



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:03 PM GMT

PDB ID : 1VQK
Title : The structure of CCDA-PHE-CAP-BIO bound to the a site of the ribosomal subunit of haloarcula marismortui
Authors : Schmeing, T.M.; Steitz, T.A.
Deposited on : 2004-12-16
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

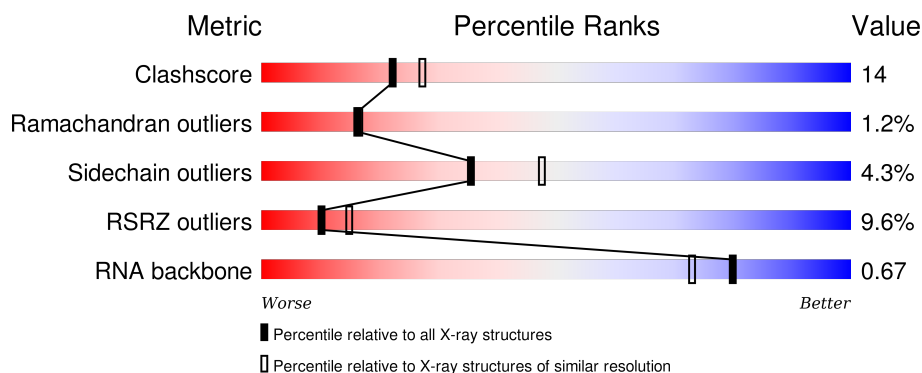
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)
RNA backbone	2183	1011 (2.84-1.76)

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

Mol	Chain	Length	Quality of chain
1	0	2922	<div> <div>3%</div> <div>65%</div> <div>24%</div> <div>5%</div> <div>6%</div> </div>
2	9	122	<div> <div>7%</div> <div>57%</div> <div>34%</div> <div>8%</div> <div>.</div> </div>
3	4	5	<div> <div>20%</div> <div>40%</div> <div>60%</div> </div>
4	A	240	<div> <div>8%</div> <div>63%</div> <div>32%</div> <div>.</div> <div>.</div> </div>
5	B	338	<div> <div>4%</div> <div>59%</div> <div>35%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
6	C	246	
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	195	
16	N	187	
17	O	116	
18	P	149	
19	Q	96	
20	R	155	
21	S	85	
22	T	120	
23	U	66	
24	V	71	
25	W	154	
26	X	92	
27	Y	241	
28	Z	83	
29	1	57	
30	2	50	

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Mol	Chain	Length	Quality of chain
31	3	92	
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	8001	-	-	-	X
33	MG	0	8008	-	-	-	X
33	MG	0	8012	-	-	-	X
33	MG	0	8013	-	-	-	X
33	MG	0	8017	-	-	-	X
33	MG	0	8020	-	-	-	X
33	MG	0	8027	-	-	-	X
33	MG	0	8038	-	-	-	X
33	MG	0	8057	-	-	-	X
33	MG	0	8080	-	-	-	X
33	MG	0	8084	-	-	-	X
33	MG	0	8097	-	-	-	X
33	MG	0	8107	-	-	-	X
34	K	0	9001	-	-	-	X
35	NA	0	9115	-	-	-	X
35	NA	0	9118	-	-	-	X
35	NA	0	9120	-	-	-	X
35	NA	0	9125	-	-	-	X
35	NA	0	9127	-	-	-	X
35	NA	0	9132	-	-	-	X
35	NA	0	9150	-	-	-	X
35	NA	0	9156	-	-	-	X
35	NA	0	9159	-	-	-	X
35	NA	0	9161	-	-	-	X
35	NA	0	9162	-	-	-	X
35	NA	0	9164	-	-	-	X
35	NA	0	9168	-	-	-	X
35	NA	0	9171	-	-	-	X
35	NA	0	9172	-	-	-	X
35	NA	0	9173	-	-	-	X
35	NA	0	9174	-	-	-	X
35	NA	0	9177	-	-	-	X
35	NA	0	9185	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	NA	9	9183	-	-	-	X
37	SR	0	9406	-	-	-	X
37	SR	0	9475	-	-	-	X
37	SR	0	9482	-	-	-	X
37	SR	0	9500	-	-	-	X
37	SR	0	9515	-	-	-	X
37	SR	B	9521	-	-	-	X

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 99036 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			

- 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'-R(*CP*CP*(DA)*(PHE)*(ACA))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	4	5	Total	C	N	O	P	0	0	0
			73	40	12	19	2			

- 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	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			
			735	450	141	144	0	0	0

- 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		
			1149	713	209	223	4	0	0

- 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		
			641	389	111	138	3	0	0

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

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

- 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		
			410	244	75	86	5	0	0

- 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		
			499	304	94	100	1	0	0

- 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		
			1196	737	209	244	6	0	0

- 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	87	Total	Mg	0	0
			87	87		
33	Y	1	Total	Mg	0	0
			1	1		
33	K	1	Total	Mg	0	0
			1	1		
33	B	1	Total	Mg	0	0
			1	1		
33	A	1	Total	Mg	0	0
			1	1		
33	T	1	Total	Mg	0	0
			1	1		
33	9	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	2	Total	K	0	0
			2	2		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	64	Total	Na	0	0
			64	64		
35	J	1	Total	Na	0	0
			1	1		
35	Q	1	Total	Na	0	0
			1	1		
35	D	1	Total	Na	0	0
			1	1		
35	C	1	Total	Na	0	0
			1	1		
35	3	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	R	3	Total 3	Na 3	0	0
35	9	1	Total 1	Na 1	0	0
35	S	1	Total 1	Na 1	0	0
35	M	1	Total 1	Na 1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	10	Total 10	Cl 10	0	0
36	J	3	Total 3	Cl 3	0	0
36	B	1	Total 1	Cl 1	0	0
36	A	1	Total 1	Cl 1	0	0
36	N	1	Total 1	Cl 1	0	0
36	O	1	Total 1	Cl 1	0	0
36	R	1	Total 1	Cl 1	0	0
36	Y	1	Total 1	Cl 1	0	0
36	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 STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	0	98	Total 98	Sr 98	0	0
37	1	2	Total 2	Sr 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	H	1	Total 1	Sr 1	0	0
37	B	2	Total 2	Sr 2	0	0
37	3	1	Total 1	Sr 1	0	0
37	A	3	Total 3	Sr 3	0	0
37	R	1	Total 1	Sr 1	0	0
37	9	3	Total 3	Sr 3	0	0
37	L	1	Total 1	Sr 1	0	0
37	S	1	Total 1	Sr 1	0	0
37	F	1	Total 1	Sr 1	0	0

- Molecule 38 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	O	1	Total 1	Cd 1	0	0
38	Z	1	Total 1	Cd 1	0	0
38	1	1	Total 1	Cd 1	0	0
38	3	1	Total 1	Cd 1	0	0
38	U	1	Total 1	Cd 1	0	0

- Molecule 39 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	0	5769	Total 5769	O 5769	0	0
39	9	140	Total 140	O 140	0	0
39	A	121	Total 121	O 121	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	B	144	Total 144	O 144	0	0
39	C	177	Total 177	O 177	0	0
39	D	48	Total 48	O 48	0	0
39	E	44	Total 44	O 44	0	0
39	F	27	Total 27	O 27	0	0
39	G	17	Total 17	O 17	0	0
39	H	69	Total 69	O 69	0	0
39	J	52	Total 52	O 52	0	0
39	K	57	Total 57	O 57	0	0
39	L	81	Total 81	O 81	0	0
39	M	130	Total 130	O 130	0	0
39	N	61	Total 61	O 61	0	0
39	O	40	Total 40	O 40	0	0
39	P	64	Total 64	O 64	0	0
39	Q	49	Total 49	O 49	0	0
39	R	82	Total 82	O 82	0	0
39	S	32	Total 32	O 32	0	0
39	T	37	Total 37	O 37	0	0
39	U	29	Total 29	O 29	0	0
39	V	14	Total 14	O 14	0	0
39	W	69	Total 69	O 69	0	0

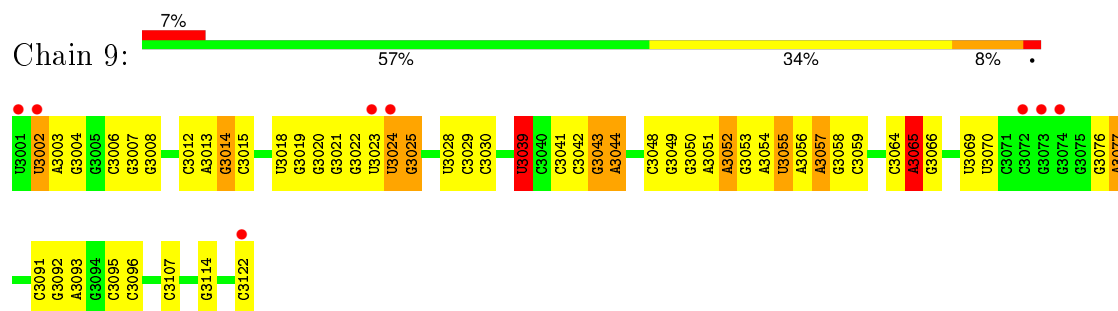
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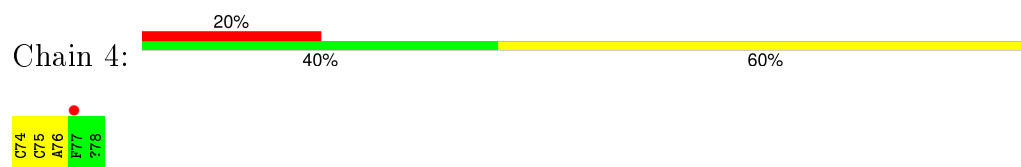
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	X	24	Total 24	O 24	0	0
39	Y	96	Total 96	O 96	0	0
39	Z	31	Total 31	O 31	0	0
39	1	50	Total 50	O 50	0	0
39	2	40	Total 40	O 40	0	0
39	3	67	Total 67	O 67	0	0
39	I	7	Total 7	O 7	0	0

A2840	G2748	G2632	C2510	G2412	G2271	U2133	G1985	G1878	A1759	A1642	C1477	G1299	G1190
A2841	U2749	A2633	A2511	A2413	G2272	G2134	U1996	U1879	U1766	U1654	U1478	G1311	A1191
G2842	G2750	A2634	A2521	A2414	A2291	A2135	U2003	C1882	G1767	G1655	C1495	G1314	A1192
G2851	G2754	A2635	G2524	A2415	A2302	C	G2005	G1902	C1768	A1656	G1496	U1314	A1193
A2852	U2756	A2637	G2525	G2417	C2309	U	C2006	U1903	C1769	A1659	A1501	A1328	G1195
U2853	A2761	C2644	C2526	G2418	C2309	G	U2007	A1919	A1778	G1660	A1502	A1331	C1196
A2856	C2762	U2645	U2531	U2419	C2313	G	U2008	C1920	A1779	C1666	U1503	A1332	U1198
C2857	U2649	G2420	U2532	G2420	G2314	G	A2011	C1921	C1786	A1667	A1504	U1333	A1199
U2858	C2765	U2422	C2533	G2421	G2315	G	U2012	A1922	C1787	U1668	U1505	C1334	C1201
U2866	U2652	U2422	C2534	G2422	G2316	U	G2013	G1926	U1768	U1668	U1506	C1335	A1202
G2867	A2653	G2426	U2535	G2426	C2317	C	G2014	G1927	G1789	G1681	A1522	G1203	G1203
G2868	C2536	C2427	C2537	C2427	U2320	A	A2015	A1928	G1794	A1682	G1523	G1340	C1204
G2869	A2538	U2435	A2538	U2435	A2321	A	U2016	G1929	G1795	A1683	U1524	A1341	U1205
G2876	U2541	C2443	U2541	C2443	U2326	A	U2032	U1937	A1796	A1684	G1525	C1342	U1206
G2877	U2545	G2452	U2545	G2452	C2329	G	G2033	G1938	A1797	A1685	A1526	C1343	A1207
U2878	U2545	G2453	U2545	G2453	U2330	U	U2034	U1939	C1798	G1686	A1527	U1350	C1208
A2879	C2548	A2456	C2548	A2456	U2330	G	C2035	C1940	G1799	C1687	G1528	G1351	G1210
A2883	G2785	U2457	C2552	U2457	G2338	A	U2042	A1941	G1809	C1692	G1552	A1352	G1211
G2884	G2786	U2457	A2553	U2457	A	G	U2043	C1943	C1818	G1700	G1555	C1360	G1212
A2890	U2791	G2462	U2563	G2462	C	U	U2044	C1946	G1819	A1701	U1559	G1363	G1216
C2894	A2792	A2465	C2564	A2465	A	A	G2053	G1947	G1820	U1702	U	U1218	G1217
G2895	G2793	A2466	C2565	A2466	G	U	A2054	G1948	A1821	A1710	C1562	A1372	U1219
A2896	U2795	A2467	C2565	A2467	C	G	G2061	G1949	A1822	C1714	C1564	G1377	G1226
G2897	U2796	A2468	A2568	A2468	C2346	A	A2062	G1950	A1829	C1715	G1564	G1378	C1229
A2898	A2681	C2472	A2569	A2468	C2347	G	U2063	U	C1834	A1717	A1574	C1384	A1230
G2900	C2682	U2472	G2578	C2472	U2348	G	U2064	A	U1835	G1718	C1573	A1232	A1231
C2901	A2694	C2476	G2578	C2476	A2353	C	A2067	C	A1836	U1722	A1574	A1406	U1234
A2902	U2698	G2480	U2586	G2480	C2354	G	G2068	C	U1837	G1723	G1592	A1407	A1233
C2903	G2697	G2481	U2587	G2481	C2355	U	A	U	U1838	G1724	C1593	U1408	G1235
A2906	G2698	G2482	G2588	G2482	A2356	C	G2072	A	A1839	U1724	C1594	U1409	A1236
G2907	A2810	A2483	U2589	A2483	A2356	G	A2074	G	A1840	G1725	G1595	U1237	U1237
A2908	G2812	C2487	C2591	A2483	A2361	A	A2074	C	A1845	G1730	U1596	U1419	C1238
G2909	A2813	C2487	G2592	C2487	A2362	U	A2081	A	U1846	C1731	A1597	G1239	G1239
A2910	G2814	C2487	G2592	C2487	A2363	C	A2081	C	A1847	A1732	A1598	U1422	A1242
C2911	G2815	A2490	A2599	A2490	A2364	C	A2089	C	G1848	A1736	A1603	C1423	A1243
A2912	U2711	G2491	A2600	G2491	G2365	C	A2090	U1964	G1849	U1736	A1604	C1426	G1243
C2913	G2712	U2492	A2601	U2492	C2369	A	G2091	C1965	C1853	G1739	G1605	U1244	U1244
A2914	G2715	C2493	G2602	C2493	A2369	G	A2096	U1967	C1856	U1741	A1615	G1430	A1246
A	G2716	U2499	C2608	U2499	A2372	U	A2096	C	C1856	U1741	A1615	U1435	A1252
C	C2717	C2500	C2608	C2500	U2373	A	A2100	G1971	C1861	G1744	U1625	C1253	C1253
C	C2718	G2501	G2611	G2501	G2379	C	A2101	U1972	G1862	G1745	A1626	C1451	C1268
A	C2720	C2502	A2612	C2502	C2388	C	G2102	A1973	G1863	G1745	G1627	C1462	C1268
U	G2826	A2503	G2613	A2503	C2388	G	A2103	G1979	U1748	U1748	A1630	A1463	U1278
C	G2827	G2504	G2613	A2504	C2388	G	A2103	U1980	G1667	G1752	A1630	A1463	U1278
A	G2828	G2505	G2618	A2505	A2398	C	G2110	A1981	G1668	G1752	A1630	A1463	U1279
U	G2829	A2606	C2626	A2606	G2399	C	G2111	C	G1668	G1752	A1630	A1463	U1279
	U2726	G2507	C2627	A2607	G2401	U	A2112	U1992	G1873	A1755	C1633	A1470	C1289
	C2747	C2508	G2627	A2608	A2402	A	G2113	A1994	G1877	G1756	G1634	C1474	U1298
		A2509		A2509	A2402	G							

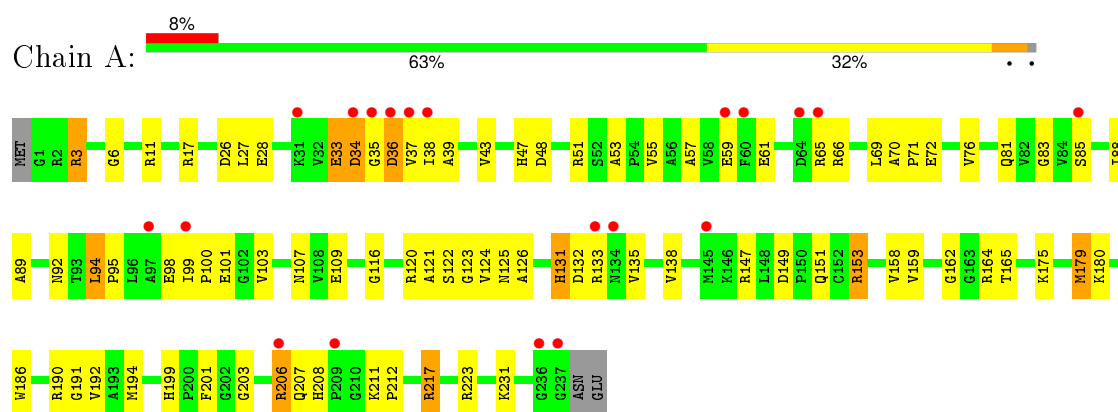
- Molecule 2: 5S ribosomal RNA



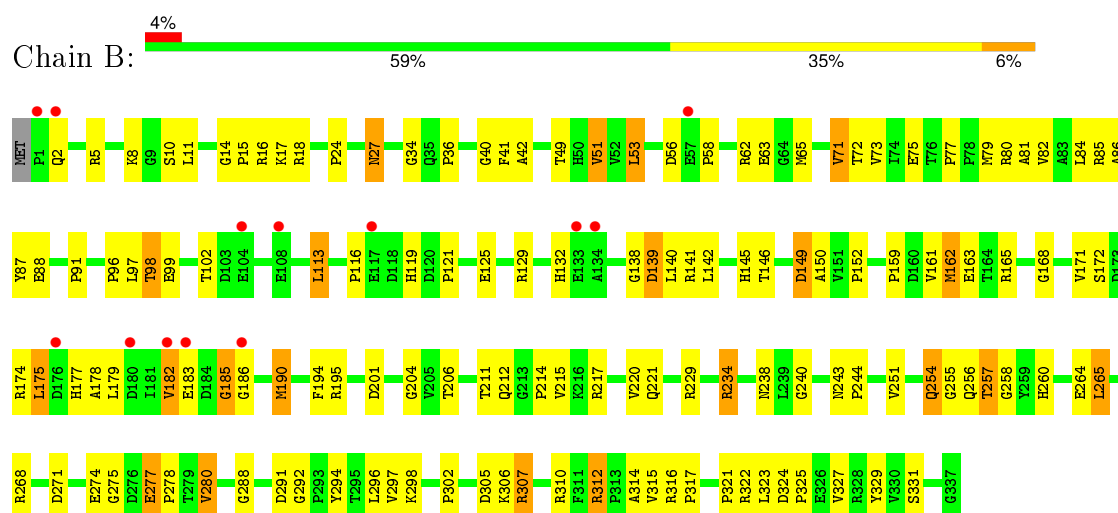
- Molecule 3: 5'-R(*CP*CP*(DA)*(PHE)*(ACA))-3'



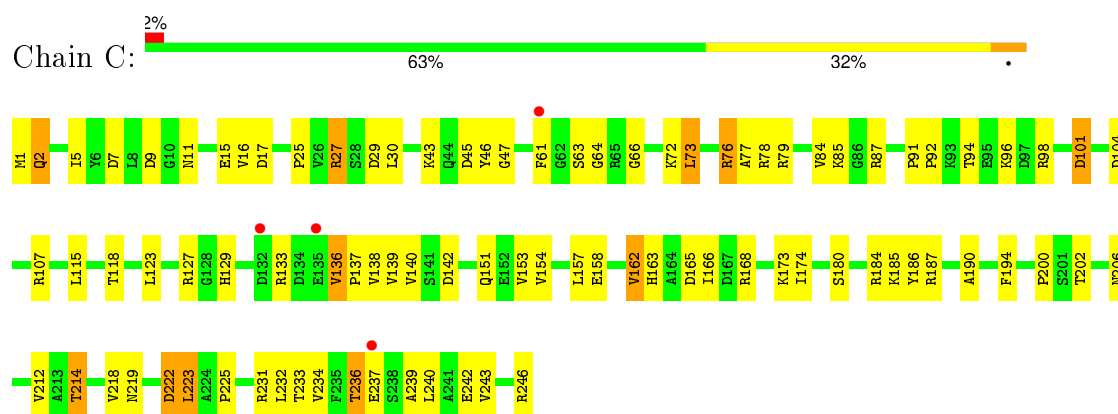
- Molecule 4: 50S ribosomal protein L2P



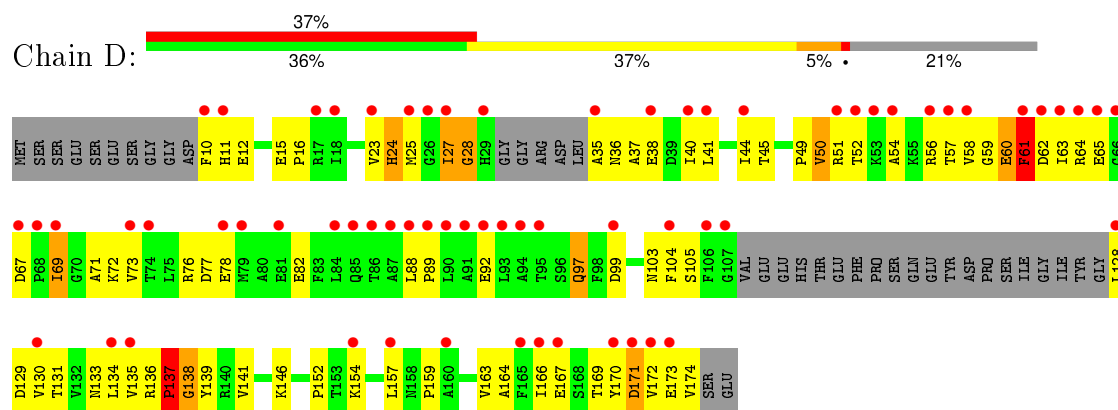
- Molecule 5: 50S ribosomal protein L3P



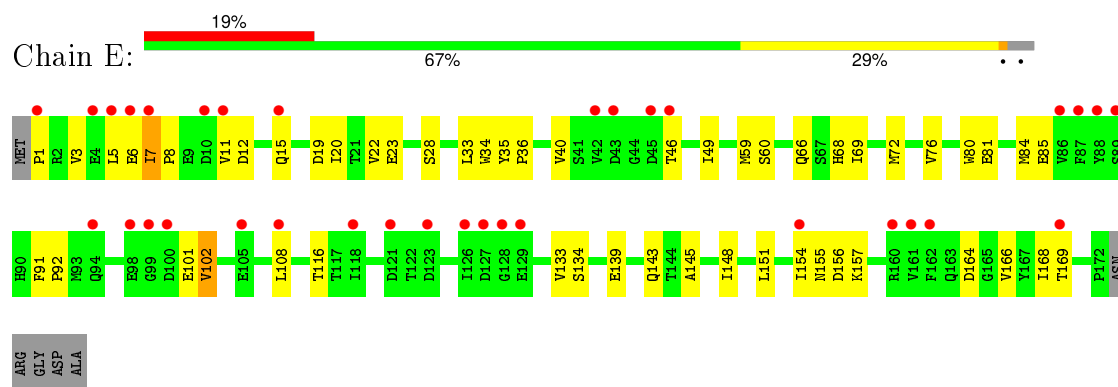
- Molecule 6: 50S ribosomal protein L4E



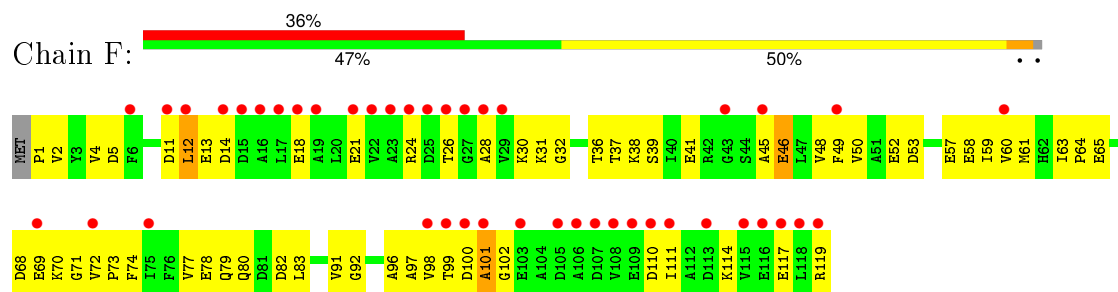
• Molecule 7: 50S ribosomal protein L5P



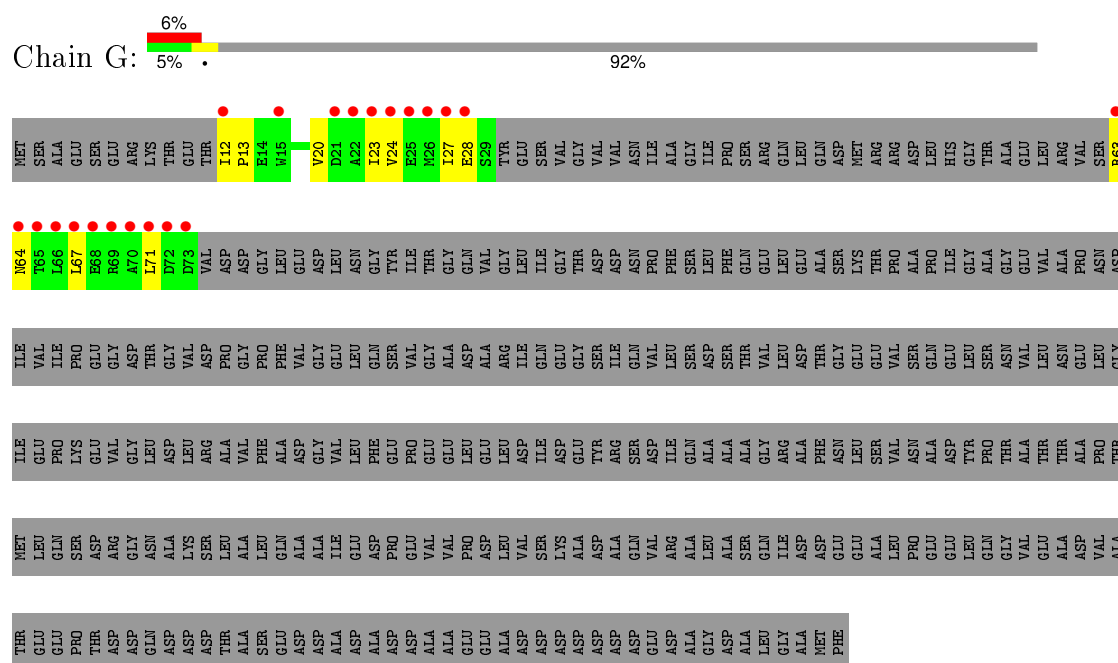
• Molecule 8: 50S ribosomal protein L6P



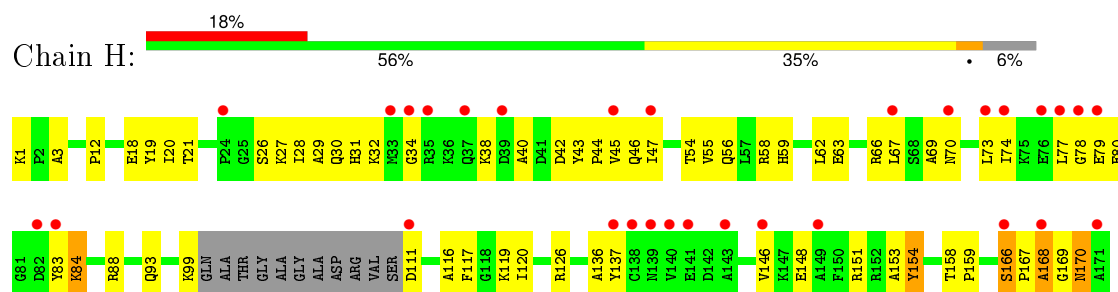
• Molecule 9: 50S ribosomal protein L7AE



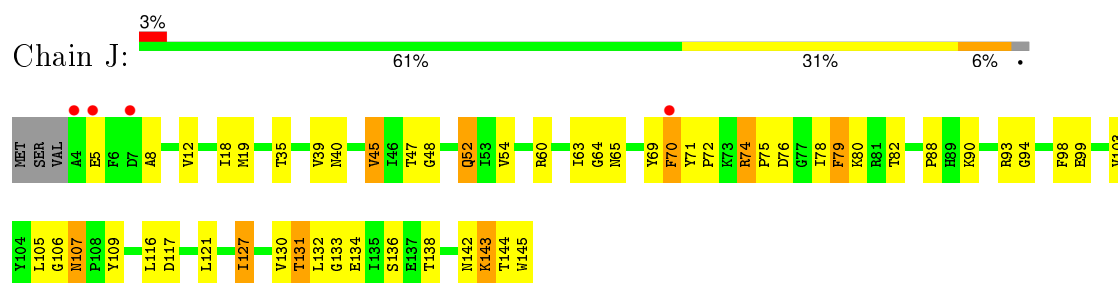
• Molecule 10: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG



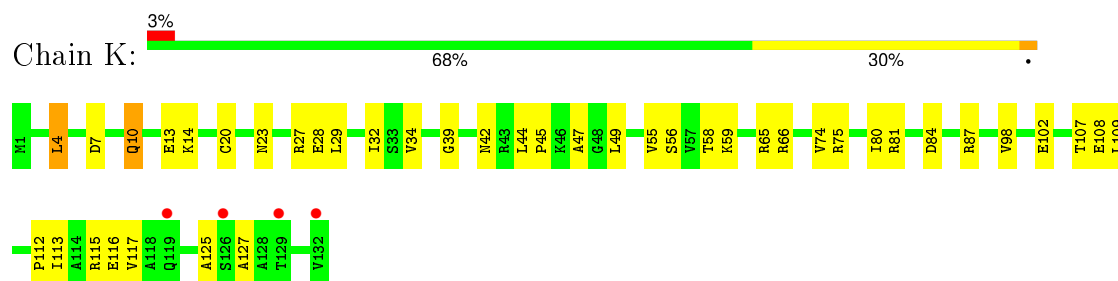
- Molecule 11: 50S RIBOSOMAL PROTEIN L10E



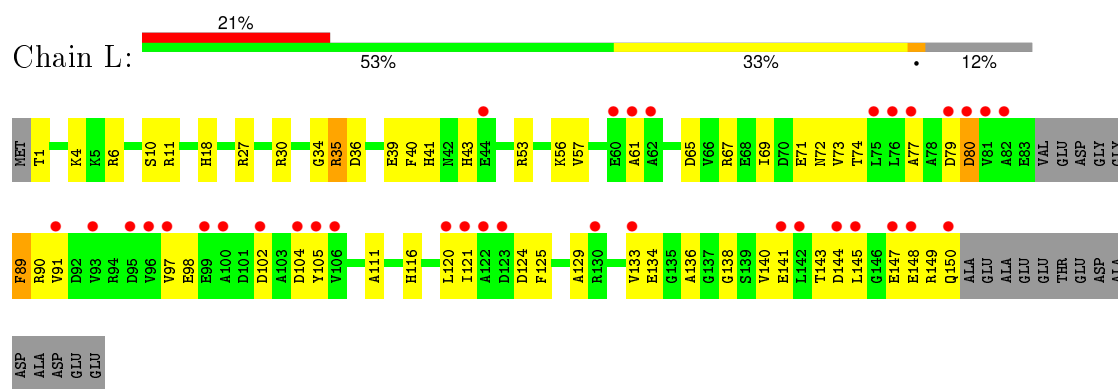
- Molecule 12: 50S ribosomal protein L13P



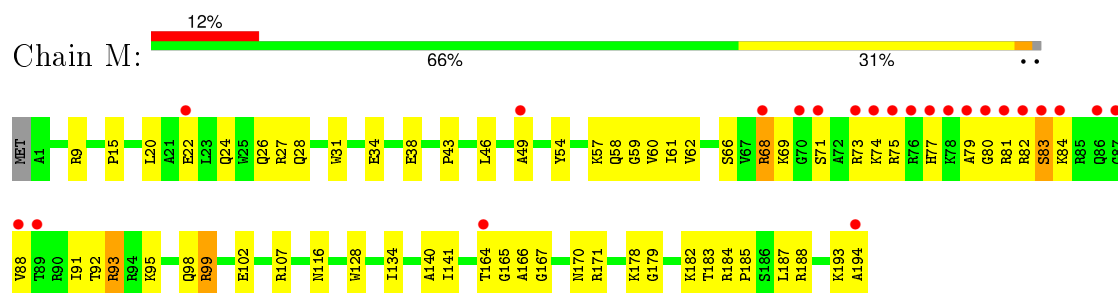
- Molecule 13: 50S ribosomal protein L14P



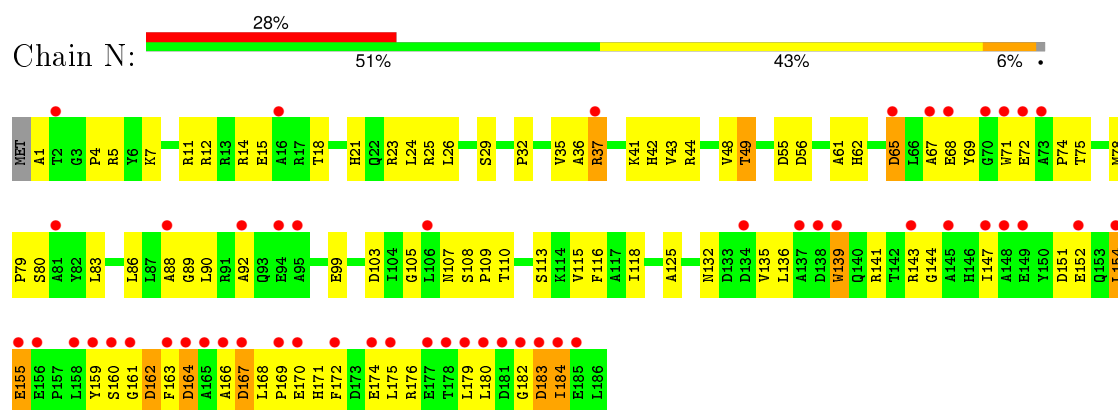
- Molecule 14: 50S ribosomal protein L15P



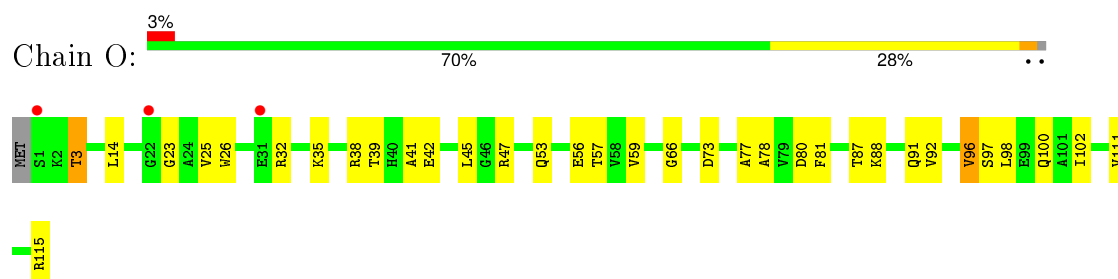
- Molecule 15: 50S Ribosomal Protein L15E



- Molecule 16: 50S ribosomal protein L18P

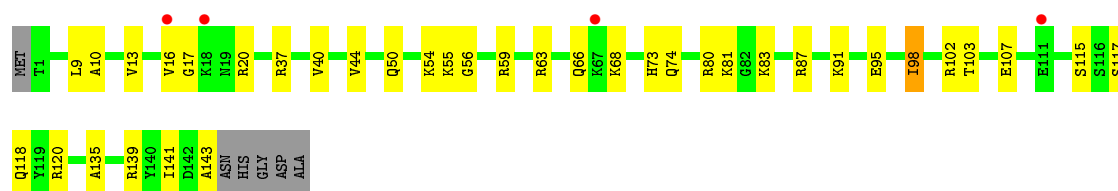


- Molecule 17: 50S ribosomal protein L18e

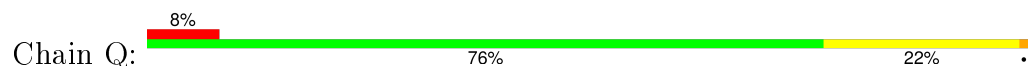


- Molecule 18: 50S ribosomal protein L19E





- Molecule 19: 50S ribosomal protein L21e



- Molecule 20: 50S ribosomal protein L22P



- Molecule 21: 50S ribosomal protein L23P



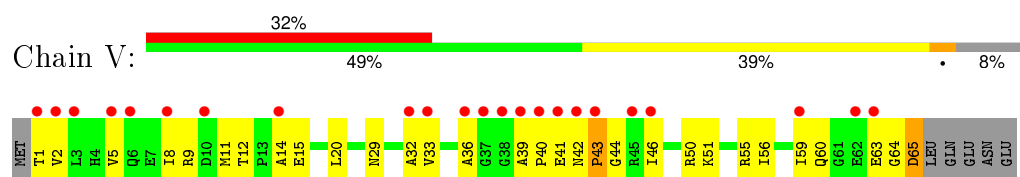
- Molecule 22: 50S ribosomal protein L24P



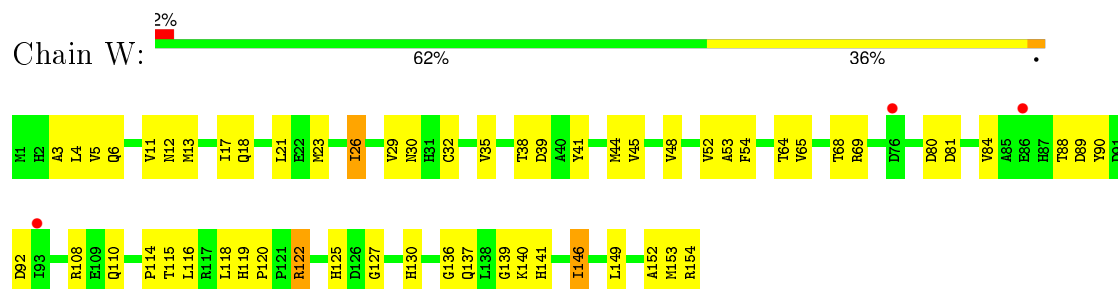
- Molecule 23: 50S ribosomal protein L24E



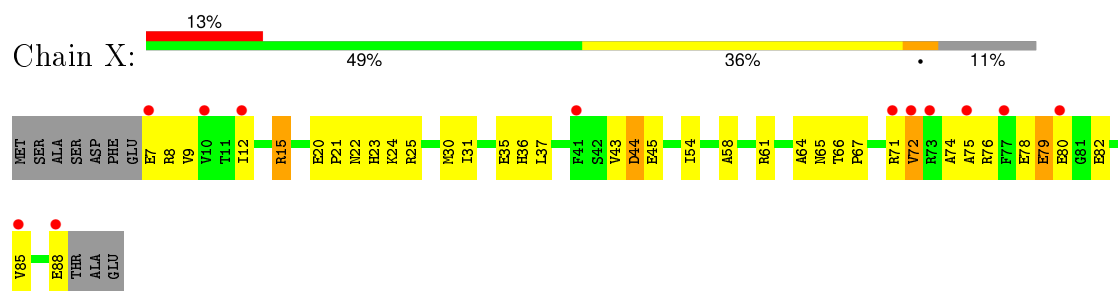
- Molecule 24: 50S ribosomal protein L29P



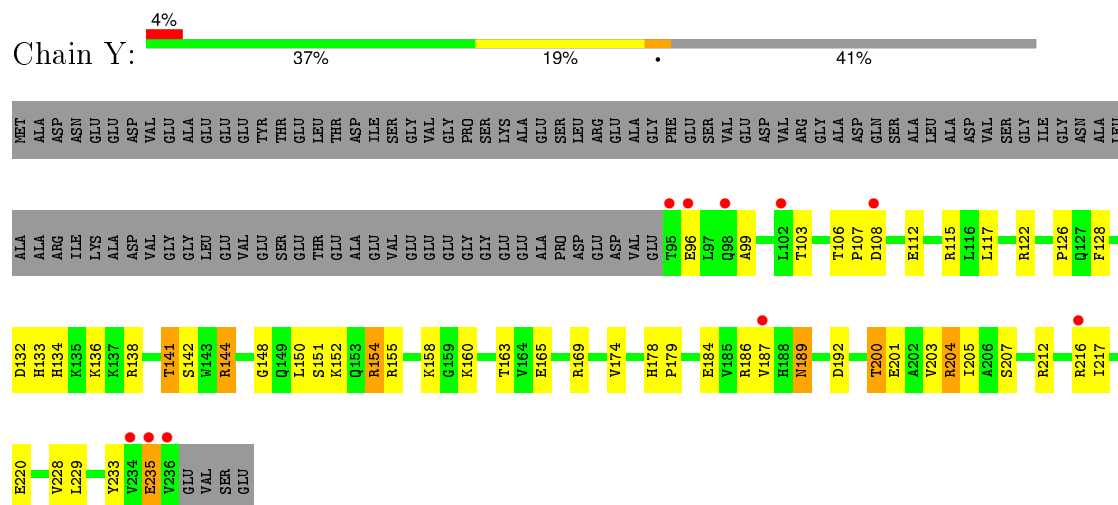
- Molecule 25: 50S ribosomal protein L30P



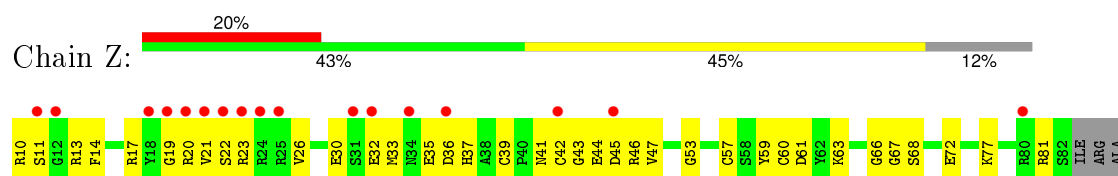
- Molecule 26: 50S ribosomal protein L31e



- Molecule 27: 50S ribosomal protein L32E



- Molecule 28: 50S ribosomal protein L37Ae



ALA
LEU
SER
GLU
ASP
GLU
GLU

- Molecule 29: 50S ribosomal protein L37e

Chain 1:  72% 26% .

MET T1 Q8 G9 K10 K11 H16 T17 K18 C19 R20 R21 K25 H28 K31 C37 D47 E56

- Molecule 30: 50S ribosomal protein L39e

Chain 2:  12% 56% 34% 8% .

MET G1 K5 K9 R10 M18 S19 R20 V21 P22 V25 M26 L27 K28 T29 D30 R31 GLU VAL GLN R35 R39 R40 H41 R44 M45 D48 E49

- Molecule 31: 50S ribosomal protein L44E

Chain 3:  5% 70% 29% .

H1 Q2 M3 R6 H17 E19 R20 E21 V25 R29 K35 R38 E41 R42 M48 P56 R60 P61 T62 T65 P66 L67 R68 Y69 R70 E73 A77 R80 R84 L88 E89 F90 Q91 E92

- Molecule 32: 50S RIBOSOMAL PROTEIN L11P

Chain I:  16% 41% 27% 57%

MET ALA GLY THR ILE GLU VAL LEU VAL PRO GLY GLY ALA ASN PRO GLY PRO PRO LEU GLY PRO GLU LEU GLY PRO THR PRO VAL ASP VAL GLN ALA VAL VAL GLN ILE ASN ASP GLN THR ALA PHE ASP GLY THR GLU VAL VAL VAL THR LYS VAL ASP TYR ASP ASP GLY

SER PHE GLU ILE GLU VAL G71 V72 P73 P74 P75 A76 E77 L78 I79 K80 D81 E82 A83 G84 P85 E86 T87 G88 S89 G90 E91 P92 Q93 E94 D95 P96 A98 D99 L100 S101 Y102 D103 Q104 V105 K106 Q107 I108 A109 E110 Q111 K112 H113 P114 D115 L116 L117 S118 Y119 D120 L121 T122 N123 A124

A125 K126 E127 V128 V129 T131 C132 T133 S134 L135 G136 V137 T138 I139 E140 GLY GLU ASN PRO ARG GLU PHE LYS GLU ARG ILE ASP ALA GLY GLU TYR ASP VAL PHE ALA ALA GLU ALA

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.87Å 298.57Å 575.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 49.73 – 2.30	Depositor EDS
% Data completeness (in resolution range)	89.5 (50.00-2.30) 89.6 (49.73-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.250 0.207 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	43.4	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 61.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 797435 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	99036	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMG, CL, SR, NA, K, ACA, CD, OMU, UR3, 1MA, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.37	0/65959	0.70	26/102870 (0.0%)
2	9	0.33	0/2905	0.71	1/4528 (0.0%)
3	4	0.52	0/75	0.73	0/110
4	A	0.34	0/1786	0.66	0/2408
5	B	0.33	0/2690	0.66	0/3652
6	C	0.38	0/1884	0.64	1/2551 (0.0%)
7	D	0.29	0/1111	0.54	0/1498
8	E	0.32	0/1382	0.57	0/1880
9	F	0.31	0/901	0.54	0/1224
10	G	0.27	0/241	0.47	0/324
11	H	0.33	0/1287	0.64	0/1725
12	J	0.35	0/1136	0.61	0/1530
13	K	0.35	0/1001	0.67	0/1347
14	L	0.33	0/1130	0.64	0/1509
15	M	0.34	0/1584	0.60	0/2119
16	N	0.28	0/1474	0.60	0/1999
17	O	0.33	0/874	0.59	1/1181 (0.1%)
18	P	0.34	0/1147	0.56	0/1528
19	Q	0.35	0/749	0.69	0/1005
20	R	0.35	0/1172	0.67	0/1578
21	S	0.32	0/648	0.58	1/875 (0.1%)
22	T	0.31	0/958	0.63	0/1289
23	U	0.35	0/417	0.58	0/562
24	V	0.27	0/502	0.53	0/675
25	W	0.34	0/1219	0.60	0/1655
26	X	0.33	0/664	0.60	0/895
27	Y	0.36	0/1146	0.65	0/1536
28	Z	0.34	0/589	0.61	0/787
29	1	0.43	0/438	0.66	0/578
30	2	0.35	0/401	0.60	0/529
31	3	0.38	0/771	0.58	0/1024
32	I	0.28	0/526	0.50	0/716

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.36	0/98767	0.67	30/147687 (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	39
2	9	0	2
All	All	1	41

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1563	G	C2'-C3'-O3'	9.69	130.83	109.50
2	9	3039	U	N1-C1'-C2'	7.45	123.68	114.00
1	0	1942	A	C5'-C4'-C3'	7.27	127.63	116.00
1	0	1819	G	C5'-C4'-C3'	6.86	126.98	116.00
1	0	1592	G	N9-C1'-C2'	6.67	122.67	114.00
1	0	871	G	C5'-C4'-O4'	-6.63	101.14	109.10
1	0	1819	G	C1'-O4'-C4'	-6.35	104.82	109.90
1	0	1979	G	C2'-C3'-O3'	6.29	123.77	113.70
1	0	777	U	O4'-C1'-N1	6.26	113.21	108.20
1	0	2313	C	C5'-C4'-O4'	5.93	116.22	109.10
1	0	1504	A	C1'-O4'-C4'	-5.91	105.17	109.90
1	0	206	G	C5'-C4'-C3'	-5.84	106.66	116.00
1	0	1819	G	C4'-C3'-C2'	-5.79	96.81	102.60
1	0	1615	A	C5'-C4'-C3'	5.69	125.10	116.00
1	0	1352	A	OP1-P-O3'	5.62	117.57	105.20
1	0	2291	A	N9-C1'-C2'	5.46	121.11	114.00
1	0	2467	A	C1'-O4'-C4'	-5.43	105.56	109.90
1	0	841	A	C1'-O4'-C4'	-5.37	105.61	109.90
1	0	1504	A	N9-C1'-C2'	5.30	120.89	114.00
1	0	1942	A	C1'-O4'-C4'	-5.28	105.68	109.90
1	0	1352	A	C2'-C3'-O3'	5.26	122.12	113.70
1	0	1120	U	C5'-C4'-C3'	-5.23	107.63	116.00
1	0	2313	C	C5'-C4'-C3'	5.21	124.33	116.00
17	O	66	GLY	N-CA-C	5.19	126.08	113.10
21	S	27	ALA	N-CA-C	-5.19	96.99	111.00
6	C	73	LEU	CA-CB-CG	-5.12	103.52	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1165	G	C1'-O4'-C4'	-5.11	105.81	109.90
1	0	921	G	N9-C1'-C2'	5.07	120.58	114.00
1	0	389	G	C5'-C4'-C3'	-5.03	107.95	116.00
1	0	69	A	C5'-C4'-O4'	-5.01	103.09	109.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1563	G	C3'

All (41) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1078	A	Sidechain
1	0	1080	C	Sidechain
1	0	1340	G	Sidechain
1	0	1430	G	Sidechain
1	0	1718	G	Sidechain
1	0	1744	G	Sidechain
1	0	1794	G	Sidechain
1	0	1809	G	Sidechain
1	0	1819	G	Sidechain
1	0	182	G	Sidechain
1	0	1829	A	Sidechain
1	0	1845	A	Sidechain
1	0	1861	C	Sidechain
1	0	1863	G	Sidechain
1	0	1867	G	Sidechain
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	2316	G	Sidechain
1	0	24	G	Sidechain
1	0	2465	A	Sidechain
1	0	2493	C	Sidechain
1	0	2503	A	Sidechain
1	0	2506	A	Sidechain
1	0	2552	C	Sidechain
1	0	2599	A	Sidechain
1	0	2632	G	Sidechain
1	0	2793	A	Sidechain
1	0	2842	G	Sidechain
1	0	396	U	Sidechain

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Mol	Chain	Res	Type	Group
1	0	462	A	Sidechain
1	0	469	G	Sidechain
1	0	471	G	Sidechain
1	0	482	G	Sidechain
1	0	518	G	Sidechain
1	0	792	G	Sidechain
1	0	795	G	Sidechain
1	0	817	G	Sidechain
1	0	868	G	Sidechain
1	0	952	G	Sidechain
2	9	3039	U	Sidechain
2	9	3065	A	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59021	0	29813	722	0
2	9	2600	0	1326	50	0
3	4	73	0	44	2	0
4	A	1753	0	1766	101	0
5	B	2625	0	2532	145	0
6	C	1859	0	1816	106	0
7	D	1094	0	1085	79	0
8	E	1357	0	1266	45	0
9	F	890	0	843	57	0
10	G	240	0	231	11	0
11	H	1266	0	1268	68	0
12	J	1120	0	1098	68	0
13	K	992	0	1031	53	0
14	L	1118	0	1076	61	0
15	M	1560	0	1568	63	0
16	N	1445	0	1401	97	0
17	O	865	0	873	40	0
18	P	1136	0	1123	35	0
19	Q	735	0	729	18	0
20	R	1149	0	1122	37	0
21	S	641	0	605	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	T	950	0	923	47	0
23	U	410	0	364	26	0
24	V	499	0	511	38	0
25	W	1196	0	1137	82	0
26	X	654	0	653	35	0
27	Y	1130	0	1133	57	0
28	Z	578	0	539	28	0
29	1	431	0	426	22	0
30	2	396	0	413	26	0
31	3	755	0	728	26	0
32	I	519	0	500	51	0
33	0	87	0	0	0	0
33	9	1	0	0	0	0
33	A	1	0	0	0	0
33	B	1	0	0	0	0
33	K	1	0	0	0	0
33	T	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	2	0	0	0	0
35	0	64	0	0	0	0
35	3	1	0	0	0	0
35	9	1	0	0	0	0
35	C	1	0	0	0	0
35	D	1	0	0	0	0
35	J	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	3	0	0	0	0
35	S	1	0	0	0	0
36	0	10	0	0	0	0
36	3	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	J	3	0	0	1	0
36	L	1	0	0	0	0
36	M	1	0	0	0	0
36	N	1	0	0	1	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
36	Y	1	0	0	0	0
37	0	98	0	0	0	0
37	1	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	3	1	0	0	0	0
37	9	3	0	0	0	0
37	A	3	0	0	0	0
37	B	2	0	0	0	0
37	F	1	0	0	0	0
37	H	1	0	0	0	0
37	L	1	0	0	0	0
37	R	1	0	0	0	0
37	S	1	0	0	0	0
38	1	1	0	0	0	0
38	3	1	0	0	0	0
38	O	1	0	0	0	0
38	U	1	0	0	0	0
38	Z	1	0	0	0	0
39	0	5769	0	0	106	0
39	1	50	0	0	2	0
39	2	40	0	0	3	0
39	3	67	0	0	4	0
39	9	140	0	0	6	0
39	A	121	0	0	11	0
39	B	144	0	0	18	0
39	C	177	0	0	18	0
39	D	48	0	0	10	0
39	E	44	0	0	1	0
39	F	27	0	0	4	0
39	G	17	0	0	1	0
39	H	69	0	0	7	0
39	I	7	0	0	1	0
39	J	52	0	0	4	0
39	K	57	0	0	6	0
39	L	81	0	0	14	0
39	M	130	0	0	3	0
39	N	61	0	0	9	0
39	O	40	0	0	5	0
39	P	64	0	0	2	0
39	Q	49	0	0	5	0
39	R	82	0	0	3	0
39	S	32	0	0	1	0
39	T	37	0	0	3	0
39	U	29	0	0	3	0
39	V	14	0	0	2	0
39	W	69	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	X	24	0	0	6	0
39	Y	96	0	0	9	0
39	Z	31	0	0	2	0
All	All	99036	0	59943	2083	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (2083) 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)
25:W:21:LEU:HD21	25:W:48:VAL:HG11	1.29	1.14
26:X:37:LEU:HD13	26:X:85:VAL:HG21	1.29	1.10
6:C:236:THR:HG22	6:C:239:ALA:H	1.19	1.07
1:O:656:G:H5'	17:O:3:THR:HG22	1.38	1.05
1:O:1160:G:H5'	1:O:1161:A:H5'	1.40	1.04
22:T:9:LYS:HE3	22:T:13:ARG:NH1	1.72	1.03
2:9:3076:G:H3'	2:9:3077:A:H5''	1.41	1.02
9:F:91:VAL:HG12	9:F:92:GLY:H	1.25	1.00
28:Z:46:ARG:HD2	28:Z:59:TYR:HB2	1.42	0.99
22:T:71:VAL:HG11	22:T:90:PRO:HB3	1.38	0.99
20:R:99:ALA:HB1	20:R:109:MET:HE1	1.45	0.98
6:C:127:ARG:NH2	6:C:225:PRO:HG2	1.78	0.97
18:P:115:SER:H	18:P:118:GLN:HE21	1.12	0.96
1:O:156:C:H5''	15:M:171:ARG:HD3	1.47	0.95
13:K:81:ARG:HB2	13:K:87:ARG:HH11	1.32	0.94
13:K:39:GLY:HA2	39:K:4183:HOH:O	1.68	0.94
12:J:93:ARG:HH11	12:J:93:ARG:HB3	1.29	0.93
7:D:57:THR:HG23	7:D:63:ILE:HA	1.51	0.93
25:W:137:GLN:HE21	25:W:141:HIS:HE1	1.15	0.93
13:K:29:LEU:HB3	13:K:55:VAL:HG11	1.51	0.93
5:B:307:ARG:HH11	5:B:307:ARG:HG3	1.34	0.92
24:V:12:THR:HG22	24:V:15:GLU:HG3	1.50	0.92
21:S:57:THR:HG22	21:S:59:ASP:H	1.34	0.92
25:W:6:GLN:HB2	25:W:26:ILE:HD12	1.52	0.91
2:9:3056:A:H2'	2:9:3057:A:H5''	1.52	0.89
1:O:2506:A:HO2'	1:O:2507:G:H8	0.92	0.89
8:E:20:ILE:HD11	8:E:40:VAL:HG11	1.54	0.89
5:B:212:GLN:HB2	5:B:257:THR:HG21	1.53	0.89
21:S:51:GLN:HE21	21:S:53:ASN:HD21	1.21	0.89
13:K:74:VAL:HG13	13:K:113:ILE:HG23	1.55	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2717:C:H2'	1:0:2718:C:H5''	1.54	0.89
8:E:36:PRO:HD3	12:J:127:ILE:HD12	1.53	0.88
1:0:1593:C:OP1	18:P:117:SER:HB3	1.74	0.88
13:K:10:GLN:H	13:K:10:GLN:HE21	0.89	0.88
8:E:15:GLN:HG3	8:E:20:ILE:HG12	1.56	0.88
13:K:10:GLN:N	13:K:10:GLN:HE21	1.71	0.88
6:C:104:ASP:HA	6:C:107:ARG:HH12	1.37	0.87
1:0:542:A:H5'	1:0:542:A:H8	1.40	0.87
1:0:2717:C:C2'	1:0:2718:C:H5''	2.04	0.87
13:K:10:GLN:H	13:K:10:GLN:NE2	1.73	0.87
4:A:81:GLN:HB2	4:A:92:ASN:ND2	1.89	0.87
5:B:238:ASN:HD22	5:B:240:GLY:H	1.17	0.87
1:0:1603:A:H5'	1:0:1605:G:O4'	1.74	0.87
6:C:1:MET:HG2	6:C:2:GLN:H	1.40	0.87
28:Z:11:SER:HB3	28:Z:23:ARG:HB2	1.57	0.87
1:0:1242:A:H5'	12:J:82:THR:HG23	1.55	0.86
1:0:1372:A:H3'	39:0:7681:HOH:O	1.75	0.86
13:K:74:VAL:HG11	13:K:113:ILE:HG12	1.57	0.86
1:0:288:A:H61	1:0:364:C:H42	1.21	0.86
5:B:162:MET:HE2	5:B:310:ARG:HD3	1.57	0.86
25:W:122:ARG:HH11	25:W:122:ARG:HG2	1.40	0.86
16:N:144:GLY:O	16:N:147:ILE:HG22	1.76	0.86
6:C:115:LEU:HD13	6:C:223:LEU:HD21	1.58	0.85
1:0:2812:A:H2	1:0:2814:A:H62	1.21	0.85
7:D:25:MET:HE2	7:D:41:LEU:HG	1.58	0.84
7:D:58:VAL:HB	7:D:62:ASP:HB3	1.58	0.84
1:0:1835:U:H5	1:0:1840:A:N7	1.75	0.84
7:D:28:GLY:HA2	7:D:69:ILE:HG23	1.59	0.84
1:0:2541:U:H3	1:0:2618:G:H1	1.24	0.84
18:P:115:SER:OG	18:P:118:GLN:HG3	1.77	0.83
1:0:2073:G:H5''	39:0:4410:HOH:O	1.77	0.83
1:0:289:G:H22	1:0:363:A:H2	1.22	0.83
25:W:122:ARG:NH2	25:W:154:ARG:HG2	1.93	0.83
27:Y:235:GLU:H	27:Y:235:GLU:CD	1.80	0.83
2:9:3039:U:H1'	2:9:3044:A:H61	1.43	0.83
15:M:164:THR:HG22	15:M:166:ALA:H	1.43	0.83
16:N:113:SER:HB2	39:N:9356:HOH:O	1.77	0.83
1:0:2840:A:OP1	5:B:211:THR:HG23	1.78	0.82
15:M:99:ARG:HH21	15:M:170:ASN:HD22	1.26	0.82
6:C:5:ILE:HD11	6:C:16:VAL:HG23	1.61	0.82
24:V:1:THR:HG23	24:V:2:VAL:H	1.44	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:83:LEU:HD13	16:N:175:LEU:HD23	1.61	0.82
25:W:88:THR:HB	39:W:6679:HOH:O	1.80	0.82
4:A:206:ARG:HD3	4:A:206:ARG:H	1.44	0.81
1:0:2506:A:O2'	1:0:2507:G:H8	1.62	0.81
15:M:134:ILE:HG23	15:M:141:ILE:HD13	1.62	0.81
39:0:5402:HOH:O	12:J:47:THR:HB	1.80	0.81
1:0:560:C:H42	1:0:597:A:H61	1.25	0.81
1:0:1116:U:HO2'	1:0:1118:A:H2	0.82	0.81
4:A:192:VAL:HB	39:A:9578:HOH:O	1.79	0.81
13:K:81:ARG:HB2	13:K:87:ARG:NH1	1.95	0.81
5:B:162:MET:CE	5:B:310:ARG:HD3	2.09	0.81
4:A:211:LYS:HG2	4:A:212:PRO:HD2	1.60	0.81
13:K:4:LEU:HD22	13:K:116:GLU:HB3	1.60	0.81
25:W:6:GLN:HB2	25:W:26:ILE:CD1	2.11	0.80
1:0:1377:C:H6	1:0:1377:C:H5'	1.44	0.80
20:R:8:ALA:HB1	20:R:13:THR:HG21	1.63	0.80
4:A:192:VAL:HG22	39:A:9618:HOH:O	1.81	0.80
1:0:1041:U:H5'	39:L:9489:HOH:O	1.80	0.80
11:H:46:GLN:HB3	11:H:167:PRO:HD2	1.64	0.80
25:W:125:HIS:HD2	25:W:127:GLY:H	1.30	0.80
1:0:1474:C:H6	1:0:1474:C:H5'	1.46	0.79
25:W:13:MET:HE1	25:W:18:GLN:HA	1.63	0.79
31:3:65:THR:HG22	31:3:67:LEU:HG	1.64	0.79
5:B:36:PRO:HA	5:B:168:GLY:HA3	1.64	0.79
1:0:1116:U:O2'	1:0:1118:A:H2	1.64	0.79
26:X:30:MET:HE1	26:X:58:ALA:HB3	1.65	0.79
1:0:2005:G:H3'	1:0:2005:G:OP2	1.83	0.78
6:C:5:ILE:HD11	6:C:16:VAL:CG2	2.14	0.78
1:0:1165:G:H4'	1:0:1174:A:O2'	1.84	0.78
7:D:25:MET:HE1	7:D:37:ALA:HB1	1.66	0.78
22:T:71:VAL:HG11	22:T:90:PRO:CB	2.13	0.78
1:0:2054:A:N3	20:R:128:ARG:NH2	2.32	0.78
30:2:41:HIS:H	30:2:45:ASN:HD22	1.32	0.78
5:B:58:PRO:HA	5:B:63:GLU:OE1	1.83	0.78
18:P:115:SER:H	18:P:118:GLN:NE2	1.82	0.78
1:0:381:G:H5''	39:M:9376:HOH:O	1.85	0.78
6:C:236:THR:HG22	6:C:239:ALA:N	1.97	0.77
9:F:91:VAL:HG12	9:F:92:GLY:N	1.99	0.77
18:P:115:SER:N	18:P:118:GLN:HE21	1.82	0.77
13:K:14:LYS:HB2	13:K:45:PRO:HG2	1.66	0.77
1:0:1701:A:H4'	1:0:1702:U:H5''	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1205:U:H2'	1:0:1206:U:H5''	1.67	0.77
1:0:2635:A:O2'	1:0:2636:C:H5'	1.85	0.76
22:T:41:ARG:HG2	22:T:41:ARG:HH11	1.50	0.76
31:3:70:ARG:HG2	31:3:77:ALA:HB2	1.66	0.76
1:0:1166:A:H61	1:0:1180:U:H3	1.31	0.76
5:B:53:LEU:HD11	5:B:327:VAL:HG22	1.65	0.76
25:W:21:LEU:CD2	25:W:48:VAL:HG11	2.13	0.76
20:R:25:PHE:CE2	20:R:29:LYS:HE2	2.20	0.76
1:0:962:C:H1'	16:N:5:ARG:NH1	2.00	0.76
32:I:132:CYS:HB3	32:I:137:VAL:HB	1.68	0.76
1:0:545:G:H8	1:0:545:G:H5'	1.49	0.76
1:0:559:U:H5'	1:0:559:U:H6	1.51	0.76
12:J:19:MET:HE3	12:J:132:LEU:HD11	1.68	0.76
7:D:135:VAL:HG21	7:D:139:TYR:CD1	2.20	0.76
16:N:37:ARG:HG3	36:N:9307:CL:CL	2.23	0.76
15:M:102:GLU:OE1	15:M:164:THR:HG21	1.86	0.75
1:0:2534:C:H1'	39:0:4089:HOH:O	1.86	0.75
13:K:107:THR:HG22	13:K:108:GLU:HG3	1.68	0.75
1:0:1119:G:N2	1:0:1246:A:C2	2.53	0.75
1:0:1206:U:H6	1:0:1206:U:H5'	1.51	0.75
1:0:871:G:H8	1:0:871:G:H5''	1.49	0.75
1:0:1175:G:H1'	1:0:1193:A:H2'	1.67	0.75
4:A:199:HIS:HD2	4:A:201:PHE:H	1.33	0.75
6:C:236:THR:CG2	6:C:239:ALA:H	1.99	0.75
4:A:191:GLY:HA2	4:A:194:MET:CE	2.17	0.75
4:A:33:GLU:CD	4:A:33:GLU:H	1.89	0.75
8:E:15:GLN:HG2	8:E:19:ASP:O	1.85	0.75
1:0:544:G:H2'	1:0:545:G:H5''	1.69	0.75
39:0:6067:HOH:O	5:B:298:LYS:HG2	1.86	0.75
4:A:153:ARG:HH11	4:A:153:ARG:HB2	1.52	0.75
1:0:871:G:C8	1:0:871:G:C5'	2.69	0.75
5:B:179:LEU:O	5:B:183:GLU:HG2	1.86	0.74
16:N:110:THR:HB	16:N:113:SER:OG	1.87	0.74
16:N:49:THR:HG22	16:N:56:ASP:HB2	1.69	0.74
32:I:99:ASP:OD1	32:I:138:THR:HB	1.88	0.74
13:K:32:ILE:HD11	13:K:56:SER:HB2	1.69	0.74
27:Y:154:ARG:HH12	27:Y:155:ARG:HG3	1.53	0.74
9:F:96:ALA:HA	39:F:3111:HOH:O	1.88	0.74
14:L:73:VAL:HG23	14:L:74:THR:H	1.52	0.74
18:P:59:ARG:NH2	18:P:66:GLN:HE22	1.85	0.74
1:0:871:G:H8	1:0:871:G:C5'	2.01	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1973:A:H5'	1:0:1973:A:H8	1.52	0.74
15:M:107:ARG:HH11	15:M:107:ARG:HG3	1.51	0.74
25:W:88:THR:HG23	25:W:110:GLN:NE2	2.02	0.73
1:0:1159:G:H21	1:0:1189:A:H8	1.36	0.73
9:F:46:GLU:OE1	9:F:100:ASP:HA	1.89	0.73
1:0:656:G:C5'	17:O:3:THR:HG22	2.17	0.73
1:0:1667:A:H8	1:0:1667:A:H5'	1.54	0.73
11:H:27:LYS:H	11:H:59:HIS:HD2	1.35	0.73
6:C:107:ARG:NH1	6:C:107:ARG:HB3	2.03	0.73
1:0:656:G:H5'	17:O:3:THR:CG2	2.17	0.73
25:W:68:THR:HG23	25:W:69:ARG:HG2	1.70	0.73
1:0:2491:G:H1'	39:O:7375:HOH:O	1.88	0.73
25:W:4:LEU:HD22	25:W:52:VAL:HG21	1.70	0.73
1:0:506:G:H22	1:0:509:A:C5'	2.02	0.73
1:0:2851:G:C2'	1:0:2852:A:H5'	2.18	0.73
21:S:57:THR:HG22	21:S:59:ASP:N	2.02	0.72
16:N:80:SER:HB2	39:N:9335:HOH:O	1.89	0.72
1:0:1299:G:O6	14:L:6:ARG:HD3	1.89	0.72
22:T:49:GLU:HB3	22:T:59:GLU:HG2	1.70	0.72
7:D:58:VAL:HG12	7:D:60:GLU:HG2	1.71	0.72
13:K:58:THR:HG22	13:K:59:LYS:HG3	1.70	0.72
1:0:2749:U:H5'	39:O:8471:HOH:O	1.89	0.72
1:0:1160:G:C5'	1:0:1161:A:H5'	2.15	0.72
1:0:481:U:H5''	39:O:6188:HOH:O	1.89	0.72
4:A:192:VAL:HG12	4:A:207:GLN:HB3	1.71	0.72
7:D:23:VAL:HG22	7:D:73:VAL:HB	1.70	0.72
1:0:1118:A:H3'	1:0:1118:A:H8	1.55	0.72
1:0:1116:U:O2'	1:0:1118:A:C2	2.41	0.72
5:B:141:ARG:HD2	5:B:163:GLU:OE2	1.90	0.72
2:9:3014:G:H8	2:9:3014:G:H5'	1.55	0.71
4:A:94:LEU:HD12	4:A:98:GLU:HB2	1.71	0.71
27:Y:165:GLU:HB3	39:Y:9394:HOH:O	1.90	0.71
1:0:541:C:H2'	1:0:542:A:H5''	1.72	0.71
25:W:137:GLN:HE21	25:W:141:HIS:CE1	2.04	0.71
11:H:30:GLN:H	11:H:66:ARG:NH1	1.87	0.71
4:A:35:GLY:O	4:A:36:ASP:HB3	1.89	0.71
10:G:12:ILE:N	10:G:13:PRO:HD3	2.06	0.71
1:0:1700:C:H5''	1:0:1701:A:OP2	1.91	0.71
32:I:110:GLU:HA	32:I:113:HIS:CE1	2.25	0.71
1:0:506:G:H22	1:0:509:A:H5''	1.54	0.71
12:J:74:ARG:NH1	12:J:76:ASP:HB2	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:50:VAL:HG13	9:F:60:VAL:HG11	1.73	0.71
20:R:99:ALA:HB1	20:R:109:MET:CE	2.19	0.71
1:0:541:C:C2'	1:0:542:A:H5''	2.20	0.71
4:A:191:GLY:HA2	4:A:194:MET:HE2	1.71	0.71
9:F:13:GLU:OE2	9:F:78:GLU:HG2	1.90	0.71
23:U:17:THR:HG22	23:U:18:GLY:N	2.06	0.71
14:L:80:ASP:HB2	14:L:90:ARG:O	1.91	0.71
1:0:1166:A:H1'	1:0:1192:A:C2	2.26	0.70
12:J:45:VAL:HG11	12:J:121:LEU:HD22	1.73	0.70
26:X:71:ARG:HD3	39:X:2171:HOH:O	1.90	0.70
9:F:53:ASP:OD1	9:F:80:GLN:HB2	1.91	0.70
2:9:3039:U:H1'	2:9:3044:A:N6	2.06	0.70
1:0:2716:G:H5''	5:B:206:THR:HG21	1.73	0.70
5:B:268:ARG:NH2	5:B:325:PRO:HG3	2.06	0.70
1:0:2765:C:H4'	39:0:6067:HOH:O	1.92	0.70
20:R:18:LEU:HB2	20:R:143:VAL:CG1	2.21	0.70
18:P:91:LYS:O	18:P:95:GLU:HG3	1.91	0.70
27:Y:189:ASN:HA	27:Y:217:ILE:HD11	1.72	0.70
7:D:23:VAL:HG21	7:D:45:THR:HG21	1.73	0.70
1:0:949:U:H4'	19:Q:95:GLU:HA	1.72	0.70
16:N:12:ARG:HD3	16:N:18:THR:OG1	1.92	0.70
4:A:48:ASP:HB3	39:A:9587:HOH:O	1.91	0.70
1:0:2586:U:H3	1:0:2592:G:H22	1.39	0.70
1:0:2042:U:H1'	39:0:7798:HOH:O	1.90	0.70
4:A:192:VAL:CG1	4:A:207:GLN:HB3	2.22	0.70
1:0:1979:G:H2'	39:0:3890:HOH:O	1.90	0.70
1:0:1838:U:O2'	1:0:2644:C:H5'	1.91	0.70
27:Y:200:THR:HG22	27:Y:201:GLU:HG3	1.72	0.70
6:C:2:GLN:HB3	39:C:9191:HOH:O	1.90	0.70
1:0:1878:G:H1'	39:0:6649:HOH:O	1.90	0.70
1:0:796:A:HO2'	28:Z:10:ARG:N	1.89	0.70
1:0:470:U:O2'	29:1:16:HIS:HD2	1.75	0.70
13:K:109:LEU:HD13	13:K:113:ILE:HD11	1.73	0.70
6:C:194:PHE:CD2	6:C:234:VAL:HG11	2.26	0.70
15:M:69:LYS:O	15:M:73:ARG:NH2	2.25	0.70
1:0:2073:G:OP2	1:0:2490:A:H5'	1.92	0.70
1:0:1183:C:N4	1:0:1184:C:H41	1.90	0.70
12:J:19:MET:HE1	12:J:132:LEU:HD21	1.74	0.70
28:Z:22:SER:O	28:Z:26:VAL:HG23	1.92	0.70
8:E:20:ILE:CD1	8:E:40:VAL:HG11	2.21	0.69
39:0:7927:HOH:O	5:B:211:THR:HG21	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:141:THR:HG23	39:Y:9389:HOH:O	1.92	0.69
1:0:1118:A:H3'	1:0:1118:A:C8	2.27	0.69
1:0:1206:U:H2'	1:0:1207:A:O4'	1.92	0.69
24:V:39:ALA:N	24:V:40:PRO:HD2	2.08	0.69
5:B:307:ARG:NH1	5:B:307:ARG:HG3	2.02	0.69
6:C:104:ASP:HA	6:C:107:ARG:NH1	2.07	0.69
25:W:125:HIS:CD2	25:W:127:GLY:H	2.11	0.69
14:L:148:GLU:HB2	39:L:9485:HOH:O	1.91	0.69
2:9:3029:C:O3'	7:D:138:GLY:HA2	1.92	0.69
6:C:1:MET:HG2	6:C:2:GLN:N	2.08	0.69
15:M:134:ILE:CG2	15:M:141:ILE:HD13	2.23	0.69
4:A:51:ARG:HB2	39:A:9587:HOH:O	1.90	0.69
39:0:8484:HOH:O	5:B:2:GLN:HG3	1.91	0.69
16:N:48:VAL:CG1	16:N:55:ASP:HB3	2.23	0.69
1:0:280:C:H2'	1:0:281:U:O4'	1.93	0.69
20:R:18:LEU:HD12	20:R:143:VAL:HG11	1.75	0.69
1:0:282:C:H1'	1:0:368:C:N4	2.07	0.69
2:9:3056:A:C2'	2:9:3057:A:H5''	2.23	0.69
8:E:35:TYR:HA	12:J:127:ILE:HD12	1.75	0.69
5:B:5:ARG:NH1	5:B:8:LYS:HE2	2.08	0.69
18:P:9:LEU:O	18:P:13:VAL:HG12	1.93	0.69
1:0:2578:G:H5'	1:0:2578:G:H8	1.57	0.69
22:T:9:LYS:HE3	22:T:13:ARG:CZ	2.22	0.68
1:0:1666:C:H2'	1:0:1667:A:H5'	1.75	0.68
5:B:201:ASP:HB2	5:B:312:ARG:HD2	1.75	0.68
1:0:2468:A:H61	31:3:48:ASN:HD21	1.38	0.68
1:0:2533:C:H5'	1:0:2533:C:H6	1.57	0.68
29:1:18:LYS:HB2	30:2:49:GLU:HG2	1.76	0.68
9:F:37:THR:O	9:F:41:GLU:HG3	1.94	0.68
25:W:81:ASP:OD1	25:W:92:ASP:HB2	1.94	0.68
1:0:1160:G:H5'	1:0:1161:A:C5'	2.19	0.68
26:X:9:VAL:HG22	26:X:88:GLU:OE2	1.94	0.68
5:B:140:LEU:HA	39:B:9576:HOH:O	1.91	0.68
5:B:190:MET:HE2	5:B:194:PHE:HD1	1.57	0.68
17:O:32:ARG:HD3	17:O:32:ARG:O	1.93	0.68
1:0:541:C:H2'	1:0:542:A:C5'	2.23	0.68
1:0:2890:A:H1'	23:U:56:ARG:NH2	2.08	0.68
1:0:93:C:H5''	24:V:1:THR:HB	1.76	0.68
11:H:166:SER:HB3	11:H:167:PRO:HD3	1.74	0.68
5:B:125:GLU:O	5:B:129:ARG:HG3	1.94	0.68
4:A:81:GLN:HB2	4:A:92:ASN:HD21	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:111:C:O2'	29:1:20:ARG:HG2	1.94	0.68
20:R:39:THR:HB	20:R:42:GLU:HG3	1.74	0.68
25:W:88:THR:HG22	25:W:89:ASP:N	2.09	0.67
4:A:95:PRO:HG2	4:A:98:GLU:HG2	1.75	0.67
9:F:63:ILE:HB	9:F:64:PRO:HD3	1.75	0.67
17:O:32:ARG:NE	17:O:35:LYS:HD2	2.08	0.67
1:0:1474:C:C6	1:0:1474:C:H5'	2.28	0.67
1:0:281:U:H2'	1:0:282:C:O4'	1.94	0.67
27:Y:144:ARG:CZ	39:Y:9412:HOH:O	2.42	0.67
32:I:89:SER:HB2	32:I:95:ASP:HB2	1.76	0.67
6:C:78:ARG:HH11	6:C:78:ARG:HG3	1.59	0.67
25:W:122:ARG:HH11	25:W:122:ARG:CG	2.08	0.67
1:0:2346:C:O2'	7:D:52:THR:HG21	1.94	0.67
8:E:116:THR:HG22	8:E:151:LEU:HD22	1.77	0.67
21:S:10:VAL:HG11	24:V:36:ALA:HA	1.77	0.67
6:C:27:ARG:HG3	6:C:29:ASP:OD1	1.95	0.67
14:L:143:THR:HG22	14:L:144:ASP:N	2.09	0.67
32:I:102:VAL:HG12	32:I:106:LYS:HE3	1.76	0.67
1:0:1209:C:H2'	1:0:1210:G:H8	1.60	0.67
1:0:1184:C:H4'	32:I:126:LYS:HB3	1.77	0.67
9:F:2:VAL:HG22	9:F:57:GLU:OE1	1.95	0.66
1:0:553:G:P	27:Y:204:ARG:HH22	2.18	0.66
11:H:166:SER:CB	11:H:167:PRO:CD	2.73	0.66
12:J:75:PRO:HG2	12:J:105:LEU:HD21	1.76	0.66
28:Z:11:SER:CB	28:Z:23:ARG:HB2	2.25	0.66
1:0:1189:A:H3'	39:0:8231:HOH:O	1.95	0.66
16:N:7:LYS:HE3	19:Q:21:ARG:O	1.94	0.66
13:K:98:VAL:HG13	13:K:102:GLU:HA	1.76	0.66
5:B:102:THR:HG23	5:B:182:VAL:HG12	1.78	0.66
24:V:12:THR:HG22	24:V:15:GLU:CG	2.24	0.66
4:A:69:LEU:HD23	4:A:107:ASN:HB2	1.76	0.66
5:B:275:GLY:O	5:B:291:ASP:HA	1.95	0.66
25:W:21:LEU:HD22	25:W:26:ILE:CD1	2.25	0.66
25:W:80:ASP:O	25:W:84:VAL:HG23	1.94	0.66
1:0:380:A:OP2	15:M:9:ARG:HD2	1.96	0.66
1:0:797:A:C4'	28:Z:10:ARG:N	2.59	0.66
29:1:25:LYS:HD2	30:2:49:GLU:N	2.11	0.66
1:0:657:G:OP1	6:C:27:ARG:NH2	2.26	0.66
5:B:102:THR:HG21	5:B:182:VAL:O	1.96	0.66
1:0:2779:G:H21	8:E:143:GLN:NE2	1.94	0.66
1:0:544:G:C2'	1:0:545:G:H5''	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3013:A:O2'	2:9:3014:G:H5''	1.95	0.66
8:E:68:HIS:O	8:E:72:MET:HG3	1.94	0.66
15:M:80:GLY:O	15:M:81:ARG:HD2	1.95	0.66
5:B:8:LYS:HG3	5:B:220:VAL:HG12	1.78	0.65
4:A:100:PRO:HG2	4:A:103:VAL:HG21	1.77	0.65
11:H:170:ASN:HD22	11:H:170:ASN:N	1.95	0.65
1:0:871:G:C8	1:0:871:G:H5'	2.30	0.65
11:H:3:ALA:HA	11:H:58:ARG:NH1	2.10	0.65
1:0:338:C:H4'	6:C:174:ILE:CD1	2.26	0.65
7:D:154:LYS:HD2	7:D:154:LYS:H	1.61	0.65
11:H:46:GLN:HE21	11:H:137:TYR:HE2	1.45	0.65
27:Y:154:ARG:NH1	27:Y:155:ARG:HG3	2.11	0.65
19:Q:25:PRO:HB2	39:Q:4350:HOH:O	1.96	0.65
1:0:2363:G:O2'	19:Q:11:ARG:HG3	1.97	0.65
14:L:91:VAL:HG13	14:L:120:LEU:HD23	1.78	0.65
12:J:93:ARG:NH1	12:J:93:ARG:HB3	2.08	0.65
7:D:65:GLU:HA	39:D:6752:HOH:O	1.97	0.65
15:M:183:THR:HG22	15:M:194:ALA:HB1	1.78	0.65
1:0:1244:U:OP1	12:J:18:ILE:HD13	1.97	0.65
4:A:125:ASN:HB3	4:A:158:VAL:HG12	1.78	0.65
16:N:164:ASP:CG	16:N:167:ASP:HA	2.15	0.65
12:J:19:MET:CE	12:J:132:LEU:HD11	2.26	0.65
1:0:709:G:O2'	17:O:25:VAL:HG12	1.96	0.65
11:H:56:GLN:HE21	11:H:126:ARG:HE	1.43	0.65
1:0:1426:C:H2'	39:O:3209:HOH:O	1.96	0.65
9:F:58:GLU:OE1	15:M:27:ARG:NH2	2.25	0.65
1:0:1641:A:H2'	1:0:1642:A:H5'	1.78	0.65
13:K:29:LEU:HB3	13:K:55:VAL:CG1	2.26	0.65
1:0:447:A:P	22:T:1:SER:HB2	2.37	0.65
5:B:51:VAL:CG2	5:B:327:VAL:HG13	2.26	0.65
29:1:25:LYS:HD2	30:2:49:GLU:H	1.60	0.65
22:T:26:THR:HA	22:T:39:ASN:HB3	1.79	0.65
9:F:77:VAL:HG21	9:F:83:LEU:HD13	1.77	0.65
21:S:51:GLN:NE2	21:S:53:ASN:HD21	1.94	0.64
4:A:199:HIS:CD2	4:A:201:PHE:H	2.13	0.64
15:M:107:ARG:NH1	15:M:107:ARG:HG3	2.11	0.64
4:A:66:ARG:HH11	4:A:66:ARG:HB2	1.62	0.64
1:0:1184:C:H1'	39:O:7937:HOH:O	1.95	0.64
24:V:56:ILE:O	24:V:60:GLN:HG3	1.96	0.64
7:D:159:PRO:O	7:D:163:VAL:HG23	1.96	0.64
23:U:47:ARG:HG3	39:U:4381:HOH:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2718:C:H6	1:0:2718:C:H5'	1.63	0.64
1:0:2661:U:H3	1:0:2812:A:H62	1.44	0.64
25:W:13:MET:HE3	25:W:17:ILE:HG22	1.79	0.64
1:0:1201:C:H2'	1:0:1202:A:H5'	1.79	0.64
23:U:52:THR:HG22	23:U:54:THR:N	2.13	0.64
18:P:80:ARG:HG2	18:P:87:ARG:CZ	2.27	0.64
26:X:37:LEU:CD1	26:X:85:VAL:HG21	2.19	0.64
1:0:1205:U:H2'	1:0:1206:U:C5'	2.27	0.64
32:I:105:VAL:HG11	32:I:129:VAL:HG22	1.80	0.64
1:0:2780:C:H1'	8:E:143:GLN:HE21	1.62	0.64
15:M:187:LEU:CD2	15:M:194:ALA:HB3	2.27	0.64
1:0:2420:G:O2'	1:0:2421:G:H5'	1.97	0.64
28:Z:17:ARG:HD3	39:Z:9219:HOH:O	1.97	0.64
27:Y:126:PRO:HG2	27:Y:128:PHE:CE1	2.33	0.64
1:0:962:C:H1'	16:N:5:ARG:HH12	1.63	0.64
5:B:62:ARG:HA	5:B:65:MET:CE	2.28	0.64
16:N:163:PHE:HZ	16:N:171:HIS:HD1	1.44	0.64
25:W:48:VAL:HG12	25:W:48:VAL:O	1.98	0.64
22:T:71:VAL:HG12	22:T:72:ILE:N	2.13	0.64
26:X:25:ARG:HD3	26:X:64:ALA:O	1.98	0.64
22:T:38:ARG:NH1	39:T:6217:HOH:O	2.31	0.64
25:W:13:MET:CE	25:W:17:ILE:HG22	2.28	0.64
1:0:1205:U:C2'	1:0:1206:U:H5''	2.27	0.64
8:E:8:PRO:HB2	8:E:11:VAL:HG23	1.80	0.64
1:0:1119:G:H22	1:0:1246:A:H2	1.40	0.63
11:H:56:GLN:NE2	11:H:126:ARG:HE	1.96	0.63
11:H:20:ILE:HG23	11:H:120:ILE:HD11	1.80	0.63
1:0:2507:G:H2'	1:0:2510:C:H42	1.62	0.63
6:C:129:HIS:CE1	6:C:231:ARG:HA	2.34	0.63
13:K:74:VAL:CG1	13:K:113:ILE:HG12	2.26	0.63
1:0:1666:C:O2'	1:0:1667:A:H5''	1.98	0.63
9:F:12:LEU:HD21	9:F:111:ILE:HG23	1.79	0.63
16:N:132:ASN:O	16:N:135:VAL:HG12	1.97	0.63
1:0:2896:A:N3	1:0:2896:A:H2'	2.14	0.63
6:C:139:VAL:HG13	39:C:9254:HOH:O	1.98	0.63
15:M:164:THR:HG22	15:M:166:ALA:N	2.11	0.63
32:I:125:ALA:O	32:I:129:VAL:HG23	1.99	0.63
1:0:2748:G:H2'	39:0:8049:HOH:O	1.99	0.63
16:N:23:ARG:HH11	16:N:23:ARG:HG2	1.63	0.63
1:0:1168:C:H5''	32:I:87:THR:HG23	1.81	0.63
1:0:1687:C:O2	29:I:9:GLY:HA2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:59:HIS:HA	11:H:62:LEU:HD23	1.79	0.63
1:0:1182:C:H1'	1:0:1192:A:H8	1.63	0.63
27:Y:144:ARG:HG3	27:Y:144:ARG:HH11	1.63	0.63
1:0:1563:G:H4'	39:0:4808:HOH:O	1.98	0.63
14:L:40:PHE:HB3	39:L:9458:HOH:O	1.99	0.63
17:O:32:ARG:HE	17:O:35:LYS:HD2	1.62	0.63
4:A:88:ILE:HD13	4:A:100:PRO:HD3	1.81	0.63
30:2:22:PRO:HG2	30:2:25:VAL:CG2	2.29	0.63
20:R:106:GLY:HA2	20:R:109:MET:HE3	1.80	0.63
1:0:1766:U:O2	1:0:1778:A:H5'	1.99	0.63
5:B:254:GLN:HG2	5:B:255:GLY:N	2.13	0.63
5:B:102:THR:CG2	5:B:182:VAL:HG12	2.29	0.62
16:N:164:ASP:OD1	16:N:167:ASP:HA	1.99	0.62
1:0:1377:C:H5'	1:0:1377:C:C6	2.30	0.62
7:D:138:GLY:N	39:D:7597:HOH:O	2.32	0.62
15:M:79:ALA:HB3	15:M:81:ARG:NH1	2.14	0.62
6:C:236:THR:HG21	39:C:9180:HOH:O	1.98	0.62
18:P:10:ALA:HA	18:P:13:VAL:CG1	2.29	0.62
11:H:27:LYS:N	11:H:59:HIS:HD2	1.98	0.62
24:V:56:ILE:HG22	24:V:60:GLN:HE21	1.63	0.62
31:3:25:VAL:HG22	31:3:68:LYS:HG3	1.82	0.62
1:0:2878:U:H2'	1:0:2879:A:O4'	1.99	0.62
5:B:212:GLN:HB2	5:B:257:THR:CG2	2.26	0.62
1:0:1116:U:H3	1:0:1246:A:H62	1.47	0.62
5:B:18:ARG:HG3	5:B:256:GLN:HG3	1.80	0.62
7:D:58:VAL:CG1	7:D:60:GLU:HG2	2.29	0.62
12:J:74:ARG:NH1	12:J:105:LEU:HD11	2.14	0.62
11:H:166:SER:CB	11:H:167:PRO:HD3	2.30	0.62
11:H:154:TYR:HB2	39:H:9555:HOH:O	1.99	0.62
7:D:170:TYR:O	7:D:171:ASP:HB3	1.99	0.62
26:X:76:ARG:HH11	26:X:76:ARG:HG3	1.63	0.62
2:9:3020:G:O2'	2:9:3021:G:H5'	1.99	0.62
18:P:59:ARG:HH22	18:P:66:GLN:HE22	1.48	0.61
27:Y:144:ARG:HH11	27:Y:144:ARG:CG	2.11	0.61
32:I:92:PRO:C	32:I:94:GLU:H	2.02	0.61
1:0:282:C:O2'	1:0:283:U:H5'	2.00	0.61
24:V:43:PRO:O	24:V:46:ILE:HG22	2.00	0.61
5:B:215:VAL:HB	5:B:234:ARG:HH12	1.65	0.61
16:N:143:ARG:HH21	16:N:169:PRO:HB2	1.65	0.61
16:N:179:LEU:HD23	16:N:184:ILE:HD12	1.82	0.61
9:F:50:VAL:CG1	9:F:60:VAL:HG11	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:396:U:O2'	1:0:418:C:H4'	2.00	0.61
4:A:121:ALA:O	4:A:124:VAL:HG22	2.01	0.61
20:R:18:LEU:HB2	20:R:143:VAL:HG12	1.81	0.61
1:0:902:G:N7	14:L:18:HIS:HD2	1.98	0.61
13:K:81:ARG:HD3	13:K:87:ARG:NH1	2.15	0.61
32:I:110:GLU:HA	32:I:113:HIS:NE2	2.16	0.61
1:0:2502:C:H2'	1:0:2503:A:H5'	1.82	0.61
16:N:86:LEU:HD21	16:N:180:LEU:CD1	2.31	0.61
22:T:115:GLU:HG3	22:T:116:ASP:N	2.16	0.61
25:W:84:VAL:HG12	39:W:6679:HOH:O	2.00	0.61
23:U:17:THR:CG2	23:U:18:GLY:N	2.64	0.61
24:V:64:GLY:O	24:V:65:ASP:HB2	2.00	0.61
1:0:156:C:H5''	15:M:171:ARG:CD	2.27	0.61
1:0:1118:A:H62	1:0:1244:U:H3	1.47	0.61
1:0:1701:A:H4'	1:0:1702:U:C5'	2.31	0.61
32:I:102:VAL:O	32:I:106:LYS:HG3	2.00	0.61
25:W:52:VAL:HG22	25:W:53:ALA:H	1.64	0.61
24:V:39:ALA:C	24:V:41:GLU:H	2.03	0.61
11:H:3:ALA:HA	11:H:58:ARG:HH12	1.65	0.61
22:T:71:VAL:CG1	22:T:90:PRO:HB3	2.24	0.61
6:C:107:ARG:NE	39:C:9264:HOH:O	2.31	0.61
14:L:133:VAL:HA	39:L:9470:HOH:O	2.01	0.61
1:0:164:G:H4'	14:L:30:ARG:HD3	1.82	0.61
12:J:74:ARG:HB3	12:J:74:ARG:HH11	1.64	0.60
22:T:48:VAL:HG22	22:T:96:VAL:HG22	1.82	0.60
1:0:2769:C:H2'	1:0:2770:G:O4'	1.99	0.60
5:B:5:ARG:HH11	5:B:8:LYS:HE2	1.65	0.60
1:0:2064:U:H5'	1:0:2652:U:H4'	1.82	0.60
25:W:130:HIS:O	25:W:136:GLY:HA3	2.01	0.60
16:N:110:THR:HB	16:N:113:SER:HG	1.64	0.60
6:C:16:VAL:HG12	6:C:17:ASP:H	1.65	0.60
32:I:138:THR:HG22	32:I:139:ILE:H	1.65	0.60
1:0:2851:G:H2'	1:0:2852:A:H5'	1.82	0.60
15:M:31:TRP:HA	15:M:34:GLU:HG3	1.83	0.60
1:0:621:C:H5'	27:Y:132:ASP:OD2	2.02	0.60
1:0:1528:A:H2'	1:0:1529:G:O4'	2.02	0.60
5:B:71:VAL:HG11	5:B:296:LEU:HD22	1.82	0.60
6:C:118:THR:O	6:C:136:VAL:HG13	2.00	0.60
27:Y:189:ASN:HD22	27:Y:189:ASN:C	2.04	0.60
29:1:10:LYS:HG3	39:1:9488:HOH:O	2.00	0.60
6:C:236:THR:HA	39:C:9257:HOH:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:25:MET:SD	7:D:40:ILE:HD11	2.42	0.60
25:W:88:THR:HG22	25:W:90:TYR:HD1	1.66	0.60
12:J:74:ARG:HH12	12:J:76:ASP:HB2	1.65	0.60
4:A:125:ASN:CB	4:A:158:VAL:HG12	2.31	0.60
1:O:681:G:N3	1:O:681:G:H5'	2.17	0.60
5:B:16:ARG:NH1	39:B:9615:HOH:O	2.33	0.60
1:O:1201:C:H5''	39:O:6761:HOH:O	2.02	0.60
2:9:3029:C:H2'	2:9:3030:C:H5'	1.83	0.60
12:J:131:THR:HG22	12:J:134:GLU:H	1.65	0.60
12:J:93:ARG:HH11	12:J:93:ARG:CB	2.07	0.60
11:H:166:SER:HB2	11:H:167:PRO:CD	2.32	0.60
1:O:2748:G:H5'	39:O:8049:HOH:O	2.00	0.60
27:Y:187:VAL:HG12	27:Y:205:ILE:HA	1.83	0.60
30:2:22:PRO:HG2	30:2:25:VAL:HG23	1.84	0.60
16:N:61:ALA:HB3	16:N:88:ALA:HB2	1.84	0.60
2:9:3014:G:C8	2:9:3014:G:H5'	2.35	0.60
18:P:40:VAL:O	18:P:44:VAL:HG23	2.01	0.60
31:3:18:GLN:OE1	31:3:73:GLU:HB3	2.02	0.60
32:I:134:SER:O	32:I:135:LEU:HD23	2.02	0.60
1:O:960:G:H4'	39:O:7904:HOH:O	2.00	0.60
1:O:2291:A:C8	1:O:2309:C:H5'	2.37	0.60
1:O:1555:G:H4'	1:O:1630:A:H2	1.67	0.60
6:C:140:VAL:HB	39:C:9257:HOH:O	2.01	0.59
1:O:380:A:H2'	39:O:7718:HOH:O	2.01	0.59
17:O:32:ARG:HH21	17:O:35:LYS:HZ1	1.50	0.59
1:O:2502:C:C2'	1:O:2503:A:H5'	2.32	0.59
1:O:272:A:H5'	1:O:273:G:OP2	2.02	0.59
12:J:74:ARG:O	12:J:78:ILE:HG12	2.02	0.59
32:I:78:LEU:HD12	32:I:112:LYS:NZ	2.16	0.59
20:R:111:ILE:HG23	20:R:145:LEU:HD11	1.84	0.59
1:O:263:U:O4'	9:F:59:ILE:HD13	2.02	0.59
28:Z:37:HIS:HB2	28:Z:47:VAL:HB	1.83	0.59
16:N:139:TRP:HA	16:N:139:TRP:CE3	2.37	0.59
14:L:35:ARG:HB2	14:L:35:ARG:HH11	1.67	0.59
9:F:91:VAL:CG1	9:F:92:GLY:H	2.08	0.59
5:B:85:ARG:NH1	39:B:9633:HOH:O	2.35	0.59
17:O:42:GLU:HB2	39:O:2176:HOH:O	2.02	0.59
5:B:297:VAL:HB	39:B:9604:HOH:O	2.01	0.59
15:M:77:HIS:HD2	15:M:79:ALA:O	1.85	0.59
1:O:834:G:H4'	1:O:835:U:OP2	2.03	0.59
16:N:62:HIS:HB3	16:N:65:ASP:OD1	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:542:A:H5'	1:0:542:A:C8	2.28	0.59
7:D:136:ARG:HH12	7:D:157:LEU:HA	1.65	0.59
14:L:73:VAL:HG23	14:L:74:THR:N	2.17	0.59
16:N:176:ARG:HG3	16:N:180:LEU:HD13	1.84	0.59
5:B:96:PRO:HG3	39:B:9633:HOH:O	2.00	0.59
24:V:1:THR:HG23	24:V:2:VAL:N	2.16	0.59
16:N:154:LEU:O	16:N:155:GLU:HB3	2.03	0.59
1:0:2100:A:H4'	6:C:64:GLY:O	2.02	0.59
25:W:88:THR:HG23	25:W:110:GLN:HE21	1.68	0.59
32:I:113:HIS:N	32:I:114:PRO:HD2	2.18	0.59
13:K:98:VAL:CG1	13:K:102:GLU:HA	2.33	0.59
1:0:2795:C:O2'	1:0:2796:U:H5'	2.03	0.59
1:0:2003:U:H4'	1:0:2004:U:H5	1.68	0.59
1:0:516:A:H5'	39:0:6188:HOH:O	2.03	0.59
20:R:111:ILE:HG23	20:R:145:LEU:CD1	2.33	0.59
1:0:2721:U:H4'	13:K:87:ARG:HG3	1.84	0.59
1:0:870:G:H2'	1:0:871:G:H5''	1.85	0.59
39:0:9698:HOH:O	5:B:214:PRO:HD2	2.03	0.59
1:0:316:A:N3	1:0:336:G:O2'	2.35	0.59
21:S:51:GLN:HE21	21:S:53:ASN:ND2	1.95	0.59
23:U:14:GLU:OE1	23:U:15:PRO:HD2	2.03	0.59
1:0:2851:G:O2'	1:0:2852:A:H5'	2.03	0.59
14:L:35:ARG:HB2	14:L:35:ARG:NH1	2.18	0.59
1:0:1328:A:OP1	27:Y:169:ARG:HD2	2.02	0.59
1:0:1819:G:H2'	1:0:1820:G:H4'	1.84	0.59
1:0:2676:C:H4'	12:J:70:PHE:CD1	2.38	0.59
13:K:23:ASN:HD21	13:K:107:THR:HB	1.68	0.58
9:F:46:GLU:O	9:F:73:PRO:HD2	2.03	0.58
9:F:58:GLU:CD	15:M:27:ARG:HH22	2.05	0.58
39:0:9972:HOH:O	29:1:1:THR:HA	2.03	0.58
5:B:88:GLU:HB3	5:B:97:LEU:HD12	1.84	0.58
1:0:2505:G:O2'	1:0:2506:A:H5'	2.04	0.58
4:A:33:GLU:O	4:A:34:ASP:HB2	2.03	0.58
16:N:69:TYR:HE2	16:N:184:ILE:HG13	1.67	0.58
7:D:59:GLY:O	7:D:61:PHE:N	2.36	0.58
1:0:545:G:C8	1:0:545:G:H5'	2.35	0.58
17:O:53:GLN:HG2	17:O:56:GLU:OE1	2.03	0.58
15:M:68:ARG:NH2	15:M:73:ARG:HD3	2.18	0.58
24:V:39:ALA:N	24:V:40:PRO:CD	2.66	0.58
26:X:12:ILE:HD12	26:X:36:HIS:ND1	2.19	0.58
39:0:3154:HOH:O	18:P:81:LYS:HG2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:20:G:H21	20:R:117:HIS:HD2	1.48	0.58
1:O:289:G:N2	1:O:363:A:H2	1.96	0.58
11:H:63:GLU:HA	39:H:9544:HOH:O	2.03	0.58
20:R:18:LEU:HD12	20:R:143:VAL:CG1	2.32	0.58
14:L:143:THR:HG22	14:L:144:ASP:H	1.68	0.58
1:O:2676:C:H4'	12:J:70:PHE:CE1	2.39	0.58
1:O:877:G:H5'	1:O:878:G:OP1	2.03	0.58
1:O:969:G:H1	1:O:999:C:H42	1.49	0.58
1:O:2726:U:O2'	26:X:22:ASN:ND2	2.37	0.58
4:A:57:ALA:HB1	4:A:65:ARG:HE	1.69	0.58
16:N:169:PRO:O	16:N:172:PHE:HB3	2.03	0.58
1:O:2426:G:H1'	39:O:6621:HOH:O	2.03	0.58
1:O:2081:A:H4'	12:J:69:TYR:CE1	2.39	0.58
22:T:112:LEU:CD2	22:T:119:ALA:HB3	2.33	0.58
1:O:625:U:H5'	39:O:3784:HOH:O	2.04	0.58
11:H:111:ASP:HA	39:H:9510:HOH:O	2.02	0.58
1:O:558:C:C2'	1:O:559:U:H5''	2.34	0.58
26:X:71:ARG:HB3	26:X:88:GLU:OE1	2.03	0.58
6:C:236:THR:H	6:C:239:ALA:HB3	1.68	0.58
20:R:96:VAL:HG13	20:R:106:GLY:HA3	1.86	0.58
8:E:20:ILE:HD12	8:E:33:LEU:HD12	1.86	0.58
5:B:238:ASN:ND2	5:B:240:GLY:H	1.95	0.58
10:G:20:VAL:O	10:G:24:VAL:HG23	2.03	0.58
21:S:73:ASP:OD1	21:S:76:GLU:HG3	2.04	0.58
25:W:21:LEU:HB3	25:W:26:ILE:HG12	1.85	0.58
14:L:104:ASP:HB2	39:L:9460:HOH:O	2.03	0.58
5:B:238:ASN:HD22	5:B:240:GLY:N	1.95	0.58
1:O:1181:A:H5'	32:I:94:GLU:OE2	2.04	0.58
1:O:1352:A:O2'	1:O:1353:C:OP1	2.20	0.58
1:O:1384:C:H5'	26:X:30:MET:HG2	1.85	0.57
1:O:1268:C:O2'	27:Y:169:ARG:HB2	2.04	0.57
5:B:221:GLN:HE22	13:K:42:ASN:HD22	1.51	0.57
4:A:26:ASP:O	4:A:28:GLU:N	2.36	0.57
24:V:55:ARG:O	24:V:59:ILE:HG12	2.04	0.57
1:O:558:C:O2'	1:O:559:U:H5''	2.04	0.57
22:T:49:GLU:OE2	22:T:97:ARG:HD2	2.04	0.57
1:O:447:A:OP2	22:T:1:SER:HB2	2.04	0.57
24:V:20:LEU:HD22	24:V:60:GLN:HE22	1.69	0.57
17:O:57:THR:O	17:O:111:VAL:HG23	2.03	0.57
5:B:190:MET:HE2	5:B:194:PHE:CD1	2.39	0.57
39:O:9983:HOH:O	4:A:180:LYS:HG2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:195:ARG:HG2	5:B:323:LEU:HD22	1.86	0.57
32:I:78:LEU:HD12	32:I:112:LYS:HZ2	1.68	0.57
22:T:112:LEU:HD23	22:T:119:ALA:HB3	1.86	0.57
26:X:31:ILE:O	26:X:35:GLU:HG3	2.05	0.57
16:N:170:GLU:O	16:N:174:GLU:HG3	2.04	0.57
27:Y:112:GLU:OE2	27:Y:115:ARG:NH1	2.37	0.57
1:O:2726:U:O2	1:O:2749:U:O5'	2.22	0.57
27:Y:203:VAL:CG1	27:Y:228:VAL:HG22	2.35	0.57
7:D:172:VAL:HG12	7:D:173:GLU:N	2.18	0.57
9:F:21:GLU:O	9:F:24:ARG:HG3	2.05	0.57
5:B:185:GLY:HA2	39:B:9632:HOH:O	2.04	0.57
14:L:67:ARG:O	14:L:71:GLU:HG3	2.04	0.57
1:O:1552:G:N2	1:O:1634:G:H1'	2.19	0.57
6:C:236:THR:HG22	6:C:239:ALA:CB	2.34	0.57
1:O:558:C:H2'	1:O:559:U:C5'	2.34	0.57
1:O:1943:C:H4'	4:A:211:LYS:O	2.05	0.57
31:3:3:MET:HB2	31:3:88:LEU:HD11	1.85	0.57
14:L:136:ALA:HB3	39:L:9470:HOH:O	2.03	0.57
1:O:2421:G:H1'	39:O:4289:HOH:O	2.03	0.57
1:O:1066:U:H2'	1:O:1067:A:C8	2.40	0.57
31:3:62:THR:HB	39:3:9482:HOH:O	2.04	0.57
15:M:164:THR:CG2	15:M:165:GLY:N	2.68	0.57
1:O:1189:A:O2'	1:O:1208:C:H2'	2.04	0.57
1:O:308:U:H5'	22:T:97:ARG:NH2	2.19	0.57
16:N:139:TRP:HA	16:N:139:TRP:HE3	1.70	0.57
1:O:538:C:OP2	27:Y:134:HIS:HE1	1.88	0.57
2:9:3069:U:OP1	16:N:4:PRO:HG3	2.05	0.57
1:O:871:G:C8	1:O:871:G:H5''	2.34	0.57
10:G:12:ILE:N	10:G:13:PRO:CD	2.68	0.57
1:O:1218:U:H2'	1:O:1219:U:C6	2.40	0.57
14:L:36:ASP:HB2	39:L:9433:HOH:O	2.05	0.57
39:9:4707:HOH:O	16:N:147:ILE:HD12	2.05	0.57
12:J:39:VAL:HG13	12:J:106:GLY:O	2.05	0.57
1:O:256:C:H2'	1:O:257:G:O4'	2.05	0.57
7:D:146:LYS:NZ	16:N:107:ASN:HD21	2.02	0.57
17:O:39:THR:O	17:O:115:ARG:NH2	2.37	0.57
4:A:33:GLU:CD	4:A:33:GLU:N	2.57	0.56
4:A:107:ASN:OD1	4:A:120:ARG:HD2	2.04	0.56
1:O:2270:G:H4'	4:A:223:ARG:HH12	1.70	0.56
6:C:214:THR:HG23	39:C:9242:HOH:O	2.03	0.56
1:O:138:U:H5''	1:O:139:C:OP2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:S:77:VAL:O	21:S:80:ARG:HG2	2.05	0.56
1:O:244:C:OP2	9:F:38:LYS:HE3	2.05	0.56
9:F:39:SER:HB3	9:F:45:ALA:HB2	1.85	0.56
18:P:16:VAL:HG12	18:P:17:GLY:N	2.20	0.56
8:E:34:TRP:O	12:J:127:ILE:HD11	2.05	0.56
7:D:54:ALA:HB2	7:D:69:ILE:HD12	1.87	0.56
26:X:21:PRO:HG2	26:X:24:LYS:HD3	1.85	0.56
2:9:3002:U:OP2	2:9:3003:A:H5'	2.06	0.56
13:K:55:VAL:HG12	13:K:56:SER:N	2.19	0.56
1:O:775:G:OP1	29:1:16:HIS:HE1	1.89	0.56
6:C:194:PHE:HA	6:C:234:VAL:HG13	1.86	0.56
15:M:182:LYS:O	15:M:194:ALA:HB2	2.06	0.56
1:O:1634:G:H3'	39:O:4478:HOH:O	2.05	0.56
1:O:2563:U:H2'	1:O:2565:C:O5'	2.05	0.56
5:B:145:HIS:HD2	5:B:146:THR:O	1.89	0.56
15:M:60:VAL:C	15:M:61:ILE:HD12	2.25	0.56
25:W:65:VAL:HA	25:W:68:THR:HG22	1.87	0.56
11:H:56:GLN:HE22	11:H:93:GLN:HG2	1.70	0.56
9:F:1:PRO:H3	9:F:4:VAL:HG23	1.71	0.56
11:H:148:GLU:HA	11:H:148:GLU:OE1	2.05	0.56
25:W:88:THR:HG22	25:W:89:ASP:H	1.69	0.56
5:B:51:VAL:HG23	5:B:329:TYR:O	2.06	0.56
2:9:3014:G:O2'	16:N:1:ALA:HB2	2.05	0.56
1:O:2064:U:H5'	1:O:2652:U:O3'	2.05	0.56
1:O:2032:U:H2'	1:O:2033:G:C5'	2.35	0.56
1:O:151:A:H2'	1:O:152:A:O4'	2.05	0.56
1:O:432:G:O2'	1:O:433:C:H5'	2.06	0.56
23:U:5:GLU:HG2	23:U:10:GLY:O	2.05	0.56
5:B:264:GLU:OE2	5:B:302:PRO:HD3	2.05	0.56
6:C:154:VAL:O	6:C:158:GLU:HG3	2.06	0.56
11:H:38:LYS:HE2	11:H:42:ASP:HB2	1.88	0.56
25:W:4:LEU:HD11	25:W:45:VAL:HG12	1.87	0.56
22:T:49:GLU:CB	22:T:59:GLU:HG2	2.34	0.56
26:X:25:ARG:HG2	39:X:5356:HOH:O	2.06	0.56
12:J:107:ASN:HD22	12:J:109:TYR:H	1.53	0.56
1:O:185:G:H4'	1:O:186:A:H4'	1.87	0.56
7:D:54:ALA:CB	7:D:69:ILE:HD12	2.35	0.56
1:O:1118:A:H8	1:O:1119:G:H5''	1.71	0.56
12:J:75:PRO:HG2	12:J:105:LEU:CD2	2.35	0.56
32:I:138:THR:HG22	32:I:139:ILE:N	2.20	0.56
1:O:1187:U:O2'	1:O:1189:A:H2	1.89	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:316:A:H5'	22:T:54:ASP:OD2	2.03	0.56
10:G:24:VAL:O	10:G:28:GLU:HB2	2.05	0.56
1:0:2694:A:H4'	8:E:91:PHE:HE1	1.70	0.56
23:U:39:ASN:ND2	23:U:44:ARG:HH11	2.03	0.56
1:0:558:C:H2'	1:0:559:U:H5'	1.88	0.56
6:C:162:VAL:HG22	6:C:232:LEU:HD21	1.88	0.56
39:0:9738:HOH:O	15:M:82:ARG:HD2	2.06	0.56
39:9:1361:HOH:O	16:N:41:LYS:HE3	2.05	0.56
28:Z:30:GLU:HA	28:Z:33:MET:HE3	1.88	0.55
12:J:107:ASN:ND2	12:J:109:TYR:H	2.04	0.55
4:A:135:VAL:HG11	4:A:147:ARG:NH1	2.21	0.55
10:G:67:LEU:O	10:G:71:LEU:HG	2.05	0.55
25:W:108:ARG:HG3	25:W:114:PRO:HG3	1.88	0.55
2:9:3076:G:C3'	2:9:3077:A:H5''	2.27	0.55
5:B:53:LEU:CD1	5:B:327:VAL:HG22	2.36	0.55
9:F:58:GLU:HA	9:F:61:MET:HE2	1.88	0.55
26:X:61:ARG:HB2	26:X:65:ASN:HB2	1.87	0.55
1:0:1736:A:H1'	39:0:8143:HOH:O	2.07	0.55
4:A:36:ASP:OD2	4:A:85:SER:HB2	2.06	0.55
1:0:1926:G:H2'	1:0:1927:A:C8	2.41	0.55
30:2:49:GLU:HB2	39:2:131:HOH:O	2.06	0.55
4:A:89:ALA:HB3	39:A:9608:HOH:O	2.05	0.55
9:F:48:VAL:HG23	9:F:74:PHE:CB	2.36	0.55
13:K:4:LEU:CD2	13:K:116:GLU:HB3	2.35	0.55
1:0:1778:A:H2'	1:0:1779:A:H5'	1.88	0.55
5:B:305:ASP:O	5:B:306:LYS:HB2	2.07	0.55
1:0:2456:A:H2'	1:0:2457:U:C6	2.42	0.55
1:0:291:C:H2'	1:0:292:G:O4'	2.06	0.55
5:B:329:TYR:CE2	23:U:15:PRO:HG2	2.41	0.55
15:M:71:SER:HB2	15:M:92:THR:HG22	1.89	0.55
1:0:475:G:H5'	6:C:73:LEU:HD23	1.87	0.55
25:W:21:LEU:HD22	25:W:26:ILE:HD11	1.88	0.55
12:J:75:PRO:HD3	12:J:136:SER:OG	2.05	0.55
10:G:12:ILE:HD12	39:G:692:HOH:O	2.06	0.55
16:N:11:ARG:HG3	16:N:14:ARG:NH1	2.21	0.55
14:L:57:VAL:HG12	14:L:57:VAL:O	2.07	0.55
4:A:123:GLY:HA3	4:A:162:GLY:HA2	1.87	0.55
27:Y:154:ARG:HH12	27:Y:155:ARG:CG	2.17	0.55
1:0:1973:A:H5'	1:0:1973:A:C8	2.39	0.55
1:0:960:G:N3	1:0:960:G:H2'	2.21	0.55
1:0:1789:G:O6	18:P:73:HIS:HE1	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:246:ARG:NH1	6:C:246:ARG:HB3	2.22	0.55
27:Y:106:THR:HG23	27:Y:107:PRO:HD2	1.88	0.55
8:E:20:ILE:CD1	8:E:33:LEU:HD12	2.37	0.55
4:A:194:MET:HE1	4:A:199:HIS:HB2	1.88	0.55
27:Y:189:ASN:ND2	27:Y:192:ASP:H	2.05	0.55
22:T:32:ARG:NH1	22:T:38:ARG:HH12	2.05	0.55
1:O:625:U:H5'	1:O:1044:C:N4	2.21	0.55
17:O:14:LEU:CD2	17:O:102:ILE:HD11	2.37	0.55
1:O:441:A:H1'	1:O:442:A:N7	2.21	0.55
7:D:135:VAL:HG22	7:D:136:ARG:H	1.72	0.55
4:A:191:GLY:HA2	4:A:194:MET:HE3	1.89	0.55
2:9:3051:A:H5'	16:N:160:SER:HB3	1.89	0.55
39:O:8105:HOH:O	31:3:60:LYS:HG3	2.06	0.55
5:B:307:ARG:HB3	39:B:9650:HOH:O	2.06	0.54
1:O:1882:C:OP1	4:A:192:VAL:HG23	2.07	0.54
1:O:1183:C:H2'	39:O:6772:HOH:O	2.07	0.54
15:M:68:ARG:HD3	15:M:68:ARG:O	2.08	0.54
5:B:258:GLY:H	5:B:260:HIS:CE1	2.25	0.54
9:F:60:VAL:HG12	9:F:60:VAL:O	2.06	0.54
31:3:42:ARG:HH11	31:3:42:ARG:HG3	1.72	0.54
1:O:2769:C:O2'	1:O:2770:G:H5'	2.07	0.54
16:N:11:ARG:O	16:N:15:GLU:HG3	2.07	0.54
2:9:3051:A:H5'	16:N:160:SER:CB	2.37	0.54
22:T:78:THR:HB	22:T:87:VAL:O	2.08	0.54
1:O:2827:A:H2'	1:O:2828:G:O4'	2.06	0.54
1:O:2866:U:H4'	1:O:2867:G:H5'	1.89	0.54
16:N:115:VAL:HG22	39:N:9356:HOH:O	2.07	0.54
32:I:139:ILE:HG22	32:I:140:GLU:N	2.23	0.54
1:O:1189:A:H1'	1:O:1209:C:O4'	2.07	0.54
7:D:24:HIS:HB2	7:D:72:LYS:CB	2.37	0.54
1:O:2591:C:H2'	1:O:2592:G:O4'	2.07	0.54
12:J:107:ASN:HD22	12:J:107:ASN:C	2.11	0.54
1:O:2533:C:C6	1:O:2533:C:H5'	2.42	0.54
4:A:153:ARG:CB	4:A:153:ARG:HH11	2.21	0.54
11:H:21:THR:O	11:H:120:ILE:HD12	2.08	0.54
16:N:154:LEU:HG	16:N:155:GLU:H	1.71	0.54
23:U:14:GLU:O	23:U:17:THR:HB	2.08	0.54
1:O:1878:G:O2'	1:O:1879:U:OP2	2.25	0.54
1:O:797:A:H4'	28:Z:10:ARG:N	2.22	0.54
5:B:72:THR:HB	39:B:9604:HOH:O	2.07	0.54
1:O:474:C:O3'	6:C:73:LEU:HD21	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1681:G:H5''	1:0:1682:A:H5'	1.89	0.54
26:X:43:VAL:HG12	26:X:44:ASP:N	2.23	0.54
1:0:1626:A:H2'	1:0:1627:G:O4'	2.08	0.54
5:B:40:GLY:HA3	39:B:9645:HOH:O	2.08	0.54
1:0:2717:C:O2'	1:0:2718:C:H5''	2.07	0.54
1:0:1666:C:H2'	1:0:1667:A:C5'	2.36	0.54
1:0:2769:C:C2'	1:0:2770:G:H5'	2.38	0.54
7:D:50:VAL:O	7:D:71:ALA:HA	2.07	0.54
1:0:1350:U:H2'	1:0:1351:G:O4'	2.07	0.54
1:0:2670:G:O2'	1:0:2671:U:H5'	2.08	0.54
28:Z:72:GLU:OE1	28:Z:77:LYS:HE2	2.07	0.54
4:A:190:ARG:NH2	4:A:207:GLN:OE1	2.40	0.54
11:H:46:GLN:NE2	11:H:137:TYR:HE2	2.05	0.54
1:0:1209:C:H2'	1:0:1210:G:C8	2.42	0.54
25:W:4:LEU:O	25:W:32:CYS:HA	2.08	0.54
5:B:62:ARG:HA	5:B:65:MET:HE2	1.90	0.54
5:B:254:GLN:HG3	39:B:9530:HOH:O	2.08	0.54
17:O:59:VAL:HG23	17:O:111:VAL:CG2	2.37	0.54
31:3:60:LYS:HG3	31:3:61:PRO:HD2	1.88	0.54
27:Y:99:ALA:HB2	27:Y:233:TYR:CE2	2.42	0.54
12:J:8:ALA:HA	12:J:35:THR:HG22	1.90	0.54
1:0:1595:G:O2'	1:0:1596:U:H5'	2.08	0.54
22:T:12:ARG:NH1	39:T:3035:HOH:O	2.40	0.54
25:W:21:LEU:HD13	25:W:26:ILE:HD11	1.90	0.53
15:M:59:GLY:HA3	15:M:141:ILE:HD12	1.89	0.53
5:B:17:LYS:O	5:B:260:HIS:HD2	1.91	0.53
1:0:1406:A:H4'	1:0:1407:A:H5''	1.90	0.53
5:B:56:ASP:OD1	5:B:322:ARG:HB3	2.08	0.53
1:0:1625:U:H4'	39:0:5232:HOH:O	2.08	0.53
1:0:2817:G:P	39:0:8476:HOH:O	2.66	0.53
1:0:949:U:O2'	19:Q:40:HIS:HE1	1.91	0.53
23:U:49:LEU:HG	39:U:3805:HOH:O	2.07	0.53
1:0:1594:C:OP2	18:P:120:ARG:HD2	2.08	0.53
6:C:107:ARG:HH11	6:C:107:ARG:HB3	1.71	0.53
5:B:195:ARG:HD2	5:B:324:ASP:OD1	2.07	0.53
1:0:2265:U:H2'	1:0:2266:A:C8	2.43	0.53
39:0:7381:HOH:O	15:M:178:LYS:HB2	2.07	0.53
31:3:3:MET:O	31:3:90:PHE:HA	2.09	0.53
5:B:51:VAL:HG23	5:B:327:VAL:HG13	1.90	0.53
1:0:2645:U:OP2	1:0:2645:U:C6	2.61	0.53
6:C:78:ARG:HG3	6:C:78:ARG:NH1	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2694:A:H4'	8:E:91:PHE:CE1	2.44	0.53
1:0:2894:C:O2'	1:0:2895:C:H5'	2.08	0.53
12:J:47:THR:HG22	12:J:48:GLY:N	2.23	0.53
7:D:172:VAL:HG12	7:D:173:GLU:H	1.74	0.53
24:V:42:ASN:HB3	39:V:7247:HOH:O	2.08	0.53
30:2:18:ASN:ND2	30:2:40:ARG:H	2.06	0.53
7:D:92:GLU:HB2	39:D:3862:HOH:O	2.07	0.53
31:3:65:THR:HG23	31:3:88:LEU:HD22	1.91	0.53
5:B:51:VAL:HG22	5:B:53:LEU:HD13	1.90	0.53
27:Y:187:VAL:HG23	27:Y:192:ASP:CB	2.38	0.53
1:0:1168:C:H5''	32:I:87:THR:CG2	2.38	0.53
1:0:1419:U:H2'	1:0:1685:A:C2	2.43	0.53
6:C:25:PRO:HG2	39:C:9126:HOH:O	2.08	0.53
26:X:7:GLU:HA	26:X:74:ALA:O	2.09	0.53
5:B:86:ALA:HA	39:B:9576:HOH:O	2.09	0.53
1:0:2676:C:H6	1:0:2676:C:H5''	1.73	0.53
1:0:2456:A:H2'	1:0:2457:U:H6	1.73	0.53
11:H:136:ALA:HB3	11:H:146:VAL:HG21	1.90	0.53
12:J:103:VAL:HG12	39:J:5907:HOH:O	2.09	0.53
5:B:18:ARG:HE	5:B:256:GLN:NE2	2.06	0.53
4:A:203:GLY:HA2	39:A:9531:HOH:O	2.08	0.53
1:0:951:A:C2'	1:0:952:G:H5'	2.38	0.53
5:B:51:VAL:HG21	5:B:327:VAL:HG13	1.90	0.53
14:L:80:ASP:CB	14:L:90:ARG:HB3	2.38	0.53
6:C:233:THR:HG22	6:C:234:VAL:N	2.23	0.53
22:T:89:ARG:O	22:T:89:ARG:HG3	2.09	0.53
1:0:2320:U:H4'	1:0:2321:A:O4'	2.08	0.53
22:T:92:ASP:OD1	22:T:94:SER:HB3	2.08	0.53
1:0:1501:A:OP2	18:P:37:ARG:HD2	2.08	0.53
1:0:2912:C:H2'	1:0:2913:A:O4'	2.09	0.53
13:K:55:VAL:CG1	13:K:56:SER:N	2.72	0.53
11:H:45:VAL:HA	11:H:167:PRO:O	2.09	0.53
5:B:141:ARG:HG2	5:B:165:ARG:HA	1.90	0.53
5:B:62:ARG:HA	5:B:65:MET:HE3	1.90	0.53
6:C:246:ARG:NH1	39:C:9176:HOH:O	2.40	0.53
18:P:103:THR:O	18:P:107:GLU:HG3	2.08	0.53
29:1:21:ARG:HD2	29:1:37:CYS:SG	2.48	0.53
1:0:1724:U:H5''	39:0:4320:HOH:O	2.08	0.53
23:U:4:ARG:HH11	23:U:4:ARG:HG2	1.74	0.53
1:0:2548:C:OP2	5:B:5:ARG:NH2	2.41	0.52
24:V:56:ILE:HG22	24:V:60:GLN:NE2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:2419:U:H5''	1:O:2420:G:H5'	1.91	0.52
5:B:321:PRO:HA	39:B:9655:HOH:O	2.09	0.52
15:M:107:ARG:NH1	39:M:9383:HOH:O	2.42	0.52
9:F:50:VAL:HG21	9:F:63:ILE:HG21	1.91	0.52
1:O:564:G:H1'	39:O:6837:HOH:O	2.09	0.52
22:T:41:ARG:NH1	22:T:41:ARG:HG2	2.22	0.52
32:I:93:GLN:HA	32:I:96:PHE:HE2	1.74	0.52
6:C:47:GLY:HA2	6:C:92:PRO:HB2	1.90	0.52
1:O:248:A:H5'	1:O:249:G:OP2	2.10	0.52
10:G:64:ASN:N	10:G:64:ASN:HD22	2.05	0.52
25:W:6:GLN:CB	25:W:26:ILE:HD12	2.33	0.52
25:W:122:ARG:CG	25:W:122:ARG:NH1	2.70	0.52
7:D:136:ARG:HB3	7:D:137:PRO:HD2	1.90	0.52
20:R:18:LEU:HB2	20:R:143:VAL:HG13	1.91	0.52
4:A:69:LEU:HD23	4:A:107:ASN:CB	2.40	0.52
1:O:2508:C:H2'	39:O:7264:HOH:O	2.09	0.52
19:Q:32:GLU:HA	19:Q:71:TYR:OH	2.09	0.52
6:C:127:ARG:CZ	6:C:225:PRO:HG2	2.39	0.52
32:I:129:VAL:O	32:I:129:VAL:HG12	2.10	0.52
14:L:145:LEU:O	14:L:148:GLU:HG3	2.08	0.52
1:O:121:U:OP2	30:2:10:ARG:NH2	2.38	0.52
17:O:59:VAL:CG2	17:O:111:VAL:HG21	2.39	0.52
9:F:48:VAL:HG12	9:F:97:ALA:HB2	1.91	0.52
1:O:848:C:H5'	39:O:7760:HOH:O	2.10	0.52
4:A:109:GLU:HG2	4:A:116:GLY:N	2.25	0.52
1:O:2541:U:O2	1:O:2618:G:N2	2.43	0.52
32:I:106:LYS:O	32:I:110:GLU:HG3	2.09	0.52
1:O:119:A:H2'	1:O:120:A:H5''	1.92	0.52
4:A:88:ILE:HG22	4:A:88:ILE:O	2.09	0.52
16:N:154:LEU:O	16:N:155:GLU:CB	2.58	0.52
1:O:2816:A:H2'	39:O:8476:HOH:O	2.10	0.52
14:L:97:VAL:HG12	14:L:98:GLU:O	2.09	0.52
1:O:1234:U:N3	5:B:244:PRO:HB3	2.25	0.52
16:N:162:ASP:HA	39:N:9331:HOH:O	2.10	0.52
22:T:69:LYS:O	22:T:71:VAL:HG23	2.10	0.52
14:L:91:VAL:CG1	14:L:120:LEU:HD23	2.39	0.52
1:O:1527:A:H1'	1:O:1528:A:C8	2.45	0.52
4:A:179:MET:HA	4:A:179:MET:CE	2.39	0.52
1:O:1462:C:H2'	1:O:1463:A:C8	2.45	0.52
24:V:8:ILE:HG21	24:V:59:ILE:HG13	1.91	0.52
15:M:164:THR:HG22	15:M:165:GLY:N	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:98:GLN:O	15:M:102:GLU:HG3	2.10	0.52
4:A:94:LEU:HB2	4:A:95:PRO:HD2	1.90	0.52
5:B:41:PHE:CD1	5:B:79:MET:HE2	2.45	0.52
15:M:24:GLN:NE2	15:M:27:ARG:HH11	2.08	0.52
1:O:2896:A:H5''	39:X:5399:HOH:O	2.09	0.52
1:O:1218:U:H2'	1:O:1219:U:H6	1.74	0.52
25:W:38:THR:HG22	25:W:39:ASP:N	2.24	0.52
21:S:33:SER:OG	21:S:36:GLU:HG3	2.10	0.52
12:J:80:LYS:NZ	39:J:7377:HOH:O	2.42	0.52
1:O:737:A:H2'	1:O:738:G:O4'	2.09	0.52
5:B:41:PHE:CD2	5:B:190:MET:HE3	2.45	0.52
8:E:23:GLU:HG2	8:E:28:SER:HB3	1.91	0.52
1:O:1211:G:O2'	1:O:1212:C:H5'	2.10	0.52
1:O:2101:A:H2'	6:C:63:SER:OG	2.10	0.52
13:K:28:GLU:HB3	13:K:59:LYS:HB2	1.91	0.52
18:P:10:ALA:HA	18:P:13:VAL:HG12	1.92	0.52
16:N:152:GLU:C	16:N:154:LEU:H	2.13	0.52
14:L:53:ARG:NH2	14:L:57:VAL:HG12	2.25	0.52
16:N:42:HIS:CE1	16:N:75:THR:HG1	2.28	0.52
17:O:97:SER:OG	17:O:100:GLN:HG3	2.10	0.52
1:O:1946:C:H2'	1:O:1971:G:C8	2.45	0.52
28:Z:53:GLY:HA2	28:Z:67:GLY:O	2.10	0.52
15:M:99:ARG:NH2	15:M:170:ASN:HD22	2.00	0.51
1:O:1741:U:H3'	39:O:3369:HOH:O	2.09	0.51
6:C:142:ASP:OD1	6:C:237:GLU:HB3	2.10	0.51
16:N:49:THR:HG22	16:N:56:ASP:CB	2.40	0.51
16:N:18:THR:HG21	39:N:9346:HOH:O	2.08	0.51
15:M:24:GLN:O	15:M:28:GLN:HG3	2.11	0.51
20:R:44:VAL:O	20:R:48:GLU:HG3	2.10	0.51
6:C:163:HIS:HD2	39:C:9243:HOH:O	1.92	0.51
7:D:57:THR:HG23	7:D:63:ILE:CA	2.31	0.51
1:O:1835:U:C5	1:O:1840:A:N7	2.67	0.51
15:M:79:ALA:HB3	15:M:81:ARG:HH12	1.72	0.51
9:F:48:VAL:HG23	9:F:74:PHE:HB3	1.92	0.51
12:J:90:LYS:HB2	36:J:9302:CL:CL	2.46	0.51
15:M:15:PRO:HA	15:M:20:LEU:HD23	1.92	0.51
1:O:1477:C:H5'	1:O:1868:G:C5'	2.40	0.51
7:D:23:VAL:CG2	7:D:73:VAL:HB	2.41	0.51
25:W:110:GLN:HE21	25:W:110:GLN:HA	1.76	0.51
4:A:36:ASP:O	4:A:38:ILE:N	2.42	0.51
1:O:776:A:OP1	29:1:28:HIS:HE1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:284:C:H4'	1:0:285:A:H8	1.74	0.51
13:K:20:CYS:HB2	13:K:29:LEU:HG	1.92	0.51
6:C:115:LEU:O	6:C:118:THR:HB	2.10	0.51
39:0:8484:HOH:O	5:B:2:GLN:CG	2.53	0.51
12:J:39:VAL:HG11	12:J:107:ASN:CG	2.30	0.51
1:0:2032:U:H2'	1:0:2033:G:H5''	1.92	0.51
1:0:1363:G:OP1	6:C:76:ARG:NH2	2.43	0.51
1:0:407:A:H5'	39:0:6556:HOH:O	2.10	0.51
6:C:118:THR:HG22	6:C:137:PRO:HB3	1.92	0.51
20:R:18:LEU:HG	20:R:91:LEU:HD13	1.92	0.51
18:P:55:LYS:HG2	18:P:56:GLY:N	2.25	0.51
20:R:29:LYS:NZ	39:R:9449:HOH:O	2.44	0.51
14:L:90:ARG:NH2	14:L:121:ILE:HD11	2.25	0.51
14:L:120:LEU:HD12	14:L:133:VAL:HG21	1.92	0.51
5:B:62:ARG:HG2	5:B:65:MET:HE3	1.92	0.51
1:0:2883:A:H2'	1:0:2884:G:O4'	2.11	0.51
1:0:2717:C:H2'	1:0:2718:C:C5'	2.35	0.51
4:A:36:ASP:C	4:A:38:ILE:H	2.14	0.51
16:N:86:LEU:HD21	16:N:180:LEU:HD12	1.92	0.51
1:0:1067:A:H5'	39:0:4922:HOH:O	2.10	0.51
1:0:2270:G:H4'	4:A:223:ARG:NH1	2.25	0.51
1:0:2443:C:H5'	14:L:57:VAL:HG21	1.93	0.51
9:F:49:PHE:HE1	9:F:98:VAL:HG23	1.76	0.51
1:0:2626:C:H2'	1:0:2627:G:C8	2.46	0.51
1:0:1919:A:H4'	39:0:5416:HOH:O	2.10	0.51
11:H:54:THR:O	11:H:55:VAL:HG13	2.11	0.51
1:0:559:U:H2'	1:0:560:C:O4'	2.11	0.51
22:T:40:VAL:HG22	22:T:41:ARG:N	2.26	0.51
8:E:11:VAL:HG12	8:E:12:ASP:N	2.26	0.51
1:0:2524:G:H21	1:0:2526:C:N4	2.08	0.51
1:0:1966:U:H2'	1:0:1967:U:H2'	1.93	0.51
19:Q:3:SER:HB3	39:Q:5998:HOH:O	2.11	0.51
1:0:2711:U:H1'	39:0:4035:HOH:O	2.09	0.51
1:0:1278:A:H4'	1:0:1279:U:C4	2.46	0.51
1:0:69:A:H5'	1:0:69:A:C8	2.45	0.51
6:C:142:ASP:CG	6:C:237:GLU:HB3	2.31	0.51
13:K:7:ASP:OD2	13:K:81:ARG:NH2	2.44	0.51
9:F:58:GLU:HA	9:F:61:MET:HG3	1.93	0.51
1:0:1333:U:H2'	1:0:1334:C:C6	2.46	0.51
21:S:57:THR:CG2	21:S:58:MET:N	2.74	0.50
5:B:41:PHE:CG	5:B:79:MET:HE2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:7:ILE:HD11	8:E:11:VAL:C	2.32	0.50
12:J:99:GLU:HA	39:J:7377:HOH:O	2.09	0.50
1:0:1853:C:OP1	4:A:231:LYS:HG3	2.12	0.50
1:0:2821:C:H4'	5:B:116:PRO:HG3	1.92	0.50
12:J:54:VAL:HG11	12:J:138:THR:HG21	1.93	0.50
26:X:7:GLU:HA	26:X:75:ALA:HA	1.92	0.50
15:M:167:GLY:O	15:M:171:ARG:HG3	2.11	0.50
25:W:110:GLN:NE2	25:W:110:GLN:HA	2.26	0.50
1:0:1165:G:H1'	1:0:1174:A:H1'	1.94	0.50
2:9:3008:G:O6	16:N:11:ARG:NH1	2.39	0.50
1:0:1363:G:P	6:C:76:ARG:HH22	2.35	0.50
11:H:116:ALA:O	11:H:117:PHE:C	2.50	0.50
32:I:72:VAL:CG1	32:I:73:PRO:HD2	2.41	0.50
1:0:90:A:H2'	1:0:91:G:O4'	2.11	0.50
9:F:26:THR:HG21	9:F:102:GLY:C	2.32	0.50
26:X:78:GLU:HG2	26:X:79:GLU:OE2	2.11	0.50
5:B:175:LEU:O	5:B:175:LEU:HD23	2.11	0.50
6:C:16:VAL:HG12	6:C:17:ASP:N	2.25	0.50
1:0:1198:U:H2'	1:0:1200:A:OP2	2.11	0.50
7:D:104:PHE:CE2	7:D:166:ILE:HD13	2.46	0.50
26:X:72:VAL:HG22	26:X:85:VAL:HG12	1.92	0.50
11:H:58:ARG:HG3	11:H:58:ARG:HH11	1.75	0.50
1:0:475:G:C5'	6:C:73:LEU:HD23	2.42	0.50
1:0:926:A:O2'	14:L:41:HIS:HD2	1.94	0.50
31:3:35:TRP:HB2	39:3:9488:HOH:O	2.09	0.50
1:0:1120:U:H5''	1:0:1120:U:C6	2.46	0.50
1:0:362:G:H2'	1:0:363:A:C8	2.46	0.50
5:B:310:ARG:HD2	39:B:9588:HOH:O	2.10	0.50
1:0:2812:A:C2	1:0:2814:A:N6	2.68	0.50
1:0:1118:A:C8	1:0:1118:A:C3'	2.89	0.50
23:U:9:CYS:O	23:U:52:THR:HG23	2.10	0.50
1:0:474:C:O3'	6:C:73:LEU:CD2	2.60	0.50
1:0:485:A:N3	1:0:487:G:H5''	2.26	0.50
7:D:51:ARG:HD3	39:D:7636:HOH:O	2.11	0.50
1:0:1592:G:O2'	1:0:1593:C:O4'	2.29	0.50
28:Z:19:GLY:O	28:Z:23:ARG:HG2	2.11	0.50
32:I:100:LEU:O	32:I:139:ILE:HG23	2.11	0.50
12:J:107:ASN:HD21	12:J:109:TYR:HB2	1.77	0.50
6:C:162:VAL:CG2	6:C:232:LEU:HD21	2.42	0.50
28:Z:42:CYS:SG	28:Z:43:GLY:N	2.85	0.50
25:W:119:HIS:HD2	25:W:120:PRO:O	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1119:G:H8	12:J:52:GLN:NE2	2.10	0.50
1:0:1979:G:O2'	1:0:1980:U:OP1	2.30	0.50
1:0:1167:G:H2'	1:0:1168:C:O4'	2.11	0.50
1:0:482:G:H4'	1:0:508:A:N1	2.27	0.50
1:0:1252:A:H2'	1:0:1253:C:O4'	2.12	0.50
7:D:10:PHE:CE1	7:D:11:HIS:HB3	2.47	0.50
6:C:118:THR:CG2	6:C:137:PRO:HB3	2.41	0.50
12:J:76:ASP:HA	39:J:5907:HOH:O	2.11	0.50
1:0:1972:U:H2'	1:0:1973:A:H5'	1.94	0.50
1:0:447:A:O2'	1:0:448:G:H5'	2.12	0.50
39:K:7438:HOH:O	23:U:20:MET:HE1	2.11	0.50
8:E:154:ILE:HD11	8:E:157:LYS:HB2	1.92	0.50
24:V:59:ILE:O	24:V:63:GLU:HG2	2.11	0.50
4:A:153:ARG:NH1	4:A:153:ARG:HB2	2.24	0.50
1:0:1189:A:H1'	1:0:1209:C:C1'	2.41	0.50
11:H:3:ALA:CA	11:H:58:ARG:HH12	2.24	0.50
1:0:2815:G:OP2	12:J:99:GLU:HG2	2.12	0.50
1:0:920:C:H5''	1:0:921:G:O5'	2.12	0.50
1:0:87:C:H2'	30:2:28:LYS:O	2.12	0.50
7:D:167:GLU:C	7:D:169:THR:H	2.14	0.50
7:D:41:LEU:HA	7:D:44:ILE:HG22	1.94	0.49
2:9:3044:A:O4'	7:D:76:ARG:NE	2.44	0.49
25:W:88:THR:HG22	25:W:90:TYR:CD1	2.47	0.49
4:A:65:ARG:C	4:A:66:ARG:HG3	2.32	0.49
17:O:78:ALA:C	17:O:98:LEU:HD13	2.32	0.49
1:0:1477:C:O2'	1:0:1478:U:H5'	2.12	0.49
1:0:1942:A:H3'	39:0:7828:HOH:O	2.12	0.49
5:B:314:ALA:HB3	5:B:317:PRO:HG3	1.93	0.49
1:0:1132:A:N6	1:0:1229:C:H2'	2.27	0.49
1:0:155:C:OP2	15:M:188:ARG:HD3	2.11	0.49
1:0:1119:G:N2	1:0:1246:A:N1	2.60	0.49
11:H:40:ALA:HB1	11:H:137:TYR:CE2	2.47	0.49
1:0:1159:G:H1	1:0:1208:C:H42	1.60	0.49
16:N:164:ASP:OD2	16:N:167:ASP:HA	2.11	0.49
2:9:3054:A:H2	39:9:3535:HOH:O	1.94	0.49
1:0:1921:A:O2'	1:0:1922:A:H5'	2.12	0.49
1:0:449:A:N7	6:C:43:LYS:HG2	2.26	0.49
1:0:1119:G:H8	12:J:52:GLN:HE22	1.59	0.49
11:H:27:LYS:H	11:H:59:HIS:CD2	2.23	0.49
16:N:183:ASP:O	16:N:184:ILE:O	2.30	0.49
11:H:73:LEU:HD21	11:H:146:VAL:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:894:A:N1	6:C:87:ARG:NH2	2.61	0.49
4:A:132:ASP:OD1	4:A:133:ARG:N	2.42	0.49
1:0:317:A:OP1	22:T:52:ARG:O	2.30	0.49
1:0:1666:C:C2'	1:0:1667:A:C5'	2.91	0.49
27:Y:187:VAL:HG23	27:Y:192:ASP:HB3	1.93	0.49
11:H:169:GLY:HA3	39:H:9553:HOH:O	2.11	0.49
1:0:292:G:H2'	1:0:358:G:N2	2.27	0.49
6:C:219:ASN:O	6:C:222:ASP:OD1	2.30	0.49
5:B:49:THR:CG2	5:B:280:VAL:HG23	2.43	0.49
1:0:821:U:H2'	1:0:822:C:H6	1.77	0.49
26:X:30:MET:HE1	26:X:58:ALA:CB	2.40	0.49
32:I:74:PRO:C	32:I:112:LYS:HZ1	2.15	0.49
4:A:131:HIS:O	4:A:132:ASP:HB2	2.11	0.49
1:0:2786:G:H2'	39:0:7679:HOH:O	2.12	0.49
16:N:167:ASP:C	16:N:168:LEU:HG	2.33	0.49
25:W:108:ARG:HE	25:W:114:PRO:HG3	1.77	0.49
1:0:2453:G:H5''	39:L:9438:HOH:O	2.11	0.49
1:0:820:G:O2'	1:0:856:G:H4'	2.13	0.49
31:3:70:ARG:HB3	39:3:9504:HOH:O	2.13	0.49
4:A:33:GLU:OE1	4:A:33:GLU:N	2.45	0.49
1:0:1667:A:H2'	1:0:1668:U:C6	2.48	0.49
1:0:470:U:O2'	29:1:16:HIS:CD2	2.62	0.49
8:E:49:ILE:HD11	8:E:69:ILE:HD12	1.94	0.49
4:A:223:ARG:CZ	39:A:9556:HOH:O	2.60	0.49
1:0:951:A:O2'	1:0:952:G:H5'	2.13	0.49
1:0:204:A:C2'	1:0:205:U:H5'	2.43	0.49
32:I:116:LEU:HD22	32:I:127:GLU:OE1	2.12	0.49
39:0:9730:HOH:O	5:B:229:ARG:HD2	2.13	0.49
25:W:115:THR:HB	39:W:6871:HOH:O	2.12	0.49
6:C:107:ARG:CB	6:C:107:ARG:HH11	2.25	0.49
25:W:88:THR:CG2	25:W:90:TYR:HD1	2.24	0.49
24:V:39:ALA:O	24:V:41:GLU:N	2.41	0.49
20:R:39:THR:HB	20:R:42:GLU:CG	2.42	0.49
6:C:200:PRO:HB3	6:C:212:VAL:HG23	1.95	0.49
7:D:128:LEU:HB2	39:D:6007:HOH:O	2.13	0.49
1:0:2090:G:H2'	1:0:2091:G:C8	2.47	0.49
5:B:113:LEU:HD21	5:B:161:VAL:HG21	1.95	0.49
23:U:17:THR:CG2	23:U:18:GLY:H	2.25	0.49
1:0:1878:G:O2'	1:0:1879:U:C6	2.62	0.49
23:U:52:THR:HG22	23:U:54:THR:H	1.76	0.49
1:0:2895:C:H4'	39:X:4132:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:34:VAL:HG22	13:K:47:ALA:HB2	1.94	0.49
12:J:142:ASN:O	12:J:144:THR:N	2.45	0.49
1:0:299:U:H5'	39:0:7818:HOH:O	2.12	0.49
12:J:45:VAL:HG11	12:J:121:LEU:CD2	2.42	0.49
2:9:3028:U:H2'	2:9:3029:C:C6	2.47	0.49
1:0:2521:A:OP2	11:H:3:ALA:HB3	2.13	0.49
9:F:14:ASP:O	9:F:18:GLU:HG3	2.12	0.49
5:B:81:ALA:O	5:B:186:GLY:HA3	2.12	0.49
1:0:2365:G:H5''	39:Q:6597:HOH:O	2.11	0.49
28:Z:36:ASP:HB3	28:Z:45:ASP:HB3	1.95	0.49
2:9:3004:G:H21	16:N:44:ARG:NH1	2.10	0.49
16:N:37:ARG:NH2	16:N:105:GLY:HA3	2.27	0.48
25:W:52:VAL:HG22	25:W:53:ALA:N	2.27	0.48
7:D:146:LYS:NZ	16:N:107:ASN:ND2	2.61	0.48
18:P:16:VAL:HG13	18:P:20:ARG:NH1	2.28	0.48
7:D:35:ALA:O	7:D:38:GLU:HG3	2.13	0.48
1:0:392:U:H5''	15:M:193:LYS:HB3	1.95	0.48
1:0:399:C:H5'	15:M:179:GLY:O	2.13	0.48
17:O:41:ALA:HA	39:O:5104:HOH:O	2.12	0.48
13:K:125:ALA:C	13:K:127:ALA:H	2.15	0.48
1:0:1654:U:H2'	4:A:47:HIS:HD2	1.76	0.48
24:V:29:ASN:O	24:V:33:VAL:HG23	2.13	0.48
7:D:57:THR:HA	39:D:5728:HOH:O	2.13	0.48
31:3:20:HIS:HA	31:3:70:ARG:O	2.13	0.48
1:0:1180:U:H2'	1:0:1181:A:C8	2.47	0.48
25:W:4:LEU:HD23	25:W:54:PHE:HB3	1.95	0.48
11:H:169:GLY:C	11:H:170:ASN:HD22	2.15	0.48
11:H:170:ASN:ND2	11:H:170:ASN:N	2.57	0.48
24:V:64:GLY:O	24:V:65:ASP:CB	2.59	0.48
12:J:131:THR:HB	12:J:134:GLU:OE1	2.13	0.48
12:J:70:PHE:CG	12:J:70:PHE:O	2.65	0.48
1:0:2507:G:H2'	1:0:2510:C:N4	2.28	0.48
5:B:217:ARG:HG3	5:B:257:THR:HG22	1.94	0.48
1:0:541:C:H2'	1:0:542:A:H5'	1.94	0.48
16:N:1:ALA:HB3	39:N:9368:HOH:O	2.13	0.48
27:Y:203:VAL:HG12	27:Y:228:VAL:HG22	1.94	0.48
16:N:24:LEU:HD13	19:Q:26:PRO:HB3	1.94	0.48
15:M:187:LEU:HD23	15:M:194:ALA:HB3	1.94	0.48
1:0:1654:U:H2'	4:A:47:HIS:CD2	2.48	0.48
1:0:1056:U:H2'	1:0:1057:A:O4'	2.12	0.48
18:P:98:ILE:HD12	18:P:102:ARG:NE	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:O:5842:HOH:O	25:W:122:ARG:NH2	2.47	0.48
1:O:1299:G:H5'	39:O:4654:HOH:O	2.13	0.48
1:O:2748:G:H4'	1:O:2749:U:C5'	2.43	0.48
27:Y:126:PRO:HG2	27:Y:128:PHE:CZ	2.48	0.48
1:O:1745:G:H22	1:O:2033:G:H5'	1.78	0.48
1:O:475:G:OP1	6:C:73:LEU:HD22	2.13	0.48
21:S:33:SER:O	21:S:37:VAL:HG23	2.13	0.48
1:O:2414:A:H2'	1:O:2415:A:C8	2.49	0.48
1:O:2253:G:O2'	1:O:2254:G:H5'	2.14	0.48
1:O:2649:A:H5'	1:O:2649:A:H8	1.78	0.48
22:T:71:VAL:CG1	22:T:72:ILE:N	2.76	0.48
25:W:122:ARG:NH2	39:W:5817:HOH:O	2.46	0.48
32:I:131:THR:O	32:I:135:LEU:HG	2.13	0.48
4:A:179:MET:HG2	4:A:186:TRP:CB	2.44	0.48
9:F:11:ASP:O	9:F:14:ASP:HB2	2.14	0.48
1:O:603:A:H5''	1:O:604:G:OP1	2.12	0.48
1:O:1902:G:H2'	1:O:1903:U:O4'	2.14	0.48
15:M:99:ARG:HH21	15:M:170:ASN:ND2	2.02	0.48
17:O:59:VAL:HG21	17:O:111:VAL:HG21	1.95	0.48
15:M:57:LYS:HE2	15:M:140:ALA:O	2.13	0.48
11:H:34:GLY:HA3	11:H:84:LYS:HA	1.94	0.48
2:9:3039:U:O2'	2:9:3042:C:C5	2.65	0.48
1:O:558:C:C2'	1:O:559:U:C5'	2.92	0.48
7:D:136:ARG:NH1	7:D:157:LEU:HA	2.27	0.48
25:W:54:PHE:CZ	25:W:140:LYS:HB2	2.48	0.48
31:3:6:ARG:NH1	31:3:21:GLU:HB2	2.28	0.48
8:E:84:MET:HE1	8:E:148:ILE:HD12	1.96	0.48
1:O:2831:C:O3'	20:R:71:LYS:HE2	2.14	0.48
39:O:4952:HOH:O	15:M:83:SER:HB3	2.14	0.48
1:O:1203:G:O2'	1:O:1204:C:H5'	2.13	0.48
12:J:19:MET:HE2	12:J:79:PHE:HA	1.94	0.48
32:I:105:VAL:HG11	32:I:129:VAL:CG2	2.44	0.48
4:A:53:ALA:HB3	39:A:9587:HOH:O	2.14	0.48
30:2:10:ARG:HD2	30:2:49:GLU:OE2	2.13	0.48
11:H:146:VAL:HG22	39:H:9541:HOH:O	2.14	0.48
16:N:78:MET:HB2	16:N:79:PRO:HD3	1.96	0.48
25:W:29:VAL:O	25:W:30:ASN:HB2	2.14	0.48
22:T:71:VAL:HG13	22:T:91:LEU:O	2.13	0.48
2:9:3057:A:C8	7:D:141:VAL:HG21	2.48	0.48
4:A:26:ASP:CG	4:A:26:ASP:O	2.53	0.48
1:O:137:U:H2'	1:O:139:C:C5	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:932:U:H2'	1:0:933:C:C6	2.49	0.48
25:W:149:LEU:HG	25:W:153:MET:CE	2.44	0.48
1:0:343:C:O2'	1:0:344:C:H5'	2.12	0.48
28:Z:32:GLU:HA	28:Z:35:GLU:HG3	1.95	0.48
1:0:2781:U:H1'	8:E:139:GLU:OE2	2.14	0.48
16:N:36:ALA:HB1	16:N:118:ILE:HD12	1.95	0.48
16:N:43:VAL:HG13	16:N:118:ILE:HD11	1.94	0.48
1:0:500:G:H21	20:R:98:ASN:HD21	1.60	0.48
25:W:139:GLY:O	25:W:141:HIS:HD2	1.95	0.48
7:D:49:PRO:HA	7:D:73:VAL:HG22	1.96	0.48
25:W:88:THR:CG2	25:W:89:ASP:N	2.75	0.48
12:J:75:PRO:HB3	12:J:132:LEU:HB3	1.95	0.48
32:I:113:HIS:N	32:I:114:PRO:CD	2.77	0.48
22:T:48:VAL:HG23	22:T:98:VAL:HA	1.96	0.48
1:0:2443:C:O3'	14:L:56:LYS:HE3	2.14	0.48
1:0:2681:A:H4'	1:0:2682:C:H5'	1.96	0.48
6:C:61:PHE:HB3	39:C:9250:HOH:O	2.12	0.48
1:0:329:A:OP2	6:C:206:ASN:HB2	2.14	0.48
17:O:80:ASP:OD1	17:O:81:PHE:N	2.46	0.48
27:Y:117:LEU:HA	27:Y:174:VAL:HG11	1.96	0.48
1:0:1130:U:H2'	1:0:1131:G:O4'	2.14	0.48
6:C:153:VAL:O	6:C:157:LEU:HG	2.14	0.48
39:9:5851:HOH:O	16:N:115:VAL:HG13	2.13	0.47
1:0:2748:G:C5'	39:0:8049:HOH:O	2.59	0.47
8:E:7:ILE:HD11	8:E:11:VAL:O	2.14	0.47
1:0:2003:U:H4'	1:0:2004:U:C5	2.46	0.47
6:C:157:LEU:HD13	6:C:166:ILE:HD11	1.95	0.47
27:Y:150:LEU:HB3	39:Y:9358:HOH:O	2.13	0.47
27:Y:178:HIS:CG	27:Y:179:PRO:HD2	2.49	0.47
15:M:43:PRO:HG3	15:M:62:VAL:HG21	1.96	0.47
2:9:3049:G:H5''	39:9:4707:HOH:O	2.14	0.47
1:0:1118:A:C8	1:0:1119:G:H5''	2.48	0.47
1:0:757:C:OP1	14:L:27:ARG:HD2	2.13	0.47
1:0:486:A:H1'	39:0:7288:HOH:O	2.13	0.47
4:A:70:ALA:HA	4:A:71:PRO:HD3	1.77	0.47
11:H:79:GLU:C	11:H:80:GLU:HG3	2.35	0.47
1:0:1717:A:H5''	18:P:54:LYS:HB2	1.95	0.47
27:Y:122:ARG:NH2	39:Y:9335:HOH:O	2.48	0.47
1:0:1506:U:H6	1:0:1506:U:H5'	1.79	0.47
6:C:127:ARG:HD3	6:C:129:HIS:HE1	1.80	0.47
1:0:2072:G:H3'	1:0:2073:G:C5'	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:36:PRO:HB3	5:B:174:ARG:CB	2.44	0.47
10:G:27:ILE:HD13	10:G:71:LEU:HD23	1.97	0.47
17:O:14:LEU:HG	17:O:102:ILE:HD11	1.97	0.47
24:V:5:VAL:HG23	39:V:2271:HOH:O	2.13	0.47
1:0:1451:C:H5'	1:0:1505:U:C5	2.49	0.47
1:0:2825:C:H4'	1:0:2826:G:O5'	2.14	0.47
2:9:3092:G:H2'	2:9:3093:A:C8	2.50	0.47
27:Y:235:GLU:CD	27:Y:235:GLU:N	2.52	0.47
17:O:32:ARG:HB2	39:O:4656:HOH:O	2.13	0.47
8:E:101:GLU:HB2	8:E:116:THR:O	2.14	0.47
5:B:254:GLN:NE2	39:B:9589:HOH:O	2.46	0.47
10:G:23:ILE:HD13	10:G:67:LEU:HD23	1.95	0.47
1:0:1755:A:H2'	1:0:1756:G:O4'	2.14	0.47
1:0:830:G:O2'	1:0:831:U:H5'	2.14	0.47
9:F:117:GLU:C	9:F:119:ARG:H	2.18	0.47
11:H:167:PRO:O	11:H:168:ALA:HB2	2.14	0.47
32:I:89:SER:CB	32:I:95:ASP:HB2	2.44	0.47
11:H:20:ILE:HG23	11:H:120:ILE:CD1	2.43	0.47
1:0:1406:A:H4'	1:0:1407:A:C5'	2.44	0.47
1:0:952:G:N3	1:0:2302:A:H2'	2.29	0.47
9:F:5:ASP:O	9:F:119:ARG:NH1	2.47	0.47
8:E:22:VAL:HG12	8:E:76:VAL:HG11	1.97	0.47
2:9:3058:G:H1'	39:D:3839:HOH:O	2.14	0.47
1:0:2102:G:H5''	1:0:2538:A:C2	2.50	0.47
1:0:2908:A:H2'	1:0:2909:G:O4'	2.13	0.47
25:W:21:LEU:HD21	25:W:48:VAL:CG1	2.21	0.47
6:C:129:HIS:HE1	6:C:231:ARG:HA	1.78	0.47
1:0:542:A:H2'	1:0:543:G:O4'	2.15	0.47
5:B:162:MET:HE3	5:B:310:ARG:HD3	1.90	0.47
1:0:588:G:O6	25:W:154:ARG:NH1	2.48	0.47
9:F:68:ASP:C	9:F:70:LYS:H	2.18	0.47
1:0:2852:A:H5''	39:O:5787:HOH:O	2.14	0.47
13:K:28:GLU:OE2	13:K:58:THR:HG21	2.15	0.47
18:P:13:VAL:HG11	18:P:40:VAL:CG1	2.45	0.47
1:0:2032:U:C2'	1:0:2033:G:H5''	2.44	0.47
6:C:46:TYR:CE2	6:C:98:ARG:NH1	2.82	0.47
1:0:1525:G:H5'	1:0:1526:A:OP2	2.15	0.47
6:C:242:GLU:HB2	39:C:9188:HOH:O	2.14	0.47
5:B:24:PRO:HG3	5:B:204:GLY:HA2	1.95	0.47
1:0:2509:A:H2'	1:0:2510:C:O4'	2.15	0.47
16:N:74:PRO:HG2	16:N:159:TYR:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3042:C:H5'	2:9:3043:G:OP2	2.14	0.47
20:R:9:ASP:O	20:R:13:THR:HB	2.14	0.47
4:A:94:LEU:N	4:A:94:LEU:HD23	2.30	0.47
1:0:1878:G:O2'	1:0:1879:U:P	2.72	0.47
5:B:41:PHE:CG	5:B:190:MET:HE3	2.49	0.47
8:E:102:VAL:HG13	8:E:116:THR:HG23	1.95	0.47
8:E:69:ILE:HA	8:E:72:MET:CE	2.44	0.47
15:M:34:GLU:HB3	15:M:38:GLU:HG3	1.96	0.47
12:J:130:VAL:HG12	12:J:131:THR:H	1.80	0.47
1:0:2819:C:O4'	5:B:96:PRO:HB2	2.14	0.47
12:J:39:VAL:HG11	12:J:107:ASN:CB	2.44	0.47
9:F:36:THR:HG23	9:F:97:ALA:HB2	1.96	0.47
7:D:134:LEU:HD11	7:D:166:ILE:HD11	1.97	0.47
1:0:1120:U:H6	1:0:1120:U:H5''	1.80	0.47
1:0:87:C:C2	30:2:30:ASP:OD2	2.68	0.47
1:0:2649:A:C8	1:0:2649:A:H5'	2.49	0.47
1:0:603:A:H4'	1:0:604:G:O5'	2.14	0.47
8:E:1:PRO:HG2	8:E:59:MET:SD	2.54	0.47
9:F:101:ALA:HA	39:F:5413:HOH:O	2.15	0.47
13:K:13:GLU:OE1	13:K:44:LEU:HD12	2.14	0.47
1:0:1007:A:H2'	11:H:19:TYR:CZ	2.49	0.47
1:0:645:U:OP2	14:L:4:LYS:HE2	2.13	0.47
1:0:1603:A:H5''	1:0:1605:G:H5'	1.96	0.47
1:0:380:A:H4'	1:0:381:G:OP1	2.15	0.47
1:0:870:G:OP2	4:A:3:ARG:HD3	2.15	0.47
1:0:506:G:H22	1:0:509:A:H5'	1.75	0.47
1:0:2644:C:O2'	1:0:2645:U:H5'	2.14	0.47
1:0:894:A:C2	6:C:87:ARG:NH2	2.83	0.47
11:H:158:THR:HB	11:H:159:PRO:HD3	1.97	0.47
1:0:1422:U:H2'	1:0:1423:C:C6	2.50	0.47
1:0:2837:U:H2'	39:0:7345:HOH:O	2.14	0.47
8:E:80:TRP:O	8:E:134:SER:HA	2.14	0.47
1:0:2712:G:H5'	39:K:4183:HOH:O	2.14	0.47
1:0:1181:A:N1	1:0:1192:A:O2'	2.46	0.47
1:0:1972:U:H2'	1:0:1973:A:C5'	2.45	0.47
9:F:28:ALA:CB	9:F:99:THR:HG23	2.45	0.47
5:B:190:MET:CE	5:B:194:PHE:CD1	2.98	0.47
1:0:2346:C:H6	1:0:2346:C:O5'	1.96	0.47
16:N:69:TYR:CE2	16:N:184:ILE:HG13	2.48	0.47
14:L:35:ARG:HD3	14:L:35:ARG:C	2.36	0.47
1:0:1836:A:H1'	29:1:1:THR:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:241:A:C2	1:0:378:A:H4'	2.50	0.47
7:D:99:ASP:O	7:D:159:PRO:HG3	2.14	0.47
1:0:1352:A:HO2'	1:0:1353:C:P	2.36	0.47
12:J:80:LYS:HE2	12:J:98:PHE:CZ	2.50	0.47
2:9:3091:C:H2'	2:9:3092:G:O4'	2.15	0.47
4:A:126:ALA:HB1	4:A:138:VAL:CG1	2.45	0.47
15:M:66:SER:HB3	15:M:128:TRP:CD1	2.50	0.47
5:B:265:LEU:HD21	5:B:316:ARG:HD3	1.97	0.47
6:C:133:ARG:NE	6:C:138:VAL:HG22	2.30	0.47
1:0:2364:A:H5''	19:Q:15:LYS:HD3	1.96	0.47
14:L:61:ALA:HB2	14:L:105:TYR:CZ	2.50	0.47
2:9:3039:U:HO2'	2:9:3042:C:H5	1.55	0.46
1:0:1201:C:C2'	1:0:1202:A:H5'	2.45	0.46
9:F:99:THR:O	9:F:100:ASP:HB2	2.15	0.46
30:2:22:PRO:HG2	30:2:25:VAL:HG21	1.97	0.46
29:1:28:HIS:CE1	29:1:31:LYS:HE2	2.49	0.46
1:0:2252:A:H2'	1:0:2253:G:O4'	2.16	0.46
16:N:67:ALA:HA	16:N:71:TRP:HB3	1.97	0.46
17:O:73:ASP:HA	17:O:92:VAL:O	2.14	0.46
2:9:3048:C:H4'	16:N:141:ARG:HH21	1.80	0.46
5:B:14:GLY:HA2	5:B:15:PRO:C	2.35	0.46
1:0:1242:A:OP2	12:J:60:ARG:NH2	2.45	0.46
2:9:3049:G:O2'	2:9:3050:G:H5'	2.14	0.46
31:3:70:ARG:CG	31:3:77:ALA:HB2	2.42	0.46
27:Y:151:SER:HB3	27:Y:154:ARG:HB3	1.98	0.46
14:L:145:LEU:O	14:L:145:LEU:HD23	2.15	0.46
39:0:4570:HOH:O	22:T:82:THR:HA	2.15	0.46
4:A:72:GLU:HG3	28:Z:66:GLY:HA2	1.96	0.46
1:0:1331:A:OP2	27:Y:142:SER:OG	2.32	0.46
39:0:5295:HOH:O	16:N:21:HIS:HD2	1.97	0.46
5:B:132:HIS:CE1	5:B:171:VAL:HG21	2.51	0.46
1:0:2338:G:H2'	7:D:129:ASP:OD1	2.15	0.46
1:0:1095:U:O2	25:W:120:PRO:HG2	2.16	0.46
7:D:135:VAL:HG22	7:D:136:ARG:N	2.29	0.46
4:A:194:MET:CE	4:A:199:HIS:HB2	2.45	0.46
1:0:2748:G:H4'	1:0:2749:U:H5'	1.95	0.46
11:H:66:ARG:HD3	39:H:9544:HOH:O	2.14	0.46
1:0:2346:C:H4'	7:D:52:THR:CG2	2.46	0.46
5:B:277:GLU:N	5:B:278:PRO:HD2	2.30	0.46
23:U:6:CYS:HB2	23:U:32:CYS:HB3	1.97	0.46
17:O:38:ARG:NH1	39:O:7674:HOH:O	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:14:LYS:HG3	13:K:32:ILE:O	2.15	0.46
39:O:6852:HOH:O	8:E:35:TYR:HB2	2.16	0.46
1:O:2635:A:C2'	1:O:2636:C:H5'	2.45	0.46
28:Z:26:VAL:O	28:Z:30:GLU:HG3	2.16	0.46
14:L:143:THR:CG2	14:L:144:ASP:N	2.76	0.46
19:Q:25:PRO:HA	19:Q:26:PRO:HD3	1.81	0.46
1:O:709:G:O2'	17:O:25:VAL:CG1	2.61	0.46
1:O:1435:U:H5'	39:O:3209:HOH:O	2.14	0.46
11:H:47:ILE:HD12	11:H:146:VAL:CG1	2.45	0.46
1:O:407:A:H2'	1:O:408:A:C8	2.51	0.46
1:O:920:C:H4'	1:O:921:G:C2	2.51	0.46
1:O:1748:U:H4'	39:O:7993:HOH:O	2.14	0.46
1:O:1053:G:OP1	11:H:12:PRO:HG3	2.15	0.46
27:Y:133:HIS:HD2	39:Y:9382:HOH:O	1.97	0.46
1:O:1098:A:H2'	1:O:1099:G:O4'	2.15	0.46
17:O:47:ARG:HG3	17:O:47:ARG:HH11	1.80	0.46
25:W:88:THR:CG2	25:W:89:ASP:H	2.28	0.46
14:L:134:GLU:HG3	39:L:9453:HOH:O	2.15	0.46
5:B:81:ALA:HB1	5:B:142:LEU:HD13	1.97	0.46
1:O:2906:A:H5'	1:O:2907:C:O4'	2.15	0.46
7:D:36:ASN:HB3	39:D:1655:HOH:O	2.16	0.46
1:O:653:C:H2'	1:O:654:A:C8	2.51	0.46
1:O:333:G:O2'	1:O:334:G:H5'	2.16	0.46
14:L:89:PHE:CD1	14:L:89:PHE:N	2.83	0.46
2:9:3024:U:H3'	2:9:3025:G:H5'	1.97	0.46
13:K:87:ARG:NH1	39:K:4066:HOH:O	2.49	0.46
8:E:35:TYR:HA	12:J:127:ILE:CD1	2.44	0.46
32:I:89:SER:HB3	32:I:97:VAL:CG2	2.46	0.46
1:O:2362:A:H2'	1:O:2363:G:C8	2.51	0.46
26:X:25:ARG:HD2	39:X:3861:HOH:O	2.16	0.46
7:D:173:GLU:HG3	7:D:174:VAL:N	2.30	0.46
1:O:2415:A:O2'	16:N:29:SER:HB3	2.15	0.46
20:R:114:VAL:HA	20:R:144:GLU:O	2.15	0.46
1:O:2044:G:OP1	26:X:23:HIS:HE1	1.98	0.46
1:O:684:G:H2'	1:O:685:C:C6	2.51	0.46
27:Y:136:LYS:HE3	27:Y:138:ARG:NH1	2.30	0.46
6:C:129:HIS:HD2	6:C:165:ASP:OD2	1.98	0.46
1:O:1173:A:H4'	1:O:1174:A:C8	2.51	0.46
14:L:121:ILE:HG12	14:L:141:GLU:HB2	1.98	0.46
1:O:40:C:H6	1:O:40:C:O5'	1.99	0.46
1:O:2824:C:H5''	1:O:2825:C:H5'	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:271:C:H41	1:0:378:A:H2	1.64	0.46
1:0:2784:A:H1'	8:E:60:SER:OG	2.15	0.46
16:N:32:PRO:HD2	16:N:99:GLU:O	2.16	0.46
39:0:6254:HOH:O	13:K:87:ARG:CZ	2.64	0.46
4:A:94:LEU:HD12	4:A:98:GLU:CB	2.43	0.46
1:0:136:C:H2'	1:0:137:U:O4'	2.15	0.46
5:B:80:ARG:HB2	5:B:145:HIS:CE1	2.51	0.46
1:0:2911:C:O2'	1:0:2912:C:H5'	2.16	0.46
1:0:1786:C:OP1	18:P:74:GLN:HG2	2.16	0.46
19:Q:64:GLU:HG3	19:Q:74:ASP:OD2	2.16	0.46
1:0:2472:C:O2'	1:0:2634:G:H4'	2.15	0.46
1:0:899:C:H5'	39:0:3799:HOH:O	2.16	0.46
1:0:1342:C:O2'	1:0:1343:C:H5'	2.15	0.46
24:V:12:THR:HG23	24:V:14:ALA:N	2.31	0.46
24:V:1:THR:CG2	24:V:2:VAL:H	2.15	0.46
11:H:63:GLU:O	11:H:67:LEU:HB2	2.16	0.46
5:B:41:PHE:HA	5:B:79:MET:HE1	1.96	0.46
6:C:27:ARG:HG2	6:C:30:LEU:HG	1.97	0.46
1:0:710:G:H5'	17:O:25:VAL:CG1	2.46	0.46
16:N:86:LEU:O	16:N:90:LEU:HG	2.15	0.46
17:O:96:VAL:HG13	17:O:100:GLN:HB2	1.98	0.46
29:1:28:HIS:CD2	29:1:31:LYS:HG3	2.50	0.46
13:K:34:VAL:CG2	13:K:47:ALA:HB2	2.46	0.46
5:B:75:GLU:C	5:B:77:PRO:HD3	2.36	0.46
1:0:2348:C:H1'	7:D:131:THR:HG21	1.98	0.46
1:0:602:A:O2'	1:0:605:C:H4'	2.15	0.46
16:N:151:ASP:OD1	16:N:166:ALA:HA	2.16	0.46
15:M:49:ALA:C	15:M:54:TYR:HB3	2.36	0.46
8:E:85:GLU:HG3	8:E:169:THR:OG1	2.16	0.46
25:W:21:LEU:HD22	25:W:26:ILE:HD13	1.96	0.46
32:I:113:HIS:HE1	32:I:121:LEU:HD22	1.81	0.46
14:L:1:THR:HB	14:L:6:ARG:NH1	2.31	0.46
5:B:312:ARG:HD3	5:B:315:VAL:HG13	1.97	0.46
1:0:834:G:H3'	1:0:835:U:H4'	1.98	0.46
1:0:123:U:H1'	39:0:7856:HOH:O	2.16	0.46
12:J:71:TYR:CD1	12:J:72:PRO:HD2	2.51	0.46
8:E:81:GLU:HA	8:E:133:VAL:O	2.15	0.46
4:A:39:ALA:HB3	4:A:61:GLU:OE2	2.16	0.46
4:A:217:ARG:CG	4:A:217:ARG:HH11	2.29	0.46
29:1:56:GLU:HG2	29:1:56:GLU:OXT	2.16	0.46
1:0:1183:C:H5	1:0:1192:A:OP1	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:23:ARG:NH1	16:N:23:ARG:HG2	2.31	0.45
14:L:129:ALA:O	14:L:133:VAL:HG23	2.16	0.45
22:T:38:ARG:HG3	22:T:38:ARG:HH11	1.81	0.45
16:N:86:LEU:HD12	16:N:125:ALA:HB2	1.98	0.45
1:O:2064:U:H4'	1:O:2653:A:OP1	2.15	0.45
1:O:1200:A:H3'	39:O:6295:HOH:O	2.16	0.45
1:O:392:U:C5'	15:M:193:LYS:HB3	2.46	0.45
1:O:2679:G:H2'	1:O:2681:A:OP2	2.15	0.45
11:H:78:GLY:C	11:H:80:GLU:H	2.20	0.45
5:B:265:LEU:CD2	5:B:316:ARG:HD3	2.46	0.45
1:O:1847:A:OP1	4:A:175:LYS:HG3	2.16	0.45
5:B:294:TYR:HE2	39:B:9647:HOH:O	1.99	0.45
1:O:288:A:H2'	1:O:289:G:C8	2.50	0.45
2:9:3050:G:H5''	16:N:159:TYR:HE1	1.81	0.45
14:L:73:VAL:HG21	14:L:116:HIS:CD2	2.51	0.45
1:O:121:U:O4	29:1:18:LYS:HG2	2.15	0.45
17:O:59:VAL:CG2	17:O:111:VAL:CG2	2.94	0.45
9:F:48:VAL:CG2	9:F:74:PHE:HB3	2.46	0.45
1:O:1025:C:H5'	25:W:23:MET:O	2.16	0.45
1:O:1503:U:H2'	1:O:1504:A:O4'	2.16	0.45
1:O:236:A:H8	1:O:236:A:OP1	1.99	0.45
20:R:84:ALA:O	20:R:88:PHE:HD1	1.99	0.45
20:R:132:ARG:CZ	39:R:9492:HOH:O	2.63	0.45
1:O:622:G:P	27:Y:148:GLY:HA3	2.56	0.45
9:F:52:GLU:OE1	9:F:78:GLU:OE1	2.34	0.45
22:T:32:ARG:NH1	22:T:38:ARG:NH1	2.63	0.45
32:I:72:VAL:HG13	32:I:73:PRO:HD2	1.98	0.45
32:I:118:SER:HB2	32:I:123:ASN:HB2	1.98	0.45
25:W:11:VAL:O	25:W:12:ASN:HB2	2.16	0.45
12:J:63:ILE:HG22	12:J:64:GLY:N	2.30	0.45
1:O:968:G:H1'	11:H:32:LYS:HD2	1.98	0.45
7:D:64:ARG:NE	7:D:67:ASP:HB3	2.32	0.45
1:O:2356:A:H5'	39:O:6178:HOH:O	2.16	0.45
15:M:74:LYS:HG3	15:M:75:ARG:N	2.31	0.45
1:O:2748:G:H8	39:O:8049:HOH:O	2.00	0.45
1:O:2779:G:H21	8:E:143:GLN:HE22	1.64	0.45
26:X:76:ARG:NH1	26:X:76:ARG:HG3	2.31	0.45
7:D:10:PHE:CG	7:D:11:HIS:N	2.85	0.45
1:O:56:G:H5''	24:V:50:ARG:NH1	2.32	0.45
8:E:6:GLU:HA	8:E:46:THR:HG22	1.97	0.45
6:C:84:VAL:HG12	6:C:85:LYS:HG2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:1335:C:OP2	27:Y:207:SER:HB3	2.16	0.45
1:O:259:G:H21	15:M:58:GLN:NE2	2.15	0.45
13:K:49:LEU:HD12	13:K:80:ILE:HD13	1.97	0.45
1:O:1603:A:H5'	1:O:1605:G:C4'	2.46	0.45
2:9:3042:C:O2	7:D:76:ARG:NH1	2.48	0.45
4:A:94:LEU:HG	4:A:99:ILE:HD11	1.97	0.45
11:H:28:ILE:HG23	39:H:9544:HOH:O	2.16	0.45
30:2:35:ARG:HB2	39:2:2691:HOH:O	2.16	0.45
1:O:157:G:H4'	15:M:95:LYS:HE2	1.98	0.45
26:X:66:THR:HG23	26:X:67:PRO:HD2	1.99	0.45
1:O:2015:A:H2'	1:O:2016:U:O4'	2.17	0.45
1:O:810:G:H1'	39:O:7740:HOH:O	2.17	0.45
2:9:3107:C:H5	39:9:3167:HOH:O	1.99	0.45
16:N:108:SER:HA	16:N:109:PRO:HD3	1.81	0.45
5:B:84:LEU:HB2	5:B:182:VAL:HG21	1.99	0.45
5:B:178:ALA:O	5:B:182:VAL:HG23	2.16	0.45
1:O:2421:G:H2'	39:O:4659:HOH:O	2.16	0.45
18:P:50:GLN:HG2	39:P:204:HOH:O	2.16	0.45
5:B:87:TYR:O	5:B:138:GLY:N	2.35	0.45
12:J:88:PRO:O	12:J:94:GLY:HA3	2.17	0.45
27:Y:212:ARG:HD2	39:Y:9402:HOH:O	2.16	0.45
8:E:15:GLN:NE2	8:E:40:VAL:O	2.50	0.45
7:D:40:ILE:HG13	7:D:41:LEU:N	2.32	0.45
16:N:143:ARG:HE	16:N:143:ARG:HB3	1.56	0.45
1:O:999:C:H2'	1:O:1000:C:O4'	2.17	0.45
4:A:123:GLY:HA2	4:A:159:VAL:O	2.17	0.45
23:U:4:ARG:NH1	23:U:4:ARG:HG2	2.31	0.45
5:B:243:ASN:HA	5:B:244:PRO:C	2.37	0.45
1:O:88:G:N7	30:2:28:LYS:HD2	2.31	0.45
21:S:11:THR:H	21:S:14:ALA:HB3	1.81	0.45
1:O:2398:A:H2'	1:O:2399:G:O4'	2.16	0.45
25:W:139:GLY:O	25:W:141:HIS:CD2	2.70	0.45
1:O:1592:G:H2'	1:O:1593:C:C6	2.52	0.45
1:O:1192:A:H3'	1:O:1193:A:H5'	1.99	0.45
27:Y:148:GLY:O	27:Y:154:ARG:HD3	2.17	0.45
29:1:18:LYS:HB2	30:2:49:GLU:CG	2.45	0.45
14:L:144:ASP:O	14:L:147:GLU:HB2	2.17	0.45
7:D:103:ASN:ND2	7:D:134:LEU:H	2.14	0.45
31:3:6:ARG:NH1	31:3:21:GLU:HG3	2.32	0.45
14:L:10:SER:O	14:L:11:ARG:HB3	2.17	0.45
1:O:328:U:O4'	6:C:202:THR:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2809:G:H2'	1:0:2810:G:O4'	2.17	0.45
1:0:1151:G:OP1	10:G:63:ARG:NH1	2.50	0.45
14:L:72:ASN:HB2	39:L:9478:HOH:O	2.16	0.45
1:0:812:A:H2'	1:0:813:C:C6	2.51	0.45
1:0:2857:C:H2'	1:0:2858:U:C6	2.52	0.45
22:T:20:HIS:HB3	22:T:41:ARG:HD2	1.98	0.45
39:O:7282:HOH:O	16:N:4:PRO:HD2	2.17	0.45
20:R:114:VAL:HG13	20:R:114:VAL:O	2.17	0.45
1:0:95:A:H5''	1:0:97:G:O4'	2.17	0.45
1:0:793:A:H5''	18:P:83:LYS:HG2	1.99	0.45
22:T:3:GLN:HA	22:T:4:PRO:HD3	1.82	0.45
1:0:371:U:H2'	1:0:372:A:H8	1.82	0.45
24:V:51:LYS:O	24:V:55:ARG:HG3	2.17	0.45
32:I:99:ASP:O	32:I:100:LEU:HD23	2.17	0.45
1:0:1667:A:C8	1:0:1667:A:H5'	2.42	0.45
7:D:170:TYR:O	7:D:171:ASP:CB	2.65	0.45
1:0:1555:G:H4'	1:0:1630:A:C2	2.51	0.45
27:Y:115:ARG:NE	39:Y:9356:HOH:O	2.50	0.45
2:9:3054:A:O2'	2:9:3055:U:H5'	2.16	0.45
1:0:2699:A:H2'	1:0:2700:G:O4'	2.15	0.45
1:0:1994:A:P	13:K:66:ARG:HH22	2.40	0.45
6:C:142:ASP:OD1	6:C:236:THR:HG23	2.18	0.44
25:W:122:ARG:HH22	25:W:154:ARG:HG2	1.79	0.44
7:D:60:GLU:O	7:D:60:GLU:HG3	2.17	0.44
1:0:1834:C:H2'	1:0:1840:A:N6	2.32	0.44
16:N:49:THR:CG2	16:N:56:ASP:HB2	2.45	0.44
1:0:2866:U:C4	23:U:50:GLU:HB3	2.52	0.44
1:0:497:A:H2'	1:0:498:A:C5'	2.47	0.44
1:0:1787:C:OP1	18:P:68:LYS:HE2	2.18	0.44
6:C:218:VAL:N	39:C:9229:HOH:O	2.50	0.44
21:S:81:ILE:HG23	39:S:9494:HOH:O	2.17	0.44
14:L:124:ASP:OD1	14:L:149:ARG:NH2	2.50	0.44
1:0:2568:A:H5''	1:0:2702:A:O2'	2.17	0.44
6:C:180:SER:HB2	39:C:9251:HOH:O	2.17	0.44
25:W:88:THR:HG23	25:W:110:GLN:HB3	1.99	0.44
22:T:49:GLU:OE2	22:T:51:LEU:HD21	2.17	0.44
11:H:29:ALA:C	11:H:30:GLN:HG3	2.37	0.44
1:0:2545:U:OP2	5:B:2:GLN:NE2	2.50	0.44
1:0:2890:A:H1'	23:U:56:ARG:CZ	2.46	0.44
4:A:65:ARG:HH11	4:A:65:ARG:HG2	1.82	0.44
23:U:52:THR:CG2	23:U:54:THR:HB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:16:VAL:HG13	18:P:20:ARG:CZ	2.47	0.44
15:M:22:GLU:HG2	15:M:26:GLN:NE2	2.32	0.44
6:C:168:ARG:NH2	6:C:190:ALA:O	2.50	0.44
9:F:60:VAL:O	9:F:60:VAL:CG1	2.64	0.44
20:R:39:THR:HG22	20:R:41:GLY:H	1.83	0.44
14:L:134:GLU:HA	14:L:138:GLY:O	2.17	0.44
24:V:5:VAL:CG1	24:V:9:ARG:NH1	2.81	0.44
39:O:6811:HOH:O	27:Y:158:LYS:HD3	2.18	0.44
1:O:415:A:O2'	1:O:416:G:H5'	2.18	0.44
18:P:135:ALA:HB1	18:P:139:ARG:HH12	1.82	0.44
1:O:629:A:H2'	1:O:630:A:O4'	2.17	0.44
1:O:366:U:H2'	1:O:367:G:O4'	2.17	0.44
32:I:87:THR:HG22	32:I:88:GLY:N	2.32	0.44
4:A:69:LEU:HD23	4:A:107:ASN:CG	2.37	0.44
5:B:71:VAL:CG1	5:B:296:LEU:HD22	2.48	0.44
4:A:101:GLU:OE2	4:A:131:HIS:HB2	2.18	0.44
13:K:65:ARG:NE	39:K:5358:HOH:O	2.46	0.44
1:O:1666:C:C2'	1:O:1667:A:H5''	2.47	0.44
1:O:1878:G:C1'	39:O:6649:HOH:O	2.60	0.44
1:O:338:C:H4'	6:C:174:ILE:HD11	1.99	0.44
15:M:187:LEU:HD22	15:M:194:ALA:HB3	1.99	0.44
1:O:40:C:H4'	39:O:7503:HOH:O	2.17	0.44
1:O:2101:A:OP2	6:C:66:GLY:HA2	2.18	0.44
22:T:52:ARG:O	22:T:53:GLY:O	2.35	0.44
1:O:2480:G:H3'	39:O:4764:HOH:O	2.16	0.44
1:O:2505:G:C2'	1:O:2506:A:H5'	2.48	0.44
13:K:109:LEU:HD13	13:K:113:ILE:CD1	2.45	0.44
2:9:3049:G:H2'	2:9:3050:G:O4'	2.18	0.44
4:A:207:GLN:O	4:A:208:HIS:HB3	2.17	0.44
25:W:5:VAL:O	25:W:52:VAL:CG2	2.65	0.44
5:B:5:ARG:HD2	5:B:8:LYS:NZ	2.33	0.44
1:O:1641:A:C2'	1:O:1642:A:H5'	2.46	0.44
22:T:48:VAL:CG1	22:T:96:VAL:HG21	2.47	0.44
16:N:152:GLU:HA	16:N:152:GLU:OE1	2.18	0.44
1:O:2907:C:H2'	1:O:2908:A:O4'	2.17	0.44
1:O:236:A:H4'	1:O:237:G:H5'	2.00	0.44
1:O:1086:A:C6	25:W:11:VAL:HG11	2.53	0.44
14:L:65:ASP:CG	14:L:111:ALA:HB3	2.37	0.44
30:2:20:ARG:HG3	30:2:21:VAL:N	2.33	0.44
1:O:2506:A:O2'	1:O:2507:G:O5'	2.35	0.44
9:F:70:LYS:C	9:F:72:VAL:H	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:154:LYS:HD2	7:D:154:LYS:N	2.28	0.44
22:T:24:ARG:HH21	22:T:39:ASN:HD22	1.65	0.44
25:W:118:LEU:HD12	25:W:153:MET:HE3	1.99	0.44
14:L:149:ARG:O	14:L:150:GLN:HB2	2.17	0.44
1:O:12:U:H2'	1:O:13:G:H5'	2.00	0.44
31:3:69:TYR:CZ	31:3:80:ARG:HD2	2.53	0.44
1:O:2718:C:H5'	1:O:2718:C:C6	2.48	0.44
4:A:36:ASP:HA	4:A:83:GLY:HA3	1.99	0.44
1:O:120:A:H5'	29:1:20:ARG:HH21	1.82	0.44
11:H:3:ALA:CB	11:H:58:ARG:HH12	2.30	0.44
8:E:23:GLU:HG2	8:E:28:SER:CB	2.47	0.44
6:C:107:ARG:NH1	39:C:9236:HOH:O	2.51	0.44
7:D:37:ALA:O	7:D:40:ILE:HG12	2.18	0.44
4:A:3:ARG:H	4:A:3:ARG:HG2	1.66	0.44
9:F:50:VAL:CG2	9:F:63:ILE:HG21	2.47	0.44
16:N:23:ARG:NH1	39:N:9346:HOH:O	2.51	0.44
5:B:56:ASP:HB3	5:B:322:ARG:HH21	1.83	0.44
10:G:64:ASN:N	10:G:64:ASN:ND2	2.66	0.44
5:B:171:VAL:HG23	5:B:172:SER:N	2.33	0.44
32:I:124:ALA:O	32:I:128:VAL:HG23	2.18	0.44
1:O:566:A:H2'	1:O:567:U:O4'	2.17	0.44
7:D:78:GLU:O	7:D:82:GLU:HG3	2.17	0.44
16:N:72:GLU:HG2	16:N:72:GLU:O	2.17	0.44
1:O:2541:U:O2'	3:4:76:DA:H4'	2.17	0.43
32:I:102:VAL:HG23	32:I:140:GLU:O	2.18	0.43
1:O:1298:U:H2'	1:O:1299:G:C8	2.52	0.43
27:Y:189:ASN:HD22	27:Y:192:ASP:H	1.64	0.43
5:B:138:GLY:O	5:B:139:ASP:O	2.36	0.43
16:N:89:GLY:O	16:N:92:ALA:HB3	2.18	0.43
1:O:1314:U:H2'	39:O:6410:HOH:O	2.18	0.43
28:Z:13:ARG:NH1	39:Z:9218:HOH:O	2.51	0.43
9:F:65:GLU:O	9:F:69:GLU:HG2	2.18	0.43
22:T:47:THR:HB	22:T:100:ASP:HB3	1.99	0.43
8:E:145:ALA:HB1	8:E:168:ILE:CD1	2.48	0.43
25:W:26:ILE:O	25:W:26:ILE:HG13	2.18	0.43
25:W:122:ARG:NH1	25:W:152:ALA:O	2.51	0.43
12:J:132:LEU:HA	12:J:132:LEU:HD23	1.85	0.43
27:Y:187:VAL:CG2	27:Y:192:ASP:HB2	2.48	0.43
16:N:167:ASP:O	16:N:168:LEU:HG	2.17	0.43
5:B:234:ARG:HH11	5:B:234:ARG:HB3	1.83	0.43
23:U:20:MET:CG	23:U:28:THR:HG23	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:125:PHE:CE1	14:L:140:VAL:HG13	2.53	0.43
1:0:2531:U:O2'	1:0:2532:A:H5'	2.17	0.43
1:0:2720:C:O2	13:K:87:ARG:NH2	2.51	0.43
1:0:1180:U:H1'	39:0:3831:HOH:O	2.18	0.43
14:L:145:LEU:C	14:L:145:LEU:HD23	2.38	0.43
5:B:41:PHE:HA	5:B:79:MET:CE	2.49	0.43
39:0:5535:HOH:O	11:H:58:ARG:HG3	2.18	0.43
28:Z:72:GLU:HB3	28:Z:77:LYS:HE3	2.00	0.43
22:T:79:LEU:HG	22:T:89:ARG:HB2	2.00	0.43
6:C:79:ARG:O	6:C:87:ARG:HG2	2.18	0.43
1:0:2415:A:H2'	1:0:2416:G:H5'	2.00	0.43
1:0:2036:C:O4'	13:K:44:LEU:HG	2.18	0.43
5:B:139:ASP:HB3	39:B:9547:HOH:O	2.17	0.43
20:R:34:GLU:HG2	20:R:46:TYR:OH	2.17	0.43
5:B:149:ASP:HB2	39:B:9577:HOH:O	2.18	0.43
1:0:2807:U:P	5:B:27:ASN:HD21	2.40	0.43
1:0:2372:A:H2'	1:0:2373:U:C6	2.53	0.43
9:F:110:ASP:O	9:F:114:LYS:HG3	2.18	0.43
16:N:116:PHE:HB3	16:N:136:LEU:HD23	2.00	0.43
25:W:122:ARG:HG2	25:W:152:ALA:O	2.17	0.43
7:D:25:MET:CE	7:D:41:LEU:HG	2.39	0.43
7:D:49:PRO:HB3	39:D:5828:HOH:O	2.19	0.43
32:I:88:GLY:C	32:I:97:VAL:HG21	2.38	0.43
1:0:2338:G:OP1	7:D:97:GLN:HG2	2.19	0.43
27:Y:184:GLU:HG2	27:Y:229:LEU:HD11	2.00	0.43
1:0:635:A:H2'	1:0:636:G:H5''	2.00	0.43
1:0:360:A:H2'	1:0:361:C:O4'	2.18	0.43
1:0:462:A:H2'	39:0:5450:HOH:O	2.17	0.43
1:0:450:C:OP1	6:C:184:ARG:NH2	2.38	0.43
7:D:25:MET:CE	7:D:40:ILE:HD11	2.49	0.43
7:D:25:MET:HE1	7:D:37:ALA:O	2.18	0.43
13:K:115:ARG:HG3	13:K:116:GLU:N	2.32	0.43
11:H:28:ILE:HA	11:H:63:GLU:OE1	2.18	0.43
16:N:48:VAL:HG11	16:N:55:ASP:HB3	2.00	0.43
14:L:143:THR:CG2	14:L:144:ASP:H	2.31	0.43
5:B:73:VAL:HG22	5:B:296:LEU:CD2	2.48	0.43
5:B:305:ASP:O	5:B:306:LYS:CB	2.66	0.43
1:0:1741:U:O2'	1:0:2723:G:H4'	2.19	0.43
5:B:24:PRO:CG	5:B:204:GLY:HA2	2.48	0.43
1:0:2698:G:H2'	1:0:2699:A:C8	2.53	0.43
1:0:2898:G:H4'	5:B:288:GLY:HA2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2589:U:H2'	1:0:2590:U:C6	2.53	0.43
25:W:48:VAL:CG1	25:W:48:VAL:O	2.66	0.43
1:0:558:C:H2'	1:0:559:U:H5''	1.98	0.43
2:9:3014:G:H2'	2:9:3015:C:H5'	2.01	0.43
2:9:3029:C:C2'	2:9:3030:C:H5'	2.48	0.43
14:L:133:VAL:HB	39:L:9453:HOH:O	2.19	0.43
31:3:38:ARG:CB	31:3:42:ARG:HH12	2.31	0.43
31:3:38:ARG:HB3	31:3:42:ARG:HH12	1.84	0.43
1:0:2663:U:O2	39:0:8476:HOH:O	2.20	0.43
1:0:2820:A:H2'	1:0:2821:C:C6	2.53	0.43
5:B:91:PRO:O	12:J:144:THR:HG21	2.18	0.43
26:X:66:THR:HG22	26:X:67:PRO:O	2.18	0.43
14:L:150:GLN:HB3	39:L:9466:HOH:O	2.19	0.43
4:A:17:ARG:HD2	39:A:9527:HOH:O	2.18	0.43
13:K:49:LEU:HD12	13:K:80:ILE:HG21	2.00	0.43
24:V:8:ILE:CG2	24:V:59:ILE:HG13	2.48	0.43
8:E:20:ILE:HD11	8:E:40:VAL:CG1	2.39	0.43
32:I:139:ILE:CG2	32:I:140:GLU:N	2.82	0.43
30:2:48:ASP:O	30:2:49:GLU:HB2	2.18	0.43
1:0:969:G:H1	1:0:999:C:N4	2.16	0.43
7:D:146:LYS:HZ3	16:N:107:ASN:HD21	1.66	0.43
9:F:48:VAL:HG12	9:F:97:ALA:CB	2.47	0.43
18:P:37:ARG:HG2	18:P:37:ARG:HH11	1.84	0.43
1:0:249:G:O2'	1:0:250:C:H5'	2.19	0.43
1:0:2237:G:H1'	1:0:2238:A:C8	2.54	0.43
1:0:2353:A:H4'	1:0:2354:A:O5'	2.17	0.43
1:0:2011:A:H4'	1:0:2012:U:O5'	2.19	0.43
24:V:8:ILE:HA	24:V:11:MET:HE2	2.00	0.43
7:D:60:GLU:O	7:D:61:PHE:C	2.56	0.43
25:W:5:VAL:O	25:W:52:VAL:HG23	2.19	0.43
1:0:681:G:N7	39:0:7461:HOH:O	2.36	0.43
17:O:14:LEU:HD23	17:O:102:ILE:HD11	1.99	0.43
1:0:40:C:N3	1:0:441:A:H2	2.16	0.43
6:C:45:ASP:OD2	6:C:98:ARG:HD2	2.19	0.43
1:0:1992:U:OP2	13:K:66:ARG:HD2	2.18	0.43
1:0:2587:OMU:H2'	1:0:2589:U:H5''	2.00	0.43
1:0:941:G:C5	1:0:942:U:C4	3.07	0.43
1:0:2499:U:H2'	1:0:2500:C:H6	1.84	0.43
4:A:164:ARG:CZ	39:A:9571:HOH:O	2.66	0.43
1:0:644:G:N3	1:0:644:G:H5'	2.34	0.43
39:0:5842:HOH:O	25:W:119:HIS:CG	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1174:A:C5	1:0:1201:C:H4'	2.54	0.43
25:W:3:ALA:O	25:W:54:PHE:HA	2.19	0.43
11:H:154:TYR:C	11:H:154:TYR:CD1	2.92	0.43
4:A:26:ASP:OD2	4:A:28:GLU:HG3	2.18	0.43
6:C:151:GLN:O	6:C:154:VAL:HB	2.18	0.43
1:0:204:A:H2'	1:0:205:U:H5'	1.99	0.43
1:0:1057:A:H2'	1:0:1058:A:C8	2.54	0.43
12:J:63:ILE:CG2	12:J:64:GLY:N	2.82	0.43
1:0:1470:A:OP1	15:M:93:ARG:HD2	2.18	0.43
5:B:119:HIS:O	5:B:121:PRO:HD3	2.19	0.43
11:H:83:TYR:C	11:H:83:TYR:CD1	2.91	0.43
1:0:802:G:H2'	1:0:803:C:C6	2.54	0.43
3:4:74:C:H2'	3:4:75:C:H5'	2.01	0.43
1:0:1160:G:HO2'	1:0:1190:G:H8	1.63	0.43
2:9:3050:G:H5''	16:N:159:TYR:CE1	2.54	0.43
17:O:25:VAL:HG23	17:O:26:TRP:N	2.33	0.43
12:J:131:THR:HG22	12:J:133:GLY:N	2.34	0.43
1:0:1477:C:H5'	1:0:1868:G:H5''	2.00	0.43
16:N:71:TRP:HB2	39:N:9338:HOH:O	2.18	0.43
1:0:1236:A:C8	12:J:63:ILE:HD11	2.54	0.43
1:0:2697:A:H2'	1:0:2698:G:O4'	2.19	0.43
26:X:45:GLU:HG3	39:X:6178:HOH:O	2.19	0.43
1:0:286:U:H2'	1:0:287:C:C6	2.54	0.43
13:K:49:LEU:HD22	13:K:117:VAL:CG2	2.49	0.42
1:0:364:C:H2'	1:0:365:G:O4'	2.19	0.42
1:0:1299:G:N2	39:0:5248:HOH:O	2.51	0.42
22:T:38:ARG:HG3	22:T:38:ARG:NH1	2.34	0.42
15:M:61:ILE:N	15:M:61:ILE:HD12	2.33	0.42
1:0:2452:G:H5'	39:3:9488:HOH:O	2.17	0.42
1:0:2416:G:O2'	16:N:25:ARG:HG2	2.19	0.42
20:R:132:ARG:NH2	39:R:9492:HOH:O	2.52	0.42
23:U:11:THR:HG22	23:U:53:ASP:OD2	2.19	0.42
6:C:185:LYS:HD3	6:C:186:TYR:CE1	2.54	0.42
27:Y:186:ARG:HG2	27:Y:186:ARG:HH11	1.84	0.42
26:X:80:GLU:O	26:X:80:GLU:HG2	2.19	0.42
7:D:27:ILE:HG22	7:D:28:GLY:N	2.32	0.42
14:L:80:ASP:HB2	14:L:90:ARG:HB3	2.01	0.42
1:0:396:U:OP2	31:3:38:ARG:HD2	2.18	0.42
32:I:75:THR:HA	32:I:112:LYS:NZ	2.34	0.42
1:0:1351:G:OP1	6:C:96:LYS:NZ	2.41	0.42
1:0:92:G:H4'	24:V:44:GLY:HA3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:2:18:ASN:HD21	30:2:40:ARG:H	1.66	0.42
11:H:119:LYS:HB2	11:H:119:LYS:HE3	1.81	0.42
1:0:669:G:O2'	1:0:670:G:H5'	2.19	0.42
1:0:526:U:H2'	1:0:527:U:C6	2.54	0.42
2:9:3059:C:O5'	2:9:3059:C:H6	2.02	0.42
16:N:103:ASP:OD1	16:N:103:ASP:C	2.58	0.42
32:I:129:VAL:HG13	32:I:139:ILE:HD11	2.01	0.42
5:B:42:ALA:H	5:B:79:MET:HE2	1.85	0.42
19:Q:11:ARG:HD3	39:Q:5620:HOH:O	2.18	0.42
1:0:2769:C:H2'	1:0:2770:G:C5'	2.48	0.42
16:N:152:GLU:C	16:N:154:LEU:N	2.72	0.42
24:V:42:ASN:O	24:V:44:GLY:N	2.52	0.42
1:0:1200:A:H4'	39:0:7822:HOH:O	2.19	0.42
6:C:157:LEU:CD1	6:C:166:ILE:HD11	2.49	0.42
30:2:20:ARG:HD2	30:2:39:ARG:NH2	2.34	0.42
1:0:2238:A:O2'	1:0:2239:C:H5'	2.18	0.42
1:0:200:U:H2'	39:0:4038:HOH:O	2.18	0.42
19:Q:77:ASP:HB3	19:Q:82:LYS:HE3	2.01	0.42
26:X:74:ALA:CB	26:X:85:VAL:HG22	2.49	0.42
28:Z:57:CYS:SG	28:Z:59:TYR:HB3	2.59	0.42
5:B:36:PRO:CA	5:B:168:GLY:HA3	2.44	0.42
14:L:77:ALA:C	14:L:79:ASP:H	2.23	0.42
27:Y:187:VAL:HB	27:Y:203:VAL:CG2	2.50	0.42
4:A:51:ARG:HH21	4:A:55:VAL:HG23	1.84	0.42
1:0:2421:G:H4'	39:0:5345:HOH:O	2.18	0.42
12:J:39:VAL:CG1	12:J:40:ASN:N	2.82	0.42
1:0:2036:C:C1'	13:K:44:LEU:HG	2.50	0.42
6:C:218:VAL:HG12	39:C:9229:HOH:O	2.18	0.42
2:9:3064:C:C2'	2:9:3065:A:H5'	2.49	0.42
1:0:2487:C:H5	39:0:5455:HOH:O	2.02	0.42
8:E:166:VAL:HG12	39:E:3134:HOH:O	2.18	0.42
24:V:8:ILE:HA	24:V:11:MET:CE	2.50	0.42
32:I:92:PRO:C	32:I:94:GLU:N	2.70	0.42
25:W:64:THR:O	25:W:68:THR:HG22	2.20	0.42
14:L:79:ASP:O	14:L:80:ASP:O	2.37	0.42
1:0:185:G:C4'	1:0:186:A:H4'	2.50	0.42
1:0:1477:C:C5'	1:0:1868:G:H5"	2.50	0.42
1:0:69:A:H5'	1:0:69:A:H8	1.85	0.42
6:C:98:ARG:NH1	39:C:9163:HOH:O	2.51	0.42
1:0:666:A:H2'	1:0:667:C:O4'	2.20	0.42
1:0:2900:G:H2'	1:0:2901:C:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:426:G:H2'	1:0:427:C:O4'	2.19	0.42
1:0:889:C:H2'	1:0:890:C:C6	2.55	0.42
20:R:69:LYS:HB2	20:R:72:VAL:HG23	2.00	0.42
1:0:1821:A:O2'	1:0:1822:A:H5'	2.20	0.42
9:F:79:GLN:HG3	9:F:82:ASP:OD2	2.18	0.42
13:K:115:ARG:HG2	13:K:116:GLU:OE1	2.19	0.42
9:F:30:LYS:HE2	9:F:99:THR:HG21	2.01	0.42
1:0:120:A:H2'	1:0:120:A:N3	2.35	0.42
1:0:1044:C:H5''	39:0:9648:HOH:O	2.19	0.42
17:O:77:ALA:HA	17:O:96:VAL:O	2.20	0.42
1:0:1099:G:H2'	1:0:1100:G:O4'	2.20	0.42
30:2:35:ARG:HG2	39:2:6391:HOH:O	2.19	0.42
1:0:2568:A:H2'	1:0:2569:A:O4'	2.20	0.42
13:K:27:ARG:HD2	39:K:4747:HOH:O	2.18	0.42
1:0:23:G:C6	1:0:24:G:N1	2.88	0.42
27:Y:108:ASP:N	27:Y:108:ASP:OD1	2.49	0.42
6:C:236:THR:HG22	6:C:239:ALA:HB2	2.01	0.42
25:W:125:HIS:HE1	39:W:3071:HOH:O	2.02	0.42
1:0:319:A:H4'	1:0:338:C:C5	2.54	0.42
16:N:24:LEU:HD22	39:Q:2847:HOH:O	2.19	0.42
1:0:960:G:N3	1:0:960:G:C2'	2.82	0.42
1:0:1328:A:C8	27:Y:169:ARG:HD3	2.54	0.42
15:M:82:ARG:O	15:M:84:LYS:N	2.52	0.42
1:0:440:C:H2'	1:0:441:A:C8	2.55	0.42
1:0:1236:A:H2'	1:0:1237:U:O4'	2.19	0.42
1:0:371:U:H2'	1:0:372:A:C8	2.55	0.42
32:I:80:LYS:HD3	32:I:86:GLU:O	2.20	0.42
1:0:27:U:H2'	1:0:28:G:O4'	2.20	0.42
1:0:697:G:H4'	1:0:730:G:O3'	2.19	0.42
26:X:54:ILE:HD11	26:X:85:VAL:HG12	2.02	0.42
39:0:3171:HOH:O	25:W:119:HIS:HE1	2.03	0.42
6:C:136:VAL:HG22	6:C:137:PRO:HA	2.01	0.42
27:Y:96:GLU:O	27:Y:235:GLU:HA	2.20	0.42
7:D:76:ARG:O	7:D:77:ASP:HB2	2.20	0.42
11:H:28:ILE:HG21	11:H:31:HIS:CE1	2.54	0.42
1:0:1168:C:H4'	39:I:5128:HOH:O	2.19	0.42
31:3:17:HIS:O	31:3:18:GLN:HG3	2.20	0.42
6:C:7:ASP:OD1	6:C:11:ASN:HB2	2.20	0.42
39:0:4983:HOH:O	4:A:11:ARG:CZ	2.68	0.42
12:J:143:LYS:HG3	12:J:145:TRP:CE2	2.55	0.42
1:0:1289:C:H3'	39:0:6930:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2072:G:C6	1:0:2533:C:H1'	2.55	0.42
2:9:3014:G:C2'	16:N:1:ALA:HB2	2.50	0.42
1:0:1878:G:O2'	1:0:1879:U:C5	2.66	0.42
27:Y:99:ALA:HB2	27:Y:233:TYR:CZ	2.55	0.42
1:0:2820:A:OP1	5:B:98:THR:HG22	2.20	0.42
1:0:1131:G:C6	1:0:1230:A:C4	3.08	0.42
19:Q:64:GLU:HG3	19:Q:74:ASP:CG	2.40	0.42
1:0:65:C:O2'	1:0:66:G:H5'	2.19	0.42
1:0:1081:A:H5''	39:0:3751:HOH:O	2.19	0.42
31:3:91:GLN:O	31:3:92:GLU:HB2	2.19	0.42
1:0:2133:U:H4'	1:0:2134:G:H5'	2.01	0.42
6:C:165:ASP:O	6:C:168:ARG:HB3	2.20	0.42
24:V:11:MET:HB3	24:V:15:GLU:HB2	2.00	0.42
1:0:1181:A:H2'	1:0:1182:C:H5'	2.02	0.42
12:J:19:MET:CE	12:J:132:LEU:HD21	2.48	0.42
4:A:34:ASP:OD1	4:A:35:GLY:N	2.38	0.42
4:A:36:ASP:HB2	4:A:83:GLY:HA3	2.02	0.42
14:L:69:ILE:HA	39:L:9478:HOH:O	2.20	0.42
1:0:2329:C:O2'	1:0:2330:U:H5'	2.20	0.42
25:W:41:TYR:CD2	25:W:44:MET:HE3	2.55	0.42
39:0:4845:HOH:O	19:Q:55:ARG:HD2	2.19	0.42
1:0:1714:C:O2'	1:0:1715:C:H5'	2.20	0.42
2:9:3006:C:H4'	16:N:35:VAL:HG11	2.02	0.42
6:C:123:LEU:HD23	6:C:123:LEU:HA	1.83	0.42
24:V:12:THR:HG23	24:V:14:ALA:H	1.84	0.41
25:W:122:ARG:CG	25:W:152:ALA:O	2.68	0.41
1:0:1180:U:O2'	32:I:92:PRO:HD2	2.20	0.41
29:1:10:LYS:N	39:1:9488:HOH:O	2.42	0.41
12:J:130:VAL:HG12	12:J:131:THR:N	2.35	0.41
7:D:173:GLU:O	7:D:174:VAL:C	2.59	0.41
1:0:2908:A:C2'	1:0:2909:G:H5'	2.49	0.41
1:0:2587:OMU:H6	1:0:2587:OMU:O5'	2.20	0.41
6:C:7:ASP:OD2	6:C:9:ASP:HB2	2.21	0.41
1:0:1495:C:H2'	1:0:1496:G:C8	2.54	0.41
4:A:76:VAL:HG23	28:Z:63:LYS:HB3	2.01	0.41
1:0:1311:G:O6	6:C:173:LYS:HE3	2.20	0.41
17:O:45:LEU:CD1	17:O:88:LYS:HD2	2.50	0.41
19:Q:53:HIS:HA	19:Q:54:PRO:HD3	1.95	0.41
11:H:43:TYR:HA	11:H:44:PRO:HD3	1.78	0.41
1:0:2112:A:H2'	1:0:2113:G:C8	2.55	0.41
1:0:2672:C:O2'	1:0:2673:U:H5'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Q:30:VAL:O	19:Q:30:VAL:HG12	2.19	0.41
11:H:40:ALA:HB1	11:H:137:TYR:CD2	2.55	0.41
1:0:1202:A:H2'	1:0:1203:G:O4'	2.20	0.41
9:F:72:VAL:HA	9:F:73:PRO:HD3	1.90	0.41
11:H:26:SER:HA	11:H:59:HIS:CD2	2.55	0.41
22:T:21:LYS:HA	22:T:24:ARG:HG3	2.02	0.41
5:B:254:GLN:HG2	5:B:255:GLY:H	1.81	0.41
26:X:20:GLU:CD	26:X:21:PRO:HD2	2.40	0.41
8:E:91:PHE:HA	8:E:92:PRO:HD3	1.87	0.41
6:C:184:ARG:HB3	39:C:9169:HOH:O	2.19	0.41
11:H:70:ASN:O	11:H:74:ILE:HG13	2.20	0.41
13:K:75:ARG:HD3	13:K:112:PRO:O	2.21	0.41
2:9:3018:U:H2'	2:9:3019:G:H8	1.85	0.41
15:M:59:GLY:HA3	15:M:141:ILE:CD1	2.49	0.41
25:W:65:VAL:CG1	25:W:116:LEU:HD13	2.50	0.41
1:0:664:U:O4	1:0:681:G:H5''	2.20	0.41
9:F:49:PHE:CD1	9:F:49:PHE:N	2.88	0.41
1:0:2089:A:O2'	1:0:2090:G:H5'	2.19	0.41
12:J:71:TYR:CG	12:J:72:PRO:HD2	2.55	0.41
11:H:99:LYS:HD3	11:H:119:LYS:HD3	2.01	0.41
1:0:764:C:H2'	1:0:765:G:O4'	2.20	0.41
30:2:5:LYS:O	30:2:9:LYS:HG3	2.20	0.41
17:O:87:THR:O	17:O:91:GLN:HG3	2.19	0.41
1:0:517:U:H1'	39:0:8135:HOH:O	2.20	0.41
1:0:2388:C:H5'	19:Q:83:THR:O	2.20	0.41
1:0:2427:C:OP2	31:3:84:ARG:HD2	2.18	0.41
2:9:3057:A:O2'	7:D:152:PRO:HD2	2.20	0.41
1:0:2715:G:N2	5:B:264:GLU:OE1	2.53	0.41
1:0:559:U:H5'	1:0:559:U:C6	2.41	0.41
20:R:25:PHE:CE2	20:R:29:LYS:CE	2.99	0.41
32:I:139:ILE:C	32:I:140:GLU:HG3	2.40	0.41
14:L:80:ASP:HB3	14:L:90:ARG:HB3	2.02	0.41
1:0:1838:U:H1'	1:0:2644:C:O4'	2.21	0.41
21:S:10:VAL:HG11	24:V:36:ALA:CA	2.48	0.41
1:0:1164:U:OP1	32:I:74:PRO:HA	2.20	0.41
1:0:2326:U:H4'	1:0:2412:G:C4'	2.50	0.41
1:0:2067:A:H2'	1:0:2068:G:O4'	2.20	0.41
18:P:141:ILE:C	18:P:143:ALA:H	2.22	0.41
1:0:907:A:H2'	1:0:908:A:C8	2.55	0.41
13:K:80:ILE:O	13:K:87:ARG:HA	2.20	0.41
1:0:1119:G:H2'	12:J:52:GLN:NE2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:37:ARG:CZ	16:N:105:GLY:HA3	2.51	0.41
6:C:30:LEU:HA	6:C:30:LEU:HD23	1.90	0.41
5:B:62:ARG:CB	5:B:65:MET:HE3	2.50	0.41
32:I:75:THR:HA	32:I:112:LYS:HZ3	1.86	0.41
1:O:2032:U:H2'	1:O:2033:G:H5'	2.01	0.41
1:O:926:A:H5'	14:L:39:GLU:OE2	2.20	0.41
1:O:1342:C:C2'	1:O:1343:C:H5'	2.50	0.41
2:9:3052:A:O2'	2:9:3053:G:H5'	2.20	0.41
1:O:612:U:H2'	1:O:613:C:C6	2.56	0.41
1:O:1759:A:N3	1:O:1818:C:H2'	2.35	0.41
20:R:106:GLY:HA2	20:R:109:MET:CE	2.46	0.41
32:I:132:CYS:C	32:I:134:SER:N	2.74	0.41
1:O:1189:A:H1'	1:O:1209:C:H1'	2.02	0.41
26:X:9:VAL:HG13	26:X:88:GLU:OE1	2.21	0.41
29:1:18:LYS:CB	30:2:49:GLU:HG2	2.47	0.41
1:O:710:G:H5'	17:O:25:VAL:HG13	2.03	0.41
4:A:66:ARG:HH11	4:A:66:ARG:CB	2.30	0.41
16:N:61:ALA:CB	16:N:88:ALA:HB2	2.48	0.41
4:A:135:VAL:HG21	4:A:147:ARG:HG2	2.02	0.41
17:O:97:SER:H	17:O:100:GLN:NE2	2.18	0.41
1:O:821:U:H2'	1:O:822:C:C6	2.56	0.41
9:F:31:LYS:HE3	39:F:2623:HOH:O	2.20	0.41
30:2:44:ARG:HA	30:2:44:ARG:HD3	1.78	0.41
5:B:146:THR:O	5:B:159:PRO:HB3	2.21	0.41
1:O:500:G:O2'	20:R:94:ASN:ND2	2.54	0.41
5:B:294:TYR:C	5:B:294:TYR:CD1	2.93	0.41
1:O:2326:U:H4'	1:O:2412:G:H4'	2.03	0.41
1:O:816:G:H5'	1:O:1598:A:H4'	2.02	0.41
25:W:146:ILE:HA	25:W:146:ILE:HD13	1.88	0.41
1:O:1603:A:C5'	1:O:1605:G:H5'	2.50	0.41
13:K:107:THR:HG22	13:K:108:GLU:CG	2.43	0.41
9:F:28:ALA:HB3	9:F:99:THR:O	2.20	0.41
27:Y:187:VAL:HB	27:Y:203:VAL:HG22	2.02	0.41
20:R:39:THR:CG2	20:R:107:GLU:O	2.68	0.41
4:A:66:ARG:CB	4:A:66:ARG:NH1	2.84	0.41
22:T:75:GLU:O	22:T:76:ASP:HB2	2.21	0.41
1:O:1573:A:H2'	1:O:1574:C:O4'	2.21	0.41
1:O:671:A:O2'	1:O:672:G:H2'	2.21	0.41
18:P:63:ARG:NH2	39:P:191:HOH:O	2.54	0.41
1:O:1226:G:H5'	39:O:5101:HOH:O	2.20	0.41
1:O:565:A:OP2	1:O:592:G:N1	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:150:ALA:O	5:B:152:PRO:HD3	2.21	0.41
1:0:2314:G:C2'	1:0:2315:C:H5'	2.51	0.41
1:0:2717:C:H5'	5:B:302:PRO:HA	2.02	0.41
7:D:44:ILE:HG23	7:D:45:THR:HG23	2.03	0.41
4:A:206:ARG:N	4:A:206:ARG:HD3	2.23	0.41
1:0:1119:G:N2	1:0:1246:A:H2	2.09	0.41
1:0:1739:G:H1'	1:0:2726:U:O4	2.20	0.41
1:0:797:A:O4'	28:Z:10:ARG:N	2.54	0.41
1:0:2578:G:H5'	1:0:2578:G:C8	2.45	0.41
1:0:2361:A:H2'	1:0:2362:A:C8	2.55	0.41
1:0:2503:A:OP1	11:H:151:ARG:NH2	2.49	0.41
5:B:271:ASP:HB3	5:B:296:LEU:HD12	2.03	0.41
18:P:16:VAL:CG1	18:P:20:ARG:CZ	2.99	0.41
23:U:44:ARG:HB3	39:U:3805:HOH:O	2.20	0.41
5:B:260:HIS:HE1	39:B:9585:HOH:O	2.03	0.41
1:0:1940:C:H4'	39:0:7828:HOH:O	2.19	0.41
1:0:1132:A:H2'	1:0:1133:A:C8	2.56	0.41
5:B:49:THR:HG21	5:B:280:VAL:HG23	2.03	0.41
5:B:277:GLU:N	5:B:278:PRO:CD	2.84	0.41
14:L:89:PHE:N	39:L:9468:HOH:O	2.54	0.41
1:0:123:U:O2'	1:0:124:C:H5'	2.20	0.41
1:0:1849:G:H1'	1:0:2011:A:N1	2.35	0.41
17:O:45:LEU:HD12	17:O:88:LYS:HD2	2.02	0.41
1:0:1659:A:H2'	1:0:1660:G:O4'	2.19	0.41
1:0:1768:C:H2'	1:0:1769:C:O4'	2.20	0.41
4:A:43:VAL:HG21	4:A:59:GLU:HG3	2.03	0.41
1:0:177:A:H2'	1:0:178:U:O4'	2.21	0.41
1:0:2481:G:H5''	39:0:5116:HOH:O	2.20	0.41
1:0:2103:A:N3	1:0:2103:A:H2'	2.35	0.41
1:0:750:A:O3'	6:C:101:ASP:HB2	2.21	0.41
39:0:8066:HOH:O	15:M:91:ILE:HG12	2.21	0.41
1:0:2053:G:H4'	20:R:136:TRP:CE2	2.56	0.41
22:T:88:PRO:HB3	39:T:6320:HOH:O	2.20	0.41
1:0:2435:U:H1'	39:0:5981:HOH:O	2.21	0.41
1:0:887:G:H2'	1:0:888:U:C6	2.55	0.41
20:R:4:TYR:CZ	20:R:15:LYS:HB3	2.55	0.41
28:Z:39:CYS:SG	28:Z:41:ASN:HB3	2.60	0.41
4:A:6:GLY:HA3	39:A:9550:HOH:O	2.20	0.41
1:0:2506:A:O2'	1:0:2507:G:P	2.78	0.41
1:0:289:G:N1	1:0:363:A:C2	2.83	0.41
1:0:1166:A:H1'	1:0:1192:A:N3	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:X:9:VAL:HG13	26:X:88:GLU:OE2	2.21	0.41
27:Y:189:ASN:ND2	27:Y:189:ASN:C	2.73	0.41
15:M:73:ARG:HG3	39:M:9411:HOH:O	2.21	0.41
17:O:26:TRP:HA	17:O:26:TRP:CE3	2.56	0.41
4:A:122:SER:O	4:A:124:VAL:HG13	2.21	0.41
29:1:8:GLN:HE22	29:1:11:LYS:NZ	2.19	0.41
1:0:2061:C:C2'	1:0:2062:A:H5'	2.51	0.41
21:S:29:ASP:OD1	21:S:31:ARG:NH1	2.54	0.41
8:E:5:LEU:HD21	8:E:66:GLN:HG3	2.03	0.41
1:0:1065:G:H5'	39:0:4141:HOH:O	2.20	0.41
7:D:105:SER:HA	7:D:130:VAL:O	2.21	0.41
1:0:162:C:H2'	1:0:163:U:H5'	2.02	0.41
2:9:3095:C:O2'	2:9:3096:C:H5'	2.21	0.41
21:S:8:PRO:HD2	24:V:32:ALA:HA	2.04	0.41
17:O:23:GLY:C	39:O:3062:HOH:O	2.59	0.41
7:D:12:GLU:O	7:D:15:GLU:HG2	2.21	0.41
1:0:262:A:OP2	9:F:91:VAL:HG11	2.21	0.40
5:B:217:ARG:HG3	5:B:257:THR:CG2	2.51	0.40
9:F:32:GLY:N	39:F:3111:HOH:O	2.54	0.40
24:V:39:ALA:C	24:V:41:GLU:N	2.71	0.40
4:A:123:GLY:HA3	4:A:162:GLY:CA	2.49	0.40
17:O:98:LEU:O	17:O:102:ILE:HG13	2.21	0.40
1:0:1149:U:H5''	1:0:1151:G:O4'	2.21	0.40
4:A:164:ARG:HB2	28:Z:68:SER:OG	2.21	0.40
1:0:2791:U:H1'	1:0:2792:A:H5''	2.03	0.40
39:0:5961:HOH:O	14:L:34:GLY:HA2	2.20	0.40
7:D:88:LEU:N	7:D:89:PRO:CD	2.84	0.40
1:0:2856:A:OP1	26:X:15:ARG:NH2	2.52	0.40
28:Z:60:CYS:O	28:Z:61:ASP:HB2	2.21	0.40
28:Z:11:SER:O	28:Z:14:PHE:HB2	2.21	0.40
6:C:5:ILE:HG13	6:C:15:GLU:HA	2.03	0.40
5:B:174:ARG:HA	5:B:177:HIS:HB3	2.02	0.40
30:2:41:HIS:HD2	30:2:44:ARG:H	1.69	0.40
4:A:65:ARG:NH1	4:A:65:ARG:HG2	2.36	0.40
5:B:85:ARG:HB2	5:B:99:GLU:HG2	2.03	0.40
27:Y:112:GLU:OE1	27:Y:112:GLU:HA	2.21	0.40
18:P:16:VAL:CG1	18:P:17:GLY:N	2.83	0.40
11:H:47:ILE:HD12	11:H:146:VAL:HG13	2.03	0.40
1:0:920:C:H5'	1:0:921:G:C4	2.56	0.40
1:0:64:G:H2'	1:0:65:C:O4'	2.21	0.40
1:0:2793:A:H2'	1:0:2794:G:H5'	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:790:A:H1'	1:0:1710:A:H2'	2.03	0.40
12:J:12:VAL:HG21	12:J:116:LEU:HD11	2.03	0.40
27:Y:216:ARG:HD2	39:Y:9370:HOH:O	2.20	0.40
31:3:70:ARG:HG2	31:3:70:ARG:HH11	1.86	0.40
5:B:331:SER:OG	23:U:14:GLU:OE2	2.33	0.40
1:0:484:A:N1	1:0:506:G:H4'	2.36	0.40
1:0:797:A:H5'	28:Z:10:ARG:N	2.36	0.40
6:C:194:PHE:CD2	6:C:234:VAL:CG1	3.01	0.40
6:C:234:VAL:HG13	6:C:234:VAL:O	2.21	0.40
1:0:2361:A:H8	1:0:2361:A:H5'	1.86	0.40
15:M:183:THR:CG2	15:M:194:ALA:HB1	2.50	0.40
16:N:182:GLY:O	16:N:183:ASP:C	2.60	0.40
26:X:12:ILE:HD12	26:X:36:HIS:CG	2.56	0.40
1:0:2868:C:H2'	1:0:2869:G:O4'	2.22	0.40
1:0:1937:U:O2'	1:0:1938:G:H5'	2.21	0.40
1:0:2379:G:N3	1:0:2418:G:H2'	2.36	0.40
15:M:184:ARG:HG3	15:M:185:PRO:HA	2.03	0.40
1:0:2401:A:H2'	1:0:2402:A:C8	2.57	0.40
1:0:2780:C:H1'	8:E:143:GLN:NE2	2.33	0.40
23:U:52:THR:HG21	23:U:54:THR:HB	2.03	0.40
7:D:36:ASN:HA	39:D:7500:HOH:O	2.22	0.40
1:0:2568:A:C2'	1:0:2569:A:H5'	2.51	0.40
30:2:20:ARG:HD2	30:2:39:ARG:HH21	1.85	0.40
11:H:77:LEU:HD12	11:H:83:TYR:CD2	2.57	0.40
9:F:79:GLN:HB2	9:F:82:ASP:OD2	2.22	0.40
27:Y:152:LYS:HB3	27:Y:160:LYS:HG3	2.03	0.40
1:0:2611:G:H5'	1:0:2613:G:C8	2.57	0.40
11:H:69:ALA:HB2	11:H:153:ALA:HB2	2.04	0.40
1:0:295:C:H2'	1:0:296:G:O4'	2.21	0.40
1:0:297:U:H1'	39:0:4518:HOH:O	2.21	0.40
5:B:274:GLU:HA	5:B:292:GLY:O	2.21	0.40
1:0:2754:G:H2'	1:0:2755:G:O4'	2.22	0.40
2:9:3012:C:H5'	2:9:3070:U:O4'	2.22	0.40
1:0:622:G:O2'	1:0:623:U:H5'	2.20	0.40
16:N:23:ARG:HD2	39:N:9357:HOH:O	2.20	0.40
1:0:1838:U:H1'	1:0:2644:C:H5'	2.04	0.40
1:0:2756:U:O2	1:0:2896:A:H2	2.05	0.40
5:B:10:SER:O	5:B:16:ARG:NH1	2.52	0.40
1:0:1819:G:H2'	1:0:1820:G:C4'	2.51	0.40
4:A:149:ASP:OD1	4:A:151:GLN:HB2	2.22	0.40
6:C:72:LYS:HG2	6:C:77:ALA:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1795:G:H2'	1:0:1796:A:O4'	2.22	0.40
1:0:1797:A:H2'	1:0:1799:G:O5'	2.21	0.40
1:0:1185:U:H2'	1:0:1186:C:C6	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	235/240 (98%)	209 (89%)	23 (10%)	3 (1%)	15	15
5	B	335/338 (99%)	314 (94%)	17 (5%)	4 (1%)	16	16
6	C	244/246 (99%)	229 (94%)	15 (6%)	0	100	100
7	D	134/177 (76%)	105 (78%)	17 (13%)	12 (9%)	1	0
8	E	170/178 (96%)	165 (97%)	5 (3%)	0	100	100
9	F	117/120 (98%)	100 (86%)	15 (13%)	2 (2%)	11	10
10	G	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
11	H	156/171 (91%)	140 (90%)	14 (9%)	2 (1%)	15	15
12	J	140/145 (97%)	131 (94%)	6 (4%)	3 (2%)	9	7
13	K	130/132 (98%)	123 (95%)	7 (5%)	0	100	100
14	L	141/165 (86%)	118 (84%)	22 (16%)	1 (1%)	26	31
15	M	192/195 (98%)	182 (95%)	8 (4%)	2 (1%)	19	21
16	N	184/187 (98%)	163 (89%)	12 (6%)	9 (5%)	3	1
17	O	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
18	P	141/149 (95%)	139 (99%)	2 (1%)	0	100	100
19	Q	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
20	R	148/155 (96%)	141 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	S	79/85 (93%)	76 (96%)	2 (2%)	1 (1%)	15	15
22	T	117/120 (98%)	109 (93%)	7 (6%)	1 (1%)	21	24
23	U	51/66 (77%)	48 (94%)	3 (6%)	0	100	100
24	V	63/71 (89%)	59 (94%)	3 (5%)	1 (2%)	12	11
25	W	152/154 (99%)	148 (97%)	4 (3%)	0	100	100
26	X	80/92 (87%)	73 (91%)	7 (9%)	0	100	100
27	Y	140/241 (58%)	138 (99%)	2 (1%)	0	100	100
28	Z	71/83 (86%)	61 (86%)	7 (10%)	3 (4%)	3	1
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%)	1 (1%)	1 (1%)	17	18
32	I	68/162 (42%)	55 (81%)	12 (18%)	1 (2%)	13	12
All	All	3705/4431 (84%)	3430 (93%)	229 (6%)	46 (1%)	16	16

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	27	LEU
4	A	37	VAL
5	B	139	ASP
7	D	137	PRO
9	F	101	ALA
11	H	166	SER
11	H	168	ALA
14	L	80	ASP
16	N	154	LEU
16	N	184	ILE
28	Z	81	ARG
4	A	34	ASP
7	D	27	ILE
7	D	60	GLU
7	D	171	ASP
12	J	143	LYS
15	M	83	SER
16	N	162	ASP
16	N	183	ASP
22	T	53	GLY
24	V	43	PRO

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Mol	Chain	Res	Type
7	D	28	GLY
7	D	56	ARG
7	D	61	PHE
12	J	5	GLU
16	N	155	GLU
16	N	164	ASP
28	Z	20	ARG
31	3	56	PRO
5	B	185	GLY
7	D	97	GLN
7	D	164	ALA
9	F	71	GLY
12	J	65	ASN
16	N	68	GLU
16	N	167	ASP
32	I	76	ALA
5	B	34	GLY
7	D	138	GLY
21	S	46	ASP
5	B	182	VAL
7	D	69	ILE
28	Z	21	VAL
16	N	161	GLY
7	D	16	PRO
15	M	88	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	179/182 (98%)	169 (94%)	10 (6%)	26	35
5	B	282/283 (100%)	261 (93%)	21 (7%)	17	21
6	C	193/193 (100%)	178 (92%)	15 (8%)	16	19
7	D	117/148 (79%)	112 (96%)	5 (4%)	35	47
8	E	152/156 (97%)	145 (95%)	7 (5%)	33	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	F	93/94 (99%)	91 (98%)	2 (2%)	60	77
10	G	27/283 (10%)	27 (100%)	0	100	100
11	H	132/138 (96%)	126 (96%)	6 (4%)	34	46
12	J	118/121 (98%)	109 (92%)	9 (8%)	16	20
13	K	106/106 (100%)	103 (97%)	3 (3%)	51	68
14	L	113/127 (89%)	109 (96%)	4 (4%)	43	58
15	M	158/159 (99%)	153 (97%)	5 (3%)	46	62
16	N	149/150 (99%)	144 (97%)	5 (3%)	44	59
17	O	93/94 (99%)	91 (98%)	2 (2%)	60	77
18	P	113/117 (97%)	112 (99%)	1 (1%)	84	93
19	Q	79/80 (99%)	75 (95%)	4 (5%)	29	39
20	R	117/122 (96%)	114 (97%)	3 (3%)	54	71
21	S	71/74 (96%)	69 (97%)	2 (3%)	51	68
22	T	105/106 (99%)	101 (96%)	4 (4%)	40	54
23	U	44/52 (85%)	44 (100%)	0	100	100
24	V	51/57 (90%)	50 (98%)	1 (2%)	63	79
25	W	130/130 (100%)	126 (97%)	4 (3%)	47	64
26	X	66/74 (89%)	60 (91%)	6 (9%)	12	13
27	Y	120/196 (61%)	110 (92%)	10 (8%)	14	17
28	Z	60/68 (88%)	59 (98%)	1 (2%)	68	83
29	1	46/47 (98%)	45 (98%)	1 (2%)	60	77
30	2	42/46 (91%)	41 (98%)	1 (2%)	57	74
31	3	79/79 (100%)	78 (99%)	1 (1%)	76	87
32	I	58/130 (45%)	58 (100%)	0	100	100
All	All	3093/3612 (86%)	2960 (96%)	133 (4%)	35	47

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	3	ARG
4	A	33	GLU
4	A	36	ASP
4	A	94	LEU
4	A	131	HIS

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Mol	Chain	Res	Type
4	A	153	ARG
4	A	165	THR
4	A	179	MET
4	A	206	ARG
4	A	217	ARG
5	B	11	LEU
5	B	27	ASN
5	B	51	VAL
5	B	53	LEU
5	B	71	VAL
5	B	82	VAL
5	B	98	THR
5	B	113	LEU
5	B	149	ASP
5	B	162	MET
5	B	175	LEU
5	B	190	MET
5	B	234	ARG
5	B	251	VAL
5	B	254	GLN
5	B	257	THR
5	B	265	LEU
5	B	277	GLU
5	B	280	VAL
5	B	307	ARG
5	B	312	ARG
6	C	2	GLN
6	C	27	ARG
6	C	76	ARG
6	C	91	PRO
6	C	94	THR
6	C	101	ASP
6	C	136	VAL
6	C	162	VAL
6	C	187	ARG
6	C	214	THR
6	C	222	ASP
6	C	223	LEU
6	C	236	THR
6	C	240	LEU
6	C	243	VAL
7	D	24	HIS

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Mol	Chain	Res	Type
7	D	50	VAL
7	D	61	PHE
7	D	133	ASN
7	D	137	PRO
8	E	3	VAL
8	E	7	ILE
8	E	102	VAL
8	E	108	LEU
8	E	155	ASN
8	E	156	ASP
8	E	164	ASP
9	F	12	LEU
9	F	46	GLU
11	H	1	LYS
11	H	18	GLU
11	H	84	LYS
11	H	88	ARG
11	H	154	TYR
11	H	170	ASN
12	J	45	VAL
12	J	52	GLN
12	J	70	PHE
12	J	74	ARG
12	J	79	PHE
12	J	107	ASN
12	J	117	ASP
12	J	127	ILE
12	J	131	THR
13	K	4	LEU
13	K	10	GLN
13	K	84	ASP
14	L	35	ARG
14	L	43	HIS
14	L	89	PHE
14	L	102	ASP
15	M	46	LEU
15	M	68	ARG
15	M	93	ARG
15	M	99	ARG
15	M	116	ASN
16	N	26	LEU
16	N	37	ARG

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Mol	Chain	Res	Type
16	N	49	THR
16	N	65	ASP
16	N	139	TRP
17	O	3	THR
17	O	96	VAL
18	P	98	ILE
19	Q	16	ASN
19	Q	18	PRO
19	Q	57	ASP
19	Q	95	GLU
20	R	13	THR
20	R	82	GLU
20	R	132	ARG
21	S	3	ASP
21	S	71	ASP
22	T	39	ASN
22	T	48	VAL
22	T	89	ARG
22	T	96	VAL
24	V	65	ASP
25	W	26	ILE
25	W	35	VAL
25	W	122	ARG
25	W	146	ILE
26	X	8	ARG
26	X	15	ARG
26	X	44	ASP
26	X	72	VAL
26	X	79	GLU
26	X	82	GLU
27	Y	103	THR
27	Y	141	THR
27	Y	144	ARG
27	Y	154	ARG
27	Y	163	THR
27	Y	189	ASN
27	Y	200	THR
27	Y	204	ARG
27	Y	220	GLU
27	Y	235	GLU
28	Z	44	GLU
29	1	47	ASP

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Mol	Chain	Res	Type
30	2	18	ASN
31	3	56	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	199	HIS
5	B	2	GLN
5	B	27	ASN
5	B	145	HIS
5	B	191	ASN
5	B	221	GLN
5	B	238	ASN
5	B	256	GLN
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	103	ASN
7	D	133	ASN
8	E	90	HIS
8	E	106	ASN
8	E	119	HIS
8	E	143	GLN
10	G	64	ASN
11	H	31	HIS
11	H	56	GLN
11	H	59	HIS
11	H	170	ASN
12	J	25	GLN
12	J	52	GLN
12	J	107	ASN
12	J	126	ASN
13	K	10	GLN
14	L	18	HIS
14	L	41	HIS
14	L	42	ASN
14	L	43	HIS
15	M	24	GLN
15	M	26	GLN

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Mol	Chain	Res	Type
15	M	58	GLN
15	M	77	HIS
15	M	137	ASN
15	M	143	ASN
15	M	170	ASN
16	N	93	GLN
16	N	107	ASN
16	N	153	GLN
17	O	53	GLN
17	O	100	GLN
18	P	50	GLN
18	P	66	GLN
18	P	73	HIS
18	P	88	GLN
18	P	89	ASN
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	53	ASN
22	T	37	GLN
22	T	39	ASN
22	T	73	HIS
23	U	39	ASN
23	U	48	ASN
24	V	60	GLN
25	W	12	ASN
25	W	28	HIS
25	W	110	GLN
25	W	119	HIS
25	W	125	HIS
25	W	141	HIS
26	X	22	ASN
26	X	23	HIS
27	Y	133	HIS
27	Y	134	HIS
27	Y	149	GLN
27	Y	189	ASN

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Mol	Chain	Res	Type
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	30	GLN
31	3	48	ASN
32	I	93	GLN
32	I	104	GLN
32	I	113	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	238 (8%)	33 (1%)
2	9	121/122 (99%)	16 (13%)	2 (1%)
3	4	1/5 (20%)	0	0
All	All	2867/3049 (94%)	254 (8%)	35 (1%)

All (254) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G
1	0	86	A
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	141	C
1	0	151	A
1	0	166	A
1	0	186	A
1	0	191	A

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Mol	Chain	Res	Type
1	0	192	A
1	0	219	G
1	0	237	G
1	0	249	G
1	0	271	C
1	0	272	A
1	0	273	G
1	0	283	U
1	0	284	C
1	0	308	U
1	0	309	C
1	0	318	C
1	0	336	G
1	0	337	A
1	0	358	G
1	0	381	G
1	0	397	A
1	0	417	G
1	0	457	U
1	0	461	C
1	0	473	A
1	0	487	G
1	0	498	A
1	0	511	A
1	0	514	G
1	0	537	G
1	0	538	C
1	0	539	G
1	0	542	A
1	0	545	G
1	0	553	G
1	0	559	U
1	0	581	G
1	0	588	G
1	0	604	G
1	0	620	A
1	0	632	A
1	0	644	G
1	0	660	A
1	0	688	A
1	0	698	A
1	0	701	U

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Mol	Chain	Res	Type
1	0	735	C
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	868	G
1	0	869	G
1	0	871	G
1	0	875	A
1	0	877	G
1	0	878	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	1100	G
1	0	1109	U
1	0	1110	G
1	0	1119	G
1	0	1130	U
1	0	1137	G
1	0	1164	U
1	0	1165	G
1	0	1166	A
1	0	1174	A
1	0	1175	G
1	0	1185	U
1	0	1192	A

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Mol	Chain	Res	Type
1	0	1193	A
1	0	1206	U
1	0	1208	C
1	0	1216	G
1	0	1237	U
1	0	1238	C
1	0	1239	G
1	0	1279	U
1	0	1289	C
1	0	1342	C
1	0	1353	C
1	0	1360	C
1	0	1377	C
1	0	1378	G
1	0	1407	A
1	0	1409	G
1	0	1474	C
1	0	1505	U
1	0	1506	U
1	0	1524	U
1	0	1525	G
1	0	1526	A
1	0	1528	A
1	0	1562	C
1	0	1564	C
1	0	1592	G
1	0	1625	U
1	0	1626	A
1	0	1633	C
1	0	1634	G
1	0	1656	A
1	0	1667	A
1	0	1682	A
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1701	A
1	0	1722	U
1	0	1723	G
1	0	1725	C
1	0	1730	G
1	0	1731	C

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Mol	Chain	Res	Type
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	1873	G
1	0	1879	U
1	0	1919	A
1	0	1942	A
1	0	1967	U
1	0	1971	G
1	0	1973	A
1	0	1979	G
1	0	1980	U
1	0	1996	U
1	0	2004	U
1	0	2006	C
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
1	0	2272	G
1	0	2291	A
1	0	2317	C
1	0	2321	A

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Mol	Chain	Res	Type
1	0	2354	A
1	0	2361	A
1	0	2369	A
1	0	2379	G
1	0	2422	U
1	0	2462	G
1	0	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	2536	C
1	0	2537	G
1	0	2541	U
1	0	2553	A
1	0	2564	G
1	0	2589	U
1	0	2601	A
1	0	2602	G
1	0	2608	C
1	0	2611	G
1	0	2613	G
1	0	2634	G
1	0	2644	C
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	2762	C
1	0	2768	A
1	0	2783	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	2812	A
1	0	2825	C
1	0	2852	A
1	0	2853	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	3007	G
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 (35) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	69	A
1	0	129	A
1	0	169	A
1	0	338	C
1	0	603	A
1	0	644	G
1	0	699	C
1	0	834	G
1	0	857	A
1	0	871	G
1	0	877	G

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Mol	Chain	Res	Type
1	0	1232	A
1	0	1237	U
1	0	1246	A
1	0	1352	A
1	0	1506	U
1	0	1563	G
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1856	C
1	0	1942	A
1	0	1979	G
1	0	2011	A
1	0	2313	C
1	0	2467	A
1	0	2526	C
1	0	2536	C
1	0	2649	A
1	0	2718	C
1	0	2761	A
1	0	2791	U
1	0	2852	A
2	9	3055	U
2	9	3065	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	OMU	0	2587	1	12,22,23	1.01	1 (8%)	19,31,34	3.16	2 (10%)
1	OMG	0	2588	1,3	17,26,27	1.06	1 (5%)	21,38,41	2.53	3 (14%)
1	UR3	0	2619	1	12,22,23	0.86	1 (8%)	16,32,35	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	0	2621	1	13,21,22	1.65	2 (15%)	18,30,33	6.05	4 (22%)
1	1MA	0	628	1,35	14,25,26	0.96	1 (7%)	15,37,40	1.15	1 (6%)

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

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C5-C1'	-4.96	1.47	1.52
1	0	2619	UR3	C6-C5	-2.12	1.33	1.38
1	0	2587	OMU	C4-N3	2.44	1.37	1.33
1	0	628	1MA	C6-N6	2.59	1.33	1.29
1	0	2621	PSU	C4-N3	2.79	1.38	1.33
1	0	2588	OMG	C6-N1	3.24	1.39	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	N1-C2-N3	-21.21	114.80	128.33
1	0	2588	OMG	C5-C6-N1	-8.81	111.54	123.59
1	0	628	1MA	C2-N3-C4	-3.60	110.83	116.40
1	0	2587	OMU	C5-C4-N3	-3.30	114.66	123.12
1	0	2588	OMG	N3-C2-N1	-2.22	124.06	127.44
1	0	2621	PSU	C5-C1'-C2'	-2.05	111.87	115.52
1	0	2621	PSU	C6-N1-C2	2.58	119.62	115.47
1	0	2588	OMG	C6-N1-C2	6.59	125.08	115.94
1	0	2587	OMU	C4-N3-C2	13.10	127.12	114.14
1	0	2621	PSU	C4-N3-C2	13.76	127.14	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 311 ligands modelled in this entry, 311 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	0	2749/2922 (94%)	-0.02	98 (3%) 46 55	22, 45, 89, 149	0
2	9	122/122 (100%)	0.23	8 (6%) 22 29	38, 63, 87, 149	0
3	4	4/5 (80%)	1.66	1 (25%) 1 1	61, 64, 71, 74	0
4	A	237/240 (98%)	0.63	20 (8%) 14 19	28, 50, 82, 104	0
5	B	337/338 (99%)	0.35	13 (3%) 43 52	28, 50, 75, 86	0
6	C	246/246 (100%)	0.16	4 (1%) 74 80	25, 46, 68, 80	0
7	D	140/177 (79%)	2.25	65 (46%) 0 0	58, 88, 120, 130	0
8	E	172/178 (96%)	0.99	34 (19%) 1 2	40, 62, 80, 86	0
9	F	119/120 (99%)	1.45	43 (36%) 0 0	44, 71, 100, 110	0
10	G	29/348 (8%)	3.08	21 (72%) 0 0	71, 89, 99, 100	0
11	H	160/171 (93%)	0.93	30 (18%) 2 2	43, 61, 93, 101	0
12	J	142/145 (97%)	0.17	4 (2%) 56 66	36, 47, 67, 89	0
13	K	132/132 (100%)	0.06	4 (3%) 54 63	33, 46, 67, 72	0
14	L	145/165 (87%)	1.05	35 (24%) 1 1	27, 64, 110, 120	0
15	M	194/195 (99%)	0.69	23 (11%) 6 9	31, 44, 77, 87	0
16	N	186/187 (99%)	1.28	52 (27%) 1 1	43, 63, 108, 113	0
17	O	115/116 (99%)	0.23	3 (2%) 59 68	39, 53, 67, 75	0
18	P	143/149 (95%)	0.27	4 (2%) 56 66	38, 51, 65, 76	0
19	Q	95/96 (98%)	0.32	8 (8%) 14 19	38, 47, 61, 76	0
20	R	150/155 (96%)	0.09	4 (2%) 58 67	29, 43, 61, 71	0
21	S	81/85 (95%)	0.56	8 (9%) 9 14	42, 58, 80, 95	0
22	T	119/120 (99%)	0.77	10 (8%) 14 19	40, 54, 81, 110	0
23	U	53/66 (80%)	0.36	2 (3%) 44 53	40, 50, 68, 79	0
24	V	65/71 (91%)	2.05	23 (35%) 0 0	52, 76, 110, 116	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	154/154 (100%)	0.21	3 (1%) 70 76	37, 49, 69, 78	0
26	X	82/92 (89%)	0.96	12 (14%) 3 5	40, 53, 82, 101	0
27	Y	142/241 (58%)	0.36	10 (7%) 19 27	29, 42, 63, 85	0
28	Z	73/83 (87%)	0.99	17 (23%) 1 1	48, 70, 85, 92	0
29	1	56/57 (98%)	-0.25	0 100 100	26, 32, 39, 49	0
30	2	46/50 (92%)	0.68	6 (13%) 5 7	33, 51, 67, 80	0
31	3	92/92 (100%)	0.43	5 (5%) 29 38	33, 55, 70, 83	0
32	I	70/162 (43%)	6.48	66 (94%) 0 0	111, 123, 141, 143	0
All	All	6650/7480 (88%)	0.43	636 (9%) 10 15	22, 50, 95, 149	0

All (636) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	I	71	GLY	17.4
7	D	63	ILE	15.8
24	V	1	THR	15.1
32	I	133	THR	14.1
32	I	79	ILE	13.7
16	N	166	ALA	12.3
32	I	76	ALA	11.8
32	I	96	PHE	11.7
32	I	88	GLY	11.6
24	V	39	ALA	11.4
32	I	116	LEU	11.0
7	D	57	THR	10.9
24	V	40	PRO	10.9
32	I	105	VAL	10.8
32	I	118	SER	10.6
32	I	113	HIS	10.4
22	T	119	ALA	10.4
32	I	85	PHE	10.3
32	I	75	THR	9.9
32	I	87	THR	9.9
7	D	61	PHE	9.8
32	I	102	VAL	9.6
32	I	137	VAL	9.5
4	A	237	GLY	9.3
32	I	121	LEU	9.3
26	X	88	GLU	9.0

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Mol	Chain	Res	Type	RSRZ
32	I	81	ASP	8.4
32	I	109	ALA	8.4
32	I	108	ILE	8.3
32	I	132	CYS	8.2
32	I	93	GLN	8.2
32	I	129	VAL	8.2
2	9	3001	U	8.1
4	A	37	VAL	8.1
15	M	70	GLY	7.9
32	I	125	ALA	7.8
32	I	104	GLN	7.8
7	D	90	LEU	7.6
32	I	77	GLU	7.6
30	2	49	GLU	7.5
1	0	1951	G	7.3
1	0	282	C	7.2
32	I	107	GLN	7.2
24	V	38	GLY	7.0
32	I	78	LEU	7.0
32	I	91	GLU	7.0
32	I	89	SER	7.0
10	G	23	ILE	6.8
32	I	111	GLN	6.8
28	Z	11	SER	6.6
1	0	1177	A	6.5
32	I	117	LEU	6.4
32	I	97	VAL	6.4
32	I	114	PRO	6.4
32	I	74	PRO	6.3
10	G	26	MET	6.3
15	M	79	ALA	6.3
22	T	118	SER	6.3
1	0	1199	A	6.2
7	D	170	TYR	6.0
15	M	74	LYS	5.9
32	I	86	GLU	5.9
32	I	103	ASP	5.9
10	G	27	ILE	5.8
14	L	106	VAL	5.8
2	9	3024	U	5.7
16	N	68	GLU	5.6
1	0	2637	A	5.6

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Mol	Chain	Res	Type	RSRZ
26	X	80	GLU	5.6
9	F	16	ALA	5.5
1	0	285	A	5.5
1	0	1172	G	5.5
32	I	98	ALA	5.4
32	I	126	LYS	5.3
8	E	45	ASP	5.3
7	D	44	ILE	5.3
1	0	280	C	5.3
1	0	1173	A	5.3
9	F	110	ASP	5.3
30	2	35	ARG	5.3
1	0	960	G	5.3
21	S	81	ILE	5.3
7	D	10	PHE	5.2
32	I	122	THR	5.2
16	N	163	PHE	5.2
1	0	999	C	5.2
14	L	75	LEU	5.2
1	0	2238	A	5.2
14	L	97	VAL	5.2
1	0	1948	G	5.1
16	N	175	LEU	5.1
1	0	10	U	5.1
7	D	69	ILE	5.1
32	I	123	ASN	5.0
24	V	37	GLY	5.0
9	F	119	ARG	5.0
4	A	35	GLY	5.0
1	0	514	G	5.0
7	D	64	ARG	4.9
12	J	70	PHE	4.9
32	I	83	ALA	4.9
28	Z	24	ARG	4.9
10	G	71	LEU	4.9
32	I	120	ASP	4.8
8	E	87	PHE	4.8
1	0	2748	G	4.8
32	I	124	ALA	4.8
32	I	138	THR	4.8
7	D	62	ASP	4.8
32	I	106	LYS	4.8

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Mol	Chain	Res	Type	RSRZ
1	0	2004	U	4.8
2	9	3023	U	4.8
1	0	2769	C	4.8
7	D	92	GLU	4.8
1	0	272	A	4.8
1	0	288	A	4.7
1	0	497	A	4.7
2	9	3002	U	4.7
32	I	115	ASP	4.7
10	G	24	VAL	4.6
1	0	1965	C	4.6
12	J	4	ALA	4.6
28	Z	20	ARG	4.6
9	F	106	ALA	4.6
14	L	76	LEU	4.6
10	G	22	ALA	4.6
1	0	1200	A	4.5
9	F	117	GLU	4.5
16	N	161	GLY	4.5
7	D	11	HIS	4.5
6	C	61	PHE	4.4
1	0	2237	G	4.4
7	D	73	VAL	4.4
1	0	970	U	4.4
27	Y	235	GLU	4.4
11	H	111	ASP	4.4
14	L	91	VAL	4.4
8	E	6	GLU	4.4
1	0	1202	A	4.3
32	I	136	GLY	4.3
9	F	22	VAL	4.3
28	Z	22	SER	4.3
1	0	1525	G	4.3
7	D	66	GLY	4.3
24	V	36	ALA	4.3
14	L	145	LEU	4.3
26	X	85	VAL	4.3
7	D	166	ILE	4.3
16	N	165	ALA	4.3
31	3	92	GLU	4.2
9	F	28	ALA	4.2
11	H	171	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
10	G	66	LEU	4.2
16	N	147	ILE	4.2
4	A	133	ARG	4.2
24	V	41	GLU	4.2
1	0	1171	A	4.2
7	D	18	ILE	4.2
32	I	119	TYR	4.1
16	N	184	ILE	4.1
11	H	34	GLY	4.1
7	D	107	GLY	4.1
19	Q	95	GLU	4.1
1	0	1950	G	4.1
7	D	93	LEU	4.1
7	D	173	GLU	4.1
1	0	2511	A	4.1
1	0	2508	C	4.0
16	N	154	LEU	4.0
32	I	112	LYS	4.0
23	U	47	ARG	4.0
7	D	172	VAL	4.0
11	H	146	VAL	4.0
1	0	1198	U	4.0
10	G	69	ARG	4.0
22	T	116	ASP	4.0
27	Y	95	THR	4.0
7	D	40	ILE	4.0
8	E	86	VAL	3.9
26	X	10	VAL	3.9
28	Z	21	VAL	3.9
16	N	155	GLU	3.9
32	I	135	LEU	3.9
7	D	51	ARG	3.9
11	H	73	LEU	3.9
32	I	95	ASP	3.9
3	4	77	PHE	3.9
32	I	80	LYS	3.9
8	E	154	ILE	3.9
11	H	37	GLN	3.9
7	D	134	LEU	3.8
16	N	95	ALA	3.8
11	H	35	ARG	3.8
15	M	78	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
7	D	171	ASP	3.8
8	E	100	ASP	3.8
9	F	15	ASP	3.8
11	H	74	ILE	3.8
7	D	26	GLY	3.8
27	Y	108	ASP	3.8
4	A	99	ILE	3.8
17	O	22	GLY	3.7
32	I	72	VAL	3.7
7	D	104	PHE	3.7
9	F	107	ASP	3.7
22	T	112	LEU	3.7
24	V	8	ILE	3.7
10	G	21	ASP	3.7
10	G	70	ALA	3.7
14	L	60	GLU	3.7
16	N	180	LEU	3.7
1	0	2747	C	3.7
32	I	110	GLU	3.7
22	T	82	THR	3.7
10	G	12	ILE	3.7
32	I	90	GLY	3.7
11	H	143	ALA	3.7
9	F	25	ASP	3.7
32	I	127	GLU	3.7
16	N	172	PHE	3.7
7	D	88	LEU	3.6
10	G	67	LEU	3.6
4	A	38	ILE	3.6
2	9	3122	C	3.6
14	L	80	ASP	3.6
9	F	118	LEU	3.6
9	F	99	THR	3.6
1	0	284	C	3.6
7	D	91	ALA	3.6
11	H	47	ILE	3.6
9	F	108	VAL	3.6
4	A	36	ASP	3.6
9	F	49	PHE	3.6
28	Z	25	ARG	3.5
8	E	43	ASP	3.5
7	D	167	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	0	281	U	3.5
1	0	1169	U	3.5
24	V	59	ILE	3.5
4	A	97	ALA	3.5
26	X	7	GLU	3.5
32	I	94	GLU	3.5
14	L	99	GLU	3.5
32	I	99	ASP	3.5
32	I	134	SER	3.5
8	E	4	GLU	3.4
7	D	23	VAL	3.4
15	M	86	GLN	3.4
1	0	283	U	3.4
4	A	236	GLY	3.4
8	E	160	ARG	3.4
14	L	105	TYR	3.4
4	A	31	LYS	3.4
16	N	139	TRP	3.4
1	0	1168	C	3.4
10	G	25	GLU	3.4
11	H	83	TYR	3.4
8	E	10	ASP	3.4
16	N	181	ASP	3.4
7	D	85	GLN	3.4
4	A	85	SER	3.4
11	H	82	ASP	3.4
16	N	183	ASP	3.4
26	X	71	ARG	3.3
1	0	1163	G	3.3
32	I	82	GLU	3.3
9	F	100	ASP	3.3
14	L	102	ASP	3.3
1	0	735	C	3.3
1	0	1000	C	3.3
27	Y	236	VAL	3.3
1	0	2645	U	3.3
1	0	969	G	3.3
24	V	43	PRO	3.3
32	I	84	GLY	3.3
19	Q	76	VAL	3.3
11	H	138	CYS	3.3
8	E	108	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
27	Y	234	VAL	3.3
1	0	716	G	3.2
7	D	81	GLU	3.2
22	T	115	GLU	3.2
1	0	1966	U	3.2
1	0	1967	U	3.2
14	L	130	ARG	3.2
16	N	185	GLU	3.2
1	0	1170	U	3.2
5	B	1	PRO	3.2
7	D	130	VAL	3.2
9	F	98	VAL	3.2
14	L	93	VAL	3.2
1	0	279	C	3.2
1	0	295	C	3.2
24	V	63	GLU	3.2
14	L	100	ALA	3.2
16	N	71	TRP	3.2
11	H	78	GLY	3.2
7	D	106	PHE	3.2
1	0	2103	A	3.2
15	M	71	SER	3.2
21	S	20	PHE	3.1
28	Z	12	GLY	3.1
5	B	57	GLU	3.1
32	I	92	PRO	3.1
9	F	103	GLU	3.1
8	E	128	GLY	3.1
7	D	56	ARG	3.1
13	K	132	VAL	3.1
16	N	178	THR	3.1
1	0	1947	G	3.1
16	N	152	GLU	3.1
7	D	27	ILE	3.1
8	E	89	SER	3.1
9	F	17	LEU	3.0
14	L	79	ASP	3.0
1	0	370	G	3.0
16	N	145	ALA	3.0
15	M	84	LYS	3.0
16	N	158	LEU	3.0
6	C	132	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
27	Y	98	GLN	3.0
1	0	358	G	3.0
10	G	73	ASP	3.0
31	3	62	THR	3.0
1	0	138	U	3.0
16	N	72	GLU	3.0
1	0	362	G	3.0
1	0	1178	G	3.0
21	S	2	TRP	3.0
31	3	41	GLU	3.0
1	0	1929	G	3.0
28	Z	42	CYS	3.0
32	I	140	GLU	3.0
7	D	135	VAL	3.0
14	L	121	ILE	3.0
7	D	79	MET	3.0
16	N	37	ARG	3.0
10	G	15	TRP	2.9
25	W	76	ASP	2.9
9	F	115	VAL	2.9
14	L	81	VAL	2.9
24	V	2	VAL	2.9
24	V	14	ALA	2.9
16	N	159	TYR	2.9
25	W	86	GLU	2.9
15	M	75	ARG	2.9
15	M	89	THR	2.9
1	0	1165	G	2.9
14	L	104	ASP	2.9
16	N	137	ALA	2.9
1	0	1189	A	2.9
8	E	127	ASP	2.9
15	M	87	GLY	2.9
14	L	148	GLU	2.9
27	Y	216	ARG	2.9
1	0	2344	G	2.9
15	M	83	SER	2.9
7	D	35	ALA	2.9
7	D	84	LEU	2.9
28	Z	36	ASP	2.9
4	A	65	ARG	2.8
19	Q	18	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
14	L	62	ALA	2.8
22	T	117	ASP	2.8
8	E	88	TYR	2.8
10	G	63	ARG	2.8
8	E	5	LEU	2.8
24	V	6	GLN	2.8
1	0	1625	U	2.8
7	D	38	GLU	2.8
24	V	10	ASP	2.8
32	I	139	ILE	2.8
28	Z	45	ASP	2.8
11	H	70	ASN	2.8
1	0	1181	A	2.8
8	E	161	VAL	2.8
16	N	149	GLU	2.8
27	Y	96	GLU	2.8
9	F	19	ALA	2.8
14	L	61	ALA	2.8
16	N	94	GLU	2.8
26	X	77	PHE	2.7
10	G	68	GLU	2.7
8	E	94	GLN	2.7
1	0	372	A	2.7
1	0	1180	U	2.7
1	0	1179	C	2.7
15	M	88	VAL	2.7
7	D	165	PHE	2.7
14	L	147	GLU	2.7
16	N	177	GLU	2.7
7	D	68	PRO	2.7
16	N	81	ALA	2.7
16	N	160	SER	2.7
32	I	128	VAL	2.7
11	H	24	PRO	2.7
1	0	1164	U	2.7
26	X	73	ARG	2.7
5	B	183	GLU	2.7
7	D	17	ARG	2.7
16	N	138	ASP	2.7
16	N	164	ASP	2.7
1	0	1195	G	2.7
8	E	129	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
10	G	72	ASP	2.7
9	F	12	LEU	2.7
1	0	289	G	2.7
1	0	2345	A	2.7
7	D	154	LYS	2.7
11	H	67	LEU	2.6
15	M	77	HIS	2.6
22	T	59	GLU	2.6
16	N	67	ALA	2.6
28	Z	19	GLY	2.6
8	E	121	ASP	2.6
15	M	76	ARG	2.6
4	A	64	ASP	2.6
24	V	46	ILE	2.6
1	0	1190	G	2.6
7	D	89	PRO	2.6
1	0	717	C	2.6
8	E	15	GLN	2.6
9	F	11	ASP	2.6
1	0	1196	C	2.6
15	M	73	ARG	2.6
15	M	164	THR	2.6
4	A	145	MET	2.6
7	D	95	THR	2.6
24	V	33	VAL	2.6
1	0	1174	A	2.5
8	E	98	GLU	2.5
11	H	39	ASP	2.5
7	D	41	LEU	2.5
16	N	179	LEU	2.5
20	R	104	PHE	2.5
1	0	1279	U	2.5
5	B	134	ALA	2.5
7	D	160	ALA	2.5
11	H	168	ALA	2.5
14	L	120	LEU	2.5
16	N	134	ASP	2.5
1	0	1208	C	2.5
14	L	150	GLN	2.5
15	M	80	GLY	2.5
16	N	156	GLU	2.5
21	S	70	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
9	F	23	ALA	2.5
7	D	52	THR	2.5
10	G	65	THR	2.5
8	E	118	ILE	2.5
1	0	369	G	2.5
30	2	39	ARG	2.5
7	D	54	ALA	2.5
28	Z	18	TYR	2.5
1	0	1192	A	2.4
1	0	1981	A	2.4
5	B	186	GLY	2.4
9	F	24	ARG	2.4
26	X	41	PHE	2.4
11	H	79	GLU	2.4
30	2	44	ARG	2.4
16	N	169	PRO	2.4
11	H	137	TYR	2.4
8	E	42	VAL	2.4
1	0	2239	C	2.4
1	0	1197	G	2.4
2	9	3073	G	2.4
6	C	135	GLU	2.4
9	F	18	GLU	2.4
9	F	43	GLY	2.4
9	F	109	GLU	2.4
16	N	170	GLU	2.4
20	R	7	GLU	2.4
28	Z	31	SER	2.4
4	A	34	ASP	2.4
7	D	99	ASP	2.4
9	F	101	ALA	2.4
19	Q	17	LYS	2.4
7	D	87	ALA	2.4
8	E	99	GLY	2.4
8	E	123	ASP	2.4
26	X	72	VAL	2.4
13	K	126	SER	2.4
4	A	60	PHE	2.4
12	J	5	GLU	2.4
24	V	45	ARG	2.4
7	D	157	LEU	2.4
22	T	35	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
9	F	21	GLU	2.4
24	V	5	VAL	2.4
1	0	1203	G	2.4
11	H	141	GLU	2.3
19	Q	64	GLU	2.3
11	H	139	ASN	2.3
1	0	373	G	2.3
1	0	1175	G	2.3
1	0	1527	A	2.3
28	Z	23	ARG	2.3
18	P	16	VAL	2.3
11	H	149	ALA	2.3
14	L	82	ALA	2.3
16	N	148	ALA	2.3
16	N	167	ASP	2.3
23	U	4	ARG	2.3
7	D	65	GLU	2.3
28	Z	32	GLU	2.3
9	F	113	ASP	2.3
32	I	73	PRO	2.3
8	E	169	THR	2.3
14	L	122	ALA	2.3
1	0	365	G	2.3
14	L	144	ASP	2.3
4	A	209	PRO	2.3
7	D	53	LYS	2.3
18	P	67	LYS	2.3
26	X	75	ALA	2.3
16	N	182	GLY	2.3
30	2	20	ARG	2.3
7	D	29	HIS	2.3
1	0	1949	G	2.3
4	A	206	ARG	2.3
5	B	104	GLU	2.3
6	C	237	GLU	2.3
28	Z	80	ARG	2.3
7	D	58	VAL	2.3
9	F	60	VAL	2.3
14	L	96	VAL	2.3
27	Y	187	VAL	2.3
1	0	290	C	2.3
21	S	72	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
5	B	108	GLU	2.3
1	0	1964	U	2.2
8	E	11	VAL	2.2
5	B	180	ASP	2.2
5	B	117	GLU	2.2
5	B	133	GLU	2.2
9	F	69	GLU	2.2
27	Y	102	LEU	2.2
1	0	809	G	2.2
1	0	2507	G	2.2
8	E	46	THR	2.2
9	F	26	THR	2.2
8	E	126	ILE	2.2
14	L	77	ALA	2.2
11	H	45	VAL	2.2
11	H	140	VAL	2.2
11	H	166	SER	2.2
14	L	141	GLU	2.2
17	O	1	SER	2.2
31	3	6	ARG	2.2
7	D	25	MET	2.2
16	N	2	THR	2.2
16	N	73	ALA	2.2
21	S	45	TYR	2.2
7	D	74	THR	2.2
21	S	78	ALA	2.2
20	R	96	VAL	2.2
17	O	31	GLU	2.2
24	V	62	GLU	2.2
8	E	7	ILE	2.2
25	W	93	ILE	2.2
8	E	162	PHE	2.2
9	F	6	PHE	2.2
1	0	804	C	2.2
14	L	44	GLU	2.2
7	D	86	THR	2.2
7	D	67	ASP	2.1
14	L	95	ASP	2.1
14	L	123	ASP	2.1
5	B	182	VAL	2.1
8	E	105	GLU	2.1
10	G	28	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
4	A	134	ASN	2.1
11	H	77	LEU	2.1
16	N	106	LEU	2.1
5	B	176	ASP	2.1
19	Q	81	GLU	2.1
24	V	42	ASN	2.1
15	M	82	ARG	2.1
16	N	65	ASP	2.1
5	B	2	GLN	2.1
16	N	92	ALA	2.1
9	F	75	ILE	2.1
19	Q	84	ILE	2.1
20	R	150	PRO	2.1
22	T	77	VAL	2.1
12	J	7	ASP	2.1
15	M	81	ARG	2.1
1	0	1522	A	2.1
14	L	142	LEU	2.1
2	9	3072	C	2.1
16	N	16	ALA	2.1
16	N	88	ALA	2.1
24	V	32	ALA	2.1
28	Z	34	ASN	2.1
9	F	111	ILE	2.1
7	D	78	GLU	2.1
2	9	3074	G	2.1
1	0	1526	A	2.1
7	D	94	ALA	2.1
16	N	70	GLY	2.1
18	P	18	LYS	2.1
16	N	174	GLU	2.1
15	M	68	ARG	2.1
9	F	14	ASP	2.1
7	D	128	LEU	2.1
13	K	129	THR	2.1
10	G	64	ASN	2.1
30	2	26	MET	2.1
1	0	278	A	2.1
19	Q	20	ASP	2.1
8	E	1	PRO	2.1
9	F	72	VAL	2.1
9	F	116	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
14	L	133	VAL	2.1
18	P	111	GLU	2.0
21	S	77	VAL	2.1
9	F	27	GLY	2.0
11	H	33	MET	2.0
24	V	3	LEU	2.0
15	M	194	ALA	2.0
13	K	119	GLN	2.0
1	0	1201	C	2.0
11	H	76	GLU	2.0
31	3	29	ARG	2.0
9	F	105	ASP	2.0
15	M	49	ALA	2.0
1	0	371	U	2.0
15	M	22	GLU	2.0
16	N	143	ARG	2.0
26	X	12	ILE	2.0
9	F	29	VAL	2.0
4	A	59	GLU	2.0
9	F	45	ALA	2.0
1	0	361	C	2.0
1	0	1176	C	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	1MA	0	628	23/24	0.98	0.14	-	31,33,36,39	0
1	OMU	0	2587	21/22	0.98	0.12	-	35,37,38,39	0
1	OMG	0	2588	24/25	0.97	0.12	-	32,34,38,40	0
1	PSU	0	2621	20/21	0.98	0.12	-	33,36,44,45	0
1	UR3	0	2619	21/22	0.98	0.14	-	42,46,49,51	0

6.3 Carbohydrates [i](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
35	NA	0	9164	1/1	0.62	0.57	84.72	67,67,67,67	0
37	SR	0	9500	1/1	0.17	1.75	75.02	200,200,200,200	0
35	NA	0	9125	1/1	0.90	1.02	61.89	106,106,106,106	0
35	NA	0	9120	1/1	0.94	0.31	32.27	61,61,61,61	0
37	SR	B	9521	1/1	0.21	0.72	25.64	200,200,200,200	0
33	MG	0	8084	1/1	0.92	0.54	25.46	109,109,109,109	0
35	NA	0	9185	1/1	0.81	0.56	25.07	54,54,54,54	0
35	NA	0	9161	1/1	0.95	0.31	24.87	57,57,57,57	0
35	NA	0	9177	1/1	0.93	0.40	23.02	70,70,70,70	0
35	NA	0	9168	1/1	0.84	0.28	21.30	72,72,72,72	0
35	NA	0	9172	1/1	0.82	0.42	19.83	68,68,68,68	0
35	NA	0	9150	1/1	0.87	0.33	19.39	54,54,54,54	0
35	NA	0	9173	1/1	0.90	0.39	18.81	66,66,66,66	0
35	NA	0	9162	1/1	0.98	0.29	17.10	51,51,51,51	0
37	SR	0	9406	1/1	1.00	0.17	15.65	33,33,33,33	0
35	NA	0	9132	1/1	0.85	0.38	13.99	61,61,61,61	0
35	NA	0	9115	1/1	0.95	0.25	13.20	43,43,43,43	0
33	MG	0	8038	1/1	0.99	0.27	10.83	13,13,13,13	0
35	NA	0	9174	1/1	0.84	0.24	10.73	67,67,67,67	0
33	MG	0	8001	1/1	0.97	0.22	10.33	17,17,17,17	0
35	NA	0	9118	1/1	0.94	0.22	10.06	41,41,41,41	0
33	MG	0	8008	1/1	0.99	0.22	9.53	14,14,14,14	0
33	MG	0	8012	1/1	0.99	0.26	9.24	37,37,37,37	0
34	K	0	9001	1/1	0.87	0.49	8.97	95,95,95,95	0
33	MG	0	8013	1/1	0.85	0.38	8.90	16,16,16,16	0
35	NA	0	9171	1/1	0.52	0.24	7.00	63,63,63,63	0
37	SR	0	9482	1/1	0.94	0.19	6.31	118,118,118,118	0
35	NA	9	9183	1/1	0.82	0.23	6.11	72,72,72,72	0
35	NA	0	9156	1/1	0.97	0.20	5.87	55,55,55,55	0
33	MG	0	8057	1/1	0.88	0.41	5.73	79,79,79,79	0
33	MG	0	8017	1/1	0.98	0.18	5.50	20,20,20,20	0
33	MG	0	8097	1/1	0.94	0.20	4.91	55,55,55,55	0
33	MG	0	8080	1/1	0.92	0.24	4.79	48,48,48,48	0
35	NA	0	9127	1/1	0.94	0.19	4.35	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	0	8107	1/1	0.82	0.22	3.32	68,68,68,68	0
35	NA	0	9159	1/1	0.93	0.17	2.78	56,56,56,56	0
33	MG	0	8027	1/1	0.95	0.19	2.77	30,30,30,30	0
37	SR	0	9515	1/1	0.99	0.18	2.40	100,100,100,100	0
37	SR	0	9475	1/1	0.97	0.14	2.30	77,77,77,77	0
33	MG	0	8020	1/1	0.97	0.19	2.19	30,30,30,30	0
35	NA	0	9165	1/1	0.94	0.21	1.50	41,41,41,41	0
37	SR	H	9486	1/1	0.96	0.18	1.45	121,121,121,121	0
35	NA	0	9117	1/1	0.99	0.16	1.35	32,32,32,32	0
37	SR	0	9407	1/1	0.98	0.14	1.34	42,42,42,42	0
35	NA	0	9105	1/1	0.98	0.15	1.26	41,41,41,41	0
33	MG	0	8074	1/1	0.99	0.21	1.20	20,20,20,20	0
37	SR	0	9410	1/1	1.00	0.15	1.16	34,34,34,34	0
33	MG	0	8054	1/1	0.80	0.13	1.14	58,58,58,58	0
36	CL	0	9316	1/1	0.93	0.17	1.12	74,74,74,74	0
33	MG	A	8066	1/1	0.96	0.18	1.02	53,53,53,53	0
35	NA	R	9186	1/1	0.92	0.15	0.99	64,64,64,64	0
33	MG	0	8056	1/1	0.98	0.18	0.96	47,47,47,47	0
36	CL	B	9319	1/1	0.92	0.16	0.91	59,59,59,59	0
35	NA	0	9178	1/1	0.91	0.15	0.81	54,54,54,54	0
34	K	0	9002	1/1	0.91	0.19	0.55	86,86,86,86	0
33	MG	0	8003	1/1	0.96	0.18	0.54	29,29,29,29	0
35	NA	0	9182	1/1	0.82	0.13	0.49	84,84,84,84	0
35	NA	0	9124	1/1	0.90	0.15	0.36	51,51,51,51	0
35	NA	C	9104	1/1	0.97	0.17	0.23	27,27,27,27	0
33	MG	0	8004	1/1	0.99	0.12	0.20	27,27,27,27	0
37	SR	1	9419	1/1	0.99	0.12	0.11	38,38,38,38	0
35	NA	0	9166	1/1	0.91	0.11	-0.12	65,65,65,65	0
33	MG	0	8096	1/1	0.97	0.13	-0.36	44,44,44,44	0
33	MG	0	8002	1/1	0.98	0.13	-0.38	22,22,22,22	0
35	NA	0	9139	1/1	0.96	0.13	-0.50	57,57,57,57	0
36	CL	M	9318	1/1	0.99	0.16	-0.53	37,37,37,37	0
37	SR	F	9595	1/1	0.97	0.14	-0.57	95,95,95,95	0
37	SR	A	9437	1/1	0.97	0.13	-0.57	64,64,64,64	0
35	NA	J	9146	1/1	0.83	0.13	-0.60	62,62,62,62	0
36	CL	J	9321	1/1	0.98	0.12	-0.67	58,58,58,58	0
37	SR	0	9490	1/1	0.96	0.12	-0.72	105,105,105,105	0
35	NA	0	9135	1/1	0.92	0.14	-0.77	46,46,46,46	0
37	SR	0	9509	1/1	0.97	0.12	-0.78	83,83,83,83	0
33	MG	0	8110	1/1	0.98	0.14	-0.82	46,46,46,46	0
37	SR	0	9424	1/1	0.99	0.15	-0.86	43,43,43,43	0
38	CD	U	9201	1/1	0.99	0.09	-0.98	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	R	9137	1/1	0.95	0.11	-1.00	32,32,32,32	0
37	SR	0	9534	1/1	0.96	0.11	-1.00	106,106,106,106	0
35	NA	Q	9148	1/1	0.98	0.13	-1.01	50,50,50,50	0
38	CD	Z	9203	1/1	0.99	0.07	-1.22	75,75,75,75	0
33	MG	T	8073	1/1	0.94	0.15	-1.24	42,42,42,42	0
33	MG	0	8015	1/1	0.96	0.10	-1.25	29,29,29,29	0
33	MG	0	8088	1/1	0.93	0.06	-1.36	43,43,43,43	0
35	NA	M	9147	1/1	0.98	0.10	-1.42	38,38,38,38	0
35	NA	R	9138	1/1	0.99	0.08	-1.50	52,52,52,52	0
37	SR	0	9451	1/1	0.99	0.09	-1.50	63,63,63,63	0
33	MG	0	8060	1/1	0.95	0.10	-1.55	81,81,81,81	0
37	SR	L	9409	1/1	1.00	0.12	-1.84	36,36,36,36	0
33	MG	0	8067	1/1	0.98	0.12	-1.88	36,36,36,36	0
37	SR	0	9457	1/1	0.99	0.09	-1.99	47,47,47,47	0
36	CL	0	9312	1/1	1.00	0.09	-2.08	45,45,45,45	0
37	SR	0	9442	1/1	0.98	0.11	-2.13	59,59,59,59	0
38	CD	3	9204	1/1	0.99	0.06	-2.15	58,58,58,58	0
33	MG	0	8032	1/1	0.89	0.11	-2.19	36,36,36,36	0
36	CL	3	9304	1/1	0.95	0.11	-2.20	59,59,59,59	0
36	CL	0	9315	1/1	0.96	0.10	-2.43	54,54,54,54	0
36	CL	O	9308	1/1	0.98	0.06	-2.45	67,67,67,67	0
35	NA	0	9131	1/1	0.96	0.11	-2.57	47,47,47,47	0
33	MG	Y	8109	1/1	0.98	0.10	-2.58	38,38,38,38	0
37	SR	0	9455	1/1	0.98	0.10	-2.68	61,61,61,61	0
37	SR	3	9439	1/1	0.99	0.06	-2.75	63,63,63,63	0
37	SR	A	9436	1/1	0.99	0.06	-2.83	57,57,57,57	0
37	SR	0	9468	1/1	0.70	0.05	-2.85	115,115,115,115	0
37	SR	0	9473	1/1	0.99	0.04	-3.12	69,69,69,69	0
37	SR	0	9506	1/1	0.96	0.07	-3.35	86,86,86,86	0
35	NA	0	9123	1/1	0.99	0.10	-3.36	37,37,37,37	0
35	NA	0	9143	1/1	0.97	0.07	-3.38	38,38,38,38	0
37	SR	0	9444	1/1	1.00	0.09	-3.46	47,47,47,47	0
37	SR	0	9453	1/1	0.98	0.09	-3.83	68,68,68,68	0
38	CD	1	9202	1/1	1.00	0.04	-3.86	51,51,51,51	0
33	MG	0	8044	1/1	0.99	0.06	-4.33	42,42,42,42	0
37	SR	0	9483	1/1	0.98	0.08	-4.37	67,67,67,67	0
37	SR	0	9498	1/1	0.99	0.06	-4.95	63,63,63,63	0
37	SR	0	9428	1/1	1.00	0.07	-4.99	43,43,43,43	0
36	CL	0	9305	1/1	0.98	0.07	-5.11	52,52,52,52	0
33	MG	0	8019	1/1	0.96	0.05	-5.22	53,53,53,53	0
37	SR	0	9532	1/1	0.99	0.05	-5.42	100,100,100,100	0
33	MG	0	8112	1/1	0.99	0.04	-5.59	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	0	8039	1/1	0.96	0.04	-6.54	56,56,56,56	0
37	SR	0	9416	1/1	1.00	0.09	-7.63	45,45,45,45	0
37	SR	0	9456	1/1	0.98	0.06	-8.94	67,67,67,67	0
37	SR	9	9588	1/1	0.86	0.14	-	122,122,122,122	0
36	CL	0	9303	1/1	0.98	0.17	-	49,49,49,49	0
35	NA	0	9126	1/1	0.83	0.14	-	55,55,55,55	0
37	SR	0	9422	1/1	0.99	0.12	-	53,53,53,53	0
33	MG	0	8075	1/1	0.93	0.06	-	37,37,37,37	0
37	SR	0	9425	1/1	0.99	0.09	-	71,71,71,71	0
33	MG	0	8021	1/1	0.87	0.24	-	51,51,51,51	0
37	SR	0	9495	1/1	0.95	0.11	-	88,88,88,88	0
33	MG	K	8069	1/1	0.99	0.21	-	23,23,23,23	0
35	NA	0	9141	1/1	0.87	0.12	-	61,61,61,61	0
35	NA	0	9158	1/1	0.95	0.10	-	62,62,62,62	0
35	NA	0	9130	1/1	0.96	0.09	-	45,45,45,45	0
33	MG	0	8050	1/1	0.71	0.24	-	94,94,94,94	0
35	NA	0	9170	1/1	0.90	0.32	-	75,75,75,75	0
37	SR	0	9423	1/1	0.99	0.10	-	51,51,51,51	0
33	MG	0	8108	1/1	0.39	0.28	-	115,115,115,115	0
35	NA	0	9154	1/1	0.92	0.20	-	51,51,51,51	0
36	CL	R	9306	1/1	0.99	0.16	-	46,46,46,46	0
37	SR	0	9508	1/1	0.99	0.08	-	83,83,83,83	0
35	NA	0	9106	1/1	0.96	0.19	-	37,37,37,37	0
33	MG	0	8029	1/1	0.98	0.22	-	27,27,27,27	0
37	SR	0	9474	1/1	0.96	0.09	-	96,96,96,96	0
37	SR	0	9415	1/1	1.00	0.11	-	50,50,50,50	0
33	MG	0	8030	1/1	0.93	0.04	-	34,34,34,34	0
35	NA	0	9129	1/1	-0.07	0.43	-	88,88,88,88	0
37	SR	0	9529	1/1	0.90	0.10	-	116,116,116,116	0
37	SR	0	9449	1/1	0.99	0.09	-	59,59,59,59	0
37	SR	0	9478	1/1	0.98	0.07	-	70,70,70,70	0
33	MG	0	8059	1/1	0.77	0.27	-	60,60,60,60	0
33	MG	0	8022	1/1	0.73	0.55	-	113,113,113,113	0
37	SR	0	9420	1/1	0.99	0.15	-	60,60,60,60	0
33	MG	0	8058	1/1	0.92	0.47	-	85,85,85,85	0
37	SR	0	9501	1/1	0.50	0.33	-	200,200,200,200	0
37	SR	0	9488	1/1	0.98	0.13	-	78,78,78,78	0
33	MG	0	8061	1/1	0.63	0.13	-	81,81,81,81	0
37	SR	0	9505	1/1	0.93	0.14	-	104,104,104,104	0
37	SR	0	9570	1/1	0.97	0.07	-	96,96,96,96	0
37	SR	0	9452	1/1	0.89	0.19	-	114,114,114,114	0
35	NA	0	9175	1/1	0.93	0.19	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
37	SR	0	9629	1/1	0.97	0.10	-	69,69,69,69	0
37	SR	0	9440	1/1	0.99	0.04	-	63,63,63,63	0
37	SR	0	9443	1/1	0.99	0.10	-	59,59,59,59	0
35	NA	0	9140	1/1	0.86	0.34	-	61,61,61,61	0
37	SR	0	9484	1/1	0.29	0.16	-	150,150,150,150	0
37	SR	0	9626	1/1	0.95	0.30	-	140,140,140,140	0
36	CL	0	9317	1/1	0.99	0.08	-	49,49,49,49	0
37	SR	0	9480	1/1	0.99	0.06	-	86,86,86,86	0
35	NA	0	9111	1/1	0.77	0.21	-	57,57,57,57	0
35	NA	0	9136	1/1	0.97	0.11	-	31,31,31,31	0
35	NA	0	9102	1/1	0.95	0.20	-	58,58,58,58	0
37	SR	0	9568	1/1	0.98	0.08	-	75,75,75,75	0
37	SR	0	9601	1/1	0.06	1.54	-	200,200,200,200	0
33	MG	0	8106	1/1	0.99	0.03	-	37,37,37,37	0
33	MG	0	8052	1/1	0.62	0.30	-	72,72,72,72	0
38	CD	O	9205	1/1	0.95	0.05	-	85,85,85,85	0
33	MG	0	8041	1/1	0.94	0.12	-	47,47,47,47	0
35	NA	0	9134	1/1	0.95	0.07	-	47,47,47,47	0
33	MG	0	8045	1/1	0.94	0.22	-	75,75,75,75	0
35	NA	0	9113	1/1	0.80	0.15	-	64,64,64,64	0
35	NA	0	9110	1/1	0.85	0.20	-	49,49,49,49	0
35	NA	D	9151	1/1	0.91	0.12	-	63,63,63,63	0
37	SR	0	9445	1/1	0.99	0.10	-	62,62,62,62	0
37	SR	0	9426	1/1	0.98	0.08	-	66,66,66,66	0
37	SR	0	9461	1/1	0.99	0.04	-	73,73,73,73	0
37	SR	0	9405	1/1	0.97	0.14	-	54,54,54,54	0
37	SR	0	9414	1/1	0.98	0.12	-	53,53,53,53	0
37	SR	0	9448	1/1	0.98	0.07	-	62,62,62,62	0
36	CL	0	9311	1/1	0.97	0.09	-	56,56,56,56	0
37	SR	0	9408	1/1	0.99	0.15	-	38,38,38,38	0
33	MG	0	8065	1/1	0.87	0.32	-	92,92,92,92	0
33	MG	0	8063	1/1	0.96	0.07	-	74,74,74,74	0
33	MG	0	8068	1/1	0.98	0.14	-	47,47,47,47	0
35	NA	0	9116	1/1	0.97	0.27	-	45,45,45,45	0
35	NA	0	9108	1/1	0.96	0.12	-	34,34,34,34	0
33	MG	0	8070	1/1	0.99	0.18	-	21,21,21,21	0
33	MG	0	8089	1/1	0.94	0.12	-	61,61,61,61	0
37	SR	R	9418	1/1	0.99	0.15	-	53,53,53,53	0
37	SR	0	9438	1/1	0.98	0.09	-	63,63,63,63	0
36	CL	L	9310	1/1	0.96	0.09	-	56,56,56,56	0
35	NA	0	9114	1/1	0.97	0.19	-	51,51,51,51	0
33	MG	0	8046	1/1	0.96	0.08	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	CL	J	9301	1/1	0.96	0.09	-	55,55,55,55	0
33	MG	0	8036	1/1	0.96	0.09	-	63,63,63,63	0
37	SR	0	9462	1/1	0.99	0.12	-	66,66,66,66	0
37	SR	0	9447	1/1	0.96	0.10	-	66,66,66,66	0
33	MG	0	8072	1/1	0.95	0.25	-	74,74,74,74	0
33	MG	0	8090	1/1	0.87	0.25	-	81,81,81,81	0
37	SR	0	9466	1/1	0.96	0.04	-	87,87,87,87	0
33	MG	0	8079	1/1	0.97	0.14	-	30,30,30,30	0
33	MG	0	8031	1/1	0.98	0.13	-	48,48,48,48	0
37	SR	0	9467	1/1	0.97	0.10	-	74,74,74,74	0
37	SR	0	9450	1/1	0.99	0.08	-	64,64,64,64	0
37	SR	0	9517	1/1	0.97	0.06	-	96,96,96,96	0
33	MG	0	8037	1/1	0.98	0.06	-	40,40,40,40	0
37	SR	9	9503	1/1	0.96	0.03	-	109,109,109,109	0
37	SR	S	9470	1/1	0.99	0.14	-	95,95,95,95	0
37	SR	0	9431	1/1	0.96	0.14	-	55,55,55,55	0
37	SR	0	9441	1/1	0.98	0.08	-	54,54,54,54	0
35	NA	0	9107	1/1	0.93	0.23	-	58,58,58,58	0
36	CL	J	9302	1/1	0.92	0.11	-	55,55,55,55	0
33	MG	0	8114	1/1	0.78	0.17	-	83,83,83,83	0
37	SR	0	9427	1/1	0.98	0.12	-	53,53,53,53	0
33	MG	0	8042	1/1	0.90	0.06	-	53,53,53,53	0
37	SR	0	9432	1/1	0.98	0.12	-	63,63,63,63	0
33	MG	0	8082	1/1	0.68	0.48	-	103,103,103,103	0
35	NA	0	9179	1/1	0.92	0.82	-	84,84,84,84	0
33	MG	0	8014	1/1	0.77	0.30	-	78,78,78,78	0
33	MG	B	8055	1/1	0.85	0.26	-	104,104,104,104	0
37	SR	1	9460	1/1	0.98	0.12	-	49,49,49,49	0
33	MG	0	8099	1/1	0.93	0.17	-	77,77,77,77	0
37	SR	0	9465	1/1	0.97	0.08	-	96,96,96,96	0
36	CL	0	9322	1/1	0.94	0.10	-	54,54,54,54	0
33	MG	0	8028	1/1	0.98	0.10	-	34,34,34,34	0
33	MG	0	8115	1/1	0.94	0.14	-	53,53,53,53	0
35	NA	0	9163	1/1	0.82	0.32	-	77,77,77,77	0
33	MG	0	8085	1/1	0.92	0.41	-	102,102,102,102	0
37	SR	0	9547	1/1	0.71	0.52	-	200,200,200,200	0
37	SR	0	9454	1/1	0.97	0.09	-	73,73,73,73	0
33	MG	0	8043	1/1	0.94	0.07	-	47,47,47,47	0
37	SR	0	9429	1/1	0.99	0.11	-	63,63,63,63	0
37	SR	0	9413	1/1	0.99	0.12	-	44,44,44,44	0
37	SR	0	9566	1/1	0.98	0.07	-	75,75,75,75	0
35	NA	0	9149	1/1	0.95	0.14	-	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	0	8103	1/1	0.87	0.31	-	79,79,79,79	0
35	NA	0	9101	1/1	0.93	0.16	-	43,43,43,43	0
33	MG	0	8116	1/1	0.97	0.04	-	51,51,51,51	0
37	SR	0	9434	1/1	0.99	0.15	-	58,58,58,58	0
37	SR	0	9417	1/1	0.98	0.13	-	53,53,53,53	0
37	SR	0	9477	1/1	0.97	0.10	-	82,82,82,82	0
37	SR	0	9522	1/1	0.93	0.06	-	104,104,104,104	0
37	SR	9	9481	1/1	0.98	0.06	-	83,83,83,83	0
37	SR	B	9458	1/1	0.98	0.09	-	73,73,73,73	0
33	MG	0	8102	1/1	0.92	0.15	-	70,70,70,70	0
35	NA	0	9181	1/1	0.82	0.12	-	48,48,48,48	0
33	MG	0	8040	1/1	0.87	0.34	-	94,94,94,94	0
33	MG	0	8104	1/1	0.79	0.33	-	83,83,83,83	0
36	CL	0	9313	1/1	0.98	0.11	-	51,51,51,51	0
37	SR	0	9459	1/1	0.96	0.07	-	96,96,96,96	0
37	SR	0	9590	1/1	0.72	0.09	-	142,142,142,142	0
33	MG	0	8098	1/1	0.92	0.08	-	43,43,43,43	0
36	CL	N	9307	1/1	0.93	0.12	-	54,54,54,54	0
35	NA	0	9122	1/1	0.34	0.45	-	98,98,98,98	0
33	MG	0	8051	1/1	0.95	0.29	-	22,22,22,22	0
33	MG	0	8117	1/1	0.98	0.11	-	39,39,39,39	0
33	MG	0	8094	1/1	0.54	0.39	-	82,82,82,82	0
35	NA	0	9152	1/1	0.83	0.37	-	67,67,67,67	0
37	SR	A	9497	1/1	0.98	0.11	-	85,85,85,85	0
33	MG	0	8005	1/1	0.98	0.09	-	29,29,29,29	0
35	NA	0	9184	1/1	0.55	0.29	-	86,86,86,86	0
37	SR	0	9581	1/1	0.73	0.07	-	134,134,134,134	0
37	SR	0	9469	1/1	0.99	0.04	-	85,85,85,85	0
37	SR	0	9464	1/1	0.98	0.06	-	80,80,80,80	0
33	MG	0	8083	1/1	0.92	0.07	-	51,51,51,51	0
33	MG	0	8101	1/1	0.81	0.12	-	51,51,51,51	0
33	MG	0	8092	1/1	0.57	1.62	-	83,83,83,83	0
35	NA	0	9167	1/1	0.97	0.06	-	50,50,50,50	0
37	SR	0	9435	1/1	0.99	0.07	-	68,68,68,68	0
33	MG	0	8025	1/1	0.90	0.34	-	23,23,23,23	0
37	SR	0	9489	1/1	0.94	0.08	-	87,87,87,87	0
35	NA	3	9169	1/1	0.93	0.41	-	102,102,102,102	0
35	NA	0	9128	1/1	0.99	0.13	-	40,40,40,40	0
33	MG	0	8026	1/1	0.99	0.18	-	26,26,26,26	0
37	SR	0	9539	1/1	0.81	0.37	-	167,167,167,167	0
33	MG	0	8024	1/1	0.88	0.91	-	90,90,90,90	0
33	MG	0	8076	1/1	0.95	0.21	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	0	9155	1/1	0.96	0.23	-	54,54,54,54	0
33	MG	0	8093	1/1	0.95	0.14	-	42,42,42,42	0
35	NA	S	9112	1/1	0.46	0.16	-	74,74,74,74	0
33	MG	9	8095	1/1	0.87	0.24	-	44,44,44,44	0
33	MG	0	8091	1/1	0.90	0.07	-	56,56,56,56	0
36	CL	Y	9320	1/1	0.97	0.10	-	42,42,42,42	0
37	SR	0	9430	1/1	1.00	0.14	-	41,41,41,41	0
33	MG	0	8047	1/1	0.65	0.52	-	94,94,94,94	0
37	SR	0	9585	1/1	0.97	0.08	-	86,86,86,86	0
37	SR	0	9446	1/1	0.97	0.10	-	80,80,80,80	0
36	CL	A	9309	1/1	0.99	0.17	-	64,64,64,64	0
37	SR	0	9545	1/1	0.99	0.05	-	67,67,67,67	0
33	MG	0	8009	1/1	0.95	0.07	-	31,31,31,31	0
35	NA	0	9157	1/1	0.93	0.16	-	41,41,41,41	0
37	SR	0	9560	1/1	0.97	0.08	-	97,97,97,97	0
35	NA	0	9160	1/1	0.94	0.15	-	42,42,42,42	0
37	SR	0	9504	1/1	0.91	0.10	-	92,92,92,92	0
37	SR	0	9537	1/1	0.60	0.17	-	152,152,152,152	0
33	MG	0	8113	1/1	0.92	0.08	-	45,45,45,45	0
37	SR	0	9421	1/1	0.97	0.10	-	65,65,65,65	0
37	SR	0	9412	1/1	0.98	0.12	-	43,43,43,43	0
37	SR	0	9433	1/1	0.97	0.11	-	73,73,73,73	0
37	SR	0	9411	1/1	0.99	0.16	-	42,42,42,42	0
36	CL	0	9314	1/1	0.97	0.06	-	47,47,47,47	0
37	SR	0	9530	1/1	0.95	0.12	-	94,94,94,94	0

6.5 Other polymers

There are no such residues in this entry.