



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 01:53 pm BST

PDB ID : 1VQ5
Title : The structure of the transition state analogue "RAA" bound to the large ribosomal subunit of haloarcula marismortui
Authors : Schmeing, T.M.; Steitz, T.A.
Deposited on : 2004-12-16
Resolution : 2.60 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 : 2.11
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) : 2.11

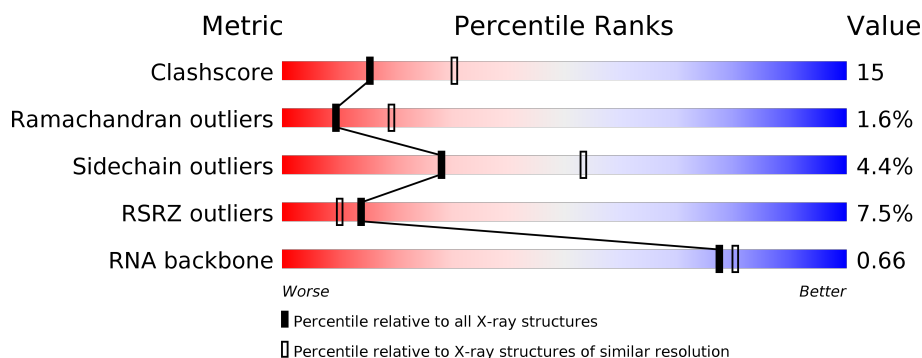
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)
RNA backbone	3102	1040 (2.90-2.30)

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	0	2922	<div> <div>2%</div> <div> <div></div> <div>61%</div> <div>28%</div> <div>5%</div> <div>6%</div> </div> </div>
2	9	122	<div> <div>3%</div> <div> <div></div> <div>58%</div> <div>32%</div> <div>10%</div> </div> </div>
3	4	8	<div> <div></div> <div> <div></div> <div>38%</div> <div>63%</div> </div> </div>
4	A	240	<div> <div>6%</div> <div> <div></div> <div>60%</div> <div>34%</div> <div>• •</div> </div> </div>
5	B	338	<div> <div>9%</div> <div> <div></div> <div>50%</div> <div>45%</div> <div>5%</div> </div> </div>
6	C	246	<div> <div>2%</div> <div> <div></div> <div>59%</div> <div>35%</div> <div>6%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
7	D	177	
8	E	178	
9	F	120	
10	G	348	
11	H	171	
12	J	145	
13	K	132	
14	L	165	
15	M	194	
16	N	187	
17	O	116	
18	P	149	
19	Q	96	
20	R	155	
21	S	85	
22	T	120	
23	U	66	
24	V	71	
25	W	154	
26	X	92	
27	Y	241	
28	Z	83	
29	1	57	
30	2	50	
31	3	92	

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Mol	Chain	Length	Quality of chain
32	I	162	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	MG	0	8049	-	-	-	X
33	MG	0	8092	-	-	-	X
35	NA	0	9121	-	-	-	X
35	NA	0	9155	-	-	-	X
35	NA	0	9162	-	-	-	X
35	NA	0	9177	-	-	-	X
35	NA	0	9182	-	-	-	X
35	NA	0	9184	-	-	-	X
35	NA	B	9158	-	-	-	X
35	NA	R	9186	-	-	-	X

2 Entry composition [i](#)

There are 38 unique types of molecules in this entry. The entry contains 99060 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S ribosomal rna.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	2754	Total	C	N	O	P	0	0	0
			59021	26350	10878	19048	2745			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	628	1MA	A	modified residue	GB 3377779
0	2587	OMU	U	modified residue	GB 3377779
0	2588	OMG	G	modified residue	GB 3377779
0	2619	UR3	U	modified residue	GB 3377779
0	2621	PSU	U	modified residue	GB 3377779

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

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

- Molecule 3 is a RNA chain called 5'-D*(DC)P*(DC)P*(5AA)P*(2OP)P*(PO2)P*AP*C*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	4	8	Total	C	N	O	P	0	0	0
			126	61	23	37	5			

- Molecule 4 is a protein called 50S ribosomal protein L2P.

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

- Molecule 5 is a protein called 50S ribosomal protein L3P.

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

- Molecule 6 is a protein called 50S ribosomal protein L4E.

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

- Molecule 7 is a protein called 50S ribosomal protein L5P.

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

- Molecule 8 is a protein called 50S ribosomal protein L6P.

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

- Molecule 9 is a protein called 50S ribosomal protein L7AE.

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

- Molecule 10 is a protein called ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG.

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

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L10E.

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	M	194	Total	C	N	O	S	0	0	0
			1560	943	332	284	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	13	GLU	LYS	CONFLICT	GB 55231501
M	194	ALA	GLY	CONFLICT	GB 55231501

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L11P.

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

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	106	Total	Mg	0	0
			106	106		
33	Y	1	Total	Mg	0	0
			1	1		
33	K	1	Total	Mg	0	0
			1	1		
33	B	2	Total	Mg	0	0
			2	2		
33	A	2	Total	Mg	0	0
			2	2		
33	4	1	Total	Mg	0	0
			1	1		
33	T	1	Total	Mg	0	0
			1	1		
33	2	1	Total	Mg	0	0
			1	1		
33	9	2	Total	Mg	0	0
			2	2		
33	3	1	Total	Mg	0	0
			1	1		

- Molecule 34 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	0	3	Total K 3 3	0	0

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

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

- Molecule 36 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	0	10	Total Cl 10 10	0	0
36	J	3	Total Cl 3 3	0	0
36	B	1	Total Cl 1 1	0	0
36	A	1	Total Cl 1 1	0	0
36	N	1	Total Cl 1 1	0	0

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

- Molecule 37 is CADMIUM ION (three-letter code: CD) (formula: Cd).

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

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	0	5820	Total 5820	O 5820	0	0
38	9	133	Total 133	O 133	0	0
38	4	8	Total 8	O 8	0	0
38	A	117	Total 117	O 117	0	0
38	B	150	Total 150	O 150	0	0
38	C	165	Total 165	O 165	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	D	49	Total 49	O 49	0	0
38	E	47	Total 47	O 47	0	0
38	F	21	Total 21	O 21	0	0
38	G	16	Total 16	O 16	0	0
38	H	66	Total 66	O 66	0	0
38	J	52	Total 52	O 52	0	0
38	K	54	Total 54	O 54	0	0
38	L	83	Total 83	O 83	0	0
38	M	118	Total 118	O 118	0	0
38	N	66	Total 66	O 66	0	0
38	O	39	Total 39	O 39	0	0
38	P	65	Total 65	O 65	0	0
38	Q	52	Total 52	O 52	0	0
38	R	85	Total 85	O 85	0	0
38	S	31	Total 31	O 31	0	0
38	T	39	Total 39	O 39	0	0
38	U	25	Total 25	O 25	0	0
38	V	13	Total 13	O 13	0	0
38	W	68	Total 68	O 68	0	0
38	X	27	Total 27	O 27	0	0
38	Y	92	Total 92	O 92	0	0

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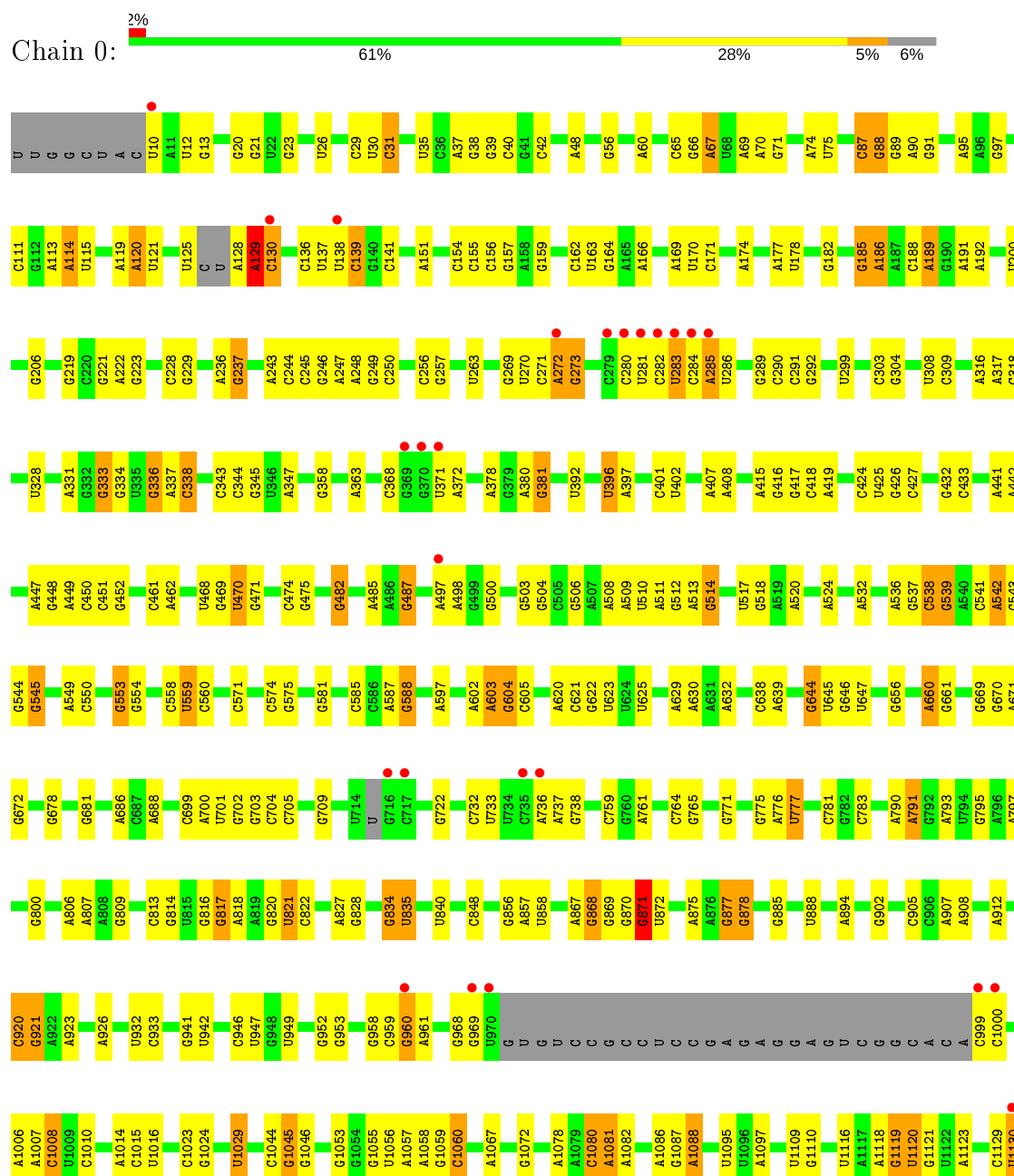
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	Z	30	Total 30	O 30	0	0
38	1	59	Total 59	O 59	0	0
38	2	42	Total 42	O 42	0	0
38	3	74	Total 74	O 74	0	0
38	I	10	Total 10	O 10	0	0

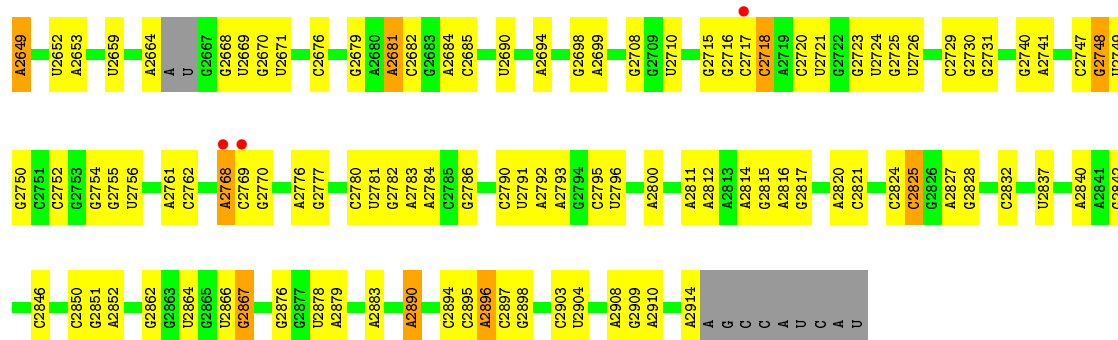
3 Residue-property plots

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

- Molecule 1: 23S ribosomal rna



C2526	U2527	C2533	C2534	C2535	C2536	C2537	U2541	C2542	C2548	C2551	C2552	A2553	U2563	C2564	C2565	C2577	C2578	U2586	U2587	C2588	U2589	U2590	C2591	C2592	U2597	U2598	A2601	C2602	C2603	A2604	U2607	C2608	C2613	C2614	U2619	U2620	C2630	C2634	A2637	C2643	C2644	U2645										
G2421	U2422	C2423	G2426	C2427	G2428	G2438	C2439	C2443	U2444	U2445	U2446	A2455	A2456	U2457	G2462	C2467	A2468	A2469	C2472	C2476	G2480	A2483	C2487	A2490	C2491	U2492	C2493	C2502	A2503	A2504	G2505	A2506	C2507	C2508	A2509	C2510	A2511	U2512	C2515	U2516	A2521	G2524	C2525									
C2329	U2330	C2331	G2338	A	C	A	A	A	A	A	A	A2353	A2354	C2355	A2356	C2357	A2361	A2362	C2363	A2364	C2365	A2369	A2372	U2373	U2377	U2378	C2379	C2380	C2381	G2385	U2387	C2388	C2392	A2401	A2402	C2403	G2404	A2408	G2412	A2413	A2414	A2415	G2418	U2419	C2420							
C	G	G	U	G	C	U	C	C	C	C	C	C2241	U2242	C2243	C2248	G2249	G2250	G2251	A2252	G2253	C2254	A2255	G2256	G2257	A2258	U2265	A2266	G2267	C2268	G2269	G2270	G2271	G2272	C2281	U2282	A2291	A2300	A2301	A2302	C2309	G2312	C2313	C2314	C2315	G2316	C2317	U2320	A2321	G2324			
A	G	A	C	A	C	U	U	A	A	A	A	G	C	C	C	C	C	C	C	C	C	A	U	U	U	U	C	C	A	A	A	A	A	A	A	A	A	A	A	A	A	A	U									
A2067	G2068	G2072	C2073	A2074	U2078	G2079	G2080	A2081	G2093	A2096	A2101	G2102	C2105	C2106	G2110	U2115	U2116	G2134	A2135	G2136	A	C	C	A	G	U	U	C	C	A	A	A	A	U	G	U	U	U	U	U	U	G										
G1806	A1811	C1819	G1820	A1829	C1830	C1834	U1835	A1839	A1840	A1845	U1846	G1847	G1848	G1849	G1855	C1856	G1863	G1867	G1868	G1877	G1878	U1879	C1880	A1881	A1904	U1905	A1919	C1920	A1921	A1922	G1926	A1927	A1930	A1931	G1932	G1933	A1934	C1940	A1941	A1942	C1943	G1948	G1949									
G1950	G1951	U	A	A	C	U	A	U	A	G	A	C	C	C	U1964	G1971	U1972	A1973	G1976	U1977	A1978	G1979	U1986	A1997	U2004	U2008	A2011	U2012	G2013	G2014	A2015	U2016	U2028	C2029	A2030	G2033	U2034	C2035	C2036	U2043	G2044	G2050	A2054	C2061	A2062	U2064						
A1701	U1702	A1710	A1711	A1712	G1713	C1714	C1715	A1716	A1717	G1718	U1722	G1723	U1724	C1725	G1730	C1731	A1732	A1733	C1734	U1741	A1742	G1743	G1745	A1755	G1756	U1761	U1766	U1771	C1772	G1773	G1774	A1778	A1779	G1785	C1786	C1787	U1788	G1789	C1790	U1791	C1798	G1805										
U1595	U1596	A1598	A1603	G1604	G1605	C1613	G1614	A1624	U1625	A1626	A1631	A1632	C1633	G1634	U1635	G1636	A1637	A1641	A1642	C1643	C1644	U1654	G1655	A1656	A1657	A1658	G1663	A1664	G1665	C1666	U1668	A1669	G1670	C1675	C1679	G1681	A1682	G1683	A1684	A1685	C1686	C1687	C1692	G1697	U1698							
C1450	C1451	G1453	A1458	C1462	A1463	C1474	C1477	U1478	C1483	G1484	A1485	A1494	C1495	G1496	U1500	U1503	A1504	U1505	U1506	C1513	C1514	U1524	G1525	A1526	A1527	A1528	G1529	G1535	C1536	U1544	C1545	A1559	U1561	C1562	C1563	C1564	U1567	G1568	G1592	C1593	C1594											
A1328	A1331	U1333	C1334	C1335	U1336	G1340	C1342	C1343	G1351	A1352	C1353	C1360	G1363	A1372	A1375	G1376	C1377	U1380	G1385	G1391	A1392	G1398	A1399	A1406	U1407	U1408	G1409	G1417	U1418	U1419	C1420	C1423	A1424	A1427	A1434	U1435	C1436	U1440	G1441	A1442												
C1209	G1210	C1213	G1214	A1215	G1216	G1224	C1225	C1229	U1234	G1235	A1236	U1237	C1238	G1239	A1242	C1243	U1244	G1245	A1246	U1249	C1250	C1251	A1252	C1253	C1268	G1269	U1270	C1273	A1278	U1279	C1289	G1290	A1294	G1299	G1300	U1304	C1305	A1307	A1308	U1309	U1310	G1311	U1314									
G1131	A1132	G1135	U1136	G1137	A1150	G1151	G1158	G1159	G1160	A1161	G1162	G1163	U1164	G1165	A1166	G1167	C1168	U1169	U1170	A1171	G1172	A1173	A1174	C1176	A1177	G1178	C1179	U1180	A1181	C1182	C1183	U1184	U1185	C1186	U1187	A1188	G1189	G1190	A1191	A1192	A1193	A1194	G1195	U1198	A1199	A1200	A1202	G1203	C1204	U1205	U1206	C1208



• Molecule 2: 5S ribosomal RNA



• Molecule 3: 5'-D*(DC)P*(DC)P*(5AA)P*(2OP)P*(PO2)P*AP*C*C)-3'

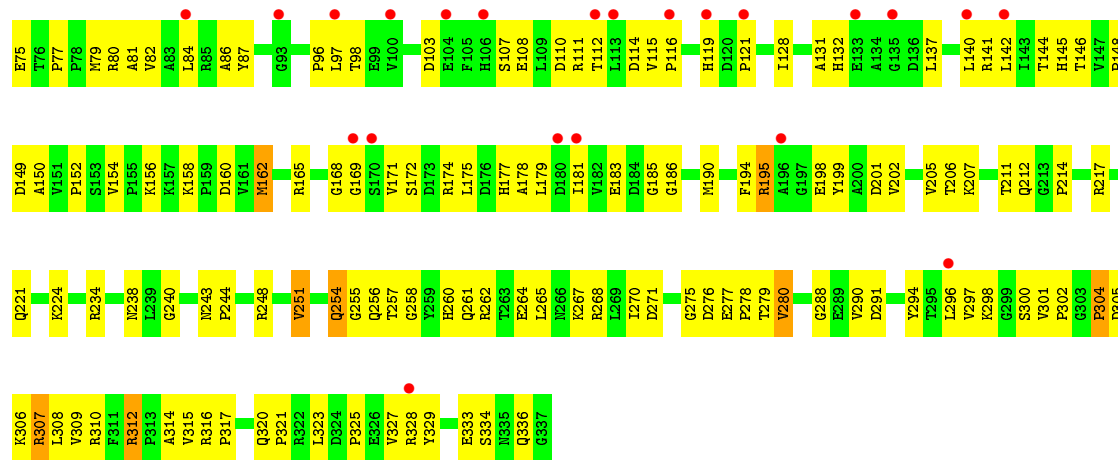


• Molecule 4: 50S ribosomal protein L2P

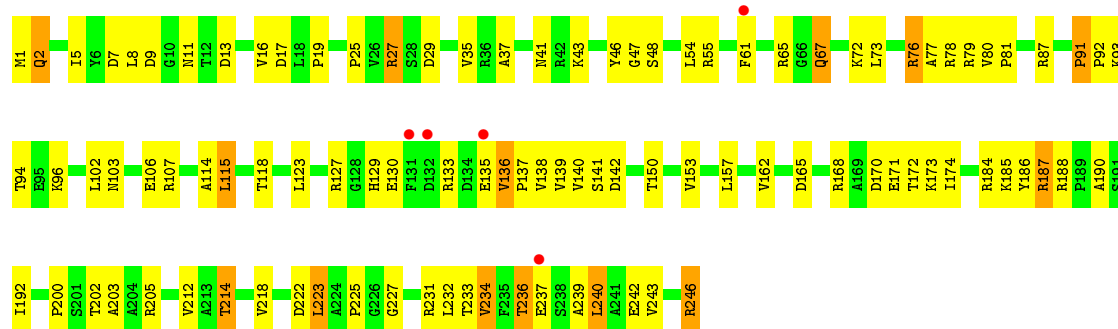


• Molecule 5: 50S ribosomal protein L3P

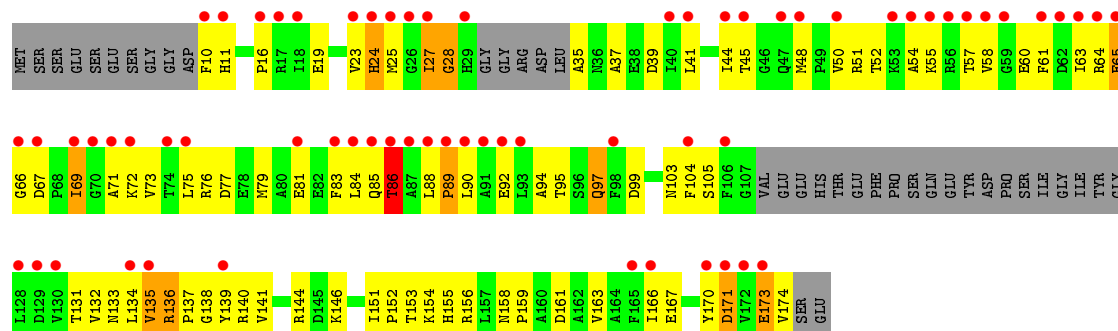




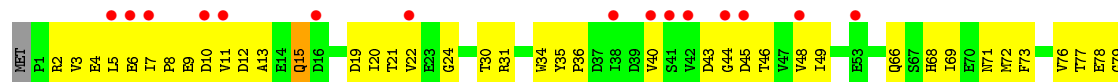
• Molecule 6: 50S ribosomal protein L4E

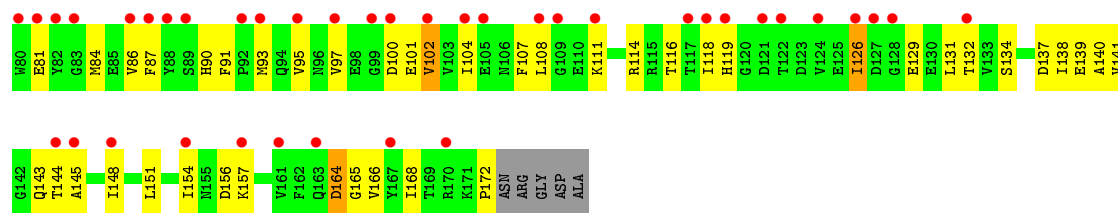


• Molecule 7: 50S ribosomal protein L5P

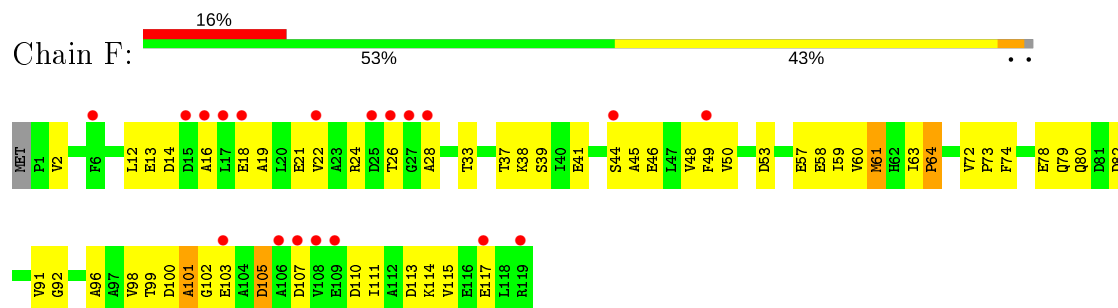


• Molecule 8: 50S ribosomal protein L6P

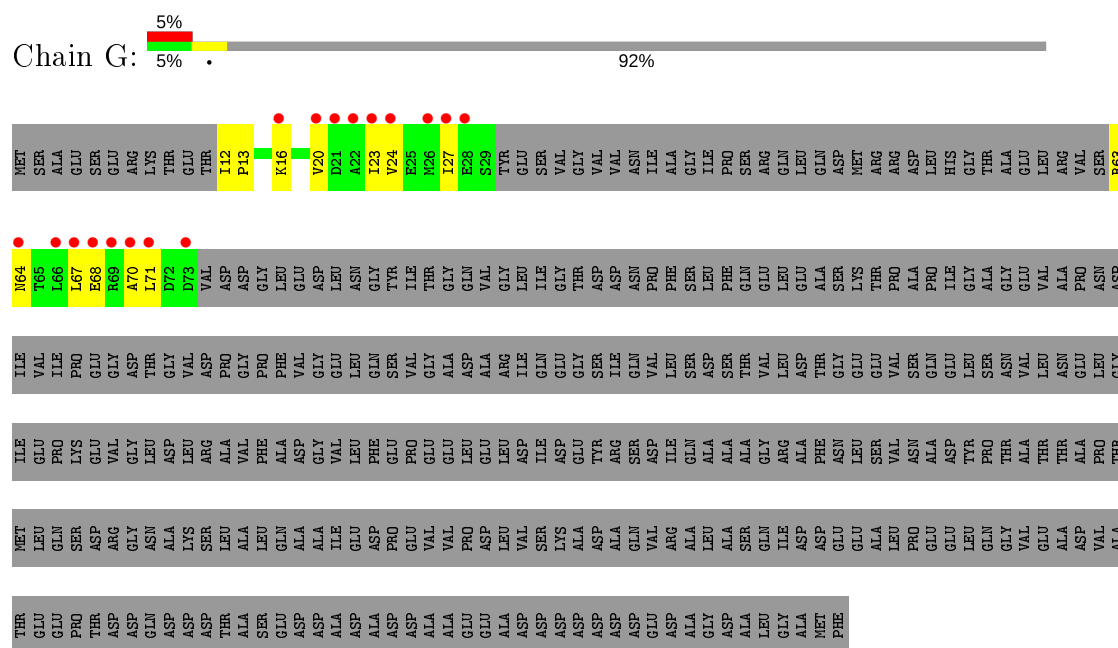




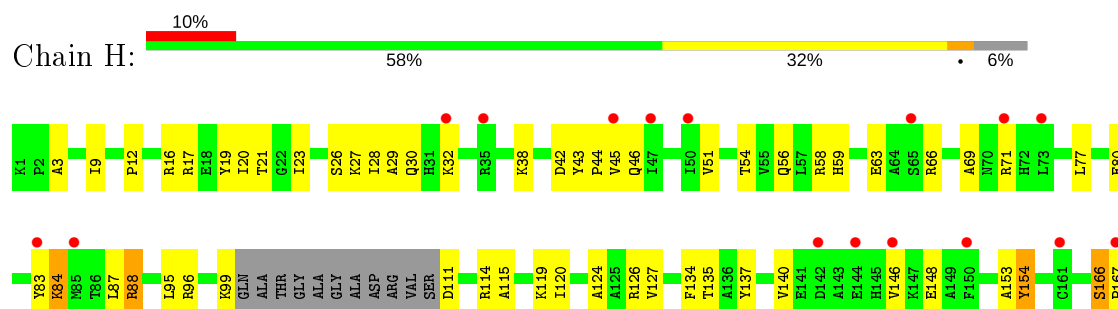
• Molecule 9: 50S ribosomal protein L7AE

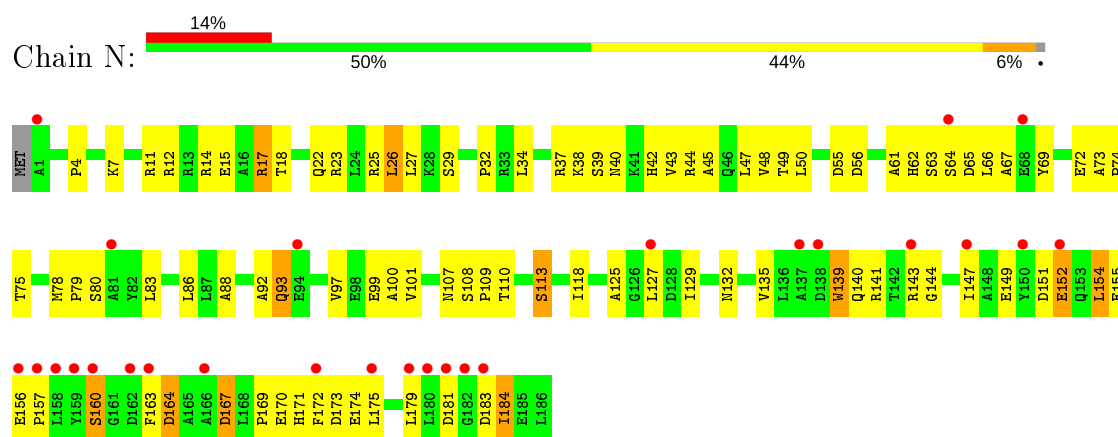


• Molecule 10: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG

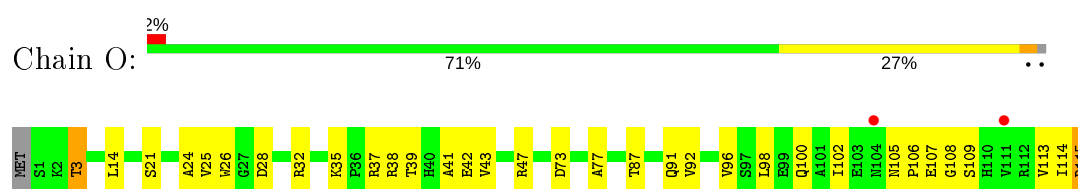


• Molecule 11: 50S RIBOSOMAL PROTEIN L10E

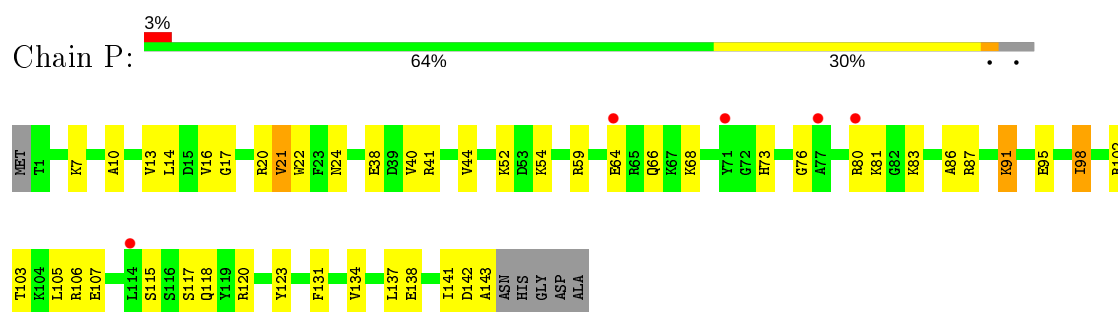




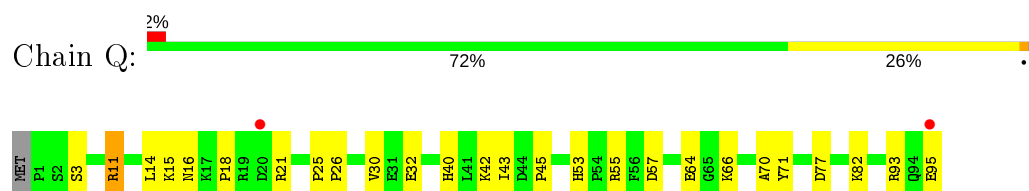
- Molecule 17: 50S ribosomal protein L18e



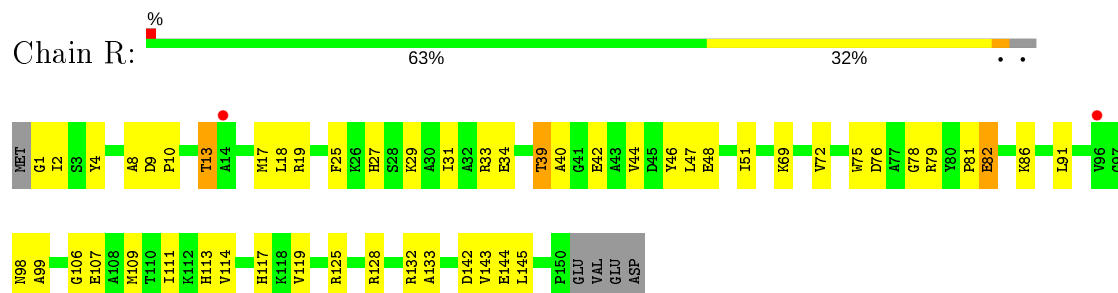
- Molecule 18: 50S ribosomal protein L19E



- Molecule 19: 50S ribosomal protein L21e



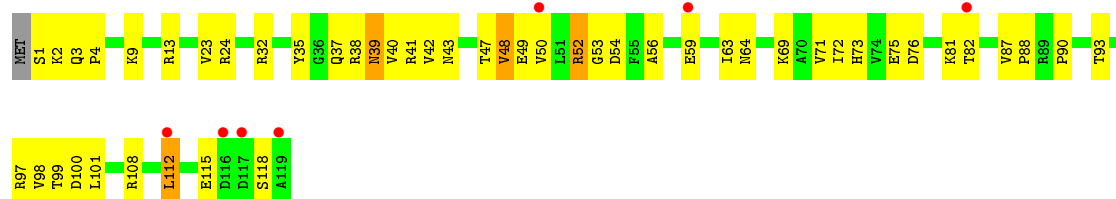
- Molecule 20: 50S ribosomal protein L22P



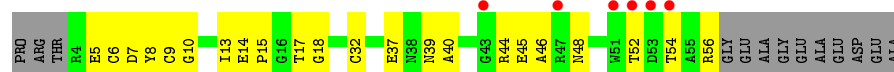
- Molecule 21: 50S ribosomal protein L23P



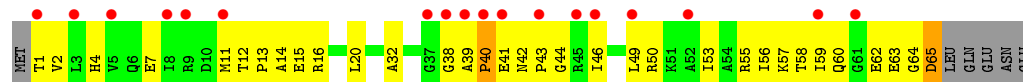
• Molecule 22: 50S ribosomal protein L24P



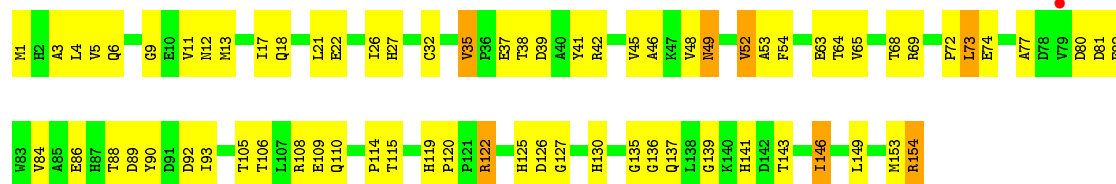
• Molecule 23: 50S ribosomal protein L24E



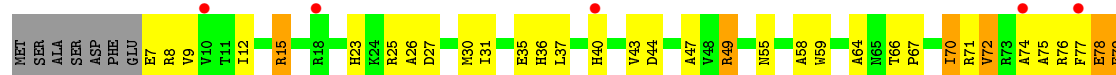
• Molecule 24: 50S ribosomal protein L29P

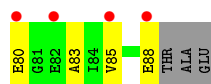


• Molecule 25: 50S ribosomal protein L30P

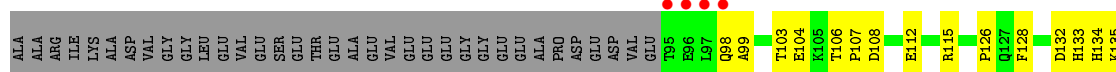
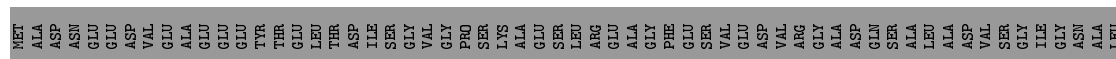


• Molecule 26: 50S ribosomal protein L31e

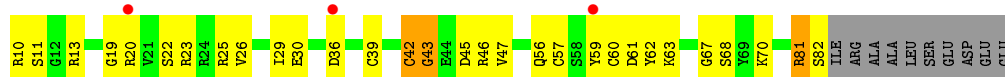




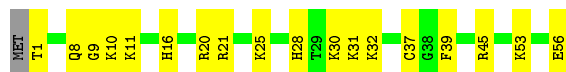
- Molecule 27: 50S ribosomal protein L32E



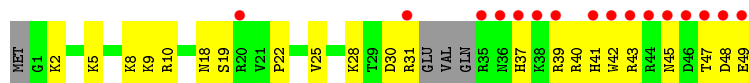
- Molecule 28: 50S ribosomal protein L37Ae



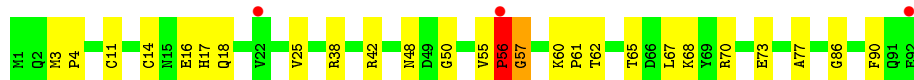
- Molecule 29: 50S ribosomal protein L37e



- Molecule 30: 50S ribosomal protein L39e



- Molecule 31: 50S ribosomal protein L44E



- Molecule 32: 50S RIBOSOMAL PROTEIN L11P



•	A125	•	SER	•	MET
•	K126	•	PHE	•	ALA
•	E127	•	GLU	•	GLY
•	V128	•	ILE	•	THR
•	V129	•	GLU	•	ILE
•	G130	•	VAL	•	GLU
•	T131	•	G71	•	VAL
•	C132	•	V72	•	LEU
•	T133	•	P73	•	VAL
•	S134	•	P74	•	PRO
•	L135	•	T75	•	GLY
•	G136	•	A76	•	GLY
•	V137	•	E77	•	GLU
•	T138	•	L78	•	ALA
•	I139	•	I79	•	ASN
•	E140	•	K30	•	PRO
		•	D81	•	GLY
		•	E82	•	PRO
		•	A83	•	PRO
		•	G84	•	LEU
		•	F85	•	GLY
		•	E86	•	PRO
		•	T87	•	GLU
		•	G88	•	LEU
		•	S89	•	GLY
		•	G90	•	PRO
		•	E91	•	THR
		•	P92	•	PRO
		•	Q93	•	VAL
		•	E94	•	ASP
		•	D95	•	VAL
		•	F96	•	GLN
		•	V97	•	ALA
		•	A98	•	VAL
			D99		VAL
			L100		GLN
			S101		GLU
		•	V102	•	ILE
		•	D103	•	ASN
		•	Q104	•	ASP
		•	V105	•	GLN
		•	K106	•	THR
		•	Q107	•	ALA
		•	I108	•	ALA
		•	A109	•	PHE
		•	E110	•	ASP
		•	Q111	•	GLY
		•	K112	•	THR
		•	H113	•	GLU
		•	P114	•	VAL
		•	D115	•	PRO
		•	L116	•	VAL
		•	L117	•	THR
		•	S118	•	VAL
		•	Y119	•	LYS
		•	D120	•	TYR
		•	L121	•	ASP
		•	T122	•	ASP
		•	N123	•	ASP
		•	A124	•	GLY

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.79Å 300.61Å 573.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 49.67 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-2.60) 90.1 (49.67-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.83 (at 2.48Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.197 , 0.237 0.238 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	53.1	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 55.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	99060	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% 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, NA, K, PO2, CD, 5AA, DCZ, OMU, UR3, 2OP, 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	0	0.38	0/65959	0.69	20/102870 (0.0%)
2	9	0.33	0/2905	0.70	1/4528 (0.0%)
3	4	0.53	0/83	0.82	0/119
4	A	0.33	0/1786	0.64	0/2408
5	B	0.32	0/2690	0.63	0/3652
6	C	0.39	0/1884	0.66	0/2551
7	D	0.29	0/1111	0.53	0/1498
8	E	0.31	0/1382	0.57	0/1880
9	F	0.30	0/901	0.53	0/1224
10	G	0.29	0/241	0.45	0/324
11	H	0.34	0/1287	0.63	0/1725
12	J	0.35	0/1136	0.60	0/1530
13	K	0.35	0/1001	0.67	0/1347
14	L	0.33	0/1130	0.64	0/1509
15	M	0.35	0/1584	0.61	0/2119
16	N	0.28	0/1474	0.62	0/1999
17	O	0.34	0/874	0.59	0/1181
18	P	0.33	0/1147	0.54	0/1528
19	Q	0.37	0/749	0.68	0/1005
20	R	0.35	0/1172	0.64	0/1578
21	S	0.33	0/648	0.58	0/875
22	T	0.32	0/958	0.65	1/1289 (0.1%)
23	U	0.34	0/417	0.56	0/562
24	V	0.28	0/502	0.51	0/675
25	W	0.33	0/1219	0.62	0/1655
26	X	0.34	0/664	0.59	0/895
27	Y	0.36	0/1146	0.65	0/1536
28	Z	0.37	0/589	0.65	0/787
29	1	0.41	0/438	0.64	0/578
30	2	0.32	0/401	0.55	0/529
31	3	0.38	0/771	0.59	0/1024
32	I	0.29	0/526	0.53	0/716

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.37	0/98775	0.67	22/147696 (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
1	0	1	52
25	W	0	1
All	All	1	53

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1563	G	C2'-C3'-O3'	9.50	130.40	109.50
1	0	1942	A	C5'-C4'-C3'	7.87	128.58	116.00
2	9	3039	U	N1-C1'-C2'	6.80	122.84	114.00
1	0	871	G	C5'-C4'-O4'	-6.76	100.98	109.10
1	0	1819	G	C5'-C4'-C3'	6.21	125.94	116.00
1	0	2467	A	C1'-O4'-C4'	-5.92	105.17	109.90
1	0	2316	G	C5'-C4'-C3'	-5.90	106.56	116.00
1	0	1504	A	C1'-O4'-C4'	-5.79	105.27	109.90
1	0	1120	U	C5'-C4'-C3'	-5.77	106.77	116.00
1	0	1504	A	N9-C1'-C2'	5.76	121.49	114.00
1	0	2291	A	N9-C1'-C2'	5.72	121.43	114.00
1	0	1829	A	N9-C1'-C2'	-5.59	105.85	112.00
1	0	2313	C	C5'-C4'-O4'	5.55	115.76	109.10
1	0	1942	A	C5'-C4'-O4'	5.42	115.60	109.10
1	0	206	G	C5'-C4'-C3'	-5.39	107.38	116.00
1	0	129	A	C2'-C3'-O3'	5.34	122.25	113.70
1	0	1165	G	C1'-O4'-C4'	-5.17	105.76	109.90
22	T	52	ARG	N-CA-C	5.15	124.91	111.00
1	0	1942	A	C4'-C3'-C2'	-5.14	97.46	102.60
1	0	2607	U	N1-C1'-C2'	5.13	120.67	114.00
1	0	2313	C	C5'-C4'-C3'	5.07	124.11	116.00
1	0	1971	G	N9-C1'-C2'	5.01	120.51	114.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1563	G	C3'

All (53) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1055	G	Sidechain
1	0	1078	A	Sidechain
1	0	1340	G	Sidechain
1	0	1342	C	Sidechain
1	0	1351	G	Sidechain
1	0	1417	G	Sidechain
1	0	1458	A	Sidechain
1	0	1718	G	Sidechain
1	0	174	A	Sidechain
1	0	1819	G	Sidechain
1	0	1829	A	Sidechain
1	0	1839	A	Sidechain
1	0	1845	A	Sidechain
1	0	1848	G	Sidechain
1	0	1863	G	Sidechain
1	0	1867	G	Sidechain
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	189	A	Sidechain
1	0	2312	G	Sidechain
1	0	2316	G	Sidechain
1	0	2412	G	Sidechain
1	0	2493	C	Sidechain
1	0	2503	A	Sidechain
1	0	2506	A	Sidechain
1	0	2551	C	Sidechain
1	0	2552	C	Sidechain
1	0	2564	G	Sidechain
1	0	26	U	Sidechain
1	0	2607	U	Sidechain
1	0	2620	U	Sidechain
1	0	2630	G	Sidechain
1	0	2643	G	Sidechain
1	0	2793	A	Sidechain
1	0	2842	G	Sidechain
1	0	333	G	Sidechain
1	0	396	U	Sidechain
1	0	469	G	Sidechain

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Mol	Chain	Res	Type	Group
1	0	470	U	Sidechain
1	0	471	G	Sidechain
1	0	48	A	Sidechain
1	0	482	G	Sidechain
1	0	518	G	Sidechain
1	0	554	G	Sidechain
1	0	722	G	Sidechain
1	0	771	G	Sidechain
1	0	781	C	Sidechain
1	0	791	A	Sidechain
1	0	817	G	Sidechain
1	0	867	A	Sidechain
1	0	868	G	Sidechain
1	0	888	U	Sidechain
25	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	0	59021	0	29813	777	1
2	9	2600	0	1326	52	1
3	4	126	0	75	5	0
4	A	1753	0	1766	106	0
5	B	2625	0	2533	158	1
6	C	1859	0	1816	111	0
7	D	1094	0	1085	93	0
8	E	1357	0	1266	78	0
9	F	890	0	843	51	0
10	G	240	0	231	11	0
11	H	1266	0	1268	60	0
12	J	1120	0	1098	62	0
13	K	992	0	1031	51	1
14	L	1118	0	1076	53	0
15	M	1560	0	1568	62	0
16	N	1445	0	1401	109	0
17	O	865	0	873	29	0
18	P	1136	0	1123	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	Q	735	0	729	23	0
20	R	1149	0	1122	55	0
21	S	641	0	605	19	0
22	T	950	0	923	50	0
23	U	410	0	364	21	0
24	V	499	0	511	34	0
25	W	1196	0	1137	95	0
26	X	654	0	653	44	0
27	Y	1130	0	1133	53	0
28	Z	578	0	539	24	0
29	1	431	0	426	27	0
30	2	396	0	413	29	0
31	3	755	0	728	19	0
32	I	519	0	500	58	0
33	0	106	0	0	0	0
33	2	1	0	0	0	0
33	3	1	0	0	0	0
33	4	1	0	0	0	0
33	9	2	0	0	0	0
33	A	2	0	0	0	0
33	B	2	0	0	0	0
33	K	1	0	0	0	0
33	T	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	3	0	0	0	0
35	0	71	0	0	0	0
35	9	2	0	0	0	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	C	1	0	0	0	0
35	H	2	0	0	0	0
35	J	1	0	0	0	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	3	0	0	0	0
35	S	1	0	0	0	0
36	0	10	0	0	1	0
36	3	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	J	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	L	1	0	0	0	0
36	M	1	0	0	0	0
36	N	1	0	0	0	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
36	Y	1	0	0	0	0
37	1	1	0	0	0	0
37	3	1	0	0	0	0
37	O	1	0	0	0	0
37	U	1	0	0	0	0
37	Z	1	0	0	0	0
38	0	5820	0	0	111	0
38	1	59	0	0	2	0
38	2	42	0	0	2	0
38	3	74	0	0	3	0
38	4	8	0	0	0	0
38	9	133	0	0	3	0
38	A	117	0	0	9	0
38	B	150	0	0	16	0
38	C	165	0	0	15	0
38	D	49	0	0	11	0
38	E	47	0	0	7	0
38	F	21	0	0	3	0
38	G	16	0	0	0	0
38	H	66	0	0	6	0
38	I	10	0	0	2	0
38	J	52	0	0	1	0
38	K	54	0	0	3	0
38	L	83	0	0	10	0
38	M	118	0	0	3	0
38	N	66	0	0	8	0
38	O	39	0	0	4	0
38	P	65	0	0	3	0
38	Q	52	0	0	5	0
38	R	85	0	0	4	0
38	S	31	0	0	3	0
38	T	39	0	0	1	0
38	U	25	0	0	0	0
38	V	13	0	0	2	0
38	W	68	0	0	6	0
38	X	27	0	0	2	0
38	Y	92	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	Z	30	0	0	2	0
All	All	99060	0	59975	2235	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (2235) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1160:G:H5'	1:0:1161:A:H5'	1.26	1.12
15:M:164:THR:HG22	15:M:167:GLY:H	1.13	1.09
1:0:156:C:H5''	15:M:171:ARG:HD3	1.35	1.08
11:H:46:GLN:HB3	11:H:167:PRO:HD2	1.30	1.08
11:H:166:SER:HB2	11:H:167:PRO:HD3	1.35	1.07
24:V:12:THR:HG22	24:V:15:GLU:HG3	1.31	1.07
26:X:37:LEU:HD13	26:X:85:VAL:HG21	1.37	1.06
22:T:71:VAL:HG11	22:T:90:PRO:HB3	1.36	1.06
7:D:25:MET:HE3	7:D:37:ALA:HB1	1.33	1.05
22:T:9:LYS:HE3	22:T:13:ARG:NH1	1.75	1.02
2:9:3076:G:H3'	2:9:3077:A:H5''	1.39	1.02
6:C:236:THR:HG22	6:C:239:ALA:H	1.24	1.01
1:0:1242:A:H5'	12:J:82:THR:HG23	1.41	1.01
27:Y:187:VAL:HG23	27:Y:192:ASP:HB2	1.43	0.99
1:0:2717:C:H2'	1:0:2718:C:H5''	1.42	0.99
1:0:1119:G:H2'	12:J:52:GLN:NE2	1.77	0.98
12:J:74:ARG:HB3	12:J:74:ARG:HH11	1.29	0.97
30:2:41:HIS:H	30:2:45:ASN:HD22	0.98	0.97
1:0:1119:G:H2'	12:J:52:GLN:HE22	1.32	0.95
4:A:211:LYS:HB3	4:A:212:PRO:HD2	1.49	0.94
1:0:2717:C:C2'	1:0:2718:C:H5''	1.98	0.93
1:0:870:G:H2'	1:0:871:G:H5''	1.48	0.93
1:0:871:G:C8	1:0:871:G:H5'	2.02	0.93
13:K:29:LEU:HB3	13:K:55:VAL:HG11	1.51	0.93
13:K:10:GLN:H	13:K:10:GLN:NE2	1.66	0.92
1:0:1474:C:H6	1:0:1474:C:H5'	1.34	0.92
1:0:541:C:H2'	1:0:542:A:H5''	1.52	0.92
32:I:132:CYS:HB3	32:I:137:VAL:HB	1.49	0.91
16:N:17:ARG:HB3	16:N:17:ARG:HH11	1.34	0.91
13:K:10:GLN:H	13:K:10:GLN:HE21	0.94	0.90
1:0:2812:A:H2	1:0:2814:A:H62	1.17	0.89
20:R:99:ALA:HB1	20:R:109:MET:HE1	1.55	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:871:G:H8	1:0:871:G:H5'	1.36	0.89
18:P:115:SER:H	18:P:118:GLN:HE21	0.93	0.89
1:0:1667:A:H8	1:0:1667:A:H5'	1.38	0.89
6:C:236:THR:HG22	6:C:239:ALA:N	1.87	0.88
2:9:3056:A:H2'	2:9:3057:A:H5''	1.54	0.88
16:N:83:LEU:HD13	16:N:175:LEU:HD23	1.56	0.88
25:W:21:LEU:HD22	25:W:26:ILE:HD11	1.53	0.88
1:0:1835:U:H5	1:0:1840:A:N7	1.72	0.88
28:Z:10:ARG:HA	38:Z:9215:HOH:O	1.74	0.88
22:T:101:LEU:HD13	22:T:112:LEU:HD11	1.54	0.87
1:0:1751:G:H2'	1:0:1752:G:H5''	1.54	0.87
1:0:2364:A:H5''	19:Q:15:LYS:HD3	1.56	0.87
6:C:1:MET:HG2	6:C:2:GLN:H	1.37	0.87
13:K:10:GLN:N	13:K:10:GLN:HE21	1.71	0.87
24:V:1:THR:HG23	24:V:2:VAL:H	1.40	0.86
1:0:1160:G:C5'	1:0:1161:A:H5'	2.04	0.86
1:0:2506:A:HO2'	1:0:2507:G:H8	0.87	0.86
5:B:264:GLU:HG2	5:B:267:LYS:HE2	1.57	0.86
6:C:5:ILE:HD11	6:C:16:VAL:HG23	1.57	0.86
6:C:127:ARG:NH2	6:C:225:PRO:HG2	1.89	0.86
5:B:307:ARG:HB2	5:B:307:ARG:HH11	1.39	0.85
4:A:35:GLY:O	4:A:36:ASP:HB3	1.76	0.85
20:R:8:ALA:HB1	20:R:13:THR:HG21	1.57	0.85
25:W:13:MET:HE2	25:W:18:GLN:HA	1.57	0.85
16:N:48:VAL:CG1	16:N:55:ASP:HB3	2.06	0.85
25:W:72:PRO:HG2	25:W:77:ALA:HB3	1.57	0.85
15:M:99:ARG:HD2	15:M:167:GLY:HA2	1.59	0.85
1:0:542:A:H5'	1:0:542:A:H8	1.41	0.85
1:0:545:G:H8	1:0:545:G:H5'	1.42	0.84
4:A:153:ARG:HH11	4:A:153:ARG:HB2	1.41	0.84
18:P:115:SER:N	18:P:118:GLN:HE21	1.75	0.84
16:N:144:GLY:O	16:N:147:ILE:HG22	1.77	0.84
25:W:4:LEU:HD22	25:W:52:VAL:HG21	1.56	0.84
1:0:2586:U:H3	1:0:2592:G:H22	1.25	0.84
15:M:166:ALA:HA	15:M:169:ARG:NH1	1.93	0.84
28:Z:46:ARG:HD2	28:Z:59:TYR:HB2	1.58	0.84
7:D:57:THR:HG23	7:D:63:ILE:HA	1.60	0.83
13:K:62:PRO:HG3	13:K:65:ARG:HH21	1.43	0.83
18:P:115:SER:H	18:P:118:GLN:NE2	1.76	0.83
26:X:30:MET:HE1	26:X:55:ASN:HA	1.58	0.83
5:B:62:ARG:HA	5:B:65:MET:HE2	1.57	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:164:THR:HG22	15:M:167:GLY:N	1.91	0.83
16:N:48:VAL:HG11	16:N:55:ASP:HB3	1.59	0.83
2:9:3006:C:H5''	16:N:37:ARG:NH1	1.94	0.83
4:A:191:GLY:HA2	4:A:194:MET:CE	2.09	0.82
15:M:102:GLU:OE1	15:M:164:THR:HG21	1.79	0.82
24:V:12:THR:HG23	24:V:14:ALA:H	1.42	0.82
25:W:137:GLN:HE21	25:W:141:HIS:HE1	1.27	0.82
11:H:56:GLN:HE21	11:H:126:ARG:HE	1.25	0.82
1:0:1159:G:H21	1:0:1189:A:H8	1.27	0.82
1:0:21:G:H5'	20:R:2:ILE:HA	1.61	0.82
1:0:2904:U:H4'	26:X:8:ARG:NH1	1.95	0.82
23:U:9:CYS:HA	23:U:52:THR:HG23	1.62	0.82
11:H:166:SER:HB2	11:H:167:PRO:CD	2.10	0.82
30:2:41:HIS:N	30:2:45:ASN:HD22	1.77	0.82
5:B:36:PRO:HA	5:B:168:GLY:HA3	1.60	0.82
1:0:282:C:H1'	1:0:368:C:N4	1.94	0.81
1:0:381:G:H5''	38:0:4610:HOH:O	1.79	0.81
4:A:192:VAL:HG12	4:A:207:GLN:HB3	1.62	0.81
1:0:2506:A:O2'	1:0:2507:G:H8	1.64	0.81
12:J:107:ASN:ND2	12:J:109:TYR:H	1.79	0.81
1:0:21:G:C5'	20:R:2:ILE:HA	2.12	0.80
25:W:88:THR:HB	38:W:6679:HOH:O	1.80	0.80
7:D:154:LYS:HD2	7:D:154:LYS:H	1.46	0.80
20:R:39:THR:HG22	20:R:42:GLU:H	1.46	0.80
5:B:217:ARG:HG3	5:B:257:THR:HG22	1.62	0.80
1:0:2533:C:H5'	1:0:2533:C:H6	1.46	0.80
1:0:506:G:H22	1:0:509:A:H5''	1.47	0.79
5:B:201:ASP:HB2	5:B:312:ARG:HD2	1.63	0.79
25:W:4:LEU:HD23	25:W:54:PHE:HB3	1.63	0.79
1:0:541:C:C2'	1:0:542:A:H5''	2.10	0.79
32:I:102:VAL:HG12	32:I:106:LYS:HE3	1.61	0.79
1:0:1160:G:H5'	1:0:1161:A:C5'	2.10	0.79
5:B:27:ASN:H	5:B:27:ASN:HD22	1.30	0.79
13:K:81:ARG:HB2	13:K:87:ARG:HH11	1.47	0.79
1:0:1165:G:H4'	1:0:1174:A:O2'	1.83	0.79
7:D:134:LEU:HD11	7:D:166:ILE:HD11	1.64	0.79
16:N:12:ARG:HD3	16:N:18:THR:OG1	1.82	0.79
25:W:38:THR:HG22	25:W:39:ASP:H	1.47	0.79
18:P:115:SER:OG	18:P:118:GLN:HG3	1.83	0.78
7:D:88:LEU:HB2	7:D:89:PRO:HD3	1.65	0.78
1:0:1450:C:H4'	1:0:1451:C:OP2	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:93:GLN:HE21	16:N:93:GLN:HA	1.47	0.78
6:C:236:THR:H	6:C:239:ALA:HB3	1.49	0.78
4:A:36:ASP:OD2	4:A:85:SER:HB2	1.84	0.77
1:O:2291:A:C8	1:O:2309:C:H5'	2.19	0.77
12:J:45:VAL:HG23	12:J:130:VAL:O	1.83	0.77
29:1:8:GLN:HE22	29:1:11:LYS:NZ	1.83	0.77
7:D:136:ARG:HD2	7:D:155:HIS:O	1.83	0.77
25:W:80:ASP:O	25:W:84:VAL:HG23	1.84	0.77
9:F:91:VAL:HG12	9:F:92:GLY:H	1.49	0.77
1:O:559:U:H5'	1:O:559:U:H6	1.49	0.77
27:Y:235:GLU:H	27:Y:235:GLU:CD	1.86	0.77
25:W:21:LEU:HD22	25:W:26:ILE:CD1	2.15	0.77
1:O:2748:G:H2'	38:O:7745:HOH:O	1.84	0.76
4:A:131:HIS:O	4:A:132:ASP:HB2	1.86	0.76
1:O:877:G:H5'	1:O:878:G:OP1	1.85	0.76
5:B:238:ASN:HD22	5:B:240:GLY:H	1.33	0.76
1:O:1244:U:OP1	12:J:18:ILE:HD13	1.85	0.76
6:C:115:LEU:HD21	6:C:243:VAL:HG13	1.64	0.76
1:O:1162:G:H1'	32:I:117:LEU:HD11	1.67	0.76
1:O:871:G:H8	1:O:871:G:C5'	1.99	0.76
1:O:870:G:C2'	1:O:871:G:H5''	2.16	0.76
7:D:135:VAL:HG22	7:D:136:ARG:H	1.51	0.76
1:O:56:G:H5''	24:V:50:ARG:HH12	1.49	0.76
21:S:57:THR:HG22	21:S:59:ASP:H	1.52	0.75
25:W:6:GLN:HB2	25:W:26:ILE:HD12	1.67	0.75
15:M:183:THR:HG22	15:M:194:ALA:HB1	1.67	0.75
7:D:28:GLY:HA2	7:D:69:ILE:HG23	1.66	0.75
25:W:88:THR:HG23	25:W:110:GLN:HE21	1.50	0.75
25:W:122:ARG:HH11	25:W:122:ARG:HG2	1.51	0.75
5:B:179:LEU:O	5:B:183:GLU:HG2	1.87	0.75
5:B:212:GLN:HB2	5:B:257:THR:HG21	1.69	0.75
6:C:139:VAL:HG13	38:C:9244:HOH:O	1.85	0.75
1:O:1641:A:H2'	1:O:1642:A:H5'	1.69	0.75
25:W:88:THR:HG22	25:W:89:ASP:H	1.49	0.75
1:O:1372:A:H3'	38:O:7407:HOH:O	1.87	0.74
1:O:2862:G:H4'	5:B:336:GLN:O	1.87	0.74
11:H:166:SER:CB	11:H:167:PRO:HD3	2.13	0.74
31:3:70:ARG:HG2	31:3:77:ALA:HB2	1.69	0.74
24:V:39:ALA:N	24:V:40:PRO:HD2	2.02	0.74
38:O:6419:HOH:O	4:A:223:ARG:HG3	1.86	0.74
25:W:68:THR:HG23	25:W:69:ARG:HG2	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:187:VAL:HG23	27:Y:192:ASP:CB	2.18	0.74
28:Z:11:SER:HB3	28:Z:23:ARG:HB2	1.68	0.74
2:9:3006:C:OP1	16:N:37:ARG:NH1	2.21	0.74
1:0:2908:A:H2'	1:0:2909:G:O4'	1.88	0.74
29:1:10:LYS:HG3	38:1:9236:HOH:O	1.87	0.74
26:X:25:ARG:HD3	26:X:64:ALA:O	1.88	0.74
23:U:14:GLU:OE1	23:U:15:PRO:HD2	1.88	0.74
1:0:2904:U:H4'	26:X:8:ARG:HH12	1.50	0.74
1:0:1116:U:HO2'	1:0:1118:A:H2	1.34	0.74
1:0:2756:U:H3	1:0:2896:A:H2	1.34	0.73
18:P:59:ARG:NH2	18:P:66:GLN:HE22	1.85	0.73
20:R:99:ALA:HB1	20:R:109:MET:CE	2.17	0.73
11:H:46:GLN:HB3	11:H:167:PRO:CD	2.15	0.73
20:R:18:LEU:HD12	20:R:143:VAL:HG11	1.68	0.73
1:0:1299:G:O6	14:L:6:ARG:HD3	1.89	0.73
9:F:91:VAL:HG12	9:F:92:GLY:N	2.03	0.73
16:N:17:ARG:NH1	16:N:17:ARG:HB3	2.03	0.73
2:9:3014:G:H5'	2:9:3014:G:H8	1.54	0.73
31:3:60:LYS:HG3	31:3:61:PRO:HD2	1.70	0.73
2:9:3029:C:H2'	2:9:3030:C:H5'	1.70	0.73
16:N:151:ASP:O	16:N:154:LEU:HB2	1.88	0.73
25:W:13:MET:HE1	25:W:17:ILE:HG22	1.71	0.73
11:H:58:ARG:HG3	11:H:58:ARG:HH11	1.53	0.73
12:J:131:THR:HG22	12:J:134:GLU:H	1.53	0.73
25:W:21:LEU:HD13	25:W:26:ILE:HD11	1.70	0.73
22:T:63:ILE:HD11	22:T:75:GLU:HB2	1.70	0.72
1:0:2716:G:H5''	5:B:206:THR:HG21	1.71	0.72
7:D:146:LYS:NZ	16:N:107:ASN:HD21	1.87	0.72
1:0:793:A:H5''	18:P:83:LYS:HG2	1.71	0.72
1:0:281:U:H2'	1:0:282:C:O4'	1.89	0.72
11:H:27:LYS:H	11:H:59:HIS:HD2	1.37	0.72
1:0:182:G:H5'	38:0:5431:HOH:O	1.90	0.72
4:A:199:HIS:HD2	4:A:201:PHE:H	1.34	0.72
14:L:133:VAL:HA	38:L:9371:HOH:O	1.88	0.72
1:0:1116:U:O2'	1:0:1118:A:H2	1.72	0.72
1:0:1119:G:N2	1:0:1246:A:C2	2.58	0.72
1:0:2270:G:H4'	4:A:223:ARG:HH12	1.54	0.72
1:0:506:G:H22	1:0:509:A:C5'	2.03	0.72
26:X:43:VAL:HG12	26:X:44:ASP:H	1.55	0.72
5:B:195:ARG:HG2	5:B:323:LEU:HD22	1.71	0.72
2:9:3039:U:H1'	2:9:3044:A:H61	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:9:ILE:HD12	11:H:54:THR:HG22	1.71	0.71
22:T:49:GLU:OE2	22:T:97:ARG:HD2	1.90	0.71
4:A:88:ILE:HD13	4:A:100:PRO:HD3	1.72	0.71
1:O:1184:C:H1'	38:O:7672:HOH:O	1.89	0.71
1:O:1701:A:H4'	1:O:1702:U:H5''	1.72	0.71
4:A:191:GLY:HA2	4:A:194:MET:HE2	1.72	0.71
8:E:81:GLU:HG2	8:E:134:SER:HB3	1.72	0.71
30:2:41:HIS:H	30:2:45:ASN:ND2	1.82	0.71
13:K:81:ARG:HD3	13:K:87:ARG:NH1	2.06	0.71
27:Y:154:ARG:NH1	27:Y:155:ARG:HG3	2.06	0.71
1:O:1116:U:H3	1:O:1246:A:H62	1.35	0.71
20:R:25:PHE:CE2	20:R:29:LYS:HE2	2.25	0.71
1:O:871:G:C8	1:O:871:G:C5'	2.74	0.71
4:A:100:PRO:HG2	4:A:103:VAL:HG21	1.73	0.71
12:J:74:ARG:CB	12:J:74:ARG:HH11	2.01	0.71
13:K:74:VAL:CG1	13:K:113:ILE:HG12	2.20	0.71
5:B:168:GLY:H	5:B:174:ARG:HD3	1.56	0.71
1:O:272:A:H5'	1:O:273:G:OP2	1.90	0.71
1:O:380:A:H2'	38:O:7446:HOH:O	1.90	0.71
1:O:188:C:H5''	15:M:163:LEU:HD21	1.73	0.70
32:I:99:ASP:OD1	32:I:138:THR:HB	1.90	0.70
16:N:113:SER:HB2	38:N:9360:HOH:O	1.89	0.70
11:H:56:GLN:NE2	11:H:126:ARG:HE	1.89	0.70
12:J:93:ARG:HH11	12:J:93:ARG:HB3	1.55	0.70
13:K:74:VAL:HG11	13:K:113:ILE:HG12	1.72	0.70
15:M:187:LEU:CD2	15:M:194:ALA:HB3	2.21	0.70
16:N:47:LEU:HD11	16:N:127:LEU:HD21	1.74	0.70
26:X:43:VAL:HG12	26:X:44:ASP:N	2.05	0.70
1:O:2533:C:C6	1:O:2533:C:H5'	2.25	0.70
4:A:191:GLY:HA2	4:A:194:MET:HE3	1.72	0.70
7:D:99:ASP:HA	38:D:5675:HOH:O	1.92	0.70
16:N:169:PRO:O	16:N:172:PHE:HB3	1.91	0.70
1:O:2054:A:N3	20:R:128:ARG:NH2	2.39	0.70
28:Z:26:VAL:O	28:Z:30:GLU:HG3	1.91	0.70
4:A:33:GLU:O	4:A:34:ASP:HB2	1.90	0.70
6:C:115:LEU:HD13	6:C:223:LEU:HD21	1.72	0.70
6:C:162:VAL:HG12	6:C:192:ILE:HD11	1.72	0.70
6:C:246:ARG:HH11	6:C:246:ARG:HB3	1.56	0.70
5:B:62:ARG:HA	5:B:65:MET:CE	2.21	0.70
26:X:72:VAL:HG22	26:X:85:VAL:HG12	1.74	0.70
1:O:1118:A:H3'	1:O:1118:A:H8	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2256:G:H2'	1:0:2257:G:H5'	1.74	0.70
1:0:450:C:OP1	6:C:184:ARG:NH2	2.25	0.70
4:A:153:ARG:NH1	4:A:153:ARG:HB2	2.07	0.70
20:R:17:MET:HE1	20:R:19:ARG:NH2	2.07	0.70
18:P:59:ARG:HH22	18:P:66:GLN:HE22	1.38	0.69
2:9:3006:C:H5''	16:N:37:ARG:HH12	1.57	0.69
27:Y:154:ARG:HH12	27:Y:155:ARG:HG3	1.55	0.69
7:D:99:ASP:HB3	7:D:103:ASN:H	1.55	0.69
22:T:32:ARG:NH1	22:T:38:ARG:HH12	1.90	0.69
18:P:103:THR:HA	18:P:106:ARG:NH1	2.06	0.69
31:3:25:VAL:HG22	31:3:68:LYS:HG3	1.73	0.69
8:E:3:VAL:HG22	8:E:49:ILE:HB	1.75	0.69
22:T:41:ARG:HH11	22:T:41:ARG:HG2	1.56	0.69
25:W:88:THR:HG23	25:W:110:GLN:HB3	1.75	0.69
13:K:29:LEU:HB3	13:K:55:VAL:CG1	2.22	0.69
1:0:1559:A:H1'	38:0:6128:HOH:O	1.93	0.69
1:0:1118:A:H3'	1:0:1118:A:C8	2.28	0.69
1:0:1667:A:C8	1:0:1667:A:H5'	2.25	0.69
5:B:258:GLY:H	5:B:260:HIS:CE1	2.11	0.69
4:A:121:ALA:O	4:A:124:VAL:HG22	1.92	0.69
1:0:474:C:O3'	6:C:73:LEU:HD21	1.93	0.69
22:T:24:ARG:HH21	22:T:39:ASN:HD22	1.41	0.69
1:0:1209:C:H2'	1:0:1210:G:H8	1.56	0.69
1:0:1603:A:H5'	1:0:1605:G:O4'	1.93	0.68
1:0:2679:G:H2'	1:0:2681:A:OP2	1.93	0.68
15:M:24:GLN:NE2	15:M:27:ARG:HH11	1.90	0.68
17:O:32:ARG:HD3	17:O:32:ARG:O	1.92	0.68
23:U:52:THR:HG22	23:U:54:THR:H	1.58	0.68
1:0:1979:G:H2'	38:0:3601:HOH:O	1.92	0.68
4:A:153:ARG:CB	4:A:153:ARG:HH11	2.05	0.68
8:E:97:VAL:HG12	38:E:4191:HOH:O	1.93	0.68
20:R:18:LEU:HB2	20:R:143:VAL:HG12	1.75	0.68
25:W:84:VAL:HG12	38:W:6679:HOH:O	1.93	0.68
1:0:2851:G:O2'	1:0:2852:A:H5'	1.92	0.68
16:N:164:ASP:CG	16:N:167:ASP:HA	2.14	0.68
5:B:18:ARG:HG3	5:B:256:GLN:HG3	1.73	0.68
5:B:320:GLN:NE2	5:B:321:PRO:HD2	2.09	0.68
38:0:3542:HOH:O	32:I:92:PRO:HD2	1.93	0.68
1:0:603:A:H5''	1:0:604:G:OP1	1.94	0.68
5:B:141:ARG:HG2	5:B:165:ARG:HA	1.76	0.68
25:W:81:ASP:OD1	25:W:92:ASP:HB2	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:151:SER:HB3	27:Y:154:ARG:HB3	1.75	0.68
1:0:2426:G:H1'	38:0:6350:HOH:O	1.92	0.67
1:0:2769:C:C2'	1:0:2770:G:H5'	2.23	0.67
4:A:192:VAL:CG1	4:A:207:GLN:HB3	2.23	0.67
4:A:200:PRO:HG2	4:A:225:VAL:HG21	1.76	0.67
9:F:63:ILE:HB	9:F:64:PRO:HD3	1.76	0.67
20:R:111:ILE:HG23	20:R:145:LEU:HD11	1.75	0.67
1:0:56:G:H5''	24:V:50:ARG:NH1	2.07	0.67
25:W:119:HIS:HD2	25:W:120:PRO:O	1.77	0.67
4:A:95:PRO:HG2	4:A:98:GLU:HG2	1.76	0.67
1:0:2840:A:OP1	5:B:211:THR:HG23	1.94	0.67
5:B:140:LEU:HA	38:B:9380:HOH:O	1.95	0.67
5:B:7:ARG:NH1	5:B:11:LEU:HD21	2.09	0.67
16:N:7:LYS:HE3	19:Q:21:ARG:O	1.95	0.67
5:B:108:GLU:HB3	5:B:111:ARG:HD2	1.75	0.67
5:B:41:PHE:HB3	5:B:190:MET:HE1	1.75	0.67
1:0:1751:G:C2'	1:0:1752:G:H5''	2.24	0.67
1:0:2827:A:H2'	1:0:2828:G:O4'	1.95	0.67
7:D:95:THR:OG1	7:D:174:VAL:HG22	1.95	0.67
1:0:1474:C:C6	1:0:1474:C:H5'	2.23	0.66
2:9:3056:A:C2'	2:9:3057:A:H5''	2.24	0.66
1:0:1441:G:H1'	38:0:7965:HOH:O	1.96	0.66
4:A:179:MET:HG2	4:A:186:TRP:CB	2.25	0.66
7:D:25:MET:HE1	7:D:41:LEU:HG	1.77	0.66
12:J:54:VAL:HG11	12:J:138:THR:HG21	1.77	0.66
6:C:140:VAL:HB	38:C:9247:HOH:O	1.95	0.66
14:L:37:LYS:HG2	38:L:9335:HOH:O	1.95	0.66
20:R:18:LEU:HD12	20:R:143:VAL:CG1	2.25	0.66
1:0:1205:U:H2'	1:0:1206:U:H5''	1.78	0.66
1:0:1377:C:H6	1:0:1377:C:H5'	1.61	0.66
13:K:62:PRO:HG3	13:K:65:ARG:NH2	2.09	0.66
28:Z:36:ASP:HB3	28:Z:45:ASP:HB3	1.77	0.66
1:0:1328:A:OP1	27:Y:169:ARG:HD2	1.95	0.66
1:0:1189:A:H1'	1:0:1209:C:O4'	1.95	0.66
3:4:176:A:O4'	3:4:175:C:H2'	1.95	0.66
14:L:79:ASP:HB3	38:L:9356:HOH:O	1.95	0.66
1:0:560:C:H42	1:0:597:A:H61	1.41	0.66
1:0:88:G:H5'	1:0:88:G:H8	1.61	0.66
21:S:57:THR:HG22	21:S:59:ASP:N	2.11	0.66
23:U:14:GLU:O	23:U:17:THR:HB	1.96	0.66
1:0:2578:G:H5'	1:0:2578:G:H8	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:164:THR:CG2	15:M:167:GLY:H	2.00	0.65
1:O:21:G:H5''	20:R:1:GLY:O	1.96	0.65
5:B:51:VAL:CG2	5:B:327:VAL:HG13	2.25	0.65
25:W:38:THR:HG22	25:W:39:ASP:N	2.12	0.65
27:Y:200:THR:HG22	27:Y:201:GLU:HG3	1.78	0.65
8:E:7:ILE:HG22	8:E:45:ASP:O	1.95	0.65
13:K:74:VAL:HG12	13:K:75:ARG:HG3	1.79	0.65
1:O:447:A:OP2	22:T:1:SER:HB2	1.96	0.65
29:1:25:LYS:HG3	30:2:49:GLU:H	1.60	0.65
8:E:22:VAL:HG12	8:E:76:VAL:HG11	1.78	0.65
32:I:101:SER:H	32:I:104:GLN:NE2	1.94	0.65
12:J:19:MET:HE2	12:J:132:LEU:HD11	1.79	0.65
1:O:2878:U:H2'	1:O:2879:A:O4'	1.95	0.65
9:F:58:GLU:HA	9:F:61:MET:HG3	1.78	0.65
17:O:32:ARG:HE	17:O:35:LYS:HD2	1.61	0.65
24:V:12:THR:HG22	24:V:15:GLU:CG	2.17	0.65
26:X:78:GLU:HG2	26:X:79:GLU:H	1.60	0.65
1:O:545:G:C8	1:O:545:G:H5'	2.30	0.65
4:A:210:GLY:HA3	38:A:9379:HOH:O	1.97	0.65
29:1:21:ARG:HD2	29:1:37:CYS:SG	2.36	0.65
5:B:275:GLY:O	5:B:291:ASP:HA	1.97	0.65
7:D:44:ILE:HG12	7:D:83:PHE:HE1	1.62	0.65
15:M:134:ILE:HG23	15:M:141:ILE:HD13	1.79	0.65
6:C:16:VAL:HG12	6:C:17:ASP:H	1.61	0.65
16:N:100:ALA:O	16:N:129:ILE:HG23	1.98	0.65
16:N:86:LEU:HD12	16:N:125:ALA:HB2	1.79	0.65
25:W:65:VAL:HA	25:W:68:THR:HG22	1.79	0.65
1:O:21:G:H4'	20:R:2:ILE:HG22	1.80	0.64
11:H:51:VAL:HG21	11:H:127:VAL:HG11	1.79	0.64
1:O:1667:A:H2'	1:O:1668:U:C6	2.32	0.64
4:A:192:VAL:HG13	38:A:9350:HOH:O	1.96	0.64
1:O:1666:C:O2'	1:O:1667:A:H5''	1.96	0.64
1:O:777:U:O2'	29:1:11:LYS:HG2	1.97	0.64
16:N:38:LYS:HE2	16:N:107:ASN:ND2	2.11	0.64
11:H:21:THR:O	11:H:120:ILE:HD12	1.98	0.64
16:N:38:LYS:HE2	16:N:107:ASN:HD21	1.63	0.64
1:O:544:G:H2'	1:O:545:G:H5''	1.78	0.64
25:W:106:THR:OG1	25:W:109:GLU:HG3	1.98	0.64
1:O:1654:U:H2'	4:A:47:HIS:HD2	1.61	0.64
8:E:15:GLN:HG3	8:E:20:ILE:HG12	1.79	0.64
8:E:69:ILE:HA	8:E:72:MET:CE	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:O:4899:HOH:O	17:O:39:THR:HB	1.97	0.64
18:P:64:GLU:HG2	38:P:169:HOH:O	1.98	0.64
4:A:190:ARG:NH2	4:A:207:GLN:OE1	2.31	0.64
4:A:57:ALA:HB1	4:A:65:ARG:HE	1.63	0.64
6:C:16:VAL:HG12	6:C:17:ASP:N	2.12	0.64
5:B:297:VAL:HB	38:B:9407:HOH:O	1.97	0.64
15:M:34:GLU:HB3	15:M:38:GLU:HG3	1.80	0.64
1:O:2073:G:H5''	38:O:4124:HOH:O	1.98	0.64
1:O:2587:OMU:H2'	1:O:2589:U:H5''	1.79	0.64
7:D:86:THR:C	7:D:89:PRO:HD2	2.17	0.64
32:I:125:ALA:O	32:I:129:VAL:HG23	1.97	0.64
1:O:2676:C:H4'	12:J:70:PHE:CE1	2.32	0.63
1:O:1189:A:H1'	1:O:1209:C:C1'	2.27	0.63
29:1:8:GLN:HE22	29:1:11:LYS:HZ2	1.44	0.63
4:A:179:MET:HA	4:A:179:MET:CE	2.28	0.63
4:A:32:VAL:HG22	4:A:38:ILE:HG13	1.80	0.63
6:C:118:THR:HG22	6:C:137:PRO:HB3	1.81	0.63
6:C:246:ARG:NH1	6:C:246:ARG:HB3	2.13	0.63
10:G:16:LYS:O	10:G:20:VAL:HG23	1.98	0.63
2:9:3051:A:H5'	16:N:160:SER:HB3	1.81	0.63
14:L:143:THR:HG22	14:L:144:ASP:N	2.11	0.63
24:V:64:GLY:O	24:V:65:ASP:HB2	1.96	0.63
2:9:3039:U:H1'	2:9:3044:A:N6	2.13	0.63
5:B:81:ALA:O	5:B:186:GLY:HA3	1.99	0.63
1:O:338:C:H4'	6:C:174:ILE:CD1	2.29	0.63
9:F:53:ASP:OD1	9:F:80:GLN:HB2	1.97	0.63
1:O:1116:U:O2'	1:O:1118:A:C2	2.51	0.63
1:O:282:C:O2'	1:O:283:U:H5'	1.98	0.63
5:B:221:GLN:HE22	13:K:42:ASN:HD22	1.45	0.63
10:G:64:ASN:N	10:G:64:ASN:HD22	1.94	0.63
11:H:27:LYS:H	11:H:59:HIS:CD2	2.16	0.63
2:9:3041:C:H4'	7:D:48:MET:HB2	1.80	0.63
12:J:52:GLN:HG3	12:J:53:ILE:N	2.13	0.63
25:W:21:LEU:HD21	25:W:48:VAL:CG1	2.29	0.63
1:O:1058:A:H2'	1:O:1060:C:H5''	1.79	0.63
30:2:40:ARG:HA	30:2:45:ASN:ND2	2.14	0.63
1:O:542:A:H5'	1:O:542:A:C8	2.29	0.62
7:D:146:LYS:NZ	16:N:107:ASN:ND2	2.46	0.62
16:N:110:THR:HB	16:N:113:SER:OG	1.98	0.62
23:U:5:GLU:HG3	23:U:10:GLY:O	1.99	0.62
25:W:21:LEU:CD2	25:W:26:ILE:HD11	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:162:MET:HE3	5:B:308:LEU:HD21	1.81	0.62
16:N:163:PHE:HZ	16:N:171:HIS:HD1	1.45	0.62
1:0:2256:G:C2'	1:0:2257:G:H5'	2.30	0.62
30:2:40:ARG:HD2	30:2:47:THR:HG22	1.80	0.62
16:N:139:TRP:HA	16:N:139:TRP:CE3	2.35	0.62
22:T:38:ARG:HG3	22:T:38:ARG:HH11	1.64	0.62
28:Z:11:SER:CB	28:Z:23:ARG:HB2	2.28	0.62
1:0:111:C:O2'	29:1:20:ARG:HG2	1.99	0.62
2:9:3054:A:O2'	2:9:3055:U:H5'	1.99	0.62
6:C:200:PRO:HB3	6:C:212:VAL:HG23	1.82	0.62
27:Y:103:THR:HG22	27:Y:104:GLU:OE2	1.98	0.62
1:0:1625:U:H4'	38:0:4948:HOH:O	1.97	0.62
9:F:2:VAL:HG22	9:F:57:GLU:OE1	2.00	0.62
27:Y:112:GLU:CD	27:Y:115:ARG:HH12	2.01	0.62
1:0:2534:C:H1'	38:0:3800:HOH:O	1.99	0.62
1:0:1206:U:H6	1:0:1206:U:H5'	1.65	0.62
1:0:1634:G:H3'	38:0:4189:HOH:O	2.00	0.62
1:0:2251:G:H2'	1:0:2252:A:C8	2.34	0.62
5:B:145:HIS:HD2	5:B:146:THR:O	1.81	0.62
12:J:130:VAL:HG12	12:J:131:THR:N	2.15	0.62
1:0:2780:C:H1'	8:E:143:GLN:HE21	1.65	0.62
1:0:299:U:H5'	38:0:7546:HOH:O	1.99	0.62
1:0:31:C:H2'	38:0:7888:HOH:O	1.99	0.62
2:9:3001:U:H5''	2:9:3003:A:OP1	2.00	0.62
21:S:11:THR:H	21:S:14:ALA:HB3	1.65	0.62
23:U:52:THR:HG22	23:U:54:THR:N	2.15	0.62
1:0:1819:G:H2'	1:0:1820:G:H4'	1.82	0.62
4:A:199:HIS:CD2	4:A:201:PHE:H	2.16	0.62
15:M:28:GLN:O	15:M:32:ARG:HG3	2.00	0.62
26:X:76:ARG:HH11	26:X:76:ARG:HG3	1.64	0.62
16:N:23:ARG:HH11	16:N:23:ARG:HG2	1.65	0.61
1:0:2256:G:H2'	1:0:2257:G:C5'	2.30	0.61
1:0:541:C:H2'	1:0:542:A:C5'	2.26	0.61
1:0:1684:A:H1'	30:2:43:ARG:HH22	1.63	0.61
6:C:129:HIS:CE1	6:C:231:ARG:HA	2.36	0.61
16:N:179:LEU:HD23	16:N:184:ILE:HD12	1.82	0.61
16:N:61:ALA:HB3	16:N:88:ALA:HB2	1.80	0.61
1:0:470:U:O2'	29:1:16:HIS:HD2	1.83	0.61
16:N:152:GLU:C	16:N:154:LEU:H	2.04	0.61
20:R:111:ILE:HG23	20:R:145:LEU:CD1	2.30	0.61
1:0:1166:A:H1'	1:0:1192:A:C2	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:84:LEU:HD23	5:B:142:LEU:HD23	1.82	0.61
7:D:25:MET:HE3	7:D:37:ALA:CB	2.22	0.61
1:0:119:A:H2'	1:0:120:A:H5''	1.81	0.61
7:D:138:GLY:N	38:D:7597:HOH:O	2.33	0.61
32:I:76:ALA:O	32:I:80:LYS:HG3	2.01	0.61
21:S:33:SER:O	21:S:37:VAL:HG23	1.99	0.61
1:0:2491:G:H1'	38:0:7098:HOH:O	1.99	0.61
2:9:3014:G:H5'	2:9:3014:G:C8	2.34	0.61
16:N:154:LEU:O	16:N:155:GLU:HB3	2.00	0.61
1:0:20:G:H21	20:R:117:HIS:HD2	1.48	0.61
27:Y:144:ARG:CZ	38:Y:9407:HOH:O	2.48	0.61
1:0:656:G:OP2	17:O:37:ARG:HD2	2.01	0.61
16:N:80:SER:HB2	38:N:9335:HOH:O	2.01	0.61
1:0:1527:A:H1'	1:0:1528:A:C8	2.35	0.61
5:B:144:THR:HB	38:B:9426:HOH:O	2.00	0.61
38:0:4951:HOH:O	5:B:300:SER:HB3	1.99	0.61
18:P:16:VAL:CG1	18:P:20:ARG:HB2	2.31	0.61
1:0:1080:C:H4'	1:0:1081:A:OP1	2.00	0.61
1:0:2649:A:H5'	1:0:2649:A:H8	1.66	0.61
1:0:969:G:H1	1:0:999:C:H42	1.49	0.61
5:B:254:GLN:HG2	5:B:255:GLY:N	2.14	0.61
8:E:81:GLU:HG2	8:E:134:SER:CB	2.30	0.61
32:I:92:PRO:C	32:I:94:GLU:H	2.02	0.61
15:M:187:LEU:HD23	15:M:194:ALA:HB3	1.81	0.61
1:0:538:C:OP2	27:Y:134:HIS:HE1	1.84	0.60
4:A:211:LYS:HB3	4:A:212:PRO:CD	2.27	0.60
22:T:9:LYS:HE3	22:T:13:ARG:HH11	1.63	0.60
1:0:1180:U:H4'	32:I:91:GLU:HG2	1.82	0.60
1:0:1182:C:H1'	1:0:1192:A:H8	1.64	0.60
1:0:1535:G:H2'	1:0:1536:C:C6	2.36	0.60
1:0:247:A:H2'	38:0:4218:HOH:O	2.01	0.60
1:0:285:A:H2'	1:0:286:U:O4'	2.00	0.60
1:0:797:A:H4'	28:Z:10:ARG:N	2.16	0.60
5:B:305:ASP:O	5:B:306:LYS:HB2	2.01	0.60
1:0:902:G:N7	14:L:18:HIS:HD2	2.00	0.60
1:0:2346:C:O5'	1:0:2346:C:H6	1.84	0.60
8:E:84:MET:HE1	8:E:148:ILE:HD12	1.81	0.60
8:E:93:MET:HE1	8:E:165:GLY:N	2.16	0.60
13:K:34:VAL:HG22	13:K:47:ALA:HB2	1.83	0.60
23:U:39:ASN:ND2	23:U:44:ARG:HH11	1.98	0.60
38:0:5117:HOH:O	12:J:47:THR:HB	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:132:ASN:O	16:N:135:VAL:HG12	2.01	0.60
18:P:80:ARG:HG2	18:P:87:ARG:CZ	2.32	0.60
1:0:157:G:H4'	15:M:95:LYS:HE3	1.84	0.60
1:0:2896:A:H5''	38:0:6357:HOH:O	2.01	0.60
9:F:50:VAL:CG1	9:F:60:VAL:HG11	2.31	0.60
11:H:9:ILE:HG23	11:H:126:ARG:CZ	2.32	0.60
1:0:1118:A:H62	1:0:1244:U:H3	1.48	0.60
1:0:1741:U:H5'	1:0:1742:A:OP1	2.01	0.60
11:H:29:ALA:HB3	11:H:66:ARG:HH12	1.67	0.60
18:P:105:LEU:HD21	18:P:137:LEU:HD21	1.84	0.60
5:B:74:ILE:HD13	5:B:309:VAL:HG21	1.84	0.60
6:C:27:ARG:HG3	6:C:29:ASP:OD1	2.02	0.60
17:O:105:ASN:HD21	17:O:109:SER:H	1.49	0.60
25:W:35:VAL:HG23	25:W:41:TYR:CD2	2.36	0.60
8:E:13:ALA:HB2	8:E:22:VAL:HG22	1.84	0.60
12:J:75:PRO:HG2	12:J:105:LEU:CD2	2.32	0.60
19:Q:26:PRO:O	19:Q:30:VAL:HG23	2.02	0.60
27:Y:144:ARG:HH11	27:Y:144:ARG:CG	2.14	0.60
5:B:168:GLY:N	5:B:174:ARG:HD3	2.16	0.60
6:C:162:VAL:HG13	6:C:232:LEU:HD21	1.83	0.60
32:I:72:VAL:HG13	32:I:73:PRO:HD2	1.84	0.60
29:1:28:HIS:CE1	29:1:31:LYS:HE2	2.37	0.60
1:0:447:A:P	22:T:1:SER:HB2	2.42	0.60
1:0:1500:U:P	18:P:41:ARG:HH22	2.24	0.59
1:0:2524:G:H21	1:0:2526:C:N4	2.00	0.59
1:0:2720:C:O2	13:K:87:ARG:NH2	2.35	0.59
4:A:39:ALA:HB3	4:A:61:GLU:OE2	2.02	0.59
5:B:103:ASP:HB2	38:B:9394:HOH:O	2.02	0.59
7:D:23:VAL:O	7:D:23:VAL:HG23	2.02	0.59
27:Y:154:ARG:HH12	27:Y:155:ARG:CG	2.14	0.59
1:0:2505:G:O2'	1:0:2506:A:H5'	2.02	0.59
2:9:3013:A:O2'	2:9:3014:G:H5''	2.03	0.59
4:A:105:VAL:HG11	4:A:154:ALA:HB1	1.83	0.59
4:A:36:ASP:HA	4:A:83:GLY:HA3	1.84	0.59
5:B:36:PRO:CA	5:B:168:GLY:HA3	2.32	0.59
38:0:7663:HOH:O	5:B:211:THR:HG21	2.01	0.59
1:0:2769:C:H2'	1:0:2770:G:H5'	1.82	0.59
30:2:22:PRO:HG2	30:2:25:VAL:HG23	1.84	0.59
30:2:40:ARG:HG3	30:2:45:ASN:HB3	1.82	0.59
20:R:119:VAL:O	20:R:119:VAL:HG12	2.00	0.59
27:Y:106:THR:HG23	27:Y:107:PRO:HD2	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1972:U:H2'	1:0:1973:A:H5'	1.83	0.59
2:9:3114:G:O6	16:N:11:ARG:HD3	2.02	0.59
1:0:2414:A:H2'	1:0:2415:A:C8	2.37	0.59
1:0:2851:G:C2'	1:0:2852:A:H5'	2.32	0.59
1:0:820:G:H5''	38:0:3356:HOH:O	2.01	0.59
1:0:558:C:C2'	1:0:559:U:H5''	2.33	0.59
6:C:236:THR:HA	38:C:9247:HOH:O	2.03	0.59
7:D:146:LYS:HZ3	16:N:107:ASN:HD21	1.50	0.59
32:I:102:VAL:CG1	32:I:106:LYS:HE3	2.30	0.59
16:N:49:THR:HG22	16:N:56:ASP:HB2	1.85	0.59
22:T:69:LYS:O	22:T:71:VAL:HG23	2.03	0.59
7:D:135:VAL:HG22	7:D:136:ARG:N	2.17	0.59
9:F:61:MET:HB3	15:M:19:GLN:OE1	2.01	0.59
28:Z:22:SER:O	28:Z:26:VAL:HG23	2.02	0.59
1:0:407:A:H2'	1:0:408:A:C8	2.38	0.59
1:0:2630:G:O6	4:A:206:ARG:NH2	2.36	0.59
2:9:3092:G:H2'	2:9:3093:A:C8	2.38	0.59
12:J:107:ASN:HD22	12:J:108:PRO:N	2.01	0.59
13:K:14:LYS:HB2	13:K:45:PRO:HG2	1.84	0.59
1:0:1187:U:O2'	1:0:1189:A:H2	1.86	0.58
1:0:2241:C:H2'	1:0:2242:U:C6	2.38	0.58
1:0:2502:C:C2'	1:0:2503:A:H5'	2.33	0.58
1:0:681:G:N3	1:0:681:G:H5'	2.18	0.58
7:D:135:VAL:HG21	7:D:139:TYR:CD1	2.38	0.58
12:J:75:PRO:HG2	12:J:105:LEU:HD21	1.83	0.58
13:K:109:LEU:HD13	13:K:113:ILE:HD11	1.85	0.58
14:L:143:THR:HG22	14:L:145:LEU:H	1.67	0.58
5:B:137:LEU:HD11	5:B:140:LEU:HD21	1.85	0.58
7:D:86:THR:O	7:D:90:LEU:HG	2.04	0.58
17:O:47:ARG:HG3	17:O:47:ARG:HH11	1.68	0.58
18:P:134:VAL:O	18:P:138:GLU:HG3	2.03	0.58
1:0:952:G:OP1	19:Q:42:LYS:HE2	2.03	0.58
25:W:21:LEU:HD21	25:W:48:VAL:HG11	1.85	0.58
26:X:80:GLU:HB3	38:X:5564:HOH:O	2.02	0.58
5:B:154:VAL:HG12	5:B:156:LYS:HG2	1.85	0.58
14:L:54:PRO:HG2	14:L:57:VAL:HG21	1.85	0.58
1:0:1594:C:OP2	18:P:120:ARG:HD2	2.02	0.58
1:0:2812:A:C2	1:0:2814:A:N6	2.69	0.58
9:F:50:VAL:HG21	9:F:63:ILE:HG21	1.85	0.58
20:R:9:ASP:O	20:R:13:THR:HB	2.02	0.58
24:V:11:MET:HB3	24:V:15:GLU:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1175:G:H1'	1:0:1193:A:H2'	1.85	0.58
1:0:449:A:N7	6:C:43:LYS:HG2	2.19	0.58
8:E:69:ILE:HA	8:E:72:MET:HE3	1.84	0.58
11:H:45:VAL:HA	11:H:167:PRO:O	2.03	0.58
11:H:56:GLN:HE21	11:H:126:ARG:NE	2.00	0.58
23:U:17:THR:HG22	23:U:18:GLY:N	2.18	0.58
27:Y:189:ASN:HA	27:Y:217:ILE:HD11	1.85	0.58
4:A:76:VAL:HG23	28:Z:63:LYS:HB3	1.85	0.58
1:0:1060:C:H6	1:0:1060:C:H5'	1.69	0.58
1:0:1835:U:C5	1:0:1840:A:N7	2.64	0.58
4:A:36:ASP:C	4:A:38:ILE:H	2.07	0.58
5:B:307:ARG:CB	5:B:307:ARG:HH11	2.12	0.58
15:M:24:GLN:HE22	15:M:27:ARG:HH11	1.52	0.58
1:0:130:C:H2'	38:O:3467:HOH:O	2.02	0.58
7:D:58:VAL:CG1	7:D:60:GLU:HG2	2.34	0.58
13:K:98:VAL:HG13	13:K:99:ASP:N	2.18	0.58
16:N:170:GLU:O	16:N:174:GLU:HG3	2.03	0.58
1:0:1593:C:OP1	18:P:117:SER:HB3	2.04	0.58
23:U:13:ILE:HG12	23:U:32:CYS:HB3	1.84	0.58
23:U:46:ALA:HB1	23:U:52:THR:HG21	1.86	0.58
27:Y:189:ASN:HD22	27:Y:189:ASN:C	2.07	0.58
1:0:280:C:H2'	1:0:281:U:O4'	2.03	0.58
17:O:14:LEU:HD23	17:O:102:ILE:HD11	1.86	0.58
13:K:32:ILE:HD11	13:K:56:SER:HB3	1.85	0.58
15:M:60:VAL:C	15:M:61:ILE:HD12	2.23	0.58
26:X:31:ILE:O	26:X:35:GLU:HG3	2.03	0.58
27:Y:98:GLN:HG3	27:Y:236:VAL:HB	1.84	0.58
5:B:314:ALA:HB3	5:B:317:PRO:HG3	1.86	0.57
12:J:107:ASN:HD21	12:J:109:TYR:HB2	1.68	0.57
12:J:19:MET:CE	12:J:132:LEU:HD11	2.34	0.57
24:V:58:THR:O	24:V:62:GLU:HG3	2.03	0.57
1:0:1342:C:C2'	1:0:1343:C:H5'	2.34	0.57
2:9:3029:C:C2'	2:9:3030:C:H5'	2.34	0.57
17:O:14:LEU:CD2	17:O:102:ILE:HD11	2.33	0.57
17:O:96:VAL:HA	38:O:4258:HOH:O	2.03	0.57
18:P:10:ALA:HA	18:P:13:VAL:HG12	1.86	0.57
27:Y:144:ARG:HH11	27:Y:144:ARG:HG3	1.69	0.57
1:0:1010:C:H4'	16:N:4:PRO:HB2	1.84	0.57
1:0:1377:C:H5'	1:0:1377:C:C6	2.39	0.57
1:0:95:A:H5''	1:0:97:G:O4'	2.03	0.57
2:9:3076:G:C3'	2:9:3077:A:H5''	2.25	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:42:GLU:HB2	38:O:2176:HOH:O	2.05	0.57
1:O:1118:A:H8	1:O:1119:G:H5''	1.70	0.57
1:O:2541:U:H5'	38:O:9721:HOH:O	2.04	0.57
1:O:1189:A:H3'	38:O:7881:HOH:O	2.03	0.57
1:O:316:A:N3	1:O:336:G:O2'	2.37	0.57
4:A:109:GLU:HG2	4:A:116:GLY:N	2.19	0.57
5:B:58:PRO:HA	5:B:63:GLU:OE1	2.05	0.57
24:V:55:ARG:O	24:V:59:ILE:HG12	2.02	0.57
1:O:558:C:H2'	1:O:559:U:C5'	2.34	0.57
6:C:1:MET:HG2	6:C:2:GLN:N	2.12	0.57
8:E:8:PRO:HB2	8:E:11:VAL:HG23	1.87	0.57
32:I:93:GLN:HA	32:I:96:PHE:CE2	2.40	0.57
1:O:2676:C:H4'	12:J:70:PHE:HE1	1.70	0.57
17:O:87:THR:O	17:O:91:GLN:HG3	2.03	0.57
21:S:33:SER:OG	21:S:36:GLU:HG3	2.05	0.57
1:O:558:C:O2'	1:O:559:U:H5''	2.05	0.57
2:9:3028:U:H5''	16:N:40:ASN:ND2	2.20	0.57
8:E:6:GLU:HA	8:E:46:THR:HG22	1.85	0.57
11:H:169:GLY:C	11:H:170:ASN:HD22	2.08	0.57
1:O:2769:C:H2'	1:O:2770:G:C5'	2.35	0.57
21:S:57:THR:CG2	21:S:58:MET:N	2.67	0.57
28:Z:42:CYS:SG	28:Z:43:GLY:N	2.78	0.57
5:B:321:PRO:HA	38:B:9461:HOH:O	2.05	0.57
25:W:4:LEU:HD22	25:W:52:VAL:CG2	2.32	0.57
1:O:1185:U:H2'	1:O:1186:C:C6	2.40	0.57
32:I:113:HIS:N	32:I:114:PRO:HD2	2.20	0.57
16:N:139:TRP:HA	16:N:139:TRP:HE3	1.68	0.57
20:R:132:ARG:HG2	20:R:133:ALA:N	2.20	0.57
5:B:329:TYR:CE2	23:U:15:PRO:HG2	2.40	0.57
1:O:1205:U:H2'	1:O:1206:U:C5'	2.35	0.56
1:O:90:A:H2'	1:O:91:G:O4'	2.04	0.56
7:D:65:GLU:HG3	38:D:6752:HOH:O	2.05	0.56
12:J:74:ARG:NH1	12:J:76:ASP:HB2	2.19	0.56
14:L:136:ALA:HB3	38:L:9371:HOH:O	2.05	0.56
24:V:39:ALA:N	24:V:40:PRO:CD	2.68	0.56
27:Y:132:ASP:OD1	27:Y:135:LYS:HD2	2.05	0.56
1:O:1352:A:H5''	1:O:1353:C:OP2	2.05	0.56
1:O:2420:G:O2'	1:O:2421:G:H5'	2.06	0.56
29:1:45:ARG:HB3	38:1:9223:HOH:O	2.05	0.56
6:C:170:ASP:O	6:C:171:GLU:HG3	2.05	0.56
6:C:5:ILE:HD11	6:C:16:VAL:CG2	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:55:VAL:HG12	13:K:56:SER:N	2.20	0.56
16:N:164:ASP:OD2	16:N:167:ASP:HA	2.05	0.56
1:0:1209:C:H2'	1:0:1210:G:C8	2.40	0.56
1:0:328:U:O4'	6:C:202:THR:HG22	2.04	0.56
6:C:47:GLY:HA2	6:C:92:PRO:HB2	1.86	0.56
8:E:5:LEU:HD21	8:E:66:GLN:HG3	1.86	0.56
10:G:12:ILE:N	10:G:13:PRO:HD3	2.20	0.56
20:R:39:THR:HG23	20:R:107:GLU:O	2.05	0.56
1:0:2502:C:H2'	1:0:2503:A:H5'	1.85	0.56
29:1:25:LYS:HD2	30:2:48:ASP:HA	1.87	0.56
7:D:25:MET:CE	7:D:41:LEU:HG	2.35	0.56
18:P:103:THR:O	18:P:107:GLU:HG3	2.05	0.56
25:W:88:THR:HG23	25:W:110:GLN:NE2	2.18	0.56
1:0:138:U:H5''	1:0:139:C:OP2	2.05	0.56
10:G:20:VAL:O	10:G:24:VAL:HG23	2.05	0.56
12:J:130:VAL:HG12	12:J:131:THR:H	1.71	0.56
1:0:1687:C:O2	29:1:9:GLY:HA2	2.06	0.56
1:0:200:U:H2'	38:0:3748:HOH:O	2.05	0.56
1:0:2468:A:H61	31:3:48:ASN:HD21	1.52	0.56
11:H:58:ARG:HG3	11:H:58:ARG:NH1	2.20	0.56
32:I:129:VAL:HG13	32:I:139:ILE:HD11	1.88	0.56
1:0:1242:A:OP2	12:J:60:ARG:NH2	2.36	0.56
1:0:1679:C:H5'	38:0:9638:HOH:O	2.06	0.56
1:0:2649:A:C8	1:0:2649:A:H5'	2.41	0.56
2:9:3020:G:O2'	2:9:3021:G:H5'	2.06	0.56
6:C:153:VAL:O	6:C:157:LEU:HG	2.06	0.56
20:R:44:VAL:O	20:R:48:GLU:HG3	2.06	0.56
1:0:1667:A:H2'	1:0:1668:U:H6	1.69	0.56
30:2:41:HIS:O	30:2:45:ASN:HB2	2.06	0.56
20:R:39:THR:HB	20:R:42:GLU:HG3	1.86	0.56
1:0:1086:A:N6	25:W:11:VAL:HG11	2.21	0.56
1:0:2320:U:H4'	1:0:2321:A:O4'	2.05	0.56
1:0:65:C:O2'	1:0:66:G:H5'	2.05	0.56
1:0:462:A:C2	30:2:37:HIS:HB3	2.41	0.56
7:D:153:THR:O	7:D:156:ARG:HB2	2.06	0.56
1:0:1163:G:H5'	32:I:115:ASP:O	2.06	0.56
16:N:37:ARG:NE	38:N:9333:HOH:O	2.35	0.56
5:B:30:PRO:HB2	5:B:39:GLN:NE2	2.21	0.56
5:B:62:ARG:HG2	5:B:65:MET:HE3	1.88	0.56
14:L:93:VAL:HG21	14:L:122:ALA:HB2	1.88	0.56
21:S:43:GLU:HB3	38:S:7106:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:122:ARG:HH21	25:W:154:ARG:HD2	1.70	0.56
1:0:1834:C:H2'	1:0:1840:A:N6	2.20	0.56
8:E:126:ILE:HB	8:E:131:LEU:HD23	1.88	0.56
1:0:1053:G:OP1	11:H:12:PRO:HG3	2.05	0.55
1:0:2690:U:O2'	8:E:111:LYS:HE3	2.06	0.55
1:0:2909:G:H2'	1:0:2910:A:H8	1.70	0.55
1:0:317:A:H5''	22:T:52:ARG:HD2	1.88	0.55
4:A:192:VAL:HB	38:A:9388:HOH:O	2.06	0.55
38:0:7252:HOH:O	4:A:211:LYS:HG2	2.05	0.55
4:A:88:ILE:HG22	4:A:88:ILE:O	2.06	0.55
8:E:84:MET:HE1	8:E:148:ILE:CD1	2.36	0.55
1:0:1167:G:H4'	32:I:135:LEU:HD22	1.88	0.55
1:0:2795:C:O2'	1:0:2796:U:H5'	2.05	0.55
32:I:138:THR:HG22	32:I:139:ILE:N	2.22	0.55
38:0:5492:HOH:O	13:K:39:GLY:HA2	2.06	0.55
16:N:34:LEU:HA	16:N:47:LEU:HD23	1.86	0.55
25:W:26:ILE:O	25:W:26:ILE:HG13	2.06	0.55
26:X:9:VAL:HG22	26:X:88:GLU:OE2	2.05	0.55
1:0:1213:C:O2'	1:0:1214:G:H5'	2.07	0.55
1:0:1441:G:O2'	1:0:1442:A:H5'	2.06	0.55
31:3:17:HIS:O	31:3:18:GLN:HG3	2.07	0.55
8:E:45:ASP:OD2	8:E:46:THR:HG23	2.06	0.55
20:R:18:LEU:HB2	20:R:143:VAL:CG1	2.36	0.55
31:3:62:THR:HG23	31:3:86:GLY:HA2	1.88	0.55
4:A:105:VAL:CG1	4:A:154:ALA:HB1	2.37	0.55
11:H:3:ALA:HA	11:H:58:ARG:NH1	2.21	0.55
14:L:90:ARG:NH2	14:L:121:ILE:HD11	2.21	0.55
19:Q:11:ARG:HD3	38:Q:5620:HOH:O	2.05	0.55
1:0:2812:A:H2	1:0:2814:A:N6	1.97	0.55
5:B:214:PRO:HD2	38:B:9320:HOH:O	2.06	0.55
5:B:57:GLU:O	5:B:63:GLU:HB2	2.06	0.55
14:L:133:VAL:HB	38:L:9355:HOH:O	2.07	0.55
38:0:4281:HOH:O	22:T:82:THR:HA	2.05	0.55
1:0:1189:A:H1'	1:0:1209:C:H1'	1.87	0.55
1:0:2533:C:H6	1:0:2533:C:C5'	2.18	0.55
1:0:503:G:H2'	1:0:504:G:H8	1.72	0.55
8:E:11:VAL:HG12	8:E:12:ASP:N	2.22	0.55
8:E:81:GLU:O	8:E:172:PRO:HD3	2.07	0.55
25:W:5:VAL:HG22	25:W:32:CYS:HB2	1.87	0.55
1:0:1342:C:O2'	1:0:1343:C:H5'	2.05	0.55
1:0:1506:U:H6	1:0:1506:U:H5'	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2526:C:O2'	1:0:2527:U:H5'	2.07	0.55
1:0:2896:A:OP1	26:X:15:ARG:NH1	2.40	0.55
1:0:820:G:H3'	38:0:3356:HOH:O	2.05	0.55
6:C:25:PRO:HG2	38:C:9123:HOH:O	2.06	0.55
22:T:9:LYS:CE	22:T:13:ARG:NH1	2.62	0.55
1:0:2241:C:H2'	1:0:2242:U:H6	1.70	0.55
1:0:2824:C:H5''	1:0:2825:C:H5'	1.88	0.55
6:C:218:VAL:HG12	38:C:9220:HOH:O	2.04	0.55
32:I:93:GLN:HA	32:I:96:PHE:HE2	1.72	0.55
25:W:88:THR:HG22	25:W:89:ASP:N	2.21	0.55
38:0:6533:HOH:O	27:Y:158:LYS:HD3	2.06	0.55
1:0:2909:G:H2'	1:0:2910:A:C8	2.42	0.55
18:P:131:PHE:CD1	18:P:137:LEU:HD13	2.42	0.55
1:0:316:A:H5'	22:T:54:ASP:OD2	2.06	0.55
1:0:558:C:H2'	1:0:559:U:H5'	1.89	0.55
1:0:816:G:H5'	1:0:1598:A:H4'	1.89	0.55
1:0:2694:A:H4'	8:E:91:PHE:CE1	2.41	0.55
25:W:1:MET:N	25:W:37:GLU:HG3	2.22	0.55
1:0:159:G:OP1	15:M:74:LYS:HE3	2.07	0.54
1:0:1778:A:H2'	1:0:1779:A:H5'	1.89	0.54
1:0:2781:U:H2'	1:0:2782:G:H5'	1.88	0.54
11:H:170:ASN:HD22	11:H:170:ASN:N	2.04	0.54
17:O:106:PRO:HG2	17:O:107:GLU:OE1	2.07	0.54
1:0:2890:A:H1'	23:U:56:ARG:NH2	2.22	0.54
25:W:52:VAL:HG22	25:W:53:ALA:H	1.72	0.54
25:W:82:GLU:O	25:W:86:GLU:HG3	2.07	0.54
30:2:22:PRO:HG2	30:2:25:VAL:CG2	2.37	0.54
5:B:36:PRO:HA	5:B:168:GLY:CA	2.33	0.54
11:H:99:LYS:HD3	11:H:119:LYS:HD3	1.90	0.54
2:9:3006:C:C5'	16:N:37:ARG:NH1	2.69	0.54
4:A:97:ALA:HB2	4:A:150:PRO:HB2	1.90	0.54
1:0:1120:U:H5'	1:0:1121:G:OP2	2.07	0.54
1:0:2506:A:O2'	1:0:2507:G:O5'	2.26	0.54
25:W:13:MET:HE2	25:W:18:GLN:CA	2.34	0.54
1:0:544:G:C2'	1:0:545:G:H5''	2.37	0.54
1:0:969:G:H1	1:0:999:C:N4	2.05	0.54
8:E:95:VAL:O	8:E:126:ILE:HD12	2.08	0.54
15:M:57:LYS:HE2	15:M:140:ALA:O	2.07	0.54
16:N:43:VAL:HG13	16:N:118:ILE:HD11	1.89	0.54
16:N:44:ARG:HG3	16:N:45:ALA:N	2.22	0.54
1:0:10:U:O4	1:0:532:A:OP2	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1202:A:H2'	1:0:1203:G:H5'	1.88	0.54
1:0:2248:C:H3'	38:0:5709:HOH:O	2.07	0.54
7:D:51:ARG:HD3	38:D:7636:HOH:O	2.07	0.54
9:F:21:GLU:O	9:F:24:ARG:HG2	2.08	0.54
1:0:2504:A:H4'	11:H:71:ARG:HH11	1.72	0.54
24:V:39:ALA:O	24:V:41:GLU:N	2.36	0.54
5:B:71:VAL:HG11	5:B:296:LEU:HB3	1.89	0.54
6:C:35:VAL:HG21	6:C:227:GLY:HA2	1.90	0.54
8:E:77:THR:OG1	8:E:78:GLU:N	2.40	0.54
1:0:2081:A:H4'	12:J:69:TYR:CE1	2.43	0.54
26:X:78:GLU:HG2	26:X:79:GLU:N	2.22	0.54
8:E:132:THR:O	8:E:132:THR:HG23	2.08	0.54
1:0:2721:U:H4'	13:K:87:ARG:HG3	1.90	0.54
9:F:38:LYS:NZ	15:M:3:SER:HA	2.22	0.54
25:W:139:GLY:O	25:W:141:HIS:HD2	1.90	0.54
1:0:1596:U:H2'	1:0:1598:A:OP2	2.08	0.54
1:0:2755:G:H1'	38:0:4963:HOH:O	2.08	0.54
31:3:62:THR:HB	38:3:9351:HOH:O	2.08	0.54
13:K:62:PRO:CG	13:K:65:ARG:HH21	2.17	0.54
18:P:141:ILE:C	18:P:143:ALA:H	2.12	0.54
22:T:35:TYR:CG	22:T:112:LEU:HD22	2.43	0.54
1:0:1666:C:H2'	1:0:1667:A:H5'	1.89	0.54
1:0:2064:U:H5'	1:0:2652:U:O3'	2.08	0.54
1:0:396:U:O2'	1:0:418:C:H4'	2.08	0.54
7:D:50:VAL:O	7:D:71:ALA:HA	2.08	0.54
21:S:77:VAL:O	21:S:80:ARG:HG2	2.07	0.54
25:W:137:GLN:NE2	25:W:141:HIS:HE1	2.02	0.54
25:W:13:MET:CE	25:W:17:ILE:HG22	2.38	0.54
1:0:2385:G:H2'	1:0:2386:U:C6	2.43	0.53
1:0:1787:C:H4'	1:0:2883:A:O4'	2.08	0.53
2:9:3069:U:OP1	16:N:4:PRO:HG3	2.08	0.53
32:I:116:LEU:HD22	32:I:127:GLU:OE1	2.09	0.53
26:X:37:LEU:CD1	26:X:85:VAL:HG21	2.25	0.53
27:Y:112:GLU:OE2	27:Y:115:ARG:NH1	2.36	0.53
1:0:625:U:H5''	1:0:1044:C:N4	2.22	0.53
1:0:1351:G:OP1	6:C:96:LYS:NZ	2.38	0.53
1:0:2443:C:O3'	14:L:56:LYS:HE3	2.08	0.53
2:9:3064:C:H2'	2:9:3065:A:H5'	1.90	0.53
1:0:1943:C:H4'	4:A:211:LYS:O	2.08	0.53
38:0:4905:HOH:O	4:A:6:GLY:HA3	2.08	0.53
5:B:112:THR:OG1	5:B:158:LYS:HG2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:50:VAL:HG13	9:F:60:VAL:HG11	1.90	0.53
25:W:5:VAL:HG11	25:W:153:MET:HE3	1.90	0.53
1:O:1418:U:OP1	30:2:42:TRP:HB3	2.08	0.53
1:O:960:G:N3	1:O:960:G:H2'	2.23	0.53
6:C:233:THR:HG22	6:C:234:VAL:N	2.24	0.53
8:E:84:MET:HG2	8:E:168:ILE:HD13	1.90	0.53
15:M:122:GLN:OE1	15:M:127:LYS:HE2	2.09	0.53
16:N:73:ALA:HB1	16:N:74:PRO:CD	2.39	0.53
24:V:1:THR:HG23	24:V:2:VAL:N	2.17	0.53
1:O:1166:A:H61	1:O:1180:U:H3	1.56	0.53
1:O:2241:C:O2'	1:O:2242:U:H5'	2.09	0.53
1:O:2768:A:H2'	1:O:2769:C:O4'	2.07	0.53
1:O:380:A:OP2	15:M:9:ARG:HD2	2.09	0.53
31:3:73:GLU:HB3	38:3:9363:HOH:O	2.07	0.53
5:B:280:VAL:HG13	5:B:334:SER:HA	1.89	0.53
17:O:73:ASP:HA	17:O:92:VAL:O	2.07	0.53
1:O:396:U:OP2	31:3:38:ARG:HD2	2.07	0.53
1:O:818:A:O2'	28:Z:13:ARG:HD3	2.08	0.53
4:A:32:VAL:HG12	4:A:34:ASP:H	1.72	0.53
4:A:36:ASP:O	4:A:38:ILE:N	2.40	0.53
5:B:175:LEU:C	5:B:175:LEU:HD23	2.28	0.53
12:J:47:THR:HG22	12:J:48:GLY:H	1.74	0.53
13:K:125:ALA:C	13:K:127:ALA:H	2.12	0.53
15:M:134:ILE:CG2	15:M:141:ILE:HD13	2.39	0.53
38:O:5796:HOH:O	15:M:58:GLN:HG3	2.08	0.53
18:P:143:ALA:HA	38:P:190:HOH:O	2.08	0.53
1:O:121:U:OP2	30:2:10:ARG:NH2	2.28	0.53
2:9:3044:A:O4'	7:D:76:ARG:NE	2.41	0.53
4:A:81:GLN:HB2	4:A:92:ASN:ND2	2.23	0.53
18:P:20:ARG:NH1	18:P:54:LYS:HD3	2.23	0.53
1:O:2265:U:H2'	1:O:2266:A:C8	2.44	0.53
9:F:48:VAL:HG23	9:F:74:PHE:CB	2.39	0.53
10:G:67:LEU:O	10:G:71:LEU:HG	2.08	0.53
26:X:71:ARG:HB3	26:X:88:GLU:OE1	2.09	0.53
1:O:1766:U:O2	1:O:1778:A:H5'	2.09	0.53
1:O:588:G:O6	25:W:154:ARG:NH1	2.42	0.53
5:B:175:LEU:O	5:B:175:LEU:HD23	2.07	0.53
5:B:248:ARG:O	5:B:251:VAL:HG13	2.08	0.53
9:F:96:ALA:HA	38:F:3111:HOH:O	2.08	0.53
25:W:149:LEU:HG	25:W:153:MET:HE2	1.90	0.53
1:O:790:A:H2'	1:O:791:A:O4'	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:132:ASP:OD1	4:A:133:ARG:N	2.42	0.53
7:D:25:MET:CE	7:D:37:ALA:HB1	2.23	0.53
20:R:34:GLU:HG2	20:R:46:TYR:OH	2.09	0.53
23:U:9:CYS:CA	23:U:52:THR:HG23	2.36	0.53
1:0:1299:G:N7	14:L:6:ARG:NH1	2.56	0.53
1:0:1477:C:H5'	1:0:1868:G:C5'	2.39	0.53
1:0:1847:A:OP1	4:A:175:LYS:HG3	2.08	0.53
1:0:2073:G:OP2	1:0:2490:A:H5'	2.09	0.53
1:0:644:G:N3	1:0:644:G:H5'	2.23	0.53
3:4:74:DCZ:C2'	3:4:75:DC:H5'	2.38	0.53
7:D:167:GLU:OE2	7:D:173:GLU:HG2	2.09	0.53
7:D:27:ILE:HD11	7:D:37:ALA:HB2	1.90	0.53
8:E:13:ALA:CB	8:E:22:VAL:HG22	2.39	0.53
32:I:131:THR:HG22	32:I:131:THR:O	2.09	0.53
22:T:50:VAL:HG12	22:T:56:ALA:HA	1.91	0.53
1:0:1406:A:H4'	1:0:1407:A:H5''	1.90	0.52
1:0:185:G:O3'	1:0:186:A:H4'	2.09	0.52
1:0:244:C:OP2	9:F:38:LYS:HE3	2.09	0.52
16:N:62:HIS:HB3	16:N:65:ASP:OD1	2.09	0.52
25:W:108:ARG:HE	25:W:114:PRO:CG	2.23	0.52
1:0:797:A:C4'	28:Z:10:ARG:N	2.71	0.52
1:0:1477:C:H5'	1:0:1868:G:H5'	1.90	0.52
1:0:1741:U:O2'	1:0:2723:G:H4'	2.09	0.52
1:0:2423:C:H5''	38:0:7262:HOH:O	2.08	0.52
22:T:38:ARG:HG3	22:T:38:ARG:NH1	2.24	0.52
24:V:42:ASN:HB3	38:V:7247:HOH:O	2.09	0.52
1:0:2781:U:C2'	1:0:2782:G:H5'	2.40	0.52
7:D:170:TYR:O	7:D:171:ASP:HB3	2.10	0.52
32:I:139:ILE:C	32:I:140:GLU:HG3	2.28	0.52
27:Y:133:HIS:HD2	38:Y:9379:HOH:O	1.93	0.52
1:0:1632:A:H2'	1:0:1633:C:H5'	1.91	0.52
1:0:468:U:H3'	38:0:7773:HOH:O	2.10	0.52
5:B:87:TYR:CE2	5:B:96:PRO:HG3	2.44	0.52
9:F:19:ALA:O	9:F:22:VAL:HG22	2.09	0.52
32:I:72:VAL:CG1	32:I:73:PRO:HD2	2.40	0.52
14:L:114:VAL:HG11	38:L:9371:HOH:O	2.08	0.52
16:N:179:LEU:HD23	16:N:184:ILE:CD1	2.39	0.52
25:W:88:THR:CG2	25:W:110:GLN:NE2	2.73	0.52
1:0:1130:U:H2'	1:0:1131:G:O4'	2.09	0.52
1:0:2072:G:C6	1:0:2533:C:H1'	2.45	0.52
1:0:2769:C:O2'	1:0:2770:G:H5'	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:74:VAL:HG13	13:K:113:ILE:HG23	1.92	0.52
2:9:3051:A:H5'	16:N:160:SER:CB	2.39	0.52
17:O:77:ALA:HB1	17:O:98:LEU:HD12	1.89	0.52
27:Y:99:ALA:HB2	27:Y:233:TYR:CZ	2.44	0.52
4:A:94:LEU:HG	4:A:99:ILE:HD11	1.92	0.52
5:B:190:MET:HE2	5:B:194:PHE:CD1	2.44	0.52
5:B:71:VAL:HG11	5:B:296:LEU:HD22	1.92	0.52
7:D:85:GLN:O	7:D:86:THR:HG23	2.09	0.52
8:E:137:ASP:O	8:E:141:VAL:HG23	2.09	0.52
21:S:56:ASN:O	30:2:8:LYS:NZ	2.35	0.52
29:1:8:GLN:HE22	29:1:11:LYS:HZ1	1.57	0.52
31:3:14:CYS:HB3	31:3:16:GLU:HG2	1.90	0.52
4:A:1:GLY:HA2	4:A:197:VAL:HG23	1.91	0.52
5:B:177:HIS:O	5:B:181:ILE:HG13	2.09	0.52
6:C:140:VAL:HG12	6:C:141:SER:N	2.24	0.52
32:I:75:THR:N	32:I:112:LYS:HZ1	2.08	0.52
12:J:45:VAL:HG22	12:J:46:ILE:N	2.24	0.52
14:L:21:ARG:N	38:L:9329:HOH:O	2.43	0.52
16:N:72:GLU:HG2	16:N:72:GLU:O	2.10	0.52
23:U:17:THR:CG2	23:U:18:GLY:N	2.72	0.52
24:V:39:ALA:C	24:V:41:GLU:H	2.13	0.52
25:W:4:LEU:O	25:W:32:CYS:HA	2.10	0.52
27:Y:155:ARG:NH1	38:Y:9358:HOH:O	2.42	0.52
1:0:958:G:H2'	1:0:959:C:C6	2.45	0.52
5:B:320:GLN:HE21	5:B:321:PRO:HD2	1.75	0.52
14:L:53:ARG:NH2	14:L:57:VAL:HG12	2.25	0.52
7:D:146:LYS:HZ1	16:N:107:ASN:HD21	1.58	0.52
24:V:64:GLY:O	24:V:65:ASP:CB	2.57	0.52
1:0:1669:A:H2'	1:0:1670:G:C8	2.45	0.52
1:0:1701:A:H5'	38:0:6532:HOH:O	2.10	0.52
30:2:39:ARG:HG2	38:2:3143:HOH:O	2.09	0.52
7:D:163:VAL:HA	38:D:6326:HOH:O	2.10	0.52
7:D:67:ASP:O	7:D:69:ILE:HG13	2.10	0.52
8:E:107:PHE:CE2	8:E:108:LEU:HD13	2.44	0.52
18:P:105:LEU:CD2	18:P:137:LEU:HD21	2.39	0.52
1:0:1234:U:N3	5:B:244:PRO:HB3	2.25	0.52
1:0:447:A:OP1	22:T:2:LYS:HG2	2.10	0.52
1:0:447:A:O2'	1:0:448:G:H5'	2.10	0.52
4:A:86:ALA:HB3	4:A:94:LEU:HD13	1.92	0.52
5:B:148:PRO:HB2	5:B:156:LYS:O	2.10	0.52
7:D:88:LEU:C	7:D:90:LEU:H	2.13	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:113:ASP:O	9:F:117:GLU:HG3	2.10	0.52
12:J:26:VAL:HG13	12:J:36:VAL:HG11	1.92	0.52
24:V:16:ARG:NH2	24:V:63:GLU:HG3	2.25	0.52
1:0:2769:C:H2'	1:0:2770:G:O4'	2.10	0.51
31:3:3:MET:O	31:3:90:PHE:HA	2.09	0.51
12:J:74:ARG:O	12:J:78:ILE:HG12	2.11	0.51
1:0:2054:A:H2	20:R:128:ARG:HH22	1.51	0.51
1:0:524:A:H5''	20:R:29:LYS:HD3	1.93	0.51
1:0:848:C:H5'	38:0:7491:HOH:O	2.09	0.51
3:4:74:DCZ:H2'1	3:4:75:DC:O4'	2.10	0.51
4:A:76:VAL:CG2	28:Z:63:LYS:HB3	2.40	0.51
5:B:217:ARG:CG	5:B:257:THR:HG22	2.37	0.51
5:B:52:VAL:C	5:B:53:LEU:HD12	2.30	0.51
16:N:47:LEU:HD12	16:N:92:ALA:HB1	1.92	0.51
21:S:81:ILE:HG12	38:S:4527:HOH:O	2.10	0.51
22:T:48:VAL:HG23	22:T:98:VAL:HA	1.93	0.51
1:0:2252:A:C6	1:0:2253:G:H1'	2.45	0.51
26:X:43:VAL:HG12	26:X:47:ALA:HB3	1.91	0.51
1:0:2717:C:O2'	1:0:2718:C:H5''	2.11	0.51
2:9:3049:G:O2'	2:9:3050:G:H5'	2.10	0.51
6:C:129:HIS:HE1	6:C:231:ARG:HA	1.76	0.51
16:N:78:MET:HB2	16:N:79:PRO:HD3	1.92	0.51
16:N:32:PRO:HD2	16:N:99:GLU:O	2.10	0.51
26:X:12:ILE:HD12	26:X:36:HIS:ND1	2.26	0.51
26:X:30:MET:CE	26:X:55:ASN:HA	2.37	0.51
26:X:78:GLU:CG	26:X:79:GLU:H	2.23	0.51
1:0:1375:A:H2'	1:0:1376:G:H5'	1.93	0.51
1:0:2597:U:H2'	1:0:2598:U:H5'	1.93	0.51
1:0:669:G:O2'	1:0:670:G:H5'	2.10	0.51
8:E:95:VAL:HG22	8:E:104:ILE:HG12	1.92	0.51
8:E:126:ILE:HB	8:E:131:LEU:CD2	2.41	0.51
12:J:108:PRO:HG2	12:J:109:TYR:CD1	2.45	0.51
17:O:26:TRP:HA	17:O:26:TRP:CE3	2.46	0.51
22:T:41:ARG:NH1	22:T:41:ARG:HG2	2.25	0.51
1:0:1641:A:C2'	1:0:1642:A:H5'	2.39	0.51
1:0:512:G:O3'	1:0:513:A:H8	1.94	0.51
5:B:108:GLU:HA	5:B:110:ASP:OD1	2.11	0.51
5:B:265:LEU:HD21	5:B:316:ARG:HD3	1.92	0.51
11:H:170:ASN:N	11:H:170:ASN:ND2	2.59	0.51
32:I:134:SER:O	32:I:135:LEU:HD23	2.11	0.51
16:N:149:GLU:O	16:N:152:GLU:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:126:ASP:HB3	25:W:135:GLY:O	2.10	0.51
1:0:1119:G:H22	1:0:1246:A:H2	1.50	0.51
1:0:1787:C:H2'	1:0:1788:U:H6	1.75	0.51
1:0:474:C:O3'	6:C:73:LEU:CD2	2.59	0.51
1:0:553:G:OP2	27:Y:204:ARG:NH2	2.37	0.51
2:9:3039:U:HO2'	2:9:3042:C:H5	1.55	0.51
2:9:3057:A:C8	7:D:141:VAL:HG21	2.46	0.51
5:B:42:ALA:HB1	5:B:308:LEU:HD11	1.92	0.51
32:I:131:THR:O	32:I:135:LEU:HG	2.10	0.51
12:J:51:GLU:O	12:J:55:GLU:HG3	2.10	0.51
1:0:1559:A:OP2	1:0:1559:A:H8	1.94	0.51
1:0:517:U:H1'	38:0:7782:HOH:O	2.10	0.51
4:A:43:VAL:HG21	4:A:59:GLU:HG3	1.93	0.51
1:0:2338:G:OP1	7:D:97:GLN:HG2	2.10	0.51
9:F:79:GLN:HG3	9:F:82:ASP:OD2	2.11	0.51
11:H:167:PRO:O	11:H:168:ALA:HB2	2.11	0.51
23:U:6:CYS:C	23:U:8:TYR:H	2.14	0.51
26:X:43:VAL:CG1	26:X:47:ALA:HB3	2.40	0.51
1:0:1123:A:C6	1:0:1238:C:H5'	2.46	0.51
1:0:834:G:H4'	1:0:835:U:OP2	2.11	0.51
1:0:920:C:H4'	1:0:921:G:C2	2.45	0.51
4:A:179:MET:HA	4:A:179:MET:HE3	1.93	0.51
5:B:150:ALA:O	5:B:152:PRO:HD3	2.10	0.51
8:E:166:VAL:HG12	38:E:3134:HOH:O	2.10	0.51
13:K:118:ALA:HA	13:K:125:ALA:HB2	1.93	0.51
16:N:11:ARG:HG3	16:N:14:ARG:NH1	2.26	0.51
20:R:33:ARG:NH1	38:R:9345:HOH:O	2.44	0.51
24:V:4:HIS:HB3	38:V:6622:HOH:O	2.10	0.51
25:W:46:ALA:O	25:W:49:ASN:HB2	2.10	0.51
1:0:289:G:H22	1:0:363:A:H2	1.57	0.51
4:A:212:PRO:HB2	38:A:9353:HOH:O	2.10	0.51
1:0:2591:C:OP1	5:B:1:PRO:HG3	2.11	0.51
6:C:79:ARG:O	6:C:87:ARG:HG2	2.10	0.51
7:D:84:LEU:C	7:D:86:THR:H	2.13	0.51
8:E:131:LEU:HD12	8:E:166:VAL:HG11	1.92	0.51
38:0:7104:HOH:O	15:M:178:LYS:HB2	2.09	0.51
19:Q:77:ASP:HB3	19:Q:82:LYS:HE3	1.91	0.51
1:0:1086:A:C6	25:W:11:VAL:HG11	2.45	0.51
1:0:1123:A:C2	1:0:1129:C:H4'	2.46	0.50
1:0:1236:A:H2'	1:0:1237:U:O4'	2.12	0.50
1:0:1289:C:H3'	38:0:6650:HOH:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:37:VAL:HG22	38:A:9391:HOH:O	2.11	0.50
1:0:1181:A:H5'	32:I:94:GLU:OE2	2.10	0.50
12:J:93:ARG:NH1	12:J:93:ARG:HB3	2.23	0.50
19:Q:32:GLU:O	19:Q:93:ARG:NH2	2.44	0.50
21:S:6:LYS:O	21:S:7:HIS:HB3	2.11	0.50
1:0:1044:C:H3'	1:0:1045:G:H5''	1.93	0.50
1:0:1940:C:H4'	38:0:7555:HOH:O	2.11	0.50
1:0:2717:C:H2'	1:0:2718:C:C5'	2.29	0.50
4:A:88:ILE:HD13	4:A:100:PRO:CD	2.38	0.50
22:T:73:HIS:CD2	22:T:88:PRO:HG3	2.46	0.50
1:0:702:G:O2'	1:0:703:G:H5'	2.11	0.50
29:1:28:HIS:CD2	29:1:30:LYS:HB2	2.46	0.50
2:9:3002:U:OP2	2:9:3003:A:H5'	2.12	0.50
4:A:131:HIS:O	4:A:132:ASP:CB	2.59	0.50
6:C:236:THR:HG21	38:C:9171:HOH:O	2.11	0.50
8:E:137:ASP:OD1	8:E:139:GLU:HB2	2.11	0.50
9:F:91:VAL:CG1	9:F:92:GLY:H	2.21	0.50
11:H:28:ILE:HG23	38:H:9179:HOH:O	2.11	0.50
14:L:73:VAL:HG11	14:L:118:LEU:HD21	1.93	0.50
26:X:74:ALA:HB2	26:X:85:VAL:HG13	1.92	0.50
1:0:1132:A:N6	1:0:1229:C:H2'	2.27	0.50
1:0:1423:C:O2'	1:0:1424:A:H5'	2.11	0.50
1:0:343:C:O2'	1:0:344:C:H5'	2.11	0.50
7:D:64:ARG:NE	7:D:67:ASP:HB3	2.27	0.50
9:F:37:THR:O	9:F:41:GLU:HG3	2.10	0.50
11:H:148:GLU:HA	11:H:148:GLU:OE1	2.12	0.50
15:M:164:THR:HG23	15:M:165:GLY:N	2.25	0.50
18:P:134:VAL:O	18:P:137:LEU:HB3	2.11	0.50
25:W:141:HIS:HB2	25:W:146:ILE:HG12	1.93	0.50
8:E:84:MET:HE3	8:E:148:ILE:HG21	1.94	0.50
14:L:143:THR:CG2	14:L:144:ASP:N	2.74	0.50
38:9:7568:HOH:O	16:N:107:ASN:HB3	2.11	0.50
18:P:120:ARG:NH2	18:P:123:TYR:CD2	2.79	0.50
25:W:21:LEU:CD1	25:W:26:ILE:HD11	2.40	0.50
27:Y:107:PRO:HB3	27:Y:182:PHE:CD2	2.47	0.50
1:0:441:A:H1'	1:0:442:A:N7	2.27	0.50
29:1:28:HIS:O	29:1:32:LYS:N	2.44	0.50
30:2:40:ARG:CD	30:2:47:THR:HG22	2.42	0.50
1:0:2898:G:H4'	5:B:288:GLY:HA2	1.94	0.50
5:B:7:ARG:HG2	5:B:7:ARG:HH11	1.77	0.50
8:E:101:GLU:HB2	8:E:116:THR:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:46:LEU:HG	38:M:9416:HOH:O	2.10	0.50
1:0:2668:G:H2'	1:0:2669:U:C6	2.47	0.50
1:0:920:C:H5'	1:0:921:G:C4	2.46	0.50
38:0:3205:HOH:O	12:J:46:ILE:HA	2.12	0.50
16:N:143:ARG:HA	16:N:172:PHE:CD2	2.47	0.50
16:N:47:LEU:HD13	16:N:97:VAL:HG11	1.93	0.50
21:S:57:THR:HG22	21:S:58:MET:N	2.26	0.50
24:V:38:GLY:C	24:V:40:PRO:HD2	2.32	0.50
27:Y:235:GLU:CD	27:Y:235:GLU:N	2.62	0.50
1:0:1201:C:H5''	38:0:6487:HOH:O	2.12	0.50
1:0:1375:A:C2'	1:0:1376:G:H5'	2.41	0.50
2:9:3049:G:H2'	2:9:3050:G:O4'	2.12	0.50
5:B:279:THR:OG1	5:B:290:VAL:HB	2.12	0.50
1:0:475:G:C5'	6:C:73:LEU:HD23	2.42	0.50
10:G:64:ASN:N	10:G:64:ASN:ND2	2.59	0.50
11:H:83:TYR:C	11:H:83:TYR:CD1	2.85	0.50
16:N:143:ARG:NH1	16:N:173:ASP:OD1	2.45	0.50
27:Y:187:VAL:CG2	27:Y:192:ASP:HB2	2.28	0.50
1:0:2064:U:H4'	1:0:2653:A:OP1	2.11	0.50
5:B:132:HIS:HB2	5:B:137:LEU:HD22	1.94	0.50
7:D:146:LYS:HZ3	16:N:107:ASN:ND2	2.07	0.50
20:R:27:HIS:O	20:R:31:ILE:HG13	2.12	0.50
22:T:71:VAL:HG11	22:T:90:PRO:CB	2.25	0.50
25:W:63:GLU:HG2	25:W:93:ILE:HG22	1.93	0.50
9:F:46:GLU:OE2	9:F:100:ASP:HA	2.12	0.49
9:F:58:GLU:OE1	15:M:27:ARG:NH2	2.33	0.49
30:2:5:LYS:O	30:2:9:LYS:HG3	2.12	0.49
4:A:36:ASP:HB2	4:A:85:SER:H	1.77	0.49
5:B:294:TYR:HE2	38:B:9454:HOH:O	1.95	0.49
5:B:66:GLU:OE1	5:B:328:ARG:HD2	2.12	0.49
7:D:54:ALA:HB2	7:D:69:ILE:HD12	1.93	0.49
7:D:94:ALA:HB3	7:D:97:GLN:HG3	1.94	0.49
8:E:119:HIS:O	8:E:140:ALA:HB1	2.12	0.49
1:0:2036:C:O4'	13:K:44:LEU:HG	2.12	0.49
26:X:43:VAL:HG22	26:X:76:ARG:NH1	2.27	0.49
1:0:1014:A:H2'	1:0:1015:C:H5'	1.93	0.49
1:0:2710:U:H1'	38:0:7824:HOH:O	2.12	0.49
2:9:3023:U:O2'	2:9:3024:U:H4'	2.12	0.49
6:C:61:PHE:HB3	38:C:9242:HOH:O	2.13	0.49
7:D:23:VAL:HG21	7:D:45:THR:HG21	1.94	0.49
1:0:2521:A:OP2	11:H:3:ALA:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:67:ARG:HB2	14:L:112:GLY:HA3	1.94	0.49
18:P:13:VAL:HG21	18:P:41:ARG:HG2	1.94	0.49
19:Q:16:ASN:HB2	38:Q:6597:HOH:O	2.11	0.49
19:Q:32:GLU:HA	19:Q:71:TYR:OH	2.12	0.49
25:W:5:VAL:HG11	25:W:153:MET:CE	2.41	0.49
1:O:1503:U:H2'	1:O:1504:A:O4'	2.12	0.49
30:2:40:ARG:HH11	30:2:40:ARG:HG2	1.77	0.49
4:A:179:MET:HG2	4:A:186:TRP:CG	2.47	0.49
4:A:94:LEU:N	4:A:94:LEU:HD23	2.27	0.49
6:C:133:ARG:NE	6:C:138:VAL:HG22	2.27	0.49
8:E:24:GLY:HA3	8:E:76:VAL:HB	1.94	0.49
38:O:3592:HOH:O	13:K:9:THR:HA	2.11	0.49
16:N:34:LEU:HD22	16:N:129:ILE:HD13	1.94	0.49
27:Y:106:THR:CG2	27:Y:107:PRO:HD2	2.43	0.49
27:Y:234:VAL:HG12	27:Y:235:GLU:N	2.27	0.49
14:L:73:VAL:HG23	14:L:74:THR:N	2.28	0.49
16:N:47:LEU:CD1	16:N:97:VAL:HG11	2.42	0.49
26:X:9:VAL:HG13	26:X:88:GLU:OE1	2.12	0.49
27:Y:184:GLU:OE1	27:Y:204:ARG:NH1	2.45	0.49
27:Y:200:THR:HG22	27:Y:201:GLU:CG	2.42	0.49
1:O:1462:C:H2'	1:O:1463:A:C8	2.48	0.49
1:O:1787:C:OP1	18:P:68:LYS:HE2	2.13	0.49
1:O:1820:G:C6	1:O:2030:A:C2	3.00	0.49
1:O:2392:C:H4'	38:Q:2875:HOH:O	2.13	0.49
1:O:263:U:O4'	9:F:59:ILE:HD13	2.12	0.49
7:D:154:LYS:H	7:D:154:LYS:CD	2.19	0.49
9:F:101:ALA:HA	38:F:5413:HOH:O	2.13	0.49
9:F:16:ALA:HA	9:F:111:ILE:HD13	1.94	0.49
11:H:63:GLU:HA	38:H:9179:HOH:O	2.12	0.49
14:L:35:ARG:HD3	14:L:35:ARG:C	2.33	0.49
22:T:49:GLU:HB3	22:T:59:GLU:HG2	1.95	0.49
26:X:71:ARG:HD3	38:X:2171:HOH:O	2.12	0.49
1:O:1733:A:H4'	5:B:212:GLN:HA	1.94	0.49
1:O:256:C:H2'	1:O:257:G:O4'	2.12	0.49
1:O:705:C:H2'	1:O:705:C:O2	2.13	0.49
31:3:55:VAL:HB	31:3:56:PRO:HD2	1.94	0.49
1:O:1845:A:O3'	4:A:187:PRO:HB2	2.12	0.49
32:I:118:SER:HB2	32:I:123:ASN:HB2	1.94	0.49
1:O:661:G:C5	1:O:686:A:C2	3.01	0.49
5:B:221:GLN:HE22	13:K:42:ASN:ND2	2.10	0.49
5:B:82:VAL:HG12	5:B:82:VAL:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:48:VAL:HG22	22:T:97:ARG:O	2.13	0.49
25:W:26:ILE:HG22	38:W:5420:HOH:O	2.12	0.49
1:0:1202:A:H2'	1:0:1203:G:C5'	2.43	0.49
1:0:2894:C:O2'	1:0:2895:C:H5'	2.12	0.49
29:1:28:HIS:HD2	29:1:30:LYS:H	1.60	0.49
2:9:3064:C:C2'	2:9:3065:A:H5'	2.42	0.49
38:0:9532:HOH:O	4:A:11:ARG:HD3	2.12	0.49
4:A:220:PRO:HD2	4:A:223:ARG:HD3	1.95	0.49
6:C:7:ASP:OD2	6:C:9:ASP:HB2	2.12	0.49
2:9:3057:A:O2'	7:D:152:PRO:HD2	2.13	0.49
1:0:2694:A:H4'	8:E:91:PHE:HE1	1.78	0.49
25:W:139:GLY:O	25:W:141:HIS:CD2	2.66	0.49
27:Y:178:HIS:CG	27:Y:179:PRO:HD2	2.48	0.49
1:0:1118:A:C3'	1:0:1118:A:C8	2.91	0.49
1:0:2252:A:C5	1:0:2253:G:H1'	2.47	0.49
1:0:585:C:H5''	38:0:5151:HOH:O	2.13	0.49
38:0:5676:HOH:O	4:A:164:ARG:CZ	2.60	0.49
5:B:314:ALA:CB	5:B:317:PRO:HG3	2.43	0.49
13:K:81:ARG:HB2	13:K:87:ARG:NH1	2.24	0.49
1:0:1878:G:H1'	38:0:6378:HOH:O	2.11	0.48
9:F:107:ASP:O	9:F:111:ILE:HG13	2.12	0.48
9:F:111:ILE:O	9:F:115:VAL:HG23	2.13	0.48
15:M:78:LYS:HD3	38:M:9434:HOH:O	2.13	0.48
17:O:113:VAL:O	17:O:114:ILE:HD13	2.13	0.48
17:O:26:TRP:HA	17:O:26:TRP:HE3	1.76	0.48
22:T:71:VAL:HG12	22:T:72:ILE:N	2.27	0.48
25:W:22:GLU:HG2	25:W:27:HIS:CD2	2.48	0.48
1:0:1427:A:H61	1:0:1440:U:C1'	2.25	0.48
1:0:1701:A:H4'	1:0:1702:U:C5'	2.42	0.48
1:0:221:G:H2'	1:0:222:A:C8	2.48	0.48
4:A:215:ILE:HG13	4:A:216:SER:N	2.28	0.48
4:A:32:VAL:HG12	4:A:34:ASP:N	2.27	0.48
8:E:9:GLU:HG3	8:E:10:ASP:N	2.28	0.48
32:I:75:THR:OG1	32:I:112:LYS:NZ	2.45	0.48
14:L:104:ASP:O	14:L:105:TYR:HB3	2.12	0.48
1:0:926:A:H5'	14:L:39:GLU:OE2	2.13	0.48
15:M:166:ALA:HA	15:M:169:ARG:HH12	1.73	0.48
17:O:77:ALA:HA	17:O:96:VAL:O	2.13	0.48
1:0:1135:G:H5'	38:0:6188:HOH:O	2.12	0.48
1:0:1904:A:H2'	1:0:1905:U:O4'	2.13	0.48
1:0:2762:C:H3'	38:0:3673:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:282:C:H1'	1:0:368:C:H42	1.74	0.48
1:0:74:A:H2'	1:0:75:U:C6	2.48	0.48
1:0:800:G:H4'	38:0:7283:HOH:O	2.13	0.48
1:0:941:G:C5	1:0:942:U:C4	3.01	0.48
8:E:15:GLN:HG2	8:E:19:ASP:O	2.13	0.48
11:H:28:ILE:HA	11:H:63:GLU:OE1	2.12	0.48
20:R:39:THR:HB	20:R:42:GLU:CG	2.43	0.48
21:S:23:LYS:HE2	38:S:3430:HOH:O	2.12	0.48
22:T:41:ARG:NH1	22:T:42:VAL:O	2.46	0.48
25:W:21:LEU:HB3	25:W:26:ILE:CG1	2.43	0.48
1:0:1165:G:H1'	1:0:1174:A:H1'	1.96	0.48
1:0:1352:A:N1	6:C:48:SER:HB3	2.27	0.48
1:0:2730:G:O2'	1:0:2731:G:H5'	2.13	0.48
29:1:28:HIS:CD2	29:1:31:LYS:HG3	2.48	0.48
8:E:2:ARG:HH21	8:E:48:VAL:HG21	1.77	0.48
9:F:14:ASP:O	9:F:18:GLU:HG3	2.13	0.48
32:I:75:THR:CA	32:I:112:LYS:HZ1	2.27	0.48
32:I:96:PHE:HA	32:I:136:GLY:CA	2.44	0.48
19:Q:14:LEU:HD21	19:Q:43:ILE:HD12	1.95	0.48
24:V:56:ILE:O	24:V:60:GLN:HG3	2.14	0.48
1:0:1717:A:H5''	18:P:54:LYS:HB2	1.96	0.48
1:0:2356:A:H2'	1:0:2357:G:O4'	2.13	0.48
1:0:536:A:H3'	38:0:5327:HOH:O	2.12	0.48
1:0:602:A:O2'	1:0:605:C:H4'	2.13	0.48
5:B:254:GLN:NE2	38:B:9390:HOH:O	2.46	0.48
8:E:154:ILE:HD11	8:E:157:LYS:HB2	1.94	0.48
8:E:15:GLN:NE2	8:E:40:VAL:O	2.46	0.48
12:J:74:ARG:HH12	12:J:76:ASP:HB2	1.79	0.48
22:T:75:GLU:O	22:T:76:ASP:HB2	2.12	0.48
26:X:30:MET:CE	26:X:58:ALA:HB3	2.44	0.48
28:Z:60:CYS:O	28:Z:61:ASP:HB2	2.13	0.48
1:0:1666:C:H2'	1:0:1667:A:C5'	2.44	0.48
1:0:827:A:H2'	1:0:828:G:O4'	2.14	0.48
5:B:84:LEU:HD23	5:B:142:LEU:CD2	2.42	0.48
1:0:1363:G:OP1	6:C:76:ARG:NH2	2.45	0.48
8:E:69:ILE:HA	8:E:72:MET:HE2	1.95	0.48
11:H:88:ARG:NH1	11:H:135:THR:OG1	2.40	0.48
12:J:133:GLY:O	12:J:137:GLU:HG3	2.14	0.48
14:L:54:PRO:HG2	14:L:57:VAL:CG2	2.42	0.48
1:0:317:A:OP1	22:T:52:ARG:O	2.30	0.48
1:0:1201:C:H2'	1:0:1202:A:H5'	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1829:A:H2'	1:0:1830:C:H5'	1.96	0.48
4:A:105:VAL:HG12	4:A:106:CYS:N	2.28	0.48
5:B:75:GLU:C	5:B:77:PRO:HD3	2.34	0.48
7:D:27:ILE:HD11	7:D:37:ALA:CB	2.44	0.48
8:E:31:ARG:HH12	8:E:68:HIS:CG	2.32	0.48
11:H:154:TYR:CD1	11:H:154:TYR:C	2.87	0.48
32:I:87:THR:HG22	32:I:88:GLY:N	2.28	0.48
32:I:96:PHE:HD2	32:I:136:GLY:HA2	1.79	0.48
21:S:37:VAL:O	21:S:41:VAL:HG23	2.13	0.48
27:Y:144:ARG:CG	27:Y:144:ARG:NH1	2.76	0.48
1:0:1785:G:OP1	18:P:76:GLY:HA3	2.13	0.48
6:C:138:VAL:O	6:C:234:VAL:HA	2.13	0.48
9:F:48:VAL:CG2	9:F:74:PHE:HB3	2.43	0.48
17:O:38:ARG:NH1	38:O:7674:HOH:O	2.47	0.48
19:Q:3:SER:HB3	38:Q:5998:HOH:O	2.13	0.48
1:0:1087:G:H4'	1:0:1088:A:OP1	2.14	0.48
1:0:1029:U:O2'	1:0:1273:C:OP1	2.27	0.48
1:0:1333:U:H2'	1:0:1334:C:C6	2.49	0.48
1:0:1544:U:H2'	1:0:1545:C:H6	1.79	0.48
1:0:1790:C:H2'	1:0:1791:U:H6	1.79	0.48
1:0:1380:U:O4	1:0:2043:U:H4'	2.13	0.48
1:0:2685:C:H1'	38:0:3745:HOH:O	2.13	0.48
1:0:2718:C:H6	1:0:2718:C:H5'	1.78	0.48
6:C:136:VAL:HG22	6:C:137:PRO:HA	1.95	0.48
12:J:39:VAL:HG12	12:J:40:ASN:ND2	2.29	0.48
14:L:6:ARG:NH2	38:L:9347:HOH:O	2.45	0.48
14:L:80:ASP:HB2	14:L:90:ARG:O	2.14	0.48
26:X:49:ARG:HG3	26:X:49:ARG:O	2.09	0.48
1:0:1130:U:H5'	38:0:7873:HOH:O	2.13	0.48
1:0:1300:G:H1'	38:0:4964:HOH:O	2.14	0.48
1:0:2613:G:O2'	1:0:2614:C:H5'	2.14	0.48
7:D:10:PHE:CD1	7:D:11:HIS:N	2.82	0.48
24:V:49:LEU:O	24:V:53:ILE:HG13	2.14	0.48
38:0:6937:HOH:O	27:Y:165:GLU:HB3	2.13	0.48
1:0:1202:A:C2'	1:0:1203:G:H5'	2.43	0.47
1:0:170:U:H2'	1:0:171:C:H5'	1.95	0.47
1:0:2255:A:O2'	1:0:2256:G:H5'	2.14	0.47
1:0:2256:G:O2'	1:0:2257:G:H5'	2.14	0.47
8:E:100:ASP:HB2	38:E:2789:HOH:O	2.13	0.47
1:0:1681:G:H5''	1:0:1682:A:H5'	1.95	0.47
1:0:378:A:OP1	15:M:9:ARG:NH2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3039:U:H3'	2:9:3040:C:H5''	1.96	0.47
6:C:118:THR:CG2	6:C:137:PRO:HB3	2.44	0.47
6:C:236:THR:CG2	6:C:239:ALA:H	2.12	0.47
9:F:91:VAL:CG1	9:F:92:GLY:N	2.74	0.47
12:J:135:ILE:O	12:J:139:LEU:HG	2.13	0.47
25:W:4:LEU:HD11	25:W:45:VAL:HG12	1.96	0.47
1:0:2361:A:H2'	1:0:2362:A:C8	2.49	0.47
5:B:195:ARG:CZ	5:B:323:LEU:HD13	2.44	0.47
5:B:310:ARG:HD2	38:B:9452:HOH:O	2.14	0.47
1:0:1097:A:H5''	25:W:125:HIS:NE2	2.30	0.47
1:0:1180:U:H2'	1:0:1181:A:C8	2.49	0.47
1:0:2782:G:O6	1:0:2790:C:H5''	2.14	0.47
1:0:415:A:O2'	1:0:416:G:H5'	2.15	0.47
4:A:105:VAL:HG11	4:A:154:ALA:CB	2.44	0.47
5:B:128:ILE:O	5:B:131:ALA:HB3	2.14	0.47
6:C:37:ALA:O	6:C:41:ASN:ND2	2.48	0.47
12:J:46:ILE:O	12:J:46:ILE:HG12	2.13	0.47
14:L:125:PHE:CE1	14:L:140:VAL:HG13	2.49	0.47
18:P:83:LYS:O	18:P:86:ALA:HB3	2.13	0.47
19:Q:18:PRO:O	19:Q:21:ARG:HB2	2.15	0.47
1:0:1919:A:H4'	38:0:5131:HOH:O	2.13	0.47
1:0:2403:C:H3'	38:0:5482:HOH:O	2.15	0.47
1:0:2507:G:H2'	1:0:2510:C:H42	1.78	0.47
1:0:2541:U:H4'	1:0:2542:C:OP1	2.13	0.47
1:0:821:U:H2'	1:0:822:C:H6	1.79	0.47
38:0:9672:HOH:O	29:1:1:THR:HA	2.13	0.47
6:C:2:GLN:HB3	38:C:9181:HOH:O	2.14	0.47
8:E:116:THR:HG22	8:E:151:LEU:HD22	1.96	0.47
16:N:27:LEU:HD22	16:N:50:LEU:HD13	1.96	0.47
16:N:73:ALA:HB1	16:N:74:PRO:HD2	1.97	0.47
1:0:1878:G:O2'	1:0:1879:U:P	2.72	0.47
1:0:2897:C:H2'	1:0:2898:G:H8	1.79	0.47
6:C:234:VAL:HG22	6:C:234:VAL:O	2.14	0.47
7:D:173:GLU:HG3	7:D:174:VAL:N	2.30	0.47
7:D:39:ASP:HB2	38:D:5583:HOH:O	2.15	0.47
9:F:101:ALA:HB3	9:F:105:ASP:OD1	2.15	0.47
16:N:22:GLN:HG2	16:N:26:LEU:HD22	1.97	0.47
16:N:37:ARG:NH2	38:N:9333:HOH:O	2.47	0.47
18:P:10:ALA:O	18:P:13:VAL:HG12	2.14	0.47
20:R:39:THR:HB	20:R:42:GLU:CD	2.35	0.47
21:S:39:ASP:HB3	21:S:43:GLU:OE2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1406:A:H4'	1:0:1407:A:C5'	2.44	0.47
1:0:1654:U:H2'	4:A:47:HIS:CD2	2.46	0.47
1:0:37:A:H2'	1:0:38:G:C8	2.49	0.47
13:K:34:VAL:CG2	13:K:47:ALA:HB2	2.45	0.47
28:Z:25:ARG:O	28:Z:29:ILE:HG13	2.15	0.47
1:0:1666:C:C2'	1:0:1667:A:H5''	2.45	0.47
1:0:177:A:H2'	1:0:178:U:O4'	2.14	0.47
1:0:587:A:H5''	38:0:7501:HOH:O	2.15	0.47
3:4:74:DCZ:H2'1	3:4:75:DC:H5'	1.96	0.47
5:B:162:MET:CE	5:B:308:LEU:HD21	2.44	0.47
8:E:79:GLY:HA3	38:E:7046:HOH:O	2.15	0.47
8:E:86:VAL:CG1	8:E:129:GLU:HA	2.44	0.47
32:I:113:HIS:NE2	32:I:121:LEU:HD22	2.29	0.47
15:M:61:ILE:N	15:M:61:ILE:HD12	2.29	0.47
16:N:164:ASP:OD1	16:N:167:ASP:HA	2.15	0.47
1:0:1495:C:H2'	1:0:1496:G:C8	2.50	0.47
1:0:475:G:OP1	6:C:73:LEU:HD22	2.15	0.47
1:0:660:A:H4'	1:0:661:G:O5'	2.15	0.47
5:B:16:ARG:NH1	38:B:9418:HOH:O	2.47	0.47
5:B:238:ASN:HD22	5:B:240:GLY:N	2.07	0.47
19:Q:66:LYS:HB2	19:Q:70:ALA:O	2.15	0.47
24:V:42:ASN:O	24:V:44:GLY:N	2.48	0.47
1:0:12:U:H2'	1:0:13:G:H5'	1.96	0.47
1:0:1972:U:H2'	1:0:1973:A:C5'	2.45	0.47
6:C:55:ARG:NH2	29:1:56:GLU:OE2	2.39	0.47
31:3:57:GLY:HA2	38:3:9327:HOH:O	2.15	0.47
2:9:3055:U:H4'	2:9:3056:A:C8	2.50	0.47
5:B:277:GLU:N	5:B:278:PRO:HD2	2.29	0.47
38:0:5785:HOH:O	5:B:298:LYS:HD3	2.14	0.47
9:F:13:GLU:OE2	9:F:78:GLU:HG2	2.14	0.47
12:J:75:PRO:HD3	12:J:136:SER:OG	2.15	0.47
12:J:22:VAL:O	12:J:26:VAL:HG23	2.15	0.47
1:0:1183:C:N4	1:0:1184:C:H41	2.13	0.47
1:0:2361:A:H5''	38:0:9323:HOH:O	2.15	0.47
1:0:2428:G:N7	31:3:60:LYS:NZ	2.63	0.47
2:9:3055:U:H4'	2:9:3056:A:H8	1.79	0.47
9:F:38:LYS:HZ3	15:M:3:SER:HA	1.80	0.47
18:P:103:THR:HB	38:P:180:HOH:O	2.15	0.47
20:R:18:LEU:HG	20:R:91:LEU:HD13	1.96	0.47
1:0:1118:A:C8	1:0:1119:G:H5''	2.49	0.46
1:0:2011:A:H4'	1:0:2012:U:O5'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:558:C:C2'	1:0:559:U:C5'	2.92	0.46
2:9:3048:C:H4'	16:N:141:ARG:HH21	1.79	0.46
5:B:258:GLY:H	5:B:260:HIS:HE1	1.56	0.46
5:B:25:ARG:HA	5:B:310:ARG:HH21	1.80	0.46
6:C:130:GLU:HA	6:C:130:GLU:OE1	2.15	0.46
6:C:185:LYS:HD3	6:C:186:TYR:CE1	2.50	0.46
7:D:35:ALA:N	38:D:5576:HOH:O	2.47	0.46
8:E:73:PHE:O	8:E:76:VAL:HG22	2.14	0.46
9:F:26:THR:HG21	9:F:103:GLU:HG3	1.97	0.46
32:I:138:THR:HG22	32:I:139:ILE:H	1.79	0.46
16:N:34:LEU:HD13	16:N:47:LEU:HD21	1.97	0.46
18:P:59:ARG:HH22	18:P:66:GLN:NE2	2.09	0.46
25:W:11:VAL:O	25:W:12:ASN:HB2	2.14	0.46
1:0:553:G:P	27:Y:204:ARG:HH22	2.38	0.46
1:0:1172:G:H1'	38:0:5254:HOH:O	2.15	0.46
1:0:1427:A:H61	1:0:1440:U:H1'	1.80	0.46
1:0:485:A:N3	1:0:487:G:H5''	2.30	0.46
31:3:18:GLN:OE1	31:3:73:GLU:HB3	2.15	0.46
4:A:35:GLY:O	4:A:36:ASP:CB	2.56	0.46
1:0:2846:C:H4'	5:B:156:LYS:HB3	1.98	0.46
1:0:2548:C:OP2	5:B:5:ARG:NH2	2.48	0.46
12:J:39:VAL:HG13	12:J:106:GLY:O	2.15	0.46
15:M:59:GLY:HA3	15:M:141:ILE:CD1	2.46	0.46
16:N:69:TYR:CE2	16:N:184:ILE:HD11	2.50	0.46
18:P:13:VAL:HG13	18:P:14:LEU:N	2.31	0.46
25:W:130:HIS:O	25:W:136:GLY:HA3	2.14	0.46
26:X:15:ARG:HB3	26:X:15:ARG:HH11	1.80	0.46
1:0:2694:A:H5''	8:E:90:HIS:CE1	2.51	0.46
1:0:2748:G:H1'	38:0:8206:HOH:O	2.14	0.46
31:3:3:MET:HG3	31:3:4:PRO:HD2	1.97	0.46
2:9:3050:G:H2'	2:9:3051:A:C8	2.50	0.46
8:E:114:ARG:HB3	8:E:151:LEU:HD11	1.97	0.46
8:E:87:PHE:O	8:E:93:MET:HE3	2.15	0.46
32:I:106:LYS:O	32:I:110:GLU:HG3	2.15	0.46
38:0:3949:HOH:O	17:O:3:THR:HG21	2.15	0.46
25:W:108:ARG:HE	25:W:114:PRO:HG2	1.80	0.46
1:0:2301:A:H5''	1:0:2302:A:H5'	1.98	0.46
1:0:2866:U:H4'	1:0:2867:G:H5'	1.97	0.46
1:0:29:C:O2'	1:0:30:U:H5'	2.16	0.46
1:0:424:C:H2'	1:0:425:U:C6	2.50	0.46
1:0:776:A:OP1	29:1:28:HIS:HE1	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:242:GLU:HG3	38:C:9178:HOH:O	2.15	0.46
10:G:64:ASN:O	10:G:68:GLU:HG3	2.16	0.46
11:H:9:ILE:HG12	11:H:56:GLN:CG	2.46	0.46
32:I:75:THR:HA	32:I:112:LYS:HZ1	1.79	0.46
38:O:9868:HOH:O	25:W:119:HIS:HE1	1.97	0.46
1:O:1385:G:O3'	26:X:49:ARG:NH1	2.48	0.46
28:Z:81:ARG:O	28:Z:82:SER:C	2.53	0.46
1:O:1119:G:H8	12:J:52:GLN:NE2	2.13	0.46
1:O:236:A:H4'	1:O:237:G:H5'	1.97	0.46
1:O:2487:C:H5	38:O:5168:HOH:O	1.98	0.46
1:O:775:G:OP1	29:1:16:HIS:HE1	1.99	0.46
6:C:200:PRO:HB3	6:C:212:VAL:CG2	2.45	0.46
9:F:39:SER:HB3	9:F:45:ALA:HB2	1.98	0.46
1:O:2708:G:N2	13:K:1:MET:O	2.47	0.46
16:N:110:THR:HB	16:N:113:SER:HG	1.79	0.46
17:O:21:SER:HB3	17:O:107:GLU:HA	1.96	0.46
23:U:9:CYS:HA	23:U:52:THR:CG2	2.39	0.46
25:W:149:LEU:HG	25:W:153:MET:CE	2.46	0.46
1:O:1278:A:H4'	1:O:1279:U:C4	2.50	0.46
1:O:2064:U:H5'	1:O:2652:U:H4'	1.98	0.46
1:O:482:G:H4'	1:O:508:A:N1	2.31	0.46
14:L:145:LEU:O	14:L:148:GLU:HG3	2.15	0.46
18:P:40:VAL:O	18:P:44:VAL:HG23	2.15	0.46
20:R:113:HIS:O	20:R:145:LEU:HD12	2.15	0.46
21:S:8:PRO:HD2	24:V:32:ALA:HA	1.98	0.46
24:V:1:THR:O	24:V:4:HIS:CE1	2.69	0.46
24:V:57:LYS:HA	24:V:60:GLN:HE21	1.81	0.46
1:O:1205:U:C2'	1:O:1206:U:H5''	2.45	0.46
1:O:1427:A:N6	1:O:1440:U:H1'	2.31	0.46
1:O:2269:C:C2'	1:O:2270:G:H5'	2.46	0.46
1:O:2324:G:H4'	1:O:2418:G:O2'	2.15	0.46
1:O:2415:A:N3	16:N:26:LEU:HD13	2.31	0.46
1:O:558:C:H2'	1:O:559:U:H5''	1.97	0.46
1:O:87:C:H2'	30:2:28:LYS:O	2.16	0.46
5:B:154:VAL:CG1	5:B:156:LYS:HG2	2.45	0.46
5:B:145:HIS:HA	5:B:160:ASP:O	2.15	0.46
6:C:142:ASP:OD1	6:C:236:THR:HG23	2.16	0.46
11:H:154:TYR:HD1	11:H:154:TYR:C	2.18	0.46
13:K:22:ASP:HB2	38:K:5264:HOH:O	2.14	0.46
1:O:1086:A:OP1	25:W:9:GLY:N	2.43	0.46
1:O:1236:A:C8	12:J:63:ILE:HD11	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2445:U:H2'	1:0:2446:G:C8	2.51	0.46
1:0:2670:G:O2'	1:0:2671:U:H5'	2.16	0.46
15:M:64:ARG:HD2	38:M:9383:HOH:O	2.15	0.46
16:N:154:LEU:C	16:N:156:GLU:H	2.19	0.46
1:0:21:G:H5''	20:R:2:ILE:HA	1.96	0.46
28:Z:39:CYS:HA	28:Z:47:VAL:HG21	1.97	0.46
1:0:1878:G:O2'	1:0:1879:U:C6	2.67	0.46
1:0:2832:C:H5	38:0:7432:HOH:O	1.98	0.46
1:0:88:G:H2'	1:0:89:G:C8	2.51	0.46
36:0:9303:CL:CL	30:2:2:LYS:HE3	2.52	0.46
29:1:25:LYS:HD2	30:2:49:GLU:N	2.30	0.46
4:A:123:GLY:HA3	4:A:162:GLY:HA2	1.98	0.46
4:A:165:THR:O	4:A:165:THR:HG22	2.15	0.46
6:C:162:VAL:CG1	6:C:192:ILE:HD11	2.44	0.46
9:F:48:VAL:HG23	9:F:74:PHE:HB2	1.97	0.46
9:F:57:GLU:HB2	15:M:23:LEU:HD11	1.97	0.46
12:J:52:GLN:HG3	12:J:53:ILE:H	1.80	0.46
1:0:1613:C:H2'	1:0:1614:G:O4'	2.15	0.46
1:0:960:G:N3	1:0:960:G:C2'	2.79	0.46
30:2:40:ARG:HG3	30:2:45:ASN:CB	2.44	0.46
7:D:140:ARG:O	7:D:144:ARG:HG2	2.16	0.46
9:F:33:THR:HG21	9:F:59:ILE:O	2.16	0.46
12:J:107:ASN:HD22	12:J:107:ASN:C	2.16	0.46
1:0:793:A:C5'	18:P:83:LYS:HG2	2.41	0.46
1:0:2365:G:H4'	19:Q:45:PRO:O	2.16	0.46
20:R:119:VAL:O	20:R:119:VAL:CG1	2.63	0.46
22:T:35:TYR:CD2	22:T:112:LEU:HD22	2.51	0.46
25:W:21:LEU:HD21	25:W:48:VAL:HG13	1.98	0.46
1:0:2472:C:O2'	1:0:2634:G:H4'	2.16	0.45
32:I:96:PHE:HA	32:I:136:GLY:HA3	1.97	0.45
15:M:72:ALA:HB2	15:M:93:ARG:HG2	1.98	0.45
20:R:17:MET:CE	20:R:19:ARG:CZ	2.94	0.45
38:0:4054:HOH:O	22:T:9:LYS:HD3	2.16	0.45
25:W:65:VAL:HA	25:W:68:THR:CG2	2.45	0.45
1:0:289:G:N2	1:0:363:A:H2	2.15	0.45
4:A:36:ASP:C	4:A:38:ILE:N	2.69	0.45
7:D:166:ILE:HB	38:D:6326:HOH:O	2.15	0.45
7:D:81:GLU:C	7:D:83:PHE:H	2.20	0.45
8:E:102:VAL:HG11	8:E:148:ILE:HG12	1.98	0.45
32:I:102:VAL:O	32:I:106:LYS:HG3	2.17	0.45
13:K:75:ARG:CZ	38:K:4172:HOH:O	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:69:LYS:HG2	15:M:127:LYS:HG3	1.98	0.45
16:N:34:LEU:HD22	16:N:129:ILE:CD1	2.45	0.45
26:X:43:VAL:CG1	26:X:44:ASP:H	2.24	0.45
1:0:1120:U:H5''	1:0:1120:U:C6	2.51	0.45
1:0:1168:C:H4'	38:I:5128:HOH:O	2.15	0.45
1:0:2372:A:H2'	1:0:2373:U:C6	2.52	0.45
1:0:500:G:H21	20:R:98:ASN:HD21	1.62	0.45
5:B:97:LEU:HD21	38:B:9444:HOH:O	2.17	0.45
1:0:894:A:C2	6:C:87:ARG:NH2	2.84	0.45
8:E:154:ILE:HD11	8:E:157:LYS:HE2	1.97	0.45
20:R:17:MET:HE1	20:R:19:ARG:CZ	2.47	0.45
21:S:52:VAL:C	21:S:53:ASN:HD22	2.20	0.45
22:T:32:ARG:CZ	22:T:38:ARG:NH1	2.80	0.45
1:0:1309:U:O2'	1:0:1310:U:H5'	2.15	0.45
1:0:156:C:H5''	15:M:171:ARG:CD	2.24	0.45
1:0:2300:A:H4'	1:0:2301:A:O5'	2.16	0.45
5:B:202:VAL:HG11	5:B:301:VAL:HG13	1.99	0.45
32:I:112:LYS:O	32:I:116:LEU:HG	2.16	0.45
13:K:75:ARG:O	13:K:93:ASN:HA	2.16	0.45
14:L:34:GLY:C	14:L:36:ASP:H	2.20	0.45
1:0:2415:A:C2	16:N:25:ARG:HB3	2.52	0.45
20:R:132:ARG:CZ	38:R:9383:HOH:O	2.65	0.45
22:T:49:GLU:HG3	22:T:97:ARG:HB3	1.97	0.45
1:0:1095:U:O2	25:W:120:PRO:HG2	2.16	0.45
1:0:2467:A:H1'	38:0:5014:HOH:O	2.17	0.45
1:0:2563:U:H2'	1:0:2565:C:O5'	2.16	0.45
1:0:270:U:H1'	38:0:4020:HOH:O	2.16	0.45
1:0:952:G:N3	1:0:2302:A:H2'	2.31	0.45
4:A:36:ASP:CG	4:A:85:SER:HB2	2.36	0.45
7:D:159:PRO:O	7:D:163:VAL:HG23	2.16	0.45
12:J:47:THR:O	12:J:53:ILE:HD11	2.17	0.45
26:X:7:GLU:HA	26:X:74:ALA:O	2.16	0.45
1:0:2385:G:H2'	1:0:2386:U:H6	1.80	0.45
1:0:2619:UR3:H6	1:0:2619:UR3:O5'	2.17	0.45
1:0:290:C:O2'	1:0:291:C:H5'	2.15	0.45
1:0:678:G:OP2	6:C:107:ARG:NH2	2.50	0.45
6:C:165:ASP:O	6:C:168:ARG:HB3	2.17	0.45
9:F:46:GLU:O	9:F:73:PRO:HD2	2.17	0.45
15:M:98:GLN:O	15:M:102:GLU:HG3	2.17	0.45
26:X:75:ALA:O	26:X:83:ALA:HA	2.16	0.45
1:0:1314:U:H2'	38:0:6137:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:136:C:H2'	1:0:137:U:O4'	2.17	0.45
1:0:1711:A:O2'	1:0:1712:A:H5'	2.17	0.45
1:0:2004:U:H4'	38:0:5579:HOH:O	2.16	0.45
1:0:2729:C:O2'	1:0:2730:G:H5'	2.17	0.45
1:0:2816:A:H5''	1:0:2817:G:H5'	1.99	0.45
4:A:192:VAL:HG12	4:A:192:VAL:O	2.17	0.45
5:B:51:VAL:HG21	5:B:327:VAL:HG13	1.99	0.45
6:C:214:THR:HG23	38:C:9234:HOH:O	2.15	0.45
38:0:3990:HOH:O	8:E:143:GLN:HG2	2.16	0.45
9:F:72:VAL:HA	9:F:73:PRO:HD3	1.86	0.45
15:M:167:GLY:O	15:M:171:ARG:HG3	2.17	0.45
27:Y:126:PRO:HG2	27:Y:128:PHE:CZ	2.52	0.45
1:0:2281:C:C2'	1:0:2282:U:H5'	2.46	0.45
1:0:559:U:H2'	1:0:560:C:O4'	2.17	0.45
1:0:703:G:O2'	1:0:704:C:H5'	2.17	0.45
1:0:907:A:H2'	1:0:908:A:H8	1.81	0.45
5:B:51:VAL:O	5:B:51:VAL:HG13	2.16	0.45
5:B:86:ALA:HA	38:B:9380:HOH:O	2.16	0.45
6:C:172:THR:HG22	6:C:188:ARG:CZ	2.47	0.45
8:E:118:ILE:HG23	8:E:144:THR:HG21	1.99	0.45
8:E:43:ASP:O	8:E:45:ASP:N	2.47	0.45
14:L:66:VAL:HG23	14:L:67:ARG:N	2.32	0.45
16:N:140:GLN:HA	16:N:143:ARG:HD3	1.99	0.45
38:0:7005:HOH:O	16:N:4:PRO:HD2	2.16	0.45
16:N:93:GLN:NE2	16:N:93:GLN:HA	2.23	0.45
17:O:47:ARG:HG3	17:O:47:ARG:NH1	2.31	0.45
26:X:66:THR:HG22	26:X:67:PRO:O	2.17	0.45
26:X:74:ALA:CB	26:X:85:VAL:HG22	2.46	0.45
1:0:1007:A:H2'	11:H:19:TYR:CZ	2.52	0.45
1:0:1163:G:H2'	1:0:1164:U:C5	2.52	0.45
1:0:23:G:H1'	1:0:520:A:N6	2.32	0.45
1:0:243:A:H61	1:0:269:G:H1'	1.81	0.45
5:B:276:ASP:HB3	5:B:291:ASP:OD1	2.17	0.45
12:J:107:ASN:HD22	12:J:108:PRO:CD	2.29	0.45
12:J:47:THR:HG22	12:J:48:GLY:N	2.31	0.45
13:K:30:LYS:O	13:K:55:VAL:HG13	2.17	0.45
18:P:142:ASP:O	18:P:143:ALA:O	2.35	0.45
24:V:46:ILE:HA	24:V:49:LEU:HD12	1.99	0.45
1:0:2698:G:H2'	1:0:2699:A:O4'	2.16	0.45
1:0:451:C:O2'	1:0:452:G:H5'	2.17	0.45
1:0:920:C:H5''	1:0:921:G:O5'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3106:C:O2'	2:9:3107:C:H5'	2.16	0.45
6:C:133:ARG:HG2	6:C:135:GLU:O	2.17	0.45
7:D:23:VAL:HG21	7:D:45:THR:CG2	2.46	0.45
7:D:81:GLU:O	7:D:85:GLN:HG3	2.17	0.45
8:E:34:TRP:HA	38:E:4572:HOH:O	2.17	0.45
9:F:49:PHE:HE1	9:F:98:VAL:HG23	1.82	0.45
38:0:5725:HOH:O	10:G:12:ILE:HA	2.16	0.45
14:L:64:ILE:HG13	14:L:68:GLU:OE1	2.15	0.45
18:P:98:ILE:HD12	18:P:102:ARG:NE	2.32	0.45
1:0:1289:C:O2'	1:0:1290:G:H5'	2.16	0.44
1:0:1304:U:H2'	1:0:1305:C:C6	2.52	0.44
1:0:249:G:O2'	1:0:250:C:H5'	2.16	0.44
1:0:432:G:O2'	1:0:433:C:H5'	2.17	0.44
31:3:65:THR:CG2	31:3:67:LEU:HG	2.47	0.44
8:E:15:GLN:CG	8:E:20:ILE:HG12	2.47	0.44
32:I:132:CYS:C	32:I:134:SER:H	2.19	0.44
12:J:99:GLU:HA	38:J:9371:HOH:O	2.17	0.44
14:L:12:THR:HG21	14:L:16:GLY:O	2.17	0.44
16:N:39:SER:HB3	16:N:42:HIS:H	1.82	0.44
16:N:63:SER:HB2	16:N:75:THR:HB	1.99	0.44
19:Q:25:PRO:HB2	38:Q:4350:HOH:O	2.16	0.44
1:0:1056:U:H2'	1:0:1057:A:O4'	2.16	0.44
1:0:1200:A:H4'	38:0:7550:HOH:O	2.17	0.44
1:0:1657:A:H2'	1:0:1658:A:C8	2.52	0.44
1:0:1942:A:O2'	1:0:1943:C:H5'	2.17	0.44
1:0:2781:U:H2'	1:0:2782:G:C5'	2.47	0.44
1:0:816:G:C6	1:0:817:G:N1	2.85	0.44
29:1:37:CYS:SG	29:1:39:PHE:HB2	2.57	0.44
4:A:135:VAL:HG21	4:A:147:ARG:HG2	2.00	0.44
5:B:198:GLU:HA	38:B:9461:HOH:O	2.15	0.44
7:D:24:HIS:HB2	7:D:72:LYS:HB3	1.99	0.44
8:E:43:ASP:HA	38:E:5864:HOH:O	2.16	0.44
38:0:9937:HOH:O	9:F:38:LYS:HE2	2.17	0.44
38:0:9851:HOH:O	18:P:81:LYS:HG2	2.18	0.44
25:W:38:THR:O	25:W:42:ARG:HB2	2.17	0.44
1:0:1943:C:O4'	4:A:212:PRO:HA	2.17	0.44
1:0:2061:C:C2'	1:0:2062:A:H5'	2.48	0.44
1:0:2438:G:H2'	1:0:2439:C:O4'	2.17	0.44
1:0:35:U:H5'	6:C:47:GLY:O	2.17	0.44
4:A:100:PRO:HG2	4:A:103:VAL:CG2	2.45	0.44
4:A:53:ALA:HB3	38:A:9400:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:2715:G:O2'	5:B:262:ARG:HD2	2.17	0.44
6:C:133:ARG:NE	6:C:135:GLU:O	2.50	0.44
8:E:31:ARG:NH1	8:E:68:HIS:CG	2.86	0.44
14:L:121:ILE:HG12	14:L:141:GLU:HB2	1.99	0.44
22:T:64:ASN:HB3	22:T:73:HIS:HB2	1.98	0.44
1:O:1167:G:H2'	1:O:1168:C:O4'	2.17	0.44
1:O:1174:A:C5	1:O:1201:C:H4'	2.52	0.44
1:O:1249:U:H2'	1:O:1250:C:C6	2.52	0.44
1:O:2036:C:C4'	13:K:44:LEU:HG	2.47	0.44
38:O:7568:HOH:O	4:A:177:HIS:HE1	2.01	0.44
5:B:301:VAL:HG13	5:B:302:PRO:HD2	1.98	0.44
7:D:158:ASN:HB2	7:D:161:ASP:OD2	2.16	0.44
11:H:46:GLN:NE2	11:H:137:TYR:HE2	2.15	0.44
11:H:38:LYS:HE2	11:H:42:ASP:HB2	1.98	0.44
32:I:92:PRO:O	32:I:94:GLU:HG3	2.16	0.44
12:J:39:VAL:HG11	12:J:107:ASN:HB2	1.99	0.44
13:K:90:PHE:CD1	13:K:90:PHE:N	2.86	0.44
16:N:18:THR:HG21	38:N:9348:HOH:O	2.17	0.44
22:T:53:GLY:HA3	38:T:6384:HOH:O	2.16	0.44
27:Y:112:GLU:OE1	27:Y:115:ARG:NH1	2.50	0.44
1:O:113:A:OP2	1:O:114:A:H2'	2.18	0.44
1:O:1544:U:H2'	1:O:1545:C:C6	2.53	0.44
1:O:2061:C:H2'	1:O:2062:A:H5'	2.00	0.44
1:O:2403:C:H2'	1:O:2404:G:O5'	2.17	0.44
6:C:246:ARG:NE	38:C:9220:HOH:O	2.51	0.44
8:E:21:THR:HG23	8:E:30:THR:OG1	2.17	0.44
9:F:50:VAL:HG11	9:F:60:VAL:HG11	1.99	0.44
11:H:77:LEU:HD12	11:H:83:TYR:CD2	2.52	0.44
32:I:101:SER:OG	32:I:104:GLN:HG3	2.18	0.44
32:I:110:GLU:HA	32:I:113:HIS:CD2	2.52	0.44
14:L:77:ALA:HB3	38:L:9328:HOH:O	2.18	0.44
16:N:154:LEU:HD12	16:N:156:GLU:O	2.17	0.44
16:N:15:GLU:HB3	16:N:17:ARG:HG3	1.99	0.44
18:P:141:ILE:O	18:P:143:ALA:N	2.41	0.44
20:R:114:VAL:HG13	20:R:114:VAL:O	2.18	0.44
25:W:88:THR:CG2	25:W:110:GLN:HE21	2.22	0.44
26:X:70:ILE:HG23	26:X:70:ILE:O	2.17	0.44
1:O:1067:A:H5'	38:O:4638:HOH:O	2.18	0.44
1:O:1632:A:C2'	1:O:1633:C:H5'	2.47	0.44
1:O:656:G:H5'	17:O:3:THR:CG2	2.48	0.44
1:O:968:G:H1'	11:H:32:LYS:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:968:G:O2'	1:0:969:G:H5'	2.17	0.44
6:C:16:VAL:CG1	6:C:17:ASP:N	2.80	0.44
7:D:64:ARG:CD	7:D:67:ASP:HB3	2.47	0.44
11:H:38:LYS:HE2	11:H:42:ASP:CB	2.47	0.44
16:N:11:ARG:NH2	38:N:9316:HOH:O	2.51	0.44
20:R:40:ALA:O	20:R:44:VAL:HG23	2.18	0.44
22:T:48:VAL:HG22	22:T:97:ARG:C	2.38	0.44
27:Y:189:ASN:ND2	27:Y:192:ASP:H	2.16	0.44
1:0:1307:A:H2'	1:0:1308:A:C8	2.53	0.44
1:0:2015:A:H2'	1:0:2016:U:O4'	2.17	0.44
1:0:1811:A:C2	1:0:2752:C:H1'	2.52	0.44
30:2:10:ARG:HH11	30:2:49:GLU:CD	2.21	0.44
4:A:130:THR:HG22	4:A:131:HIS:N	2.32	0.44
5:B:212:GLN:HG2	5:B:257:THR:OG1	2.17	0.44
6:C:102:LEU:HD12	38:C:9117:HOH:O	2.16	0.44
6:C:129:HIS:HD2	6:C:165:ASP:OD2	2.01	0.44
6:C:65:ARG:HG3	6:C:67:GLN:HB2	2.00	0.44
7:D:173:GLU:O	7:D:174:VAL:C	2.56	0.44
7:D:44:ILE:HG12	7:D:83:PHE:CE1	2.49	0.44
7:D:76:ARG:O	7:D:77:ASP:HB2	2.16	0.44
9:F:12:LEU:HD21	9:F:111:ILE:HG23	1.99	0.44
13:K:114:ALA:HB3	13:K:117:VAL:HG23	2.00	0.44
1:0:926:A:O2'	14:L:41:HIS:CD2	2.70	0.44
24:V:12:THR:CG2	24:V:15:GLU:HG3	2.22	0.44
25:W:122:ARG:NH1	25:W:122:ARG:HG2	2.25	0.44
1:0:1587:U:H2'	1:0:1588:G:O4'	2.18	0.44
1:0:1829:A:H5''	38:0:3389:HOH:O	2.16	0.44
1:0:425:U:H4'	38:0:7160:HOH:O	2.17	0.44
2:9:3042:C:O2	7:D:76:ARG:NH1	2.50	0.44
5:B:14:GLY:HA3	38:B:9410:HOH:O	2.17	0.44
6:C:233:THR:HG22	6:C:234:VAL:H	1.83	0.44
6:C:19:PRO:HD2	6:C:240:LEU:HD21	2.00	0.44
16:N:108:SER:HA	16:N:109:PRO:HD3	1.75	0.44
16:N:15:GLU:OE1	16:N:17:ARG:HD2	2.17	0.44
16:N:63:SER:O	16:N:66:LEU:HB2	2.17	0.44
16:N:64:SER:C	16:N:66:LEU:H	2.21	0.44
23:U:52:THR:CG2	23:U:54:THR:HB	2.48	0.44
25:W:73:LEU:O	25:W:74:GLU:HG2	2.18	0.44
28:Z:56:GLN:HA	28:Z:62:TYR:O	2.17	0.44
1:0:1204:C:H1'	38:0:5023:HOH:O	2.18	0.44
1:0:2329:C:O2'	1:0:2330:U:H5'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:248:A:H5'	1:0:249:G:OP2	2.18	0.44
1:0:2511:A:H2'	1:0:2512:U:O4'	2.18	0.44
5:B:268:ARG:NH2	5:B:325:PRO:HG3	2.33	0.44
5:B:312:ARG:HD3	5:B:315:VAL:HG13	2.00	0.44
5:B:7:ARG:HD3	5:B:9:GLY:O	2.18	0.44
8:E:71:ASN:HD22	8:E:138:ILE:HD13	1.83	0.44
16:N:37:ARG:HD3	16:N:37:ARG:HA	1.75	0.44
18:P:91:LYS:O	18:P:95:GLU:HG3	2.18	0.44
22:T:43:ASN:HD22	22:T:108:ARG:NH2	2.15	0.44
25:W:143:THR:N	38:W:3520:HOH:O	2.51	0.44
26:X:76:ARG:NH1	26:X:76:ARG:HG3	2.31	0.44
1:0:1224:G:H2'	1:0:1225:C:C6	2.52	0.43
1:0:1926:G:H2'	1:0:1927:A:C8	2.53	0.43
1:0:2684:A:H2'	1:0:2685:C:C6	2.53	0.43
1:0:958:G:H2'	1:0:959:C:H6	1.82	0.43
1:0:999:C:H2'	1:0:1000:C:O4'	2.18	0.43
5:B:24:PRO:HA	5:B:261:GLN:OE1	2.18	0.43
5:B:304:PRO:HD2	5:B:307:ARG:NH1	2.32	0.43
6:C:136:VAL:HA	6:C:137:PRO:C	2.39	0.43
6:C:5:ILE:CD1	6:C:16:VAL:HG23	2.40	0.43
6:C:72:LYS:HG2	6:C:77:ALA:HA	1.99	0.43
7:D:44:ILE:HG23	7:D:45:THR:HG23	2.00	0.43
13:K:14:LYS:HG3	13:K:32:ILE:O	2.18	0.43
16:N:154:LEU:HD11	16:N:157:PRO:HA	1.99	0.43
17:O:96:VAL:HG12	17:O:100:GLN:HB2	1.99	0.43
25:W:105:THR:HG23	25:W:106:THR:N	2.31	0.43
25:W:64:THR:O	25:W:68:THR:HG22	2.18	0.43
27:Y:126:PRO:HG2	27:Y:128:PHE:CE1	2.53	0.43
1:0:162:C:H2'	1:0:163:U:H5'	2.01	0.43
1:0:1666:C:C2'	1:0:1667:A:C5'	2.96	0.43
1:0:806:A:H2'	1:0:807:A:O4'	2.18	0.43
2:9:3049:G:C2'	2:9:3050:G:H5'	2.48	0.43
4:A:43:VAL:HG21	4:A:59:GLU:OE2	2.18	0.43
5:B:175:LEU:O	5:B:178:ALA:HB3	2.18	0.43
7:D:54:ALA:CB	7:D:69:ILE:HD12	2.48	0.43
9:F:110:ASP:O	9:F:114:LYS:HG3	2.18	0.43
16:N:154:LEU:O	16:N:155:GLU:CB	2.65	0.43
16:N:42:HIS:CB	16:N:62:HIS:HE1	2.31	0.43
19:Q:25:PRO:HA	19:Q:26:PRO:HD3	1.81	0.43
22:T:81:LYS:HD2	22:T:87:VAL:HG11	1.99	0.43
1:0:1015:C:H2'	1:0:1016:U:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1398:G:H2'	1:0:1399:A:C8	2.53	0.43
1:0:1504:A:H5'	38:0:4704:HOH:O	2.17	0.43
1:0:1682:A:H2'	38:0:3108:HOH:O	2.18	0.43
1:0:1849:G:H1'	1:0:2011:A:N1	2.33	0.43
1:0:2684:A:H1'	38:0:3235:HOH:O	2.18	0.43
1:0:2724:U:H2'	1:0:2725:G:O4'	2.18	0.43
1:0:333:G:O2'	1:0:334:G:H5'	2.18	0.43
1:0:946:C:H2'	1:0:947:U:C6	2.53	0.43
5:B:51:VAL:HG13	5:B:53:LEU:CD1	2.48	0.43
6:C:168:ARG:NH2	6:C:190:ALA:O	2.51	0.43
7:D:58:VAL:HG12	7:D:60:GLU:HG2	2.00	0.43
1:0:1168:C:H5''	32:I:87:THR:HG23	2.00	0.43
32:I:92:PRO:C	32:I:94:GLU:N	2.70	0.43
14:L:130:ARG:O	14:L:134:GLU:HG3	2.18	0.43
20:R:114:VAL:HA	20:R:144:GLU:O	2.18	0.43
1:0:1250:C:O2'	1:0:1251:C:H5'	2.18	0.43
1:0:1450:C:O2'	1:0:1494:A:H5'	2.17	0.43
1:0:1528:A:H2'	1:0:1529:G:O4'	2.18	0.43
1:0:1595:G:O2'	1:0:1596:U:H5'	2.19	0.43
1:0:1973:A:H5'	1:0:1973:A:H8	1.83	0.43
1:0:2338:G:H1'	7:D:105:SER:OG	2.18	0.43
1:0:2455:A:H2'	1:0:2456:A:O4'	2.18	0.43
1:0:2756:U:N3	1:0:2896:A:H2	2.08	0.43
1:0:574:C:H2'	1:0:575:G:O4'	2.19	0.43
1:0:2717:C:OP1	5:B:207:LYS:HG3	2.18	0.43
5:B:51:VAL:HG13	5:B:53:LEU:HD11	2.00	0.43
13:K:55:VAL:CG1	13:K:56:SER:N	2.81	0.43
14:L:73:VAL:HG21	14:L:116:HIS:CD2	2.54	0.43
16:N:23:ARG:NH1	16:N:23:ARG:HG2	2.33	0.43
20:R:99:ALA:CB	20:R:109:MET:HE1	2.39	0.43
24:V:12:THR:HG23	24:V:14:ALA:N	2.21	0.43
27:Y:112:GLU:CD	27:Y:115:ARG:NH1	2.70	0.43
1:0:2504:A:H2'	1:0:2505:G:O4'	2.18	0.43
1:0:926:A:O2'	14:L:41:HIS:HD2	2.01	0.43
6:C:7:ASP:OD1	6:C:11:ASN:O	2.37	0.43
14:L:59:GLU:HG2	14:L:104:ASP:CG	2.39	0.43
20:R:47:LEU:O	20:R:51:ILE:HG13	2.18	0.43
29:1:8:GLN:NE2	29:1:11:LYS:NZ	2.59	0.43
38:0:7762:HOH:O	31:3:60:LYS:HG3	2.17	0.43
4:A:51:ARG:NH1	4:A:120:ARG:O	2.51	0.43
5:B:79:MET:O	5:B:80:ARG:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:145:ALA:HB1	8:E:168:ILE:HD11	2.01	0.43
11:H:87:LEU:HD13	11:H:134:PHE:CE2	2.53	0.43
1:O:2365:G:P	19:Q:15:LYS:HG3	2.59	0.43
20:R:4:TYR:HA	20:R:144:GLU:OE2	2.19	0.43
22:T:32:ARG:NH1	22:T:38:ARG:NH1	2.63	0.43
1:O:120:A:H2'	1:O:120:A:N3	2.34	0.43
1:O:1878:G:O2'	1:O:1879:U:OP2	2.35	0.43
1:O:2456:A:H2'	1:O:2457:U:C6	2.54	0.43
1:O:475:G:H5'	6:C:73:LEU:HD23	2.00	0.43
1:O:622:G:O2'	1:O:623:U:H5'	2.19	0.43
5:B:27:ASN:N	5:B:27:ASN:HD22	2.01	0.43
8:E:156:ASP:N	8:E:156:ASP:OD1	2.51	0.43
8:E:31:ARG:HH12	8:E:68:HIS:CD2	2.37	0.43
15:M:182:LYS:HD2	15:M:193:LYS:HB2	1.99	0.43
24:V:20:LEU:HD22	24:V:60:GLN:HE22	1.84	0.43
1:O:1189:A:O2'	1:O:1208:C:H2'	2.18	0.43
1:O:1419:U:H5'	1:O:1420:C:OP2	2.18	0.43
1:O:1636:G:O2'	1:O:1637:A:H5'	2.18	0.43
1:O:1930:A:H2'	1:O:1931:A:C8	2.53	0.43
1:O:2379:G:H5'	1:O:2381:C:O4'	2.18	0.43
1:O:2587:OMU:HM23	1:O:2589:U:C6	2.54	0.43
1:O:392:U:O2'	15:M:182:LYS:HE2	2.18	0.43
1:O:644:G:H1'	38:O:6645:HOH:O	2.19	0.43
4:A:114:ASP:C	4:A:114:ASP:OD1	2.56	0.43
5:B:52:VAL:O	5:B:53:LEU:HD12	2.19	0.43
5:B:69:VAL:HA	5:B:70:PRO:HD3	1.86	0.43
6:C:150:THR:HA	6:C:203:ALA:O	2.18	0.43
7:D:152:PRO:O	7:D:156:ARG:HG2	2.18	0.43
10:G:23:ILE:O	10:G:27:ILE:HG13	2.19	0.43
14:L:93:VAL:CG2	14:L:122:ALA:HB2	2.48	0.43
18:P:38:GLU:HA	18:P:41:ARG:HH11	1.83	0.43
1:O:245:C:H2'	1:O:246:G:H5'	2.01	0.43
2:9:3003:A:H2	2:9:3021:G:N3	2.17	0.43
38:O:7650:HOH:O	4:A:211:LYS:NZ	2.51	0.43
6:C:236:THR:O	6:C:239:ALA:N	2.51	0.43
7:D:170:TYR:CD1	7:D:170:TYR:N	2.86	0.43
13:K:113:ILE:HG22	13:K:114:ALA:O	2.19	0.43
15:M:59:GLY:C	15:M:141:ILE:HD11	2.39	0.43
1:O:154:C:P	15:M:188:ARG:HH12	2.41	0.43
15:M:182:LYS:O	15:M:194:ALA:HB2	2.18	0.43
16:N:49:THR:CG2	16:N:56:ASP:HB2	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:912:A:C4	1:0:1294:A:C2	3.07	0.43
1:0:2134:G:C6	1:0:2258:A:C8	3.07	0.43
1:0:222:A:H2'	1:0:223:G:O4'	2.18	0.43
1:0:2780:C:H2'	1:0:2781:U:C6	2.54	0.43
1:0:303:C:H2'	1:0:304:G:O4'	2.19	0.43
5:B:14:GLY:HA2	5:B:15:PRO:C	2.40	0.43
5:B:17:LYS:O	5:B:260:HIS:HD2	2.02	0.43
1:0:2715:G:N2	5:B:264:GLU:OE1	2.52	0.43
11:H:80:GLU:HA	38:H:9183:HOH:O	2.18	0.43
13:K:113:ILE:HD12	13:K:128:ALA:HB2	2.01	0.43
15:M:31:TRP:HA	15:M:34:GLU:HG3	2.01	0.43
1:0:709:G:O2'	17:O:25:VAL:CG1	2.67	0.43
18:P:22:TRP:CH2	18:P:24:ASN:HA	2.54	0.43
18:P:38:GLU:HA	18:P:41:ARG:NH1	2.34	0.43
26:X:76:ARG:O	26:X:77:PHE:HB3	2.18	0.43
38:0:9991:HOH:O	27:Y:163:THR:HG23	2.19	0.43
28:Z:57:CYS:SG	28:Z:59:TYR:HB3	2.59	0.43
1:0:1675:C:H5''	30:2:5:LYS:HD2	2.01	0.42
1:0:737:A:H2'	1:0:738:G:O4'	2.19	0.42
4:A:94:LEU:HG	4:A:99:ILE:CD1	2.49	0.42
5:B:79:MET:C	5:B:80:ARG:HG3	2.39	0.42
6:C:91:PRO:O	6:C:93:LYS:HG3	2.19	0.42
8:E:145:ALA:O	8:E:148:ILE:HB	2.19	0.42
9:F:28:ALA:HB3	9:F:99:THR:HG23	2.01	0.42
1:0:1008:C:H5''	11:H:16:ARG:HH12	1.84	0.42
32:I:124:ALA:O	32:I:128:VAL:HG23	2.19	0.42
32:I:132:CYS:CB	32:I:137:VAL:HB	2.35	0.42
32:I:92:PRO:HG3	38:I:6825:HOH:O	2.18	0.42
14:L:24:ALA:HB2	14:L:30:ARG:HD2	2.01	0.42
16:N:61:ALA:CB	16:N:88:ALA:HB2	2.48	0.42
1:0:1309:U:H2'	1:0:1310:U:O4'	2.19	0.42
1:0:2067:A:H2'	1:0:2068:G:O4'	2.19	0.42
1:0:2251:G:H2'	1:0:2252:A:H8	1.81	0.42
1:0:2815:G:N7	12:J:80:LYS:NZ	2.65	0.42
1:0:2820:A:H2'	1:0:2821:C:O4'	2.18	0.42
1:0:638:C:H2'	1:0:639:A:C8	2.54	0.42
1:0:795:G:N3	1:0:817:G:C2	2.87	0.42
4:A:107:ASN:OD1	4:A:120:ARG:HD2	2.20	0.42
7:D:23:VAL:CG2	7:D:23:VAL:O	2.66	0.42
8:E:3:VAL:CG2	8:E:49:ILE:HB	2.47	0.42
38:E:2512:HOH:O	12:J:127:ILE:HD11	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:43:PRO:HG3	15:M:62:VAL:HG21	2.01	0.42
24:V:12:THR:OG1	24:V:13:PRO:HD2	2.19	0.42
24:V:7:GLU:O	24:V:11:MET:HG3	2.18	0.42
1:0:2467:A:O2'	1:0:2468:A:H2'	2.19	0.42
1:0:920:C:H4'	1:0:921:G:N2	2.33	0.42
5:B:207:LYS:HG2	5:B:304:PRO:HB3	2.01	0.42
8:E:35:TYR:CD2	8:E:36:PRO:HD2	2.54	0.42
11:H:20:ILE:HG23	11:H:120:ILE:HD11	2.00	0.42
12:J:130:VAL:CG1	12:J:131:THR:N	2.82	0.42
14:L:59:GLU:HG2	14:L:104:ASP:OD2	2.19	0.42
16:N:34:LEU:HA	16:N:47:LEU:CD2	2.49	0.42
19:Q:64:GLU:HA	19:Q:64:GLU:OE1	2.19	0.42
27:Y:108:ASP:N	27:Y:108:ASP:OD1	2.53	0.42
1:0:2255:A:C6	1:0:2256:G:C5	3.08	0.42
1:0:2314:G:C2'	1:0:2315:C:H5'	2.49	0.42
1:0:2564:G:OP2	1:0:2565:C:H5''	2.19	0.42
2:9:3034:A:H2'	2:9:3035:C:O4'	2.19	0.42
5:B:305:ASP:O	5:B:306:LYS:CB	2.66	0.42
6:C:236:THR:O	6:C:237:GLU:C	2.58	0.42
7:D:104:PHE:CE2	7:D:132:VAL:HB	2.55	0.42
13:K:22:ASP:O	13:K:110:LYS:HE3	2.20	0.42
15:M:24:GLN:O	15:M:28:GLN:HG3	2.19	0.42
20:R:72:VAL:CG1	20:R:75:TRP:HB3	2.49	0.42
23:U:37:GLU:O	23:U:40:ALA:HB3	2.20	0.42
1:0:2346:C:O2'	7:D:52:THR:HG21	2.19	0.42
1:0:764:C:H2'	1:0:765:G:O4'	2.20	0.42
4:A:88:ILE:CD1	4:A:100:PRO:HD3	2.45	0.42
5:B:277:GLU:N	5:B:278:PRO:CD	2.83	0.42
6:C:13:ASP:OD1	6:C:13:ASP:O	2.37	0.42
6:C:16:VAL:CG1	6:C:17:ASP:H	2.30	0.42
7:D:95:THR:HG1	7:D:174:VAL:HG22	1.81	0.42
7:D:81:GLU:C	7:D:83:PHE:N	2.73	0.42
11:H:43:TYR:HA	11:H:44:PRO:HD3	1.79	0.42
18:P:7:LYS:HD3	18:P:21:VAL:CG2	2.49	0.42
20:R:125:ARG:HG2	38:R:9344:HOH:O	2.19	0.42
25:W:38:THR:CG2	25:W:39:ASP:N	2.82	0.42
1:0:1151:G:OP1	10:G:63:ARG:NH1	2.53	0.42
1:0:2044:G:OP1	26:X:23:HIS:HE1	2.03	0.42
1:0:2524:G:H21	1:0:2526:C:H41	1.68	0.42
1:0:2761:A:H2'	38:0:5903:HOH:O	2.18	0.42
1:0:37:A:H2'	1:0:38:G:H8	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:514:G:OP1	1:0:514:G:H2'	2.20	0.42
1:0:67:A:H5''	1:0:69:A:C8	2.55	0.42
2:9:3052:A:O2'	2:9:3053:G:H5'	2.20	0.42
5:B:55:ASN:HB3	5:B:63:GLU:HA	2.01	0.42
7:D:66:GLY:O	7:D:67:ASP:HB3	2.18	0.42
7:D:99:ASP:CB	7:D:103:ASN:HB2	2.50	0.42
8:E:108:LEU:HD11	8:E:164:ASP:HB2	2.02	0.42
11:H:69:ALA:HB2	11:H:153:ALA:HB2	2.00	0.42
19:Q:93:ARG:NH1	19:Q:93:ARG:HG3	2.35	0.42
20:R:17:MET:HE3	20:R:19:ARG:NE	2.34	0.42
22:T:71:VAL:CG1	22:T:72:ILE:N	2.82	0.42
27:Y:144:ARG:NH2	38:Y:9407:HOH:O	2.51	0.42
28:Z:39:CYS:HA	28:Z:47:VAL:CG2	2.50	0.42
1:0:1160:G:O2'	1:0:1190:G:H1'	2.19	0.42
1:0:1206:U:H2'	1:0:1207:A:O4'	2.19	0.42
1:0:1380:U:H5'	38:0:9533:HOH:O	2.20	0.42
1:0:1409:G:H5'	38:0:4024:HOH:O	2.19	0.42
1:0:1483:C:O2'	1:0:1484:G:H5'	2.19	0.42
1:0:347:A:O2'	6:C:205:ARG:NH2	2.53	0.42
1:0:371:U:H2'	1:0:372:A:H8	1.84	0.42
1:0:820:G:O2'	1:0:856:G:H4'	2.19	0.42
1:0:783:C:OP1	4:A:180:LYS:HE3	2.19	0.42
5:B:307:ARG:CG	5:B:307:ARG:HH11	2.33	0.42
7:D:88:LEU:O	7:D:90:LEU:N	2.53	0.42
9:F:99:THR:O	9:F:100:ASP:HB2	2.19	0.42
12:J:39:VAL:CG1	12:J:107:ASN:HB2	2.50	0.42
16:N:42:HIS:CG	16:N:62:HIS:HE1	2.37	0.42
26:X:15:ARG:HB3	26:X:15:ARG:NH1	2.34	0.42
26:X:30:MET:HE2	26:X:58:ALA:HB3	2.02	0.42
27:Y:186:ARG:HG2	27:Y:186:ARG:HH11	1.85	0.42
27:Y:187:VAL:HB	27:Y:203:VAL:CG2	2.49	0.42
1:0:1771:U:O2	28:Z:19:GLY:HA2	2.19	0.42
1:0:1058:A:H2'	1:0:1060:C:C5'	2.48	0.42
1:0:1525:G:H5'	1:0:1526:A:OP2	2.20	0.42
1:0:1634:G:H2'	1:0:1635:U:C6	2.54	0.42
1:0:236:A:H8	1:0:236:A:OP1	2.03	0.42
4:A:109:GLU:HG2	4:A:116:GLY:H	1.83	0.42
4:A:130:THR:HG22	4:A:131:HIS:O	2.19	0.42
1:0:1881:A:OP1	4:A:199:HIS:HE1	2.02	0.42
5:B:270:ILE:O	5:B:271:ASP:HB2	2.19	0.42
6:C:237:GLU:HB2	38:C:9226:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:27:ILE:HD12	10:G:70:ALA:HB1	2.01	0.42
11:H:66:ARG:HD3	38:H:9179:HOH:O	2.19	0.42
32:I:99:ASP:O	32:I:100:LEU:HD23	2.20	0.42
22:T:3:GLN:HA	22:T:4:PRO:HD3	1.84	0.42
25:W:6:GLN:HB2	25:W:26:ILE:CD1	2.45	0.42
26:X:36:HIS:CE1	26:X:40:HIS:CD2	3.08	0.42
1:0:125:U:H2'	38:0:4064:HOH:O	2.18	0.42
1:0:1331:A:OP2	27:Y:142:SER:OG	2.34	0.42
1:0:1335:C:H2'	1:0:1336:U:C6	2.55	0.42
1:0:1697:G:O2'	1:0:1698:U:H5'	2.20	0.42
1:0:2105:C:H2'	1:0:2106:C:C6	2.54	0.42
1:0:2266:A:H2'	1:0:2267:G:C8	2.55	0.42
1:0:42:C:H1'	38:0:4957:HOH:O	2.19	0.42
1:0:645:U:O2	1:0:761:A:H2	2.03	0.42
4:A:87:GLU:HB3	38:A:9415:HOH:O	2.20	0.42
6:C:27:ARG:CG	6:C:27:ARG:HH11	2.32	0.42
1:0:475:G:OP1	6:C:73:LEU:CD2	2.68	0.42
32:I:112:LYS:C	32:I:114:PRO:HD2	2.40	0.42
32:I:129:VAL:HG13	32:I:139:ILE:CD1	2.49	0.42
12:J:42:GLU:O	12:J:131:THR:HG23	2.20	0.42
14:L:120:LEU:HD12	14:L:133:VAL:HG21	2.01	0.42
1:0:164:G:O3'	14:L:30:ARG:HB2	2.20	0.42
5:B:329:TYR:HE2	23:U:15:PRO:HG2	1.81	0.42
1:0:1184:C:O2'	1:0:1185:U:OP2	2.31	0.42
1:0:621:C:H5'	27:Y:132:ASP:OD2	2.20	0.42
1:0:700:A:C2	14:L:71:GLU:HG2	2.55	0.42
1:0:813:C:H2'	1:0:814:G:O4'	2.20	0.42
5:B:280:VAL:HG22	5:B:333:GLU:O	2.19	0.42
1:0:2837:U:H1'	5:B:307:ARG:HH12	1.85	0.42
9:F:99:THR:HA	38:F:3461:HOH:O	2.19	0.42
11:H:3:ALA:HA	11:H:58:ARG:HH12	1.85	0.42
32:I:132:CYS:C	32:I:134:SER:N	2.73	0.42
12:J:107:ASN:HD22	12:J:108:PRO:HD2	1.85	0.42
25:W:21:LEU:O	25:W:26:ILE:HG12	2.20	0.42
26:X:78:GLU:CG	26:X:79:GLU:N	2.82	0.42
27:Y:153:GLN:HG3	27:Y:160:LYS:O	2.20	0.42
1:0:1181:A:N1	1:0:1192:A:O2'	2.50	0.41
1:0:1252:A:H2'	1:0:1253:C:O4'	2.19	0.41
1:0:2269:C:H2'	1:0:2270:G:C5'	2.50	0.41
1:0:2330:U:H4'	1:0:2331:C:OP1	2.20	0.41
1:0:704:C:H2'	1:0:705:C:H6	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:2:19:SER:HB3	38:2:4479:HOH:O	2.20	0.41
5:B:243:ASN:HA	5:B:244:PRO:C	2.39	0.41
8:E:4:GLU:HG2	8:E:48:VAL:HG22	2.02	0.41
11:H:166:SER:HB3	38:H:9143:HOH:O	2.20	0.41
16:N:73:ALA:HB2	16:N:163:PHE:CE2	2.55	0.41
20:R:82:GLU:O	20:R:86:LYS:HG3	2.20	0.41
1:0:1046:G:N3	1:0:1082:A:H2	2.18	0.41
1:0:1453:G:N2	1:0:1675:C:C2	2.87	0.41
1:0:419:A:H1'	1:0:1921:A:C2	2.55	0.41
1:0:1921:A:C6	1:0:1922:A:C2	3.08	0.41
1:0:1948:G:O2'	1:0:1949:G:H5'	2.21	0.41
1:0:2028:U:H2'	1:0:2029:C:C6	2.55	0.41
1:0:2604:A:H5'	38:0:6052:HOH:O	2.19	0.41
1:0:401:C:H2'	1:0:402:U:C6	2.55	0.41
1:0:39:G:H2'	1:0:40:C:O4'	2.20	0.41
1:0:629:A:H2'	1:0:630:A:O4'	2.20	0.41
4:A:161:GLY:O	28:Z:68:SER:OG	2.34	0.41
4:A:48:ASP:HA	4:A:49:PRO:HD3	1.83	0.41
1:0:2821:C:O2'	5:B:114:ASP:O	2.36	0.41
6:C:140:VAL:CG1	6:C:141:SER:N	2.83	0.41
6:C:27:ARG:NH1	6:C:27:ARG:CG	2.83	0.41
6:C:54:LEU:HD23	6:C:79:ARG:HG3	2.01	0.41
7:D:23:VAL:HG22	7:D:73:VAL:HB	2.02	0.41
11:H:17:ARG:HD3	11:H:23:ILE:CD1	2.50	0.41
11:H:46:GLN:HE21	11:H:137:TYR:HE2	1.68	0.41
14:L:67:ARG:O	14:L:71:GLU:HG3	2.20	0.41
16:N:157:PRO:HA	38:N:9323:HOH:O	2.21	0.41
16:N:67:ALA:C	16:N:69:TYR:N	2.74	0.41
18:P:16:VAL:HG12	18:P:17:GLY:N	2.35	0.41
20:R:119:VAL:HG21	20:R:142:ASP:CG	2.40	0.41
21:S:29:ASP:OD1	21:S:31:ARG:HG3	2.21	0.41
1:0:128:A:O2'	1:0:129:A:H5'	2.20	0.41
1:0:1377:C:C5'	1:0:1377:C:H6	2.32	0.41
1:0:1398:G:O2'	1:0:1399:A:H5'	2.20	0.41
1:0:138:U:OP2	1:0:139:C:H5	2.03	0.41
1:0:1701:A:H5''	1:0:1702:U:H3'	2.01	0.41
1:0:2363:G:O3'	19:Q:11:ARG:NH1	2.53	0.41
29:1:53:LYS:HD3	29:1:53:LYS:HA	1.92	0.41
4:A:82:VAL:HG13	4:A:93:THR:HB	2.01	0.41
5:B:258:GLY:N	5:B:260:HIS:CE1	2.85	0.41
6:C:27:ARG:NH1	6:C:27:ARG:HG2	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:181:GLU:N	15:M:181:GLU:OE1	2.48	0.41
18:P:141:ILE:C	18:P:143:ALA:N	2.73	0.41
20:R:9:ASP:HA	20:R:10:PRO:HD2	1.92	0.41
22:T:43:ASN:ND2	22:T:108:ARG:CZ	2.83	0.41
25:W:110:GLN:NE2	25:W:110:GLN:HA	2.35	0.41
1:0:1023:C:O2'	1:0:1024:G:H5'	2.20	0.41
1:0:1333:U:H2'	1:0:1334:C:H6	1.85	0.41
1:0:1641:A:H2'	1:0:1642:A:C5'	2.45	0.41
1:0:2270:G:H4'	4:A:223:ARG:NH1	2.29	0.41
1:0:671:A:O2'	1:0:672:G:H2'	2.20	0.41
1:0:932:U:H2'	1:0:933:C:C6	2.56	0.41
30:2:30:ASP:O	30:2:31:ARG:HB2	2.20	0.41
4:A:217:ARG:HG3	38:A:9325:HOH:O	2.20	0.41
5:B:119:HIS:O	5:B:121:PRO:HD3	2.20	0.41
7:D:151:ILE:HA	7:D:152:PRO:HD3	1.95	0.41
12:J:93:ARG:HH11	12:J:93:ARG:CB	2.27	0.41
13:K:9:THR:O	13:K:10:GLN:C	2.58	0.41
17:O:21:SER:OG	17:O:106:PRO:HB2	2.20	0.41
25:W:115:THR:HG23	38:W:5420:HOH:O	2.21	0.41
25:W:125:HIS:CD2	25:W:127:GLY:H	2.38	0.41
1:0:1734:C:OP1	5:B:234:ARG:NH1	2.50	0.41
1:0:2269:C:H2'	1:0:2270:G:H5'	2.01	0.41
1:0:2401:A:H2'	1:0:2402:A:C8	2.55	0.41
1:0:2821:C:H4'	5:B:116:PRO:HG3	2.01	0.41
1:0:426:G:H2'	1:0:427:C:O4'	2.21	0.41
1:0:538:C:H5''	1:0:539:G:C8	2.55	0.41
1:0:870:G:C3'	1:0:871:G:H5''	2.50	0.41
8:E:11:VAL:HG13	8:E:76:VAL:HG21	2.03	0.41
9:F:50:VAL:CG2	9:F:63:ILE:HG21	2.50	0.41
13:K:113:ILE:HG22	13:K:114:ALA:N	2.34	0.41
13:K:75:ARG:HE	13:K:94:ALA:HB3	1.85	0.41
16:N:183:ASP:O	16:N:184:ILE:O	2.38	0.41
25:W:122:ARG:NH1	25:W:122:ARG:CG	2.82	0.41
1:0:1080:C:H6	1:0:1080:C:O5'	2.04	0.41
1:0:137:U:H2'	1:0:139:C:C5	2.56	0.41
1:0:1528:A:H62	1:0:1663:G:H21	1.67	0.41
1:0:2078:U:O2'	1:0:2079:G:H5'	2.21	0.41
1:0:2768:A:O2'	1:0:2769:C:H5'	2.21	0.41
1:0:2783:A:H2'	1:0:2784:A:C8	2.56	0.41
1:0:470:U:O2'	29:1:16:HIS:CD2	2.69	0.41
1:0:485:A:O2'	1:0:487:G:H5'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:820:G:H5'	1:0:821:U:H5'	2.03	0.41
1:0:946:C:H2'	1:0:947:U:H6	1.84	0.41
5:B:255:GLY:O	5:B:257:THR:HG23	2.21	0.41
6:C:236:THR:HG22	6:C:239:ALA:CB	2.50	0.41
6:C:78:ARG:HH11	6:C:78:ARG:HG3	1.85	0.41
8:E:68:HIS:O	8:E:72:MET:HG3	2.20	0.41
9:F:26:THR:HB	9:F:102:GLY:HA3	2.03	0.41
12:J:42:GLU:HG2	12:J:43:ARG:HG3	2.03	0.41
16:N:101:VAL:HG12	38:N:9328:HOH:O	2.19	0.41
25:W:48:VAL:CG1	25:W:48:VAL:O	2.68	0.41
1:0:1185:U:H2'	1:0:1186:C:H6	1.84	0.41
1:0:1269:G:H2'	1:0:1270:U:C6	2.56	0.41
1:0:1391:G:H2'	1:0:1392:A:H5'	2.02	0.41
1:0:1744:G:H2'	1:0:1745:G:H5'	2.02	0.41
1:0:2377:U:O5'	1:0:2377:U:H6	2.03	0.41
1:0:2754:G:O2'	1:0:2755:G:H5'	2.21	0.41
1:0:736:A:H2'	1:0:737:A:O4'	2.21	0.41
5:B:16:ARG:HD3	38:B:9410:HOH:O	2.19	0.41
6:C:114:ALA:HB1	6:C:223:LEU:HB3	2.03	0.41
19:Q:53:HIS:ND1	19:Q:55:ARG:HB2	2.36	0.41
1:0:1500:U:OP2	18:P:41:ARG:NH2	2.54	0.41
1:0:2353:A:H4'	1:0:2354:A:O5'	2.20	0.41
1:0:2413:A:H2'	1:0:2414:A:O4'	2.20	0.41
1:0:821:U:H2'	1:0:822:C:C6	2.56	0.41
1:0:958:G:O2'	1:0:959:C:H5'	2.20	0.41
31:3:48:ASN:ND2	31:3:50:GLY:H	2.17	0.41
5:B:51:VAL:O	5:B:53:LEU:HD13	2.21	0.41
7:D:92:GLU:HB2	38:D:3862:HOH:O	2.19	0.41
11:H:95:LEU:HD11	11:H:124:ALA:HB2	2.03	0.41
11:H:9:ILE:HG22	11:H:9:ILE:O	2.20	0.41
16:N:29:SER:OG	16:N:101:VAL:HG21	2.20	0.41
18:P:16:VAL:CG1	18:P:17:GLY:N	2.84	0.41
25:W:108:ARG:HE	25:W:114:PRO:HG3	1.86	0.41
1:0:1268:C:O2'	27:Y:169:ARG:HB2	2.20	0.41
1:0:1194:A:O2'	1:0:1195:G:H5'	2.21	0.41
1:0:1755:A:H2'	1:0:1756:G:O4'	2.20	0.41
1:0:189:A:OP1	15:M:171:ARG:NH2	2.53	0.41
1:0:2387:U:H2'	1:0:2388:C:C6	2.56	0.41
1:0:281:U:O2'	1:0:282:C:H5'	2.20	0.41
1:0:542:A:H2'	1:0:543:G:O4'	2.21	0.41
2:9:3060:C:O2'	2:9:3061:C:H5'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:199:TYR:CE2	5:B:268:ARG:HB2	2.56	0.41
1:0:2718:C:P	5:B:45:LYS:HZ1	2.44	0.41
6:C:46:TYR:CE1	6:C:92:PRO:HB3	2.56	0.41
11:H:146:VAL:HG22	38:H:9176:HOH:O	2.21	0.41
11:H:38:LYS:O	11:H:84:LYS:HE2	2.21	0.41
32:I:113:HIS:N	32:I:114:PRO:CD	2.83	0.41
1:0:1180:U:H4'	32:I:91:GLU:OE2	2.21	0.41
12:J:131:THR:HG22	12:J:133:GLY:N	2.35	0.41
1:0:926:A:C4'	14:L:39:GLU:HG2	2.51	0.41
15:M:59:GLY:HA3	15:M:141:ILE:HD11	2.03	0.41
17:O:24:ALA:O	17:O:28:ASP:HB2	2.20	0.41
17:O:32:ARG:HH11	17:O:115:ARG:HH21	1.69	0.41
22:T:47:THR:HB	22:T:100:ASP:HB3	2.01	0.41
22:T:23:VAL:C	22:T:93:THR:HG21	2.41	0.41
22:T:40:VAL:HG22	22:T:41:ARG:N	2.36	0.41
25:W:21:LEU:CD2	25:W:48:VAL:HG11	2.50	0.41
1:0:907:A:H2'	1:0:908:A:C8	2.54	0.41
2:9:3107:C:H5	38:9:3167:HOH:O	2.03	0.41
2:9:3114:G:H2'	2:9:3115:C:C6	2.56	0.41
4:A:33:GLU:O	4:A:34:ASP:CB	2.61	0.41
5:B:175:LEU:C	5:B:175:LEU:CD2	2.89	0.41
5:B:224:LYS:HA	5:B:224:LYS:HD3	1.94	0.41
5:B:5:ARG:HH11	5:B:8:LYS:HE2	1.86	0.41
6:C:123:LEU:HA	6:C:123:LEU:HD23	1.94	0.41
6:C:133:ARG:HD2	38:C:9206:HOH:O	2.20	0.41
6:C:223:LEU:HA	6:C:223:LEU:HD12	1.94	0.41
7:D:105:SER:HB2	7:D:131:THR:HG23	2.01	0.41
17:O:41:ALA:HA	38:O:5104:HOH:O	2.21	0.41
23:U:45:GLU:HB2	23:U:48:ASN:ND2	2.36	0.41
25:W:3:ALA:O	25:W:54:PHE:HA	2.21	0.41
27:Y:187:VAL:CG1	27:Y:205:ILE:HA	2.51	0.41
28:Z:67:GLY:N	28:Z:70:LYS:O	2.53	0.41
1:0:1173:A:H4'	1:0:1174:A:C8	2.56	0.41
1:0:1477:C:O2'	1:0:1478:U:H5'	2.21	0.41
1:0:1419:U:H2'	1:0:1685:A:C2	2.55	0.41
1:0:1773:G:N2	1:0:1774:G:C8	2.88	0.41
1:0:1976:G:O2'	1:0:1977:U:H5'	2.21	0.41
1:0:2265:U:H2'	1:0:2266:A:H8	1.86	0.41
7:D:10:PHE:CG	7:D:11:HIS:N	2.89	0.41
32:I:78:LEU:HD13	32:I:108:ILE:HG23	2.03	0.41
1:0:155:C:OP2	15:M:188:ARG:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:2365:G:OP1	19:Q:15:LYS:HG3	2.21	0.41
21:S:17:ASP:HB3	21:S:23:LYS:HB2	2.02	0.41
25:W:153:MET:O	25:W:154:ARG:C	2.59	0.41
28:Z:13:ARG:NH1	38:Z:9218:HOH:O	2.53	0.41
1:O:1158:G:O2'	1:O:1159:G:H5'	2.21	0.40
1:O:1714:C:O2'	1:O:1715:C:H5'	2.21	0.40
1:O:1761:U:H5'	18:P:81:LYS:O	2.22	0.40
1:O:1933:G:O2'	1:O:1934:A:H5'	2.20	0.40
1:O:228:C:H2'	1:O:229:G:H5'	2.03	0.40
1:O:571:C:H6	1:O:571:C:O5'	2.03	0.40
1:O:732:C:O2'	1:O:733:U:H5'	2.21	0.40
2:9:3059:C:H5'	38:9:5233:HOH:O	2.21	0.40
4:A:165:THR:CG2	4:A:165:THR:O	2.69	0.40
4:A:211:LYS:HB2	38:A:9413:HOH:O	2.21	0.40
38:O:9988:HOH:O	6:C:214:THR:HB	2.20	0.40
7:D:55:LYS:HA	38:D:6752:HOH:O	2.21	0.40
7:D:57:THR:HG23	7:D:63:ILE:CA	2.42	0.40
13:K:44:LEU:HA	13:K:45:PRO:HD2	1.96	0.40
13:K:89:LYS:HA	38:K:7064:HOH:O	2.21	0.40
15:M:134:ILE:O	15:M:136:PRO:HD3	2.21	0.40
1:O:380:A:C2	15:M:13:GLU:HB3	2.56	0.40
15:M:9:ARG:HB2	15:M:47:ASP:OD2	2.20	0.40
16:N:181:ASP:O	16:N:184:ILE:HG22	2.21	0.40
1:O:1789:G:O6	18:P:73:HIS:HE1	2.04	0.40
22:T:47:THR:HG22	22:T:99:THR:OG1	2.21	0.40
25:W:72:PRO:CG	25:W:77:ALA:HB3	2.39	0.40
1:O:1513:C:O2'	1:O:1514:C:H5'	2.21	0.40
1:O:1562:C:N4	38:O:6128:HOH:O	2.55	0.40
1:O:1643:C:O2'	1:O:1644:C:H5'	2.22	0.40
1:O:1741:U:H3'	38:O:3074:HOH:O	2.21	0.40
1:O:1855:G:H4'	1:O:1856:C:O5'	2.21	0.40
1:O:1943:C:H5''	4:A:209:PRO:HG3	2.03	0.40
1:O:1996:U:O2'	1:O:1997:A:H5'	2.21	0.40
1:O:2619:UR3:H5'	3:4:76:5AA:H103	2.03	0.40
1:O:2740:G:H2'	1:O:2741:A:O4'	2.21	0.40
5:B:171:VAL:HG23	5:B:172:SER:N	2.35	0.40
38:O:7751:HOH:O	5:B:2:GLN:HG3	2.21	0.40
5:B:80:ARG:HA	5:B:186:GLY:O	2.21	0.40
1:O:1311:G:O6	6:C:173:LYS:HE3	2.22	0.40
6:C:187:ARG:NH2	38:C:9162:HOH:O	2.51	0.40
32:I:119:TYR:CD1	32:I:119:TYR:N	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:89:PHE:CD1	14:L:89:PHE:N	2.89	0.40
26:X:26:ALA:HB1	26:X:59:TRP:CE2	2.56	0.40
1:0:1167:G:H4'	32:I:135:LEU:CD2	2.51	0.40
1:0:1434:A:H2'	1:0:1436:C:C5	2.56	0.40
1:0:1631:A:H2'	1:0:1632:A:C8	2.56	0.40
1:0:2115:U:H2'	1:0:2116:U:C6	2.56	0.40
1:0:2266:A:OP2	15:M:90:ARG:NH2	2.52	0.40
1:0:2379:G:N7	1:0:2408:A:N1	2.70	0.40
1:0:291:C:H2'	1:0:292:G:O4'	2.21	0.40
1:0:646:G:H2'	1:0:647:U:C6	2.56	0.40
1:0:790:A:H1'	1:0:1710:A:O2'	2.22	0.40
2:9:3029:C:H2'	2:9:3030:C:C5'	2.45	0.40
5:B:205:VAL:O	5:B:307:ARG:NE	2.54	0.40
6:C:118:THR:O	6:C:136:VAL:HG13	2.21	0.40
7:D:75:LEU:HD22	7:D:79:MET:HB3	2.02	0.40
8:E:144:THR:O	8:E:148:ILE:HG13	2.21	0.40
9:F:99:THR:HG23	9:F:99:THR:O	2.21	0.40
11:H:54:THR:HA	11:H:127:VAL:O	2.22	0.40
11:H:26:SER:HA	11:H:59:HIS:HD2	1.85	0.40
13:K:22:ASP:OD1	13:K:22:ASP:C	2.60	0.40
13:K:78:LYS:HA	13:K:79:PRO:HD3	1.95	0.40
14:L:122:ALA:HB3	14:L:125:PHE:CZ	2.56	0.40
14:L:125:PHE:CZ	14:L:140:VAL:HG13	2.57	0.40
1:0:949:U:O2'	19:Q:40:HIS:HE1	2.03	0.40
1:0:2050:G:OP1	20:R:79:ARG:HB3	2.21	0.40
23:U:39:ASN:HD22	23:U:44:ARG:HH11	1.68	0.40
25:W:125:HIS:HE1	38:W:3071:HOH:O	2.05	0.40
25:W:48:VAL:HG12	25:W:48:VAL:O	2.21	0.40
1:0:1167:G:H3'	38:0:7702:HOH:O	2.20	0.40
1:0:1624:A:H4'	1:0:1626:A:H5''	2.03	0.40
1:0:1744:G:C2'	1:0:1745:G:H5'	2.51	0.40
1:0:1805:G:O2'	1:0:1806:G:H5'	2.21	0.40
1:0:2314:G:O2'	1:0:2315:C:H5'	2.22	0.40
1:0:2776:A:H2'	1:0:2777:G:O4'	2.20	0.40
1:0:549:A:O2'	1:0:550:C:H5'	2.21	0.40
2:9:3012:C:H5'	2:9:3070:U:O4'	2.21	0.40
4:A:186:TRP:CD1	4:A:187:PRO:HA	2.56	0.40
5:B:183:GLU:OE1	5:B:183:GLU:HA	2.21	0.40
5:B:33:ASP:HB3	5:B:34:GLY:H	1.57	0.40
7:D:19:GLU:HG3	38:D:6165:HOH:O	2.21	0.40
7:D:64:ARG:HG2	7:D:67:ASP:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:99:ASP:HB2	7:D:103:ASN:HB2	2.04	0.40
14:L:53:ARG:NH2	14:L:57:VAL:CG1	2.84	0.40
14:L:68:GLU:HG3	38:L:9342:HOH:O	2.22	0.40
16:N:183:ASP:O	16:N:184:ILE:C	2.59	0.40
20:R:132:ARG:NH1	38:R:9383:HOH:O	2.54	0.40
20:R:69:LYS:HE2	20:R:78:GLY:O	2.21	0.40
22:T:37:GLN:OE1	22:T:118:SER:HA	2.21	0.40
24:V:59:ILE:O	24:V:63:GLU:HG2	2.21	0.40
25:W:137:GLN:HG3	25:W:137:GLN:O	2.21	0.40
25:W:73:LEU:HA	25:W:73:LEU:HD12	1.74	0.40
1:O:2093:G:H5''	38:B:9327:HOH:O	2.21	0.40
1:O:2515:C:H2'	1:O:2516:G:O4'	2.21	0.40
29:1:28:HIS:CD2	29:1:31:LYS:H	2.39	0.40
30:2:40:ARG:NH1	30:2:40:ARG:HG2	2.37	0.40
5:B:115:VAL:HA	5:B:116:PRO:HD3	1.88	0.40
38:O:9429:HOH:O	6:C:103:ASN:HB3	2.20	0.40
6:C:173:LYS:O	6:C:186:TYR:HA	2.22	0.40
6:C:80:VAL:HA	6:C:81:PRO:HD3	1.95	0.40
8:E:20:ILE:HD11	8:E:40:VAL:CG1	2.51	0.40
11:H:114:ARG:O	11:H:115:ALA:C	2.60	0.40
12:J:107:ASN:HD22	12:J:109:TYR:H	1.64	0.40
12:J:11:ILE:HD11	12:J:109:TYR:CD2	2.57	0.40
15:M:69:LYS:HG3	15:M:126:GLN:CA	2.52	0.40
15:M:184:ARG:HG3	15:M:185:PRO:HA	2.04	0.40
15:M:40:ILE:HG21	15:M:64:ARG:NH2	2.36	0.40
1:O:2659:U:H4'	20:R:76:ASP:HB3	2.03	0.40
22:T:24:ARG:HH21	22:T:39:ASN:ND2	2.14	0.40
1:O:56:G:C5'	24:V:50:ARG:HH12	2.27	0.40
25:W:137:GLN:HE21	25:W:141:HIS:CE1	2.18	0.40
27:Y:144:ARG:NH1	38:Y:9373:HOH:O	2.54	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3020:G:OP1	5:B:195:ARG:NH2[7_545]	1.98	0.22
1:O:1171:A:N3	1:O:1964:U:O5'[3_655]	2.13	0.07
13:K:63:GLU:CB	13:K:63:GLU:CB[3_655]	2.13	0.07

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	235/240 (98%)	206 (88%)	24 (10%)	5 (2%)	7	13
5	B	335/338 (99%)	294 (88%)	35 (10%)	6 (2%)	8	16
6	C	244/246 (99%)	217 (89%)	26 (11%)	1 (0%)	34	57
7	D	134/177 (76%)	97 (72%)	25 (19%)	12 (9%)	1	0
8	E	170/178 (96%)	156 (92%)	13 (8%)	1 (1%)	25	47
9	F	117/120 (98%)	106 (91%)	7 (6%)	4 (3%)	3	5
10	G	25/348 (7%)	23 (92%)	2 (8%)	0	100	100
11	H	156/171 (91%)	142 (91%)	11 (7%)	3 (2%)	8	15
12	J	140/145 (97%)	130 (93%)	8 (6%)	2 (1%)	11	22
13	K	130/132 (98%)	119 (92%)	8 (6%)	3 (2%)	6	11
14	L	141/165 (86%)	120 (85%)	19 (14%)	2 (1%)	11	22
15	M	192/194 (99%)	178 (93%)	14 (7%)	0	100	100
16	N	184/187 (98%)	167 (91%)	11 (6%)	6 (3%)	4	6
17	O	113/116 (97%)	104 (92%)	8 (7%)	1 (1%)	17	35
18	P	141/149 (95%)	135 (96%)	6 (4%)	0	100	100
19	Q	93/96 (97%)	87 (94%)	6 (6%)	0	100	100
20	R	148/155 (96%)	138 (93%)	8 (5%)	2 (1%)	11	22
21	S	79/85 (93%)	75 (95%)	4 (5%)	0	100	100
22	T	117/120 (98%)	107 (92%)	10 (8%)	0	100	100
23	U	51/66 (77%)	47 (92%)	3 (6%)	1 (2%)	7	14
24	V	63/71 (89%)	55 (87%)	6 (10%)	2 (3%)	4	6
25	W	152/154 (99%)	146 (96%)	5 (3%)	1 (1%)	22	43
26	X	80/92 (87%)	70 (88%)	8 (10%)	2 (2%)	5	9
27	Y	140/241 (58%)	139 (99%)	1 (1%)	0	100	100
28	Z	71/83 (86%)	60 (84%)	7 (10%)	4 (6%)	2	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
30	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
31	3	90/92 (98%)	88 (98%)	0	2 (2%)	6	12
32	I	68/162 (42%)	51 (75%)	17 (25%)	0	100	100
All	All	3705/4430 (84%)	3350 (90%)	295 (8%)	60 (2%)	9	19

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	34	ASP
4	A	132	ASP
9	F	101	ALA
11	H	168	ALA
12	J	5	GLU
16	N	154	LEU
16	N	184	ILE
28	Z	81	ARG
4	A	37	VAL
5	B	34	GLY
5	B	169	GLY
6	C	8	LEU
7	D	65	GLU
7	D	137	PRO
7	D	173	GLU
9	F	44	SER
11	H	166	SER
24	V	43	PRO
5	B	107	SER
7	D	86	THR
11	H	140	VAL
13	K	126	SER
14	L	80	ASP
14	L	143	THR
16	N	113	SER
16	N	164	ASP
23	U	7	ASP
26	X	78	GLU
28	Z	42	CYS
5	B	185	GLY
7	D	171	ASP
8	E	44	GLY

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Mol	Chain	Res	Type
9	F	61	MET
9	F	64	PRO
12	J	143	LYS
16	N	167	ASP
26	X	70	ILE
31	3	56	PRO
5	B	2	GLN
7	D	89	PRO
16	N	160	SER
25	W	49	ASN
28	Z	20	ARG
31	3	57	GLY
7	D	16	PRO
7	D	97	GLN
28	Z	43	GLY
4	A	211	LYS
4	A	236	GLY
7	D	28	GLY
24	V	40	PRO
7	D	27	ILE
17	O	108	GLY
20	R	106	GLY
7	D	69	ILE
7	D	135	VAL
13	K	39	GLY
20	R	81	PRO
5	B	30	PRO
13	K	111	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	
4	A	179/182 (98%)	169 (94%)	10 (6%)	21	42
5	B	282/283 (100%)	265 (94%)	17 (6%)	19	39
6	C	193/193 (100%)	176 (91%)	17 (9%)	10	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	D	117/148 (79%)	112 (96%)	5 (4%)	29	54
8	E	152/156 (97%)	148 (97%)	4 (3%)	46	72
9	F	93/94 (99%)	92 (99%)	1 (1%)	73	88
10	G	27/283 (10%)	27 (100%)	0	100	100
11	H	132/138 (96%)	126 (96%)	6 (4%)	27	52
12	J	118/121 (98%)	109 (92%)	9 (8%)	13	26
13	K	106/106 (100%)	101 (95%)	5 (5%)	26	50
14	L	113/127 (89%)	107 (95%)	6 (5%)	22	45
15	M	158/158 (100%)	151 (96%)	7 (4%)	28	53
16	N	149/150 (99%)	144 (97%)	5 (3%)	37	63
17	O	93/94 (99%)	90 (97%)	3 (3%)	39	65
18	P	113/117 (97%)	109 (96%)	4 (4%)	36	62
19	Q	79/80 (99%)	76 (96%)	3 (4%)	33	59
20	R	117/122 (96%)	114 (97%)	3 (3%)	46	72
21	S	71/74 (96%)	69 (97%)	2 (3%)	43	69
22	T	105/106 (99%)	101 (96%)	4 (4%)	33	59
23	U	44/52 (85%)	44 (100%)	0	100	100
24	V	51/57 (90%)	50 (98%)	1 (2%)	55	78
25	W	130/130 (100%)	124 (95%)	6 (5%)	27	51
26	X	66/74 (89%)	61 (92%)	5 (8%)	13	26
27	Y	120/196 (61%)	111 (92%)	9 (8%)	13	27
28	Z	60/68 (88%)	60 (100%)	0	100	100
29	1	46/47 (98%)	46 (100%)	0	100	100
30	2	42/46 (91%)	41 (98%)	1 (2%)	49	74
31	3	79/79 (100%)	76 (96%)	3 (4%)	33	59
32	I	58/130 (45%)	57 (98%)	1 (2%)	60	81
All	All	3093/3611 (86%)	2956 (96%)	137 (4%)	28	53

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	3	ARG
4	A	33	GLU

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Mol	Chain	Res	Type
4	A	36	ASP
4	A	69	LEU
4	A	78	ASP
4	A	94	LEU
4	A	120	ARG
4	A	125	ASN
4	A	179	MET
4	A	217	ARG
5	B	5	ARG
5	B	7	ARG
5	B	11	LEU
5	B	27	ASN
5	B	33	ASP
5	B	49	THR
5	B	63	GLU
5	B	98	THR
5	B	149	ASP
5	B	162	MET
5	B	195	ARG
5	B	251	VAL
5	B	254	GLN
5	B	280	VAL
5	B	304	PRO
5	B	307	ARG
5	B	312	ARG
6	C	2	GLN
6	C	27	ARG
6	C	67	GLN
6	C	76	ARG
6	C	91	PRO
6	C	94	THR
6	C	106	GLU
6	C	115	LEU
6	C	136	VAL
6	C	187	ARG
6	C	214	THR
6	C	222	ASP
6	C	223	LEU
6	C	234	VAL
6	C	236	THR
6	C	240	LEU
6	C	246	ARG

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Mol	Chain	Res	Type
7	D	24	HIS
7	D	61	PHE
7	D	86	THR
7	D	133	ASN
7	D	136	ARG
8	E	15	GLN
8	E	102	VAL
8	E	126	ILE
8	E	164	ASP
9	F	105	ASP
11	H	30	GLN
11	H	84	LYS
11	H	88	ARG
11	H	96	ARG
11	H	111	ASP
11	H	154	TYR
12	J	16	ASP
12	J	46	ILE
12	J	52	GLN
12	J	74	ARG
12	J	76	ASP
12	J	79	PHE
12	J	107	ASN
12	J	112	ASP
12	J	131	THR
13	K	7	ASP
13	K	10	GLN
13	K	49	LEU
13	K	98	VAL
13	K	129	THR
14	L	4	LYS
14	L	30	ARG
14	L	35	ARG
14	L	99	GLU
14	L	102	ASP
14	L	104	ASP
15	M	23	LEU
15	M	46	LEU
15	M	68	ARG
15	M	93	ARG
15	M	99	ARG
15	M	116	ASN

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Mol	Chain	Res	Type
15	M	164	THR
16	N	17	ARG
16	N	26	LEU
16	N	93	GLN
16	N	139	TRP
16	N	152	GLU
17	O	3	THR
17	O	43	VAL
17	O	115	ARG
18	P	21	VAL
18	P	52	LYS
18	P	91	LYS
18	P	98	ILE
19	Q	11	ARG
19	Q	57	ASP
19	Q	95	GLU
20	R	13	THR
20	R	39	THR
20	R	82	GLU
21	S	10	VAL
21	S	53	ASN
22	T	39	ASN
22	T	48	VAL
22	T	112	LEU
22	T	115	GLU
24	V	65	ASP
25	W	35	VAL
25	W	52	VAL
25	W	73	LEU
25	W	122	ARG
25	W	146	ILE
25	W	154	ARG
26	X	15	ARG
26	X	27	ASP
26	X	49	ARG
26	X	72	VAL
26	X	79	GLU
27	Y	141	THR
27	Y	144	ARG
27	Y	163	THR
27	Y	174	VAL
27	Y	186	ARG

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Mol	Chain	Res	Type
27	Y	189	ASN
27	Y	203	VAL
27	Y	204	ARG
27	Y	235	GLU
30	2	18	ASN
31	3	11	CYS
31	3	42	ARG
31	3	56	PRO
32	I	86	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (85) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	29	HIS
4	A	92	ASN
4	A	176	HIS
4	A	199	HIS
5	B	27	ASN
5	B	145	HIS
5	B	221	GLN
5	B	238	ASN
5	B	260	HIS
5	B	320	GLN
5	B	332	ASN
6	C	2	GLN
6	C	39	GLN
6	C	129	HIS
7	D	47	GLN
7	D	97	GLN
7	D	103	ASN
7	D	133	ASN
8	E	71	ASN
8	E	90	HIS
8	E	106	ASN
8	E	143	GLN
10	G	64	ASN
11	H	31	HIS
11	H	56	GLN
11	H	59	HIS
11	H	70	ASN
11	H	170	ASN
12	J	52	GLN

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Mol	Chain	Res	Type
12	J	107	ASN
13	K	10	GLN
14	L	18	HIS
14	L	41	HIS
14	L	42	ASN
15	M	24	GLN
15	M	26	GLN
15	M	58	GLN
15	M	143	ASN
15	M	170	ASN
16	N	40	ASN
16	N	93	GLN
16	N	107	ASN
18	P	50	GLN
18	P	66	GLN
18	P	73	HIS
18	P	88	GLN
18	P	118	GLN
19	Q	16	ASN
19	Q	40	HIS
20	R	61	GLN
20	R	94	ASN
20	R	98	ASN
20	R	113	HIS
20	R	117	HIS
21	S	25	GLN
21	S	53	ASN
22	T	39	ASN
22	T	43	ASN
22	T	73	HIS
23	U	39	ASN
23	U	48	ASN
24	V	29	ASN
24	V	60	GLN
25	W	2	HIS
25	W	110	GLN
25	W	119	HIS
25	W	125	HIS
25	W	141	HIS
26	X	23	HIS
27	Y	133	HIS
27	Y	134	HIS

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Mol	Chain	Res	Type
27	Y	149	GLN
27	Y	189	ASN
29	1	8	GLN
29	1	16	HIS
29	1	28	HIS
30	2	16	ASN
30	2	18	ASN
30	2	41	HIS
30	2	45	ASN
31	3	2	GLN
31	3	15	ASN
31	3	30	GLN
31	3	48	ASN
32	I	104	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	235 (8%)	32 (1%)
2	9	121/122 (99%)	15 (12%)	1 (0%)
3	4	0/8	-	-
All	All	2866/3052 (93%)	250 (8%)	33 (1%)

All (250) RNA backbone outliers are listed below:

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

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Mol	Chain	Res	Type
1	0	185	G
1	0	186	A
1	0	191	A
1	0	192	A
1	0	219	G
1	0	237	G
1	0	271	C
1	0	272	A
1	0	273	G
1	0	283	U
1	0	284	C
1	0	285	A
1	0	308	U
1	0	309	C
1	0	318	C
1	0	331	A
1	0	336	G
1	0	337	A
1	0	345	G
1	0	358	G
1	0	381	G
1	0	397	A
1	0	417	G
1	0	461	C
1	0	487	G
1	0	497	A
1	0	498	A
1	0	510	U
1	0	511	A
1	0	514	G
1	0	537	G
1	0	538	C
1	0	539	G
1	0	542	A
1	0	545	G
1	0	553	G
1	0	559	U
1	0	581	G
1	0	588	G
1	0	604	G
1	0	620	A
1	0	632	A

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Mol	Chain	Res	Type
1	0	644	G
1	0	660	A
1	0	688	A
1	0	701	U
1	0	759	C
1	0	777	U
1	0	809	G
1	0	821	U
1	0	835	U
1	0	840	U
1	0	857	A
1	0	858	U
1	0	868	G
1	0	869	G
1	0	871	G
1	0	872	U
1	0	875	A
1	0	877	G
1	0	878	G
1	0	885	G
1	0	905	C
1	0	920	C
1	0	921	G
1	0	923	A
1	0	953	G
1	0	960	G
1	0	961	A
1	0	1006	A
1	0	1008	C
1	0	1029	U
1	0	1045	G
1	0	1059	G
1	0	1060	C
1	0	1072	G
1	0	1081	A
1	0	1088	A
1	0	1109	U
1	0	1110	G
1	0	1119	G
1	0	1130	U
1	0	1131	G
1	0	1137	G

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Mol	Chain	Res	Type
1	0	1164	U
1	0	1165	G
1	0	1166	A
1	0	1174	A
1	0	1175	G
1	0	1185	U
1	0	1192	A
1	0	1193	A
1	0	1206	U
1	0	1216	G
1	0	1234	U
1	0	1237	U
1	0	1238	C
1	0	1239	G
1	0	1279	U
1	0	1289	C
1	0	1342	C
1	0	1353	C
1	0	1360	C
1	0	1377	C
1	0	1407	A
1	0	1409	G
1	0	1451	C
1	0	1474	C
1	0	1485	A
1	0	1505	U
1	0	1506	U
1	0	1524	U
1	0	1525	G
1	0	1526	A
1	0	1559	A
1	0	1564	C
1	0	1592	G
1	0	1603	A
1	0	1625	U
1	0	1626	A
1	0	1634	G
1	0	1656	A
1	0	1667	A
1	0	1682	A
1	0	1684	A
1	0	1685	A

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Mol	Chain	Res	Type
1	0	1692	C
1	0	1701	A
1	0	1710	A
1	0	1722	U
1	0	1723	G
1	0	1725	C
1	0	1730	G
1	0	1731	C
1	0	1732	A
1	0	1752	G
1	0	1778	A
1	0	1798	C
1	0	1819	G
1	0	1820	G
1	0	1829	A
1	0	1856	C
1	0	1879	U
1	0	1919	A
1	0	1942	A
1	0	1971	G
1	0	1973	A
1	0	1978	A
1	0	1979	G
1	0	1996	U
1	0	2008	U
1	0	2011	A
1	0	2012	U
1	0	2013	G
1	0	2033	G
1	0	2034	U
1	0	2064	U
1	0	2072	G
1	0	2073	G
1	0	2074	A
1	0	2096	A
1	0	2101	A
1	0	2102	G
1	0	2110	G
1	0	2238	A
1	0	2243	C
1	0	2258	A
1	0	2271	G

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Mol	Chain	Res	Type
1	0	2272	G
1	0	2291	A
1	0	2317	C
1	0	2321	A
1	0	2354	A
1	0	2361	A
1	0	2369	A
1	0	2422	U
1	0	2462	G
1	0	2469	A
1	0	2476	C
1	0	2480	G
1	0	2483	A
1	0	2507	G
1	0	2509	A
1	0	2511	A
1	0	2533	C
1	0	2537	G
1	0	2541	U
1	0	2542	C
1	0	2553	A
1	0	2564	G
1	0	2589	U
1	0	2601	A
1	0	2602	G
1	0	2608	C
1	0	2613	G
1	0	2637	A
1	0	2645	U
1	0	2649	A
1	0	2664	A
1	0	2681	A
1	0	2682	C
1	0	2726	U
1	0	2747	C
1	0	2748	G
1	0	2749	U
1	0	2750	G
1	0	2768	A
1	0	2786	G
1	0	2792	A
1	0	2800	A

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Mol	Chain	Res	Type
1	0	2811	A
1	0	2825	C
1	0	2850	C
1	0	2864	U
1	0	2867	G
1	0	2876	G
1	0	2890	A
1	0	2896	A
1	0	2903	C
1	0	2914	A
2	9	3002	U
2	9	3014	G
2	9	3022	G
2	9	3023	U
2	9	3024	U
2	9	3025	G
2	9	3041	C
2	9	3043	G
2	9	3044	A
2	9	3052	A
2	9	3057	A
2	9	3066	G
2	9	3077	A
2	9	3114	G
2	9	3122	C

All (33) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	129	A
1	0	169	A
1	0	338	C
1	0	603	A
1	0	699	C
1	0	834	G
1	0	857	A
1	0	869	G
1	0	871	G
1	0	877	G
1	0	1080	C
1	0	1237	U
1	0	1246	A

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Mol	Chain	Res	Type
1	0	1352	A
1	0	1377	C
1	0	1450	C
1	0	1563	G
1	0	1667	A
1	0	1692	C
1	0	1856	C
1	0	1942	A
1	0	2011	A
1	0	2313	C
1	0	2467	A
1	0	2526	C
1	0	2536	C
1	0	2541	U
1	0	2637	A
1	0	2649	A
1	0	2718	C
1	0	2726	U
1	0	2791	U
2	9	3065	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	PSU	0	2621	1	17,21,22	1.64	3 (17%)	20,30,33	5.44	4 (20%)
1	1MA	0	628	1	15,25,26	0.78	0	15,37,40	1.36	1 (6%)
1	OMU	0	2587	1,35	14,22,23	1.02	1 (7%)	14,31,34	1.15	1 (7%)
1	OMG	0	2588	1,3	18,26,27	1.10	2 (11%)	20,38,41	2.57	4 (20%)
1	UR3	0	2619	1	14,22,23	0.86	1 (7%)	15,32,35	0.56	0
3	5AA	4	76	1,3	18,26,27	0.74	0	15,38,41	0.75	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	1MA	0	628	1	-	0/3/25/26	0/3/3/3
1	OMU	0	2587	1,35	-	0/7/27/28	0/2/2/2
1	OMG	0	2588	1,3	-	0/5/27/28	0/3/3/3
1	UR3	0	2619	1	-	0/5/25/26	0/2/2/2
3	5AA	4	76	1,3	-	0/7/29/30	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C5-C1'	-4.95	1.48	1.52
1	0	2588	OMG	C6-N1	3.45	1.39	1.33
1	0	2621	PSU	C4-N3	3.03	1.38	1.33
1	0	2587	OMU	C4-N3	2.78	1.37	1.33
1	0	2621	PSU	C2-N1	2.66	1.43	1.38
1	0	2588	OMG	C8-N7	-2.26	1.30	1.34
1	0	2619	UR3	C6-N1	2.11	1.38	1.35

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	N1-C2-N3	-17.18	114.77	128.43
1	0	2621	PSU	C4-N3-C2	14.43	127.32	115.14
1	0	2588	OMG	C5-C6-N1	-8.58	111.70	123.43
1	0	2621	PSU	C5-C4-N3	-8.36	114.59	125.36
1	0	2588	OMG	C6-N1-C2	5.77	125.09	115.93
1	0	628	1MA	C2-N3-C4	-4.55	110.89	116.58
1	0	2587	OMU	C5-C4-N3	-3.96	114.59	123.31
1	0	2588	OMG	C2-N3-C4	-2.97	111.96	115.36
1	0	2621	PSU	C6-N1-C2	2.54	119.54	115.36
1	0	2588	OMG	N3-C2-N1	-2.49	123.90	127.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	2	0
1	0	2619	UR3	2	0
3	4	76	5AA	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 234 ligands modelled in this entry, 234 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	4	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	4	176:A	O3'	175:C	P	8.45

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	0	2749/2922 (94%)	0.03	65 (2%) 59 53	24, 51, 98, 161	0
2	9	122/122 (100%)	0.19	4 (3%) 46 39	46, 68, 96, 153	0
3	4	4/8 (50%)	-0.08	0 100 100	42, 42, 46, 46	0
4	A	237/240 (98%)	0.51	15 (6%) 20 15	31, 55, 94, 120	0
5	B	337/338 (99%)	0.97	32 (9%) 8 5	33, 65, 94, 103	0
6	C	246/246 (100%)	-0.01	5 (2%) 65 60	26, 51, 75, 86	0
7	D	140/177 (79%)	2.30	65 (46%) 0 0	64, 110, 134, 141	0
8	E	172/178 (96%)	1.66	54 (31%) 0 0	50, 81, 105, 115	0
9	F	119/120 (99%)	0.81	19 (15%) 1 1	57, 81, 107, 122	0
10	G	29/348 (8%)	2.93	17 (58%) 0 0	74, 95, 105, 107	0
11	H	160/171 (93%)	0.91	17 (10%) 6 4	42, 63, 94, 101	0
12	J	142/145 (97%)	0.68	4 (2%) 53 46	42, 59, 82, 97	0
13	K	132/132 (100%)	0.83	11 (8%) 11 8	37, 62, 86, 90	0
14	L	145/165 (87%)	0.74	19 (13%) 3 2	28, 74, 118, 131	0
15	M	194/194 (100%)	0.12	2 (1%) 82 80	33, 48, 64, 72	0
16	N	186/187 (99%)	0.83	27 (14%) 2 1	43, 69, 118, 124	0
17	O	115/116 (99%)	0.19	2 (1%) 70 66	43, 61, 79, 89	0
18	P	143/149 (95%)	0.52	5 (3%) 44 36	46, 62, 75, 81	0
19	Q	95/96 (98%)	0.35	2 (2%) 63 58	40, 50, 66, 77	0
20	R	150/155 (96%)	0.19	2 (1%) 77 73	36, 51, 72, 82	0
21	S	81/85 (95%)	0.34	4 (4%) 29 23	48, 65, 85, 94	0
22	T	119/120 (99%)	0.42	7 (5%) 22 17	44, 61, 90, 111	0
23	U	53/66 (80%)	0.97	6 (11%) 5 3	48, 63, 80, 88	0
24	V	65/71 (91%)	1.40	18 (27%) 0 0	59, 83, 117, 124	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	154/154 (100%)	0.39	1 (0%) 89 88	41, 57, 78, 88	0
26	X	82/92 (89%)	0.79	9 (10%) 5 3	49, 66, 89, 106	0
27	Y	142/241 (58%)	0.50	8 (5%) 24 19	32, 51, 74, 95	0
28	Z	73/83 (87%)	0.25	3 (4%) 37 30	45, 64, 78, 96	0
29	1	56/57 (98%)	-0.10	0 100 100	31, 38, 46, 61	0
30	2	46/50 (92%)	1.64	16 (34%) 0 0	40, 70, 123, 128	0
31	3	92/92 (100%)	0.37	3 (3%) 46 39	37, 60, 74, 89	0
32	I	70/162 (43%)	3.96	58 (82%) 0 0	108, 129, 152, 155	0
All	All	6650/7482 (88%)	0.44	500 (7%) 14 10	24, 58, 109, 161	0

All (500) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	I	93	GLN	11.8
32	I	133	THR	9.5
24	V	1	THR	8.2
7	D	88	LEU	8.1
32	I	137	VAL	8.0
7	D	69	ILE	7.7
10	G	27	ILE	7.6
32	I	114	PRO	7.1
32	I	96	PHE	6.9
32	I	71	GLY	6.8
2	9	3001	U	6.8
32	I	111	GLN	6.7
30	2	36	ASN	6.6
7	D	44	ILE	6.6
30	2	44	ARG	6.5
7	D	63	ILE	6.5
7	D	89	PRO	6.4
24	V	43	PRO	6.4
7	D	58	VAL	6.4
7	D	84	LEU	6.4
30	2	37	HIS	6.4
10	G	23	ILE	6.3
32	I	121	LEU	6.3
7	D	90	LEU	6.2
32	I	78	LEU	6.2
30	2	38	LYS	6.1

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Mol	Chain	Res	Type	RSRZ
32	I	113	HIS	6.1
32	I	81	ASP	6.0
24	V	39	ALA	5.9
4	A	37	VAL	5.9
32	I	116	LEU	5.8
7	D	57	THR	5.8
32	I	135	LEU	5.8
7	D	10	PHE	5.7
30	2	48	ASP	5.6
32	I	72	VAL	5.6
32	I	88	GLY	5.5
30	2	41	HIS	5.5
30	2	49	GLU	5.5
32	I	110	GLU	5.5
1	0	282	C	5.5
7	D	134	LEU	5.4
32	I	132	CYS	5.4
7	D	26	GLY	5.4
32	I	117	LEU	5.3
7	D	56	ARG	5.3
7	D	92	GLU	5.3
7	D	85	GLN	5.2
32	I	73	PRO	5.2
1	0	2237	G	5.2
32	I	77	GLU	5.2
7	D	65	GLU	5.2
7	D	64	ARG	5.1
10	G	24	VAL	5.1
8	E	100	ASP	5.1
1	0	1173	A	5.1
7	D	170	TYR	5.1
32	I	89	SER	5.0
32	I	102	VAL	5.0
1	0	1177	A	4.9
7	D	61	PHE	4.9
24	V	40	PRO	4.9
32	I	125	ALA	4.9
10	G	71	LEU	4.8
7	D	75	LEU	4.8
4	A	36	ASP	4.7
7	D	172	VAL	4.7
8	E	10	ASP	4.6

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Mol	Chain	Res	Type	RSRZ
14	L	80	ASP	4.6
7	D	40	ILE	4.6
2	9	3024	U	4.6
26	X	88	GLU	4.6
32	I	109	ALA	4.6
2	9	3023	U	4.6
8	E	45	ASP	4.5
30	2	42	TRP	4.5
7	D	41	LEU	4.5
7	D	70	GLY	4.5
23	U	54	THR	4.4
7	D	130	VAL	4.4
32	I	97	VAL	4.4
10	G	67	LEU	4.4
8	E	42	VAL	4.3
9	F	119	ARG	4.3
10	G	28	GLU	4.3
14	L	60	GLU	4.3
32	I	85	PHE	4.2
32	I	118	SER	4.2
1	0	1525	G	4.2
13	K	132	VAL	4.2
32	I	79	ILE	4.2
32	I	128	VAL	4.2
32	I	103	ASP	4.1
7	D	18	ILE	4.1
32	I	139	ILE	4.1
7	D	87	ALA	4.1
11	H	47	ILE	4.0
10	G	26	MET	4.0
1	0	1951	G	4.0
8	E	93	MET	3.9
16	N	147	ILE	3.9
8	E	83	GLY	3.9
32	I	107	GLN	3.9
7	D	86	THR	3.9
32	I	86	GLU	3.9
8	E	95	VAL	3.9
30	2	47	THR	3.9
8	E	92	PRO	3.9
7	D	50	VAL	3.8
28	Z	59	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
9	F	16	ALA	3.8
16	N	166	ALA	3.8
32	I	129	VAL	3.8
1	0	735	C	3.8
8	E	99	GLY	3.8
16	N	172	PHE	3.8
16	N	160	SER	3.7
22	T	112	LEU	3.7
8	E	148	ILE	3.7
32	I	75	THR	3.7
7	D	98	PHE	3.7
8	E	11	VAL	3.7
32	I	124	ALA	3.7
21	S	81	ILE	3.7
1	0	2238	A	3.7
1	0	1279	U	3.7
5	B	180	ASP	3.7
1	0	970	U	3.6
8	E	118	ILE	3.6
1	0	1199	A	3.6
32	I	91	GLU	3.6
32	I	92	PRO	3.6
9	F	18	GLU	3.6
24	V	38	GLY	3.6
10	G	20	VAL	3.6
32	I	95	ASP	3.6
5	B	104	GLU	3.6
32	I	84	GLY	3.6
18	P	77	ALA	3.5
7	D	27	ILE	3.5
27	Y	235	GLU	3.5
1	0	1172	G	3.5
5	B	119	HIS	3.5
10	G	22	ALA	3.5
26	X	85	VAL	3.5
9	F	44	SER	3.5
30	2	20	ARG	3.5
26	X	74	ALA	3.5
5	B	181	ILE	3.5
8	E	102	VAL	3.5
5	B	106	HIS	3.5
14	L	105	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
7	D	66	GLY	3.4
24	V	37	GLY	3.4
1	0	2004	U	3.4
30	2	35	ARG	3.4
8	E	48	VAL	3.4
9	F	117	GLU	3.4
9	F	27	GLY	3.4
30	2	45	ASN	3.4
22	T	50	VAL	3.4
7	D	59	GLY	3.4
1	0	960	G	3.4
10	G	64	ASN	3.4
7	D	93	LEU	3.4
7	D	55	LYS	3.4
16	N	181	ASP	3.3
1	0	280	C	3.3
7	D	104	PHE	3.3
8	E	82	TYR	3.3
11	H	83	TYR	3.3
14	L	124	ASP	3.3
16	N	68	GLU	3.3
23	U	47	ARG	3.3
16	N	64	SER	3.3
16	N	152	GLU	3.3
10	G	16	LYS	3.3
32	I	119	TYR	3.3
7	D	173	GLU	3.3
14	L	149	ARG	3.3
32	I	131	THR	3.3
5	B	64	GLY	3.3
1	0	1190	G	3.3
1	0	283	U	3.2
1	0	1198	U	3.2
10	G	73	ASP	3.2
4	A	237	GLY	3.2
16	N	163	PHE	3.2
32	I	104	GLN	3.2
7	D	11	HIS	3.2
14	L	104	ASP	3.2
22	T	117	ASP	3.2
32	I	83	ALA	3.2
7	D	106	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
5	B	116	PRO	3.2
28	Z	20	ARG	3.2
1	0	284	C	3.2
8	E	105	GLU	3.1
13	K	101	ASN	3.1
1	0	1130	U	3.1
24	V	59	ILE	3.1
1	0	1185	U	3.1
1	0	497	A	3.1
7	D	67	ASP	3.1
32	I	115	ASP	3.1
4	A	32	VAL	3.1
14	L	91	VAL	3.1
14	L	108	VAL	3.1
7	D	166	ILE	3.1
16	N	175	LEU	3.1
8	E	109	GLY	3.1
19	Q	95	GLU	3.1
30	2	43	ARG	3.0
24	V	41	GLU	3.0
8	E	22	VAL	3.0
7	D	135	VAL	3.0
8	E	170	ARG	3.0
7	D	83	PHE	3.0
32	I	106	LYS	3.0
27	Y	96	GLU	3.0
7	D	24	HIS	3.0
7	D	25	MET	3.0
8	E	122	THR	3.0
1	0	1163	G	2.9
1	0	285	A	2.9
8	E	126	ILE	2.9
32	I	87	THR	2.9
1	0	10	U	2.9
8	E	128	GLY	2.9
4	A	35	GLY	2.9
32	I	105	VAL	2.9
9	F	106	ALA	2.9
18	P	114	LEU	2.9
31	3	92	GLU	2.8
8	E	161	VAL	2.8
13	K	3	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
5	B	135	GLY	2.8
11	H	50	ILE	2.8
17	O	111	VAL	2.8
16	N	159	TYR	2.8
16	N	180	LEU	2.8
9	F	25	ASP	2.8
21	S	76	GLU	2.8
22	T	59	GLU	2.8
7	D	91	ALA	2.8
7	D	29	HIS	2.8
2	9	3002	U	2.8
8	E	88	TYR	2.8
8	E	87	PHE	2.8
7	D	16	PRO	2.8
1	0	1202	A	2.8
7	D	62	ASP	2.8
4	A	133	ARG	2.8
11	H	144	GLU	2.8
23	U	53	ASP	2.8
1	0	1174	A	2.8
9	F	17	LEU	2.8
7	D	17	ARG	2.8
21	S	16	ASN	2.7
7	D	47	GLN	2.7
7	D	23	VAL	2.7
1	0	1000	C	2.7
1	0	2249	G	2.7
32	I	94	GLU	2.7
4	A	31	LYS	2.7
9	F	107	ASP	2.7
1	0	138	U	2.7
22	T	119	ALA	2.7
8	E	44	GLY	2.7
16	N	182	GLY	2.7
8	E	108	LEU	2.7
27	Y	97	LEU	2.7
1	0	2508	C	2.7
8	E	121	ASP	2.7
22	T	116	ASP	2.7
11	H	171	ALA	2.7
14	L	81	VAL	2.7
9	F	15	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
27	Y	95	THR	2.7
31	3	22	VAL	2.6
5	B	133	GLU	2.6
16	N	157	PRO	2.6
32	I	74	PRO	2.6
5	B	97	LEU	2.6
11	H	65	SER	2.6
7	D	45	THR	2.6
8	E	154	ILE	2.6
1	0	969	G	2.6
5	B	140	LEU	2.6
24	V	45	ARG	2.6
24	V	49	LEU	2.6
32	I	136	GLY	2.6
5	B	328	ARG	2.6
8	E	145	ALA	2.6
24	V	52	ALA	2.6
10	G	21	ASP	2.6
10	G	66	LEU	2.6
9	F	26	THR	2.6
1	0	279	C	2.6
26	X	10	VAL	2.6
10	G	68	GLU	2.6
1	0	272	A	2.6
10	G	69	ARG	2.6
6	C	237	GLU	2.5
7	D	171	ASP	2.5
5	B	35	GLN	2.5
26	X	82	GLU	2.5
10	G	70	ALA	2.5
14	L	61	ALA	2.5
11	H	71	ARG	2.5
1	0	2769	C	2.5
1	0	1171	A	2.5
11	H	142	ASP	2.5
5	B	196	ALA	2.5
16	N	137	ALA	2.5
32	I	76	ALA	2.5
5	B	54	VAL	2.5
1	0	1181	A	2.5
4	A	128	LEU	2.5
5	B	142	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
9	F	103	GLU	2.5
9	F	109	GLU	2.5
16	N	138	ASP	2.5
13	K	119	GLN	2.5
16	N	183	ASP	2.5
13	K	5	GLY	2.4
7	D	74	THR	2.4
7	D	128	LEU	2.4
8	E	81	GLU	2.4
8	E	97	VAL	2.4
9	F	108	VAL	2.4
11	H	161	CYS	2.4
27	Y	141	THR	2.4
4	A	38	ILE	2.4
8	E	86	VAL	2.4
20	R	96	VAL	2.4
8	E	41	SER	2.4
11	H	45	VAL	2.4
11	H	150	PHE	2.4
32	I	90	GLY	2.4
8	E	144	THR	2.4
13	K	63	GLU	2.4
14	L	133	VAL	2.4
32	I	112	LYS	2.4
8	E	38	ILE	2.4
5	B	52	VAL	2.4
1	0	999	C	2.4
7	D	81	GLU	2.4
13	K	109	LEU	2.4
16	N	1	ALA	2.4
19	Q	20	ASP	2.4
13	K	131	ILE	2.4
8	E	6	GLU	2.4
8	E	80	TRP	2.4
30	2	31	ARG	2.4
5	B	65	MET	2.3
7	D	129	ASP	2.3
32	I	126	LYS	2.3
5	B	74	ILE	2.3
6	C	61	PHE	2.3
8	E	40	VAL	2.3
8	E	157	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
18	P	71	TYR	2.3
16	N	127	LEU	2.3
1	0	2509	A	2.3
1	0	1192	A	2.3
1	0	1200	A	2.3
5	B	51	VAL	2.3
8	E	111	LYS	2.3
8	E	16	ASP	2.3
24	V	3	LEU	2.3
8	E	104	ILE	2.3
5	B	100	VAL	2.3
13	K	88	VAL	2.3
20	R	14	ALA	2.3
23	U	52	THR	2.3
1	0	370	G	2.3
11	H	35	ARG	2.3
16	N	143	ARG	2.3
24	V	9	ARG	2.3
14	L	100	ALA	2.3
16	N	94	GLU	2.3
6	C	131	PHE	2.3
30	2	39	ARG	2.3
8	E	119	HIS	2.3
22	T	82	THR	2.3
27	Y	234	VAL	2.3
14	L	150	GLN	2.2
4	A	129	LEU	2.2
11	H	73	LEU	2.2
18	P	64	GLU	2.2
1	0	1213	C	2.2
5	B	73	VAL	2.2
8	E	124	VAL	2.2
1	0	281	U	2.2
8	E	53	GLU	2.2
11	H	167	PRO	2.2
7	D	53	LYS	2.2
7	D	71	ALA	2.2
8	E	117	THR	2.2
24	V	61	GLY	2.2
25	W	79	VAL	2.2
23	U	51	TRP	2.2
32	I	98	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
4	A	63	GLY	2.2
27	Y	98	GLN	2.2
1	0	1204	C	2.2
5	B	113	LEU	2.2
26	X	18	ARG	2.2
13	K	57	VAL	2.2
14	L	97	VAL	2.2
4	A	62	ASP	2.2
16	N	162	ASP	2.2
1	0	371	U	2.2
1	0	1625	U	2.2
1	0	1150	A	2.2
12	J	57	TYR	2.2
4	A	65	ARG	2.2
24	V	8	ILE	2.2
31	3	56	PRO	2.2
6	C	132	ASP	2.2
30	2	46	ASP	2.2
5	B	71	VAL	2.2
24	V	5	VAL	2.2
6	C	135	GLU	2.2
24	V	11	MET	2.2
8	E	132	THR	2.2
1	0	130	C	2.2
7	D	165	PHE	2.2
4	A	85	SER	2.1
14	L	106	VAL	2.1
14	L	118	LEU	2.1
1	0	2344	G	2.1
1	0	2768	A	2.1
7	D	54	ALA	2.1
7	D	139	TYR	2.1
8	E	89	SER	2.1
27	Y	193	LEU	2.1
14	L	102	ASP	2.1
1	0	716	G	2.1
1	0	736	A	2.1
1	0	2577	A	2.1
5	B	112	THR	2.1
16	N	150	TYR	2.1
1	0	2251	G	2.1
5	B	93	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
16	N	158	LEU	2.1
16	N	179	LEU	2.1
32	I	127	GLU	2.1
16	N	81	ALA	2.1
17	O	104	ASN	2.1
28	Z	36	ASP	2.1
5	B	296	LEU	2.1
14	L	96	VAL	2.1
1	0	1665	G	2.1
8	E	163	GLN	2.1
1	0	1169	U	2.1
1	0	717	C	2.1
1	0	1186	C	2.1
1	0	2717	C	2.1
15	M	164	THR	2.1
5	B	170	SER	2.1
15	M	165	GLY	2.1
23	U	43	GLY	2.1
8	E	5	LEU	2.1
14	L	59	GLU	2.1
16	N	156	GLU	2.1
11	H	85	MET	2.1
18	P	80	ARG	2.1
5	B	169	GLY	2.1
8	E	7	ILE	2.1
9	F	22	VAL	2.1
26	X	40	HIS	2.1
7	D	72	LYS	2.1
11	H	32	LYS	2.1
13	K	83	PRO	2.1
8	E	167	TYR	2.1
4	A	86	ALA	2.1
1	0	1205	U	2.0
1	0	2250	G	2.0
24	V	46	ILE	2.0
26	X	80	GLU	2.0
12	J	47	THR	2.0
12	J	6	PHE	2.0
5	B	84	LEU	2.0
1	0	1162	G	2.0
5	B	121	PRO	2.0
11	H	146	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
32	I	82	GLU	2.0
9	F	28	ALA	2.0
21	S	20	PHE	2.0
5	B	58	PRO	2.0
12	J	78	ILE	2.0
1	0	369	G	2.0
1	0	1179	C	2.0
8	E	127	ASP	2.0
7	D	48	MET	2.0
9	F	6	PHE	2.0
9	F	49	PHE	2.0
26	X	77	PHE	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
1	OMG	0	2588	24/25	0.90	0.20	30,33,38,40	0
1	UR3	0	2619	21/22	0.92	0.22	33,38,39,42	0
1	1MA	0	628	23/24	0.93	0.21	28,34,37,38	0
1	OMU	0	2587	21/22	0.93	0.17	31,35,40,41	0
3	5AA	4	76	24/25	0.93	0.23	40,44,46,47	0
1	PSU	0	2621	20/21	0.94	0.17	31,34,40,41	0

6.3 Carbohydrates ⓘ

There are no carbohydrates 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(\AA^2)	Q<0.9
33	MG	0	8063	1/1	0.30	0.19	71,71,71,71	0
35	NA	0	9184	1/1	0.32	0.89	83,83,83,83	0
33	MG	0	8116	1/1	0.46	0.18	62,62,62,62	0
33	MG	0	8091	1/1	0.50	0.07	79,79,79,79	0
33	MG	0	8068	1/1	0.53	0.07	60,60,60,60	0
35	NA	0	9110	1/1	0.53	0.34	43,43,43,43	0
35	NA	R	9186	1/1	0.56	0.43	78,78,78,78	0
35	NA	0	9177	1/1	0.59	0.45	68,68,68,68	0
35	NA	0	9124	1/1	0.59	0.22	66,66,66,66	0
33	MG	0	8090	1/1	0.60	0.31	65,65,65,65	0
35	NA	0	9102	1/1	0.61	0.25	45,45,45,45	0
36	CL	J	9302	1/1	0.63	0.21	79,79,79,79	0
35	NA	0	9170	1/1	0.64	0.29	49,49,49,49	0
33	MG	0	8103	1/1	0.64	0.26	65,65,65,65	0
35	NA	0	9155	1/1	0.64	0.49	79,79,79,79	0
35	NA	0	9182	1/1	0.64	0.49	81,81,81,81	0
35	NA	0	9129	1/1	0.66	0.25	57,57,57,57	0
33	MG	0	8025	1/1	0.66	0.14	46,46,46,46	0
35	NA	0	9157	1/1	0.67	0.11	73,73,73,73	0
33	MG	0	8058	1/1	0.68	0.16	56,56,56,56	0
33	MG	9	8052	1/1	0.68	0.12	54,54,54,54	0
33	MG	0	8101	1/1	0.69	0.40	72,72,72,72	0
35	NA	0	9105	1/1	0.69	0.26	44,44,44,44	0
36	CL	J	9301	1/1	0.69	0.20	78,78,78,78	0
35	NA	0	9176	1/1	0.69	0.33	49,49,49,49	0
33	MG	0	8059	1/1	0.70	0.15	51,51,51,51	0
33	MG	0	8053	1/1	0.70	0.16	57,57,57,57	0
33	MG	0	8113	1/1	0.70	0.20	52,52,52,52	0
33	MG	0	8034	1/1	0.71	0.13	38,38,38,38	0
33	MG	0	8117	1/1	0.72	0.15	37,37,37,37	0
33	MG	0	8084	1/1	0.72	0.13	38,38,38,38	0
35	NA	0	9111	1/1	0.73	0.21	61,61,61,61	0
36	CL	N	9307	1/1	0.73	0.33	72,72,72,72	0
35	NA	S	9112	1/1	0.73	0.28	73,73,73,73	0
35	NA	0	9121	1/1	0.73	0.82	55,55,55,55	0
35	NA	0	9162	1/1	0.75	0.56	64,64,64,64	0
35	NA	0	9133	1/1	0.76	0.15	34,34,34,34	0
33	MG	B	8056	1/1	0.76	0.10	47,47,47,47	0
36	CL	J	9321	1/1	0.77	0.18	55,55,55,55	0
33	MG	0	8092	1/1	0.77	0.45	90,90,90,90	0
33	MG	0	8021	1/1	0.78	0.17	32,32,32,32	0
33	MG	B	8055	1/1	0.78	0.20	62,62,62,62	0
33	MG	0	8093	1/1	0.78	0.20	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	NA	0	9181	1/1	0.79	0.35	56,56,56,56	0
35	NA	B	9158	1/1	0.79	0.85	70,70,70,70	0
36	CL	0	9315	1/1	0.79	0.26	80,80,80,80	0
33	MG	0	8049	1/1	0.79	0.43	81,81,81,81	0
33	MG	0	8050	1/1	0.79	0.14	69,69,69,69	0
33	MG	0	8079	1/1	0.79	0.10	29,29,29,29	0
33	MG	0	8088	1/1	0.80	0.15	38,38,38,38	0
33	MG	0	8047	1/1	0.80	0.18	86,86,86,86	0
33	MG	0	8038	1/1	0.80	0.17	32,32,32,32	0
36	CL	3	9304	1/1	0.80	0.12	61,61,61,61	0
33	MG	0	8033	1/1	0.80	0.11	38,38,38,38	0
35	NA	0	9144	1/1	0.80	0.14	33,33,33,33	0
35	NA	0	9142	1/1	0.81	0.26	47,47,47,47	0
35	NA	0	9126	1/1	0.81	0.17	41,41,41,41	0
33	MG	9	8095	1/1	0.81	0.10	77,77,77,77	0
33	MG	0	8111	1/1	0.82	0.09	52,52,52,52	0
35	NA	0	9101	1/1	0.82	0.25	40,40,40,40	0
35	NA	0	9113	1/1	0.82	0.36	67,67,67,67	0
33	MG	0	8018	1/1	0.82	0.16	42,42,42,42	0
35	NA	0	9161	1/1	0.82	0.22	56,56,56,56	0
35	NA	0	9125	1/1	0.82	0.22	59,59,59,59	0
33	MG	0	8006	1/1	0.82	0.09	37,37,37,37	0
33	MG	0	8023	1/1	0.82	0.24	52,52,52,52	0
33	MG	0	8099	1/1	0.82	0.17	53,53,53,53	0
33	MG	0	8044	1/1	0.83	0.13	55,55,55,55	0
33	MG	0	8104	1/1	0.83	0.17	55,55,55,55	0
33	MG	0	8008	1/1	0.83	0.08	37,37,37,37	0
35	NA	0	9117	1/1	0.84	0.26	61,61,61,61	0
35	NA	0	9171	1/1	0.84	0.21	52,52,52,52	0
35	NA	0	9169	1/1	0.84	0.33	60,60,60,60	0
35	NA	C	9104	1/1	0.84	0.14	40,40,40,40	0
33	MG	K	8069	1/1	0.84	0.09	52,52,52,52	0
33	MG	0	8003	1/1	0.84	0.15	31,31,31,31	0
33	MG	Y	8109	1/1	0.84	0.34	44,44,44,44	0
35	NA	0	9139	1/1	0.84	0.16	31,31,31,31	0
35	NA	0	9173	1/1	0.84	0.22	62,62,62,62	0
33	MG	0	8071	1/1	0.85	0.18	66,66,66,66	0
33	MG	0	8032	1/1	0.85	0.20	41,41,41,41	0
33	MG	0	8045	1/1	0.85	0.19	73,73,73,73	0
33	MG	0	8007	1/1	0.85	0.11	27,27,27,27	0
35	NA	0	9164	1/1	0.85	0.28	53,53,53,53	0
35	NA	9	9151	1/1	0.86	0.14	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
36	CL	L	9310	1/1	0.86	0.16	63,63,63,63	0
33	MG	0	8082	1/1	0.86	0.16	76,76,76,76	0
35	NA	H	9122	1/1	0.86	0.17	72,72,72,72	0
33	MG	3	8078	1/1	0.86	0.10	43,43,43,43	0
33	MG	0	8072	1/1	0.86	0.26	60,60,60,60	0
35	NA	0	9131	1/1	0.86	0.20	41,41,41,41	0
35	NA	0	9156	1/1	0.86	0.32	49,49,49,49	0
33	MG	0	8026	1/1	0.87	0.10	24,24,24,24	0
33	MG	0	8057	1/1	0.87	0.15	42,42,42,42	0
37	CD	U	9201	1/1	0.87	0.11	74,74,74,74	0
33	MG	0	8064	1/1	0.87	0.15	30,30,30,30	0
35	NA	0	9135	1/1	0.87	0.40	52,52,52,52	0
35	NA	R	9138	1/1	0.88	0.14	63,63,63,63	0
36	CL	0	9311	1/1	0.88	0.16	53,53,53,53	0
35	NA	0	9119	1/1	0.88	0.10	44,44,44,44	0
36	CL	0	9316	1/1	0.88	0.31	66,66,66,66	0
35	NA	0	9174	1/1	0.88	0.35	62,62,62,62	0
34	K	0	9003	1/1	0.88	0.20	64,64,64,64	0
35	NA	0	9166	1/1	0.88	0.12	69,69,69,69	0
33	MG	0	8009	1/1	0.88	0.13	30,30,30,30	0
35	NA	0	9141	1/1	0.89	0.10	45,45,45,45	0
35	NA	0	9123	1/1	0.89	0.30	44,44,44,44	0
33	MG	0	8080	1/1	0.89	0.18	41,41,41,41	0
35	NA	0	9179	1/1	0.89	0.29	70,70,70,70	0
35	NA	9	9183	1/1	0.89	0.14	60,60,60,60	0
35	NA	H	9109	1/1	0.89	0.13	34,34,34,34	0
35	NA	0	9149	1/1	0.89	0.18	38,38,38,38	0
33	MG	0	8096	1/1	0.89	0.15	53,53,53,53	0
35	NA	0	9185	1/1	0.89	0.37	51,51,51,51	0
35	NA	0	9165	1/1	0.89	0.23	47,47,47,47	0
33	MG	0	8100	1/1	0.89	0.44	70,70,70,70	0
35	NA	R	9137	1/1	0.89	0.15	44,44,44,44	0
33	MG	0	8037	1/1	0.89	0.11	45,45,45,45	0
35	NA	Q	9148	1/1	0.89	0.21	38,38,38,38	0
33	MG	0	8108	1/1	0.90	0.11	58,58,58,58	0
33	MG	0	8070	1/1	0.90	0.10	57,57,57,57	0
33	MG	0	8077	1/1	0.90	0.09	28,28,28,28	0
35	NA	0	9178	1/1	0.90	0.48	57,57,57,57	0
33	MG	0	8036	1/1	0.90	0.13	35,35,35,35	0
33	MG	0	8027	1/1	0.90	0.09	37,37,37,37	0
33	MG	0	8106	1/1	0.90	0.07	54,54,54,54	0
35	NA	A	9145	1/1	0.90	0.20	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	NA	0	9106	1/1	0.90	0.37	38,38,38,38	0
33	MG	0	8015	1/1	0.90	0.12	33,33,33,33	0
33	MG	0	8081	1/1	0.90	0.16	52,52,52,52	0
33	MG	0	8013	1/1	0.91	0.19	33,33,33,33	0
33	MG	0	8016	1/1	0.91	0.29	50,50,50,50	0
33	MG	0	8107	1/1	0.91	0.10	53,53,53,53	0
36	CL	0	9317	1/1	0.91	0.09	61,61,61,61	0
33	MG	0	8014	1/1	0.91	0.07	43,43,43,43	0
37	CD	1	9202	1/1	0.91	0.07	62,62,62,62	0
33	MG	0	8115	1/1	0.91	0.09	57,57,57,57	0
33	MG	0	8085	1/1	0.91	0.19	72,72,72,72	0
33	MG	0	8030	1/1	0.91	0.17	35,35,35,35	0
35	NA	0	9127	1/1	0.91	0.12	42,42,42,42	0
36	CL	Y	9320	1/1	0.91	0.12	52,52,52,52	0
33	MG	0	8086	1/1	0.91	0.12	50,50,50,50	0
33	MG	0	8002	1/1	0.91	0.14	39,39,39,39	0
33	MG	4	8118	1/1	0.91	0.13	41,41,41,41	0
33	MG	T	8073	1/1	0.92	0.13	59,59,59,59	0
33	MG	0	8022	1/1	0.92	0.09	35,35,35,35	0
33	MG	0	8061	1/1	0.92	0.08	37,37,37,37	0
35	NA	0	9172	1/1	0.92	0.26	62,62,62,62	0
33	MG	0	8001	1/1	0.92	0.11	35,35,35,35	0
33	MG	0	8094	1/1	0.92	0.11	73,73,73,73	0
35	NA	J	9146	1/1	0.92	0.08	42,42,42,42	0
33	MG	0	8010	1/1	0.92	0.11	28,28,28,28	0
33	MG	0	8060	1/1	0.92	0.23	46,46,46,46	0
36	CL	B	9319	1/1	0.92	0.22	55,55,55,55	0
33	MG	0	8041	1/1	0.92	0.25	79,79,79,79	0
34	K	0	9002	1/1	0.92	0.12	48,48,48,48	0
35	NA	0	9136	1/1	0.92	0.09	55,55,55,55	0
33	MG	0	8119	1/1	0.92	0.20	62,62,62,62	0
33	MG	0	8046	1/1	0.92	0.09	59,59,59,59	0
33	MG	0	8035	1/1	0.92	0.12	49,49,49,49	0
35	NA	0	9163	1/1	0.92	0.20	65,65,65,65	0
35	NA	0	9140	1/1	0.93	0.26	47,47,47,47	0
35	NA	0	9134	1/1	0.93	0.15	41,41,41,41	0
37	CD	O	9205	1/1	0.93	0.05	143,143,143,143	0
35	NA	0	9130	1/1	0.93	0.12	45,45,45,45	0
35	NA	0	9115	1/1	0.93	0.14	37,37,37,37	0
35	NA	0	9128	1/1	0.93	0.09	43,43,43,43	0
33	MG	0	8011	1/1	0.93	0.19	20,20,20,20	0
35	NA	0	9114	1/1	0.93	0.21	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
36	CL	A	9309	1/1	0.93	0.25	61,61,61,61	0
33	MG	0	8114	1/1	0.93	0.07	56,56,56,56	0
35	NA	0	9108	1/1	0.93	0.10	49,49,49,49	0
33	MG	0	8075	1/1	0.93	0.16	57,57,57,57	0
33	MG	0	8012	1/1	0.93	0.13	32,32,32,32	0
36	CL	0	9313	1/1	0.94	0.13	60,60,60,60	0
33	MG	0	8089	1/1	0.94	0.10	56,56,56,56	0
33	MG	0	8005	1/1	0.94	0.19	36,36,36,36	0
36	CL	0	9303	1/1	0.94	0.12	53,53,53,53	0
33	MG	0	8031	1/1	0.94	0.13	30,30,30,30	0
33	MG	0	8051	1/1	0.94	0.08	72,72,72,72	0
35	NA	0	9152	1/1	0.94	0.50	61,61,61,61	0
33	MG	0	8083	1/1	0.94	0.09	42,42,42,42	0
36	CL	0	9314	1/1	0.94	0.11	49,49,49,49	0
36	CL	0	9312	1/1	0.94	0.28	59,59,59,59	0
33	MG	A	8066	1/1	0.94	0.06	66,66,66,66	0
35	NA	0	9168	1/1	0.94	0.08	49,49,49,49	0
33	MG	0	8102	1/1	0.94	0.10	58,58,58,58	0
33	MG	0	8098	1/1	0.94	0.10	47,47,47,47	0
35	NA	0	9116	1/1	0.94	0.17	42,42,42,42	0
35	NA	0	9175	1/1	0.94	0.34	52,52,52,52	0
35	NA	0	9120	1/1	0.95	0.26	52,52,52,52	0
35	NA	0	9103	1/1	0.95	0.26	43,43,43,43	0
35	NA	0	9107	1/1	0.95	0.17	46,46,46,46	0
35	NA	0	9150	1/1	0.95	0.23	42,42,42,42	0
33	MG	0	8028	1/1	0.95	0.18	41,41,41,41	0
33	MG	0	8040	1/1	0.95	0.14	56,56,56,56	0
33	MG	0	8020	1/1	0.95	0.13	31,31,31,31	0
33	MG	0	8097	1/1	0.95	0.09	40,40,40,40	0
33	MG	0	8048	1/1	0.95	0.07	56,56,56,56	0
35	NA	0	9160	1/1	0.95	0.35	46,46,46,46	0
33	MG	0	8087	1/1	0.95	0.27	59,59,59,59	0
35	NA	0	9167	1/1	0.95	0.07	52,52,52,52	0
33	MG	0	8039	1/1	0.96	0.05	52,52,52,52	0
33	MG	0	8067	1/1	0.96	0.16	49,49,49,49	0
33	MG	0	8042	1/1	0.96	0.06	44,44,44,44	0
33	MG	A	8065	1/1	0.96	0.17	45,45,45,45	0
35	NA	0	9159	1/1	0.96	0.24	50,50,50,50	0
36	CL	R	9306	1/1	0.96	0.13	57,57,57,57	0
35	NA	M	9147	1/1	0.96	0.14	25,25,25,25	0
33	MG	0	8110	1/1	0.96	0.15	32,32,32,32	0
36	CL	0	9322	1/1	0.96	0.18	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	NA	L	9180	1/1	0.96	0.46	51,51,51,51	0
33	MG	0	8043	1/1	0.96	0.11	47,47,47,47	0
33	MG	0	8062	1/1	0.96	0.07	51,51,51,51	0
33	MG	0	8112	1/1	0.97	0.07	39,39,39,39	0
37	CD	Z	9203	1/1	0.97	0.09	67,67,67,67	0
33	MG	0	8004	1/1	0.97	0.09	34,34,34,34	0
35	NA	0	9154	1/1	0.97	0.14	33,33,33,33	0
33	MG	0	8029	1/1	0.97	0.07	36,36,36,36	0
33	MG	0	8024	1/1	0.97	0.17	39,39,39,39	0
35	NA	0	9153	1/1	0.97	0.19	21,21,21,21	0
33	MG	0	8017	1/1	0.97	0.14	29,29,29,29	0
35	NA	0	9118	1/1	0.97	0.22	62,62,62,62	0
33	MG	2	8076	1/1	0.97	0.14	55,55,55,55	0
35	NA	0	9143	1/1	0.98	0.17	33,33,33,33	0
37	CD	3	9204	1/1	0.98	0.06	64,64,64,64	0
34	K	0	9001	1/1	0.98	0.14	71,71,71,71	0
35	NA	0	9132	1/1	0.98	0.06	34,34,34,34	0
33	MG	0	8054	1/1	0.98	0.10	29,29,29,29	0
33	MG	0	8019	1/1	0.98	0.14	35,35,35,35	0
36	CL	M	9318	1/1	0.98	0.17	47,47,47,47	0
36	CL	O	9308	1/1	0.98	0.27	79,79,79,79	0
36	CL	0	9305	1/1	0.98	0.11	55,55,55,55	0
33	MG	0	8074	1/1	0.99	0.08	37,37,37,37	0

6.5 Other polymers

There are no such residues in this entry.