:HOH:O	2.13	0.47
10:J:90:LYS:HB2	33:J:8802:CL:CL	2.52	0.47
12:L:125:PHE:CE1	12:L:140:VAL:HG13	2.49	0.47
14:N:132:ASN:O	14:N:135:VAL:HG12	2.15	0.47
23:W:115:THR:HG23	38:W:5420:HOH:O	2.15	0.47
23:W:52:VAL:HG22	23:W:53:ALA:H	1.80	0.47
30:0:2526:C:C6	30:0:2526:C:C5'	2.95	0.47
30:0:2637:A:C5'	38:0:4941:HOH:O	2.62	0.47
30:0:2691:A:H5'	30:0:2693:U:H1'	1.96	0.47
30:0:312:U:C2	30:0:320:G:N2	2.83	0.47
1:A:8:ARG:HG2	38:A:9016:HOH:O	2.14	0.47
23:W:125:HIS:HD2	23:W:127:GLY:H	1.62	0.47
30:0:101:C:H2'	30:0:102:A:C8	2.50	0.47
30:0:222:A:H2'	30:0:223:G:O4'	2.14	0.47
30:0:308:U:C4	30:0:342:C:H1'	2.49	0.47
29:3:3:MET:O	29:3:90:PHE:HA	2.15	0.47
10:J:131:THR:HB	10:J:134:GLU:HG3	1.96	0.47
30:0:625:U:H5''	30:0:1044:C:N4	2.30	0.47
30:0:1682:A:H5''	38:0:9463:HOH:O	2.14	0.47
30:0:2241:C:O2'	30:0:2242:U:H5'	2.15	0.47
30:0:2269:C:H2'	30:0:2270:G:C5'	2.45	0.47
30:0:2506:A:O2'	30:0:2507:G:C8	2.50	0.47
30:0:251:C:H2'	30:0:252:C:H6	1.80	0.47
30:0:304:G:H1'	30:0:347:A:N6	2.29	0.47
31:9:1:U:C4'	31:9:3:A:OP1	2.62	0.47
6:F:91:VAL:HG11	30:0:262:A:OP2	2.14	0.47
8:H:54:VAL:HG13	8:H:162:PRO:HG3	1.97	0.47
23:W:88:THR:HG22	23:W:90:TYR:HD1	1.80	0.47
30:0:1165:G:H4'	30:0:1174:A:O2'	2.15	0.47
30:0:1632:A:H2'	30:0:1633:C:C5'	2.39	0.47
30:0:1667:A:H2'	30:0:1668:U:C6	2.50	0.47
30:0:2000:G:O2'	30:0:2001:G:H5'	2.15	0.47
30:0:545:G:C8	30:0:545:G:C5'	2.88	0.47
30:0:629:A:C2	30:0:2074:A:C2	3.03	0.47
30:0:685:C:O2	30:0:748:C:H4'	2.15	0.47
31:9:42:C:H5'	31:9:43:G:OP2	2.15	0.47
2:B:132:HIS:NE2	2:B:171:VAL:HG23	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1167:G:H2'	30:0:1168:C:O4'	2.15	0.47
1:A:223:ARG:NH1	30:0:2270:G:H4'	2.30	0.47
30:0:2073:G:OP2	30:0:2490:A:H5'	2.15	0.47
30:0:264:G:H1'	30:0:265:U:H5	1.80	0.47
30:0:295:C:H2'	30:0:296:G:O4'	2.15	0.47
13:M:9:ARG:HD2	30:0:380:A:OP2	2.15	0.47
30:0:638:C:H2'	30:0:639:A:C8	2.50	0.47
10:J:36:VAL:HG12	10:J:37:ALA:N	2.30	0.47
10:J:42:GLU:O	10:J:131:THR:HG23	2.15	0.47
12:L:67:ARG:HB2	12:L:112:GLY:HA3	1.96	0.47
24:X:43:VAL:HG22	24:X:76:ARG:NH1	2.30	0.47
30:0:1321:A:H2'	30:0:1322:G:C8	2.50	0.46
30:0:677:C:O2'	30:0:678:G:H5'	2.15	0.46
31:9:3:A:OP2	31:9:25:G:N2	2.47	0.46
31:9:7:G:H5'	38:9:9100:HOH:O	2.16	0.46
4:D:141:VAL:HG21	31:9:57:A:H8	1.80	0.46
11:K:34:VAL:HG22	11:K:47:ALA:HB2	1.97	0.46
17:Q:26:PRO:O	17:Q:30:VAL:HG23	2.14	0.46
30:0:1180:U:O2'	30:0:1181:A:H5'	2.15	0.46
30:0:1805:G:H2'	30:0:1806:G:H8	1.79	0.46
30:0:1477:C:C5'	30:0:1868:G:H5''	2.45	0.46
30:0:2566:A:C2	30:0:2696:G:O4'	2.68	0.46
30:0:853:C:H2'	30:0:854:G:O4'	2.15	0.46
31:9:45:A:C5	31:9:46:C:C5	3.02	0.46
1:A:53:ALA:HB3	38:A:9066:HOH:O	2.15	0.46
2:B:298:LYS:HG2	38:0:5531:HOH:O	2.15	0.46
11:K:41:LYS:O	11:K:42:ASN:HB2	2.15	0.46
17:Q:75:ILE:HB	38:Q:6286:HOH:O	2.15	0.46
23:W:119:HIS:HD2	23:W:120:PRO:O	1.98	0.46
25:Y:126:PRO:HG2	25:Y:128:PHE:CE1	2.51	0.46
25:Y:210:GLY:H	30:0:1313:A:H5''	1.80	0.46
30:0:255:A:C5	30:0:256:C:C5	3.02	0.46
30:0:319:A:H4'	30:0:338:C:C4	2.50	0.46
29:3:38:ARG:HB3	29:3:42:ARG:HH12	1.81	0.46
5:E:20:ILE:HD11	5:E:40:VAL:HG11	1.97	0.46
8:H:5:PRO:HD2	8:H:8:MET:SD	2.55	0.46
11:K:98:VAL:HG11	11:K:102:GLU:HA	1.95	0.46
13:M:99:ARG:CD	13:M:167:GLY:HA2	2.41	0.46
14:N:17:ARG:HH11	14:N:17:ARG:HB3	1.80	0.46
30:0:1139:U:H2'	30:0:1140:C:H6	1.80	0.46
30:0:1925:G:O2'	30:0:1926:G:H5'	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2249:G:C2	30:0:2253:G:C6	3.04	0.46
30:0:2250:G:C2	30:0:2251:G:H1'	2.51	0.46
12:L:57:VAL:HG21	30:0:2443:C:H5'	1.97	0.46
1:A:204:GLY:N	30:0:2634:G:OP2	2.47	0.46
30:0:2831:C:C2'	30:0:2832:C:H5'	2.45	0.46
30:0:800:G:H2'	30:0:801:U:C6	2.50	0.46
29:3:29:ARG:NH2	30:0:1925:G:C5'	2.79	0.46
31:9:65:A:N6	31:9:112:U:C6	2.83	0.46
17:Q:27:GLN:HE21	31:9:8:G:H5''	1.80	0.46
3:C:19:PRO:HG2	3:C:22:PHE:CD1	2.51	0.46
8:H:99:ARG:NH1	30:0:1055:G:OP2	2.47	0.46
20:T:26:THR:HA	20:T:39:ASN:HB3	1.97	0.46
12:L:6:ARG:HD3	30:0:1299:G:O6	2.15	0.46
30:0:1393:A:H2'	30:0:1394:C:C6	2.51	0.46
30:0:2869:G:H2'	30:0:2870:C:C6	2.50	0.46
3:C:206:ASN:HB2	30:0:329:A:OP2	2.16	0.46
30:0:369:G:H2'	30:0:370:G:H8	1.81	0.46
31:9:55:U:H4'	31:9:56:A:H8	1.80	0.46
8:H:31:ILE:HG23	38:H:229:HOH:O	2.15	0.46
9:I:107:LYS:HB3	9:I:110:ASP:HB2	1.97	0.46
30:0:1211:G:H2'	30:0:1212:C:C6	2.50	0.46
30:0:158:A:H3'	38:0:7573:HOH:O	2.15	0.46
30:0:1641:A:H2'	30:0:1642:A:C5'	2.44	0.46
30:0:1942:A:H4'	38:0:9046:HOH:O	2.16	0.46
30:0:255:A:C4	30:0:256:C:C6	3.04	0.46
30:0:2826:G:C6	30:0:2913:A:N6	2.84	0.46
30:0:365:G:C6	30:0:366:U:C4	3.04	0.46
30:0:622:G:O2'	30:0:623:U:H5'	2.15	0.46
30:0:736:A:H2'	30:0:737:A:O4'	2.16	0.46
1:A:70:ALA:HA	1:A:71:PRO:HD3	1.75	0.46
6:F:96:ALA:HA	38:F:3111:HOH:O	2.15	0.46
13:M:27:ARG:HH12	13:M:44:THR:CG2	2.28	0.46
16:P:120:ARG:NH1	30:0:1594:C:C5	2.84	0.46
21:U:44:ARG:HB3	38:U:3805:HOH:O	2.15	0.46
30:0:2379:G:N7	30:0:2408:A:N1	2.64	0.46
30:0:2433:A:H2'	30:0:2434:A:C8	2.50	0.46
30:0:2594:C:O2'	30:0:2595:U:H5'	2.16	0.46
30:0:2895:C:H2'	38:0:9573:HOH:O	2.15	0.46
30:0:451:C:O2'	30:0:452:G:H5'	2.16	0.46
11:K:29:LEU:HB3	11:K:55:VAL:HG11	1.98	0.46
12:L:18:HIS:HB2	30:0:903:U:O4	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:184:ARG:HG3	13:M:185:PRO:HA	1.98	0.46
30:0:1603:A:H5''	30:0:1604:G:H3'	1.98	0.46
30:0:1825:U:O2'	30:0:1826:C:H5'	2.15	0.46
13:M:27:ARG:NH1	13:M:44:THR:CG2	2.78	0.46
26:Z:76:THR:HG21	30:0:1652:C:H4'	1.96	0.46
30:0:1015:C:O5'	30:0:1015:C:H6	1.98	0.46
30:0:1506:U:H6	30:0:1506:U:H5'	1.81	0.46
30:0:366:U:H2'	30:0:367:G:O4'	2.16	0.46
30:0:466:A:H2'	30:0:467:G:O4'	2.15	0.46
31:9:45:A:H2'	31:9:46:C:C6	2.51	0.46
8:H:39:LYS:HA	8:H:87:LYS:NZ	2.30	0.46
30:0:1180:U:H2'	30:0:1181:A:O4'	2.16	0.46
30:0:1622:G:H2'	30:0:1623:C:H5'	1.98	0.46
30:0:1684:A:O2'	30:0:1685:A:H5''	2.16	0.46
30:0:1714:C:O2'	30:0:1715:C:H5'	2.16	0.46
30:0:1774:G:H1'	38:0:4551:HOH:O	2.14	0.46
30:0:2361:A:H2'	30:0:2362:A:C8	2.49	0.46
30:0:958:G:O2'	30:0:959:C:H5'	2.15	0.46
31:9:52:A:H2'	31:9:53:G:O4'	2.16	0.46
3:C:27:ARG:HG3	3:C:29:ASP:OD1	2.16	0.46
4:D:103:ASN:HD22	4:D:134:LEU:H	1.60	0.46
8:H:165:ARG:HD2	38:H:231:HOH:O	2.16	0.46
15:O:24:ALA:HB3	30:0:710:G:OP1	2.16	0.46
16:P:120:ARG:NH2	16:P:123:TYR:CD2	2.83	0.46
23:W:21:LEU:O	23:W:26:ILE:HG23	2.16	0.46
30:0:1165:G:H1'	30:0:1174:A:H1'	1.97	0.45
30:0:1202:A:O2'	30:0:1203:G:H5'	2.16	0.45
30:0:1278:A:H2'	30:0:1280:A:C8	2.51	0.45
30:0:1523:G:C6	30:0:1524:U:C4	3.04	0.45
30:0:2355:G:H5''	30:0:2356:A:OP2	2.16	0.45
30:0:2869:G:H2'	30:0:2870:C:H6	1.81	0.45
30:0:417:G:P	38:0:7432:HOH:O	2.74	0.45
15:O:63:LYS:NZ	30:0:659:A:N7	2.53	0.45
30:0:735:C:C5	30:0:736:A:N3	2.84	0.45
1:A:101:GLU:OE2	1:A:131:HIS:HB2	2.16	0.45
16:P:40:VAL:O	16:P:44:VAL:HG23	2.17	0.45
1:A:217:ARG:NH2	30:0:1853:C:O2'	2.49	0.45
30:0:236:A:H4'	30:0:237:G:OP1	2.15	0.45
30:0:271:C:N4	30:0:378:A:C2	2.71	0.45
30:0:496:G:H3'	38:0:7681:HOH:O	2.15	0.45
30:0:24:G:N2	30:0:518:G:H1'	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:64:G:H2'	30:0:65:C:O4'	2.16	0.45
30:0:711:G:O2'	30:0:712:C:H5'	2.17	0.45
27:1:28:HIS:CE1	27:1:31:LYS:HE2	2.51	0.45
31:9:106:U:O2'	31:9:107:C:H5'	2.15	0.45
3:C:79:ARG:O	3:C:87:ARG:HG2	2.16	0.45
9:I:114:TYR:N	9:I:114:TYR:CD1	2.84	0.45
20:T:38:ARG:NH1	38:0:6693:HOH:O	2.42	0.45
24:X:43:VAL:HG12	24:X:44:ASP:N	2.30	0.45
25:Y:234:VAL:HG12	25:Y:235:GLU:N	2.31	0.45
30:0:105:G:O2'	30:0:106:A:H5'	2.16	0.45
30:0:1201:C:H2'	30:0:1202:A:H5'	1.98	0.45
30:0:1883:U:C2'	30:0:1884:G:H5'	2.46	0.45
30:0:1909:A:N1	30:0:2128:G:H1'	2.31	0.45
30:0:2467:A:O2'	30:0:2468:A:H2'	2.17	0.45
30:0:2092:G:H2'	30:0:2613:G:OP1	2.16	0.45
2:B:26:PHE:HE1	38:B:9109:HOH:O	1.99	0.45
3:C:233:THR:HG22	3:C:234:VAL:H	1.81	0.45
4:D:170:TYR:HD1	4:D:170:TYR:N	2.14	0.45
5:E:1:PRO:HG2	5:E:59:MET:SD	2.56	0.45
6:F:36:THR:HG23	6:F:97:ALA:HB2	1.97	0.45
12:L:34:GLY:HA3	12:L:38:HIS:CE1	2.50	0.45
15:O:25:VAL:HG23	15:O:26:TRP:N	2.31	0.45
19:S:55:GLN:NE2	30:0:1446:U:H2'	2.30	0.45
20:T:21:LYS:HA	20:T:24:ARG:HG3	1.99	0.45
21:U:17:THR:CG2	21:U:18:GLY:N	2.79	0.45
23:W:73:LEU:HA	23:W:73:LEU:HD12	1.80	0.45
30:0:1015:C:H2'	30:0:1016:U:C6	2.51	0.45
30:0:1942:A:HO2'	30:0:1943:C:H5'	1.80	0.45
30:0:210:U:H2'	30:0:211:U:C6	2.51	0.45
31:9:2:U:OP2	31:9:2:U:H4'	2.16	0.45
1:A:94:LEU:HG	1:A:99:ILE:HD11	1.97	0.45
30:0:1001:U:O2'	30:0:1002:G:H5'	2.17	0.45
30:0:1268:C:H2'	30:0:1269:G:C8	2.52	0.45
30:0:1834:C:H2'	30:0:1840:A:H62	1.82	0.45
30:0:1855:G:H4'	30:0:1856:C:O5'	2.16	0.45
30:0:2895:C:O2'	30:0:2896:A:H5''	2.16	0.45
30:0:843:A:C2	30:0:846:A:C8	3.04	0.45
27:1:25:LYS:O	27:1:25:LYS:HG2	2.17	0.45
3:C:236:THR:CG2	3:C:239:ALA:H	2.21	0.45
16:P:16:VAL:CG1	16:P:20:ARG:HB2	2.46	0.45
24:X:21:PRO:HG2	24:X:24:LYS:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1634:G:C3'	38:0:3907:HOH:O	2.46	0.45
30:0:2314:G:C2'	30:0:2315:C:H5'	2.47	0.45
30:0:2456:A:H5'	38:0:5702:HOH:O	2.17	0.45
30:0:2664:A:H8	30:0:2664:A:OP1	1.99	0.45
30:0:423:A:C5	30:0:424:C:C5	3.05	0.45
30:0:682:A:H2'	30:0:683:G:O4'	2.16	0.45
30:0:945:U:H2'	30:0:946:C:C6	2.52	0.45
28:2:48:ASP:O	28:2:49:GLU:HB2	2.17	0.45
1:A:199:HIS:HD2	1:A:201:PHE:HB2	1.82	0.45
2:B:69:VAL:HA	2:B:70:PRO:HD3	1.81	0.45
4:D:141:VAL:HG21	31:9:57:A:C8	2.51	0.45
23:W:35:VAL:HG23	23:W:41:TYR:CD2	2.52	0.45
25:Y:133:HIS:HD2	38:Y:8881:HOH:O	1.98	0.45
30:0:1183:C:H42	30:0:1184:C:N4	2.10	0.45
30:0:1379:A:H1'	38:0:9695:HOH:O	2.16	0.45
30:0:1386:G:O2'	30:0:1387:G:H5'	2.17	0.45
30:0:1624:A:H4'	30:0:1626:A:H5''	1.99	0.45
30:0:2506:A:C4	38:0:6063:HOH:O	2.67	0.45
30:0:2681:A:H4'	30:0:2682:C:OP1	2.16	0.45
30:0:482:G:O4'	30:0:511:A:C2	2.69	0.45
30:0:73:U:O2'	30:0:74:G:H5'	2.17	0.45
2:B:5:ARG:NH2	30:0:2548:C:OP2	2.50	0.45
17:Q:25:PRO:HA	17:Q:26:PRO:HD3	1.83	0.45
23:W:13:MET:CE	23:W:17:ILE:HG22	2.47	0.45
30:0:1014:A:H2'	30:0:1015:C:H5'	1.99	0.45
30:0:1484:G:H2'	38:0:9106:HOH:O	2.17	0.45
1:A:190:ARG:NH1	30:0:1845:A:OP2	2.49	0.45
30:0:670:G:H2'	30:0:671:A:C8	2.51	0.45
2:B:223:ARG:HG3	2:B:232:TRP:O	2.17	0.45
12:L:61:ALA:HB2	12:L:105:TYR:CZ	2.52	0.45
14:N:40:ASN:ND2	31:9:28:U:H5''	2.31	0.45
18:R:96:VAL:HG13	18:R:106:GLY:HA3	1.99	0.45
30:0:1221:G:H8	38:0:5995:HOH:O	1.95	0.45
30:0:1400:C:O2'	30:0:1401:G:H5'	2.17	0.45
30:0:2248:C:C4	30:0:2249:G:N7	2.85	0.45
30:0:2727:A:C6	30:0:2756:U:C2	3.05	0.45
5:E:154:ILE:HD11	5:E:157:LYS:NZ	2.32	0.45
11:K:118:ALA:CA	11:K:125:ALA:HB2	2.47	0.45
25:Y:130:ARG:HB2	25:Y:142:SER:O	2.16	0.45
25:Y:170:SER:OG	25:Y:175:ARG:HG3	2.16	0.45
30:0:1191:A:C2	30:0:1207:A:C2	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1279:U:O2	30:0:1279:U:C2'	2.64	0.45
30:0:1425:G:O2'	30:0:1426:C:H5'	2.17	0.45
30:0:1537:C:H1'	38:0:6597:HOH:O	2.16	0.45
30:0:861:A:H4'	30:0:1697:G:H4'	1.99	0.45
30:0:2002:C:H2'	30:0:2003:U:H5'	1.99	0.45
30:0:2819:C:H2'	30:0:2820:A:C8	2.51	0.45
30:0:441:A:H8	30:0:441:A:O5'	1.99	0.45
27:1:20:ARG:HG2	30:0:111:C:O2'	2.17	0.45
1:A:94:LEU:HG	1:A:99:ILE:CD1	2.47	0.45
11:K:34:VAL:HB	38:K:7169:HOH:O	2.17	0.45
30:0:107:U:H2'	30:0:108:U:H5'	1.99	0.44
30:0:128:A:H3'	30:0:128:A:C8	2.52	0.44
30:0:1333:U:H2'	30:0:1334:C:C6	2.52	0.44
30:0:1771:U:O2'	30:0:1773:G:N7	2.50	0.44
30:0:2072:G:C6	30:0:2533:C:H1'	2.52	0.44
30:0:2483:A:H4'	30:0:2484:U:OP2	2.17	0.44
30:0:2812:A:H1'	38:0:5796:HOH:O	2.17	0.44
31:9:36:C:C5	31:9:37:C:C5	3.05	0.44
31:9:39:U:HO2'	31:9:42:C:H5	1.65	0.44
5:E:91:PHE:HE1	30:0:2694:A:H4'	1.82	0.44
12:L:36:ASP:HB2	38:L:8836:HOH:O	2.17	0.44
17:Q:42:LYS:HE2	30:0:952:G:OP1	2.18	0.44
24:X:74:ALA:HB2	24:X:85:VAL:HG13	2.00	0.44
30:0:790:A:H1'	30:0:1710:A:H2'	1.99	0.44
30:0:1759:A:N3	30:0:1818:C:H2'	2.33	0.44
30:0:213:G:N2	30:0:225:G:H2'	2.32	0.44
30:0:2329:C:O2'	30:0:2330:U:H5'	2.17	0.44
30:0:2543:G:H2'	30:0:2544:G:O4'	2.17	0.44
30:0:2689:A:H2'	30:0:2690:U:H5'	1.99	0.44
30:0:368:C:C2'	30:0:369:G:H5'	2.47	0.44
30:0:506:G:N2	30:0:509:A:C5'	2.72	0.44
30:0:905:C:H3'	38:0:5198:HOH:O	2.17	0.44
6:F:30:LYS:HE2	6:F:99:THR:HG21	1.99	0.44
8:H:46:TYR:HA	8:H:47:PRO:HD3	1.80	0.44
20:T:9:LYS:HD2	38:0:3766:HOH:O	2.16	0.44
23:W:4:LEU:O	23:W:32:CYS:HA	2.17	0.44
30:0:1545:C:H1'	30:0:1641:A:N6	2.33	0.44
30:0:1522:A:C2	30:0:1665:G:C6	3.05	0.44
13:M:86:GLN:NE2	30:0:2274:A:H1'	2.32	0.44
30:0:2511:A:H2'	30:0:2512:U:O4'	2.17	0.44
30:0:343:C:O2'	30:0:344:C:H5'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:579:G:H2'	30:0:580:A:C8	2.52	0.44
31:9:39:U:C2'	31:9:40:C:OP1	2.65	0.44
10:J:74:ARG:NH1	10:J:76:ASP:HB2	2.31	0.44
13:M:164:THR:CG2	13:M:167:GLY:H	2.27	0.44
20:T:9:LYS:HG3	38:0:7437:HOH:O	2.16	0.44
21:U:33:SER:O	21:U:37:GLU:HG3	2.16	0.44
30:0:1175:G:H8	30:0:1193:A:HO2'	1.64	0.44
30:0:1622:G:C2'	30:0:1623:C:H5'	2.47	0.44
30:0:2239:C:H2'	30:0:2240:U:C6	2.53	0.44
30:0:2375:A:H2'	30:0:2376:C:C6	2.53	0.44
30:0:2775:A:C6	30:0:2799:A:C8	3.06	0.44
30:0:281:U:H5	38:0:7606:HOH:O	2.01	0.44
17:Q:95:GLU:HA	30:0:949:U:H4'	1.99	0.44
30:0:999:C:O2'	30:0:1000:C:H5'	2.18	0.44
1:A:109:GLU:HG2	1:A:116:GLY:N	2.33	0.44
1:A:223:ARG:HD2	30:0:2272:G:OP1	2.17	0.44
2:B:320:GLN:NE2	2:B:321:PRO:HD2	2.29	0.44
3:C:236:THR:HG22	3:C:239:ALA:CB	2.47	0.44
5:E:169:THR:HG22	5:E:170:ARG:HG3	2.00	0.44
30:0:2238:A:O2'	30:0:2239:C:H5'	2.17	0.44
30:0:249:G:O2'	30:0:250:C:H5'	2.17	0.44
30:0:2858:U:H2'	30:0:2859:C:O4'	2.16	0.44
38:C:8546:HOH:O	30:0:457:U:H4'	2.17	0.44
25:Y:134:HIS:HE1	30:0:538:C:OP2	2.01	0.44
14:N:141:ARG:NH2	31:9:48:C:H4'	2.27	0.44
2:B:211:THR:HG21	38:0:7469:HOH:O	2.17	0.44
6:F:57:GLU:O	6:F:61:MET:HG3	2.18	0.44
13:M:164:THR:HB	38:M:8819:HOH:O	2.18	0.44
14:N:143:ARG:HB3	14:N:143:ARG:HE	1.61	0.44
19:S:57:THR:HG22	19:S:58:MET:N	2.32	0.44
16:P:54:LYS:HB2	30:0:1717:A:H5''	1.98	0.44
30:0:1790:C:H2'	30:0:1791:U:C6	2.51	0.44
30:0:1973:A:H5'	30:0:1973:A:C8	2.44	0.44
30:0:277:U:O2'	30:0:278:A:H5'	2.18	0.44
30:0:2800:A:H5'	30:0:2801:A:OP2	2.18	0.44
30:0:2812:A:N7	38:0:7529:HOH:O	2.36	0.44
31:9:1:U:H5''	31:9:3:A:OP1	2.18	0.44
2:B:280:VAL:HG13	2:B:333:GLU:O	2.18	0.44
11:K:87:ARG:NE	38:0:5721:HOH:O	2.50	0.44
30:0:1434:A:H2'	30:0:1436:C:C5	2.53	0.44
30:0:1593:C:H1'	38:0:6112:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1592:G:O2'	30:0:1593:C:O4'	2.33	0.44
30:0:1950:G:H2'	30:0:1951:G:C8	2.53	0.44
30:0:636:G:H1'	30:0:2058:G:C4	2.53	0.44
30:0:2653:A:H2'	30:0:2654:C:C6	2.53	0.44
30:0:302:A:O2'	30:0:303:C:H5'	2.17	0.44
30:0:371:U:H2'	30:0:372:A:C8	2.48	0.44
4:D:57:THR:HG23	4:D:63:ILE:HA	2.00	0.44
7:G:63:ARG:N	38:G:2569:HOH:O	2.50	0.44
13:M:99:ARG:HH21	13:M:170:ASN:HD22	1.64	0.44
23:W:122:ARG:NH2	38:0:5297:HOH:O	2.49	0.44
23:W:133:LYS:HG3	38:W:5904:HOH:O	2.18	0.44
30:0:1067:A:H3'	38:0:4304:HOH:O	2.17	0.44
30:0:1191:A:H2	30:0:1206:U:H3	1.65	0.44
18:R:132:ARG:NH2	30:0:2055:A:H4'	2.32	0.44
30:0:2252:A:C6	30:0:2253:G:H1'	2.53	0.44
30:0:2718:C:C6	30:0:2718:C:H5'	2.50	0.44
30:0:2831:C:H2'	30:0:2832:C:H5'	1.99	0.44
30:0:289:G:O2'	30:0:290:C:H5'	2.17	0.44
30:0:291:C:H2'	30:0:292:G:O4'	2.18	0.44
30:0:790:A:H2'	30:0:791:A:O4'	2.17	0.44
4:D:76:ARG:NE	31:9:44:A:O4'	2.51	0.44
7:G:63:ARG:O	7:G:67:LEU:HG	2.17	0.44
14:N:24:LEU:HD13	17:Q:26:PRO:HB3	1.98	0.44
30:0:1044:C:H5''	38:0:9029:HOH:O	2.18	0.44
30:0:1181:A:H2'	30:0:1182:C:C5'	2.48	0.44
30:0:1202:A:C2'	30:0:1203:G:H5'	2.48	0.44
25:Y:142:SER:OG	30:0:1331:G:OP2	2.32	0.44
30:0:1603:A:C5'	30:0:1605:G:C5'	2.95	0.44
30:0:2264:A:H2'	30:0:2265:U:C6	2.53	0.44
30:0:2064:U:H4'	30:0:2653:A:OP1	2.17	0.44
30:0:567:U:O2'	30:0:568:G:H5'	2.17	0.44
30:0:705:C:H2'	30:0:705:C:O2	2.17	0.44
30:0:699:C:H6	30:0:744:G:O4'	2.01	0.44
1:A:217:ARG:HH11	1:A:217:ARG:HG3	1.82	0.44
2:B:36:PRO:CA	2:B:168:GLY:HA3	2.43	0.44
14:N:164:ASP:OD1	14:N:167:ASP:HA	2.18	0.44
16:P:10:ALA:HA	16:P:13:VAL:HG12	1.99	0.44
30:0:1127:C:C5	30:0:1128:U:C4	3.06	0.43
30:0:47:G:N3	30:0:114:A:C2	2.86	0.43
30:0:1163:G:C2	30:0:1184:C:N3	2.86	0.43
30:0:129:A:H4'	30:0:130:C:OP1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2598:U:O2	30:0:2600:A:C8	2.71	0.43
30:0:825:U:H5''	30:0:826:U:OP1	2.18	0.43
28:2:41:HIS:CD2	28:2:44:ARG:H	2.33	0.43
1:A:97:ALA:HA	1:A:131:HIS:NE2	2.33	0.43
3:C:168:ARG:NH2	3:C:190:ALA:O	2.51	0.43
8:H:87:LYS:NZ	8:H:87:LYS:HB2	2.33	0.43
15:O:65:LEU:HD13	30:0:746:A:C6	2.53	0.43
25:Y:141:THR:HG23	38:Y:8888:HOH:O	2.18	0.43
30:0:134:U:C2	30:0:145:A:C2	3.07	0.43
30:0:1552:G:N2	30:0:1634:G:H1'	2.33	0.43
30:0:1947:G:H2'	30:0:1948:G:H8	1.82	0.43
18:R:128:ARG:NH2	30:0:2054:A:C2	2.86	0.43
30:0:2379:G:H5'	30:0:2381:C:O4'	2.18	0.43
30:0:2421:G:H3'	30:0:2422:U:C5'	2.47	0.43
30:0:2488:A:H2'	30:0:2489:G:O4'	2.19	0.43
30:0:2566:A:H2	30:0:2695:C:O2	2.01	0.43
30:0:677:C:P	38:0:7147:HOH:O	2.75	0.43
31:9:35:C:H5''	38:9:9080:HOH:O	2.17	0.43
4:D:154:LYS:H	4:D:154:LYS:CD	2.24	0.43
6:F:91:VAL:CG1	6:F:92:GLY:N	2.78	0.43
13:M:99:ARG:HD2	13:M:167:GLY:CA	2.45	0.43
14:N:114:LYS:O	14:N:118:ILE:HG13	2.18	0.43
18:R:104:PHE:HB3	18:R:109:MET:HE1	2.01	0.43
30:0:1115:U:O2'	30:0:1116:U:H5'	2.18	0.43
30:0:1762:C:O2'	30:0:1763:C:H5'	2.17	0.43
12:L:48:LYS:HE2	30:0:220:C:C2	2.53	0.43
30:0:2607:U:H4'	38:0:9448:HOH:O	2.18	0.43
30:0:484:A:N1	30:0:506:G:H4'	2.33	0.43
22:V:44:GLY:HA3	30:0:92:G:H4'	1.99	0.43
2:B:304:PRO:HD2	2:B:307:ARG:HE	1.83	0.43
3:C:127:ARG:HD3	3:C:129:HIS:HE1	1.83	0.43
5:E:80:TRP:O	5:E:134:SER:HA	2.18	0.43
9:I:111:LEU:CD2	30:0:1163:G:H4'	2.45	0.43
30:0:1245:C:O5'	30:0:1245:C:H6	2.01	0.43
30:0:1395:C:H2'	30:0:1396:C:C6	2.53	0.43
30:0:1700:C:H5''	30:0:1701:A:OP2	2.18	0.43
30:0:17:G:H2'	30:0:18:C:H6	1.82	0.43
30:0:2256:G:H2'	30:0:2257:G:O5'	2.17	0.43
33:0:8814:CL:CL	38:0:7753:HOH:O	2.59	0.43
31:9:34:A:H2'	31:9:35:C:O4'	2.18	0.43
14:N:41:LYS:HD3	38:9:9063:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:7:LYS:HG2	16:P:23:PHE:CE2	2.54	0.43
30:0:1896:G:C6	30:0:1897:U:C4	3.07	0.43
30:0:1964:U:H2'	30:0:1964:U:O2	2.17	0.43
30:0:1972:U:C2'	30:0:1973:A:C5'	2.96	0.43
30:0:2504:A:H2'	30:0:2505:G:H5'	2.00	0.43
6:F:59:ILE:HD13	30:0:263:U:O4'	2.18	0.43
30:0:522:U:O2'	30:0:1366:C:H5'	2.18	0.43
30:0:559:U:H2'	30:0:560:U:O4'	2.18	0.43
1:A:103:VAL:HA	1:A:104:PRO:HD3	1.83	0.43
1:A:190:ARG:NH2	1:A:207:GLN:OE1	2.52	0.43
1:A:55:VAL:HG23	1:A:68:ILE:O	2.19	0.43
1:A:95:PRO:HA	1:A:153:ARG:HA	1.99	0.43
2:B:198:GLU:HA	38:B:9119:HOH:O	2.19	0.43
2:B:271:ASP:HB3	2:B:296:LEU:HD12	1.99	0.43
3:C:93:LYS:O	3:C:98:ARG:NH2	2.51	0.43
4:D:50:VAL:HG13	31:9:41:C:O4'	2.18	0.43
8:H:61:ARG:HG3	38:0:4984:HOH:O	2.17	0.43
11:K:115:ARG:HG3	11:K:116:GLU:N	2.34	0.43
13:M:157:ASP:HB3	13:M:160:PHE:HD1	1.84	0.43
24:X:15:ARG:HH22	30:0:2856:A:P	2.41	0.43
30:0:1063:G:H8	38:0:9865:HOH:O	2.01	0.43
30:0:1187:U:C2	30:0:1189:A:OP2	2.72	0.43
30:0:1702:U:H5'	38:0:3432:HOH:O	2.18	0.43
30:0:2070:G:H2'	30:0:2072:G:OP1	2.19	0.43
30:0:2437:A:H2'	30:0:2438:G:C8	2.54	0.43
30:0:2906:A:H5'	30:0:2907:C:O4'	2.19	0.43
30:0:542:A:H2'	30:0:543:G:O4'	2.18	0.43
30:0:570:C:H2'	30:0:571:C:H5'	2.01	0.43
31:9:28:U:H2'	31:9:29:C:C6	2.54	0.43
4:D:25:MET:CE	4:D:41:LEU:HG	2.47	0.43
12:L:39:GLU:HG2	30:0:926:A:C4'	2.48	0.43
13:M:193:LYS:HB3	30:0:392:U:H4'	1.99	0.43
14:N:151:ASP:OD1	14:N:166:ALA:HA	2.19	0.43
23:W:125:HIS:HB2	23:W:137:GLN:HG2	2.00	0.43
25:Y:216:ARG:NH1	38:Y:8833:HOH:O	2.51	0.43
30:0:1198:U:C6	30:0:1200:A:OP2	2.72	0.43
30:0:17:G:H2'	30:0:18:C:C6	2.53	0.43
30:0:2115:U:H2'	30:0:2116:U:C6	2.53	0.43
30:0:243:A:H61	30:0:269:G:H1'	1.83	0.43
30:0:2587:OMU:H2'	30:0:2589:U:H5''	2.00	0.43
30:0:37:A:H2'	30:0:38:G:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:969:G:H1	30:0:999:C:H42	1.66	0.43
29:3:11:CYS:HB2	29:3:20:HIS:CE1	2.54	0.43
1:A:179:MET:HG2	1:A:186:TRP:CB	2.49	0.43
2:B:14:GLY:HA2	2:B:15:PRO:C	2.39	0.43
2:B:87:TYR:HD1	38:B:9041:HOH:O	2.01	0.43
3:C:25:PRO:HG2	38:C:8523:HOH:O	2.18	0.43
3:C:54:LEU:HD23	3:C:79:ARG:HG3	2.00	0.43
30:0:1163:G:H1	30:0:1184:C:N4	2.16	0.43
30:0:1553:C:H2'	30:0:1554:C:H6	1.84	0.43
30:0:1588:G:C6	30:0:1589:G:C6	3.07	0.43
2:B:234:ARG:NH2	30:0:2039:A:OP2	2.51	0.43
30:0:2134:G:N2	30:0:2242:U:C2	2.87	0.43
30:0:652:G:H8	38:0:3020:HOH:O	2.00	0.43
30:0:734:U:H2'	30:0:736:A:OP2	2.19	0.43
28:2:28:LYS:O	30:0:87:C:H2'	2.18	0.43
30:0:886:A:OP2	30:0:2113:G:H5'	2.19	0.43
30:0:947:U:O2'	30:0:948:G:H5'	2.19	0.43
2:B:248:ARG:NH1	38:B:9080:HOH:O	2.50	0.43
2:B:297:VAL:HB	38:B:9070:HOH:O	2.19	0.43
3:C:173:LYS:HE3	30:0:1311:G:O6	2.18	0.43
4:D:10:PHE:CG	4:D:11:HIS:N	2.87	0.43
6:F:72:VAL:HA	6:F:73:PRO:HD3	1.85	0.43
14:N:108:SER:HA	14:N:109:PRO:HD3	1.78	0.43
16:P:133:SER:HA	38:0:3512:HOH:O	2.18	0.43
23:W:13:MET:HE3	23:W:17:ILE:HG22	2.00	0.43
30:0:1186:C:N4	30:0:1187:U:C4	2.87	0.43
30:0:129:A:O2'	30:0:131:A:OP1	2.36	0.43
30:0:1942:A:H2'	30:0:1943:C:H6	1.83	0.43
30:0:297:U:H1'	38:0:3947:HOH:O	2.18	0.43
30:0:735:C:C5	30:0:736:A:C2	3.06	0.43
30:0:792:G:H4'	38:0:3424:HOH:O	2.19	0.43
27:1:37:CYS:SG	27:1:39:PHE:HB2	2.59	0.43
31:9:106:U:O5'	31:9:106:U:H6	2.01	0.43
31:9:1:U:O3'	31:9:3:A:OP1	2.36	0.43
3:C:170:ASP:OD2	30:0:330:C:H5	2.01	0.43
30:0:1883:U:O2'	30:0:1884:G:H5'	2.19	0.43
13:M:171:ARG:NH2	30:0:189:A:OP1	2.51	0.43
30:0:2712:G:O2'	30:0:2713:G:H5'	2.19	0.43
30:0:2820:A:H2'	30:0:2821:C:C6	2.54	0.43
30:0:2842:G:H2'	30:0:2843:A:C5'	2.48	0.43
8:H:22:TYR:CZ	30:0:1007:A:H2'	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:98:ILE:HD12	16:P:102:ARG:NE	2.34	0.43
19:S:57:THR:C	19:S:59:ASP:H	2.22	0.43
30:0:1052:G:H2'	30:0:1052:G:N3	2.33	0.42
30:0:1965:C:H6	30:0:1965:C:O5'	2.02	0.42
30:0:212:A:O4'	30:0:214:U:C6	2.72	0.42
17:Q:53:HIS:CD2	30:0:2389:U:H4'	2.54	0.42
30:0:2783:A:H2'	30:0:2784:A:C8	2.54	0.42
30:0:282:C:O2'	30:0:283:U:C4'	2.67	0.42
30:0:2756:U:C2	30:0:2896:A:H2	2.37	0.42
30:0:305:A:C5	30:0:329:A:C2	3.07	0.42
27:1:28:HIS:HD2	27:1:30:LYS:H	1.66	0.42
3:C:236:THR:HG22	3:C:239:ALA:HB2	2.01	0.42
3:C:78:ARG:HG3	3:C:78:ARG:NH1	2.34	0.42
5:E:69:ILE:HA	5:E:72:MET:CE	2.48	0.42
13:M:47:ASP:CG	13:M:48:LYS:N	2.72	0.42
14:N:171:HIS:CE1	38:N:8855:HOH:O	2.72	0.42
14:N:23:ARG:O	14:N:27:LEU:HG	2.18	0.42
15:O:81:PHE:HB2	15:O:86:GLU:HB2	2.01	0.42
21:U:4:ARG:N	38:U:5334:HOH:O	2.52	0.42
23:W:21:LEU:HD21	23:W:48:VAL:CG1	2.46	0.42
26:Z:47:ARG:NH1	38:Z:8704:HOH:O	2.50	0.42
30:0:128:A:O2'	30:0:129:A:C5'	2.67	0.42
3:C:184:ARG:NH1	30:0:1306:U:OP1	2.51	0.42
30:0:162:C:H2'	30:0:163:U:H5'	2.02	0.42
30:0:1706:G:C5	30:0:1707:G:C6	3.07	0.42
30:0:1921:A:C6	30:0:1922:A:C2	3.08	0.42
30:0:2332:A:H3'	30:0:2333:G:H8	1.84	0.42
30:0:834:G:H3'	30:0:835:U:H4'	2.01	0.42
30:0:867:A:H2	30:0:880:C:O2	2.02	0.42
2:B:190:MET:HE2	2:B:194:PHE:CD1	2.53	0.42
3:C:237:GLU:HA	38:C:8626:HOH:O	2.18	0.42
11:K:82:ARG:NH2	11:K:115:ARG:HG2	2.33	0.42
30:0:1249:U:H2'	30:0:1250:C:C6	2.54	0.42
30:0:128:A:C8	30:0:128:A:C3'	3.02	0.42
30:0:932:U:H1'	30:0:1296:A:H1'	2.00	0.42
30:0:1350:U:H4'	38:0:5134:HOH:O	2.18	0.42
30:0:1461:U:H2'	30:0:1462:C:C6	2.54	0.42
30:0:2121:G:O2'	30:0:2122:C:H5'	2.19	0.42
30:0:2347:C:H2'	30:0:2348:C:H6	1.83	0.42
30:0:31:C:C4'	38:0:7437:HOH:O	2.66	0.42
2:B:238:ASN:ND2	2:B:240:GLY:H	2.04	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:ILE:HG13	38:B:9070:HOH:O	2.17	0.42
14:N:164:ASP:CG	14:N:167:ASP:HA	2.39	0.42
14:N:69:TYR:CE2	14:N:184:ILE:HD11	2.55	0.42
19:S:57:THR:HG23	38:S:8979:HOH:O	2.19	0.42
30:0:1098:A:H2'	30:0:1099:G:O4'	2.19	0.42
30:0:1613:C:H2'	30:0:1614:G:O4'	2.19	0.42
30:0:1741:U:C4	30:0:2033:G:C8	3.07	0.42
6:F:59:ILE:CD1	30:0:263:U:C2	3.02	0.42
30:0:40:C:H6	30:0:40:C:O5'	2.02	0.42
30:0:699:C:C2	30:0:744:G:C2	3.07	0.42
29:3:11:CYS:HB2	29:3:20:HIS:HE1	1.85	0.42
6:F:110:ASP:O	6:F:114:LYS:HG3	2.20	0.42
15:O:105:ASN:HD21	15:O:109:SER:N	2.17	0.42
18:R:104:PHE:CB	18:R:109:MET:HE1	2.49	0.42
30:0:1020:A:H1'	38:0:7242:HOH:O	2.19	0.42
30:0:177:A:H2'	30:0:178:U:O4'	2.19	0.42
30:0:2032:U:O2'	30:0:2033:G:H5''	2.20	0.42
4:D:129:ASP:OD1	30:0:2338:G:H2'	2.20	0.42
30:0:2801:A:H2'	30:0:2801:A:N3	2.34	0.42
30:0:74:G:H2'	30:0:75:U:C6	2.54	0.42
10:J:75:PRO:HD3	10:J:136:SER:OG	2.20	0.42
14:N:71:TRP:HB2	38:N:8833:HOH:O	2.19	0.42
16:P:87:ARG:HG2	38:P:188:HOH:O	2.18	0.42
18:R:3:SER:HB2	30:0:20:G:O3'	2.19	0.42
23:W:4:LEU:HD23	23:W:4:LEU:HA	1.83	0.42
30:0:1081:A:H5''	38:0:3159:HOH:O	2.19	0.42
30:0:1482:A:O2'	30:0:1483:C:H5'	2.20	0.42
30:0:1495:C:H1'	30:0:1573:A:H1'	2.02	0.42
30:0:1760:G:H5'	30:0:1818:C:O2'	2.20	0.42
30:0:2089:A:C2'	30:0:2090:G:H5'	2.49	0.42
30:0:2754:G:C2'	30:0:2755:G:H5'	2.49	0.42
30:0:2657:G:O2'	30:0:2842:G:N7	2.47	0.42
30:0:316:A:N3	30:0:336:G:O2'	2.46	0.42
25:Y:132:ASP:OD2	30:0:621:C:H5'	2.19	0.42
30:0:69:A:C8	30:0:69:A:C5'	2.96	0.42
2:B:41:PHE:CZ	2:B:79:MET:HG3	2.55	0.42
24:X:78:GLU:HB3	38:X:5564:HOH:O	2.19	0.42
30:0:1735:C:O2'	30:0:1736:A:H5'	2.19	0.42
30:0:2523:U:O2'	30:0:2524:G:H5'	2.20	0.42
2:B:56:ASP:HB2	2:B:322:ARG:HE	1.85	0.42
4:D:18:ILE:HD13	4:D:84:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:73:LEU:HD12	9:I:107:LYS:HZ2	1.85	0.42
17:Q:28:ARG:HG2	38:Q:4350:HOH:O	2.20	0.42
30:0:1058:A:H2'	30:0:1060:C:C5'	2.48	0.42
30:0:113:A:OP2	30:0:114:A:H2'	2.19	0.42
30:0:2265:U:H2'	30:0:2266:A:C8	2.55	0.42
30:0:2421:G:H3'	30:0:2422:U:H5''	2.02	0.42
30:0:2600:A:H2'	30:0:2601:A:O4'	2.19	0.42
30:0:2809:G:H2'	30:0:2810:G:O4'	2.20	0.42
30:0:445:U:H2'	30:0:446:G:C8	2.54	0.42
30:0:583:C:H2'	30:0:584:U:C6	2.50	0.42
28:2:41:HIS:HB3	28:2:44:ARG:HB2	2.02	0.42
3:C:129:HIS:HE1	3:C:231:ARG:HA	1.84	0.42
4:D:21:VAL:HA	4:D:131:THR:O	2.19	0.42
8:H:91:ARG:NH1	8:H:138:THR:OG1	2.50	0.42
11:K:29:LEU:HD22	11:K:55:VAL:HG11	2.02	0.42
18:R:82:GLU:O	18:R:86:LYS:HG3	2.19	0.42
30:0:1307:A:H2'	30:0:1308:A:C8	2.55	0.42
30:0:1562:C:N4	38:0:5872:HOH:O	2.52	0.42
30:0:1603:A:H5'	30:0:1605:G:C5'	2.49	0.42
30:0:1644:C:O2'	30:0:1645:U:H5'	2.19	0.42
30:0:1878:G:O2'	30:0:1879:U:OP2	2.38	0.42
30:0:2255:A:O2'	30:0:2256:G:H5'	2.20	0.42
1:A:206:ARG:NH2	30:0:2630:G:O6	2.53	0.42
28:2:2:LYS:HG3	30:0:1486:A:C5	2.55	0.42
14:N:159:TYR:HE1	31:9:50:G:H5''	1.85	0.42
6:F:107:ASP:O	6:F:111:ILE:HG13	2.19	0.42
6:F:111:ILE:O	6:F:115:VAL:HG23	2.20	0.42
9:I:114:TYR:HD1	9:I:114:TYR:N	2.17	0.42
11:K:78:LYS:HA	11:K:79:PRO:HD3	1.94	0.42
14:N:37:ARG:NH2	38:N:8828:HOH:O	2.51	0.42
16:P:13:VAL:HG13	16:P:14:LEU:N	2.35	0.42
19:S:37:VAL:O	19:S:41:VAL:HG23	2.20	0.42
20:T:41:ARG:NH1	20:T:42:VAL:O	2.53	0.42
30:0:912:A:C4	30:0:1294:A:C2	3.07	0.42
30:0:634:G:O2'	30:0:1358:A:OP1	2.35	0.42
30:0:1398:G:H2'	30:0:1399:A:C8	2.55	0.42
30:0:1788:U:C2	30:0:1805:G:N2	2.88	0.42
30:0:2032:U:C2'	30:0:2033:G:C5'	2.98	0.42
30:0:2461:U:O2	30:0:2466:G:H1'	2.19	0.42
2:B:5:ARG:NH1	30:0:2547:C:OP2	2.53	0.42
30:0:2553:A:H2'	30:0:2553:A:N3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2758:G:H2'	30:0:2759:C:C6	2.55	0.42
2:B:18:ARG:HG3	2:B:256:GLN:HG3	2.01	0.42
3:C:111:VAL:HB	38:C:8522:HOH:O	2.20	0.42
8:H:12:ILE:HD12	8:H:57:THR:HG22	2.02	0.42
20:T:97:ARG:NH2	30:0:308:U:H5'	2.35	0.42
30:0:12:U:C2'	30:0:13:G:H5'	2.49	0.41
30:0:1845:A:O2'	30:0:1846:U:H5'	2.19	0.41
30:0:1942:A:C4'	38:0:9046:HOH:O	2.67	0.41
30:0:2290:U:H2'	38:0:7148:HOH:O	2.19	0.41
16:P:61:ARG:NH2	30:0:2737:C:OP2	2.43	0.41
27:1:45:ARG:HB3	38:1:8967:HOH:O	2.20	0.41
4:D:131:THR:HG21	30:0:2348:C:H1'	2.01	0.41
6:F:38:LYS:HE3	30:0:244:C:OP2	2.20	0.41
18:R:9:ASP:HA	18:R:10:PRO:HD2	1.90	0.41
22:V:44:GLY:O	22:V:48:GLU:HG2	2.20	0.41
23:W:11:VAL:O	23:W:12:ASN:HB2	2.20	0.41
30:0:1598:A:N6	33:0:8815:CL:CL	2.90	0.41
30:0:1636:G:O2'	30:0:1637:A:H5'	2.20	0.41
30:0:297:U:H2'	30:0:298:C:H6	1.83	0.41
30:0:351:A:O2'	30:0:352:A:H5'	2.20	0.41
30:0:488:U:C2'	38:0:4019:HOH:O	2.67	0.41
29:3:70:ARG:HD3	38:3:9059:HOH:O	2.19	0.41
31:9:5:G:C2'	31:9:6:C:H5'	2.49	0.41
3:C:39:GLN:O	3:C:43:LYS:HD3	2.19	0.41
4:D:151:ILE:HA	4:D:152:PRO:HD3	1.92	0.41
13:M:65:VAL:HG21	13:M:105:ALA:HB2	2.02	0.41
22:V:1:THR:HG23	22:V:2:VAL:HG23	2.02	0.41
23:W:125:HIS:CE1	30:0:1097:A:H5''	2.56	0.41
24:X:34:ARG:NH1	24:X:48:VAL:O	2.51	0.41
26:Z:63:CYS:HA	26:Z:64:PRO:HD3	1.91	0.41
10:J:88:PRO:HD3	30:0:1104:C:H4'	2.01	0.41
30:0:1375:A:C2'	30:0:1376:G:H5'	2.50	0.41
30:0:2088:C:H1'	30:0:2841:A:N1	2.35	0.41
30:0:2090:G:H2'	30:0:2091:G:C8	2.55	0.41
30:0:383:A:H2'	30:0:384:G:O4'	2.19	0.41
30:0:941:G:C6	30:0:942:U:C4	3.08	0.41
4:D:76:ARG:NH1	31:9:42:C:O2	2.50	0.41
31:9:49:G:C2'	31:9:50:G:H5'	2.50	0.41
24:X:22:ASN:HA	24:X:25:ARG:HG3	2.02	0.41
30:0:1625:U:H3'	30:0:1625:U:C6	2.54	0.41
30:0:1706:G:C6	30:0:1707:G:C6	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:GLY:HA2	30:0:2114:C:OP1	2.20	0.41
1:A:214:SER:HB2	38:0:4377:HOH:O	2.20	0.41
1:A:217:ARG:CG	1:A:217:ARG:HH11	2.33	0.41
13:M:59:GLY:HA3	13:M:141:ILE:HD12	2.02	0.41
20:T:3:GLN:HA	20:T:4:PRO:HD3	1.85	0.41
23:W:3:ALA:O	23:W:54:PHE:HA	2.20	0.41
24:X:72:VAL:HG22	24:X:85:VAL:HG12	2.03	0.41
1:A:167:LYS:HB2	26:Z:53:ILE:HD13	2.02	0.41
30:0:1069:C:H2'	30:0:1070:A:O4'	2.21	0.41
9:I:130:LEU:CD2	30:0:1167:G:H4'	2.50	0.41
30:0:1184:C:O2'	30:0:1185:U:OP2	2.35	0.41
30:0:2274:A:O2'	30:0:2275:G:H5'	2.20	0.41
30:0:2385:G:H2'	30:0:2386:U:C6	2.56	0.41
29:3:28:GLY:HA3	30:0:2435:U:OP1	2.20	0.41
30:0:2635:A:C2'	30:0:2636:C:H5'	2.50	0.41
30:0:423:A:C4	30:0:424:C:C6	3.09	0.41
30:0:69:A:H2'	30:0:70:A:OP2	2.20	0.41
30:0:724:G:O2'	30:0:725:C:H5'	2.21	0.41
30:0:920:C:H4'	30:0:921:G:N2	2.35	0.41
23:W:43:GLY:HA3	30:0:945:U:O2'	2.20	0.41
27:1:12:ASN:O	30:0:1415:G:H5'	2.20	0.41
11:K:37:TYR:HB3	38:K:7169:HOH:O	2.20	0.41
12:L:114:VAL:HG11	38:L:8874:HOH:O	2.20	0.41
15:O:21:SER:OG	15:O:106:PRO:HB2	2.20	0.41
30:0:1193:A:H2	30:0:1194:A:N6	2.16	0.41
30:0:1413:A:H2'	30:0:1414:A:O4'	2.20	0.41
30:0:1483:C:O2'	30:0:1484:G:H5'	2.21	0.41
30:0:1594:C:O2'	30:0:1607:A:H4'	2.20	0.41
30:0:1787:C:O2'	30:0:1788:U:H5'	2.20	0.41
30:0:2281:C:C2'	30:0:2282:U:H5'	2.50	0.41
30:0:2505:G:H2'	30:0:2506:A:C5'	2.48	0.41
30:0:2506:A:O2'	30:0:2507:G:P	2.79	0.41
30:0:2777:G:O2'	30:0:2778:A:H5'	2.20	0.41
30:0:307:G:H3'	38:0:6693:HOH:O	2.21	0.41
1:A:173:GLY:O	1:A:176:HIS:HB3	2.19	0.41
1:A:1:GLY:HA2	1:A:197:VAL:HG23	2.03	0.41
3:C:107:ARG:O	3:C:111:VAL:HG23	2.21	0.41
10:J:19:MET:CE	10:J:132:LEU:HD11	2.51	0.41
30:0:1381:A:N3	30:0:1382:G:H1'	2.36	0.41
30:0:1926:G:H2'	30:0:1927:A:H8	1.86	0.41
30:0:2032:U:H2'	30:0:2033:G:H5'	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2903:C:O2'	30:0:2904:U:H5'	2.21	0.41
30:0:309:C:O2	30:0:309:C:H2'	2.20	0.41
30:0:459:A:H4'	38:0:9460:HOH:O	2.20	0.41
30:0:571:C:H6	30:0:571:C:O5'	2.04	0.41
30:0:736:A:H8	38:0:7219:HOH:O	2.03	0.41
3:C:101:ASP:HB2	30:0:750:A:O3'	2.21	0.41
1:A:48:ASP:HA	1:A:49:PRO:HD3	1.85	0.41
2:B:233:ARG:NH1	2:B:233:ARG:HG2	2.35	0.41
4:D:128:LEU:N	38:D:6007:HOH:O	2.53	0.41
30:0:1829:A:H2'	30:0:1830:C:H5'	2.03	0.41
30:0:1926:G:H2'	30:0:1927:A:C8	2.55	0.41
30:0:764:C:H2'	30:0:765:G:O4'	2.20	0.41
30:0:962:C:H2'	30:0:963:C:H5'	2.03	0.41
9:I:101:LYS:O	9:I:105:GLU:HG3	2.20	0.41
30:0:1159:G:H2'	30:0:1160:G:O4'	2.21	0.41
30:0:1520:G:C6	30:0:1521:C:C4	3.08	0.41
30:0:1625:U:C3'	30:0:1625:U:C6	3.04	0.41
30:0:1626:A:H2'	30:0:1627:G:O4'	2.21	0.41
30:0:2314:G:H2'	30:0:2315:C:H5'	2.03	0.41
30:0:2316:G:H8	38:0:5663:HOH:O	2.03	0.41
30:0:243:A:H61	30:0:269:G:C1'	2.34	0.41
30:0:2506:A:O2'	30:0:2507:G:O5'	2.39	0.41
30:0:535:G:O6	30:0:2064:U:C6	2.74	0.41
30:0:653:U:H2'	30:0:654:A:C8	2.55	0.41
27:1:28:HIS:O	27:1:32:LYS:N	2.48	0.41
29:3:38:ARG:NH1	30:0:396:U:C2	2.89	0.41
2:B:60:SER:HA	2:B:61:PRO:HD3	1.87	0.41
5:E:125:GLU:HB2	5:E:132:THR:HG23	2.03	0.41
14:N:82:TYR:CD2	14:N:82:TYR:C	2.93	0.41
16:P:59:ARG:O	16:P:63:ARG:HG3	2.21	0.41
23:W:119:HIS:CG	38:0:5297:HOH:O	2.74	0.41
30:0:1298:U:H2'	30:0:1299:G:C8	2.56	0.41
12:L:6:ARG:NH1	30:0:1299:G:N7	2.69	0.41
30:0:1634:G:H2'	30:0:1635:U:C6	2.56	0.41
30:0:2354:A:C2	30:0:2367:A:C8	3.09	0.41
31:9:61:C:H2'	31:9:62:A:H8	1.85	0.41
2:B:101:TRP:HB2	2:B:119:HIS:CD2	2.56	0.41
2:B:242:TRP:CZ2	30:0:2607:U:C4	3.08	0.41
5:E:7:ILE:HG13	5:E:11:VAL:HB	2.03	0.41
5:E:68:HIS:CE1	38:E:5919:HOH:O	2.74	0.41
22:V:5:VAL:HG23	38:V:2271:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1795:G:H2'	30:0:1796:A:O4'	2.21	0.41
30:0:1871:U:O4'	30:0:1873:G:C8	2.74	0.41
30:0:1903:U:O2'	30:0:1904:A:C8	2.72	0.41
30:0:2754:G:O2'	30:0:2755:G:H5'	2.20	0.41
30:0:2765:C:H2'	30:0:2766:A:C8	2.56	0.41
30:0:491:C:O2'	30:0:492:C:H5'	2.21	0.41
30:0:506:G:N1	30:0:509:A:OP2	2.54	0.41
30:0:615:G:H2'	30:0:616:U:C6	2.56	0.41
30:0:694:A:C2'	30:0:695:C:H5'	2.51	0.41
30:0:963:C:O2	30:0:1005:A:N1	2.54	0.41
1:A:47:HIS:CD2	30:0:1654:U:H2'	2.56	0.41
2:B:225:GLY:HA3	38:B:9027:HOH:O	2.21	0.41
5:E:91:PHE:HA	5:E:92:PRO:HD3	1.90	0.41
18:R:18:LEU:HG	18:R:91:LEU:HD13	2.03	0.41
20:T:106:GLU:HG3	38:T:4913:HOH:O	2.21	0.41
30:0:106:A:H2'	30:0:107:U:O4'	2.21	0.40
30:0:1116:U:C2	30:0:1246:A:N6	2.89	0.40
30:0:1205:U:H2'	30:0:1206:U:H5'	1.94	0.40
30:0:1375:A:H2'	30:0:1376:G:H5'	2.04	0.40
30:0:1555:G:H4'	30:0:1630:A:H2	1.86	0.40
30:0:2112:A:H2'	30:0:2113:G:H8	1.85	0.40
30:0:2491:G:C1'	38:0:6878:HOH:O	2.58	0.40
30:0:304:G:H1'	30:0:347:A:H61	1.86	0.40
30:0:626:U:C4	30:0:627:G:C6	3.09	0.40
23:W:130:HIS:NE2	31:9:88:G:OP1	2.50	0.40
1:A:109:GLU:HG2	1:A:116:GLY:H	1.85	0.40
3:C:131:PHE:CD2	3:C:131:PHE:N	2.89	0.40
8:H:157:TYR:CD1	8:H:157:TYR:C	2.94	0.40
9:I:112:LEU:HG	30:0:1162:G:O2'	2.21	0.40
22:V:39:ALA:N	22:V:40:PRO:CD	2.84	0.40
23:W:130:HIS:O	23:W:136:GLY:HA3	2.21	0.40
23:W:117:ARG:HD3	30:0:1287:A:O4'	2.21	0.40
30:0:1992:U:H2'	30:0:1994:A:OP2	2.20	0.40
30:0:2564:G:OP2	30:0:2565:C:H5''	2.21	0.40
30:0:423:A:H2'	30:0:424:C:H6	1.87	0.40
30:0:499:G:O2'	30:0:500:G:H5'	2.21	0.40
1:A:38:ILE:HD13	1:A:38:ILE:HA	1.88	0.40
1:A:88:ILE:HG22	1:A:88:ILE:O	2.21	0.40
14:N:170:GLU:O	14:N:174:GLU:HG3	2.20	0.40
15:O:38:ARG:NH1	38:O:7674:HOH:O	2.53	0.40
20:T:9:LYS:HE2	20:T:13:ARG:HH12	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:35:VAL:HA	23:W:36:PRO:HD3	1.83	0.40
30:0:553:G:O4'	30:0:1325:G:H5'	2.22	0.40
30:0:1761:U:H2'	30:0:1762:C:C6	2.55	0.40
30:0:1947:G:H2'	30:0:1948:G:C8	2.56	0.40
30:0:2614:C:O2'	30:0:2615:U:H5'	2.21	0.40
30:0:570:C:H6	30:0:570:C:O5'	2.04	0.40
30:0:821:U:H2'	30:0:822:C:C6	2.57	0.40
27:1:21:ARG:HD2	27:1:39:PHE:HB2	2.04	0.40
3:C:102:LEU:HD12	3:C:102:LEU:HA	1.91	0.40
3:C:193:LEU:HD12	3:C:211:ASP:O	2.21	0.40
25:Y:145:LYS:O	25:Y:147:ARG:HG2	2.21	0.40
26:Z:77:GLY:HA2	26:Z:91:GLY:O	2.21	0.40
30:0:1311:G:C2	30:0:1312:G:C8	3.09	0.40
30:0:138:U:OP2	30:0:139:C:C5	2.70	0.40
30:0:2032:U:H2'	30:0:2033:G:H5''	2.03	0.40
30:0:2135:A:O4'	30:0:2243:C:N4	2.54	0.40
30:0:503:G:H2'	30:0:504:G:H8	1.87	0.40
30:0:939:A:N1	30:0:1027:G:O2'	2.50	0.40
30:0:1014:A:H5''	31:9:101:G:O2'	2.22	0.40
2:B:199:TYR:HE2	2:B:268:ARG:HB2	1.85	0.40
2:B:229:ARG:HD2	38:0:9111:HOH:O	2.20	0.40
4:D:23:VAL:HG12	4:D:130:VAL:HG22	2.03	0.40
4:D:22:VAL:HA	4:D:73:VAL:O	2.21	0.40
5:E:68:HIS:O	5:E:72:MET:HG3	2.22	0.40
9:I:130:LEU:HA	38:I:6825:HOH:O	2.22	0.40
12:L:145:LEU:O	12:L:148:GLU:HG3	2.21	0.40
13:M:122:GLN:OE1	13:M:127:LYS:HE2	2.22	0.40
18:R:114:VAL:HG13	18:R:114:VAL:O	2.22	0.40
18:R:18:LEU:HD12	18:R:143:VAL:HG11	2.03	0.40
25:Y:148:GLY:HA3	30:0:622:G:P	2.62	0.40
26:Z:45:VAL:HG12	38:Z:8713:HOH:O	2.21	0.40
30:0:1236:A:H2'	30:0:1237:U:O4'	2.22	0.40
13:M:188:ARG:HH11	30:0:154:C:H3'	1.86	0.40
30:0:1773:G:N2	30:0:1774:G:C8	2.90	0.40
30:0:214:U:H5'	38:0:6146:HOH:O	2.22	0.40
30:0:2509:A:C2	30:0:2510:C:H1'	2.56	0.40
30:0:2734:G:O2'	30:0:2735:U:H5'	2.22	0.40
30:0:2897:C:O2'	30:0:2898:G:H5'	2.22	0.40
30:0:695:C:H2'	30:0:696:C:C6	2.57	0.40
30:0:812:A:H2'	30:0:813:C:O4'	2.21	0.40
27:1:53:LYS:HD3	27:1:53:LYS:HA	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:115:VAL:HA	2:B:116:PRO:HD3	1.85	0.40
2:B:267:LYS:HD3	38:O:9565:HOH:O	2.22	0.40
15:O:32:ARG:HE	15:O:35:LYS:HD2	1.86	0.40
16:P:94:TRP:CZ2	16:P:98:ILE:HG13	2.57	0.40
20:T:14:ALA:HA	20:T:15:PRO:HD3	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	235/240 (98%)	211 (90%)	18 (8%)	6 (3%)	5	20
2	B	335/338 (99%)	306 (91%)	25 (8%)	4 (1%)	13	40
3	C	244/246 (99%)	224 (92%)	19 (8%)	1 (0%)	34	66
4	D	134/177 (76%)	113 (84%)	16 (12%)	5 (4%)	3	13
5	E	170/178 (96%)	161 (95%)	9 (5%)	0	100	100
6	F	117/120 (98%)	106 (91%)	8 (7%)	3 (3%)	5	20
7	G	25/348 (7%)	25 (100%)	0	0	100	100
8	H	156/177 (88%)	147 (94%)	8 (5%)	1 (1%)	25	58
9	I	68/162 (42%)	54 (79%)	13 (19%)	1 (2%)	10	34
10	J	140/145 (97%)	130 (93%)	9 (6%)	1 (1%)	22	54
11	K	130/132 (98%)	124 (95%)	5 (4%)	1 (1%)	19	51
12	L	141/165 (86%)	125 (89%)	14 (10%)	2 (1%)	11	36
13	M	192/196 (98%)	182 (95%)	9 (5%)	1 (0%)	29	61
14	N	184/187 (98%)	169 (92%)	12 (6%)	3 (2%)	9	32
15	O	113/116 (97%)	108 (96%)	5 (4%)	0	100	100
16	P	141/149 (95%)	141 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	Q	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
18	R	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
19	S	79/85 (93%)	75 (95%)	4 (5%)	0	100	100
20	T	117/120 (98%)	110 (94%)	7 (6%)	0	100	100
21	U	51/67 (76%)	45 (88%)	5 (10%)	1 (2%)	7	27
22	V	63/71 (89%)	60 (95%)	2 (3%)	1 (2%)	9	32
23	W	152/154 (99%)	146 (96%)	4 (3%)	2 (1%)	12	37
24	X	80/92 (87%)	75 (94%)	4 (5%)	1 (1%)	12	37
25	Y	140/241 (58%)	138 (99%)	2 (1%)	0	100	100
26	Z	71/116 (61%)	62 (87%)	7 (10%)	2 (3%)	5	19
27	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
28	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
29	3	90/92 (98%)	88 (98%)	2 (2%)	0	100	100
All	All	3705/4472 (83%)	3447 (93%)	222 (6%)	36 (1%)	15	45

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
4	D	137	PRO
6	F	101	ALA
14	N	154	LEU
14	N	183	ASP
14	N	184	ILE
1	A	27	LEU
8	H	19	ARG
1	A	34	ASP
10	J	65	ASN
23	W	49	ASN
23	W	77	ALA
26	Z	44	ARG
1	A	36	ASP
2	B	2	GLN
2	B	185	GLY
4	D	65	GLU
11	K	127	ALA
12	L	149	ARG

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Mol	Chain	Res	Type
13	M	71	SER
24	X	70	ILE
26	Z	65	ASN
2	B	184	ASP
4	D	56	ARG
6	F	100	ASP
12	L	82	ALA
21	U	55	ALA
22	V	43	PRO
1	A	69	LEU
3	C	201	SER
4	D	27	ILE
4	D	97	GLN
9	I	83	GLY
1	A	88	ILE
2	B	169	GLY
6	F	27	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	179/182 (98%)	170 (95%)	9 (5%)	24	57
2	B	282/283 (100%)	263 (93%)	19 (7%)	16	43
3	C	193/193 (100%)	176 (91%)	17 (9%)	10	30
4	D	117/148 (79%)	110 (94%)	7 (6%)	19	49
5	E	152/156 (97%)	149 (98%)	3 (2%)	55	82
6	F	93/94 (99%)	91 (98%)	2 (2%)	52	81
7	G	27/282 (10%)	27 (100%)	0	100	100
8	H	134/145 (92%)	129 (96%)	5 (4%)	34	68
9	I	58/130 (45%)	57 (98%)	1 (2%)	60	86
10	J	118/121 (98%)	110 (93%)	8 (7%)	16	42
11	K	106/106 (100%)	104 (98%)	2 (2%)	57	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	113/127 (89%)	110 (97%)	3 (3%)	44	77
13	M	158/160 (99%)	151 (96%)	7 (4%)	28	61
14	N	149/150 (99%)	142 (95%)	7 (5%)	26	59
15	O	93/94 (99%)	92 (99%)	1 (1%)	73	92
16	P	113/117 (97%)	111 (98%)	2 (2%)	59	85
17	Q	79/80 (99%)	76 (96%)	3 (4%)	33	67
18	R	117/122 (96%)	111 (95%)	6 (5%)	24	56
19	S	71/74 (96%)	70 (99%)	1 (1%)	67	89
20	T	105/106 (99%)	97 (92%)	8 (8%)	13	36
21	U	44/53 (83%)	43 (98%)	1 (2%)	50	80
22	V	51/57 (90%)	50 (98%)	1 (2%)	55	82
23	W	130/130 (100%)	126 (97%)	4 (3%)	40	74
24	X	66/74 (89%)	62 (94%)	4 (6%)	18	48
25	Y	120/196 (61%)	116 (97%)	4 (3%)	38	72
26	Z	60/94 (64%)	60 (100%)	0	100	100
27	1	46/47 (98%)	46 (100%)	0	100	100
28	2	42/46 (91%)	41 (98%)	1 (2%)	49	79
29	3	79/79 (100%)	78 (99%)	1 (1%)	69	90
All	All	3095/3646 (85%)	2968 (96%)	127 (4%)	30	64

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

Mol	Chain	Res	Type
1	A	3	ARG
1	A	36	ASP
1	A	37	VAL
1	A	38	ILE
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	16	ARG
2	B	27	ASN

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Mol	Chain	Res	Type
2	B	49	THR
2	B	71	VAL
2	B	97	LEU
2	B	98	THR
2	B	103	ASP
2	B	108	GLU
2	B	132	HIS
2	B	190	MET
2	B	192	ASP
2	B	234	ARG
2	B	248	ARG
2	B	251	VAL
2	B	254	GLN
2	B	264	GLU
2	B	277	GLU
3	C	27	ARG
3	C	78	ARG
3	C	94	THR
3	C	131	PHE
3	C	136	VAL
3	C	151	GLN
3	C	162	VAL
3	C	187	ARG
3	C	202	THR
3	C	211	ASP
3	C	214	THR
3	C	222	ASP
3	C	223	LEU
3	C	234	VAL
3	C	236	THR
3	C	237	GLU
3	C	243	VAL
4	D	24	HIS
4	D	36	ASN
4	D	50	VAL
4	D	137	PRO
4	D	149	ARG
4	D	161	ASP
4	D	170	TYR
5	E	7	ILE
5	E	102	VAL
5	E	156	ASP

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Mol	Chain	Res	Type
6	F	12	LEU
6	F	46	GLU
8	H	62	HIS
8	H	65	LEU
8	H	87	LYS
8	H	91	ARG
8	H	157	TYR
9	I	114	TYR
10	J	45	VAL
10	J	46	ILE
10	J	52	GLN
10	J	74	ARG
10	J	76	ASP
10	J	79	PHE
10	J	107	ASN
10	J	112	ASP
11	K	10	GLN
11	K	119	GLN
12	L	35	ARG
12	L	80	ASP
12	L	104	ASP
13	M	10	ASP
13	M	46	LEU
13	M	68	ARG
13	M	93	ARG
13	M	99	ARG
13	M	116	ASN
13	M	164	THR
14	N	17	ARG
14	N	26	LEU
14	N	49	THR
14	N	127	LEU
14	N	134	ASP
14	N	135	VAL
14	N	147	ILE
15	O	38	ARG
16	P	21	VAL
16	P	98	ILE
17	Q	11	ARG
17	Q	57	ASP
17	Q	95	GLU
18	R	13	THR

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Mol	Chain	Res	Type
18	R	39	THR
18	R	82	GLU
18	R	119	VAL
18	R	132	ARG
18	R	143	VAL
19	S	10	VAL
20	T	26	THR
20	T	39	ASN
20	T	48	VAL
20	T	73	HIS
20	T	89	ARG
20	T	96	VAL
20	T	115	GLU
20	T	117	ASP
21	U	47	ARG
22	V	22	ASP
23	W	38	THR
23	W	52	VAL
23	W	88	THR
23	W	146	ILE
24	X	27	ASP
24	X	46	ASP
24	X	79	GLU
24	X	82	GLU
25	Y	95	THR
25	Y	154	ARG
25	Y	189	ASN
25	Y	203	VAL
28	2	18	ASN
29	3	3	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	199	HIS
2	B	2	GLN
2	B	27	ASN
2	B	145	HIS
2	B	238	ASN
2	B	256	GLN
2	B	260	HIS

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Mol	Chain	Res	Type
2	B	320	GLN
3	C	2	GLN
3	C	73	GLN
3	C	129	HIS
3	C	151	GLN
4	D	103	ASN
5	E	119	HIS
5	E	143	GLN
5	E	150	GLN
7	G	17	GLN
7	G	64	ASN
8	H	34	HIS
8	H	59	GLN
8	H	62	HIS
10	J	52	GLN
10	J	107	ASN
10	J	126	ASN
10	J	142	ASN
11	K	10	GLN
11	K	42	ASN
11	K	44	HIS
11	K	67	GLN
12	L	18	HIS
12	L	41	HIS
12	L	116	HIS
13	M	58	GLN
13	M	77	HIS
13	M	137	ASN
13	M	170	ASN
14	N	93	GLN
14	N	107	ASN
14	N	132	ASN
16	P	50	GLN
16	P	66	GLN
16	P	118	GLN
17	Q	27	GLN
17	Q	40	HIS
18	R	61	GLN
18	R	94	ASN
18	R	98	ASN
18	R	113	HIS
18	R	117	HIS

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Mol	Chain	Res	Type
19	S	44	GLN
19	S	53	ASN
20	T	39	ASN
21	U	39	ASN
22	V	4	HIS
22	V	60	GLN
23	W	2	HIS
23	W	110	GLN
23	W	119	HIS
23	W	125	HIS
23	W	141	HIS
24	X	23	HIS
25	Y	133	HIS
25	Y	134	HIS
25	Y	149	GLN
25	Y	189	ASN
26	Z	61	HIS
27	1	8	GLN
27	1	16	HIS
27	1	28	HIS
28	2	41	HIS
28	2	45	ASN
29	3	15	ASN
29	3	20	HIS
29	3	48	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	242 (8%)	27 (0%)
31	9	121/122 (99%)	15 (12%)	1 (0%)
All	All	2866/3045 (94%)	257 (8%)	28 (0%)

All (257) 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

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Mol	Chain	Res	Type
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	139	C
30	0	141	C
30	0	151	A
30	0	166	A
30	0	186	A
30	0	187	A
30	0	191	A
30	0	192	A
30	0	200	C
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	336	G
30	0	337	A
30	0	358	G
30	0	381	G
30	0	397	A
30	0	417	G
30	0	461	C
30	0	487	G
30	0	498	A
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

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Mol	Chain	Res	Type
30	0	553	G
30	0	559	U
30	0	588	G
30	0	604	G
30	0	605	C
30	0	620	A
30	0	632	A
30	0	644	G
30	0	660	A
30	0	688	A
30	0	698	A
30	0	701	U
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	885	G
30	0	898	G
30	0	905	C
30	0	920	C
30	0	921	G
30	0	923	A
30	0	953	G
30	0	960	G
30	0	961	A
30	0	1006	A
30	0	1008	C
30	0	1029	U
30	0	1045	G
30	0	1059	G
30	0	1060	C

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Mol	Chain	Res	Type
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
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	1205	U
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	1279	U
30	0	1289	C
30	0	1331	G
30	0	1342	C
30	0	1353	C
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	1488	U
30	0	1505	U
30	0	1506	U
30	0	1524	U
30	0	1525	G
30	0	1526	A
30	0	1562	C

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Mol	Chain	Res	Type
30	0	1592	G
30	0	1617	C
30	0	1625	U
30	0	1626	A
30	0	1634	G
30	0	1656	A
30	0	1667	A
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	1731	C
30	0	1732	A
30	0	1752	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	1968	A
30	0	1971	G
30	0	1973	A
30	0	1978	A
30	0	1979	G
30	0	1980	U
30	0	1996	U
30	0	2004	U
30	0	2006	C
30	0	2008	U
30	0	2011	A
30	0	2012	U
30	0	2013	G
30	0	2033	G

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Mol	Chain	Res	Type
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
30	0	2243	C
30	0	2258	A
30	0	2271	G
30	0	2272	G
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	2469	A
30	0	2476	C
30	0	2483	A
30	0	2507	G
30	0	2509	A
30	0	2511	A
30	0	2513	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

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Mol	Chain	Res	Type
30	0	2613	G
30	0	2637	A
30	0	2638	G
30	0	2645	U
30	0	2649	A
30	0	2664	A
30	0	2681	A
30	0	2682	C
30	0	2718	C
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	2903	C
30	0	2914	A
31	9	2	U
31	9	14	G
31	9	22	G
31	9	23	U
31	9	24	U
31	9	25	G
31	9	40	C
31	9	41	C
31	9	43	G
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 (28) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	69	A
30	0	129	A
30	0	604	G
30	0	644	G
30	0	681	G
30	0	699	C
30	0	834	G
30	0	857	A
30	0	871	G
30	0	877	G
30	0	1080	C
30	0	1232	A
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	1979	G
30	0	2313	C
30	0	2467	A
30	0	2526	C
30	0	2536	C
30	0	2649	A
30	0	2718	C
30	0	2726	U
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	0.99	1 (7%)	14,31,34	1.14	1 (7%)
30	1MA	0	628	30	15,25,26	0.79	0	15,37,40	1.43	2 (13%)
30	OMG	0	2588	30	18,26,27	1.07	2 (11%)	20,38,41	2.57	5 (25%)
30	PSU	0	2621	30	17,21,22	1.76	3 (17%)	20,30,33	5.44	5 (25%)
30	UR3	0	2619	30	14,22,23	0.73	0	15,32,35	0.61	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	OMU	0	2587	30	-	0/7/27/28	0/2/2/2
30	1MA	0	628	30	-	0/3/25/26	0/3/3/3
30	OMG	0	2588	30	-	0/5/27/28	0/3/3/3
30	PSU	0	2621	30	-	0/7/25/26	0/2/2/2
30	UR3	0	2619	30	-	0/5/25/26	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C5-C1'	-5.68	1.47	1.52
30	0	2588	OMG	C6-N1	3.39	1.38	1.33
30	0	2621	PSU	C4-N3	2.80	1.37	1.33
30	0	2587	OMU	C4-N3	2.63	1.37	1.33
30	0	2621	PSU	C2-N1	2.44	1.43	1.38
30	0	2588	OMG	C8-N7	-2.13	1.30	1.34

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2621	PSU	N1-C2-N3	-17.38	114.61	128.43
30	0	2621	PSU	C4-N3-C2	14.15	127.09	115.14
30	0	2588	OMG	C5-C6-N1	-8.53	111.77	123.43
30	0	2621	PSU	C5-C4-N3	-8.13	114.89	125.36
30	0	2588	OMG	C6-N1-C2	5.77	125.11	115.93
30	0	628	1MA	C2-N3-C4	-4.66	110.76	116.58
30	0	2587	OMU	C5-C4-N3	-3.91	114.70	123.31
30	0	2588	OMG	C2-N3-C4	-3.12	111.79	115.36
30	0	2621	PSU	C6-N1-C2	2.69	119.79	115.36
30	0	2588	OMG	N3-C2-N1	-2.44	123.97	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2621	PSU	C5-C1'-C2'	-2.09	111.59	115.32
30	0	628	1MA	O4'-C1'-C2'	-2.09	103.88	106.93
30	0	2588	OMG	C6-C5-C4	-2.07	118.82	120.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	2587	OMU	3	0

5.5 Carbohydrates [i](#)

There are no monosaccharides 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%)	-0.39	5 (2%) 63 61	35, 59, 97, 117	0
2	B	337/338 (99%)	-0.60	1 (0%) 94 94	36, 60, 90, 100	0
3	C	246/246 (100%)	-0.58	0 100 100	30, 51, 75, 89	0
4	D	140/177 (79%)	1.08	29 (20%) 1 0	73, 108, 135, 146	0
5	E	172/178 (96%)	-0.51	1 (0%) 89 89	51, 74, 96, 104	0
6	F	119/120 (99%)	0.13	5 (4%) 36 32	55, 78, 111, 125	0
7	G	29/348 (8%)	0.48	2 (6%) 16 13	83, 103, 109, 112	0
8	H	160/177 (90%)	0.03	9 (5%) 24 20	50, 73, 106, 113	0
9	I	70/162 (43%)	3.13	45 (64%) 0 0	137, 156, 173, 174	0
10	J	142/145 (97%)	-0.57	1 (0%) 87 87	41, 58, 78, 97	0
11	K	132/132 (100%)	-0.71	0 100 100	40, 55, 79, 82	0
12	L	145/165 (87%)	0.07	7 (4%) 30 27	34, 73, 123, 136	0
13	M	194/196 (98%)	-0.71	0 100 100	35, 50, 66, 73	0
14	N	186/187 (99%)	-0.08	5 (2%) 54 50	52, 75, 123, 135	0
15	O	115/116 (99%)	-0.60	0 100 100	45, 61, 78, 84	0
16	P	143/149 (95%)	-0.64	0 100 100	46, 61, 77, 84	0
17	Q	95/96 (98%)	-0.60	0 100 100	44, 55, 71, 86	0
18	R	150/155 (96%)	-0.73	0 100 100	39, 52, 71, 86	0
19	S	81/85 (95%)	-0.51	1 (1%) 79 79	49, 65, 86, 98	0
20	T	119/120 (99%)	-0.35	5 (4%) 36 32	47, 62, 89, 123	0
21	U	53/67 (79%)	-0.62	0 100 100	48, 62, 79, 88	0
22	V	65/71 (91%)	0.69	8 (12%) 4 3	55, 80, 129, 134	0
23	W	154/154 (100%)	-0.52	1 (0%) 89 89	41, 57, 74, 88	0
24	X	82/92 (89%)	-0.19	3 (3%) 41 37	49, 67, 90, 108	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	142/241 (58%)	-0.76	1 (0%) 87 87	31, 50, 73, 94	0
26	Z	73/116 (62%)	0.73	12 (16%) 1 1	63, 87, 101, 106	0
27	1	56/57 (98%)	-0.66	0 100 100	32, 39, 45, 53	0
28	2	46/50 (92%)	-0.12	3 (6%) 18 14	41, 69, 104, 115	0
29	3	92/92 (100%)	-0.38	0 100 100	44, 68, 81, 91	0
30	0	2749/2923 (94%)	-0.67	8 (0%) 94 94	28, 53, 96, 172	0
31	9	122/122 (100%)	-0.83	2 (1%) 72 71	45, 74, 96, 153	0
All	All	6646/7517 (88%)	-0.45	154 (2%) 60 58	28, 58, 108, 174	0

All (154) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	I	74	ILE	10.1
22	V	39	ALA	8.0
22	V	1	THR	7.6
4	D	63	ILE	7.5
9	I	71	ALA	7.5
26	Z	46	SER	7.4
9	I	70	THR	7.4
9	I	72	GLU	7.4
9	I	66	GLY	7.3
22	V	43	PRO	6.9
9	I	104	ALA	6.8
14	N	166	ALA	6.5
9	I	106	GLN	6.4
9	I	100	VAL	6.0
4	D	57	THR	5.8
22	V	40	PRO	5.7
9	I	80	PHE	5.4
9	I	79	GLY	5.2
26	Z	58	ASN	5.1
4	D	85	GLN	5.0
9	I	128	THR	5.0
9	I	108	HIS	4.9
9	I	132	VAL	4.8
4	D	134	LEU	4.8
26	Z	35	SER	4.8
26	Z	44	ARG	4.8
9	I	109	PRO	4.7
9	I	113	SER	4.7

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Mol	Chain	Res	Type	RSRZ
9	I	102	GLN	4.6
9	I	112	LEU	4.5
20	T	118	SER	4.5
1	A	237	GLY	4.4
9	I	93	ALA	4.4
4	D	18	ILE	4.3
9	I	105	GLU	4.2
4	D	90	LEU	4.2
26	Z	45	VAL	4.2
9	I	99	GLN	4.1
9	I	76	ASP	4.0
31	9	1	U	4.0
9	I	69	PRO	3.9
9	I	83	GLY	3.8
9	I	92	VAL	3.8
19	S	81	ILE	3.8
14	N	155	GLU	3.8
9	I	97	VAL	3.8
6	F	106	ALA	3.8
9	I	86	GLU	3.7
9	I	110	ASP	3.7
20	T	116	ASP	3.7
30	0	1198	U	3.6
4	D	88	LEU	3.6
9	I	88	GLN	3.6
26	Z	60	ASP	3.6
9	I	78	ALA	3.6
30	0	735	C	3.5
24	X	71	ARG	3.5
9	I	111	LEU	3.5
8	H	40	GLN	3.5
12	L	60	GLU	3.4
26	Z	50	VAL	3.3
20	T	119	ALA	3.3
9	I	82	THR	3.3
4	D	64	ARG	3.3
4	D	91	ALA	3.3
4	D	84	LEU	3.3
22	V	38	GLY	3.3
9	I	103	ILE	3.2
9	I	81	GLU	3.2
9	I	75	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
9	I	98	ASP	3.2
12	L	81	VAL	3.2
4	D	102	GLY	3.2
12	L	75	LEU	3.2
26	Z	49	ARG	3.0
22	V	41	GLU	3.0
8	H	133	GLY	3.0
4	D	17	ARG	3.0
4	D	69	ILE	3.0
4	D	81	GLU	3.0
8	H	86	TYR	2.9
25	Y	235	GLU	2.9
26	Z	69	ASP	2.9
4	D	44	ILE	2.9
4	D	75	LEU	2.9
28	2	49	GLU	2.9
4	D	92	GLU	2.8
4	D	93	LEU	2.8
22	V	37	GLY	2.8
1	A	37	VAL	2.7
7	G	27	ILE	2.7
8	H	149	VAL	2.7
4	D	45	THR	2.7
1	A	91	GLY	2.6
9	I	67	VAL	2.6
4	D	135	VAL	2.6
9	I	116	LEU	2.5
4	D	165	PHE	2.5
30	0	282	C	2.5
30	0	1199	A	2.5
12	L	80	ASP	2.5
20	T	115	GLU	2.4
6	F	75	ILE	2.4
4	D	157	LEU	2.4
4	D	10	PHE	2.4
9	I	84	SER	2.4
1	A	99	ILE	2.3
26	Z	42	TYR	2.3
6	F	99	THR	2.3
4	D	172	VAL	2.3
28	2	39	ARG	2.3
4	D	89	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
4	D	130	VAL	2.3
6	F	17	LEU	2.3
28	2	35	ARG	2.3
9	I	73	LEU	2.3
9	I	114	TYR	2.3
9	I	91	PHE	2.3
9	I	94	ASP	2.3
6	F	16	ALA	2.3
4	D	166	ILE	2.3
20	T	117	ASP	2.2
30	0	1169	U	2.2
8	H	37	GLY	2.2
26	Z	68	GLU	2.2
10	J	70	PHE	2.2
22	V	2	VAL	2.2
4	D	56	ARG	2.2
4	D	171	ASP	2.2
9	I	118	ASN	2.2
14	N	138	ASP	2.2
2	B	105	PHE	2.2
24	X	85	VAL	2.2
23	W	96	LEU	2.2
30	0	1172	G	2.2
31	9	24	U	2.2
9	I	127	CYS	2.2
8	H	39	LYS	2.1
5	E	170	ARG	2.1
26	Z	55	SER	2.1
30	0	1200	A	2.1
12	L	76	LEU	2.1
8	H	76	LEU	2.1
30	0	970	U	2.1
14	N	185	GLU	2.1
1	A	103	VAL	2.1
8	H	158	ASN	2.1
12	L	100	ALA	2.0
9	I	125	GLY	2.0
8	H	35	LYS	2.0
24	X	7	GLU	2.0
12	L	106	VAL	2.0
14	N	147	ILE	2.0
7	G	24	VAL	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
30	OMG	0	2588	24/25	0.98	0.12	38,42,43,43	0
30	UR3	0	2619	21/22	0.98	0.14	43,45,48,49	0
30	OMU	0	2587	21/22	0.99	0.13	40,43,46,49	0
30	PSU	0	2621	20/21	0.99	0.14	35,38,47,48	0
30	1MA	0	628	23/24	0.99	0.15	35,38,38,39	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
34	SR	0	9006	1/1	0.11	1.24	200,200,200,200	0
34	SR	0	8922	1/1	0.41	0.22	170,170,170,170	0
34	SR	0	8994	1/1	0.41	0.98	200,200,200,200	0
35	NA	0	8522	1/1	0.54	0.38	83,83,83,83	0
35	NA	0	8562	1/1	0.55	0.80	74,74,74,74	0
34	SR	0	8991	1/1	0.58	0.09	197,197,197,197	0
32	MG	0	8089	1/1	0.58	0.12	57,57,57,57	0
35	NA	0	8546	1/1	0.60	1.30	112,112,112,112	0
34	SR	0	8919	1/1	0.61	0.13	192,192,192,192	0
34	SR	0	8986	1/1	0.61	0.17	200,200,200,200	0
35	NA	0	8555	1/1	0.64	0.49	51,51,51,51	0
34	SR	B	8987	1/1	0.67	0.49	200,200,200,200	0
35	NA	0	8570	1/1	0.71	0.13	60,60,60,60	0
35	NA	0	8518	1/1	0.71	0.48	94,94,94,94	0
35	NA	0	8563	1/1	0.71	0.36	94,94,94,94	0
34	SR	0	9001	1/1	0.71	0.10	173,173,173,173	0
35	NA	9	8572	1/1	0.72	0.33	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	SR	0	8997	1/1	0.72	0.46	200,200,200,200	0
32	MG	0	8037	1/1	0.74	0.33	90,90,90,90	0
34	SR	0	8982	1/1	0.75	1.22	200,200,200,200	0
34	SR	9	8980	1/1	0.76	0.15	200,200,200,200	0
34	SR	0	8993	1/1	0.77	0.09	182,182,182,182	0
32	MG	0	8091	1/1	0.77	0.06	62,62,62,62	0
34	SR	0	8988	1/1	0.77	0.13	173,173,173,173	0
34	SR	0	8938	1/1	0.78	0.13	192,192,192,192	0
35	NA	0	8560	1/1	0.78	0.38	83,83,83,83	0
35	NA	0	8525	1/1	0.78	0.19	78,78,78,78	0
35	NA	0	8505	1/1	0.80	1.03	49,49,49,49	0
34	SR	0	8944	1/1	0.80	0.13	182,182,182,182	0
35	NA	0	8506	1/1	0.81	0.25	68,68,68,68	0
34	SR	0	8959	1/1	0.81	0.20	174,174,174,174	0
34	SR	0	8976	1/1	0.81	0.25	200,200,200,200	0
34	SR	0	8947	1/1	0.82	0.27	200,200,200,200	0
35	NA	0	8550	1/1	0.82	0.52	61,61,61,61	0
35	NA	0	8544	1/1	0.83	0.20	75,75,75,75	0
32	MG	0	8036	1/1	0.83	0.10	50,50,50,50	0
34	SR	0	8996	1/1	0.84	1.02	200,200,200,200	0
35	NA	0	8571	1/1	0.84	0.09	77,77,77,77	0
32	MG	0	8081	1/1	0.85	0.18	74,74,74,74	0
35	NA	J	8538	1/1	0.85	0.16	60,60,60,60	0
35	NA	0	8528	1/1	0.85	0.29	58,58,58,58	0
35	NA	0	8557	1/1	0.86	0.10	52,52,52,52	0
34	SR	0	8957	1/1	0.86	0.10	196,196,196,196	0
34	SR	0	8927	1/1	0.87	0.06	151,151,151,151	0
34	SR	A	8977	1/1	0.87	0.06	161,161,161,161	0
35	NA	0	8527	1/1	0.87	0.23	71,71,71,71	0
34	SR	0	8951	1/1	0.88	0.07	142,142,142,142	0
32	MG	A	8051	1/1	0.88	0.41	72,72,72,72	0
32	MG	0	8077	1/1	0.88	0.07	49,49,49,49	0
32	MG	0	8062	1/1	0.88	0.17	50,50,50,50	0
34	SR	0	8928	1/1	0.88	0.06	135,135,135,135	0
34	SR	0	8998	1/1	0.89	0.13	175,175,175,175	0
32	MG	0	8071	1/1	0.89	0.19	71,71,71,71	0
34	SR	0	8985	1/1	0.89	0.06	143,143,143,143	0
35	NA	0	8502	1/1	0.89	0.11	65,65,65,65	0
35	NA	0	8533	1/1	0.90	0.13	67,67,67,67	0
32	MG	0	8082	1/1	0.90	0.28	69,69,69,69	0
35	NA	0	8574	1/1	0.90	0.38	55,55,55,55	0
34	SR	0	9007	1/1	0.90	1.33	200,200,200,200	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	SR	0	8968	1/1	0.90	0.08	165,165,165,165	0
32	MG	0	8075	1/1	0.90	0.03	46,46,46,46	0
34	SR	0	8979	1/1	0.90	0.20	198,198,198,198	0
35	NA	0	8559	1/1	0.90	0.15	76,76,76,76	0
35	NA	0	8548	1/1	0.90	0.17	55,55,55,55	0
35	NA	C	8503	1/1	0.91	0.16	44,44,44,44	0
35	NA	0	8530	1/1	0.91	0.28	55,55,55,55	0
34	SR	0	8983	1/1	0.91	0.45	195,195,195,195	0
32	MG	0	8072	1/1	0.91	0.10	53,53,53,53	0
32	MG	0	8087	1/1	0.91	0.08	47,47,47,47	0
35	NA	S	8510	1/1	0.91	0.06	49,49,49,49	0
35	NA	0	8541	1/1	0.91	0.22	69,69,69,69	0
32	MG	0	8059	1/1	0.91	0.06	59,59,59,59	0
34	SR	0	8915	1/1	0.91	0.09	131,131,131,131	0
35	NA	0	8519	1/1	0.92	0.12	50,50,50,50	0
34	SR	0	8989	1/1	0.92	0.14	185,185,185,185	0
35	NA	0	8509	1/1	0.92	0.15	69,69,69,69	0
33	CL	0	8811	1/1	0.92	0.11	68,68,68,68	0
35	NA	Q	8540	1/1	0.92	0.08	60,60,60,60	0
34	SR	0	8960	1/1	0.92	0.05	150,150,150,150	0
34	SR	0	8958	1/1	0.92	0.11	123,123,123,123	0
34	SR	0	8984	1/1	0.92	0.04	123,123,123,123	0
34	SR	0	8942	1/1	0.92	0.08	133,133,133,133	0
32	MG	0	8083	1/1	0.92	0.11	73,73,73,73	0
35	NA	0	8561	1/1	0.92	0.49	78,78,78,78	0
32	MG	0	8066	1/1	0.92	0.15	76,76,76,76	0
34	SR	0	8962	1/1	0.93	0.05	175,175,175,175	0
32	MG	0	8038	1/1	0.93	0.10	75,75,75,75	0
37	K	0	8401	1/1	0.93	0.13	74,74,74,74	0
35	NA	0	8547	1/1	0.93	0.61	54,54,54,54	0
35	NA	0	8529	1/1	0.93	0.05	45,45,45,45	0
34	SR	S	8961	1/1	0.93	0.10	122,122,122,122	0
33	CL	O	8808	1/1	0.93	0.07	81,81,81,81	0
32	MG	0	8090	1/1	0.93	0.33	62,62,62,62	0
34	SR	0	8974	1/1	0.93	0.13	149,149,149,149	0
32	MG	T	8057	1/1	0.93	0.07	65,65,65,65	0
32	MG	0	8052	1/1	0.93	0.07	52,52,52,52	0
35	NA	0	8566	1/1	0.93	0.25	60,60,60,60	0
32	MG	0	8006	1/1	0.94	0.14	30,30,30,30	0
34	SR	0	8946	1/1	0.94	0.23	122,122,122,122	0
34	SR	0	8966	1/1	0.94	0.08	111,111,111,111	0
35	NA	0	8565	1/1	0.94	0.94	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	NA	0	8567	1/1	0.94	0.21	80,80,80,80	0
34	SR	0	8924	1/1	0.94	0.16	135,135,135,135	0
34	SR	0	8956	1/1	0.94	0.09	155,155,155,155	0
35	NA	0	8536	1/1	0.94	0.07	65,65,65,65	0
33	CL	A	8809	1/1	0.94	0.09	74,74,74,74	0
34	SR	0	8939	1/1	0.94	0.04	160,160,160,160	0
35	NA	0	8531	1/1	0.94	0.11	44,44,44,44	0
35	NA	0	8535	1/1	0.94	0.24	53,53,53,53	0
32	MG	0	8035	1/1	0.94	0.14	68,68,68,68	0
35	NA	0	8558	1/1	0.94	0.17	50,50,50,50	0
34	SR	0	8970	1/1	0.95	0.03	128,128,128,128	0
34	SR	0	8941	1/1	0.95	0.13	116,116,116,116	0
34	SR	0	8917	1/1	0.95	0.13	111,111,111,111	0
34	SR	A	8929	1/1	0.95	0.16	137,137,137,137	0
35	NA	0	8507	1/1	0.95	0.16	42,42,42,42	0
34	SR	0	8992	1/1	0.95	0.15	137,137,137,137	0
32	MG	0	8007	1/1	0.95	0.20	38,38,38,38	0
32	MG	0	8060	1/1	0.95	0.06	61,61,61,61	0
35	NA	0	8573	1/1	0.95	0.25	77,77,77,77	0
32	MG	0	8048	1/1	0.95	0.20	26,26,26,26	0
34	SR	0	8971	1/1	0.95	0.07	180,180,180,180	0
32	MG	K	8054	1/1	0.95	0.13	50,50,50,50	0
35	NA	0	8545	1/1	0.95	0.14	41,41,41,41	0
34	SR	0	8945	1/1	0.95	0.07	112,112,112,112	0
35	NA	0	8524	1/1	0.95	0.18	58,58,58,58	0
33	CL	0	8815	1/1	0.96	0.10	78,78,78,78	0
35	NA	0	8542	1/1	0.96	0.40	66,66,66,66	0
32	MG	0	8079	1/1	0.96	0.10	55,55,55,55	0
34	SR	0	8908	1/1	0.96	0.10	110,110,110,110	0
33	CL	L	8810	1/1	0.96	0.08	61,61,61,61	0
32	MG	9	8074	1/1	0.96	0.11	77,77,77,77	0
35	NA	0	8526	1/1	0.96	0.05	57,57,57,57	0
32	MG	0	8010	1/1	0.96	0.12	35,35,35,35	0
32	MG	0	8043	1/1	0.96	0.10	49,49,49,49	0
35	NA	0	8511	1/1	0.96	0.13	59,59,59,59	0
35	NA	0	8516	1/1	0.96	0.12	42,42,42,42	0
34	SR	0	8972	1/1	0.96	0.14	141,141,141,141	0
32	MG	0	8024	1/1	0.96	0.13	55,55,55,55	0
35	NA	0	8514	1/1	0.96	0.59	48,48,48,48	0
35	NA	0	8564	1/1	0.96	0.41	81,81,81,81	0
32	MG	0	8064	1/1	0.96	0.15	37,37,37,37	0
32	MG	0	8085	1/1	0.96	0.08	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	NA	9	8543	1/1	0.96	0.18	49,49,49,49	0
32	MG	0	8061	1/1	0.96	0.21	30,30,30,30	0
32	MG	0	8046	1/1	0.96	0.13	41,41,41,41	0
35	NA	0	8554	1/1	0.96	0.89	78,78,78,78	0
33	CL	J	8801	1/1	0.96	0.17	79,79,79,79	0
32	MG	0	8092	1/1	0.96	0.25	67,67,67,67	0
34	SR	0	8995	1/1	0.96	0.17	140,140,140,140	0
32	MG	0	8039	1/1	0.96	0.26	77,77,77,77	0
35	NA	0	8537	1/1	0.96	0.11	41,41,41,41	0
35	NA	0	8515	1/1	0.96	0.14	37,37,37,37	0
32	MG	0	8021	1/1	0.96	0.10	30,30,30,30	0
32	MG	0	8063	1/1	0.96	0.17	71,71,71,71	0
35	NA	0	8534	1/1	0.96	0.24	42,42,42,42	0
35	NA	0	8569	1/1	0.96	0.19	54,54,54,54	0
34	SR	0	8969	1/1	0.97	0.10	160,160,160,160	0
35	NA	0	8549	1/1	0.97	0.27	58,58,58,58	0
35	NA	0	8551	1/1	0.97	0.24	59,59,59,59	0
33	CL	R	8806	1/1	0.97	0.13	52,52,52,52	0
34	SR	0	9002	1/1	0.97	0.08	184,184,184,184	0
34	SR	0	8937	1/1	0.97	0.21	115,115,115,115	0
32	MG	0	8078	1/1	0.97	0.32	61,61,61,61	0
33	CL	0	8812	1/1	0.97	0.06	54,54,54,54	0
34	SR	0	8933	1/1	0.97	0.17	150,150,150,150	0
32	MG	0	8067	1/1	0.97	0.20	34,34,34,34	0
32	MG	0	8031	1/1	0.97	0.39	72,72,72,72	0
34	SR	9	9003	1/1	0.97	0.01	170,170,170,170	0
32	MG	0	8001	1/1	0.97	0.09	33,33,33,33	0
33	CL	0	8805	1/1	0.97	0.06	67,67,67,67	0
34	SR	0	8911	1/1	0.97	0.08	85,85,85,85	0
34	SR	0	8954	1/1	0.97	0.12	112,112,112,112	0
34	SR	0	8963	1/1	0.97	0.04	134,134,134,134	0
33	CL	J	8802	1/1	0.97	0.09	76,76,76,76	0
35	NA	0	8520	1/1	0.97	0.08	53,53,53,53	0
34	SR	0	8948	1/1	0.97	0.12	102,102,102,102	0
33	CL	0	8816	1/1	0.97	0.18	85,85,85,85	0
33	CL	N	8807	1/1	0.97	0.10	71,71,71,71	0
35	NA	0	8556	1/1	0.97	0.40	49,49,49,49	0
35	NA	0	8568	1/1	0.97	0.49	50,50,50,50	0
34	SR	0	8921	1/1	0.97	0.12	92,92,92,92	0
35	NA	0	8521	1/1	0.97	0.08	65,65,65,65	0
35	NA	R	8532	1/1	0.97	0.08	46,46,46,46	0
37	K	0	8402	1/1	0.97	0.27	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	SR	0	8967	1/1	0.97	0.08	132,132,132,132	0
33	CL	0	8803	1/1	0.97	0.08	62,62,62,62	0
34	SR	0	8949	1/1	0.97	0.08	119,119,119,119	0
35	NA	0	8575	1/1	0.97	0.18	86,86,86,86	0
35	NA	0	8513	1/1	0.97	0.13	58,58,58,58	0
32	MG	0	8029	1/1	0.97	0.17	48,48,48,48	0
34	SR	0	8975	1/1	0.97	0.07	135,135,135,135	0
34	SR	0	8955	1/1	0.97	0.16	200,200,200,200	0
32	MG	B	8042	1/1	0.98	0.09	50,50,50,50	0
32	MG	0	8041	1/1	0.98	0.20	31,31,31,31	0
32	MG	0	8030	1/1	0.98	0.48	69,69,69,69	0
35	NA	0	8501	1/1	0.98	0.22	44,44,44,44	0
32	MG	0	8070	1/1	0.98	0.13	45,45,45,45	0
35	NA	0	8508	1/1	0.98	0.18	39,39,39,39	0
32	MG	0	8044	1/1	0.98	0.05	53,53,53,53	0
32	MG	0	8040	1/1	0.98	0.16	96,96,96,96	0
34	SR	0	8964	1/1	0.98	0.10	139,139,139,139	0
34	SR	0	8953	1/1	0.98	0.08	157,157,157,157	0
34	SR	0	8923	1/1	0.98	0.10	116,116,116,116	0
34	SR	0	8965	1/1	0.98	0.05	124,124,124,124	0
34	SR	0	8981	1/1	0.98	0.16	153,153,153,153	0
34	SR	0	8918	1/1	0.98	0.14	85,85,85,85	0
32	MG	0	8076	1/1	0.98	0.07	42,42,42,42	0
32	MG	0	8026	1/1	0.98	0.07	37,37,37,37	0
34	SR	0	8936	1/1	0.98	0.10	94,94,94,94	0
32	MG	0	8012	1/1	0.98	0.16	25,25,25,25	0
32	MG	0	8032	1/1	0.98	0.05	46,46,46,46	0
33	CL	0	8814	1/1	0.98	0.10	60,60,60,60	0
32	MG	0	8020	1/1	0.98	0.13	43,43,43,43	0
32	MG	0	8016	1/1	0.98	0.18	60,60,60,60	0
32	MG	0	8093	1/1	0.98	0.08	35,35,35,35	0
34	SR	0	8973	1/1	0.98	0.07	137,137,137,137	0
32	MG	0	8056	1/1	0.98	0.11	51,51,51,51	0
32	MG	0	8088	1/1	0.98	0.14	42,42,42,42	0
32	MG	Y	8086	1/1	0.98	0.05	46,46,46,46	0
32	MG	0	8033	1/1	0.98	0.09	49,49,49,49	0
32	MG	0	8049	1/1	0.98	0.38	68,68,68,68	0
32	MG	0	8055	1/1	0.98	0.20	46,46,46,46	0
34	SR	0	8931	1/1	0.98	0.09	117,117,117,117	0
34	SR	B	8950	1/1	0.98	0.17	132,132,132,132	0
32	MG	0	8053	1/1	0.98	0.04	59,59,59,59	0
34	SR	0	9004	1/1	0.98	0.64	200,200,200,200	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	SR	0	8901	1/1	0.98	0.10	85,85,85,85	0
33	CL	0	8822	1/1	0.98	0.55	106,106,106,106	0
33	CL	M	8818	1/1	0.98	0.10	47,47,47,47	0
35	NA	0	8523	1/1	0.98	0.12	45,45,45,45	0
34	SR	0	8920	1/1	0.98	0.05	134,134,134,134	0
34	SR	F	9005	1/1	0.98	0.07	134,134,134,134	0
32	MG	0	8050	1/1	0.98	0.12	37,37,37,37	0
34	SR	0	8909	1/1	0.98	0.14	85,85,85,85	0
34	SR	0	8926	1/1	0.98	0.10	127,127,127,127	0
32	MG	0	8068	1/1	0.99	0.09	54,54,54,54	0
35	NA	0	8512	1/1	0.99	0.42	56,56,56,56	0
33	CL	0	8817	1/1	0.99	0.10	65,65,65,65	0
34	SR	0	8904	1/1	0.99	0.19	66,66,66,66	0
33	CL	J	8821	1/1	0.99	0.13	71,71,71,71	0
34	SR	0	8990	1/1	0.99	0.10	137,137,137,137	0
32	MG	0	8069	1/1	0.99	0.16	72,72,72,72	0
32	MG	0	8008	1/1	0.99	0.15	27,27,27,27	0
32	MG	0	8019	1/1	0.99	0.18	27,27,27,27	0
36	CD	Z	8703	1/1	0.99	0.09	91,91,91,91	0
32	MG	0	8034	1/1	0.99	0.07	45,45,45,45	0
32	MG	0	8058	1/1	0.99	0.07	23,23,23,23	0
36	CD	1	8702	1/1	0.99	0.10	65,65,65,65	0
34	SR	0	8935	1/1	0.99	0.10	80,80,80,80	0
32	MG	0	8002	1/1	0.99	0.07	32,32,32,32	0
32	MG	0	8017	1/1	0.99	0.22	25,25,25,25	0
34	SR	0	8916	1/1	0.99	0.06	113,113,113,113	0
33	CL	0	8813	1/1	0.99	0.06	61,61,61,61	0
33	CL	Y	8820	1/1	0.99	0.23	51,51,51,51	0
32	MG	0	8073	1/1	0.99	0.07	83,83,83,83	0
32	MG	0	8015	1/1	0.99	0.17	36,36,36,36	0
34	SR	3	8999	1/1	0.99	0.04	106,106,106,106	0
32	MG	0	8065	1/1	0.99	0.06	49,49,49,49	0
34	SR	0	9008	1/1	0.99	0.14	89,89,89,89	0
32	MG	0	8014	1/1	0.99	0.16	35,35,35,35	0
34	SR	A	8930	1/1	0.99	0.05	104,104,104,104	0
35	NA	0	8553	1/1	0.99	0.36	68,68,68,68	0
34	SR	R	8912	1/1	0.99	0.16	86,86,86,86	0
32	MG	0	8018	1/1	0.99	0.19	46,46,46,46	0
32	MG	0	8025	1/1	0.99	0.11	35,35,35,35	0
32	MG	0	8022	1/1	0.99	0.11	32,32,32,32	0
32	MG	0	8028	1/1	0.99	0.16	27,27,27,27	0
34	SR	0	9000	1/1	0.99	0.12	177,177,177,177	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	NA	0	8504	1/1	0.99	0.16	37,37,37,37	0
35	NA	0	8517	1/1	0.99	0.21	36,36,36,36	0
34	SR	1	8952	1/1	0.99	0.13	91,91,91,91	0
34	SR	0	8940	1/1	0.99	0.08	93,93,93,93	0
32	MG	0	8009	1/1	0.99	0.20	29,29,29,29	0
34	SR	0	8910	1/1	0.99	0.04	101,101,101,101	0
34	SR	0	8903	1/1	0.99	0.18	58,58,58,58	0
34	SR	0	8905	1/1	0.99	0.28	68,68,68,68	0
32	MG	0	8084	1/1	0.99	0.15	37,37,37,37	0
34	SR	0	8943	1/1	0.99	0.07	117,117,117,117	0
32	MG	0	8080	1/1	0.99	0.36	69,69,69,69	0
32	MG	0	8023	1/1	0.99	0.14	32,32,32,32	0
32	MG	0	8045	1/1	0.99	0.11	35,35,35,35	0
32	MG	0	8013	1/1	0.99	0.03	30,30,30,30	0
33	CL	B	8819	1/1	0.99	0.10	54,54,54,54	0
35	NA	M	8539	1/1	0.99	0.10	34,34,34,34	0
36	CD	U	8701	1/1	0.99	0.11	72,72,72,72	0
34	SR	0	8934	1/1	0.99	0.11	130,130,130,130	0
32	MG	0	8005	1/1	0.99	0.17	33,33,33,33	0
34	SR	9	8978	1/1	0.99	0.08	133,133,133,133	0
32	MG	0	8027	1/1	0.99	0.09	49,49,49,49	0
33	CL	3	8804	1/1	0.99	0.06	67,67,67,67	0
32	MG	0	8047	1/1	0.99	0.28	65,65,65,65	0
36	CD	3	8704	1/1	1.00	0.07	81,81,81,81	0
34	SR	0	8907	1/1	1.00	0.14	56,56,56,56	0
32	MG	0	8004	1/1	1.00	0.17	30,30,30,30	0
32	MG	0	8011	1/1	1.00	0.16	33,33,33,33	0
35	NA	0	8552	1/1	1.00	0.28	72,72,72,72	0
36	CD	O	8705	1/1	1.00	0.07	94,94,94,94	0
32	MG	0	8003	1/1	1.00	0.18	34,34,34,34	0
34	SR	3	8932	1/1	1.00	0.12	79,79,79,79	0
34	SR	0	8914	1/1	1.00	0.27	110,110,110,110	0
34	SR	0	8902	1/1	1.00	0.11	66,66,66,66	0
34	SR	1	8913	1/1	1.00	0.09	96,96,96,96	0
34	SR	0	8925	1/1	1.00	0.12	91,91,91,91	0
34	SR	0	8906	1/1	1.00	0.21	60,60,60,60	0

6.5 Other polymers ⓘ

There are no such residues in this entry.