



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:57 PM GMT

PDB ID : 1YHQ
Title : Crystal Structure Of Azithromycin Bound To The G2099A Mutant 50S Ribosomal Subunit Of Haloarcula Marismortui
Authors : Tu, D.; Blaha, G.; Moore, P.B.; Steitz, T.A.
Deposited on : 2005-01-10
Resolution : 2.40 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

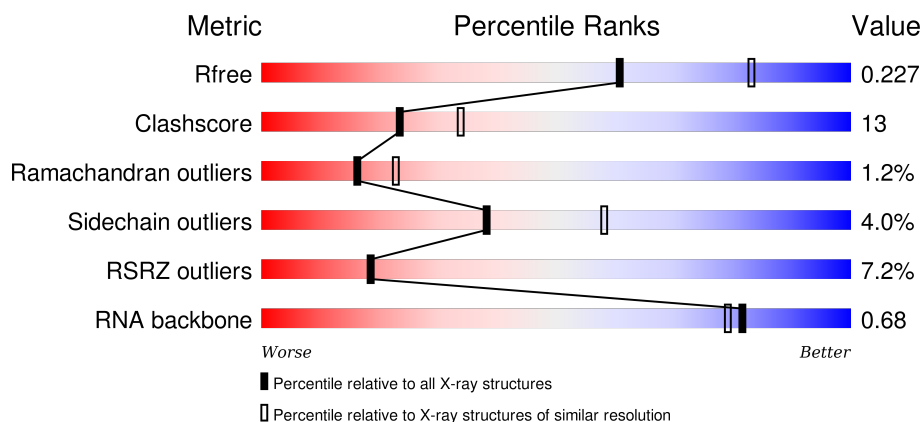
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)
RNA backbone	2183	1073 (2.90-1.90)

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>6%</div> </div>
2	9	122	<div> <div>5%</div> <div>60%</div> <div>30%</div> <div>9%</div> </div>
3	A	240	<div> <div>6%</div> <div>63%</div> <div>30%</div> <div>5%</div> </div>
4	B	338	<div> <div>3%</div> <div>60%</div> <div>36%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
5	C	246	
6	D	177	
7	E	178	
8	F	120	
9	G	348	
10	H	177	
11	I	162	
12	J	145	
13	K	132	
14	L	165	
15	M	194	
16	N	187	
17	O	116	
18	P	149	
19	Q	96	
20	R	155	
21	S	85	
22	T	120	
23	U	66	
24	V	71	
25	W	154	
26	X	92	
27	Y	241	
28	Z	83	
29	1	57	

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	NA	0	8517	-	-	-	X
35	NA	0	8521	-	-	-	X
35	NA	0	8523	-	-	-	X
35	NA	0	8527	-	-	-	X
35	NA	0	8528	-	-	-	X
35	NA	0	8534	-	-	-	X
35	NA	0	8535	-	-	-	X
35	NA	0	8542	-	-	-	X
35	NA	0	8547	-	-	-	X
35	NA	0	8550	-	-	-	X
35	NA	0	8553	-	-	-	X
35	NA	0	8555	-	-	-	X
35	NA	0	8559	-	-	-	X
35	NA	0	8560	-	-	-	X
35	NA	0	8562	-	-	-	X
35	NA	0	8563	-	-	-	X
35	NA	0	8564	-	-	-	X
35	NA	0	8565	-	-	-	X
35	NA	0	8568	-	-	-	X
35	NA	0	8571	-	-	-	X
35	NA	9	8572	-	-	-	X
35	NA	R	8575	-	-	-	X
36	CL	M	8818	-	-	-	X
37	SR	0	8903	-	-	-	X
37	SR	0	8969	-	-	-	X
37	SR	0	8992	-	-	-	X
37	SR	A	8929	-	-	-	X
37	SR	B	8987	-	-	-	X

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 99116 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	628	1MA	A	MODIFIED RESIDUE	GB 55229667
0	2099	A	G	ENGINEERED	GB 55229667
0	2587	OMU	U	MODIFIED RESIDUE	GB 55229667
0	2588	OMG	G	MODIFIED RESIDUE	GB 55229667
0	2619	UR3	U	MODIFIED RESIDUE	GB 55229667
0	2621	PSU	U	MODIFIED RESIDUE	GB 55229667

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

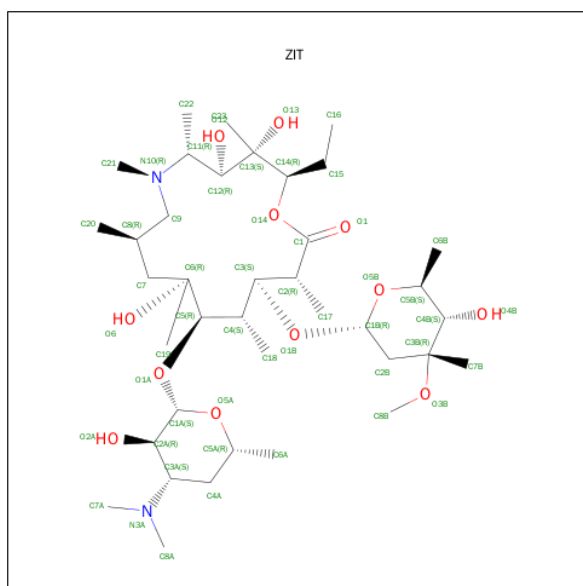
- Molecule 30 is a protein called 50S ribosomal protein L39e.

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

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

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

- Molecule 32 is AZITHROMYCIN (three-letter code: ZIT) (formula: $C_{38}H_{72}N_2O_{12}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	0	1	Total	C	N	O	0	0
			52	38	2	12		

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	0	86	Total 86 Mg 86	0	0
33	Y	1	Total 1 Mg 1	0	0
33	K	1	Total 1 Mg 1	0	0
33	B	1	Total 1 Mg 1	0	0
33	A	2	Total 2 Mg 2	0	0
33	T	1	Total 1 Mg 1	0	0
33	9	1	Total 1 Mg 1	0	0

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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	94	Total 94	Sr 94	0	0
37	1	2	Total 2	Sr 2	0	0
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	2	Total 2	Sr 2	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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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	5845	Total 5845	O 5845	0	0
39	9	145	Total 145	O 145	0	0
39	A	118	Total 118	O 118	0	0
39	B	151	Total 151	O 151	0	0
39	C	176	Total 176	O 176	0	0
39	D	49	Total 49	O 49	0	0
39	E	40	Total 40	O 40	0	0
39	F	26	Total 26	O 26	0	0
39	G	18	Total 18	O 18	0	0
39	H	72	Total 72	O 72	0	0
39	I	8	Total 8	O 8	0	0
39	J	59	Total 59	O 59	0	0
39	K	58	Total 58	O 58	0	0
39	L	72	Total 72	O 72	0	0
39	M	124	Total 124	O 124	0	0
39	N	61	Total 61	O 61	0	0
39	O	38	Total 38	O 38	0	0

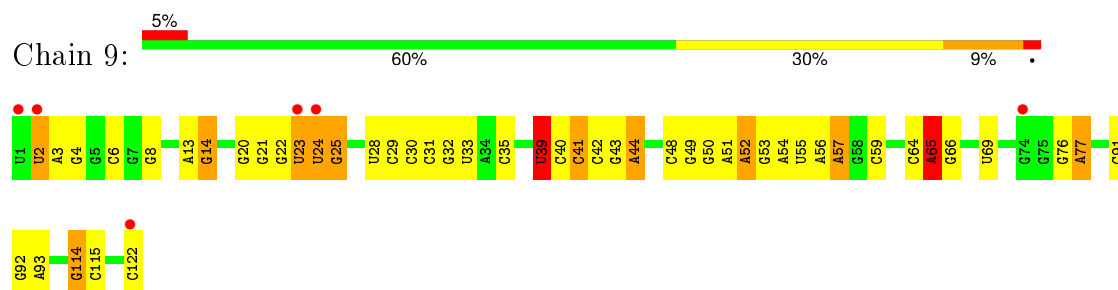
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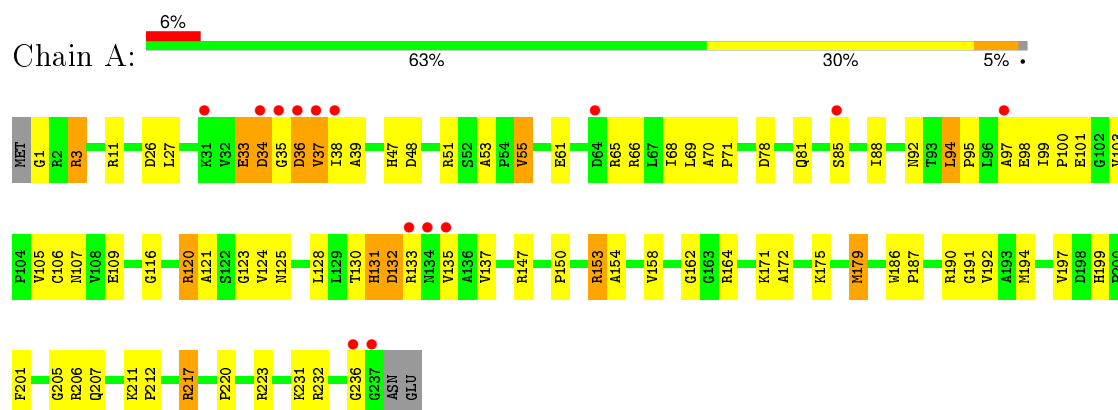
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	P	66	Total 66	O 66	0	0
39	Q	53	Total 53	O 53	0	0
39	R	87	Total 87	O 87	0	0
39	S	32	Total 32	O 32	0	0
39	T	41	Total 41	O 41	0	0
39	U	28	Total 28	O 28	0	0
39	V	12	Total 12	O 12	0	0
39	W	68	Total 68	O 68	0	0
39	X	24	Total 24	O 24	0	0
39	Y	95	Total 95	O 95	0	0
39	Z	32	Total 32	O 32	0	0
39	1	50	Total 50	O 50	0	0
39	2	44	Total 44	O 44	0	0
39	3	71	Total 71	O 71	0	0

C2867	U2756	G2634	G2516	G2421	U2290	C	G	G2005	C1882	G1739	A1603	A1427	C1289	A1191
C2868	A2761	A2635	A2521	U2422	A2291	A	G	U2008	G1902	U1740	G1604	C1439	G1290	A1192
C2869	C2762	C2636	G2524	G2426	A2300	G	U	A2011	U1903	U1741	G1605	U1440	A1291	A1193
G2876	A2768	G2638	G2525	G2427	A2301	C	G	U2012	A1919	A1742	A1615	A1441	G1295	A1194
U2878	C2769	G2642	G2526	G2428	A2302	C	C	G2013	G1940	G1752	U1625	A1442	C1299	C1196
A2879	G2770	G2643	U2527	U2435	C2309	A	C	G2014	A1941	C1753	A1626	G1452	G1300	C1197
A2883	G2779	A2649	C2533	G2442	C2313	C	G	U2015	G1925	A1754	G1627	U1458	U1304	U1198
C2884	C2780	C2443	C2534	G2443	G2316	A	U	A2016	G1926	A1755	A1626	A1458	C1305	C1201
A2890	U2781	U2652	U2535	U2444	G2317	G	G	U2031	A1927	G1756	U1657	A1470	U1306	A1202
C2894	G2783	A2653	G2536	U2445	C2320	U	U	G2032	C1940	C1762	A1630	C1474	A1307	G1203
C2895	U2787	U2661	G2537	G2446	U2320	A	C	G2033	A1941	U1766	A1634	U1474	A1308	C1204
A2896	A2664	A2664	A2321	A2453	A2321	A	G	U2034	C1942	C1767	A1641	C1477	U1314	U1205
G2900	U2791	A	C2326	A2456	C2326	U	A	C2036	C1943	C1768	A1642	C1484	A1328	A1207
C2901	A2792	U	G2336	U2457	G2336	C	U	G2044	G1946	C1769	A1653	G1484	C1208	C1208
A2902	A2793	G2667	G2337	G2462	G2337	U	A	A2054	G1947	G1773	U1654	G1497	C1209	C1209
C2903	C2795	G2670	G2338	A	A2338	G	G	U2064	G1948	G1777	U1656	U1500	U1333	G1210
A2906	U2796	C2672	A	C	C	U	U	U2064	G1950	A1778	A1657	U1500	C1334	G1211
C2907	A2800	U2673	C	C	C	A	A	G2072	U	A1779	A1658	U1503	C1335	C1212
A2908	U2807	C2676	G	G	G	G	G	G2073	A	C1786	G1665	A1504	C1343	G1216
G2909	U2808	A	A	U	A	U	U	A2074	A	C1787	C1666	U1505	U1218	U1218
C2910	G2809	C2681	G2344	G2472	G2344	C	G	U2081	C	C1798	C1667	U1506	U1219	U1219
C2911	G2810	C2682	A2345	C2476	A2345	G	G	A2089	U	G1809	U1668	G1523	A1352	C1229
C2912	A2811	A2684	C2346	G2477	C2346	U	U	G2090	A	G1819	U1677	G1524	C1353	A1230
A2913	U2812	U2694	A2353	U2478	A2353	G	G	U2091	C	G1820	U1678	G1525	C1360	A1231
A	A2813	A	A2354	A2479	A2354	U	U	G2096	C	G1829	C1679	G1526	U1232	A1232
G	G2814	G2697	C	U	C	U	A	A2096	U	G1830	C1680	G1527	U1233	A1233
C	G2815	G2698	G	C	G	C	C	A2096	C	U1835	C1681	G1529	U1234	U1234
C	G2816	G2712	U2586	C2241	C2241	C	A	A2101	U1964	A1840	A1682	U1555	C1366	G1235
A	G2817	G2713	U2587	C2242	C2242	U	A	G2102	C1965	A1845	A1683	U1559	A1372	U1237
U	G2818	G2714	U2588	C2243	C2243	C	C	G2103	U1966	U1846	A1684	U	U1238	C1238
C	G2819	G2715	U2589	C2244	C2244	C	C	C2104	U1967	C1853	A1685	C1562	C1377	G1239
A	G2820	G2716	U2590	C2245	C2245	U	U	G2110	G1970	A1840	C1687	C1574	G1378	U1242
C	G2821	G2717	U2591	C2246	C2246	A	A	G2111	U1971	A1845	C1692	A1569	A1243	A1242
C	G2822	G2718	U2592	C2247	C2247	C	C	G2112	U1972	U1846	C1697	U1561	U1244	U1244
C	G2823	G2719	U2593	C2248	C2248	C	C	G2113	A1973	U1846	G1697	C1563	C1245	C1245
C	G2824	G2720	U2594	C2249	C2249	G	C	G2114	G1976	C1853	C1700	C1564	A1393	A1246
C	G2825	G2721	U2595	C2250	C2250	C	C	G2115	U1977	C1856	A1701	C1564	U1249	U1249
C	G2826	G2722	U2596	C2251	C2251	C	C	G2116	U1978	C1857	U1702	C1574	C1250	C1250
C	G2827	G2723	U2597	C2252	C2252	U	U	G2117	G1979	A1857	A1717	A1573	A1251	A1251
C	G2828	G2724	U2598	C2253	C2253	A	A	G2118	U1980	G1863	A1717	C1574	A1252	A1252
C	G2829	G2725	U2599	C2254	C2254	C	C	G2119	U1981	G1863	A1717	C1574	C1253	C1253
C	G2830	G2726	U2600	C2255	C2255	G	G	G2120	U1982	G1863	U1722	G1589	G1268	G1268
C	G2831	G2727	U2601	C2256	C2256	C	C	G2121	U1983	G1863	U1722	G1589	G1269	G1269
C	G2832	G2728	U2602	C2257	C2257	C	C	G2122	U1984	G1863	U1722	G1589	G1270	G1270
C	G2833	G2729	U2603	C2258	C2258	C	C	G2123	U1985	G1863	U1722	G1589	G1271	G1271
C	G2834	G2730	U2604	C2259	C2259	C	C	G2124	U1986	G1863	U1722	G1589	G1272	G1272
C	G2835	G2731	U2605	C2260	C2260	C	C	G2125	U1987	G1863	U1722	G1589	G1273	G1273
C	G2836	G2732	U2606	C2261	C2261	C	C	G2126	U1988	G1863	U1722	G1589	G1274	G1274
C	G2837	G2733	U2607	C2262	C2262	C	C	G2127	U1989	G1863	U1722	G1589	G1275	G1275
C	G2838	G2734	U2608	C2263	C2263	C	C	G2128	U1990	G1863	U1722	G1589	G1276	G1276
C	G2839	G2735	U2609	C2264	C2264	C	C	G2129	U1991	G1863	U1722	G1589	G1277	G1277
C	G2840	G2736	U2610	C2265	C2265	C	C	G2130	U1992	G1863	U1722	G1589	G1278	G1278
C	G2841	G2737	U2611	C2266	C2266	C	C	G2131	U1993	G1863	U1722	G1589	G1279	G1279
C	G2842	G2738	U2612	C2267	C2267	C	C	G2132	U1994	G1863	U1722	G1589	G1280	G1280
C	G2843	G2739	U2613	C2268	C2268	C	C	G2133	U1995	G1863	U1722	G1589	G1281	G1281
C	G2844	G2740	U2614	C2269	C2269	C	C	G2134	U1996	G1863	U1722	G1589	G1282	G1282
C	G2845	G2741	U2615	C2270	C2270	C	C	G2135	U1997	G1863	U1722	G1589	G1283	G1283
C	G2846	G2742	U2616	C2271	C2271	C	C	G2136	U1998	G1863	U1722	G1589	G1284	G1284
C	G2847	G2743	U2617	C2272	C2272	C	C	G2137	U1999	G1863	U1722	G1589	G1285	G1285
C	G2848	G2744	U2618	C2273	C2273	C	C	G2138	U2000	G1863	U1722	G1589	G1286	G1286
C	G2849	G2745	U2619	C2274	C2274	C	C	G2139	U2001	G1863	U1722	G1589	G1287	G1287
C	G2850	G2746	U2620	C2275	C2275	C	C	G2140	U2002	G1863	U1722	G1589	G1288	G1288
C	G2851	G2747	U2621	C2276	C2276	C	C	G2141	U2003	G1863	U1722	G1589	G1289	G1289
C	G2852	G2748	U2622	C2277	C2277	C	C	G2142	U2004	G1863	U1722	G1589	G1290	G1290
C	G2853	G2749	U2623	C2278	C2278	C	C	G2143	U2005	G1863	U1722	G1589	G1291	G1291
C	G2854	G2750	U2624	C2279	C2279	C	C	G2144	U2006	G1863	U1722	G1589	G1292	G1292
C	G2855	G2751	U2625	C2280	C2280	C	C	G2145	U2007	G1863	U1722	G1589	G1293	G1293
C	G2856	G2752	U2626	C2281	C2281	C	C	G2146	U2008	G1863	U1722	G1589	G1294	G1294
C	G2857	G2753	U2627	C2282	C2282	C	C	G2147	U2009	G1863	U1722	G1589	G1295	G1295
C	G2858	G2754	U2628	C2283	C2283	C	C	G2148	U2010	G1863	U1722	G1589	G1296	G1296
C	G2859	G2755	U2629	C2284	C2284	C	C	G2149	U2011	G1863	U1722	G1589	G1297	G1297
C	G2860	G2756	U2630	C2285	C2285	C	C	G2150	U2012	G1863	U1722	G1589	G1298	G1298
C	G2861	G2757	U2631	C2286	C2286	C	C	G2151	U2013	G1863	U1722	G1589	G1299	G1299
C	G2862	G2758	U2632	C2287	C2287	C	C	G2152	U2014	G1863	U1722	G1589	G1300	G1300
C	G2863	G2759	U2633	C2288	C2288	C	C	G2153	U2015	G1863	U1722	G1589	G1301	G1301
C	G2864	G2760	U2634	C2289	C2289	C	C	G2154	U2016	G1863	U1722	G1589	G1302	G1302
C	G2865	G2761	U2635	C2290	C2290	C	C	G2155	U2017	G1863	U1722	G1589	G1303	G1303
C	G2866	G2762	U2636	C2291	C2291	C	C	G2156	U2018	G1863	U1722	G1589	G1304	G1304
C	G2867	G2763	U2637	C2292	C2292	C	C	G2157	U2019	G1863	U1722	G1589	G1305	G1305
C	G2868	G2764	U2638	C2293	C2293	C	C	G2158	U2020	G1863	U1722	G1589	G1306	G1306
C	G2869	G2765	U2639	C2294	C2294	C	C	G2159	U2021	G1863	U1722	G1589	G1307	G1307
C	G2870	G2766	U2640	C2295	C2295	C	C	G2160	U2022	G1863	U1722	G1589	G1308	G1308
C	G2871	G2767	U2641	C2296	C2296	C	C	G2161	U2023	G1863	U1722	G1589	G1309	G1309
C	G2872	G2768	U2642	C2297	C2297	C	C	G2162	U2024	G1863	U1722	G1589	G1310	G1310
C	G2873	G2769	U2643	C2298	C2298	C	C	G2163	U2025	G1863	U1722	G1589	G1311	G1311
C	G2874	G2770	U2644	C2299	C2299	C	C	G2164	U2026	G1863	U1722	G1589	G1312	G1312
C	G2875	G2771	U2645	C2300	C2300	C	C	G2165	U2027	G1863	U1722	G1589	G1313	G1313
C	G2876	G2772	U2646	C2301	C2301	C	C	G2166	U2028	G1863	U1722	G1589	G1314	G1314
C	G2877	G2773	U2647	C2302	C2302	C	C	G2167	U2029	G1863	U1722	G1589	G1315	G1315
C	G2878	G2774	U2648	C2303	C2303	C	C	G2168	U2030	G1863	U1722	G1589	G1316	G1316
C	G2879	G2775	U2649	C2304	C2304	C	C	G2169	U2031	G1863	U1722	G1589	G1317	G1317
C	G2880	G2776	U2650	C2305	C2305	C	C	G2170	U2032	G1863	U1722	G1589	G1318	G1318
C	G2881	G2777	U2651	C2306	C2306	C	C	G2171	U2033	G1863	U1722	G1589	G1319	G1319
C	G2882	G2778	U2652	C2307	C2307	C	C	G2172	U2034	G1863	U1722	G1589	G1320	G1320
C	G2883	G2779	U2653	C2308	C2308	C	C	G21						

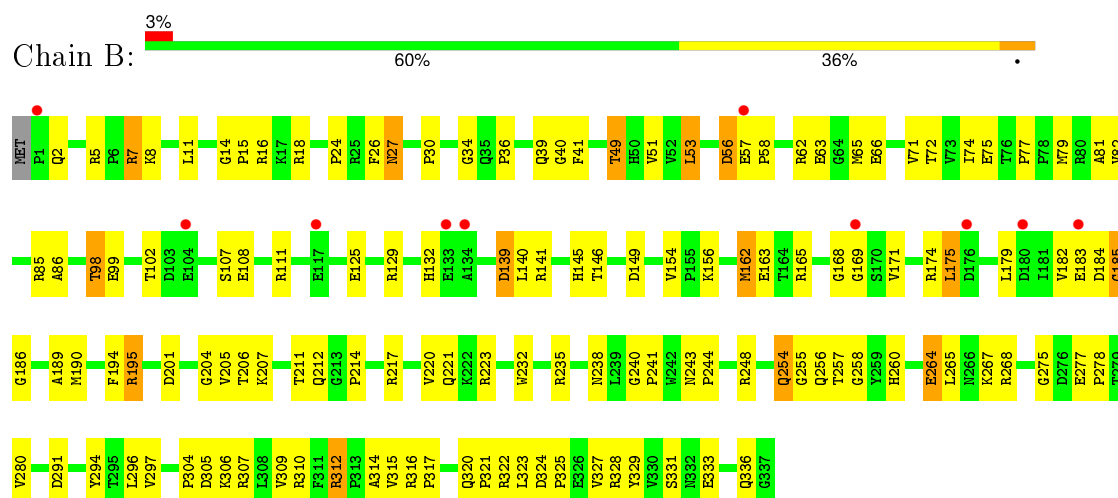
- Molecule 2: 5S Ribosomal RNA



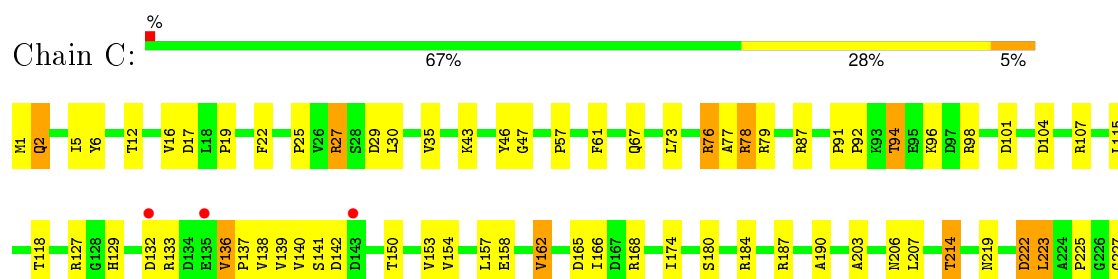
- Molecule 3: 50S ribosomal protein L2P

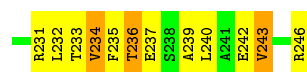


- Molecule 4: 50S ribosomal protein L3P

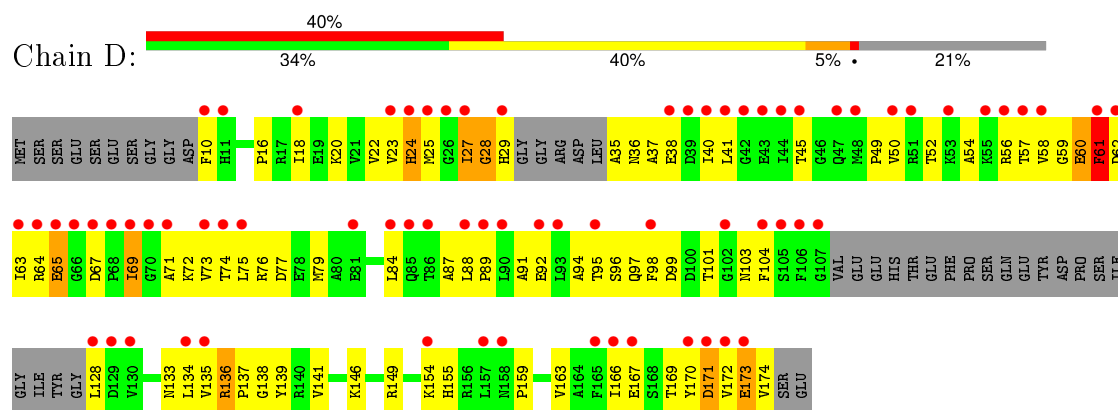


- Molecule 5: 50S ribosomal protein L4E

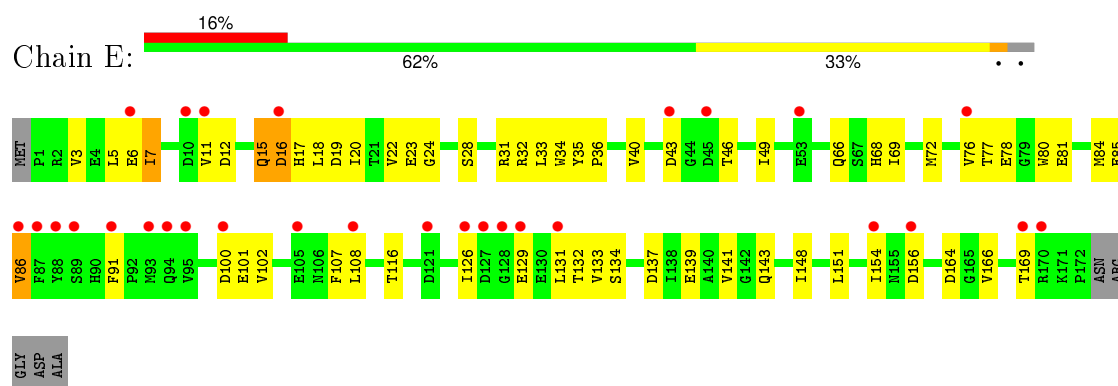




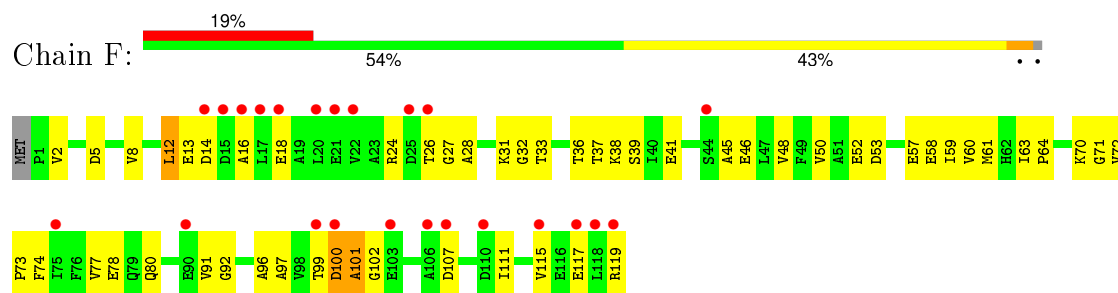
• Molecule 6: 50S ribosomal protein L5P



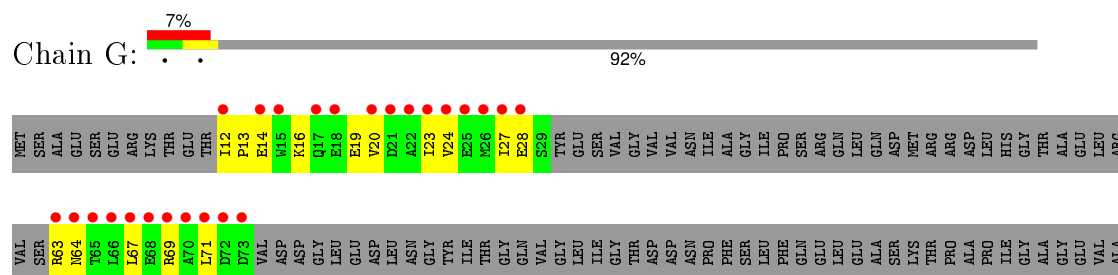
• Molecule 7: 50S ribosomal protein L6P



• Molecule 8: 50S ribosomal protein L7AE



• Molecule 9: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG



[illegible]

- Molecule 10: 50S RIBOSOMAL PROTEIN L10E

Chain H: 

[illegible]

- Molecule 11: 50S RIBOSOMAL PROTEIN L11P

Chain I:  15% 27% 43% 57%

A120	SER	MET
K121	PHE	ALA
E122	GLU	GLY
V123	ILE	THR
V124	GLU	ILE
G125	VAL	GLU
T126	G66	VAL
C127	P67	LEU
T128	P68	VAL
S129	P69	PRO
L130	T70	GLY
G131	A71	GLY
V132	E72	GLU
T133	L73	ALA
I134	I74	ASN
E135	K75	PRO
GLY	D76	GLY
GLU	E77	PRO
ASN	A78	PRO
PRO	G79	LEU
ARG	F80	GLY
GLU	B81	PRO
PHE	T82	GLU
LYS	C83	LEU
GLU	S84	GLY
ARG	G85	PRO
ILE	E86	THR
ASP	F87	PRO
ALA	O88	VAL
ALA	E89	ASP
GLY	D90	VAL
GLU	F91	GLN
TYR	N92	ALA
ASP	A93	VAL
ASP	D94	VAL
VAL	L95	GLN
PHE	S96	GLU
ALA	V97	ILE
ALA	D98	ASN
GLU	Q99	ASP
ALA	V100	GLN
GLN	K101	THR
ALA	G102	ALA
	I103	ALA
	A104	ASP
	E105	PHE
	G106	GLY
	K107	THR
	H108	GLU
	P109	VAL
	D110	PRO
	L111	VAL
	L112	THR
	S113	VAL
	I114	LYS
	D115	TYR
	L116	ASP
	T117	ASP
	M118	ASP
	A119	GLY

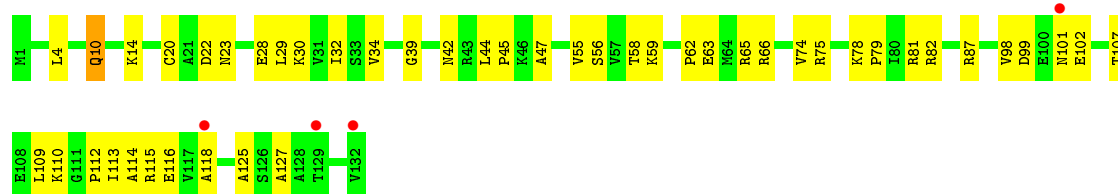
- Molecule 12: 50S ribosomal protein L13P

Chain J:  3% 66% 28% •

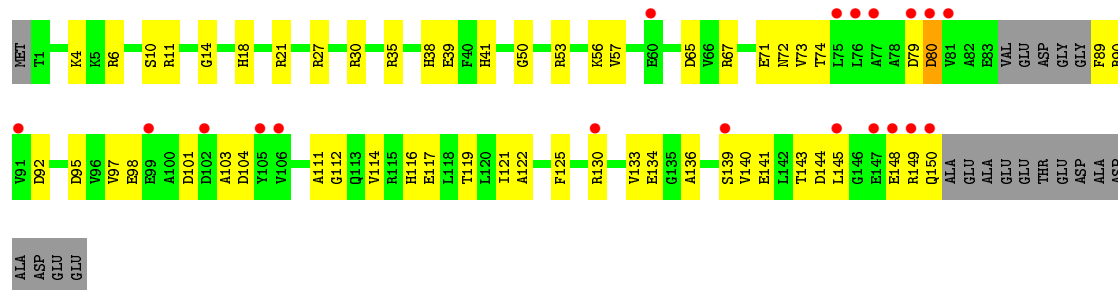
M107	P108	Y109	D110	L127	K128	F129	V130	T131	L132	G133	S136	K143	T144	V145																																
NET	SER	VAL	A4	E5	F6	D7	D13	A14	R15	I18	M19	V26	V36	E42	V45	I46	T47	G48	Q52	I53	I63	G64	V69	F70	Y71	F72	F73	R74	F75	D76	G77	I78	F79	K80	R81	T82	P88	H89	K90	R93	G94	H101	V103	V104	L105	G106

- Molecule 13: 50S ribosomal protein L14P

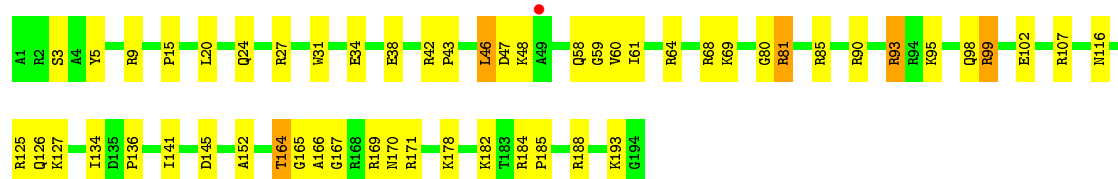
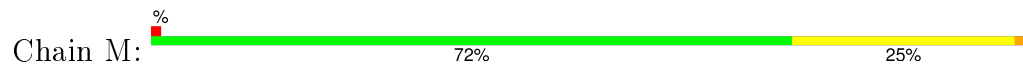
Chain K: 



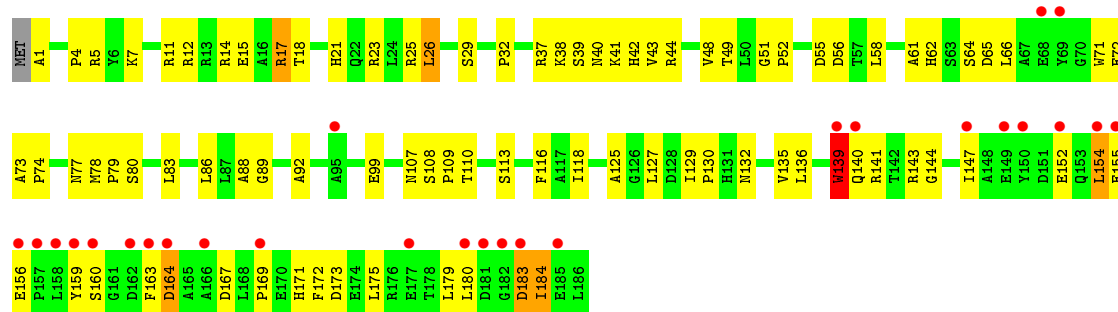
• Molecule 14: 50S ribosomal protein L15P



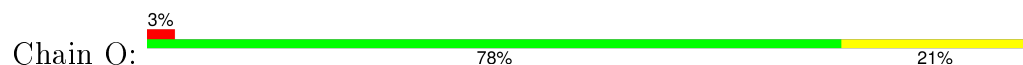
• Molecule 15: 50S Ribosomal Protein L15E



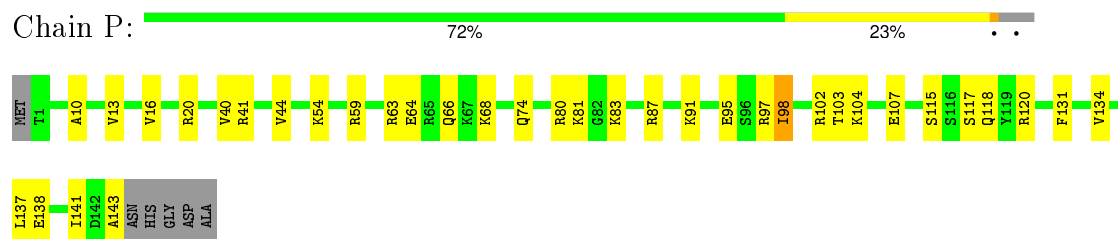
• Molecule 16: 50S ribosomal protein L18P



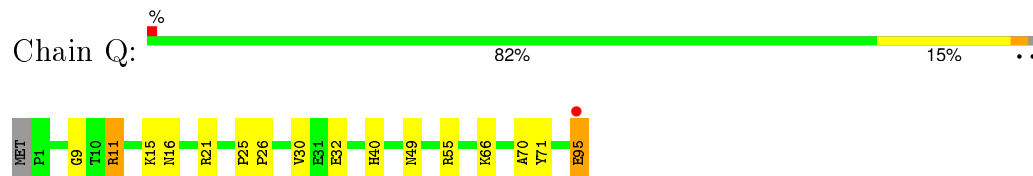
• Molecule 17: 50S ribosomal protein L18e



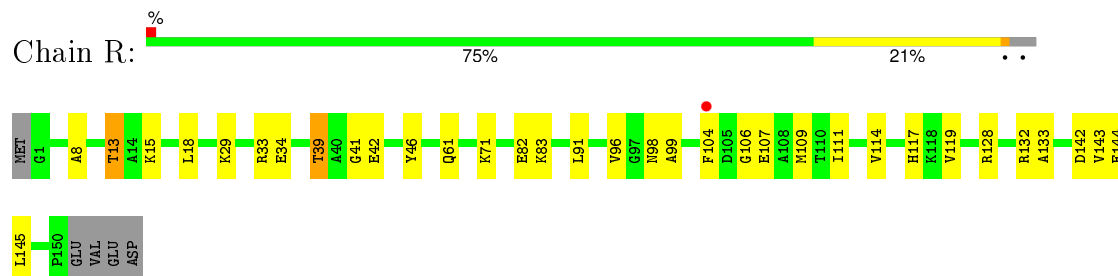
- Molecule 18: 50S ribosomal protein L19E



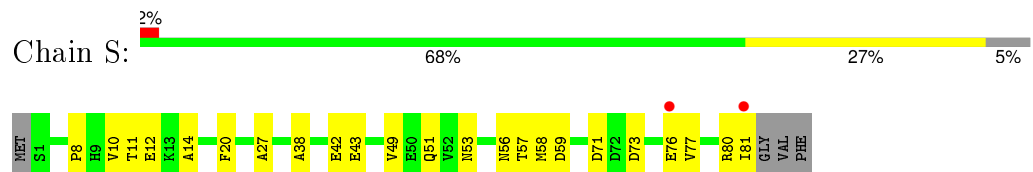
- Molecule 19: 50S ribosomal protein L21e



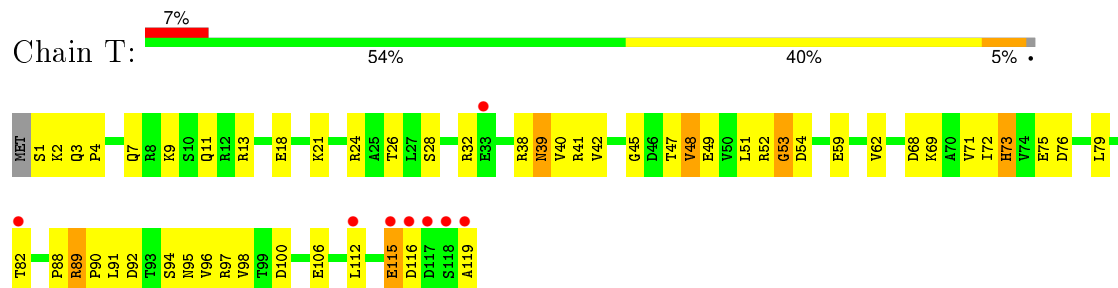
- Molecule 20: 50S ribosomal protein L22P



- Molecule 21: 50S ribosomal protein L23P

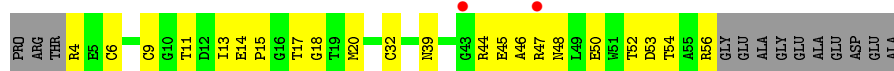


- Molecule 22: 50S ribosomal protein L24P



- Molecule 23: 50S ribosomal protein L24E





- Molecule 24: 50S ribosomal protein L29P



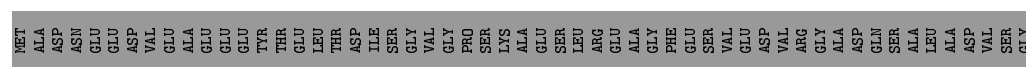
- Molecule 25: 50S ribosomal protein L30P



- Molecule 26: 50S ribosomal protein L31e



- Molecule 27: 50S ribosomal protein L32E



- Molecule 28: 50S ribosomal protein L37Ae

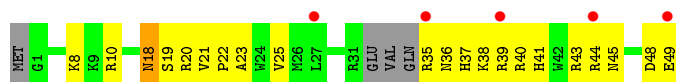




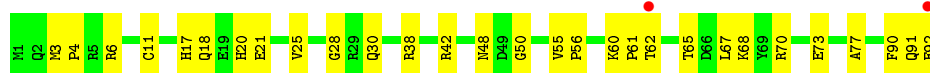
- Molecule 29: 50S ribosomal protein L37e



- Molecule 30: 50S ribosomal protein L39e



- Molecule 31: 50S ribosomal protein L44E



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	212.08Å 298.91Å 574.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.96 – 2.40 49.82 – 2.40	Depositor EDS
% Data completeness (in resolution range)	90.2 (29.96-2.40) 90.2 (49.82-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.190 , 0.229 0.190 , 0.227	Depositor DCC
R_{free} test set	6149 reflections (0.98%)	DCC
Wilson B-factor (Å ²)	41.0	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 634402 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	99116	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.53% 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, ZIT, 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	0.35	0/65957	0.69	25/102867 (0.0%)
2	9	0.32	0/2904	0.70	1/4526 (0.0%)
3	A	0.33	0/1786	0.66	0/2408
4	B	0.31	0/2690	0.64	0/3652
5	C	0.37	0/1884	0.64	0/2551
6	D	0.29	0/1111	0.53	0/1498
7	E	0.31	0/1382	0.57	0/1880
8	F	0.31	0/901	0.55	0/1224
9	G	0.27	0/241	0.47	0/324
10	H	0.35	0/1302	0.65	0/1743
11	I	0.28	0/526	0.48	0/716
12	J	0.34	0/1136	0.59	0/1530
13	K	0.33	0/1001	0.65	0/1347
14	L	0.32	0/1130	0.64	0/1509
15	M	0.33	0/1582	0.61	0/2117
16	N	0.28	0/1474	0.60	0/1999
17	O	0.32	0/874	0.59	0/1181
18	P	0.32	0/1147	0.53	0/1528
19	Q	0.34	0/749	0.69	0/1005
20	R	0.34	0/1172	0.64	0/1578
21	S	0.32	0/648	0.58	1/875 (0.1%)
22	T	0.30	0/958	0.62	0/1289
23	U	0.32	0/417	0.53	0/562
24	V	0.29	0/502	0.53	0/675
25	W	0.33	0/1219	0.62	0/1655
26	X	0.31	0/664	0.56	0/895
27	Y	0.34	0/1146	0.62	0/1536
28	Z	0.34	0/589	0.64	0/787
29	1	0.40	0/438	0.64	0/578
30	2	0.33	0/401	0.55	0/529
31	3	0.36	0/771	0.58	0/1024
All	All	0.34	0/98702	0.67	27/147588 (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	0	53
2	9	0	2
All	All	0	55

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1942	A	C5'-C4'-C3'	8.34	129.34	116.00
1	0	871	G	C5'-C4'-O4'	-7.87	99.66	109.10
2	9	39	U	N1-C1'-C2'	6.90	122.97	114.00
1	0	1979	G	C2'-C3'-O3'	6.61	124.27	113.70
1	0	1504	A	C1'-O4'-C4'	-6.48	104.71	109.90
1	0	2316	G	C5'-C4'-C3'	-6.23	106.04	116.00
1	0	1559	A	C2'-C3'-O3'	6.21	123.64	113.70
1	0	1819	G	C5'-C4'-C3'	6.18	125.89	116.00
1	0	1592	G	N9-C1'-C2'	6.17	122.02	114.00
1	0	206	G	C5'-C4'-C3'	-6.11	106.22	116.00
1	0	2291	A	N9-C1'-C2'	6.06	121.88	114.00
1	0	2726	U	N1-C1'-C2'	5.79	121.53	114.00
1	0	2313	C	C5'-C4'-O4'	5.77	116.03	109.10
1	0	2467	A	C1'-O4'-C4'	-5.72	105.32	109.90
1	0	1120	U	C5'-C4'-C3'	-5.62	107.02	116.00
1	0	777	U	O4'-C1'-N1	5.49	112.59	108.20
1	0	1504	A	N9-C1'-C2'	5.42	121.05	114.00
21	S	27	ALA	N-CA-C	-5.38	96.48	111.00
1	0	1942	A	C4'-C3'-C2'	-5.37	97.23	102.60
1	0	1819	G	C1'-O4'-C4'	-5.32	105.65	109.90
1	0	1829	A	N9-C1'-C2'	-5.31	106.16	112.00
1	0	841	A	C1'-O4'-C4'	-5.29	105.67	109.90
1	0	1452	G	C5'-C4'-C3'	-5.17	107.72	116.00
1	0	2607	U	N1-C1'-C2'	5.14	120.68	114.00
1	0	69	A	C5'-C4'-O4'	-5.13	102.95	109.10
1	0	2313	C	C5'-C4'-C3'	5.08	124.13	116.00
1	0	129	A	C2'-C3'-O3'	5.05	121.78	113.70

There are no chirality outliers.

All (55) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1039	G	Sidechain
1	0	1078	A	Sidechain
1	0	1237	U	Sidechain
1	0	1342	C	Sidechain
1	0	1417	G	Sidechain
1	0	1458	A	Sidechain
1	0	1592	G	Sidechain
1	0	1653	A	Sidechain
1	0	1777	G	Sidechain
1	0	1809	G	Sidechain
1	0	1819	G	Sidechain
1	0	1829	A	Sidechain
1	0	1845	A	Sidechain
1	0	1863	G	Sidechain
1	0	1867	G	Sidechain
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	1970	G	Sidechain
1	0	1985	U	Sidechain
1	0	221	G	Sidechain
1	0	2316	G	Sidechain
1	0	2412	G	Sidechain
1	0	246	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	2607	U	Sidechain
1	0	2630	G	Sidechain
1	0	2632	G	Sidechain
1	0	2681	A	Sidechain
1	0	270	U	Sidechain
1	0	2842	G	Sidechain
1	0	324	G	Sidechain
1	0	333	G	Sidechain
1	0	396	U	Sidechain
1	0	417	G	Sidechain
1	0	460	A	Sidechain
1	0	469	G	Sidechain
1	0	470	U	Sidechain
1	0	471	G	Sidechain
1	0	482	G	Sidechain

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Mol	Chain	Res	Type	Group
1	0	518	G	Sidechain
1	0	619	U	Sidechain
1	0	792	G	Sidechain
1	0	795	G	Sidechain
1	0	817	G	Sidechain
1	0	867	A	Sidechain
1	0	868	G	Sidechain
1	0	881	C	Sidechain
1	0	888	U	Sidechain
1	0	893	C	Sidechain
2	9	39	U	Sidechain
2	9	65	A	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59020	0	29808	686	0
2	9	2599	0	1325	53	0
3	A	1753	0	1766	109	0
4	B	2625	0	2533	125	0
5	C	1859	0	1816	97	0
6	D	1094	0	1085	91	0
7	E	1357	0	1266	55	0
8	F	890	0	843	51	0
9	G	240	0	231	18	0
10	H	1282	0	1292	53	0
11	I	519	0	500	47	0
12	J	1120	0	1098	58	0
13	K	992	0	1031	56	0
14	L	1118	0	1076	52	0
15	M	1558	0	1566	63	0
16	N	1445	0	1401	100	0
17	O	865	0	873	30	0
18	P	1136	0	1123	34	0
19	Q	735	0	728	14	0
20	R	1149	0	1122	41	0
21	S	641	0	605	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	T	950	0	923	51	0
23	U	410	0	364	24	0
24	V	499	0	511	35	0
25	W	1196	0	1137	88	0
26	X	654	0	653	42	0
27	Y	1130	0	1133	58	0
28	Z	578	0	539	19	0
29	1	431	0	426	22	0
30	2	396	0	413	25	0
31	3	755	0	728	24	0
32	0	52	0	72	0	0
33	0	86	0	0	0	0
33	9	1	0	0	0	0
33	A	2	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	65	0	0	0	0
35	9	2	0	0	0	0
35	C	1	0	0	0	0
35	H	1	0	0	0	0
35	J	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	2	0	0	0	0
35	S	1	0	0	0	0
36	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	2	0
36	L	1	0	0	0	0
36	M	1	0	0	0	0
36	N	1	0	0	0	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
36	Y	1	0	0	0	0
37	0	94	0	0	0	0
37	1	2	0	0	0	0
37	3	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	9	2	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	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	5845	0	0	120	0
39	1	50	0	0	2	0
39	2	44	0	0	3	0
39	3	71	0	0	5	0
39	9	145	0	0	4	0
39	A	118	0	0	19	0
39	B	151	0	0	25	0
39	C	176	0	0	24	0
39	D	49	0	0	19	0
39	E	40	0	0	5	0
39	F	26	0	0	7	0
39	G	18	0	0	2	0
39	H	72	0	0	12	0
39	I	8	0	0	2	0
39	J	59	0	0	2	0
39	K	58	0	0	7	0
39	L	72	0	0	15	0
39	M	124	0	0	8	0
39	N	61	0	0	12	0
39	O	38	0	0	6	0
39	P	66	0	0	4	0
39	Q	53	0	0	4	0
39	R	87	0	0	7	0
39	S	32	0	0	3	0
39	T	41	0	0	4	0
39	U	28	0	0	3	0
39	V	12	0	0	2	0
39	W	68	0	0	7	0
39	X	24	0	0	8	0
39	Y	95	0	0	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	Z	32	0	0	2	0
All	All	99116	0	59987	2007	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (2007) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1160:G:H5'	1:0:1161:A:H5'	1.18	1.10
26:X:37:LEU:HD13	26:X:85:VAL:HG21	1.32	1.09
5:C:236:THR:HG22	5:C:239:ALA:H	1.10	1.06
6:D:25:MET:HE3	6:D:37:ALA:HB1	1.34	1.04
1:0:1242:A:H5'	12:J:82:THR:HG23	1.39	1.04
2:9:6:C:H5''	16:N:37:ARG:NH1	1.74	1.03
22:T:71:VAL:HG11	22:T:90:PRO:HB3	1.41	1.01
4:B:212:GLN:HB2	4:B:257:THR:HG21	1.45	0.99
1:0:156:C:H5''	15:M:171:ARG:HD3	1.43	0.99
18:P:115:SER:H	18:P:118:GLN:HE21	1.09	0.99
6:D:154:LYS:HD2	6:D:154:LYS:H	1.27	0.98
1:0:871:G:C8	1:0:871:G:H5'	1.97	0.98
5:C:78:ARG:HG3	5:C:78:ARG:HH11	1.28	0.97
2:9:76:G:H3'	2:9:77:A:H5''	1.47	0.95
13:K:74:VAL:HG11	13:K:113:ILE:HG12	1.46	0.95
15:M:164:THR:HG22	15:M:167:GLY:H	1.32	0.95
2:9:56:A:H2'	2:9:57:A:H5''	1.46	0.95
4:B:140:LEU:HA	39:B:9048:HOH:O	1.65	0.95
5:C:127:ARG:NH2	5:C:225:PRO:HG2	1.82	0.94
25:W:137:GLN:HE21	25:W:141:HIS:HE1	1.07	0.94
4:B:86:ALA:HA	39:B:9048:HOH:O	1.68	0.93
27:Y:200:THR:HG22	27:Y:201:GLU:HG3	1.50	0.93
1:0:871:G:H8	1:0:871:G:H5'	1.30	0.93
16:N:144:GLY:O	16:N:147:ILE:HG22	1.68	0.92
12:J:19:MET:HE3	12:J:132:LEU:HD21	1.50	0.92
15:M:102:GLU:OE1	15:M:164:THR:HG21	1.69	0.92
25:W:88:THR:HB	39:W:6679:HOH:O	1.70	0.92
20:R:99:ALA:HB1	20:R:109:MET:HE1	1.50	0.92
1:0:541:C:H2'	1:0:542:A:H5''	1.52	0.92
30:2:41:HIS:H	30:2:45:ASN:HD22	1.12	0.91
13:K:10:GLN:H	13:K:10:GLN:NE2	1.67	0.91
6:D:57:THR:HG23	6:D:63:ILE:HA	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:6:GLN:HB2	25:W:26:ILE:HD12	1.52	0.91
4:B:162:MET:HE2	4:B:310:ARG:HD3	1.51	0.91
1:0:542:A:H5'	1:0:542:A:H8	1.34	0.91
21:S:57:THR:HG22	21:S:59:ASP:H	1.36	0.90
1:0:870:G:H2'	1:0:871:G:H5''	1.51	0.90
28:Z:46:ARG:HD2	28:Z:59:TYR:HB2	1.51	0.90
1:0:2717:C:C2'	1:0:2718:C:H5''	2.02	0.90
13:K:10:GLN:N	13:K:10:GLN:HE21	1.70	0.89
1:0:2717:C:H2'	1:0:2718:C:H5''	1.54	0.89
13:K:39:GLY:HA2	39:K:4183:HOH:O	1.73	0.89
4:B:238:ASN:HD22	4:B:240:GLY:H	1.18	0.89
16:N:83:LEU:HD13	16:N:175:LEU:HD23	1.53	0.89
1:0:2812:A:H2	1:0:2814:A:H62	1.19	0.89
1:0:2270:G:H4'	3:A:223:ARG:HH12	1.36	0.88
6:D:28:GLY:HA2	6:D:69:ILE:HG23	1.56	0.88
22:T:9:LYS:HE3	22:T:13:ARG:NH1	1.88	0.88
4:B:307:ARG:HH11	4:B:307:ARG:HG3	1.38	0.88
3:A:35:GLY:O	3:A:36:ASP:HB3	1.71	0.88
1:0:1160:G:C5'	1:0:1161:A:H5'	2.03	0.88
7:E:20:ILE:HD11	7:E:40:VAL:HG11	1.54	0.88
1:0:1160:G:H5'	1:0:1161:A:C5'	2.04	0.87
13:K:29:LEU:HB3	13:K:55:VAL:HG11	1.54	0.87
25:W:122:ARG:NH2	25:W:154:ARG:HB3	1.90	0.87
1:0:2506:A:HO2'	1:0:2507:G:H8	0.89	0.87
2:9:6:C:H5''	16:N:37:ARG:HH12	1.37	0.87
10:H:49:GLN:HE21	10:H:140:TYR:HE2	1.21	0.87
1:0:1835:U:H5	1:0:1840:A:N7	1.73	0.86
25:W:21:LEU:HD21	25:W:48:VAL:HG11	1.57	0.86
24:V:1:THR:HG23	24:V:2:VAL:H	1.40	0.86
11:I:127:CYS:HB3	11:I:132:VAL:HB	1.58	0.86
13:K:98:VAL:CG1	13:K:102:GLU:HA	2.04	0.85
26:X:71:ARG:HD3	39:X:2171:HOH:O	1.75	0.85
1:0:960:G:H4'	39:0:7859:HOH:O	1.75	0.85
18:P:115:SER:OG	18:P:118:GLN:HG3	1.77	0.85
31:3:65:THR:HG22	31:3:67:LEU:HG	1.59	0.85
3:A:199:HIS:HD2	3:A:201:PHE:H	1.23	0.85
13:K:81:ARG:HB2	13:K:87:ARG:HH11	1.39	0.84
5:C:236:THR:HG22	5:C:239:ALA:N	1.92	0.84
25:W:137:GLN:HE21	25:W:141:HIS:CE1	1.95	0.84
1:0:282:C:H1'	1:0:368:C:N4	1.92	0.84
10:H:170:ARG:HD2	39:H:8989:HOH:O	1.78	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:10:GLN:H	13:K:10:GLN:HE21	0.88	0.84
25:W:122:ARG:HH11	25:W:122:ARG:HG2	1.41	0.83
25:W:4:LEU:HD22	25:W:52:VAL:HG21	1.60	0.83
1:0:2716:G:H5''	4:B:206:THR:HG21	1.60	0.83
8:F:58:GLU:HA	8:F:61:MET:HE2	1.58	0.83
1:0:1116:U:HO2'	1:0:1118:A:H2	0.83	0.83
3:A:192:VAL:HG22	39:A:9095:HOH:O	1.77	0.83
17:O:42:GLU:HB2	39:O:2176:HOH:O	1.78	0.83
1:0:1667:A:H8	1:0:1667:A:H5'	1.41	0.83
1:0:1701:A:H4'	1:0:1702:U:H5''	1.60	0.83
1:0:1041:U:H5'	39:L:8881:HOH:O	1.77	0.82
1:0:506:G:H22	1:0:509:A:H5''	1.42	0.82
3:A:211:LYS:HB2	39:A:9081:HOH:O	1.78	0.82
24:V:12:THR:HG22	24:V:15:GLU:HG3	1.60	0.82
1:0:1474:C:H6	1:0:1474:C:H5'	1.43	0.82
1:0:541:C:C2'	1:0:542:A:H5''	2.09	0.81
11:I:97:VAL:HG12	11:I:101:LYS:HE3	1.59	0.81
16:N:113:SER:HB2	39:N:8856:HOH:O	1.78	0.81
25:W:88:THR:HG23	25:W:110:GLN:HE21	1.46	0.81
1:0:1300:G:H1'	39:O:5149:HOH:O	1.79	0.81
27:Y:187:VAL:HG23	39:Y:8869:HOH:O	1.79	0.81
11:I:73:LEU:HD12	11:I:107:LYS:HZ2	1.46	0.81
3:A:153:ARG:HH11	3:A:153:ARG:HB2	1.45	0.81
1:0:2890:A:H1'	23:U:56:ARG:NH2	1.96	0.80
1:0:1973:A:H5'	1:0:1973:A:H8	1.45	0.80
28:Z:10:ARG:HA	39:Z:8714:HOH:O	1.79	0.80
39:9:9098:HOH:O	16:N:23:ARG:HD3	1.80	0.80
1:0:2054:A:N3	20:R:128:ARG:NH2	2.30	0.80
1:0:2840:A:OP1	4:B:211:THR:HG23	1.82	0.80
13:K:81:ARG:HB2	13:K:87:ARG:NH1	1.96	0.79
12:J:74:ARG:HB3	12:J:74:ARG:HH11	1.46	0.79
6:D:54:ALA:HB2	6:D:69:ILE:HD12	1.63	0.79
1:0:656:G:H5'	17:O:3:THR:HG22	1.64	0.79
4:B:195:ARG:HG2	4:B:323:LEU:HD22	1.65	0.79
1:0:2586:U:H3	1:0:2592:G:H22	1.28	0.78
1:0:2488:A:H61	1:0:2534:C:H42	1.32	0.78
3:A:192:VAL:HB	39:A:9056:HOH:O	1.82	0.78
5:C:1:MET:HG2	5:C:2:GLN:H	1.46	0.78
5:C:242:GLU:HG3	39:C:8586:HOH:O	1.84	0.78
1:0:1116:U:O2'	1:0:1118:A:H2	1.65	0.78
8:F:91:VAL:HG12	8:F:92:GLY:N	1.98	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:1:25:LYS:HD2	30:2:49:GLU:H	1.46	0.78
14:L:133:VAL:HA	39:L:8865:HOH:O	1.84	0.78
11:I:73:LEU:HD12	11:I:107:LYS:NZ	1.97	0.78
25:W:88:THR:HG23	25:W:110:GLN:NE2	1.97	0.78
10:H:59:GLN:HE21	10:H:129:ARG:HE	1.30	0.77
3:A:51:ARG:HB2	39:A:9068:HOH:O	1.83	0.77
12:J:76:ASP:HA	39:J:5907:HOH:O	1.85	0.77
4:B:62:ARG:HA	4:B:65:MET:CE	2.15	0.77
4:B:179:LEU:O	4:B:183:GLU:HG2	1.84	0.77
4:B:190:MET:HE2	4:B:194:PHE:CD1	2.20	0.77
39:O:5298:HOH:O	12:J:47:THR:HB	1.84	0.77
24:V:42:ASN:HB3	39:V:7247:HOH:O	1.85	0.77
1:O:2506:A:O2'	1:O:2507:G:H8	1.68	0.76
1:O:1116:U:H3	1:O:1246:A:H62	1.33	0.76
7:E:100:ASP:HB2	39:E:2789:HOH:O	1.85	0.76
5:C:236:THR:CG2	5:C:239:ALA:H	1.95	0.76
1:O:1878:G:H1'	39:O:6568:HOH:O	1.85	0.76
1:O:381:G:H5''	39:O:4785:HOH:O	1.84	0.76
3:A:105:VAL:CG1	3:A:154:ALA:HB1	2.15	0.76
1:O:871:G:H8	1:O:871:G:C5'	1.99	0.76
8:F:91:VAL:HG12	8:F:92:GLY:H	1.48	0.76
2:9:14:G:H5'	2:9:14:G:H8	1.51	0.76
5:C:115:LEU:HD21	5:C:243:VAL:HG13	1.67	0.76
1:O:544:G:H2'	1:O:545:G:H5''	1.67	0.76
10:H:30:LYS:H	10:H:62:HIS:HD2	1.31	0.76
1:O:559:U:H5'	1:O:559:U:H6	1.51	0.76
10:H:59:GLN:NE2	10:H:129:ARG:HE	1.83	0.75
18:P:59:ARG:NH2	18:P:66:GLN:HE22	1.83	0.75
20:R:39:THR:HB	20:R:42:GLU:HG3	1.68	0.75
16:N:48:VAL:CG1	16:N:55:ASP:HB3	2.16	0.75
4:B:62:ARG:HA	4:B:65:MET:HE2	1.68	0.75
4:B:201:ASP:HB2	4:B:312:ARG:HD2	1.68	0.75
20:R:8:ALA:HB1	20:R:13:THR:HG21	1.67	0.75
3:A:194:MET:HE1	3:A:199:HIS:HB2	1.68	0.75
8:F:50:VAL:HG13	8:F:60:VAL:HG11	1.69	0.75
27:Y:212:ARG:HD2	39:Y:8899:HOH:O	1.86	0.75
1:O:870:G:C2'	1:O:871:G:H5''	2.17	0.74
4:B:162:MET:CE	4:B:310:ARG:HD3	2.17	0.74
1:O:1206:U:H6	1:O:1206:U:H5'	1.52	0.74
21:S:57:THR:HG22	21:S:59:ASP:N	2.01	0.74
3:A:199:HIS:CD2	3:A:201:PHE:H	2.04	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:236:A:H4'	1:0:237:G:H5'	1.69	0.74
4:B:36:PRO:HA	4:B:168:GLY:HA3	1.68	0.74
5:C:140:VAL:HB	39:C:8656:HOH:O	1.88	0.74
1:0:506:G:H22	1:0:509:A:C5'	2.01	0.74
1:0:545:G:H8	1:0:545:G:H5'	1.51	0.74
5:C:139:VAL:HG13	39:C:8653:HOH:O	1.86	0.74
2:9:56:A:C2'	2:9:57:A:H5''	2.18	0.74
3:A:36:ASP:OD2	3:A:85:SER:HB2	1.88	0.74
20:R:18:LEU:HD12	20:R:143:VAL:HG11	1.70	0.74
1:0:1183:C:H2'	39:0:6690:HOH:O	1.87	0.74
25:W:13:MET:HE3	25:W:17:ILE:HG22	1.70	0.74
4:B:16:ARG:NH1	39:B:9084:HOH:O	2.20	0.74
1:0:1372:A:H3'	39:0:7622:HOH:O	1.88	0.74
23:U:14:GLU:OE1	23:U:15:PRO:HD2	1.88	0.73
5:C:236:THR:HG21	39:C:8579:HOH:O	1.85	0.73
6:D:25:MET:HE1	6:D:41:LEU:HG	1.69	0.73
5:C:5:ILE:HD11	5:C:16:VAL:CG2	2.18	0.73
7:E:3:VAL:HG22	7:E:49:ILE:HB	1.70	0.73
3:A:48:ASP:HB3	39:A:9068:HOH:O	1.89	0.73
20:R:18:LEU:HB2	20:R:143:VAL:HG12	1.71	0.73
1:0:1819:G:H2'	1:0:1820:G:H4'	1.71	0.73
27:Y:235:GLU:H	27:Y:235:GLU:CD	1.92	0.73
1:0:93:C:H5''	24:V:1:THR:HB	1.69	0.73
39:0:6936:HOH:O	27:Y:141:THR:HG23	1.86	0.73
4:B:221:GLN:HE22	13:K:42:ASN:HD22	1.33	0.72
1:0:2908:A:H2'	1:0:2909:G:O4'	1.89	0.72
13:K:34:VAL:HG22	13:K:47:ALA:HB2	1.71	0.72
12:J:107:ASN:ND2	12:J:109:TYR:H	1.86	0.72
21:S:10:VAL:HG11	24:V:36:ALA:HA	1.72	0.72
1:0:2570:G:H5''	39:0:5371:HOH:O	1.88	0.72
1:0:2291:A:C8	1:0:2309:C:H5'	2.25	0.72
5:C:5:ILE:HD11	5:C:16:VAL:HG23	1.69	0.72
1:0:450:C:OP1	5:C:184:ARG:NH2	2.22	0.72
1:0:1119:G:H2'	12:J:52:GLN:NE2	2.04	0.72
4:B:18:ARG:HG3	4:B:256:GLN:HG3	1.72	0.72
25:W:125:HIS:HD2	25:W:127:GLY:H	1.36	0.72
8:F:63:ILE:HB	8:F:64:PRO:HD3	1.71	0.72
1:0:2896:A:H5''	39:0:6546:HOH:O	1.89	0.71
13:K:74:VAL:CG1	13:K:113:ILE:HG12	2.21	0.71
8:F:96:ALA:HA	39:F:3111:HOH:O	1.89	0.71
17:O:32:ARG:HD3	17:O:32:ARG:O	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:962:C:H1'	16:N:5:ARG:NH1	2.05	0.71
2:9:29:C:H2'	2:9:30:C:H5'	1.73	0.71
1:0:1603:A:H5'	1:0:1605:G:O4'	1.91	0.71
21:S:43:GLU:HB3	39:S:8990:HOH:O	1.90	0.71
25:W:6:GLN:HB2	25:W:26:ILE:CD1	2.21	0.71
1:0:1666:C:O2'	1:0:1667:A:H5''	1.91	0.71
3:A:223:ARG:HG3	39:A:9064:HOH:O	1.91	0.70
13:K:98:VAL:HG13	13:K:102:GLU:HA	1.73	0.70
1:0:481:U:H5''	39:0:6102:HOH:O	1.91	0.70
1:0:111:C:O2'	29:1:20:ARG:HG2	1.92	0.70
39:0:4698:HOH:O	30:2:38:LYS:HE3	1.90	0.70
13:K:14:LYS:HB2	13:K:45:PRO:HG2	1.73	0.70
1:0:877:G:H5'	1:0:878:G:OP1	1.92	0.70
4:B:275:GLY:O	4:B:291:ASP:HA	1.91	0.70
3:A:164:ARG:NE	39:A:9050:HOH:O	2.24	0.70
25:W:68:THR:HG23	25:W:69:ARG:HG2	1.74	0.70
2:9:39:U:H1'	2:9:44:A:H61	1.55	0.70
16:N:164:ASP:CG	16:N:167:ASP:HA	2.11	0.70
1:0:2364:A:H5''	19:Q:15:LYS:HD3	1.73	0.70
28:Z:11:SER:HB3	28:Z:23:ARG:HB2	1.73	0.70
4:B:264:GLU:HG2	4:B:267:LYS:HE2	1.73	0.70
1:0:542:A:H5'	1:0:542:A:C8	2.23	0.70
3:A:105:VAL:HG11	3:A:154:ALA:HB1	1.74	0.70
1:0:1184:C:H1'	39:0:7891:HOH:O	1.90	0.70
1:0:541:C:H2'	1:0:542:A:C5'	2.21	0.70
12:J:45:VAL:HG23	12:J:130:VAL:O	1.91	0.70
1:0:244:C:OP2	8:F:38:LYS:HE3	1.91	0.70
13:K:74:VAL:HG13	13:K:113:ILE:HG23	1.72	0.70
6:D:128:LEU:HB2	39:D:6007:HOH:O	1.90	0.70
22:T:71:VAL:HG11	22:T:90:PRO:CB	2.20	0.70
1:0:1244:U:OP1	12:J:18:ILE:HD13	1.91	0.70
12:J:74:ARG:CB	12:J:74:ARG:HH11	2.05	0.70
16:N:11:ARG:HG3	16:N:14:ARG:NH1	2.06	0.70
1:0:2635:A:O2'	1:0:2636:C:H5'	1.92	0.70
8:F:13:GLU:OE2	8:F:78:GLU:HG2	1.90	0.70
2:9:49:G:H5''	39:N:8845:HOH:O	1.92	0.69
4:B:238:ASN:HD22	4:B:240:GLY:N	1.90	0.69
1:0:281:U:H2'	1:0:282:C:O4'	1.91	0.69
10:H:102:LYS:HD3	10:H:122:LYS:HD3	1.74	0.69
10:H:32:ALA:HB3	10:H:69:ARG:HH12	1.55	0.69
1:0:1701:A:H5'	39:0:6730:HOH:O	1.90	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:39:THR:HG23	20:R:107:GLU:O	1.93	0.69
1:0:2748:G:H2'	39:0:7963:HOH:O	1.91	0.69
8:F:58:GLU:OE1	15:M:27:ARG:NH2	2.25	0.69
2:9:6:C:OP1	16:N:37:ARG:NH1	2.25	0.69
1:0:796:A:HO2'	28:Z:10:ARG:N	1.91	0.69
1:0:2780:C:H1'	7:E:143:GLN:HE21	1.58	0.69
1:0:1593:C:OP1	18:P:117:SER:HB3	1.93	0.69
1:0:2533:C:H5'	1:0:2533:C:H6	1.58	0.69
16:N:80:SER:HB2	39:N:8835:HOH:O	1.92	0.69
16:N:139:TRP:HA	16:N:139:TRP:CE3	2.28	0.69
27:Y:126:PRO:HG2	27:Y:128:PHE:CE1	2.28	0.69
1:0:1118:A:C8	1:0:1118:A:H3'	2.28	0.68
1:0:1118:A:H3'	1:0:1118:A:H8	1.58	0.68
1:0:2468:A:H61	31:3:48:ASN:HD21	1.40	0.68
1:0:1666:C:H2'	1:0:1667:A:H5'	1.75	0.68
14:L:148:GLU:HA	39:L:8864:HOH:O	1.93	0.68
4:B:58:PRO:HA	4:B:63:GLU:OE1	1.92	0.68
4:B:190:MET:HE2	4:B:194:PHE:HD1	1.59	0.68
3:A:88:ILE:HD13	3:A:100:PRO:HD3	1.76	0.68
6:D:135:VAL:HG21	6:D:139:TYR:CD1	2.29	0.68
6:D:146:LYS:NZ	16:N:107:ASN:HD21	1.92	0.68
8:F:2:VAL:HG22	8:F:57:GLU:OE1	1.94	0.68
10:H:6:ALA:HA	10:H:61:ARG:HH12	1.58	0.68
16:N:17:ARG:HB3	16:N:17:ARG:HH11	1.57	0.68
5:C:78:ARG:HG3	5:C:78:ARG:NH1	2.01	0.67
1:0:1119:G:N2	1:0:1246:A:C2	2.58	0.67
1:0:272:A:H3'	39:0:7953:HOH:O	1.93	0.67
25:W:21:LEU:HD22	25:W:26:ILE:CD1	2.25	0.67
24:V:12:THR:HG22	24:V:15:GLU:CG	2.24	0.67
1:0:2270:G:H4'	3:A:223:ARG:NH1	2.07	0.67
3:A:100:PRO:HG2	3:A:103:VAL:HG21	1.76	0.67
1:0:657:G:OP1	5:C:27:ARG:NH2	2.27	0.67
1:0:2081:A:H4'	12:J:69:TYR:CE1	2.30	0.67
16:N:7:LYS:HE3	19:Q:21:ARG:O	1.95	0.67
25:W:122:ARG:HH11	25:W:122:ARG:CG	2.07	0.67
1:0:1701:A:H4'	1:0:1702:U:C5'	2.25	0.67
6:D:23:VAL:HG21	6:D:45:THR:HG21	1.74	0.67
4:B:51:VAL:CG2	4:B:327:VAL:HG13	2.24	0.67
10:H:6:ALA:HA	10:H:61:ARG:NH1	2.09	0.67
27:Y:115:ARG:NE	39:Y:8853:HOH:O	2.27	0.67
27:Y:185:VAL:HG12	39:Y:8869:HOH:O	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:1:MET:HG2	5:C:2:GLN:N	2.10	0.67
5:C:115:LEU:HD13	5:C:223:LEU:HD21	1.76	0.67
15:M:164:THR:HG22	15:M:167:GLY:N	2.09	0.66
1:O:338:C:H4'	5:C:174:ILE:CD1	2.25	0.66
1:O:1679:C:H5'	39:O:9811:HOH:O	1.95	0.66
1:O:794:U:H3	1:O:819:A:H61	1.42	0.66
1:O:1667:A:C8	1:O:1667:A:H5'	2.29	0.66
25:W:13:MET:CE	25:W:17:ILE:HG22	2.24	0.66
1:O:558:C:C2'	1:O:559:U:H5''	2.26	0.66
12:J:74:ARG:NH1	12:J:76:ASP:HB2	2.11	0.66
5:C:2:GLN:HB3	39:C:8589:HOH:O	1.96	0.66
16:N:139:TRP:HA	16:N:139:TRP:HE3	1.61	0.66
4:B:320:GLN:HE21	4:B:321:PRO:HD2	1.61	0.66
1:O:1328:A:OP1	27:Y:169:ARG:HD2	1.96	0.66
4:B:212:GLN:HB2	4:B:257:THR:CG2	2.24	0.66
27:Y:144:ARG:NE	39:Y:8910:HOH:O	2.27	0.66
13:K:32:ILE:HD11	13:K:56:SER:HB3	1.76	0.66
14:L:136:ALA:HB3	39:L:8865:HOH:O	1.96	0.66
20:R:111:ILE:HG23	20:R:145:LEU:HD11	1.78	0.66
7:E:20:ILE:CD1	7:E:40:VAL:HG11	2.26	0.66
25:W:21:LEU:HD22	25:W:26:ILE:HD11	1.78	0.65
7:E:15:GLN:HG2	7:E:19:ASP:O	1.96	0.65
39:O:7208:HOH:O	16:N:4:PRO:HD2	1.95	0.65
10:H:83:GLU:HA	39:H:9037:HOH:O	1.96	0.65
25:W:88:THR:HG22	25:W:90:TYR:HD1	1.61	0.65
1:O:2851:G:O2'	1:O:2852:A:H5'	1.96	0.65
28:Z:11:SER:CB	28:Z:23:ARG:HB2	2.27	0.65
39:O:5438:HOH:O	15:M:125:ARG:HD3	1.96	0.65
13:K:118:ALA:HA	13:K:125:ALA:HB2	1.79	0.65
4:B:185:GLY:HA2	39:B:9103:HOH:O	1.96	0.65
25:W:21:LEU:HD21	25:W:48:VAL:CG1	2.27	0.65
6:D:166:ILE:HB	39:D:6326:HOH:O	1.97	0.65
15:M:107:ARG:HH11	15:M:107:ARG:HG3	1.61	0.65
1:O:1163:G:H5'	11:I:110:ASP:O	1.97	0.65
25:W:13:MET:HE1	25:W:18:GLN:HA	1.78	0.65
16:N:132:ASN:O	16:N:135:VAL:HG12	1.97	0.65
1:O:513:A:N3	39:O:4140:HOH:O	2.29	0.65
25:W:88:THR:HG22	25:W:89:ASP:H	1.59	0.65
25:W:88:THR:HG22	25:W:89:ASP:N	2.11	0.65
1:O:2505:G:O2'	1:O:2506:A:H5'	1.96	0.65
18:P:59:ARG:HH22	18:P:66:GLN:HE22	1.42	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:91:LYS:O	18:P:95:GLU:HG3	1.96	0.65
10:H:114:ASP:HB2	39:H:8996:HOH:O	1.96	0.65
5:C:236:THR:HA	39:C:8656:HOH:O	1.96	0.65
1:0:1183:C:N4	1:0:1184:C:H41	1.95	0.65
1:0:871:G:C8	1:0:871:G:C5'	2.74	0.64
1:0:282:C:O2'	1:0:283:U:H5'	1.96	0.64
16:N:38:LYS:HE2	16:N:107:ASN:ND2	2.12	0.64
25:W:80:ASP:O	25:W:84:VAL:HG23	1.97	0.64
20:R:99:ALA:HB1	20:R:109:MET:CE	2.26	0.64
1:0:797:A:C4'	28:Z:10:ARG:N	2.61	0.64
29:1:42:SER:HB2	39:1:8957:HOH:O	1.97	0.64
1:0:2004:U:H4'	39:0:5759:HOH:O	1.96	0.64
1:0:470:U:O2'	29:1:16:HIS:HD2	1.80	0.64
1:0:2783:A:H3'	39:0:5684:HOH:O	1.96	0.64
6:D:25:MET:SD	6:D:40:ILE:HD11	2.37	0.64
39:0:6115:HOH:O	22:T:68:ASP:HB2	1.98	0.64
2:9:39:U:H1'	2:9:44:A:N6	2.11	0.64
1:0:1165:G:H4'	1:0:1174:A:O2'	1.97	0.64
14:L:143:THR:HG22	14:L:144:ASP:N	2.12	0.64
1:0:1684:A:H1'	30:2:43:ARG:HH22	1.62	0.64
25:W:151:GLU:O	25:W:154:ARG:HB2	1.98	0.64
39:0:5912:HOH:O	9:G:12:ILE:HG23	1.98	0.64
1:0:2827:A:H2'	1:0:2828:G:O4'	1.98	0.64
21:S:51:GLN:HE21	21:S:53:ASN:HD21	1.44	0.64
25:W:149:LEU:HG	25:W:153:MET:HE2	1.80	0.64
26:X:72:VAL:HG22	26:X:85:VAL:HG12	1.77	0.64
15:M:99:ARG:HH21	15:M:170:ASN:HD22	1.45	0.64
26:X:9:VAL:HG13	26:X:88:GLU:OE1	1.97	0.64
16:N:49:THR:HG22	16:N:56:ASP:HB2	1.78	0.64
1:0:544:G:C2'	1:0:545:G:H5''	2.27	0.64
1:0:1189:A:H3'	39:0:8185:HOH:O	1.97	0.64
18:P:115:SER:N	18:P:118:GLN:HE21	1.88	0.64
6:D:170:TYR:O	6:D:171:ASP:HB3	1.98	0.64
9:G:20:VAL:O	9:G:24:VAL:HG23	1.98	0.64
1:0:1641:A:H2'	1:0:1642:A:H5'	1.79	0.64
3:A:33:GLU:CD	3:A:33:GLU:H	2.01	0.64
1:0:2721:U:H4'	13:K:87:ARG:HG3	1.80	0.64
4:B:264:GLU:HG2	4:B:267:LYS:CE	2.27	0.64
27:Y:144:ARG:NH1	39:Y:8875:HOH:O	2.26	0.64
4:B:305:ASP:O	4:B:306:LYS:HB2	1.98	0.64
24:V:39:ALA:C	24:V:41:GLU:H	1.99	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:81:ASP:OD1	25:W:92:ASP:HB2	1.97	0.64
13:K:109:LEU:HD13	13:K:113:ILE:HD11	1.79	0.63
30:2:22:PRO:HG2	30:2:25:VAL:HG23	1.79	0.63
11:I:100:VAL:HG11	11:I:124:VAL:HG22	1.80	0.63
1:0:396:U:H1'	39:0:8134:HOH:O	1.99	0.63
39:0:7310:HOH:O	15:M:178:LYS:HB2	1.97	0.63
28:Z:13:ARG:NH1	39:Z:8719:HOH:O	2.30	0.63
7:E:116:THR:HG22	7:E:151:LEU:HD22	1.80	0.63
27:Y:186:ARG:HG2	27:Y:186:ARG:HH11	1.64	0.63
1:0:2816:A:H2'	39:0:8430:HOH:O	1.97	0.63
3:A:153:ARG:CB	3:A:153:ARG:HH11	2.12	0.63
7:E:5:LEU:HD21	7:E:66:GLN:HG3	1.80	0.63
18:P:10:ALA:HA	18:P:13:VAL:HG12	1.79	0.63
2:9:6:C:C5'	16:N:37:ARG:NH1	2.57	0.63
2:9:14:G:H5'	2:9:14:G:C8	2.32	0.63
7:E:69:ILE:HA	7:E:72:MET:HE3	1.80	0.63
27:Y:106:THR:HG23	27:Y:107:PRO:HD2	1.80	0.63
7:E:81:GLU:HG2	7:E:134:SER:HB3	1.80	0.63
13:K:98:VAL:HG11	13:K:102:GLU:HA	1.78	0.63
1:0:1209:C:H2'	1:0:1210:G:H8	1.64	0.63
26:X:66:THR:HG23	26:X:67:PRO:HD2	1.81	0.63
12:J:75:PRO:HG2	12:J:105:LEU:HD21	1.80	0.63
23:U:17:THR:HG22	23:U:18:GLY:N	2.14	0.63
7:E:69:ILE:HA	7:E:72:MET:CE	2.29	0.63
25:W:65:VAL:HA	25:W:68:THR:HG22	1.80	0.63
1:0:2781:U:H1'	7:E:139:GLU:OE2	1.99	0.63
1:0:500:G:H21	20:R:98:ASN:HD21	1.45	0.63
25:W:84:VAL:HG12	39:W:6679:HOH:O	1.98	0.62
10:H:49:GLN:HG3	10:H:140:TYR:CE2	2.34	0.62
8:F:53:ASP:OD1	8:F:80:GLN:HB2	1.98	0.62
8:F:38:LYS:NZ	15:M:3:SER:HA	2.15	0.62
1:0:2426:G:H1'	39:0:6539:HOH:O	1.99	0.62
11:I:101:LYS:O	11:I:105:GLU:HG3	1.99	0.62
7:E:68:HIS:O	7:E:72:MET:HG3	1.99	0.62
3:A:95:PRO:HG2	3:A:98:GLU:HG2	1.81	0.62
4:B:41:PHE:HA	4:B:79:MET:HE2	1.82	0.62
3:A:179:MET:HG2	3:A:186:TRP:CB	2.30	0.62
23:U:14:GLU:O	23:U:17:THR:HB	2.00	0.62
1:0:2578:G:H5'	1:0:2578:G:H8	1.64	0.62
25:W:21:LEU:HD13	25:W:26:ILE:HD11	1.81	0.62
25:W:4:LEU:O	25:W:32:CYS:HA	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:7:ARG:HG2	4:B:7:ARG:HH11	1.65	0.62
20:R:18:LEU:HD12	20:R:143:VAL:CG1	2.30	0.62
6:D:99:ASP:HB3	6:D:103:ASN:H	1.64	0.62
24:V:64:GLY:O	24:V:65:ASP:HB2	2.00	0.62
1:0:1377:C:H6	1:0:1377:C:H5'	1.65	0.62
11:I:108:HIS:N	11:I:109:PRO:HD2	2.14	0.62
3:A:194:MET:CE	3:A:199:HIS:HB2	2.29	0.61
1:0:2533:C:C6	1:0:2533:C:H5'	2.34	0.61
3:A:190:ARG:NH2	3:A:207:GLN:OE1	2.32	0.61
24:V:39:ALA:N	24:V:40:PRO:HD2	2.16	0.61
1:0:2694:A:H4'	7:E:91:PHE:HE1	1.65	0.61
28:Z:36:ASP:HB3	28:Z:45:ASP:HB3	1.80	0.61
26:X:9:VAL:HG22	26:X:88:GLU:OE2	1.99	0.61
1:0:656:G:H5'	17:O:3:THR:CG2	2.30	0.61
1:0:558:C:H2'	1:0:559:U:C5'	2.30	0.61
1:0:2420:G:O2'	1:0:2421:G:H5'	2.00	0.61
5:C:25:PRO:HG2	39:C:8522:HOH:O	1.99	0.61
22:T:53:GLY:HA3	39:T:6384:HOH:O	2.00	0.61
1:0:1819:G:H5'	39:O:5176:HOH:O	2.01	0.61
5:C:236:THR:H	5:C:239:ALA:HB3	1.64	0.61
4:B:307:ARG:HD2	39:B:9123:HOH:O	2.00	0.61
1:0:1189:A:H1'	1:0:1209:C:C1'	2.30	0.61
6:D:91:ALA:HB1	39:D:5198:HOH:O	2.00	0.61
1:0:2414:A:H2'	1:0:2415:A:C8	2.36	0.61
1:0:1168:C:H4'	39:I:5128:HOH:O	2.00	0.61
1:0:1441:G:O2'	1:0:1442:A:H5'	2.00	0.61
1:0:2769:C:C2'	1:0:2770:G:H5'	2.31	0.61
1:0:2676:C:H4'	12:J:70:PHE:CE1	2.34	0.61
10:H:167:LYS:HE2	10:H:169:GLU:OE1	2.01	0.61
12:J:74:ARG:O	12:J:78:ILE:HG12	2.00	0.61
31:3:70:ARG:HG2	31:3:77:ALA:HB2	1.82	0.61
20:R:106:GLY:HA2	20:R:109:MET:HE3	1.82	0.61
7:E:49:ILE:HD11	7:E:69:ILE:HD12	1.83	0.61
27:Y:144:ARG:NH2	39:Y:8910:HOH:O	2.33	0.61
4:B:74:ILE:HD13	4:B:309:VAL:HG21	1.81	0.61
16:N:169:PRO:O	16:N:172:PHE:HB3	2.00	0.61
5:C:162:VAL:HG22	5:C:232:LEU:HD21	1.83	0.61
1:0:1189:A:H1'	1:0:1209:C:H1'	1.83	0.61
1:0:259:G:H21	15:M:58:GLN:NE2	1.99	0.61
1:0:1058:A:H2'	1:0:1060:C:H5''	1.82	0.61
14:L:79:ASP:HB3	39:L:8850:HOH:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:709:G:O2'	17:O:25:VAL:HG12	2.00	0.61
29:1:10:LYS:HG3	39:1:8979:HOH:O	2.00	0.61
4:B:312:ARG:HB2	39:B:9118:HOH:O	2.00	0.60
29:1:25:LYS:HD2	30:2:49:GLU:N	2.15	0.60
4:B:8:LYS:HG3	4:B:220:VAL:HG12	1.83	0.60
18:P:115:SER:H	18:P:118:GLN:NE2	1.89	0.60
1:O:2718:C:H6	1:O:2718:C:H5'	1.67	0.60
20:R:18:LEU:HB2	20:R:143:VAL:CG1	2.29	0.60
3:A:88:ILE:HG22	3:A:88:ILE:O	2.00	0.60
1:O:757:C:OP1	14:L:27:ARG:HD2	2.01	0.60
31:3:25:VAL:HG22	31:3:68:LYS:HG3	1.83	0.60
1:O:1119:G:H8	12:J:52:GLN:HE22	1.48	0.60
17:O:32:ARG:HE	17:O:35:LYS:HD2	1.65	0.60
17:O:87:THR:O	17:O:91:GLN:HG3	2.02	0.60
12:J:103:VAL:HG12	39:J:5907:HOH:O	2.01	0.60
4:B:145:HIS:HD2	4:B:146:THR:O	1.84	0.60
31:3:55:VAL:HG22	39:3:8937:HOH:O	2.01	0.60
1:O:2064:U:H5'	1:O:2652:U:H4'	1.83	0.60
4:B:102:THR:CG2	4:B:182:VAL:HG12	2.31	0.60
28:Z:37:HIS:HB2	28:Z:47:VAL:HB	1.82	0.60
22:T:7:GLN:O	22:T:11:GLN:HG3	2.02	0.60
1:O:69:A:H5'	1:O:69:A:C8	2.36	0.60
1:O:1701:A:H5''	1:O:1702:U:H3'	1.82	0.60
20:R:39:THR:HG22	20:R:42:GLU:H	1.65	0.60
1:O:90:A:H2'	1:O:91:G:O4'	2.02	0.60
8:F:37:THR:O	8:F:41:GLU:HG3	2.02	0.60
16:N:12:ARG:HD3	16:N:18:THR:OG1	2.01	0.60
6:D:25:MET:HE3	6:D:37:ALA:CB	2.23	0.60
25:W:141:HIS:HB2	25:W:146:ILE:HG12	1.82	0.60
14:L:145:LEU:O	14:L:148:GLU:HG3	2.02	0.60
13:K:62:PRO:HG3	13:K:65:ARG:HH21	1.67	0.60
39:O:3045:HOH:O	25:W:119:HIS:HE1	1.84	0.60
15:M:60:VAL:C	15:M:61:ILE:HD12	2.22	0.60
1:O:2005:G:H3'	1:O:2005:G:OP2	2.02	0.60
4:B:254:GLN:HG2	4:B:255:GLY:N	2.16	0.60
31:3:17:HIS:O	31:3:18:GLN:HG3	2.02	0.60
3:A:36:ASP:O	3:A:38:ILE:N	2.27	0.59
1:O:2507:G:H2'	1:O:2510:C:H42	1.66	0.59
1:O:2768:A:H2'	1:O:2769:C:O4'	2.02	0.59
4:B:41:PHE:CD1	4:B:79:MET:HE2	2.36	0.59
25:W:72:PRO:HG2	25:W:77:ALA:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:122:ARG:NH2	39:Y:8834:HOH:O	2.35	0.59
22:T:9:LYS:CE	22:T:13:ARG:NH1	2.62	0.59
11:I:105:GLU:HA	11:I:108:HIS:NE2	2.18	0.59
24:V:38:GLY:C	24:V:40:PRO:HD2	2.22	0.59
2:9:44:A:O4'	6:D:76:ARG:NE	2.35	0.59
1:0:2866:U:C4	23:U:50:GLU:HB3	2.37	0.59
26:X:74:ALA:HB2	26:X:85:VAL:HG13	1.83	0.59
16:N:37:ARG:NE	39:N:8832:HOH:O	2.35	0.59
4:B:51:VAL:HG23	4:B:329:TYR:O	2.00	0.59
1:0:121:U:OP2	30:2:10:ARG:NH2	2.31	0.59
6:D:65:GLU:HA	39:D:6752:HOH:O	2.03	0.59
11:I:129:SER:O	11:I:130:LEU:HD23	2.02	0.59
1:0:474:C:O3'	5:C:73:LEU:HD21	2.02	0.59
14:L:80:ASP:HB2	14:L:90:ARG:O	2.03	0.59
21:S:73:ASP:OD1	21:S:76:GLU:HG3	2.02	0.59
8:F:91:VAL:CG1	8:F:92:GLY:H	2.15	0.59
20:R:39:THR:HB	20:R:42:GLU:CG	2.32	0.59
6:D:159:PRO:O	6:D:163:VAL:HG23	2.02	0.59
15:M:34:GLU:HB3	15:M:38:GLU:HG3	1.84	0.59
3:A:191:GLY:HA2	3:A:194:MET:CE	2.33	0.59
15:M:24:GLN:NE2	15:M:27:ARG:HH11	2.01	0.59
1:0:1474:C:C6	1:0:1474:C:H5'	2.32	0.59
1:0:558:C:O2'	1:0:559:U:H5''	2.02	0.59
4:B:312:ARG:HD3	4:B:315:VAL:HG13	1.84	0.59
31:3:62:THR:HB	39:3:8977:HOH:O	2.01	0.59
6:D:136:ARG:HB2	39:D:7597:HOH:O	2.03	0.59
1:0:316:A:H5'	22:T:54:ASP:OD2	2.03	0.59
18:P:80:ARG:HG2	18:P:87:ARG:CZ	2.32	0.59
31:3:6:ARG:NH1	31:3:21:GLU:HG3	2.17	0.59
24:V:39:ALA:N	24:V:40:PRO:CD	2.66	0.59
4:B:102:THR:HG23	4:B:182:VAL:HG12	1.84	0.59
13:K:81:ARG:HD3	13:K:87:ARG:NH1	2.17	0.59
25:W:22:GLU:HG2	25:W:27:HIS:CD2	2.37	0.59
26:X:43:VAL:HG22	26:X:76:ARG:NH1	2.18	0.59
1:0:1080:C:H4'	1:0:1081:A:OP1	2.02	0.58
17:O:39:THR:O	17:O:115:ARG:NH2	2.36	0.58
9:G:23:ILE:O	9:G:27:ILE:HG13	2.03	0.58
1:0:2717:C:H2'	1:0:2718:C:C5'	2.30	0.58
3:A:191:GLY:HA2	3:A:194:MET:HE2	1.85	0.58
11:I:70:THR:OG1	11:I:107:LYS:HE2	2.03	0.58
12:J:131:THR:HG22	12:J:133:GLY:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:114:G:O6	16:N:11:ARG:HD3	2.03	0.58
15:M:107:ARG:NH1	39:M:8876:HOH:O	2.35	0.58
7:E:11:VAL:HG12	7:E:12:ASP:N	2.18	0.58
1:0:1119:G:H2'	12:J:52:GLN:HE22	1.66	0.58
2:9:13:A:O2'	2:9:14:G:H5''	2.03	0.58
39:0:5912:HOH:O	9:G:12:ILE:HA	2.02	0.58
5:C:98:ARG:NH1	39:C:8561:HOH:O	2.34	0.58
1:0:603:A:H5''	1:0:604:G:OP1	2.02	0.58
7:E:166:VAL:HG12	39:E:3134:HOH:O	2.02	0.58
5:C:27:ARG:HG3	5:C:29:ASP:OD1	2.02	0.58
3:A:131:HIS:O	3:A:132:ASP:HB2	2.02	0.58
1:0:164:G:H4'	14:L:30:ARG:HD3	1.86	0.58
25:W:108:ARG:HE	25:W:114:PRO:HG3	1.69	0.58
1:0:1528:A:H2'	1:0:1529:G:O4'	2.02	0.58
6:D:54:ALA:CB	6:D:69:ILE:HD12	2.32	0.58
12:J:47:THR:HG22	12:J:48:GLY:N	2.19	0.58
26:X:25:ARG:HD3	26:X:64:ALA:O	2.04	0.58
24:V:12:THR:HG23	24:V:14:ALA:H	1.68	0.58
1:0:1166:A:H61	1:0:1180:U:H3	1.51	0.58
17:O:47:ARG:HG3	17:O:47:ARG:HH11	1.68	0.58
1:0:1118:A:H62	1:0:1244:U:H3	1.52	0.58
8:F:91:VAL:CG1	8:F:92:GLY:N	2.67	0.58
8:F:50:VAL:CG1	8:F:60:VAL:HG11	2.33	0.58
25:W:125:HIS:CD2	25:W:127:GLY:H	2.20	0.58
3:A:164:ARG:CZ	39:A:9050:HOH:O	2.51	0.58
1:0:2779:G:H21	7:E:143:GLN:NE2	2.02	0.58
6:D:50:VAL:O	6:D:71:ALA:HA	2.04	0.58
14:L:72:ASN:HB2	39:L:8872:HOH:O	2.03	0.58
3:A:55:VAL:HG22	3:A:68:ILE:O	2.04	0.58
6:D:23:VAL:HG21	6:D:45:THR:CG2	2.33	0.58
1:0:125:U:H2'	39:0:4245:HOH:O	2.03	0.58
1:0:1730:G:H5'	1:0:1731:C:C5	2.38	0.58
12:J:75:PRO:HG2	12:J:105:LEU:CD2	2.34	0.58
1:0:2717:C:O2'	1:0:2718:C:H5''	2.02	0.58
1:0:558:C:H2'	1:0:559:U:H5''	1.85	0.58
1:0:396:U:O2'	1:0:418:C:H4'	2.04	0.58
7:E:35:TYR:HA	12:J:127:ILE:HD12	1.86	0.58
25:W:130:HIS:O	25:W:136:GLY:HA3	2.04	0.58
6:D:154:LYS:H	6:D:154:LYS:CD	2.06	0.57
15:M:134:ILE:HG23	15:M:141:ILE:HD13	1.86	0.57
6:D:95:THR:OG1	6:D:174:VAL:HG22	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:141:ARG:HD2	4:B:163:GLU:OE2	2.04	0.57
1:0:621:C:H5'	27:Y:132:ASP:OD2	2.04	0.57
1:0:299:U:H5'	39:0:7766:HOH:O	2.03	0.57
23:U:11:THR:HG22	23:U:53:ASP:OD2	2.04	0.57
39:0:7854:HOH:O	22:T:9:LYS:HB2	2.03	0.57
16:N:164:ASP:OD1	16:N:167:ASP:HA	2.03	0.57
25:W:38:THR:HG22	25:W:39:ASP:N	2.20	0.57
39:9:9062:HOH:O	16:N:41:LYS:HD3	2.05	0.57
14:L:133:VAL:HB	39:L:8849:HOH:O	2.03	0.57
1:0:119:A:H2'	1:0:120:A:H5''	1.87	0.57
1:0:1766:U:O2	1:0:1778:A:H5'	2.04	0.57
1:0:2346:C:O2'	6:D:52:THR:HG21	2.04	0.57
1:0:1634:G:H3'	39:0:4370:HOH:O	2.04	0.57
16:N:11:ARG:NH2	39:N:8817:HOH:O	2.38	0.57
2:9:20:G:O2'	2:9:21:G:H5'	2.04	0.57
8:F:31:LYS:HE3	39:F:2623:HOH:O	2.04	0.57
1:0:1615:A:H5'	39:0:4655:HOH:O	2.03	0.57
1:0:588:G:O6	25:W:154:ARG:NH1	2.37	0.57
5:C:107:ARG:NH1	39:C:8637:HOH:O	2.37	0.57
2:9:92:G:H2'	2:9:93:A:C8	2.40	0.57
2:9:39:U:HO2'	2:9:42:C:H5	1.52	0.57
1:0:1175:G:H1'	1:0:1193:A:H2'	1.86	0.57
11:I:124:VAL:O	11:I:124:VAL:HG12	2.05	0.57
39:0:7881:HOH:O	4:B:211:THR:HG21	2.04	0.57
14:L:148:GLU:HB2	39:L:8877:HOH:O	2.03	0.57
1:0:2320:U:H4'	1:0:2321:A:O4'	2.05	0.57
6:D:58:VAL:CG1	6:D:60:GLU:HG2	2.33	0.57
5:C:233:THR:HG22	5:C:234:VAL:N	2.18	0.57
31:3:60:LYS:HG3	31:3:61:PRO:HD2	1.85	0.57
26:X:80:GLU:HB3	39:X:5564:HOH:O	2.04	0.57
26:X:76:ARG:HH11	26:X:76:ARG:HG3	1.70	0.57
3:A:33:GLU:O	3:A:34:ASP:HB2	2.04	0.57
10:H:48:VAL:HA	10:H:170:ARG:O	2.04	0.57
1:0:1205:U:H2'	1:0:1206:U:C5'	2.34	0.57
8:F:101:ALA:HA	39:F:5413:HOH:O	2.04	0.57
1:0:280:C:H2'	1:0:281:U:O4'	2.05	0.57
4:B:214:PRO:HD2	39:B:8990:HOH:O	2.05	0.57
12:J:19:MET:CE	12:J:132:LEU:HD11	2.35	0.56
4:B:307:ARG:NH1	4:B:307:ARG:HG3	2.11	0.56
27:Y:189:ASN:HD22	27:Y:189:ASN:C	2.07	0.56
6:D:135:VAL:HG22	6:D:136:ARG:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:254:GLN:HG3	39:B:9000:HOH:O	2.05	0.56
1:O:1164:U:OP1	11:I:69:PRO:HA	2.05	0.56
1:O:263:U:O4'	8:F:59:ILE:HD13	2.05	0.56
1:O:681:G:N3	1:O:681:G:H5'	2.20	0.56
39:C:8563:HOH:O	17:O:3:THR:HG21	2.05	0.56
1:O:545:G:C8	1:O:545:G:H5'	2.37	0.56
20:R:29:LYS:HD3	39:R:8944:HOH:O	2.05	0.56
1:O:949:U:O2'	19:Q:40:HIS:HE1	1.89	0.56
10:H:23:ILE:HG23	10:H:123:ILE:HD11	1.88	0.56
4:B:125:GLU:O	4:B:129:ARG:HG3	2.05	0.56
5:C:246:ARG:NH1	39:C:8575:HOH:O	2.38	0.56
4:B:62:ARG:HA	4:B:65:MET:HE3	1.88	0.56
2:9:91:C:H2'	2:9:92:G:O4'	2.05	0.56
29:1:28:HIS:CE1	29:1:31:LYS:HE2	2.40	0.56
26:X:15:ARG:HB3	26:X:15:ARG:HH11	1.71	0.56
1:O:1299:G:O6	14:L:6:ARG:HD3	2.05	0.56
12:J:107:ASN:HD21	12:J:109:TYR:HB2	1.71	0.56
9:G:12:ILE:N	9:G:13:PRO:HD3	2.21	0.56
29:1:8:GLN:HE22	29:1:11:LYS:NZ	2.04	0.56
1:O:272:A:H5'	1:O:273:G:OP2	2.06	0.56
11:I:113:SER:HB2	11:I:118:ASN:HB2	1.88	0.56
10:H:30:LYS:N	10:H:62:HIS:HD2	2.00	0.56
1:O:1786:C:OP1	18:P:74:GLN:HG2	2.05	0.56
1:O:2820:A:OP1	4:B:98:THR:HG22	2.06	0.56
1:O:1086:A:C6	25:W:11:VAL:HG11	2.40	0.56
4:B:85:ARG:NH1	39:B:9104:HOH:O	2.38	0.56
17:O:38:ARG:NH1	39:O:7674:HOH:O	2.37	0.56
26:X:30:MET:HE1	26:X:58:ALA:HB3	1.87	0.56
22:T:71:VAL:HG12	22:T:72:ILE:N	2.21	0.56
1:O:797:A:H4'	28:Z:10:ARG:N	2.21	0.56
16:N:61:ALA:HB3	16:N:88:ALA:HB2	1.87	0.56
5:C:132:ASP:HB3	39:C:8567:HOH:O	2.06	0.56
16:N:86:LEU:HD21	16:N:180:LEU:CD1	2.36	0.56
14:L:73:VAL:HG23	14:L:74:THR:H	1.70	0.56
25:W:88:THR:HG23	25:W:110:GLN:HB3	1.88	0.56
3:A:153:ARG:NH1	3:A:153:ARG:HB2	2.17	0.56
16:N:17:ARG:NH1	16:N:17:ARG:HB3	2.21	0.56
20:R:111:ILE:HG23	20:R:145:LEU:CD1	2.36	0.56
22:T:28:SER:O	22:T:32:ARG:HG3	2.06	0.56
25:W:21:LEU:HB3	25:W:26:ILE:HG12	1.87	0.55
1:O:1835:U:C5	1:O:1840:A:N7	2.65	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:192:VAL:CG1	3:A:207:GLN:HB3	2.37	0.55
12:J:107:ASN:C	12:J:107:ASN:HD22	2.09	0.55
27:Y:144:ARG:CZ	39:Y:8910:HOH:O	2.54	0.55
30:2:22:PRO:HG2	30:2:25:VAL:CG2	2.35	0.55
17:O:73:ASP:HA	17:O:92:VAL:O	2.06	0.55
4:B:280:VAL:HG13	4:B:333:GLU:O	2.05	0.55
1:0:960:G:H2'	1:0:960:G:N3	2.22	0.55
3:A:192:VAL:HG12	3:A:207:GLN:HB3	1.86	0.55
1:0:1234:U:N3	4:B:244:PRO:HB3	2.21	0.55
8:F:99:THR:HA	39:F:3461:HOH:O	2.05	0.55
4:B:217:ARG:HG3	4:B:257:THR:HG22	1.87	0.55
27:Y:189:ASN:HA	27:Y:217:ILE:HD11	1.87	0.55
16:N:58:LEU:N	16:N:58:LEU:HD12	2.20	0.55
1:0:1182:C:H1'	1:0:1192:A:H8	1.72	0.55
1:0:1120:U:H5''	1:0:1120:U:C6	2.41	0.55
1:0:417:G:P	39:0:7848:HOH:O	2.64	0.55
1:0:20:G:H21	20:R:117:HIS:HD2	1.53	0.55
29:1:25:LYS:CD	30:2:49:GLU:H	2.18	0.55
12:J:45:VAL:HG21	12:J:129:PHE:CD1	2.41	0.55
1:0:2346:C:O5'	1:0:2346:C:H6	1.89	0.55
1:0:1363:G:OP1	5:C:76:ARG:NH2	2.39	0.55
1:0:380:A:OP2	15:M:9:ARG:HD2	2.07	0.55
2:9:2:U:OP2	2:9:3:A:H5'	2.07	0.55
1:0:447:A:P	22:T:1:SER:HB2	2.45	0.55
16:N:147:ILE:HD12	39:N:8845:HOH:O	2.06	0.55
39:0:4235:HOH:O	22:T:9:LYS:HD3	2.06	0.55
11:I:97:VAL:O	11:I:101:LYS:HG3	2.06	0.55
12:J:107:ASN:HD22	12:J:109:TYR:H	1.53	0.55
2:9:28:U:H5''	16:N:40:ASN:ND2	2.22	0.55
27:Y:151:SER:HB3	27:Y:154:ARG:HB3	1.89	0.55
27:Y:155:ARG:NH1	39:Y:8855:HOH:O	2.39	0.55
1:0:1972:U:H2'	1:0:1973:A:H5''	1.88	0.55
1:0:1973:A:H5'	1:0:1973:A:C8	2.33	0.55
3:A:69:LEU:HD23	3:A:107:ASN:HB2	1.87	0.55
26:X:25:ARG:HG2	39:X:5356:HOH:O	2.07	0.55
39:0:9846:HOH:O	29:1:1:THR:HA	2.06	0.55
6:D:154:LYS:HD2	6:D:154:LYS:N	2.08	0.55
25:W:139:GLY:O	25:W:141:HIS:HD2	1.88	0.55
1:0:319:A:H4'	1:0:338:C:C4	2.42	0.55
1:0:1384:C:H5'	26:X:30:MET:HG2	1.87	0.55
1:0:645:U:OP2	14:L:4:LYS:HE2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:O:5193:HOH:O	16:N:21:HIS:HD2	1.90	0.55
13:K:82:ARG:NH2	13:K:115:ARG:HG2	2.22	0.55
11:I:120:ALA:O	11:I:124:VAL:HG23	2.06	0.55
1:O:1116:U:O2'	1:O:1118:A:C2	2.47	0.55
1:O:447:A:OP2	22:T:1:SER:HB2	2.07	0.55
22:T:26:THR:HA	22:T:39:ASN:HB3	1.88	0.55
1:O:2694:A:H4'	7:E:91:PHE:CE1	2.42	0.55
1:O:316:A:N3	1:O:336:G:O2'	2.40	0.55
12:J:93:ARG:HH11	12:J:93:ARG:HB3	1.72	0.55
1:O:93:C:H5''	24:V:1:THR:CB	2.37	0.55
30:2:48:ASP:O	30:2:49:GLU:HB2	2.07	0.55
24:V:42:ASN:O	24:V:44:GLY:N	2.40	0.55
10:H:69:ARG:HD3	39:H:9031:HOH:O	2.07	0.55
2:9:33:U:H2'	39:9:9068:HOH:O	2.07	0.55
4:B:154:VAL:HG12	4:B:156:LYS:HG2	1.89	0.55
2:9:51:A:H5'	16:N:160:SER:HB3	1.88	0.55
6:D:88:LEU:HB2	6:D:89:PRO:HD3	1.88	0.55
5:C:115:LEU:O	5:C:118:THR:HB	2.06	0.54
16:N:49:THR:CG2	16:N:56:ASP:HB2	2.37	0.54
4:B:79:MET:HE1	39:B:9094:HOH:O	2.06	0.54
1:O:475:G:H5'	5:C:73:LEU:HD23	1.88	0.54
2:9:23:U:O2'	2:9:24:U:H4'	2.07	0.54
27:Y:133:HIS:HD2	39:Y:8880:HOH:O	1.90	0.54
1:O:2036:C:O4'	13:K:44:LEU:HG	2.07	0.54
25:W:54:PHE:CZ	25:W:140:LYS:HB2	2.42	0.54
5:C:16:VAL:HG12	5:C:17:ASP:H	1.71	0.54
1:O:69:A:H5'	1:O:69:A:H8	1.72	0.54
2:9:41:C:O4'	6:D:50:VAL:HG22	2.06	0.54
39:O:7121:HOH:O	22:T:38:ARG:NH1	2.39	0.54
24:V:55:ARG:O	24:V:59:ILE:HG12	2.08	0.54
15:M:99:ARG:HD2	15:M:167:GLY:HA2	1.88	0.54
1:O:1201:C:H2'	1:O:1202:A:H5'	1.88	0.54
1:O:2676:C:H4'	12:J:70:PHE:HE1	1.72	0.54
16:N:183:ASP:O	16:N:184:ILE:O	2.25	0.54
20:R:132:ARG:CZ	39:R:8991:HOH:O	2.55	0.54
7:E:36:PRO:HD3	12:J:127:ILE:HD12	1.89	0.54
26:X:31:ILE:O	26:X:35:GLU:HG3	2.08	0.54
5:C:214:THR:HG23	39:C:8643:HOH:O	2.07	0.54
1:O:1677:U:OP2	30:2:8:LYS:NZ	2.40	0.54
1:O:1278:A:H4'	1:O:1279:U:C4	2.43	0.54
4:B:66:GLU:OE1	4:B:328:ARG:HD2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1205:U:H2'	1:0:1206:U:H5''	1.89	0.54
18:P:103:THR:O	18:P:107:GLU:HG3	2.07	0.54
6:D:22:VAL:HG22	6:D:74:THR:HG22	1.88	0.54
5:C:79:ARG:O	5:C:87:ARG:HG2	2.08	0.54
7:E:31:ARG:NH1	39:E:5919:HOH:O	2.40	0.54
3:A:94:LEU:N	3:A:94:LEU:HD23	2.23	0.54
5:C:129:HIS:HD2	5:C:165:ASP:OD2	1.90	0.54
1:0:1625:U:H4'	39:0:5132:HOH:O	2.07	0.54
13:K:55:VAL:HG12	13:K:56:SER:N	2.22	0.54
1:0:2769:C:H2'	1:0:2770:G:H5'	1.89	0.54
25:W:108:ARG:HE	25:W:114:PRO:CG	2.20	0.54
19:Q:25:PRO:HB2	39:Q:4350:HOH:O	2.06	0.54
10:H:79:GLU:O	10:H:80:LEU:HD23	2.08	0.54
1:0:2894:C:O2'	1:0:2895:C:H5'	2.08	0.54
27:Y:178:HIS:CG	27:Y:179:PRO:HD2	2.43	0.54
1:0:1189:A:H1'	1:0:1209:C:O4'	2.08	0.54
7:E:7:ILE:HD11	7:E:11:VAL:C	2.29	0.54
26:X:25:ARG:HD2	39:X:3861:HOH:O	2.07	0.54
5:C:104:ASP:HA	5:C:107:ARG:HH12	1.71	0.54
1:0:1853:C:OP1	3:A:231:LYS:HG3	2.08	0.54
4:B:56:ASP:OD1	4:B:322:ARG:HB3	2.08	0.54
3:A:179:MET:HA	3:A:179:MET:CE	2.38	0.54
6:D:58:VAL:HG12	6:D:60:GLU:HG2	1.89	0.54
8:F:14:ASP:O	8:F:18:GLU:HG3	2.08	0.54
1:0:2862:G:H4'	4:B:336:GLN:O	2.07	0.54
13:K:66:ARG:HD3	39:K:2777:HOH:O	2.07	0.54
15:M:80:GLY:O	15:M:81:ARG:HD3	2.08	0.54
5:C:2:GLN:HB3	39:C:8535:HOH:O	2.08	0.53
4:B:329:TYR:CE2	23:U:15:PRO:HG2	2.43	0.53
6:D:23:VAL:HG22	6:D:73:VAL:HB	1.89	0.53
1:0:338:C:H4'	5:C:174:ILE:HD11	1.89	0.53
15:M:107:ARG:NH1	15:M:107:ARG:HG3	2.22	0.53
39:0:3028:HOH:O	18:P:81:LYS:HG2	2.07	0.53
1:0:902:G:N7	14:L:18:HIS:HD2	2.06	0.53
1:0:2878:U:H2'	1:0:2879:A:O4'	2.08	0.53
2:9:29:C:C2'	2:9:30:C:H5'	2.38	0.53
6:D:163:VAL:HA	39:D:6326:HOH:O	2.06	0.53
6:D:134:LEU:HD11	6:D:166:ILE:HD11	1.89	0.53
13:K:62:PRO:HG3	13:K:65:ARG:NH2	2.23	0.53
1:0:485:A:N3	1:0:487:G:H5''	2.23	0.53
1:0:200:C:H2'	39:0:3929:HOH:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1314:U:H2'	39:0:6326:HOH:O	2.07	0.53
29:1:21:ARG:HD2	29:1:37:CYS:SG	2.48	0.53
3:A:121:ALA:O	3:A:124:VAL:HG22	2.07	0.53
11:I:94:ASP:OD1	11:I:133:THR:HB	2.09	0.53
25:W:149:LEU:HG	25:W:153:MET:CE	2.38	0.53
16:N:62:HIS:HB3	16:N:65:ASP:OD1	2.09	0.53
1:0:538:C:OP2	27:Y:134:HIS:HE1	1.91	0.53
7:E:126:ILE:HB	7:E:131:LEU:CD2	2.38	0.53
16:N:43:VAL:HG13	16:N:118:ILE:HD11	1.91	0.53
1:0:2670:G:O2'	1:0:2671:U:H5'	2.08	0.53
4:B:82:VAL:HG12	4:B:82:VAL:O	2.07	0.53
24:V:1:THR:HG23	24:V:2:VAL:N	2.19	0.53
13:K:34:VAL:CG2	13:K:47:ALA:HB2	2.38	0.53
1:0:1268:C:O2'	27:Y:169:ARG:HB2	2.08	0.53
3:A:101:GLU:OE2	3:A:131:HIS:HB2	2.07	0.53
39:0:7836:HOH:O	22:T:2:LYS:HE2	2.07	0.53
30:2:23:ALA:HB3	39:2:6863:HOH:O	2.08	0.53
1:0:1594:C:OP2	18:P:120:ARG:HD2	2.08	0.53
16:N:154:LEU:O	16:N:155:GLU:HB3	2.08	0.53
26:X:8:ARG:NH1	39:X:2479:HOH:O	2.40	0.53
1:0:10:U:O4	1:0:532:A:OP2	2.26	0.53
30:2:41:HIS:HD2	30:2:44:ARG:H	1.56	0.53
1:0:905:C:OP1	27:Y:144:ARG:NH1	2.42	0.53
30:2:39:ARG:HG2	39:2:3143:HOH:O	2.09	0.53
22:T:69:LYS:O	22:T:71:VAL:HG23	2.08	0.53
6:D:65:GLU:HG3	39:D:6752:HOH:O	2.07	0.53
3:A:66:ARG:HH11	3:A:66:ARG:HB2	1.74	0.53
1:0:2243:C:H5''	39:0:4230:HOH:O	2.09	0.53
1:0:536:A:H3'	39:0:5504:HOH:O	2.09	0.53
16:N:48:VAL:HG11	16:N:55:ASP:HB3	1.90	0.53
2:9:69:U:OP1	16:N:4:PRO:HG3	2.09	0.53
23:U:52:THR:HG22	23:U:54:THR:N	2.23	0.53
1:0:156:C:H5''	15:M:171:ARG:CD	2.29	0.53
1:0:1972:U:C2'	1:0:1973:A:H5''	2.39	0.53
4:B:321:PRO:HA	39:B:9127:HOH:O	2.09	0.53
1:0:1187:U:O2'	1:0:1189:A:H2	1.92	0.53
3:A:94:LEU:HG	3:A:99:ILE:HD11	1.91	0.53
6:D:24:HIS:HB2	6:D:72:LYS:CB	2.39	0.53
8:F:38:LYS:HZ3	15:M:3:SER:HA	1.74	0.53
27:Y:112:GLU:OE2	27:Y:115:ARG:NH1	2.42	0.53
1:0:1201:C:H5''	39:0:6679:HOH:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2419:U:H5'	1:0:2420:G:H5'	1.90	0.53
26:X:43:VAL:HG12	26:X:44:ASP:N	2.24	0.53
5:C:107:ARG:NE	39:C:8661:HOH:O	2.20	0.53
10:H:165:ARG:HD2	39:H:9034:HOH:O	2.08	0.53
1:0:2812:A:C2	1:0:2814:A:N6	2.68	0.52
14:L:134:GLU:HG3	39:L:8849:HOH:O	2.08	0.52
2:9:14:G:O2'	16:N:1:ALA:HB2	2.08	0.52
5:C:118:THR:O	5:C:136:VAL:HG13	2.08	0.52
1:0:2817:G:P	39:0:8430:HOH:O	2.67	0.52
17:O:25:VAL:HG23	17:O:26:TRP:N	2.23	0.52
1:0:820:G:O2'	1:0:856:G:H4'	2.09	0.52
12:J:80:LYS:HE3	12:J:101:VAL:O	2.08	0.52
16:N:32:PRO:HD2	16:N:99:GLU:O	2.09	0.52
1:0:2712:G:H5'	39:K:4183:HOH:O	2.09	0.52
25:W:64:THR:O	25:W:68:THR:HG22	2.09	0.52
26:X:18:ARG:NH1	39:X:4132:HOH:O	2.40	0.52
1:0:2044:G:OP1	26:X:23:HIS:HE1	1.92	0.52
21:S:81:ILE:HG23	39:S:8984:HOH:O	2.10	0.52
1:0:1162:G:H1'	11:I:112:LEU:HD11	1.91	0.52
4:B:265:LEU:HD21	4:B:316:ARG:HD3	1.91	0.52
1:0:870:G:OP2	3:A:3:ARG:HD3	2.09	0.52
1:0:1119:G:H22	1:0:1246:A:H2	1.51	0.52
5:C:162:VAL:CG2	5:C:232:LEU:HD21	2.40	0.52
17:O:96:VAL:HG13	17:O:100:GLN:HB2	1.90	0.52
11:I:96:SER:H	11:I:99:GLN:NE2	2.07	0.52
7:E:154:ILE:HG13	7:E:156:ASP:OD1	2.10	0.52
11:I:87:PRO:C	11:I:89:GLU:H	2.12	0.52
1:0:1120:U:H5'	1:0:1121:G:OP2	2.08	0.52
21:S:77:VAL:O	21:S:80:ARG:HG2	2.09	0.52
14:L:101:ASP:C	14:L:103:ALA:H	2.13	0.52
1:0:711:G:H1'	39:0:7530:HOH:O	2.09	0.52
1:0:2491:G:H1'	39:0:7304:HOH:O	2.09	0.52
1:0:1972:U:H2'	1:0:1973:A:C5'	2.39	0.52
3:A:53:ALA:HB3	39:A:9068:HOH:O	2.10	0.52
17:O:32:ARG:HH21	17:O:35:LYS:NZ	2.07	0.52
15:M:134:ILE:CG2	15:M:141:ILE:HD13	2.39	0.52
27:Y:154:ARG:NH1	27:Y:155:ARG:HG3	2.24	0.52
1:0:564:G:H1'	39:0:6756:HOH:O	2.08	0.52
26:X:34:ARG:NH1	26:X:48:VAL:O	2.36	0.52
31:3:3:MET:HG3	31:3:4:PRO:HD2	1.92	0.52
1:0:1666:C:H2'	1:0:1667:A:C5'	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:108:HIS:N	11:I:109:PRO:CD	2.72	0.52
23:U:17:THR:CG2	23:U:18:GLY:N	2.73	0.52
24:V:56:ILE:O	24:V:60:GLN:HG3	2.10	0.52
7:E:84:MET:HB2	7:E:131:LEU:HB2	1.91	0.52
16:N:78:MET:HB2	16:N:79:PRO:HD3	1.90	0.52
39:O:6731:HOH:O	27:Y:158:LYS:HD3	2.10	0.52
14:L:67:ARG:O	14:L:71:GLU:HG3	2.10	0.52
30:2:41:HIS:H	30:2:45:ASN:ND2	1.95	0.52
1:0:31:C:H4'	39:O:7854:HOH:O	2.10	0.52
1:0:1119:G:H8	12:J:52:GLN:NE2	2.08	0.52
17:O:26:TRP:N	39:O:3062:HOH:O	2.42	0.52
1:0:1730:G:C5'	1:0:1731:C:C6	2.93	0.52
22:T:24:ARG:HH21	22:T:39:ASN:HD22	1.56	0.52
13:K:29:LEU:HB3	13:K:55:VAL:CG1	2.35	0.52
11:I:133:THR:HG22	11:I:134:ILE:N	2.24	0.52
6:D:135:VAL:HG22	6:D:136:ARG:N	2.25	0.52
8:F:27:GLY:HA3	8:F:101:ALA:O	2.10	0.52
1:0:949:U:H4'	19:Q:95:GLU:HA	1.90	0.52
3:A:81:GLN:HB2	3:A:92:ASN:ND2	2.24	0.52
4:B:314:ALA:HB3	4:B:317:PRO:HG3	1.92	0.52
1:0:449:A:N7	5:C:43:LYS:HG2	2.25	0.52
7:E:15:GLN:NE2	7:E:40:VAL:O	2.43	0.52
13:K:20:CYS:HB2	13:K:29:LEU:HG	1.92	0.52
25:W:122:ARG:CG	25:W:122:ARG:NH1	2.71	0.52
1:0:1700:C:H5''	1:0:1701:A:OP2	2.09	0.52
10:H:62:HIS:HA	10:H:65:LEU:HD23	1.92	0.52
5:C:27:ARG:HG2	5:C:30:LEU:HD12	1.91	0.52
25:W:5:VAL:HG11	25:W:153:MET:HE3	1.92	0.52
16:N:49:THR:CG2	16:N:58:LEU:HD11	2.40	0.52
5:C:129:HIS:CE1	5:C:231:ARG:HA	2.45	0.52
1:0:407:A:H5'	39:O:6477:HOH:O	2.10	0.52
3:A:37:VAL:HG13	39:A:9072:HOH:O	2.10	0.52
9:G:64:ASN:HD22	9:G:64:ASN:N	2.08	0.52
27:Y:187:VAL:HB	27:Y:203:VAL:HG22	1.92	0.51
1:0:1730:G:H5''	1:0:1731:C:H6	1.74	0.51
3:A:232:ARG:NH2	3:A:236:GLY:O	2.34	0.51
10:H:174:LEU:HA	39:H:9021:HOH:O	2.10	0.51
12:J:75:PRO:HD3	12:J:136:SER:OG	2.09	0.51
39:O:6168:HOH:O	13:K:87:ARG:CZ	2.57	0.51
16:N:110:THR:HB	16:N:113:SER:OG	2.11	0.51
23:U:9:CYS:HA	23:U:52:THR:HG23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:14:LEU:CD2	17:O:102:ILE:HD11	2.41	0.51
20:R:106:GLY:HA2	20:R:109:MET:CE	2.41	0.51
1:O:653:U:H2'	1:O:654:A:C8	2.44	0.51
1:O:2643:G:H5''	39:O:4401:HOH:O	2.09	0.51
12:J:74:ARG:HH12	12:J:76:ASP:HB2	1.74	0.51
1:O:2289:G:H21	1:O:2291:A:H2	1.54	0.51
25:W:65:VAL:HG12	25:W:116:LEU:HD13	1.92	0.51
1:O:775:G:OP1	29:1:16:HIS:HE1	1.94	0.51
6:D:25:MET:CE	6:D:41:LEU:HG	2.39	0.51
11:I:97:VAL:CG1	11:I:101:LYS:HE3	2.35	0.51
3:A:105:VAL:HG12	3:A:106:CYS:N	2.24	0.51
27:Y:186:ARG:HG2	27:Y:186:ARG:NH1	2.25	0.51
4:B:72:THR:HB	39:B:9073:HOH:O	2.10	0.51
4:B:141:ARG:HG2	4:B:165:ARG:HA	1.91	0.51
16:N:152:GLU:C	16:N:154:LEU:H	2.14	0.51
25:W:106:THR:OG1	25:W:109:GLU:HG3	2.11	0.51
22:T:115:GLU:HG3	22:T:116:ASP:N	2.25	0.51
1:O:1242:A:C5'	12:J:82:THR:HG23	2.27	0.51
1:O:2661:U:H3	1:O:2812:A:H62	1.59	0.51
6:D:136:ARG:HD2	6:D:155:HIS:O	2.10	0.51
24:V:20:LEU:HD22	24:V:60:GLN:HE22	1.75	0.51
1:O:136:C:H2'	1:O:137:U:O4'	2.10	0.51
3:A:97:ALA:HB2	3:A:150:PRO:HB2	1.93	0.51
6:D:58:VAL:HB	6:D:62:ASP:HB3	1.93	0.51
1:O:1947:G:H2'	1:O:1948:G:H8	1.75	0.51
1:O:834:G:H4'	1:O:835:U:OP2	2.11	0.51
2:9:35:C:H5''	39:9:9078:HOH:O	2.09	0.51
3:A:109:GLU:HG2	3:A:116:GLY:N	2.26	0.51
1:O:2748:G:H5'	39:O:7963:HOH:O	2.11	0.51
1:O:1159:G:H1	1:O:1208:C:H42	1.58	0.51
18:P:10:ALA:HA	18:P:13:VAL:CG1	2.40	0.51
16:N:154:LEU:HG	16:N:155:GLU:H	1.76	0.51
1:O:2795:C:O2'	1:O:2796:U:H5'	2.10	0.51
5:C:166:ILE:CD1	5:C:207:LEU:HD13	2.41	0.51
1:O:123:U:H5'	39:O:7091:HOH:O	2.10	0.51
2:9:54:A:O2'	2:9:55:U:H5'	2.10	0.51
16:N:179:LEU:HD23	16:N:184:ILE:HD12	1.93	0.51
27:Y:184:GLU:OE1	27:Y:204:ARG:NH1	2.44	0.51
26:X:21:PRO:HG2	26:X:24:LYS:HD3	1.91	0.51
1:O:1595:G:O2'	1:O:1596:U:H5'	2.11	0.51
28:Z:26:VAL:O	28:Z:30:GLU:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:162:C:H2'	1:0:163:U:H5'	1.93	0.51
1:0:2563:U:H2'	1:0:2565:C:O5'	2.11	0.51
1:0:1351:G:OP1	5:C:96:LYS:NZ	2.37	0.51
8:F:58:GLU:CD	15:M:27:ARG:HH22	2.14	0.51
1:0:1118:A:H8	1:0:1119:G:H5''	1.76	0.51
1:0:474:C:O3'	5:C:73:LEU:CD2	2.59	0.51
10:H:50:ILE:HG21	39:H:9028:HOH:O	2.11	0.51
11:I:84:SER:HB3	11:I:92:VAL:CG2	2.41	0.51
1:0:262:A:OP2	8:F:91:VAL:HG11	2.10	0.51
5:C:136:VAL:HG22	5:C:137:PRO:HA	1.93	0.51
22:T:32:ARG:NH1	22:T:38:ARG:HH12	2.09	0.51
1:0:392:U:O2'	15:M:182:LYS:HE2	2.11	0.51
5:C:61:PHE:HB3	39:C:8650:HOH:O	2.10	0.51
3:A:125:ASN:HB3	3:A:158:VAL:HG12	1.91	0.51
1:0:2073:G:OP2	1:0:2490:A:H5'	2.11	0.51
16:N:116:PHE:HB3	16:N:136:LEU:HD23	1.93	0.51
1:0:2301:A:H5''	1:0:2302:A:H5'	1.93	0.51
23:U:4:ARG:HH11	23:U:4:ARG:HG2	1.74	0.51
1:0:1244:U:H2'	12:J:47:THR:HG21	1.92	0.50
1:0:92:G:H4'	24:V:44:GLY:HA3	1.93	0.50
12:J:131:THR:HG22	12:J:133:GLY:H	1.76	0.50
4:B:297:VAL:HB	39:B:9073:HOH:O	2.11	0.50
31:3:18:GLN:OE1	31:3:73:GLU:HB3	2.11	0.50
13:K:28:GLU:HB3	13:K:59:LYS:HB2	1.92	0.50
1:0:2456:A:H5'	39:0:6149:HOH:O	2.10	0.50
2:9:64:C:H2'	2:9:65:A:H5'	1.93	0.50
4:B:258:GLY:H	4:B:260:HIS:CE1	2.29	0.50
26:X:37:LEU:CD1	26:X:85:VAL:HG21	2.23	0.50
2:9:48:C:H4'	16:N:141:ARG:HH21	1.76	0.50
23:U:39:ASN:ND2	23:U:44:ARG:HH11	2.08	0.50
30:2:20:ARG:HG3	30:2:21:VAL:H	1.77	0.50
1:0:2502:C:C2'	1:0:2503:A:H5'	2.40	0.50
1:0:2472:C:O2'	1:0:2634:G:H4'	2.11	0.50
2:9:76:G:C3'	2:9:77:A:H5''	2.31	0.50
21:S:10:VAL:HG11	24:V:36:ALA:CA	2.40	0.50
16:N:164:ASP:OD2	16:N:167:ASP:HA	2.10	0.50
20:R:132:ARG:NH2	39:R:8991:HOH:O	2.45	0.50
25:W:122:ARG:NH2	39:W:5817:HOH:O	2.44	0.50
3:A:105:VAL:HG11	3:A:154:ALA:CB	2.41	0.50
1:0:1470:A:OP1	15:M:93:ARG:HD2	2.12	0.50
1:0:2089:A:O2'	1:0:2090:G:H5'	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1289:C:O2'	1:0:1290:G:H5'	2.11	0.50
7:E:108:LEU:HD11	7:E:164:ASP:HB2	1.94	0.50
1:0:1118:A:C8	1:0:1118:A:C3'	2.90	0.50
10:H:30:LYS:H	10:H:62:HIS:CD2	2.21	0.50
1:0:558:C:H2'	1:0:559:U:H5'	1.93	0.50
4:B:51:VAL:HG21	4:B:327:VAL:HG13	1.92	0.50
6:D:23:VAL:CG2	6:D:73:VAL:HB	2.41	0.50
24:V:64:GLY:O	24:V:65:ASP:CB	2.59	0.50
1:0:1181:A:C2'	1:0:1182:C:H5'	2.42	0.50
23:U:46:ALA:HB1	23:U:52:THR:HG21	1.92	0.50
17:O:78:ALA:C	17:O:98:LEU:HD13	2.32	0.50
1:0:1250:C:O2'	1:0:1251:C:H5'	2.12	0.50
1:0:1299:G:H5'	39:0:4547:HOH:O	2.12	0.50
6:D:103:ASN:ND2	6:D:134:LEU:H	2.08	0.50
1:0:2769:C:H2'	1:0:2770:G:C5'	2.41	0.50
1:0:2638:G:H1'	39:0:8261:HOH:O	2.11	0.50
25:W:48:VAL:CG1	25:W:48:VAL:O	2.60	0.50
1:0:1666:C:C2'	1:0:1667:A:C5'	2.89	0.50
1:0:1163:G:H5''	11:I:110:ASP:HB3	1.94	0.50
39:0:3115:HOH:O	8:F:38:LYS:HE2	2.11	0.50
39:0:8211:HOH:O	5:C:94:THR:HG21	2.12	0.50
14:L:89:PHE:N	39:L:8863:HOH:O	2.45	0.50
5:C:77:ALA:O	5:C:78:ARG:HG3	2.11	0.50
27:Y:187:VAL:HG22	27:Y:192:ASP:CB	2.42	0.50
1:0:2756:U:H3	1:0:2896:A:H2	1.50	0.50
39:0:3724:HOH:O	11:I:87:PRO:HD3	2.11	0.50
39:0:9515:HOH:O	14:L:30:ARG:HD2	2.10	0.50
8:F:46:GLU:OE1	8:F:100:ASP:HA	2.12	0.50
3:A:65:ARG:C	3:A:66:ARG:HG3	2.32	0.50
21:S:81:ILE:HG12	39:S:8984:HOH:O	2.11	0.50
28:Z:57:CYS:SG	28:Z:59:TYR:HB3	2.52	0.49
26:X:71:ARG:HB3	26:X:88:GLU:OE1	2.11	0.49
25:W:38:THR:HG22	39:W:3580:HOH:O	2.11	0.49
5:C:246:ARG:NE	39:C:8630:HOH:O	2.26	0.49
13:K:115:ARG:HG3	13:K:116:GLU:N	2.26	0.49
2:9:64:C:C2'	2:9:65:A:H5'	2.41	0.49
11:I:126:THR:O	11:I:126:THR:HG22	2.11	0.49
25:W:88:THR:CG2	25:W:90:TYR:HD1	2.25	0.49
8:F:58:GLU:HG3	8:F:61:MET:HE1	1.94	0.49
27:Y:126:PRO:HG2	27:Y:128:PHE:CZ	2.47	0.49
9:G:16:LYS:O	9:G:20:VAL:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1377:C:H5'	1:0:1377:C:C6	2.45	0.49
1:0:2415:A:H2'	1:0:2416:G:H5'	1.93	0.49
1:0:776:A:OP1	29:1:28:HIS:HE1	1.95	0.49
30:2:20:ARG:CG	30:2:21:VAL:N	2.76	0.49
1:0:2363:G:O3'	19:Q:11:ARG:NH1	2.45	0.49
22:T:41:ARG:HG2	22:T:41:ARG:HH11	1.76	0.49
25:W:26:ILE:O	25:W:26:ILE:HG13	2.12	0.49
1:0:2812:A:H1'	39:0:6244:HOH:O	2.12	0.49
13:K:55:VAL:CG1	13:K:56:SER:N	2.75	0.49
10:H:43:ALA:HB1	10:H:140:TYR:CE2	2.47	0.49
26:X:9:VAL:HG13	26:X:88:GLU:CD	2.32	0.49
3:A:192:VAL:HG13	39:A:9022:HOH:O	2.12	0.49
10:H:6:ALA:CA	10:H:61:ARG:HH12	2.22	0.49
6:D:23:VAL:O	6:D:23:VAL:HG23	2.13	0.49
4:B:74:ILE:HG13	39:B:9073:HOH:O	2.12	0.49
15:M:31:TRP:HA	15:M:34:GLU:HG3	1.93	0.49
1:0:1200:A:H3'	39:0:6208:HOH:O	2.13	0.49
1:0:2791:U:H1'	1:0:2792:A:H5''	1.94	0.49
4:B:149:ASP:HB2	39:B:9049:HOH:O	2.13	0.49
1:0:2825:C:H4'	1:0:2826:G:O5'	2.12	0.49
1:0:343:C:O2'	1:0:344:C:H5'	2.11	0.49
14:L:125:PHE:CE1	14:L:140:VAL:HG13	2.48	0.49
27:Y:209:VAL:HG12	27:Y:214:ARG:HG3	1.94	0.49
26:X:74:ALA:CB	26:X:85:VAL:HG22	2.42	0.49
1:0:1306:U:OP1	5:C:184:ARG:HD2	2.13	0.49
31:3:48:ASN:ND2	31:3:50:GLY:H	2.10	0.49
25:W:108:ARG:HG3	25:W:114:PRO:HG3	1.94	0.49
5:C:133:ARG:NH1	39:C:8616:HOH:O	2.45	0.49
19:Q:26:PRO:O	19:Q:30:VAL:HG23	2.12	0.49
4:B:223:ARG:HG3	4:B:232:TRP:O	2.11	0.49
6:D:29:HIS:HB2	39:D:2768:HOH:O	2.11	0.49
4:B:49:THR:HG21	4:B:331:SER:O	2.13	0.49
1:0:920:C:H5''	1:0:921:G:O5'	2.13	0.49
3:A:1:GLY:HA2	3:A:197:VAL:HG23	1.95	0.49
16:N:147:ILE:HB	39:N:8845:HOH:O	2.12	0.49
1:0:2270:G:C4'	3:A:223:ARG:HH12	2.18	0.49
6:D:104:PHE:CE2	6:D:166:ILE:HD13	2.47	0.49
22:T:73:HIS:CD2	22:T:88:PRO:HG3	2.48	0.49
25:W:31:HIS:HB3	39:W:5420:HOH:O	2.12	0.49
8:F:39:SER:HB3	8:F:45:ALA:HB2	1.95	0.49
1:0:899:C:H5'	39:0:3690:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:638:C:H2'	1:0:639:A:C8	2.47	0.49
1:0:1151:G:OP1	9:G:63:ARG:NH1	2.45	0.49
25:W:65:VAL:HA	25:W:68:THR:CG2	2.42	0.49
14:L:73:VAL:HG21	14:L:116:HIS:CD2	2.48	0.49
30:2:35:ARG:HB2	39:2:2691:HOH:O	2.11	0.49
4:B:268:ARG:NH2	4:B:325:PRO:HG3	2.28	0.49
8:F:16:ALA:HA	8:F:111:ILE:HD13	1.94	0.49
5:C:19:PRO:HG2	5:C:22:PHE:CE1	2.48	0.49
6:D:18:ILE:HG12	6:D:134:LEU:CD2	2.43	0.49
1:0:1181:A:H2'	1:0:1182:C:H5'	1.94	0.49
1:0:1778:A:H2'	1:0:1779:A:H5'	1.95	0.49
22:T:62:VAL:HB	39:T:3851:HOH:O	2.13	0.49
22:T:112:LEU:HD23	22:T:119:ALA:HB3	1.95	0.49
3:A:34:ASP:OD1	3:A:35:GLY:N	2.39	0.49
10:H:61:ARG:HG3	10:H:61:ARG:HH11	1.77	0.49
4:B:102:THR:HG21	4:B:182:VAL:O	2.13	0.49
1:0:793:A:H5''	18:P:83:LYS:HG2	1.95	0.49
1:0:1426:C:H2'	39:0:3083:HOH:O	2.11	0.49
18:P:98:ILE:HD12	18:P:102:ARG:NE	2.28	0.49
15:M:99:ARG:HE	15:M:170:ASN:HD22	1.59	0.49
14:L:130:ARG:HA	39:L:8849:HOH:O	2.12	0.49
1:0:1205:U:C2'	1:0:1206:U:H5''	2.43	0.49
1:0:2521:A:OP2	10:H:6:ALA:HB3	2.13	0.49
3:A:81:GLN:HG3	3:A:92:ASN:HD21	1.77	0.49
1:0:2697:A:H2'	1:0:2698:G:O4'	2.13	0.49
27:Y:103:THR:HG22	27:Y:104:GLU:OE2	2.13	0.49
1:0:475:G:C5'	5:C:73:LEU:HD23	2.43	0.49
13:K:22:ASP:O	13:K:110:LYS:HE3	2.13	0.49
1:0:602:A:O2'	1:0:605:C:H4'	2.12	0.49
31:3:56:PRO:N	39:3:8976:HOH:O	2.45	0.49
1:0:291:C:H2'	1:0:292:G:O4'	2.13	0.49
12:J:130:VAL:HG12	12:J:131:THR:N	2.28	0.48
27:Y:107:PRO:HB3	27:Y:182:PHE:CE2	2.47	0.48
15:M:58:GLN:HG3	39:M:8905:HOH:O	2.11	0.48
2:9:92:G:H2'	2:9:93:A:H8	1.78	0.48
6:D:36:ASN:HA	39:D:7500:HOH:O	2.12	0.48
1:0:2667:G:H1'	1:0:2914:A:N3	2.27	0.48
1:0:1525:G:H5'	1:0:1526:A:OP2	2.13	0.48
1:0:1996:U:O2'	1:0:1997:A:H5'	2.13	0.48
28:Z:32:GLU:HA	28:Z:35:GLU:HG3	1.95	0.48
27:Y:216:ARG:HD2	39:Y:8868:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:V:12:THR:HG23	24:V:14:ALA:N	2.28	0.48
29:1:28:HIS:HD2	29:1:30:LYS:H	1.60	0.48
1:0:2672:C:H1'	39:B:9104:HOH:O	2.12	0.48
20:R:132:ARG:HG2	20:R:133:ALA:N	2.28	0.48
1:0:666:A:H2'	1:0:667:C:O4'	2.14	0.48
1:0:138:U:H5''	1:0:139:C:OP2	2.14	0.48
39:0:7653:HOH:O	3:A:11:ARG:HA	2.13	0.48
8:F:36:THR:HG23	8:F:97:ALA:HB2	1.94	0.48
6:D:35:ALA:N	39:D:5576:HOH:O	2.46	0.48
15:M:164:THR:HG23	15:M:165:GLY:N	2.26	0.48
12:J:19:MET:HE3	12:J:132:LEU:CD2	2.34	0.48
25:W:88:THR:HG22	25:W:90:TYR:CD1	2.46	0.48
27:Y:189:ASN:ND2	27:Y:192:ASP:H	2.11	0.48
1:0:656:G:C5'	17:O:3:THR:HG22	2.40	0.48
1:0:1942:A:H3'	39:0:7777:HOH:O	2.13	0.48
1:0:1741:U:H5'	1:0:1742:A:OP1	2.13	0.48
1:0:1477:C:H5'	1:0:1868:G:C5'	2.43	0.48
1:0:304:G:H1'	1:0:347:A:N6	2.28	0.48
7:E:85:GLU:HG3	7:E:169:THR:OG1	2.13	0.48
25:W:48:VAL:HG12	25:W:48:VAL:O	2.13	0.48
24:V:23:LEU:HD12	24:V:56:ILE:HD12	1.95	0.48
1:0:2769:C:O2'	1:0:2770:G:H5'	2.13	0.48
1:0:2064:U:H5'	1:0:2652:U:O3'	2.13	0.48
1:0:1166:A:H1'	1:0:1192:A:C2	2.48	0.48
1:0:1120:U:H6	1:0:1120:U:H5''	1.78	0.48
1:0:57:C:H5''	39:0:7195:HOH:O	2.12	0.48
22:T:49:GLU:HB3	22:T:59:GLU:HG2	1.95	0.48
1:0:462:A:H2'	39:0:5343:HOH:O	2.14	0.48
28:Z:60:CYS:O	28:Z:61:ASP:HB2	2.12	0.48
25:W:139:GLY:O	25:W:141:HIS:CD2	2.65	0.48
1:0:558:C:C2'	1:0:559:U:C5'	2.90	0.48
10:H:66:GLU:HA	39:H:9031:HOH:O	2.13	0.48
18:P:13:VAL:HG21	18:P:41:ARG:HG2	1.94	0.48
2:9:30:C:OP1	6:D:137:PRO:O	2.31	0.48
6:D:155:HIS:NE2	39:D:7597:HOH:O	2.31	0.48
7:E:133:VAL:HG12	7:E:141:VAL:HG13	1.96	0.48
9:G:23:ILE:HD13	9:G:67:LEU:HD23	1.96	0.48
10:H:141:CYS:HB2	39:H:8994:HOH:O	2.14	0.48
1:0:1053:G:OP1	10:H:15:PRO:HG3	2.13	0.48
5:C:168:ARG:NH2	5:C:190:ALA:O	2.47	0.48
12:J:13:ASP:OD1	12:J:15:ARG:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:180:SER:HB2	39:C:8651:HOH:O	2.13	0.48
6:D:149:ARG:NH2	39:D:3066:HOH:O	2.45	0.48
1:O:1010:C:H4'	16:N:4:PRO:HB2	1.95	0.48
7:E:137:ASP:OD1	7:E:139:GLU:HB2	2.13	0.48
1:O:447:A:OP1	22:T:2:LYS:HG2	2.13	0.48
22:T:40:VAL:HG22	22:T:41:ARG:N	2.29	0.48
1:O:292:G:H2'	1:O:358:G:N2	2.29	0.48
27:Y:149:GLN:NE2	39:Y:8900:HOH:O	2.41	0.48
1:O:1427:A:H61	1:O:1440:U:H1'	1.79	0.48
8:F:26:THR:HG21	8:F:102:GLY:C	2.34	0.48
15:M:64:ARG:HD2	39:M:8884:HOH:O	2.14	0.48
1:O:377:C:H5	39:O:3795:HOH:O	1.97	0.48
6:D:37:ALA:O	6:D:40:ILE:HG12	2.13	0.48
21:S:57:THR:CG2	21:S:58:MET:N	2.76	0.48
1:O:1874:U:H2'	3:A:120:ARG:HG3	1.96	0.48
1:O:1878:G:O2'	1:O:1879:U:OP2	2.31	0.48
1:O:1185:U:H2'	1:O:1186:C:C6	2.49	0.48
1:O:2036:C:C1'	13:K:44:LEU:HG	2.43	0.48
19:Q:32:GLU:HA	19:Q:71:TYR:OH	2.14	0.48
20:R:34:GLU:HG2	20:R:46:TYR:OH	2.14	0.48
3:A:36:ASP:HB2	3:A:85:SER:H	1.79	0.48
39:O:5740:HOH:O	25:W:122:ARG:NH2	2.46	0.48
4:B:195:ARG:HD2	4:B:324:ASP:OD1	2.13	0.48
2:9:8:G:O6	16:N:11:ARG:NH1	2.46	0.48
7:E:80:TRP:O	7:E:134:SER:HA	2.13	0.48
23:U:52:THR:CG2	23:U:54:THR:HB	2.44	0.48
6:D:75:LEU:HD22	6:D:79:MET:HB3	1.96	0.48
19:Q:66:LYS:HB2	19:Q:70:ALA:O	2.14	0.48
1:O:814:G:H4'	39:O:3620:HOH:O	2.12	0.48
5:C:127:ARG:CZ	5:C:225:PRO:HG2	2.42	0.48
13:K:30:LYS:O	13:K:55:VAL:HG13	2.14	0.48
1:O:654:A:OP2	17:O:38:ARG:HD3	2.14	0.48
24:V:5:VAL:CG1	24:V:9:ARG:NH1	2.77	0.48
1:O:1132:A:N6	1:O:1229:C:H2'	2.29	0.48
39:O:7437:HOH:O	19:Q:9:GLY:HA2	2.13	0.48
18:P:97:ARG:HD2	39:P:162:HOH:O	2.13	0.48
4:B:24:PRO:CG	4:B:204:GLY:HA2	2.44	0.48
1:O:644:G:N3	1:O:644:G:H5'	2.29	0.48
6:D:40:ILE:HG13	6:D:41:LEU:N	2.29	0.47
2:9:49:G:H2'	2:9:50:G:O4'	2.14	0.47
24:V:39:ALA:O	24:V:41:GLU:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:101:GLU:HB2	7:E:116:THR:O	2.13	0.47
3:A:94:LEU:HD12	3:A:98:GLU:HB2	1.95	0.47
1:0:1527:A:H1'	1:0:1528:A:C8	2.48	0.47
5:C:104:ASP:HA	5:C:107:ARG:NH1	2.29	0.47
39:0:7978:HOH:O	31:3:60:LYS:HG3	2.13	0.47
1:0:2456:A:H2'	1:0:2457:U:C6	2.49	0.47
18:P:104:LYS:HE2	18:P:138:GLU:OE2	2.14	0.47
10:H:169:GLU:C	39:H:8993:HOH:O	2.51	0.47
1:0:1882:C:OP1	3:A:192:VAL:HG23	2.14	0.47
11:I:105:GLU:HA	11:I:108:HIS:CE1	2.49	0.47
29:1:25:LYS:HD2	30:2:48:ASP:HA	1.96	0.47
1:0:1878:G:O2'	1:0:1879:U:C6	2.63	0.47
1:0:1819:G:H2'	1:0:1820:G:C4'	2.41	0.47
13:K:125:ALA:C	13:K:127:ALA:H	2.17	0.47
1:0:1730:G:C5'	1:0:1731:C:H6	2.27	0.47
22:T:32:ARG:NH1	22:T:38:ARG:NH1	2.62	0.47
1:0:1014:A:H2'	1:0:1015:C:H5'	1.95	0.47
1:0:951:A:C2'	1:0:952:G:H5'	2.44	0.47
1:0:1787:C:OP1	18:P:68:LYS:HE2	2.14	0.47
1:0:2809:G:H2'	1:0:2810:G:O4'	2.15	0.47
1:0:2443:C:O3'	14:L:56:LYS:HE3	2.13	0.47
24:V:44:GLY:O	24:V:48:GLU:HG2	2.14	0.47
1:0:396:U:OP2	31:3:38:ARG:HD2	2.15	0.47
31:3:3:MET:O	31:3:90:PHE:HA	2.14	0.47
4:B:71:VAL:HG11	4:B:296:LEU:HD22	1.96	0.47
1:0:1503:U:H2'	1:0:1504:A:O4'	2.14	0.47
13:K:63:GLU:HG2	39:K:6344:HOH:O	2.14	0.47
39:K:1387:HOH:O	23:U:20:MET:HE3	2.14	0.47
23:U:6:CYS:HB2	23:U:32:CYS:HB3	1.95	0.47
5:C:142:ASP:OD1	5:C:236:THR:HG23	2.14	0.47
3:A:220:PRO:HD2	3:A:223:ARG:HD3	1.96	0.47
26:X:9:VAL:HG13	26:X:88:GLU:OE2	2.14	0.47
27:Y:187:VAL:HG22	27:Y:192:ASP:HB2	1.95	0.47
25:W:5:VAL:HG11	25:W:153:MET:CE	2.44	0.47
1:0:1641:A:C2'	1:0:1642:A:H5'	2.44	0.47
1:0:1441:G:H1'	39:0:8267:HOH:O	2.15	0.47
29:1:28:HIS:CD2	29:1:31:LYS:HG3	2.49	0.47
16:N:65:ASP:HB3	39:N:8821:HOH:O	2.14	0.47
6:D:24:HIS:HB2	6:D:72:LYS:HB3	1.97	0.47
1:0:2787:C:H5	39:0:5098:HOH:O	1.96	0.47
3:A:130:THR:HB	3:A:137:VAL:HB	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1056:U:H2'	1:0:1057:A:O4'	2.13	0.47
1:0:1926:G:H2'	1:0:1927:A:C8	2.49	0.47
1:0:1342:C:O2'	1:0:1343:C:H5'	2.14	0.47
8:F:48:VAL:CG2	8:F:74:PHE:HB3	2.44	0.47
1:0:185:G:H4'	1:0:186:A:H4'	1.96	0.47
1:0:1667:A:H2'	1:0:1668:U:C6	2.50	0.47
1:0:2896:A:N3	1:0:2896:A:H2'	2.29	0.47
6:D:170:TYR:O	6:D:171:ASP:CB	2.61	0.47
1:0:1167:G:H2'	1:0:1168:C:O4'	2.15	0.47
23:U:44:ARG:HB3	39:U:3805:HOH:O	2.15	0.47
14:L:125:PHE:CZ	14:L:140:VAL:HG13	2.49	0.47
1:0:2133:U:H4'	1:0:2134:G:H5'	1.95	0.47
15:M:98:GLN:O	15:M:102:GLU:HG3	2.14	0.47
4:B:205:VAL:O	4:B:307:ARG:NE	2.46	0.47
1:0:282:C:H1'	1:0:368:C:H42	1.79	0.47
1:0:1943:C:O4'	3:A:212:PRO:HA	2.15	0.47
1:0:1206:U:H2'	1:0:1207:A:O4'	2.15	0.47
1:0:1419:U:H5'	1:0:1420:C:OP2	2.14	0.47
17:O:23:GLY:C	39:O:3062:HOH:O	2.52	0.47
15:M:59:GLY:HA3	15:M:141:ILE:HD12	1.97	0.47
6:D:172:VAL:HG12	6:D:173:GLU:N	2.29	0.47
29:1:8:GLN:HE22	29:1:11:LYS:HZ2	1.61	0.47
4:B:85:ARG:HB2	4:B:99:GLU:HG2	1.95	0.47
1:0:1086:A:N6	25:W:11:VAL:HG11	2.30	0.47
1:0:553:G:P	27:Y:204:ARG:HH22	2.37	0.47
24:V:5:VAL:HG23	39:V:2271:HOH:O	2.14	0.47
22:T:52:ARG:HB2	22:T:95:ASN:HB3	1.97	0.47
16:N:171:HIS:CE1	39:N:8863:HOH:O	2.68	0.47
26:X:78:GLU:HG2	26:X:79:GLU:H	1.79	0.47
1:0:737:A:H2'	1:0:738:G:O4'	2.15	0.47
1:0:2251:G:H2'	1:0:2252:A:C8	2.50	0.47
15:M:169:ARG:NH1	39:M:8871:HOH:O	2.47	0.47
1:0:1291:A:H2	39:O:5743:HOH:O	1.97	0.47
6:D:35:ALA:C	6:D:37:ALA:H	2.18	0.47
11:I:87:PRO:O	11:I:89:GLU:HG3	2.15	0.47
19:Q:25:PRO:HA	19:Q:26:PRO:HD3	1.80	0.47
11:I:67:VAL:HG13	11:I:68:PRO:HD2	1.97	0.47
4:B:81:ALA:O	4:B:186:GLY:HA3	2.14	0.47
6:D:84:LEU:HA	6:D:87:ALA:HB3	1.97	0.47
25:W:125:HIS:HE1	39:W:3071:HOH:O	1.97	0.47
1:0:1593:C:OP1	18:P:117:SER:CB	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2672:C:O2'	1:0:2673:U:H5'	2.15	0.47
2:9:51:A:H5'	16:N:160:SER:CB	2.45	0.47
1:0:553:G:OP2	27:Y:204:ARG:NH2	2.47	0.47
6:D:92:GLU:HB2	39:D:3862:HOH:O	2.14	0.47
1:0:2587:OMU:H2'	1:0:2589:U:H5''	1.96	0.47
1:0:285:A:H2'	1:0:286:U:O4'	2.15	0.47
1:0:2505:G:C2'	1:0:2506:A:H5'	2.44	0.47
25:W:4:LEU:HD23	25:W:54:PHE:HB3	1.97	0.47
39:0:6693:HOH:O	23:U:56:ARG:HD3	2.15	0.47
1:0:2591:C:H2'	1:0:2592:G:O4'	2.15	0.47
5:C:118:THR:CG2	5:C:137:PRO:HB3	2.44	0.47
1:0:1159:G:H21	1:0:1189:A:H8	1.63	0.47
11:I:75:LYS:HD3	11:I:81:GLU:O	2.15	0.47
9:G:14:GLU:HB3	39:G:4173:HOH:O	2.14	0.47
10:H:161:THR:HB	10:H:162:PRO:HD3	1.97	0.47
1:0:157:G:H4'	15:M:95:LYS:HE2	1.97	0.47
5:C:12:THR:HB	39:C:8646:HOH:O	2.14	0.47
1:0:1506:U:H6	1:0:1506:U:H5'	1.80	0.47
5:C:142:ASP:OD1	5:C:237:GLU:HB3	2.15	0.46
25:W:6:GLN:CB	25:W:26:ILE:HD12	2.34	0.46
4:B:238:ASN:ND2	4:B:240:GLY:H	2.00	0.46
1:0:2506:A:O2'	1:0:2507:G:O5'	2.34	0.46
1:0:2507:G:H2'	1:0:2510:C:N4	2.30	0.46
1:0:2769:C:H2'	1:0:2770:G:O4'	2.15	0.46
1:0:1992:U:OP2	13:K:66:ARG:HD2	2.15	0.46
16:N:152:GLU:HA	16:N:152:GLU:OE1	2.15	0.46
10:H:119:ALA:O	10:H:120:PHE:C	2.54	0.46
1:0:1130:U:H2'	1:0:1131:G:O4'	2.15	0.46
1:0:255:A:H2'	1:0:256:C:C6	2.50	0.46
1:0:12:U:H2'	1:0:13:G:H5'	1.97	0.46
1:0:1535:G:H2'	1:0:1536:C:C6	2.50	0.46
13:K:113:ILE:HG22	13:K:114:ALA:N	2.29	0.46
1:0:1666:C:C2'	1:0:1667:A:H5''	2.44	0.46
1:0:1185:U:OP1	11:I:121:LYS:HD3	2.15	0.46
1:0:2851:G:C2'	1:0:2852:A:H5'	2.45	0.46
7:E:81:GLU:HG2	7:E:134:SER:CB	2.45	0.46
16:N:143:ARG:NH1	16:N:173:ASP:OD2	2.48	0.46
4:B:241:PRO:HD2	39:B:9125:HOH:O	2.15	0.46
5:C:236:THR:HG22	5:C:239:ALA:CB	2.46	0.46
15:M:167:GLY:O	15:M:171:ARG:HG3	2.15	0.46
1:0:2716:G:H5''	4:B:206:THR:CG2	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:114:VAL:HG11	39:L:8865:HOH:O	2.14	0.46
26:X:76:ARG:O	26:X:77:PHE:HB3	2.15	0.46
3:A:109:GLU:HG2	3:A:116:GLY:H	1.81	0.46
27:Y:189:ASN:HD22	27:Y:192:ASP:H	1.63	0.46
6:D:94:ALA:HA	6:D:174:VAL:O	2.15	0.46
16:N:179:LEU:HA	16:N:184:ILE:HD12	1.97	0.46
17:O:14:LEU:HD23	17:O:102:ILE:HD11	1.98	0.46
1:O:317:A:H4'	39:O:4251:HOH:O	2.16	0.46
1:O:2807:U:P	4:B:27:ASN:HD21	2.39	0.46
1:O:2265:U:H2'	1:O:2266:A:C8	2.51	0.46
21:S:38:ALA:O	21:S:42:GLU:HG3	2.16	0.46
5:C:153:VAL:O	5:C:157:LEU:HG	2.16	0.46
28:Z:53:GLY:HA2	28:Z:67:GLY:O	2.15	0.46
5:C:140:VAL:HG12	5:C:141:SER:N	2.31	0.46
2:9:6:C:C5'	16:N:37:ARG:HH12	2.19	0.46
14:L:143:THR:HG22	14:L:144:ASP:H	1.76	0.46
1:O:1500:U:P	18:P:41:ARG:HH22	2.38	0.46
15:M:166:ALA:HA	15:M:169:ARG:NH1	2.30	0.46
1:O:1211:G:O2'	1:O:1212:C:H5'	2.15	0.46
1:O:1687:C:O2	29:1:9:GLY:HA2	2.16	0.46
14:L:21:ARG:N	39:L:8826:HOH:O	2.47	0.46
1:O:1333:U:H2'	1:O:1334:C:C6	2.51	0.46
1:O:1172:G:H1'	39:O:5430:HOH:O	2.15	0.46
20:R:82:GLU:HG3	20:R:83:LYS:N	2.30	0.46
22:T:71:VAL:HG13	22:T:91:LEU:O	2.15	0.46
12:J:19:MET:HE3	12:J:132:LEU:HD11	1.97	0.46
25:W:38:THR:HG22	25:W:39:ASP:H	1.80	0.46
1:O:2526:C:O2'	1:O:2527:U:H5'	2.16	0.46
1:O:2256:G:H2'	1:O:2257:G:C5'	2.46	0.46
1:O:426:G:H2'	1:O:427:C:O4'	2.16	0.46
25:W:21:LEU:HB3	25:W:26:ILE:CG1	2.46	0.46
10:H:49:GLN:HG3	10:H:140:TYR:CD2	2.51	0.46
3:A:51:ARG:NH1	3:A:120:ARG:O	2.49	0.46
1:O:1419:U:H2'	1:O:1685:A:C2	2.51	0.46
7:E:34:TRP:O	12:J:127:ILE:HD11	2.15	0.46
1:O:894:A:C2	5:C:87:ARG:NH2	2.83	0.46
20:R:39:THR:HG22	20:R:41:GLY:N	2.30	0.46
1:O:1603:A:H5''	1:O:1605:G:H5'	1.96	0.46
1:O:475:G:OP1	5:C:73:LEU:HD22	2.16	0.46
8:F:46:GLU:O	8:F:73:PRO:HD2	2.16	0.46
1:O:1279:U:O2	1:O:1279:U:H2'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:317:A:H5''	22:T:52:ARG:HD2	1.98	0.46
1:0:484:A:N1	1:0:506:G:H4'	2.31	0.46
27:Y:235:GLU:CD	27:Y:235:GLU:N	2.66	0.46
1:0:470:U:O2'	29:1:16:HIS:CD2	2.65	0.46
17:O:26:TRP:HB2	39:O:3062:HOH:O	2.15	0.46
1:0:1625:U:H5''	39:0:6473:HOH:O	2.16	0.46
1:0:2300:A:H4'	1:0:2301:A:O5'	2.16	0.46
5:C:19:PRO:HG2	5:C:22:PHE:CD1	2.51	0.46
1:0:1025:C:H5'	25:W:23:MET:O	2.16	0.46
1:0:1497:G:H4'	1:0:1627:G:O2'	2.16	0.46
1:0:2626:C:H2'	1:0:2627:G:C8	2.51	0.46
26:X:45:GLU:HG3	39:X:6178:HOH:O	2.15	0.46
1:0:2911:C:H2'	1:0:2912:C:C6	2.51	0.46
12:J:88:PRO:O	12:J:94:GLY:HA3	2.16	0.46
15:M:69:LYS:HG2	15:M:127:LYS:HG3	1.98	0.46
11:I:94:ASP:O	11:I:95:LEU:HD23	2.16	0.46
17:O:47:ARG:HG3	17:O:47:ARG:NH1	2.31	0.46
14:L:73:VAL:HG23	14:L:74:THR:N	2.30	0.46
16:N:163:PHE:HZ	16:N:171:HIS:HD1	1.64	0.46
1:0:2256:G:H2'	1:0:2257:G:H5'	1.98	0.46
14:L:97:VAL:HG12	14:L:98:GLU:O	2.16	0.46
1:0:1044:C:H5''	39:0:9520:HOH:O	2.15	0.46
1:0:420:U:H2'	1:0:421:C:C6	2.51	0.46
1:0:1295:G:H5''	14:L:14:GLY:O	2.16	0.46
15:M:47:ASP:CG	15:M:48:LYS:N	2.69	0.46
1:0:1717:A:H5''	18:P:54:LYS:HB2	1.97	0.46
11:I:124:VAL:HG13	11:I:134:ILE:HD11	1.99	0.45
13:K:87:ARG:NH1	39:K:4066:HOH:O	2.49	0.45
1:0:2720:C:O2	13:K:87:ARG:NH2	2.50	0.45
7:E:31:ARG:NH1	7:E:68:HIS:CG	2.84	0.45
14:L:145:LEU:O	14:L:145:LEU:HD23	2.16	0.45
25:W:38:THR:O	25:W:42:ARG:HB2	2.15	0.45
3:A:81:GLN:HB2	3:A:92:ASN:HD22	1.81	0.45
1:0:2502:C:H2'	1:0:2503:A:H5'	1.98	0.45
1:0:2266:A:OP2	15:M:90:ARG:NH2	2.49	0.45
6:D:101:THR:HG22	39:D:7400:HOH:O	2.15	0.45
4:B:14:GLY:HA2	4:B:15:PRO:C	2.36	0.45
2:9:49:G:O2'	2:9:50:G:H5'	2.16	0.45
25:W:110:GLN:NE2	25:W:110:GLN:HA	2.31	0.45
1:0:875:A:C2	3:A:194:MET:SD	3.10	0.45
5:C:118:THR:HG23	39:C:8504:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:32:ARG:HH12	22:T:38:ARG:HH12	1.64	0.45
1:0:1741:U:O2'	1:0:2723:G:H4'	2.16	0.45
4:B:24:PRO:HG3	4:B:204:GLY:HA2	1.98	0.45
24:V:7:GLU:O	24:V:11:MET:HG3	2.16	0.45
1:0:629:A:H2'	1:0:630:A:O4'	2.16	0.45
23:U:47:ARG:HG2	39:U:4381:HOH:O	2.15	0.45
11:I:134:ILE:HG22	11:I:135:GLU:N	2.31	0.45
3:A:94:LEU:HG	3:A:99:ILE:CD1	2.47	0.45
1:0:2421:G:H3'	1:0:2422:U:H5''	1.98	0.45
1:0:2415:A:O2'	16:N:29:SER:HB3	2.17	0.45
5:C:47:GLY:HA2	5:C:92:PRO:HB2	1.97	0.45
14:L:57:VAL:O	14:L:57:VAL:HG12	2.17	0.45
20:R:119:VAL:HG12	20:R:119:VAL:O	2.16	0.45
39:0:6804:HOH:O	3:A:205:GLY:HA3	2.16	0.45
4:B:294:TYR:HE2	39:B:9120:HOH:O	1.98	0.45
6:D:27:ILE:HD11	6:D:37:ALA:HB3	1.99	0.45
1:0:1589:G:N2	1:0:1605:G:H1'	2.31	0.45
1:0:2781:U:H2'	1:0:2782:G:H5'	1.99	0.45
6:D:59:GLY:O	6:D:61:PHE:N	2.47	0.45
16:N:37:ARG:CZ	39:N:8832:HOH:O	2.64	0.45
24:V:12:THR:CG2	24:V:15:GLU:HG3	2.40	0.45
1:0:1205:U:H2'	1:0:1206:U:H5'	1.99	0.45
2:9:28:U:H2'	2:9:29:C:C6	2.52	0.45
9:G:27:ILE:HD13	9:G:71:LEU:HD23	1.98	0.45
3:A:132:ASP:OD1	3:A:133:ARG:N	2.48	0.45
15:M:81:ARG:HG3	15:M:85:ARG:HB2	1.98	0.45
19:Q:11:ARG:NH1	39:Q:5620:HOH:O	2.49	0.45
20:R:119:VAL:HG21	20:R:142:ASP:CG	2.37	0.45
7:E:6:GLU:HA	7:E:46:THR:HG22	1.98	0.45
2:9:52:A:H2'	2:9:53:G:O4'	2.17	0.45
3:A:123:GLY:HA3	3:A:162:GLY:HA2	1.99	0.45
4:B:277:GLU:N	4:B:278:PRO:HD2	2.31	0.45
3:A:128:LEU:HG	39:A:9038:HOH:O	2.15	0.45
27:Y:174:VAL:HG12	27:Y:174:VAL:O	2.17	0.45
1:0:2112:A:H2'	1:0:2113:G:C8	2.52	0.45
14:L:119:THR:HG23	14:L:139:SER:OG	2.17	0.45
15:M:99:ARG:HE	15:M:170:ASN:ND2	2.15	0.45
6:D:63:ILE:HG13	6:D:64:ARG:N	2.32	0.45
4:B:304:PRO:HD2	4:B:307:ARG:NE	2.32	0.45
1:0:558:C:H5'	39:0:5710:HOH:O	2.16	0.45
4:B:305:ASP:O	4:B:306:LYS:CB	2.62	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2421:G:H3'	1:0:2422:U:C5'	2.47	0.45
1:0:2064:U:H4'	1:0:2653:A:OP1	2.16	0.45
4:B:139:ASP:HB2	4:B:165:ARG:HE	1.82	0.45
1:0:820:G:C6	3:A:171:LYS:HB2	2.52	0.45
10:H:50:ILE:HD12	10:H:149:VAL:CG1	2.47	0.45
1:0:2032:U:H5'	39:0:4980:HOH:O	2.16	0.45
17:O:21:SER:OG	17:O:106:PRO:HB2	2.17	0.45
20:R:114:VAL:HA	20:R:144:GLU:O	2.16	0.45
6:D:96:SER:C	6:D:98:PHE:H	2.20	0.45
1:0:2717:C:OP1	4:B:207:LYS:HG3	2.17	0.45
1:0:1878:G:O2'	1:0:1879:U:P	2.75	0.45
7:E:3:VAL:CG2	7:E:49:ILE:HB	2.42	0.45
14:L:143:THR:CG2	14:L:144:ASP:N	2.77	0.45
16:N:72:GLU:H	16:N:171:HIS:HE1	1.65	0.45
14:L:10:SER:O	14:L:11:ARG:HB3	2.17	0.45
1:0:1979:G:H2'	39:0:3782:HOH:O	2.16	0.45
18:P:16:VAL:CG1	18:P:20:ARG:HB2	2.46	0.45
1:0:932:U:H2'	1:0:933:C:C6	2.52	0.45
1:0:1163:G:N2	39:0:5189:HOH:O	2.49	0.45
1:0:2756:U:N3	1:0:2896:A:C2	2.75	0.45
10:H:33:GLN:H	10:H:69:ARG:HH11	1.65	0.45
16:N:143:ARG:HA	16:N:172:PHE:CD2	2.52	0.45
5:C:107:ARG:NH2	39:C:8661:HOH:O	2.47	0.45
20:R:29:LYS:HD3	39:R:8937:HOH:O	2.17	0.45
16:N:61:ALA:CB	16:N:88:ALA:HB2	2.47	0.45
13:K:4:LEU:HD22	13:K:116:GLU:HB3	1.99	0.45
2:9:24:U:H3'	2:9:25:G:H5'	1.98	0.45
14:L:67:ARG:HB2	14:L:112:GLY:HA3	1.98	0.45
13:K:58:THR:HG22	13:K:59:LYS:HG3	1.99	0.45
1:0:1406:A:H4'	1:0:1407:A:H5''	1.98	0.45
21:S:8:PRO:HD2	24:V:32:ALA:HA	1.99	0.45
1:0:2649:A:H5'	1:0:2649:A:H8	1.81	0.45
15:M:99:ARG:HH21	15:M:170:ASN:ND2	2.11	0.45
1:0:1943:C:H4'	3:A:211:LYS:O	2.16	0.45
6:D:76:ARG:O	6:D:77:ASP:HB2	2.17	0.45
5:C:27:ARG:HG2	5:C:30:LEU:CD1	2.46	0.45
1:0:2852:A:H5''	39:0:5686:HOH:O	2.17	0.45
1:0:1174:A:C5	1:0:1201:C:H4'	2.52	0.45
9:G:67:LEU:O	9:G:71:LEU:HG	2.16	0.45
7:E:18:LEU:HD13	7:E:34:TRP:CG	2.52	0.45
1:0:1947:G:H2'	1:0:1948:G:C8	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:951:A:O2'	1:0:952:G:H5'	2.17	0.45
39:K:7438:HOH:O	23:U:20:MET:HE1	2.16	0.45
31:3:30:GLN:NE2	39:3:8980:HOH:O	2.45	0.45
31:3:42:ARG:HH11	31:3:42:ARG:HG3	1.81	0.45
6:D:27:ILE:HD11	6:D:37:ALA:CB	2.47	0.45
1:0:1592:G:O2'	1:0:1593:C:O4'	2.33	0.45
1:0:1060:C:H6	1:0:1060:C:H5'	1.82	0.45
4:B:5:ARG:NH1	4:B:8:LYS:HE2	2.32	0.45
4:B:154:VAL:CG1	4:B:156:LYS:HG2	2.47	0.45
7:E:126:ILE:HB	7:E:131:LEU:HD23	1.98	0.45
10:H:149:VAL:HG13	39:H:9028:HOH:O	2.16	0.45
30:2:18:ASN:HD21	30:2:40:ARG:H	1.65	0.45
18:P:134:VAL:O	18:P:137:LEU:HB3	2.18	0.45
18:P:141:ILE:C	18:P:143:ALA:H	2.19	0.45
9:G:69:ARG:NH1	39:G:3513:HOH:O	2.50	0.45
7:E:116:THR:CG2	7:E:151:LEU:HD22	2.45	0.44
7:E:11:VAL:HG13	7:E:23:GLU:O	2.17	0.44
4:B:82:VAL:CG1	4:B:82:VAL:O	2.65	0.44
8:F:48:VAL:HG23	8:F:74:PHE:CB	2.47	0.44
5:C:35:VAL:HG21	5:C:227:GLY:HA2	1.98	0.44
1:0:2361:A:H5''	39:0:9501:HOH:O	2.17	0.44
1:0:1007:A:H2'	10:H:22:TYR:CZ	2.52	0.44
1:0:1654:U:H2'	3:A:47:HIS:HD2	1.82	0.44
3:A:192:VAL:HG12	3:A:207:GLN:CB	2.47	0.44
14:L:143:THR:HG21	39:L:8833:HOH:O	2.18	0.44
1:0:2866:U:H4'	1:0:2867:G:H5'	1.98	0.44
1:0:969:G:H1	1:0:999:C:H42	1.65	0.44
16:N:108:SER:HA	16:N:109:PRO:HD3	1.80	0.44
1:0:960:G:N3	1:0:960:G:C2'	2.80	0.44
25:W:52:VAL:HG22	25:W:53:ALA:H	1.82	0.44
5:C:16:VAL:HG12	5:C:17:ASP:N	2.31	0.44
1:0:1150:A:C2	9:G:20:VAL:HG21	2.52	0.44
1:0:380:A:H2'	39:0:7660:HOH:O	2.16	0.44
16:N:154:LEU:C	16:N:156:GLU:H	2.20	0.44
23:U:9:CYS:O	23:U:52:THR:HG23	2.16	0.44
1:0:2256:G:C2'	1:0:2257:G:H5'	2.47	0.44
1:0:1755:A:H2'	1:0:1756:G:O4'	2.17	0.44
5:C:150:THR:HA	5:C:203:ALA:O	2.17	0.44
1:0:1555:G:H4'	1:0:1630:A:H2	1.82	0.44
1:0:2003:U:H4'	1:0:2004:U:H5	1.82	0.44
25:W:38:THR:HB	39:W:5390:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:524:A:C5'	20:R:29:LYS:HE2	2.47	0.44
1:0:204:A:C2'	1:0:205:U:H5'	2.48	0.44
4:B:217:ARG:HG3	4:B:257:THR:CG2	2.48	0.44
1:0:2548:C:OP2	4:B:5:ARG:NH2	2.50	0.44
1:0:488:U:H2'	39:0:4480:HOH:O	2.17	0.44
1:0:308:U:C4	1:0:342:C:H1'	2.52	0.44
25:W:41:TYR:HA	25:W:44:MET:HE3	1.99	0.44
4:B:30:PRO:HB2	4:B:39:GLN:NE2	2.32	0.44
6:D:167:GLU:C	6:D:169:THR:H	2.21	0.44
6:D:35:ALA:C	6:D:37:ALA:N	2.71	0.44
2:9:50:G:H5''	16:N:159:TYR:HE1	1.83	0.44
12:J:74:ARG:HH12	12:J:76:ASP:CB	2.30	0.44
1:0:2756:U:N3	1:0:2896:A:H2	2.13	0.44
16:N:15:GLU:HB2	16:N:17:ARG:HG3	1.98	0.44
4:B:41:PHE:HA	4:B:79:MET:CE	2.46	0.44
5:C:46:TYR:CE2	5:C:98:ARG:NH1	2.86	0.44
29:1:28:HIS:CD2	29:1:30:LYS:HB2	2.52	0.44
7:E:84:MET:HE1	7:E:148:ILE:HD12	2.00	0.44
17:O:98:LEU:O	17:O:102:ILE:HG13	2.17	0.44
4:B:232:TRP:CD1	4:B:235:ARG:HD2	2.53	0.44
18:P:131:PHE:CD1	18:P:137:LEU:HD13	2.53	0.44
1:0:2104:C:O2	1:0:2485:A:N1	2.51	0.44
14:L:121:ILE:HG12	14:L:141:GLU:HB2	1.98	0.44
31:3:91:GLN:O	31:3:92:GLU:HB2	2.17	0.44
22:T:9:LYS:HE3	22:T:13:ARG:HH11	1.72	0.44
1:0:1882:C:O2'	1:0:2012:U:OP2	2.33	0.44
3:A:153:ARG:HD3	39:A:8995:HOH:O	2.16	0.44
1:0:559:U:H2'	1:0:560:U:O4'	2.17	0.44
6:D:146:LYS:NZ	16:N:107:ASN:ND2	2.64	0.44
25:W:11:VAL:O	25:W:12:ASN:HB2	2.16	0.44
16:N:154:LEU:O	16:N:155:GLU:CB	2.66	0.44
1:0:1131:G:C6	1:0:1230:A:C4	3.06	0.44
14:L:53:ARG:NH2	14:L:57:VAL:HG12	2.33	0.44
1:0:1137:G:H1'	39:0:4354:HOH:O	2.17	0.44
2:9:57:A:C8	6:D:141:VAL:HG21	2.53	0.44
6:D:49:PRO:HA	6:D:73:VAL:HG22	1.98	0.44
10:H:81:GLY:C	10:H:83:GLU:H	2.21	0.44
8:F:46:GLU:N	39:F:3461:HOH:O	2.51	0.44
3:A:81:GLN:H	3:A:92:ASN:ND2	2.16	0.44
1:0:2642:G:H2'	1:0:2643:G:O4'	2.18	0.44
1:0:138:U:OP2	1:0:139:C:H5	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1044:C:H3'	1:0:1045:G:H5''	1.99	0.44
22:T:75:GLU:O	22:T:76:ASP:HB2	2.18	0.44
22:T:79:LEU:HG	22:T:89:ARG:HB2	1.98	0.44
1:0:2793:A:H2'	1:0:2794:G:H5'	1.99	0.44
6:D:64:ARG:HG2	6:D:67:ASP:HB3	2.00	0.44
26:X:25:ARG:CG	39:X:5356:HOH:O	2.65	0.44
1:0:1307:A:H2'	1:0:1308:A:C8	2.53	0.44
21:S:11:THR:H	21:S:14:ALA:HB3	1.81	0.44
12:J:90:LYS:HB2	36:J:8802:CL:CL	2.54	0.44
7:E:132:THR:HB	39:E:2227:HOH:O	2.17	0.44
12:J:19:MET:HE2	12:J:132:LEU:HD11	1.99	0.43
1:0:1119:G:C8	12:J:52:GLN:NE2	2.86	0.43
23:U:17:THR:HG21	39:U:3194:HOH:O	2.17	0.43
25:W:119:HIS:HD2	25:W:120:PRO:O	2.01	0.43
9:G:19:GLU:O	9:G:23:ILE:HG13	2.18	0.43
1:0:1181:A:N1	1:0:1192:A:O2'	2.50	0.43
1:0:2524:G:H21	1:0:2526:C:N4	2.16	0.43
27:Y:95:THR:N	27:Y:236:VAL:O	2.51	0.43
1:0:1946:C:H2'	1:0:1971:G:C8	2.53	0.43
4:B:108:GLU:HB3	4:B:111:ARG:HD2	2.00	0.43
3:A:223:ARG:NE	39:A:9037:HOH:O	2.51	0.43
1:0:559:U:H5'	1:0:559:U:C6	2.41	0.43
4:B:51:VAL:HG23	4:B:327:VAL:HG13	1.98	0.43
27:Y:115:ARG:HH11	27:Y:115:ARG:HB3	1.83	0.43
1:0:392:U:C5'	15:M:193:LYS:HB3	2.49	0.43
1:0:1393:A:H2'	1:0:1394:C:C6	2.53	0.43
1:0:432:G:O2'	1:0:433:C:H5'	2.18	0.43
1:0:1252:A:H2'	1:0:1253:C:O4'	2.19	0.43
1:0:1733:A:H4'	4:B:212:GLN:HA	1.99	0.43
26:X:73:ARG:HB2	26:X:88:GLU:OE2	2.19	0.43
1:0:1119:G:C6	1:0:1244:U:C5	3.06	0.43
12:J:107:ASN:HD22	12:J:108:PRO:N	2.16	0.43
28:Z:19:GLY:O	28:Z:23:ARG:HG2	2.18	0.43
1:0:1730:G:H5'	1:0:1731:C:H5	1.81	0.43
1:0:2864:U:O2'	1:0:2865:G:H5'	2.18	0.43
10:H:168:VAL:HG13	39:H:9009:HOH:O	2.17	0.43
13:K:113:ILE:CG2	13:K:114:ALA:N	2.81	0.43
1:0:542:A:H2'	1:0:543:G:O4'	2.18	0.43
15:M:59:GLY:HA3	15:M:141:ILE:CD1	2.49	0.43
11:I:67:VAL:CG1	11:I:68:PRO:HD2	2.48	0.43
1:0:2526:C:H5'	1:0:2526:C:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:119:VAL:CG1	20:R:119:VAL:O	2.65	0.43
3:A:70:ALA:HA	3:A:71:PRO:HD3	1.81	0.43
1:0:517:U:H1'	39:0:7997:HOH:O	2.18	0.43
1:0:2115:U:H2'	1:0:2116:U:C6	2.53	0.43
10:H:57:THR:O	10:H:58:VAL:HG13	2.19	0.43
21:S:20:PHE:CD2	21:S:20:PHE:N	2.85	0.43
12:J:45:VAL:HG22	12:J:46:ILE:N	2.33	0.43
31:3:70:ARG:CG	31:3:77:ALA:HB2	2.47	0.43
1:0:2090:G:H2'	1:0:2091:G:C8	2.53	0.43
14:L:122:ALA:HB3	14:L:125:PHE:CZ	2.54	0.43
1:0:920:C:H5'	1:0:921:G:C4	2.53	0.43
16:N:73:ALA:N	39:N:8863:HOH:O	2.48	0.43
1:0:284:C:H4'	1:0:285:A:H8	1.83	0.43
1:0:2649:A:C8	1:0:2649:A:H5'	2.54	0.43
1:0:2326:C:H4'	1:0:2412:G:C4'	2.49	0.43
1:0:790:A:H2'	1:0:791:A:O4'	2.18	0.43
22:T:71:VAL:CG1	22:T:72:ILE:N	2.81	0.43
16:N:77:ASN:OD1	16:N:80:SER:HB2	2.18	0.43
27:Y:107:PRO:HB3	27:Y:182:PHE:CD2	2.54	0.43
1:0:2819:C:H2'	1:0:2820:A:C8	2.53	0.43
13:K:28:GLU:HG2	13:K:58:THR:HB	2.00	0.43
1:0:2868:C:H2'	1:0:2869:G:O4'	2.19	0.43
1:0:1484:G:H2'	39:0:9594:HOH:O	2.17	0.43
25:W:29:VAL:O	25:W:30:ASN:HB2	2.18	0.43
1:0:130:C:H5'	39:0:5666:HOH:O	2.18	0.43
7:E:77:THR:OG1	7:E:78:GLU:N	2.51	0.43
1:0:2831:C:O3'	20:R:71:LYS:HE2	2.18	0.43
3:A:39:ALA:O	3:A:61:GLU:HG3	2.18	0.43
1:0:2121:G:O2'	1:0:2122:C:H5'	2.19	0.43
4:B:175:LEU:O	4:B:175:LEU:HD23	2.19	0.43
1:0:189:A:OP1	15:M:171:ARG:NH2	2.51	0.43
16:N:71:TRP:CE3	16:N:175:LEU:HD22	2.53	0.43
5:C:235:PHE:HE2	5:C:243:VAL:HG21	1.84	0.43
1:0:920:C:H4'	1:0:921:G:C2	2.54	0.43
1:0:622:G:P	27:Y:148:GLY:HA3	2.58	0.43
22:T:92:ASP:OD1	22:T:94:SER:HB3	2.19	0.43
13:K:75:ARG:HD3	13:K:112:PRO:O	2.19	0.43
15:M:164:THR:CG2	15:M:165:GLY:N	2.82	0.43
6:D:149:ARG:HH12	16:N:15:GLU:HA	1.84	0.43
1:0:512:G:O3'	1:0:513:A:H8	2.02	0.43
1:0:137:U:OP1	1:0:259:G:O2'	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:125:ASN:CB	3:A:158:VAL:HG12	2.49	0.43
1:0:2256:G:O2'	1:0:2257:G:H5'	2.19	0.43
1:0:2031:C:H2'	1:0:2032:U:O4'	2.19	0.43
20:R:15:LYS:HE3	39:R:8984:HOH:O	2.18	0.43
1:0:2372:A:H2'	1:0:2373:U:C6	2.54	0.43
8:F:117:GLU:C	8:F:119:ARG:H	2.22	0.43
8:F:70:LYS:C	8:F:72:VAL:H	2.21	0.43
4:B:40:GLY:HA3	39:B:9118:HOH:O	2.19	0.43
4:B:53:LEU:HD11	4:B:327:VAL:HG22	2.01	0.43
4:B:41:PHE:CZ	4:B:79:MET:HG3	2.54	0.43
1:0:1853:C:O2'	3:A:217:ARG:NH2	2.52	0.43
13:K:66:ARG:HH11	13:K:66:ARG:HG2	1.84	0.43
5:C:166:ILE:HD11	5:C:207:LEU:HD13	2.01	0.43
1:0:2133:U:H4'	1:0:2134:G:C5'	2.48	0.43
1:0:2326:C:H4'	1:0:2412:G:H4'	2.01	0.43
16:N:89:GLY:O	16:N:92:ALA:HB3	2.18	0.43
1:0:1335:C:OP2	27:Y:207:SER:HB3	2.18	0.43
7:E:86:VAL:CG1	7:E:129:GLU:HA	2.49	0.43
1:0:2403:C:OP1	19:Q:49:ASN:HB3	2.19	0.43
15:M:99:ARG:CD	15:M:167:GLY:HA2	2.49	0.43
21:S:57:THR:HG22	21:S:59:ASP:HB2	2.01	0.43
8:F:60:VAL:HG12	8:F:60:VAL:O	2.19	0.43
1:0:1185:U:H5'	39:0:7891:HOH:O	2.18	0.43
1:0:1158:G:O2'	1:0:1159:G:H5'	2.19	0.43
3:A:186:TRP:CG	3:A:187:PRO:HA	2.54	0.43
4:B:314:ALA:CB	4:B:317:PRO:HG3	2.49	0.43
6:D:20:LYS:HA	6:D:75:LEU:O	2.19	0.43
1:0:2103:A:O2'	1:0:2104:C:H5'	2.19	0.43
19:Q:55:ARG:HD2	39:Q:2875:HOH:O	2.19	0.43
22:T:18:GLU:O	22:T:21:LYS:HG2	2.19	0.43
2:9:56:A:C3'	2:9:57:A:H5''	2.48	0.42
7:E:15:GLN:HG3	7:E:20:ILE:HG12	2.00	0.42
1:0:2316:G:H4'	39:0:6539:HOH:O	2.18	0.42
1:0:2768:A:O2'	1:0:2769:C:H5'	2.19	0.42
1:0:263:U:C2	8:F:59:ILE:CD1	3.02	0.42
1:0:524:A:H5'	20:R:29:LYS:HE2	2.01	0.42
8:F:111:ILE:O	8:F:115:VAL:HG23	2.18	0.42
7:E:22:VAL:O	7:E:28:SER:HA	2.19	0.42
1:0:1768:C:H2'	1:0:1769:C:O4'	2.19	0.42
1:0:56:G:H5''	24:V:50:ARG:NH1	2.33	0.42
1:0:1218:U:H2'	1:0:1219:U:C6	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:123:VAL:C	11:I:125:GLY:H	2.22	0.42
11:I:88:GLN:HA	11:I:91:PHE:HE2	1.84	0.42
1:O:451:C:O2'	1:O:452:G:H5'	2.19	0.42
6:D:37:ALA:HA	39:D:5583:HOH:O	2.19	0.42
1:O:567:U:H5''	39:O:5740:HOH:O	2.19	0.42
3:A:107:ASN:OD1	3:A:120:ARG:HD2	2.19	0.42
18:P:59:ARG:HD3	39:P:191:HOH:O	2.19	0.42
8:F:32:GLY:N	39:F:3111:HOH:O	2.52	0.42
17:O:32:ARG:HH21	17:O:35:LYS:HD2	1.84	0.42
1:O:1202:A:H2'	1:O:1203:G:O4'	2.19	0.42
3:A:37:VAL:HG22	39:A:9059:HOH:O	2.19	0.42
28:Z:22:SER:O	28:Z:26:VAL:HG23	2.19	0.42
22:T:112:LEU:CD2	22:T:119:ALA:HB3	2.49	0.42
3:A:135:VAL:N	39:A:9058:HOH:O	2.51	0.42
18:P:64:GLU:HG2	39:P:167:HOH:O	2.18	0.42
1:O:2630:G:O6	3:A:206:ARG:NH2	2.49	0.42
1:O:241:A:C2	1:O:378:A:H4'	2.54	0.42
16:N:37:ARG:NH2	39:N:8832:HOH:O	2.52	0.42
1:O:1439:C:OP1	30:2:41:HIS:HE1	2.03	0.42
1:O:2718:C:H5'	1:O:2718:C:C6	2.51	0.42
25:W:3:ALA:O	25:W:54:PHE:HA	2.19	0.42
26:X:43:VAL:HG12	26:X:44:ASP:H	1.84	0.42
20:R:61:GLN:NE2	39:R:8944:HOH:O	2.53	0.42
25:W:35:VAL:HG23	25:W:41:TYR:CD2	2.54	0.42
1:O:1573:A:H2'	1:O:1574:C:O4'	2.19	0.42
15:M:15:PRO:HA	15:M:20:LEU:HD23	2.01	0.42
1:O:1846:U:O2'	3:A:172:ALA:HB2	2.19	0.42
1:O:1287:A:O4'	25:W:117:ARG:HD3	2.20	0.42
39:O:6168:HOH:O	13:K:87:ARG:NE	2.52	0.42
5:C:246:ARG:NH2	39:C:8630:HOH:O	2.46	0.42
1:O:1948:G:H2'	1:O:1949:G:O4'	2.20	0.42
7:E:107:PHE:CZ	7:E:108:LEU:HD13	2.54	0.42
1:O:903:U:OP2	14:L:11:ARG:NH1	2.50	0.42
1:O:926:A:O2'	14:L:41:HIS:HD2	2.01	0.42
1:O:1029:U:H5'	1:O:1031:G:N7	2.34	0.42
1:O:1562:C:N4	39:O:6317:HOH:O	2.34	0.42
1:O:2353:A:H4'	1:O:2354:A:O5'	2.18	0.42
3:A:175:LYS:HE2	39:A:9040:HOH:O	2.19	0.42
1:O:1066:U:H2'	1:O:1067:A:C8	2.54	0.42
20:R:104:PHE:HB2	20:R:109:MET:HE1	2.01	0.42
4:B:162:MET:HG3	4:B:310:ARG:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:36:PRO:CA	4:B:168:GLY:HA3	2.43	0.42
10:H:66:GLU:O	10:H:70:LEU:HB2	2.20	0.42
1:0:1845:A:O3'	3:A:187:PRO:HB2	2.19	0.42
1:0:2676:C:H4'	12:J:70:PHE:CD1	2.54	0.42
4:B:139:ASP:HB2	39:B:8998:HOH:O	2.18	0.42
5:C:133:ARG:NE	5:C:138:VAL:HG22	2.34	0.42
3:A:217:ARG:CG	3:A:217:ARG:HH11	2.33	0.42
1:0:392:U:H5''	15:M:193:LYS:HB3	2.01	0.42
1:0:1940:C:H4'	39:0:7777:HOH:O	2.18	0.42
27:Y:99:ALA:HB2	27:Y:233:TYR:CE2	2.55	0.42
1:0:669:G:O2'	1:0:670:G:H5'	2.19	0.42
15:M:152:ALA:HB1	39:M:8934:HOH:O	2.20	0.42
1:0:2478:U:O2'	1:0:2479:A:H5'	2.19	0.42
1:0:646:G:H2'	1:0:647:U:C6	2.54	0.42
21:S:57:THR:CG2	21:S:59:ASP:HB2	2.50	0.42
1:0:1500:U:OP2	18:P:41:ARG:NH2	2.53	0.42
1:0:2781:U:C2'	1:0:2782:G:H5'	2.49	0.42
31:3:20:HIS:HA	31:3:70:ARG:O	2.19	0.42
26:X:41:PHE:O	26:X:43:VAL:HG23	2.19	0.42
4:B:243:ASN:HA	4:B:244:PRO:C	2.39	0.42
8:F:99:THR:O	8:F:99:THR:HG23	2.20	0.42
9:G:64:ASN:N	9:G:64:ASN:ND2	2.68	0.42
23:U:13:ILE:HG12	23:U:32:CYS:HB3	2.00	0.42
1:0:1925:G:O2'	1:0:1926:G:H5'	2.20	0.42
1:0:1626:A:H2'	1:0:1627:G:O4'	2.19	0.42
1:0:1406:A:H4'	1:0:1407:A:C5'	2.50	0.42
12:J:26:VAL:HG13	12:J:36:VAL:HG11	2.01	0.42
7:E:43:ASP:HA	39:E:5864:HOH:O	2.18	0.42
14:L:92:ASP:HB3	14:L:95:ASP:OD2	2.19	0.42
2:9:59:C:H6	2:9:59:C:O5'	2.02	0.42
6:D:146:LYS:HZ3	16:N:107:ASN:HD21	1.65	0.42
31:3:11:CYS:HB2	31:3:20:HIS:CE1	2.55	0.42
21:S:56:ASN:O	30:2:8:LYS:NZ	2.47	0.42
25:W:107:LEU:O	25:W:112:LEU:HB2	2.18	0.42
1:0:2442:G:H3'	39:0:7065:HOH:O	2.19	0.42
12:J:71:TYR:CD1	12:J:72:PRO:HD2	2.54	0.42
1:0:2754:G:H2'	1:0:2755:G:O4'	2.19	0.42
22:T:47:THR:HB	22:T:100:ASP:HB3	2.02	0.42
14:L:6:ARG:NH2	39:L:8842:HOH:O	2.47	0.42
1:0:962:C:H1'	16:N:5:ARG:HH12	1.79	0.42
24:V:60:GLN:O	24:V:65:ASP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Z:30:GLU:HA	28:Z:33:MET:HE3	2.01	0.42
25:W:19:ASP:O	25:W:23:MET:HG3	2.20	0.42
1:0:926:A:O2'	14:L:41:HIS:CD2	2.73	0.42
27:Y:99:ALA:HB2	27:Y:233:TYR:CZ	2.54	0.42
13:K:23:ASN:HD21	13:K:107:THR:HB	1.83	0.42
17:O:41:ALA:HA	39:O:5104:HOH:O	2.19	0.42
1:0:1902:G:H2'	1:0:1903:U:O4'	2.20	0.42
1:0:2401:A:H2'	1:0:2402:A:C8	2.55	0.42
23:U:45:GLU:HB2	23:U:48:ASN:ND2	2.35	0.42
5:C:78:ARG:CG	5:C:78:ARG:NH1	2.74	0.42
2:9:42:C:O2	6:D:76:ARG:NH1	2.53	0.42
1:0:2578:G:C8	1:0:2578:G:H5'	2.51	0.42
16:N:140:GLN:O	16:N:143:ARG:HB2	2.19	0.42
25:W:76:ASP:O	25:W:77:ALA:C	2.57	0.42
6:D:60:GLU:O	6:D:61:PHE:C	2.57	0.42
1:0:1162:G:H1'	11:I:112:LEU:CD1	2.49	0.42
1:0:2072:G:H3'	1:0:2073:G:C5'	2.50	0.42
27:Y:117:LEU:HD12	27:Y:174:VAL:HG11	2.02	0.42
3:A:135:VAL:HG11	3:A:147:ARG:NH1	2.35	0.42
22:T:96:VAL:HG13	22:T:97:ARG:N	2.35	0.42
5:C:219:ASN:O	5:C:222:ASP:OD1	2.37	0.42
5:C:219:ASN:N	5:C:222:ASP:OD1	2.52	0.42
1:0:441:A:H1'	1:0:442:A:N7	2.35	0.42
1:0:635:A:H2'	1:0:636:G:H5''	2.01	0.42
12:J:46:ILE:HD11	12:J:53:ILE:HG23	2.01	0.42
1:0:1684:A:O2'	1:0:1685:A:H5''	2.19	0.42
1:0:1209:C:H2'	1:0:1210:G:C8	2.51	0.42
18:P:10:ALA:CA	18:P:13:VAL:HG12	2.46	0.42
3:A:97:ALA:C	3:A:131:HIS:HE2	2.22	0.42
7:E:24:GLY:HA3	7:E:76:VAL:HB	2.02	0.42
15:M:145:ASP:HA	39:M:8909:HOH:O	2.19	0.42
1:0:214:U:H5'	39:O:6586:HOH:O	2.19	0.42
8:F:24:ARG:NH2	39:F:6800:HOH:O	2.48	0.42
16:N:64:SER:C	16:N:66:LEU:H	2.22	0.42
4:B:248:ARG:NH2	39:B:8993:HOH:O	2.50	0.42
15:M:5:TYR:HE2	15:M:46:LEU:HD13	1.84	0.42
11:I:109:PRO:HG2	11:I:110:ASP:H	1.84	0.41
3:A:105:VAL:CG1	3:A:106:CYS:N	2.82	0.41
9:G:24:VAL:O	9:G:28:GLU:HB2	2.19	0.41
5:C:138:VAL:O	5:C:234:VAL:HA	2.20	0.41
1:0:776:A:H1'	1:0:779:U:O4	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:2:36:ASN:HB3	30:2:39:ARG:HG3	2.00	0.41
1:0:304:G:H1'	1:0:347:A:H61	1.85	0.41
21:S:42:GLU:HG2	21:S:49:VAL:HG23	2.01	0.41
1:0:1754:A:H2'	1:0:1755:A:O4'	2.20	0.41
3:A:206:ARG:NH1	39:A:8979:HOH:O	2.53	0.41
1:0:482:G:H4'	1:0:508:A:N1	2.35	0.41
4:B:132:HIS:CE1	4:B:171:VAL:HG21	2.55	0.41
15:M:99:ARG:NH2	15:M:170:ASN:HD22	2.15	0.41
5:C:127:ARG:HG2	5:C:127:ARG:HH11	1.84	0.41
25:W:146:ILE:HA	25:W:146:ILE:HD13	1.89	0.41
18:P:63:ARG:NH2	39:P:191:HOH:O	2.51	0.41
1:0:2756:U:C2	1:0:2896:A:H2	2.37	0.41
1:0:1197:G:N2	39:0:6679:HOH:O	2.52	0.41
5:C:246:ARG:HB3	5:C:246:ARG:NH1	2.35	0.41
1:0:2503:A:OP1	10:H:154:ARG:NH2	2.47	0.41
10:H:154:ARG:HA	10:H:157:TYR:CE2	2.55	0.41
1:0:2252:A:C5	1:0:2253:G:H1'	2.54	0.41
20:R:114:VAL:HG13	20:R:114:VAL:O	2.20	0.41
10:H:72:ALA:HB2	10:H:156:ALA:HB2	2.02	0.41
1:0:1762:C:H4'	39:0:5120:HOH:O	2.21	0.41
1:0:2336:G:H1'	39:D:5675:HOH:O	2.19	0.41
1:0:1236:A:C8	12:J:63:ILE:HD11	2.55	0.41
1:0:2453:G:H4'	14:L:50:GLY:C	2.40	0.41
1:0:383:A:H2'	1:0:384:G:O4'	2.20	0.41
3:A:211:LYS:HD2	39:A:9081:HOH:O	2.21	0.41
12:J:42:GLU:O	12:J:131:THR:HG23	2.19	0.41
6:D:146:LYS:HZ1	16:N:107:ASN:HD21	1.64	0.41
11:I:129:SER:N	39:I:7330:HOH:O	2.47	0.41
1:0:1730:G:H5''	1:0:1731:C:C6	2.54	0.41
10:H:24:THR:O	10:H:123:ILE:HD12	2.20	0.41
16:N:154:LEU:HG	16:N:155:GLU:N	2.35	0.41
10:H:146:ALA:O	10:H:149:VAL:HG12	2.20	0.41
1:0:1657:A:H2'	1:0:1658:A:C8	2.55	0.41
1:0:2726:U:O2	1:0:2749:U:O5'	2.38	0.41
1:0:1980:U:O2	1:0:2008:U:H4'	2.20	0.41
4:B:189:ALA:HB1	39:B:9033:HOH:O	2.19	0.41
1:0:1118:A:C8	1:0:1119:G:H5''	2.54	0.41
5:C:118:THR:HG22	5:C:137:PRO:HB3	2.03	0.41
8:F:38:LYS:HZ1	15:M:3:SER:HA	1.85	0.41
7:E:81:GLU:HA	7:E:133:VAL:O	2.20	0.41
26:X:66:THR:CG2	26:X:67:PRO:HD2	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2415:A:N3	16:N:26:LEU:HD13	2.36	0.41
1:0:2547:C:OP2	4:B:5:ARG:NH1	2.53	0.41
1:0:1181:A:H2'	1:0:1182:C:C5'	2.50	0.41
13:K:78:LYS:HA	13:K:79:PRO:HD3	1.90	0.41
1:0:827:A:H2'	1:0:828:G:O4'	2.19	0.41
3:A:194:MET:CE	3:A:199:HIS:CB	2.98	0.41
20:R:18:LEU:HG	20:R:91:LEU:HD13	2.03	0.41
21:S:51:GLN:NE2	21:S:53:ASN:HD21	2.13	0.41
1:0:2416:G:O2'	16:N:25:ARG:HG2	2.19	0.41
11:I:87:PRO:HB3	11:I:129:SER:C	2.41	0.41
8:F:28:ALA:CB	8:F:99:THR:HG23	2.50	0.41
15:M:169:ARG:NH2	39:M:8852:HOH:O	2.47	0.41
1:0:1654:U:H2'	3:A:47:HIS:CD2	2.56	0.41
1:0:1739:G:O2'	1:0:1740:U:H5'	2.20	0.41
11:I:111:LEU:HD22	11:I:122:GLU:OE1	2.21	0.41
1:0:2241:C:O2'	1:0:2242:U:H5'	2.20	0.41
14:L:65:ASP:CG	14:L:111:ALA:HB3	2.40	0.41
16:N:39:SER:HB3	16:N:42:HIS:H	1.86	0.41
6:D:10:PHE:N	39:D:7345:HOH:O	2.53	0.41
10:H:86:TYR:C	10:H:86:TYR:CD1	2.93	0.41
24:V:12:THR:CG2	24:V:15:GLU:H	2.34	0.41
4:B:57:GLU:HA	4:B:58:PRO:HD2	1.96	0.41
6:D:173:GLU:O	6:D:174:VAL:C	2.59	0.41
30:2:19:SER:O	30:2:36:ASN:ND2	2.54	0.41
1:0:660:A:H4'	1:0:661:G:O5'	2.20	0.41
4:B:75:GLU:C	4:B:77:PRO:HD3	2.41	0.41
1:0:329:A:OP2	5:C:206:ASN:HB2	2.20	0.41
1:0:88:G:H2'	1:0:89:G:C8	2.55	0.41
1:0:2543:G:H2'	1:0:2544:G:O4'	2.20	0.41
1:0:702:G:O2'	1:0:703:G:H5'	2.21	0.41
1:0:249:G:O2'	1:0:250:C:H5'	2.21	0.41
5:C:154:VAL:O	5:C:158:GLU:HG3	2.21	0.41
10:H:151:GLU:HA	10:H:151:GLU:OE1	2.21	0.41
7:E:16:ASP:O	7:E:17:HIS:HB2	2.19	0.41
10:H:49:GLN:OE1	10:H:169:GLU:HB3	2.21	0.41
1:0:2054:A:H2	20:R:128:ARG:HH22	1.56	0.41
11:I:87:PRO:C	11:I:89:GLU:N	2.74	0.41
5:C:57:PRO:HG2	5:C:73:LEU:HD13	2.02	0.41
15:M:134:ILE:O	15:M:136:PRO:HD3	2.21	0.41
26:X:20:GLU:CD	26:X:21:PRO:HD2	2.41	0.41
1:0:1596:U:H2'	1:0:1598:A:OP2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:41:ARG:NH1	22:T:42:VAL:O	2.53	0.41
1:0:256:C:H2'	1:0:257:G:O4'	2.21	0.41
4:B:14:GLY:HA3	39:B:9076:HOH:O	2.21	0.41
14:L:38:HIS:CD2	14:L:39:GLU:HG3	2.55	0.41
1:0:2724:U:H2'	1:0:2725:G:O4'	2.20	0.41
1:0:1352:A:H4'	1:0:1353:C:OP2	2.20	0.41
12:J:64:GLY:HA3	36:J:8821:CL:CL	2.58	0.41
22:T:3:GLN:HA	22:T:4:PRO:HD3	1.82	0.41
1:0:2498:C:O2'	1:0:2499:U:H5'	2.20	0.41
11:I:103:ILE:HG22	11:I:103:ILE:O	2.20	0.41
22:T:71:VAL:CG1	22:T:90:PRO:HB3	2.30	0.41
1:0:1165:G:H1'	1:0:1174:A:H1'	2.03	0.41
8:F:5:ASP:O	8:F:119:ARG:NH1	2.53	0.41
1:0:95:A:H5''	1:0:97:G:O4'	2.21	0.41
1:0:2906:A:H5'	1:0:2907:C:O4'	2.21	0.41
15:M:184:ARG:HG3	15:M:185:PRO:HA	2.03	0.41
1:0:23:G:C6	1:0:24:G:N1	2.89	0.41
22:T:106:GLU:HG3	39:T:4913:HOH:O	2.21	0.41
26:X:74:ALA:HB1	26:X:85:VAL:HG22	2.03	0.41
13:K:109:LEU:CD1	13:K:113:ILE:HD11	2.48	0.41
12:J:75:PRO:HB3	12:J:132:LEU:HB3	2.02	0.41
3:A:36:ASP:CB	3:A:85:SER:H	2.34	0.41
39:0:5740:HOH:O	25:W:122:ARG:CZ	2.68	0.41
16:N:49:THR:HG22	16:N:56:ASP:CB	2.49	0.41
6:D:170:TYR:CD1	6:D:170:TYR:N	2.89	0.41
15:M:61:ILE:N	15:M:61:ILE:HD12	2.35	0.41
6:D:173:GLU:HG3	6:D:174:VAL:N	2.35	0.41
8:F:33:THR:HG21	8:F:59:ILE:O	2.20	0.41
29:1:28:HIS:O	29:1:32:LYS:N	2.47	0.41
1:0:553:G:O2'	27:Y:179:PRO:HG3	2.21	0.41
26:X:23:HIS:CD2	26:X:24:LYS:HG3	2.56	0.41
17:O:14:LEU:HG	17:O:102:ILE:HD11	2.03	0.41
13:K:28:GLU:OE2	13:K:58:THR:HG21	2.20	0.41
1:0:2089:A:C2'	1:0:2090:G:H5'	2.51	0.41
15:M:69:LYS:HG3	15:M:126:GLN:CA	2.51	0.41
22:T:48:VAL:CG2	22:T:96:VAL:HG13	2.51	0.41
15:M:46:LEU:HG	39:M:8917:HOH:O	2.19	0.41
26:X:10:VAL:HG12	26:X:11:THR:N	2.35	0.41
1:0:2883:A:H2'	1:0:2884:G:O4'	2.21	0.41
1:0:2515:C:H2'	1:0:2516:G:O4'	2.20	0.41
20:R:33:ARG:NH1	39:R:8947:HOH:O	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1976:G:O2'	1:0:1977:U:H5'	2.21	0.41
1:0:2559:C:H4'	39:0:7688:HOH:O	2.20	0.41
1:0:522:U:O2'	1:0:1366:C:H5'	2.20	0.41
1:0:2740:G:H2'	1:0:2741:A:O4'	2.21	0.41
2:9:4:G:H21	16:N:44:ARG:NH1	2.19	0.41
1:0:366:U:H2'	1:0:367:G:O4'	2.20	0.41
1:0:2884:G:H5'	39:0:4600:HOH:O	2.20	0.41
1:0:64:G:H2'	1:0:65:C:O4'	2.21	0.41
39:0:4461:HOH:O	22:T:82:THR:HA	2.21	0.41
1:0:958:G:H2'	1:0:959:C:C6	2.55	0.41
1:0:222:A:H2'	1:0:223:G:O4'	2.20	0.41
15:M:42:ARG:HA	15:M:43:PRO:HD3	1.91	0.41
1:0:1098:A:H2'	1:0:1099:G:O4'	2.21	0.41
20:R:96:VAL:HG13	20:R:106:GLY:HA3	2.03	0.41
4:B:26:PHE:CE1	4:B:310:ARG:HB3	2.56	0.41
1:0:1299:G:N2	39:0:5149:HOH:O	2.54	0.41
6:D:49:PRO:HB3	39:D:5828:HOH:O	2.21	0.41
26:X:43:VAL:HG12	26:X:47:ALA:HB3	2.02	0.41
1:0:2428:G:N7	31:3:60:LYS:NZ	2.67	0.41
24:V:51:LYS:O	24:V:55:ARG:HG3	2.21	0.41
14:L:67:ARG:HG2	14:L:67:ARG:HH11	1.86	0.41
3:A:81:GLN:CB	3:A:92:ASN:ND2	2.84	0.41
1:0:1249:U:H2'	1:0:1250:C:C6	2.56	0.41
16:N:73:ALA:HB1	16:N:74:PRO:CD	2.50	0.41
1:0:155:C:OP2	15:M:188:ARG:HD3	2.20	0.41
1:0:612:U:H2'	1:0:613:C:C6	2.56	0.41
1:0:2015:A:H2'	1:0:2016:U:O4'	2.20	0.41
11:I:95:LEU:HG	11:I:132:VAL:CG1	2.51	0.40
13:K:98:VAL:HG13	13:K:102:GLU:CA	2.46	0.40
10:H:61:ARG:HG3	10:H:61:ARG:NH1	2.36	0.40
1:0:1268:C:O2'	1:0:1269:G:H5'	2.20	0.40
1:0:1328:A:C8	27:Y:169:ARG:HD3	2.56	0.40
6:D:99:ASP:N	6:D:103:ASN:O	2.30	0.40
3:A:179:MET:HG2	3:A:186:TRP:HB2	2.01	0.40
1:0:447:A:O2'	1:0:448:G:H5'	2.22	0.40
22:T:48:VAL:HG23	22:T:98:VAL:HA	2.03	0.40
1:0:213:G:O2'	1:0:214:U:OP2	2.40	0.40
18:P:40:VAL:O	18:P:44:VAL:HG23	2.21	0.40
1:0:1773:G:C8	28:Z:16:ALA:HA	2.55	0.40
26:X:12:ILE:HD12	26:X:36:HIS:ND1	2.36	0.40
1:0:2382:A:H5'	39:3:8962:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:236:THR:C	39:C:8653:HOH:O	2.60	0.40
4:B:310:ARG:HD2	39:B:9057:HOH:O	2.20	0.40
1:O:655:U:O2'	17:O:3:THR:HB	2.21	0.40
12:J:46:ILE:HD11	12:J:53:ILE:CG2	2.51	0.40
10:H:6:ALA:CB	10:H:61:ARG:HH12	2.33	0.40
9:G:12:ILE:N	9:G:13:PRO:CD	2.84	0.40
4:B:254:GLN:NE2	39:B:9058:HOH:O	2.54	0.40
29:1:37:CYS:SG	29:1:39:PHE:HB2	2.61	0.40
22:T:45:GLY:C	39:T:3851:HOH:O	2.59	0.40
22:T:49:GLU:OE2	22:T:51:LEU:HD21	2.21	0.40
30:2:18:ASN:ND2	30:2:40:ARG:H	2.19	0.40
7:E:32:ARG:O	7:E:33:LEU:HD23	2.21	0.40
8:F:8:VAL:HG13	8:F:12:LEU:HD13	2.02	0.40
1:O:1072:G:OP2	27:Y:154:ARG:NH2	2.54	0.40
24:V:8:ILE:HG21	24:V:59:ILE:HG13	2.02	0.40
1:O:1398:G:H2'	1:O:1399:A:C8	2.56	0.40
16:N:129:ILE:HA	16:N:130:PRO:HD3	1.98	0.40
1:O:1304:U:H2'	1:O:1305:C:C6	2.56	0.40
8:F:52:GLU:HG3	8:F:77:VAL:O	2.21	0.40
1:O:59:A:H5'	39:O:4798:HOH:O	2.20	0.40
16:N:51:GLY:HA2	16:N:52:PRO:HD3	1.94	0.40
27:Y:108:ASP:N	27:Y:108:ASP:OD1	2.53	0.40
4:B:62:ARG:HG2	4:B:65:MET:HE3	2.03	0.40
1:O:1186:C:H4'	11:I:114:TYR:HE1	1.87	0.40
6:D:138:GLY:N	39:D:7597:HOH:O	2.29	0.40
6:D:38:GLU:HB3	6:D:49:PRO:HG3	2.02	0.40
16:N:86:LEU:HD12	16:N:125:ALA:HB2	2.04	0.40
8:F:107:ASP:O	8:F:111:ILE:HG13	2.21	0.40
16:N:72:GLU:H	16:N:171:HIS:CE1	2.39	0.40
1:O:1020:A:H1'	39:Q:6976:HOH:O	2.22	0.40
1:O:861:A:H4'	1:O:1697:G:H4'	2.03	0.40
1:O:2445:U:H2'	1:O:2446:G:C8	2.56	0.40
13:K:99:ASP:OD1	13:K:101:ASN:N	2.53	0.40
39:O:4832:HOH:O	3:A:212:PRO:HB2	2.20	0.40
7:E:69:ILE:HA	7:E:72:MET:HE2	2.01	0.40
2:9:114:G:H2'	2:9:115:C:C6	2.57	0.40
10:H:33:GLN:H	10:H:69:ARG:NH1	2.19	0.40
16:N:38:LYS:HB2	16:N:38:LYS:HE3	1.80	0.40
5:C:6:TYR:HE1	5:C:133:ARG:HH22	1.68	0.40
1:O:820:G:C5	3:A:171:LYS:HB2	2.57	0.40
1:O:212:A:O4'	1:O:214:U:C6	2.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:149:ARG:O	14:L:150:GLN:HB2	2.21	0.40
1:0:1039:G:H2'	1:0:1040:A:O4'	2.22	0.40
2:9:31:C:H2'	2:9:32:G:O4'	2.22	0.40
1:0:2435:U:OP1	31:3:28:GLY:HA3	2.20	0.40
1:0:2900:G:H2'	1:0:2901:C:O4'	2.22	0.40
1:0:1829:A:H2'	1:0:1830:C:H5'	2.04	0.40
1:0:278:A:H2'	1:0:279:C:O4'	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	235/240 (98%)	218 (93%)	13 (6%)	4 (2%)	11	14
4	B	335/338 (99%)	314 (94%)	14 (4%)	7 (2%)	9	10
5	C	244/246 (99%)	226 (93%)	18 (7%)	0	100	100
6	D	134/177 (76%)	103 (77%)	20 (15%)	11 (8%)	1	0
7	E	170/178 (96%)	163 (96%)	7 (4%)	0	100	100
8	F	117/120 (98%)	104 (89%)	10 (8%)	3 (3%)	7	6
9	G	25/348 (7%)	25 (100%)	0	0	100	100
10	H	156/177 (88%)	143 (92%)	13 (8%)	0	100	100
11	I	68/162 (42%)	49 (72%)	17 (25%)	2 (3%)	6	5
12	J	140/145 (97%)	130 (93%)	8 (6%)	2 (1%)	14	19
13	K	130/132 (98%)	122 (94%)	8 (6%)	0	100	100
14	L	141/165 (86%)	124 (88%)	16 (11%)	1 (1%)	26	38
15	M	192/194 (99%)	181 (94%)	11 (6%)	0	100	100
16	N	184/187 (98%)	166 (90%)	13 (7%)	5 (3%)	6	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	O	113/116 (97%)	110 (97%)	3 (3%)	0	100	100
18	P	141/149 (95%)	139 (99%)	2 (1%)	0	100	100
19	Q	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
20	R	148/155 (96%)	142 (96%)	6 (4%)	0	100	100
21	S	79/85 (93%)	74 (94%)	5 (6%)	0	100	100
22	T	117/120 (98%)	111 (95%)	5 (4%)	1 (1%)	21	30
23	U	51/66 (77%)	49 (96%)	2 (4%)	0	100	100
24	V	63/71 (89%)	58 (92%)	2 (3%)	3 (5%)	3	1
25	W	152/154 (99%)	147 (97%)	3 (2%)	2 (1%)	15	21
26	X	80/92 (87%)	73 (91%)	7 (9%)	0	100	100
27	Y	140/241 (58%)	139 (99%)	1 (1%)	0	100	100
28	Z	71/83 (86%)	61 (86%)	7 (10%)	3 (4%)	3	2
29	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
30	2	42/50 (84%)	40 (95%)	1 (2%)	1 (2%)	7	7
31	3	90/92 (98%)	85 (94%)	5 (6%)	0	100	100
All	All	3705/4436 (84%)	3437 (93%)	223 (6%)	45 (1%)	16	23

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	27	LEU
3	A	37	VAL
6	D	171	ASP
8	F	101	ALA
12	J	5	GLU
14	L	80	ASP
16	N	154	LEU
16	N	183	ASP
16	N	184	ILE
24	V	43	PRO
28	Z	81	ARG
4	B	139	ASP
6	D	27	ILE
6	D	56	ARG
6	D	65	GLU
6	D	173	GLU
12	J	143	LYS

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Mol	Chain	Res	Type
22	T	53	GLY
25	W	77	ALA
28	Z	42	CYS
3	A	34	ASP
4	B	34	GLY
4	B	169	GLY
4	B	185	GLY
6	D	61	PHE
6	D	97	GLN
11	I	91	PHE
16	N	164	ASP
6	D	16	PRO
6	D	60	GLU
8	F	100	ASP
16	N	139	TRP
4	B	2	GLN
4	B	107	SER
4	B	184	ASP
6	D	28	GLY
25	W	49	ASN
28	Z	41	ASN
30	2	37	HIS
3	A	132	ASP
8	F	71	GLY
11	I	109	PRO
24	V	40	PRO
6	D	69	ILE
24	V	39	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	179/182 (98%)	167 (93%)	12 (7%)	20	31
4	B	282/283 (100%)	268 (95%)	14 (5%)	30	48
5	C	193/193 (100%)	175 (91%)	18 (9%)	11	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	D	117/148 (79%)	113 (97%)	4 (3%)	44	65
7	E	152/156 (97%)	147 (97%)	5 (3%)	45	66
8	F	93/94 (99%)	92 (99%)	1 (1%)	80	92
9	G	27/283 (10%)	27 (100%)	0	100	100
10	H	134/145 (92%)	129 (96%)	5 (4%)	41	62
11	I	58/130 (45%)	58 (100%)	0	100	100
12	J	118/121 (98%)	110 (93%)	8 (7%)	20	31
13	K	106/106 (100%)	105 (99%)	1 (1%)	84	93
14	L	113/127 (89%)	110 (97%)	3 (3%)	52	73
15	M	158/158 (100%)	151 (96%)	7 (4%)	35	53
16	N	149/150 (99%)	145 (97%)	4 (3%)	52	73
17	O	93/94 (99%)	91 (98%)	2 (2%)	60	79
18	P	113/117 (97%)	112 (99%)	1 (1%)	84	93
19	Q	79/80 (99%)	76 (96%)	3 (4%)	40	60
20	R	117/122 (96%)	115 (98%)	2 (2%)	68	85
21	S	71/74 (96%)	69 (97%)	2 (3%)	51	72
22	T	105/106 (99%)	100 (95%)	5 (5%)	31	49
23	U	44/52 (85%)	44 (100%)	0	100	100
24	V	51/57 (90%)	49 (96%)	2 (4%)	39	59
25	W	130/130 (100%)	125 (96%)	5 (4%)	40	60
26	X	66/74 (89%)	59 (89%)	7 (11%)	8	12
27	Y	120/196 (61%)	111 (92%)	9 (8%)	17	26
28	Z	60/68 (88%)	58 (97%)	2 (3%)	45	66
29	1	46/47 (98%)	46 (100%)	0	100	100
30	2	42/46 (91%)	41 (98%)	1 (2%)	57	76
31	3	79/79 (100%)	79 (100%)	0	100	100
All	All	3095/3618 (86%)	2972 (96%)	123 (4%)	38	58

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	3	ARG
3	A	26	ASP

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Mol	Chain	Res	Type
3	A	33	GLU
3	A	36	ASP
3	A	55	VAL
3	A	78	ASP
3	A	94	LEU
3	A	120	ARG
3	A	131	HIS
3	A	153	ARG
3	A	179	MET
3	A	217	ARG
4	B	7	ARG
4	B	11	LEU
4	B	27	ASN
4	B	49	THR
4	B	53	LEU
4	B	56	ASP
4	B	98	THR
4	B	162	MET
4	B	174	ARG
4	B	175	LEU
4	B	195	ARG
4	B	254	GLN
4	B	264	GLU
4	B	312	ARG
5	C	2	GLN
5	C	27	ARG
5	C	67	GLN
5	C	76	ARG
5	C	78	ARG
5	C	91	PRO
5	C	94	THR
5	C	101	ASP
5	C	136	VAL
5	C	162	VAL
5	C	187	ARG
5	C	214	THR
5	C	222	ASP
5	C	223	LEU
5	C	234	VAL
5	C	236	THR
5	C	240	LEU
5	C	243	VAL

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Mol	Chain	Res	Type
6	D	24	HIS
6	D	61	PHE
6	D	133	ASN
6	D	136	ARG
7	E	7	ILE
7	E	15	GLN
7	E	16	ASP
7	E	86	VAL
7	E	102	VAL
8	F	12	LEU
10	H	87	LYS
10	H	91	ARG
10	H	114	ASP
10	H	157	TYR
10	H	162	PRO
12	J	7	ASP
12	J	46	ILE
12	J	52	GLN
12	J	74	ARG
12	J	76	ASP
12	J	79	PHE
12	J	107	ASN
12	J	127	ILE
13	K	10	GLN
14	L	35	ARG
14	L	104	ASP
14	L	117	GLU
15	M	46	LEU
15	M	68	ARG
15	M	81	ARG
15	M	93	ARG
15	M	99	ARG
15	M	116	ASN
15	M	164	THR
16	N	17	ARG
16	N	26	LEU
16	N	127	LEU
16	N	139	TRP
17	O	3	THR
17	O	111	VAL
18	P	98	ILE
19	Q	11	ARG

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Mol	Chain	Res	Type
19	Q	16	ASN
19	Q	95	GLU
20	R	13	THR
20	R	39	THR
21	S	12	GLU
21	S	71	ASP
22	T	39	ASN
22	T	48	VAL
22	T	73	HIS
22	T	89	ARG
22	T	115	GLU
24	V	43	PRO
24	V	65	ASP
25	W	35	VAL
25	W	52	VAL
25	W	73	LEU
25	W	122	ARG
25	W	146	ILE
26	X	15	ARG
26	X	27	ASP
26	X	46	ASP
26	X	49	ARG
26	X	72	VAL
26	X	79	GLU
26	X	82	GLU
27	Y	103	THR
27	Y	115	ARG
27	Y	141	THR
27	Y	154	ARG
27	Y	187	VAL
27	Y	189	ASN
27	Y	200	THR
27	Y	203	VAL
27	Y	220	GLU
28	Z	33	MET
28	Z	44	GLU
30	2	18	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	92	ASN

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Mol	Chain	Res	Type
3	A	199	HIS
4	B	27	ASN
4	B	145	HIS
4	B	191	ASN
4	B	221	GLN
4	B	238	ASN
4	B	260	HIS
4	B	320	GLN
4	B	332	ASN
5	C	2	GLN
5	C	39	GLN
5	C	129	HIS
6	D	47	GLN
6	D	97	GLN
6	D	103	ASN
6	D	133	ASN
7	E	15	GLN
7	E	90	HIS
7	E	106	ASN
7	E	119	HIS
7	E	143	GLN
9	G	17	GLN
9	G	64	ASN
10	H	34	HIS
10	H	59	GLN
10	H	62	HIS
10	H	73	ASN
11	I	88	GLN
11	I	99	GLN
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
15	M	24	GLN
15	M	26	GLN
15	M	58	GLN
15	M	137	ASN
15	M	170	ASN

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Mol	Chain	Res	Type
16	N	40	ASN
16	N	93	GLN
16	N	107	ASN
16	N	153	GLN
18	P	50	GLN
18	P	66	GLN
18	P	73	HIS
18	P	118	GLN
19	Q	16	ASN
19	Q	40	HIS
20	R	61	GLN
20	R	94	ASN
20	R	98	ASN
20	R	113	HIS
20	R	117	HIS
21	S	25	GLN
21	S	51	GLN
22	T	39	ASN
22	T	73	HIS
23	U	39	ASN
23	U	48	ASN
24	V	60	GLN
25	W	27	HIS
25	W	28	HIS
25	W	59	GLN
25	W	110	GLN
25	W	119	HIS
25	W	125	HIS
25	W	141	HIS
26	X	23	HIS
27	Y	133	HIS
27	Y	134	HIS
27	Y	149	GLN
27	Y	189	ASN
29	1	8	GLN
29	1	16	HIS
29	1	28	HIS
30	2	16	ASN
30	2	18	ASN
30	2	41	HIS
30	2	45	ASN
31	3	15	ASN

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Mol	Chain	Res	Type
31	3	30	GLN
31	3	48	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	226 (8%)	34 (1%)
2	9	121/122 (99%)	16 (13%)	1 (0%)
All	All	2866/3044 (94%)	242 (8%)	35 (1%)

All (242) 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	130	C
1	0	141	C
1	0	151	A
1	0	166	A
1	0	170	U
1	0	186	A
1	0	191	A
1	0	192	A
1	0	200	C
1	0	219	G
1	0	237	G
1	0	271	C
1	0	272	A
1	0	273	G
1	0	283	U
1	0	284	C
1	0	308	U
1	0	309	C

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Mol	Chain	Res	Type
1	0	318	U
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	510	U
1	0	511	A
1	0	514	G
1	0	537	G
1	0	538	C
1	0	539	G
1	0	542	A
1	0	545	G
1	0	553	G
1	0	559	U
1	0	581	G
1	0	588	G
1	0	604	G
1	0	620	A
1	0	632	A
1	0	644	G
1	0	660	A
1	0	688	A
1	0	698	A
1	0	701	U
1	0	759	C
1	0	777	U
1	0	809	G
1	0	821	U
1	0	835	U
1	0	840	U
1	0	846	A
1	0	868	G
1	0	869	G
1	0	871	G

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Mol	Chain	Res	Type
1	0	872	U
1	0	875	A
1	0	877	G
1	0	878	G
1	0	884	C
1	0	885	G
1	0	898	G
1	0	905	C
1	0	920	C
1	0	921	G
1	0	923	A
1	0	953	G
1	0	960	G
1	0	961	A
1	0	1006	A
1	0	1008	C
1	0	1029	U
1	0	1045	G
1	0	1059	G
1	0	1060	C
1	0	1072	G
1	0	1081	A
1	0	1088	A
1	0	1109	U
1	0	1110	G
1	0	1119	G
1	0	1130	U
1	0	1164	U
1	0	1165	G
1	0	1166	A
1	0	1174	A
1	0	1175	G
1	0	1185	U
1	0	1192	A
1	0	1193	A
1	0	1206	U
1	0	1216	G
1	0	1237	U
1	0	1238	C
1	0	1239	G
1	0	1279	U
1	0	1289	C

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Mol	Chain	Res	Type
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	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	1731	C
1	0	1732	A
1	0	1752	G
1	0	1778	A
1	0	1798	C
1	0	1819	G
1	0	1820	G
1	0	1829	A
1	0	1856	C
1	0	1857	A
1	0	1879	U
1	0	1919	A

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Mol	Chain	Res	Type
1	0	1942	A
1	0	1971	G
1	0	1973	A
1	0	1978	A
1	0	1979	G
1	0	1980	U
1	0	1996	U
1	0	2008	U
1	0	2011	A
1	0	2012	U
1	0	2013	G
1	0	2033	G
1	0	2034	U
1	0	2064	U
1	0	2072	G
1	0	2073	G
1	0	2074	A
1	0	2096	A
1	0	2101	A
1	0	2102	G
1	0	2103	A
1	0	2104	C
1	0	2110	G
1	0	2243	C
1	0	2258	A
1	0	2271	G
1	0	2272	G
1	0	2317	C
1	0	2321	A
1	0	2354	A
1	0	2361	A
1	0	2369	A
1	0	2379	G
1	0	2422	U
1	0	2462	G
1	0	2476	C
1	0	2483	A
1	0	2507	G
1	0	2509	A
1	0	2511	A
1	0	2533	C
1	0	2537	G

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Mol	Chain	Res	Type
1	0	2541	U
1	0	2553	A
1	0	2564	G
1	0	2589	U
1	0	2601	A
1	0	2602	G
1	0	2608	C
1	0	2613	G
1	0	2649	A
1	0	2664	A
1	0	2676	C
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	2792	A
1	0	2800	A
1	0	2811	A
1	0	2812	A
1	0	2825	C
1	0	2876	G
1	0	2890	A
1	0	2896	A
1	0	2903	C
1	0	2914	A
2	9	2	U
2	9	14	G
2	9	22	G
2	9	23	U
2	9	24	U
2	9	25	G
2	9	40	C
2	9	41	C
2	9	43	G
2	9	44	A
2	9	52	A
2	9	57	A

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Mol	Chain	Res	Type
2	9	66	G
2	9	77	A
2	9	114	G
2	9	122	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	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
1	0	1080	C
1	0	1232	A
1	0	1237	U
1	0	1246	A
1	0	1352	A
1	0	1377	C
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	2103	A
1	0	2313	C
1	0	2467	A
1	0	2526	C
1	0	2536	C
1	0	2538	A
1	0	2649	A
1	0	2718	C
1	0	2726	U
1	0	2761	A
1	0	2791	U

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Mol	Chain	Res	Type
2	9	65	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMU	0	2587	1	12,22,23	1.06	1 (8%)	19,31,34	3.14	2 (10%)
1	OMG	0	2588	1	17,26,27	1.06	1 (5%)	21,38,41	2.57	3 (14%)
1	UR3	0	2619	1	12,22,23	0.81	0	16,32,35	0.79	0
1	PSU	0	2621	1	13,21,22	1.56	2 (15%)	18,30,33	6.09	3 (16%)
1	1MA	0	628	1	14,25,26	1.00	1 (7%)	15,37,40	1.16	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	-	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	-	0/3/25/26	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C5-C1'	-4.69	1.48	1.52
1	0	2587	OMU	C4-N3	2.51	1.37	1.33
1	0	2621	PSU	C4-N3	2.63	1.38	1.33
1	0	628	1MA	C6-N6	2.64	1.33	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2588	OMG	C6-N1	3.22	1.39	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	N1-C2-N3	-21.41	114.67	128.33
1	0	2588	OMG	C5-C6-N1	-8.89	111.44	123.59
1	0	628	1MA	C2-N3-C4	-3.61	110.81	116.40
1	0	2587	OMU	C5-C4-N3	-3.23	114.84	123.12
1	0	2588	OMG	N3-C2-N1	-2.28	123.97	127.44
1	0	2621	PSU	C6-N1-C2	2.84	120.04	115.47
1	0	2588	OMG	C6-N1-C2	6.76	125.33	115.94
1	0	2587	OMU	C4-N3-C2	13.04	127.05	114.14
1	0	2621	PSU	C4-N3-C2	13.82	127.19	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 306 ligands modelled in this entry, 305 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	ZIT	0	9500	-	54,54,54	1.33	5 (9%)	76,83,83	1.06	5 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	ZIT	0	9500	-	-	0/72/107/107	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	0	9500	ZIT	C6-C5	2.13	1.60	1.55
32	0	9500	ZIT	C13-C12	2.23	1.61	1.55
32	0	9500	ZIT	O13-C13	2.51	1.48	1.44
32	0	9500	ZIT	C13-C14	3.00	1.60	1.54
32	0	9500	ZIT	C22-C11	3.48	1.58	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	0	9500	ZIT	C2B-C3B-C4B	-2.54	104.64	107.81
32	0	9500	ZIT	C4A-C3A-C2A	-2.15	106.90	110.03
32	0	9500	ZIT	O6-C6-C7	2.05	113.87	108.34
32	0	9500	ZIT	C14-O14-C1	2.07	121.61	118.12
32	0	9500	ZIT	C7-C8-C9	2.58	116.14	112.39

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.28	98 (3%) 46 47	15, 38, 82, 157	0
2	9	122/122 (100%)	0.05	6 (4%) 33 34	32, 58, 80, 139	0
3	A	237/240 (98%)	0.31	14 (5%) 26 26	19, 40, 75, 96	0
4	B	337/338 (99%)	0.24	10 (2%) 54 53	21, 47, 73, 84	0
5	C	246/246 (100%)	-0.09	3 (1%) 81 81	17, 36, 60, 69	0
6	D	140/177 (79%)	2.24	71 (50%) 0 0	51, 88, 114, 122	0
7	E	172/178 (96%)	0.95	29 (16%) 2 2	39, 61, 80, 84	0
8	F	119/120 (99%)	0.89	23 (19%) 2 1	38, 62, 88, 103	0
9	G	29/348 (8%)	3.36	25 (86%) 0 0	71, 87, 93, 95	0
10	H	160/177 (90%)	0.50	17 (10%) 8 8	31, 50, 83, 91	0
11	I	70/162 (43%)	7.19	70 (100%) 0 0	122, 135, 154, 155	0
12	J	142/145 (97%)	0.12	4 (2%) 56 55	29, 44, 65, 88	0
13	K	132/132 (100%)	-0.05	4 (3%) 54 53	24, 43, 65, 77	0
14	L	145/165 (87%)	0.67	19 (13%) 5 4	18, 56, 101, 115	0
15	M	194/194 (100%)	0.08	1 (0%) 91 91	21, 33, 49, 56	0
16	N	186/187 (99%)	0.80	27 (14%) 3 3	34, 55, 102, 112	0
17	O	115/116 (99%)	0.09	4 (3%) 48 48	30, 45, 61, 69	0
18	P	143/149 (95%)	0.00	0 100 100	30, 44, 57, 68	0
19	Q	95/96 (98%)	0.01	1 (1%) 82 82	30, 37, 54, 68	0
20	R	150/155 (96%)	-0.10	1 (0%) 89 88	25, 38, 58, 66	0
21	S	81/85 (95%)	0.17	2 (2%) 61 60	34, 50, 71, 81	0
22	T	119/120 (99%)	0.47	8 (6%) 21 21	29, 47, 76, 103	0
23	U	53/66 (80%)	0.35	2 (3%) 44 45	35, 48, 66, 78	0
24	V	65/71 (91%)	1.55	13 (20%) 1 1	43, 62, 107, 113	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	154/154 (100%)	0.02	1 (0%) 90 90	29, 43, 58, 69	0
26	X	82/92 (89%)	0.61	10 (12%) 5 5	37, 50, 78, 94	0
27	Y	142/241 (58%)	0.18	5 (3%) 48 48	21, 36, 59, 80	0
28	Z	73/83 (87%)	0.12	2 (2%) 58 57	35, 51, 68, 86	0
29	1	56/57 (98%)	-0.40	0 100 100	18, 24, 32, 43	0
30	2	46/50 (92%)	0.55	5 (10%) 7 7	26, 51, 75, 89	0
31	3	92/92 (100%)	0.28	2 (2%) 65 64	26, 48, 62, 77	0
All	All	6646/7480 (88%)	0.18	477 (7%) 18 18	15, 43, 89, 157	0

All (477) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	I	74	ILE	16.0
11	I	91	PHE	15.6
11	I	66	GLY	15.1
11	I	128	THR	14.7
11	I	88	GLN	14.2
11	I	71	ALA	14.0
24	V	1	THR	13.7
11	I	80	PHE	12.9
11	I	132	VAL	11.8
6	D	63	ILE	11.7
11	I	97	VAL	11.5
2	9	1	U	11.2
11	I	100	VAL	11.1
11	I	104	ALA	10.3
6	D	10	PHE	10.0
11	I	131	GLY	9.8
16	N	166	ALA	9.5
11	I	70	THR	9.4
24	V	39	ALA	9.3
11	I	92	VAL	9.3
11	I	86	GLU	9.1
11	I	93	ALA	8.8
11	I	103	ILE	8.6
11	I	111	LEU	8.4
11	I	108	HIS	8.3
11	I	127	CYS	8.2
3	A	37	VAL	8.0
11	I	78	ALA	8.0

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Mol	Chain	Res	Type	RSRZ
11	I	116	LEU	7.9
11	I	83	GLY	7.8
11	I	84	SER	7.8
11	I	109	PRO	7.7
24	V	40	PRO	7.7
11	I	113	SER	7.7
1	0	1198	U	7.7
11	I	82	THR	7.6
11	I	106	GLN	7.5
11	I	76	ASP	7.3
11	I	72	GLU	7.2
11	I	99	GLN	7.2
11	I	79	GLY	7.1
6	D	61	PHE	7.0
11	I	112	LEU	6.8
11	I	118	ASN	6.7
6	D	57	THR	6.7
1	0	1177	A	6.6
26	X	88	GLU	6.6
11	I	89	GLU	6.5
1	0	1951	G	6.5
11	I	98	ASP	6.4
6	D	170	TYR	6.4
11	I	87	PRO	6.4
1	0	2237	G	6.3
1	0	1172	G	6.2
11	I	124	VAL	6.2
9	G	23	ILE	6.2
11	I	129	SER	6.1
10	H	174	LEU	6.0
6	D	11	HIS	6.0
6	D	69	ILE	6.0
6	D	26	GLY	6.0
11	I	133	THR	6.0
11	I	130	LEU	5.9
3	A	237	GLY	5.9
11	I	90	ASP	5.9
11	I	73	LEU	5.8
11	I	120	ALA	5.8
1	0	1199	A	5.8
24	V	38	GLY	5.7
11	I	102	GLN	5.7

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Mol	Chain	Res	Type	RSRZ
1	0	1169	U	5.6
1	0	1192	A	5.6
1	0	1202	A	5.6
9	G	24	VAL	5.5
11	I	121	LYS	5.5
6	D	64	ARG	5.5
11	I	117	THR	5.5
11	I	68	PRO	5.4
1	0	1181	A	5.3
6	D	90	LEU	5.2
11	I	75	LYS	5.1
1	0	1163	G	5.1
1	0	1176	C	5.1
11	I	81	GLU	5.1
11	I	94	ASP	5.1
11	I	67	VAL	5.1
1	0	1168	C	5.0
14	L	80	ASP	5.0
1	0	1178	G	5.0
1	0	1173	A	4.9
9	G	71	LEU	4.9
1	0	970	U	4.8
11	I	69	PRO	4.8
9	G	27	ILE	4.8
2	9	2	U	4.7
1	0	2238	A	4.7
21	S	81	ILE	4.7
6	D	40	ILE	4.6
2	9	24	U	4.6
24	V	43	PRO	4.6
1	0	1525	G	4.6
9	G	26	MET	4.5
22	T	116	ASP	4.5
1	0	960	G	4.5
22	T	119	ALA	4.5
11	I	110	ASP	4.5
11	I	107	LYS	4.5
22	T	118	SER	4.5
11	I	95	LEU	4.5
1	0	1179	C	4.4
9	G	66	LEU	4.4
11	I	85	GLY	4.4

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Mol	Chain	Res	Type	RSRZ
7	E	127	ASP	4.4
9	G	20	VAL	4.3
11	I	119	ALA	4.3
6	D	166	ILE	4.3
4	B	57	GLU	4.3
6	D	93	LEU	4.3
6	D	58	VAL	4.3
26	X	85	VAL	4.3
1	0	1950	G	4.2
6	D	44	ILE	4.2
6	D	66	GLY	4.2
3	A	35	GLY	4.2
7	E	45	ASP	4.2
6	D	85	GLN	4.2
1	0	1200	A	4.2
1	0	2004	U	4.2
6	D	106	PHE	4.2
1	0	1948	G	4.2
7	E	87	PHE	4.2
11	I	125	GLY	4.1
9	G	73	ASP	4.1
11	I	126	THR	4.1
11	I	105	GLU	4.1
8	F	119	ARG	4.1
16	N	181	ASP	4.1
6	D	88	LEU	4.1
14	L	81	VAL	4.0
9	G	72	ASP	4.0
10	H	169	GLU	4.0
16	N	152	GLU	4.0
1	0	1170	U	4.0
1	0	1175	G	4.0
11	I	114	TYR	4.0
1	0	284	C	4.0
1	0	999	C	4.0
6	D	62	ASP	3.9
14	L	77	ALA	3.9
6	D	56	ARG	3.9
1	0	10	U	3.9
9	G	69	ARG	3.9
31	3	92	GLU	3.9
4	B	183	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
26	X	80	GLU	3.9
1	0	1180	U	3.9
6	D	68	PRO	3.9
10	H	40	GLN	3.9
1	0	1182	C	3.8
30	2	49	GLU	3.8
1	0	735	C	3.8
6	D	92	GLU	3.8
6	D	172	VAL	3.8
11	I	122	GLU	3.8
27	Y	235	GLU	3.7
6	D	27	ILE	3.7
9	G	21	ASP	3.7
1	0	1171	A	3.7
7	E	86	VAL	3.7
14	L	60	GLU	3.7
6	D	86	THR	3.6
27	Y	95	THR	3.6
10	H	172	GLU	3.6
16	N	158	LEU	3.6
11	I	115	ASP	3.6
1	0	282	C	3.6
30	2	39	ARG	3.6
14	L	75	LEU	3.6
3	A	85	SER	3.6
8	F	106	ALA	3.5
9	G	70	ALA	3.5
19	Q	95	GLU	3.5
9	G	67	LEU	3.5
26	X	7	GLU	3.5
1	0	2344	G	3.5
11	I	101	LYS	3.5
16	N	177	GLU	3.5
7	E	10	ASP	3.5
2	9	23	U	3.5
14	L	149	ARG	3.5
11	I	77	GLU	3.5
1	0	1949	G	3.5
6	D	135	VAL	3.5
6	D	18	ILE	3.4
22	T	117	ASP	3.4
9	G	18	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
9	G	65	THR	3.4
1	0	285	A	3.4
1	0	1190	G	3.4
6	D	41	LEU	3.4
8	F	118	LEU	3.4
6	D	165	PHE	3.4
11	I	123	VAL	3.3
1	0	1162	G	3.3
6	D	104	PHE	3.3
1	0	1167	G	3.3
5	C	135	GLU	3.3
16	N	183	ASP	3.3
9	G	68	GLU	3.3
8	F	25	ASP	3.3
16	N	68	GLU	3.3
24	V	41	GLU	3.3
1	0	2508	C	3.3
6	D	107	GLY	3.3
9	G	22	ALA	3.3
23	U	47	ARG	3.3
3	A	36	ASP	3.3
11	I	96	SER	3.3
1	0	1165	G	3.3
1	0	138	U	3.2
3	A	133	ARG	3.2
6	D	89	PRO	3.2
1	0	1625	U	3.2
6	D	75	LEU	3.2
6	D	157	LEU	3.2
9	G	28	GLU	3.2
1	0	1191	A	3.2
1	0	1183	C	3.2
1	0	2769	C	3.2
7	E	100	ASP	3.1
14	L	91	VAL	3.1
16	N	150	TYR	3.1
8	F	15	ASP	3.1
16	N	180	LEU	3.1
1	0	497	A	3.1
1	0	1193	A	3.1
16	N	155	GLU	3.1
8	F	22	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
6	D	38	GLU	3.1
3	A	97	ALA	3.1
1	0	1184	C	3.1
1	0	1964	U	3.1
1	0	272	A	3.1
1	0	1174	A	3.1
14	L	147	GLU	3.1
14	L	148	GLU	3.1
4	B	1	PRO	3.1
16	N	162	ASP	3.1
1	0	280	C	3.0
22	T	82	THR	3.0
1	0	283	U	3.0
22	T	115	GLU	3.0
9	G	25	GLU	3.0
14	L	150	GLN	3.0
6	D	43	GLU	3.0
6	D	67	ASP	2.9
7	E	43	ASP	2.9
27	Y	108	ASP	2.9
7	E	6	GLU	2.9
7	E	88	TYR	2.9
13	K	132	VAL	2.9
6	D	74	THR	2.9
16	N	164	ASP	2.9
16	N	139	TRP	2.9
30	2	35	ARG	2.9
1	0	1197	G	2.9
6	D	173	GLU	2.9
16	N	154	LEU	2.9
1	0	1164	U	2.9
7	E	126	ILE	2.9
9	G	15	TRP	2.9
2	9	122	C	2.9
10	H	170	ARG	2.9
7	E	121	ASP	2.9
10	H	86	TYR	2.9
21	S	76	GLU	2.8
27	Y	216	ARG	2.8
3	A	236	GLY	2.8
7	E	131	LEU	2.8
10	H	149	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
6	D	98	PHE	2.8
1	0	1196	C	2.8
4	B	180	ASP	2.8
6	D	23	VAL	2.8
1	0	1203	G	2.8
6	D	55	LYS	2.8
7	E	129	GLU	2.8
3	A	135	VAL	2.8
6	D	171	ASP	2.8
8	F	103	GLU	2.8
1	0	1279	U	2.8
7	E	95	VAL	2.8
27	Y	236	VAL	2.8
14	L	102	ASP	2.8
1	0	1947	G	2.7
1	0	1965	C	2.7
7	E	108	LEU	2.7
8	F	107	ASP	2.7
1	0	1186	C	2.7
1	0	2239	C	2.7
14	L	76	LEU	2.7
1	0	1527	A	2.7
9	G	17	GLN	2.7
1	0	1204	C	2.7
7	E	94	GLN	2.7
8	F	18	GLU	2.7
12	J	5	GLU	2.7
24	V	59	ILE	2.7
1	0	1208	C	2.7
1	0	1526	A	2.7
1	0	2637	A	2.7
8	F	16	ALA	2.7
8	F	100	ASP	2.7
12	J	4	ALA	2.7
6	D	65	GLU	2.6
3	A	34	ASP	2.6
14	L	105	TYR	2.6
7	E	154	ILE	2.6
16	N	140	GLN	2.6
8	F	14	ASP	2.6
16	N	149	GLU	2.6
26	X	77	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	0	372	A	2.6
1	0	1201	C	2.6
6	D	25	MET	2.6
8	F	90	GLU	2.6
16	N	163	PHE	2.6
6	D	29	HIS	2.6
10	H	165	ARG	2.6
1	0	1000	C	2.5
6	D	134	LEU	2.5
1	0	736	A	2.5
6	D	154	LYS	2.5
6	D	48	MET	2.5
1	0	362	G	2.5
13	K	118	ALA	2.5
1	0	1207	A	2.5
6	D	50	VAL	2.5
10	H	48	VAL	2.5
10	H	50	ILE	2.5
16	N	147	ILE	2.5
7	E	128	GLY	2.5
28	Z	11	SER	2.5
1	0	1166	A	2.5
14	L	99	GLU	2.5
10	H	76	LEU	2.5
1	0	279	C	2.5
3	A	31	LYS	2.5
24	V	37	GLY	2.5
6	D	81	GLU	2.5
10	H	144	GLU	2.5
16	N	160	SER	2.5
1	0	2511	A	2.5
6	D	130	VAL	2.5
5	C	132	ASP	2.5
14	L	79	ASP	2.5
14	L	106	VAL	2.4
1	0	1967	U	2.4
6	D	45	THR	2.4
3	A	38	ILE	2.4
9	G	14	GLU	2.4
1	0	128	A	2.4
6	D	95	THR	2.4
26	X	41	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
26	X	71	ARG	2.4
24	V	8	ILE	2.4
4	B	134	ALA	2.4
12	J	110	ASP	2.4
1	0	1185	U	2.4
1	0	1206	U	2.4
17	O	23	GLY	2.4
16	N	185	GLU	2.4
10	H	85	ASP	2.4
26	X	72	VAL	2.4
1	0	1189	A	2.4
4	B	169	GLY	2.4
24	V	10	ASP	2.4
11	I	134	ILE	2.4
31	3	62	THR	2.3
6	D	70	GLY	2.3
12	J	70	PHE	2.3
7	E	11	VAL	2.3
7	E	89	SER	2.3
24	V	2	VAL	2.3
1	0	969	G	2.3
11	I	135	GLU	2.3
24	V	63	GLU	2.3
1	0	1188	A	2.3
16	N	159	TYR	2.3
9	G	12	ILE	2.3
1	0	371	U	2.3
6	D	128	LEU	2.3
9	G	63	ARG	2.3
6	D	158	ASN	2.3
6	D	42	GLY	2.3
16	N	95	ALA	2.3
1	0	1966	U	2.3
1	0	1665	G	2.3
2	9	74	G	2.3
30	2	44	ARG	2.3
6	D	129	ASP	2.3
4	B	104	GLU	2.3
4	B	117	GLU	2.3
6	D	167	GLU	2.3
30	2	27	LEU	2.3
16	N	156	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
25	W	86	GLU	2.2
8	F	44	SER	2.2
6	D	39	ASP	2.2
1	0	1159	G	2.2
10	H	140	TYR	2.2
7	E	105	GLU	2.2
8	F	117	GLU	2.2
9	G	64	ASN	2.2
23	U	43	GLY	2.2
6	D	84	LEU	2.2
8	F	17	LEU	2.2
14	L	145	LEU	2.2
10	H	89	THR	2.2
1	0	2345	A	2.2
6	D	24	HIS	2.2
14	L	139	SER	2.2
16	N	169	PRO	2.2
26	X	10	VAL	2.2
1	0	2664	A	2.2
7	E	53	GLU	2.2
28	Z	80	ARG	2.2
7	E	156	ASP	2.2
16	N	69	TYR	2.2
14	L	130	ARG	2.2
1	0	1523	G	2.2
22	T	112	LEU	2.2
13	K	129	THR	2.2
8	F	110	ASP	2.2
8	F	21	GLU	2.2
8	F	26	THR	2.2
5	C	143	ASP	2.2
8	F	115	VAL	2.1
26	X	42	SER	2.1
6	D	51	ARG	2.1
7	E	170	ARG	2.1
4	B	176	ASP	2.1
7	E	76	VAL	2.1
22	T	33	GLU	2.1
6	D	47	GLN	2.1
1	0	370	G	2.1
1	0	1195	G	2.1
6	D	73	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
3	A	134	ASN	2.1
10	H	38	ARG	2.1
10	H	141	CYS	2.1
7	E	91	PHE	2.1
16	N	157	PRO	2.1
6	D	53	LYS	2.1
7	E	16	ASP	2.1
24	V	45	ARG	2.1
8	F	99	THR	2.1
6	D	105	SER	2.1
8	F	75	ILE	2.1
16	N	182	GLY	2.1
1	0	1158	G	2.1
17	O	24	ALA	2.0
1	0	2506	A	2.0
7	E	93	MET	2.0
3	A	64	ASP	2.0
17	O	20	SER	2.0
4	B	133	GLU	2.0
13	K	101	ASN	2.0
1	0	1161	A	2.0
7	E	169	THR	2.0
20	R	104	PHE	2.0
6	D	71	ALA	2.0
15	M	49	ALA	2.0
6	D	102	GLY	2.0
1	0	2914	A	2.0
8	F	20	LEU	2.0
17	O	1	SER	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
1	OMU	0	2587	21/22	0.98	0.12	-	26,28,29,32	0
1	UR3	0	2619	21/22	0.98	0.13	-	29,33,35,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	PSU	0	2621	20/21	0.98	0.13	-	22,25,33,33	0
1	1MA	0	628	23/24	0.98	0.15	-	22,24,25,28	0
1	OMG	0	2588	24/25	0.98	0.12	-	23,27,29,30	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	0	8555	1/1	0.82	0.49	93.70	43,43,43,43	0
35	NA	0	8542	1/1	0.85	0.43	32.60	51,51,51,51	0
35	NA	0	8563	1/1	0.84	0.39	21.85	56,56,56,56	0
35	NA	0	8565	1/1	0.89	0.29	21.02	46,46,46,46	0
37	SR	B	8987	1/1	0.14	0.48	14.67	189,189,189,189	0
35	NA	0	8553	1/1	0.93	0.24	14.54	48,48,48,48	0
37	SR	0	8969	1/1	0.97	0.25	13.74	115,115,115,115	0
35	NA	0	8550	1/1	0.92	0.21	12.73	41,41,41,41	0
35	NA	0	8564	1/1	0.86	0.37	12.07	55,55,55,55	0
35	NA	0	8517	1/1	0.94	0.21	11.56	36,36,36,36	0
35	NA	0	8562	1/1	0.72	0.27	10.20	59,59,59,59	0
35	NA	0	8560	1/1	0.98	0.36	9.84	54,54,54,54	0
35	NA	0	8521	1/1	0.87	0.24	9.60	55,55,55,55	0
35	NA	0	8571	1/1	0.55	0.25	7.35	79,79,79,79	0
37	SR	0	8903	1/1	0.99	0.17	6.41	41,41,41,41	0
35	NA	0	8528	1/1	0.98	0.20	6.38	32,32,32,32	0
35	NA	9	8572	1/1	0.89	0.29	6.06	59,59,59,59	0
37	SR	0	8992	1/1	0.97	0.22	5.02	111,111,111,111	0
35	NA	0	8568	1/1	0.91	0.24	4.60	42,42,42,42	0
35	NA	0	8535	1/1	0.94	0.26	4.20	40,40,40,40	0
37	SR	A	8929	1/1	0.68	0.25	4.05	123,123,123,123	0
35	NA	0	8547	1/1	0.94	0.19	3.81	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	0	8559	1/1	0.92	0.15	2.69	51,51,51,51	0
35	NA	0	8527	1/1	0.95	0.17	2.49	31,31,31,31	0
35	NA	0	8534	1/1	0.95	0.15	2.43	29,29,29,29	0
35	NA	0	8523	1/1	0.93	0.16	2.29	31,31,31,31	0
35	NA	R	8575	1/1	0.90	0.21	2.22	73,73,73,73	0
36	CL	M	8818	1/1	0.97	0.23	2.16	36,36,36,36	0
37	SR	0	8991	1/1	0.79	0.15	1.94	167,167,167,167	0
35	NA	M	8539	1/1	0.95	0.18	1.60	28,28,28,28	0
35	NA	0	8530	1/1	0.97	0.16	1.53	37,37,37,37	0
35	NA	0	8556	1/1	0.94	0.22	1.31	37,37,37,37	0
35	NA	0	8552	1/1	0.96	0.14	0.98	48,48,48,48	0
35	NA	0	8515	1/1	0.97	0.17	0.48	30,30,30,30	0
35	NA	0	8508	1/1	0.92	0.13	0.20	40,40,40,40	0
37	SR	0	8959	1/1	0.86	0.17	0.19	132,132,132,132	0
37	SR	0	8975	1/1	0.94	0.13	0.08	99,99,99,99	0
33	MG	A	8051	1/1	0.97	0.17	-0.01	55,55,55,55	0
35	NA	0	8569	1/1	0.91	0.13	-0.02	61,61,61,61	0
36	CL	0	8812	1/1	0.99	0.13	-0.20	39,39,39,39	0
32	ZIT	0	9500	52/52	0.95	0.14	-0.35	28,38,42,44	0
36	CL	J	8821	1/1	0.92	0.17	-0.36	52,52,52,52	0
35	NA	Q	8540	1/1	0.98	0.17	-0.37	39,39,39,39	0
35	NA	C	8503	1/1	0.92	0.14	-0.38	29,29,29,29	0
35	NA	0	8504	1/1	0.95	0.13	-0.50	26,26,26,26	0
35	NA	0	8557	1/1	0.92	0.12	-0.57	54,54,54,54	0
37	SR	0	8993	1/1	0.69	0.10	-0.73	143,143,143,143	0
37	SR	H	8972	1/1	0.84	0.12	-0.76	112,112,112,112	0
35	NA	0	8519	1/1	0.99	0.15	-0.78	36,36,36,36	0
37	SR	R	8912	1/1	0.95	0.12	-0.79	77,77,77,77	0
33	MG	0	8047	1/1	0.98	0.13	-0.84	46,46,46,46	0
35	NA	0	8520	1/1	0.98	0.09	-0.99	50,50,50,50	0
37	SR	0	8985	1/1	0.94	0.11	-1.02	104,104,104,104	0
36	CL	0	8815	1/1	0.95	0.11	-1.04	47,47,47,47	0
35	NA	0	8512	1/1	0.97	0.11	-1.05	36,36,36,36	0
33	MG	0	8044	1/1	0.97	0.15	-1.10	40,40,40,40	0
35	NA	0	8537	1/1	0.99	0.13	-1.28	32,32,32,32	0
38	CD	U	8701	1/1	0.99	0.09	-1.35	55,55,55,55	0
37	SR	0	8947	1/1	0.83	0.10	-1.46	148,148,148,148	0
37	SR	0	8922	1/1	0.55	0.12	-1.47	161,161,161,161	0
35	NA	J	8538	1/1	0.95	0.10	-1.50	48,48,48,48	0
36	CL	O	8808	1/1	0.97	0.10	-1.52	54,54,54,54	0
37	SR	0	8981	1/1	0.94	0.11	-1.52	141,141,141,141	0
38	CD	Z	8703	1/1	0.98	0.08	-1.53	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	CL	0	8816	1/1	0.98	0.11	-1.57	53,53,53,53	0
33	MG	0	8009	1/1	0.98	0.13	-1.63	26,26,26,26	0
35	NA	0	8513	1/1	0.94	0.13	-1.70	33,33,33,33	0
33	MG	0	8084	1/1	0.95	0.04	-1.70	36,36,36,36	0
33	MG	0	8008	1/1	0.97	0.12	-1.77	26,26,26,26	0
33	MG	A	8050	1/1	0.96	0.13	-1.82	33,33,33,33	0
36	CL	B	8819	1/1	0.98	0.09	-1.85	46,46,46,46	0
33	MG	0	8058	1/1	0.99	0.08	-1.92	26,26,26,26	0
37	SR	0	8964	1/1	0.90	0.09	-1.92	109,109,109,109	0
37	SR	A	8930	1/1	0.96	0.05	-2.11	82,82,82,82	0
33	MG	0	8011	1/1	0.99	0.09	-2.15	24,24,24,24	0
33	MG	T	8057	1/1	0.94	0.08	-2.42	51,51,51,51	0
33	MG	0	8028	1/1	0.98	0.11	-2.45	19,19,19,19	0
38	CD	3	8704	1/1	0.99	0.07	-2.57	53,53,53,53	0
37	SR	0	8970	1/1	0.81	0.09	-2.61	109,109,109,109	0
37	SR	0	8984	1/1	0.96	0.10	-2.63	98,98,98,98	0
37	SR	0	8943	1/1	0.86	0.09	-2.65	108,108,108,108	0
37	SR	F	9005	1/1	0.91	0.05	-2.74	106,106,106,106	0
35	NA	0	8533	1/1	0.97	0.08	-2.78	50,50,50,50	0
33	MG	0	8070	1/1	0.96	0.10	-3.02	36,36,36,36	0
33	MG	0	8045	1/1	0.97	0.09	-3.08	29,29,29,29	0
33	MG	0	8003	1/1	0.97	0.11	-3.23	23,23,23,23	0
37	SR	0	8918	1/1	0.99	0.12	-3.50	66,66,66,66	0
33	MG	0	8041	1/1	0.98	0.10	-3.68	18,18,18,18	0
33	MG	0	8052	1/1	0.95	0.09	-3.72	23,23,23,23	0
37	SR	3	8932	1/1	0.99	0.07	-3.74	58,58,58,58	0
37	SR	0	8936	1/1	0.99	0.09	-3.74	67,67,67,67	0
33	MG	0	8025	1/1	0.94	0.08	-3.80	24,24,24,24	0
33	MG	Y	8086	1/1	0.97	0.11	-3.82	35,35,35,35	0
33	MG	0	8062	1/1	0.89	0.08	-3.94	46,46,46,46	0
33	MG	0	8075	1/1	0.97	0.07	-4.06	31,31,31,31	0
37	SR	0	8904	1/1	0.99	0.08	-4.23	34,34,34,34	0
33	MG	0	8065	1/1	0.95	0.07	-4.27	45,45,45,45	0
36	CL	3	8804	1/1	0.97	0.09	-4.29	47,47,47,47	0
35	NA	0	8558	1/1	0.98	0.08	-4.53	46,46,46,46	0
33	MG	0	8014	1/1	0.99	0.09	-4.56	25,25,25,25	0
33	MG	0	8043	1/1	0.98	0.09	-4.58	46,46,46,46	0
36	CL	0	8805	1/1	0.97	0.09	-4.58	45,45,45,45	0
33	MG	0	8012	1/1	0.98	0.07	-4.59	13,13,13,13	0
33	MG	B	8042	1/1	0.97	0.05	-4.60	52,52,52,52	0
34	K	0	8402	1/1	0.99	0.09	-4.84	46,46,46,46	0
37	SR	1	8913	1/1	0.98	0.07	-4.84	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
38	CD	1	8702	1/1	0.99	0.06	-4.90	44,44,44,44	0
33	MG	0	8001	1/1	0.99	0.08	-5.57	25,25,25,25	0
33	MG	0	8034	1/1	0.98	0.08	-5.64	35,35,35,35	0
33	MG	0	8029	1/1	0.92	0.08	-5.97	40,40,40,40	0
33	MG	0	8088	1/1	0.98	0.05	-6.93	29,29,29,29	0
33	MG	0	8013	1/1	0.99	0.04	-6.97	24,24,24,24	0
33	MG	0	8040	1/1	0.93	0.09	-6.98	78,78,78,78	0
33	MG	0	8015	1/1	0.98	0.09	-7.69	31,31,31,31	0
33	MG	0	8002	1/1	0.97	0.08	-7.69	27,27,27,27	0
33	MG	0	8087	1/1	0.99	0.08	-9.06	26,26,26,26	0
33	MG	0	8006	1/1	0.99	0.06	-9.12	30,30,30,30	0
37	SR	0	8902	1/1	0.99	0.07	-9.12	49,49,49,49	0
33	MG	0	8004	1/1	0.98	0.05	-9.82	22,22,22,22	0
37	SR	0	8945	1/1	0.98	0.04	-9.98	92,92,92,92	0
37	SR	0	8910	1/1	0.96	0.04	-10.59	80,80,80,80	0
37	SR	0	8949	1/1	0.95	0.05	-11.20	93,93,93,93	0
37	SR	0	8978	1/1	0.96	0.05	-13.07	82,82,82,82	0
37	SR	0	8948	1/1	0.97	0.07	-14.93	69,69,69,69	0
37	SR	A	8977	1/1	0.89	0.07	-	143,143,143,143	0
37	SR	0	8955	1/1	0.59	0.37	-	169,169,169,169	0
33	MG	0	8007	1/1	0.97	0.10	-	24,24,24,24	0
35	NA	0	8574	1/1	0.85	0.44	-	48,48,48,48	0
35	NA	0	8511	1/1	0.96	0.11	-	59,59,59,59	0
33	MG	0	8032	1/1	0.99	0.08	-	36,36,36,36	0
33	MG	0	8053	1/1	0.93	0.09	-	58,58,58,58	0
33	MG	0	8022	1/1	0.93	0.15	-	30,30,30,30	0
33	MG	0	8021	1/1	0.97	0.09	-	28,28,28,28	0
35	NA	0	8549	1/1	0.95	0.47	-	74,74,74,74	0
33	MG	0	8079	1/1	0.89	0.08	-	40,40,40,40	0
33	MG	0	8073	1/1	0.86	0.19	-	76,76,76,76	0
35	NA	0	8551	1/1	0.93	0.20	-	39,39,39,39	0
35	NA	0	8505	1/1	0.98	0.14	-	33,33,33,33	0
37	SR	0	8958	1/1	0.96	0.07	-	83,83,83,83	0
33	MG	0	8081	1/1	0.70	0.20	-	55,55,55,55	0
37	SR	0	8960	1/1	0.73	0.09	-	128,128,128,128	0
37	SR	0	8944	1/1	0.72	0.16	-	146,146,146,146	0
33	MG	0	8072	1/1	0.97	0.09	-	37,37,37,37	0
33	MG	0	8082	1/1	0.90	0.23	-	44,44,44,44	0
37	SR	0	8920	1/1	0.95	0.08	-	96,96,96,96	0
37	SR	0	8921	1/1	0.98	0.07	-	66,66,66,66	0
37	SR	0	8927	1/1	0.80	0.12	-	133,133,133,133	0
37	SR	B	8950	1/1	0.90	0.06	-	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	0	8570	1/1	0.97	0.09	-	35,35,35,35	0
36	CL	N	8807	1/1	0.98	0.12	-	46,46,46,46	0
33	MG	0	8061	1/1	0.97	0.12	-	23,23,23,23	0
37	SR	0	9008	1/1	0.95	0.07	-	83,83,83,83	0
33	MG	0	8019	1/1	0.96	0.07	-	22,22,22,22	0
37	SR	0	8946	1/1	0.93	0.09	-	87,87,87,87	0
36	CL	Y	8820	1/1	0.97	0.17	-	35,35,35,35	0
37	SR	0	8907	1/1	0.99	0.11	-	33,33,33,33	0
37	SR	0	8937	1/1	0.96	0.09	-	94,94,94,94	0
33	MG	0	8024	1/1	0.92	0.09	-	53,53,53,53	0
35	NA	0	8522	1/1	0.91	0.28	-	46,46,46,46	0
37	SR	0	8963	1/1	0.91	0.06	-	103,103,103,103	0
37	SR	0	8999	1/1	0.94	0.04	-	78,78,78,78	0
33	MG	0	8068	1/1	0.97	0.15	-	48,48,48,48	0
33	MG	0	8071	1/1	0.86	0.36	-	54,54,54,54	0
35	NA	S	8510	1/1	0.94	0.17	-	24,24,24,24	0
35	NA	0	8573	1/1	0.88	0.09	-	55,55,55,55	0
33	MG	0	8083	1/1	0.95	0.08	-	41,41,41,41	0
35	NA	0	8506	1/1	0.79	0.18	-	50,50,50,50	0
37	SR	0	8905	1/1	0.99	0.23	-	48,48,48,48	0
33	MG	0	8067	1/1	0.96	0.09	-	29,29,29,29	0
35	NA	0	8531	1/1	0.94	0.06	-	29,29,29,29	0
37	SR	0	9007	1/1	0.91	0.27	-	154,154,154,154	0
37	SR	0	8962	1/1	0.80	0.19	-	139,139,139,139	0
33	MG	0	8010	1/1	0.98	0.09	-	29,29,29,29	0
37	SR	0	8917	1/1	0.97	0.09	-	90,90,90,90	0
33	MG	0	8038	1/1	0.92	0.12	-	65,65,65,65	0
37	SR	0	8973	1/1	0.90	0.11	-	113,113,113,113	0
33	MG	0	8037	1/1	0.79	0.22	-	77,77,77,77	0
36	CL	0	8813	1/1	0.98	0.14	-	45,45,45,45	0
33	MG	0	8076	1/1	0.94	0.08	-	28,28,28,28	0
33	MG	0	8036	1/1	0.94	0.10	-	36,36,36,36	0
35	NA	0	8536	1/1	0.72	0.14	-	46,46,46,46	0
37	SR	0	8911	1/1	0.97	0.08	-	65,65,65,65	0
35	NA	0	8548	1/1	0.78	0.09	-	50,50,50,50	0
33	MG	0	8048	1/1	0.99	0.07	-	33,33,33,33	0
37	SR	0	9000	1/1	0.79	0.18	-	150,150,150,150	0
33	MG	0	8077	1/1	0.96	0.08	-	26,26,26,26	0
33	MG	0	8090	1/1	0.98	0.09	-	49,49,49,49	0
33	MG	0	8018	1/1	0.99	0.13	-	38,38,38,38	0
33	MG	0	8016	1/1	0.96	0.06	-	35,35,35,35	0
33	MG	0	8023	1/1	0.98	0.06	-	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	0	8069	1/1	0.78	0.17	-	58,58,58,58	0
37	SR	0	8956	1/1	0.92	0.06	-	127,127,127,127	0
37	SR	0	8971	1/1	0.75	0.09	-	158,158,158,158	0
35	NA	0	8561	1/1	0.87	0.55	-	62,62,62,62	0
37	SR	9	8980	1/1	0.65	0.20	-	162,162,162,162	0
37	SR	0	8990	1/1	0.93	0.10	-	106,106,106,106	0
33	MG	0	8046	1/1	0.93	0.10	-	25,25,25,25	0
36	CL	J	8802	1/1	0.97	0.09	-	51,51,51,51	0
37	SR	0	8967	1/1	0.97	0.04	-	116,116,116,116	0
37	SR	0	8938	1/1	0.97	0.05	-	147,147,147,147	0
33	MG	9	8074	1/1	0.75	0.10	-	64,64,64,64	0
35	NA	0	8554	1/1	0.76	0.31	-	52,52,52,52	0
35	NA	0	8507	1/1	0.93	0.10	-	27,27,27,27	0
33	MG	0	8093	1/1	0.94	0.09	-	29,29,29,29	0
37	SR	0	8957	1/1	0.67	0.33	-	176,176,176,176	0
37	SR	0	8979	1/1	0.49	0.29	-	184,184,184,184	0
38	CD	O	8705	1/1	0.99	0.06	-	58,58,58,58	0
37	SR	0	8995	1/1	0.95	0.07	-	112,112,112,112	0
33	MG	0	8017	1/1	0.94	0.21	-	26,26,26,26	0
37	SR	0	8906	1/1	0.99	0.10	-	40,40,40,40	0
37	SR	0	8988	1/1	0.82	0.10	-	149,149,149,149	0
33	MG	0	8027	1/1	0.95	0.04	-	32,32,32,32	0
35	NA	0	8502	1/1	0.95	0.18	-	43,43,43,43	0
37	SR	0	8909	1/1	1.00	0.08	-	70,70,70,70	0
35	NA	0	8501	1/1	0.99	0.19	-	26,26,26,26	0
37	SR	0	8982	1/1	0.91	0.19	-	152,152,152,152	0
35	NA	0	8524	1/1	0.98	0.20	-	31,31,31,31	0
37	SR	0	8931	1/1	0.96	0.06	-	86,86,86,86	0
33	MG	0	8049	1/1	0.96	0.11	-	64,64,64,64	0
36	CL	0	8814	1/1	0.97	0.11	-	40,40,40,40	0
33	MG	0	8089	1/1	0.95	0.19	-	37,37,37,37	0
36	CL	0	8811	1/1	0.97	0.11	-	45,45,45,45	0
33	MG	0	8031	1/1	0.89	0.09	-	41,41,41,41	0
37	SR	S	8961	1/1	0.89	0.09	-	113,113,113,113	0
37	SR	0	8933	1/1	0.94	0.14	-	108,108,108,108	0
36	CL	0	8803	1/1	0.99	0.16	-	41,41,41,41	0
37	SR	0	8965	1/1	0.92	0.05	-	109,109,109,109	0
33	MG	0	8092	1/1	0.96	0.09	-	47,47,47,47	0
33	MG	0	8080	1/1	0.88	0.08	-	53,53,53,53	0
35	NA	0	8526	1/1	0.95	0.10	-	36,36,36,36	0
37	SR	0	8928	1/1	0.72	0.11	-	112,112,112,112	0
35	NA	0	8525	1/1	0.67	0.21	-	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	0	8529	1/1	0.97	0.09	-	32,32,32,32	0
33	MG	K	8054	1/1	0.97	0.10	-	34,34,34,34	0
37	SR	0	8942	1/1	0.96	0.06	-	110,110,110,110	0
37	SR	0	8983	1/1	0.71	0.15	-	149,149,149,149	0
37	SR	0	8935	1/1	0.99	0.13	-	60,60,60,60	0
36	CL	0	8817	1/1	0.99	0.08	-	46,46,46,46	0
37	SR	1	8952	1/1	0.99	0.06	-	62,62,62,62	0
35	NA	0	8566	1/1	0.97	0.15	-	44,44,44,44	0
37	SR	0	8901	1/1	0.99	0.05	-	71,71,71,71	0
33	MG	0	8039	1/1	0.89	0.13	-	60,60,60,60	0
35	NA	0	8514	1/1	0.92	0.16	-	41,41,41,41	0
33	MG	0	8056	1/1	0.94	0.17	-	49,49,49,49	0
35	NA	0	8567	1/1	0.87	0.31	-	53,53,53,53	0
35	NA	0	8546	1/1	0.93	0.25	-	63,63,63,63	0
36	CL	A	8809	1/1	0.97	0.23	-	52,52,52,52	0
33	MG	0	8064	1/1	0.99	0.04	-	34,34,34,34	0
37	SR	0	8940	1/1	0.97	0.05	-	66,66,66,66	0
37	SR	0	8976	1/1	0.43	0.25	-	159,159,159,159	0
33	MG	0	8066	1/1	0.83	0.11	-	47,47,47,47	0
37	SR	0	8994	1/1	0.94	0.27	-	168,168,168,168	0
37	SR	0	8919	1/1	0.77	0.16	-	169,169,169,169	0
37	SR	0	9004	1/1	0.61	0.23	-	176,176,176,176	0
36	CL	L	8810	1/1	0.96	0.08	-	43,43,43,43	0
33	MG	0	8091	1/1	0.98	0.12	-	42,42,42,42	0
35	NA	0	8516	1/1	0.96	0.14	-	44,44,44,44	0
37	SR	0	8951	1/1	0.85	0.05	-	137,137,137,137	0
33	MG	0	8055	1/1	0.99	0.11	-	29,29,29,29	0
37	SR	0	8916	1/1	0.91	0.06	-	95,95,95,95	0
37	SR	0	9006	1/1	-0.01	0.99	-	200,200,200,200	0
35	NA	0	8509	1/1	0.90	0.15	-	47,47,47,47	0
37	SR	0	9002	1/1	0.63	0.17	-	162,162,162,162	0
35	NA	H	8518	1/1	0.73	0.23	-	66,66,66,66	0
37	SR	0	8989	1/1	0.87	0.18	-	148,148,148,148	0
37	SR	0	8998	1/1	0.84	0.13	-	133,133,133,133	0
33	MG	0	8063	1/1	0.91	0.19	-	71,71,71,71	0
37	SR	0	8924	1/1	0.88	0.13	-	123,123,123,123	0
33	MG	0	8078	1/1	0.97	0.09	-	40,40,40,40	0
33	MG	0	8020	1/1	0.97	0.12	-	37,37,37,37	0
37	SR	0	8996	1/1	0.17	0.59	-	185,185,185,185	0
33	MG	0	8060	1/1	0.94	0.07	-	45,45,45,45	0
33	MG	0	8030	1/1	0.86	0.24	-	48,48,48,48	0
36	CL	J	8801	1/1	0.94	0.11	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
37	SR	0	8986	1/1	0.59	0.81	-	169,169,169,169	0
37	SR	0	8966	1/1	0.96	0.03	-	89,89,89,89	0
33	MG	0	8026	1/1	0.99	0.07	-	28,28,28,28	0
35	NA	9	8543	1/1	0.90	0.24	-	41,41,41,41	0
33	MG	0	8033	1/1	0.97	0.07	-	32,32,32,32	0
37	SR	0	8997	1/1	0.89	0.56	-	171,171,171,171	0
37	SR	0	8968	1/1	0.76	0.09	-	142,142,142,142	0
34	K	0	8401	1/1	0.93	0.11	-	58,58,58,58	0
37	SR	0	8926	1/1	0.94	0.06	-	95,95,95,95	0
37	SR	0	8908	1/1	0.97	0.09	-	71,71,71,71	0
37	SR	0	8915	1/1	0.96	0.06	-	85,85,85,85	0
35	NA	0	8544	1/1	0.89	0.20	-	49,49,49,49	0
37	SR	0	8953	1/1	0.96	0.07	-	121,121,121,121	0
37	SR	0	8941	1/1	0.93	0.05	-	90,90,90,90	0
33	MG	0	8035	1/1	0.95	0.07	-	52,52,52,52	0
37	SR	0	8925	1/1	0.99	0.06	-	75,75,75,75	0
33	MG	0	8059	1/1	0.99	0.04	-	27,27,27,27	0
33	MG	0	8085	1/1	0.73	0.12	-	90,90,90,90	0
36	CL	R	8806	1/1	0.97	0.16	-	40,40,40,40	0
35	NA	0	8545	1/1	0.99	0.13	-	29,29,29,29	0
37	SR	0	8939	1/1	0.91	0.09	-	108,108,108,108	0
36	CL	0	8822	1/1	0.98	0.15	-	48,48,48,48	0
37	SR	0	9001	1/1	0.36	0.26	-	160,160,160,160	0
37	SR	0	8923	1/1	0.98	0.08	-	78,78,78,78	0
37	SR	0	8914	1/1	0.97	0.10	-	88,88,88,88	0
33	MG	0	8005	1/1	0.98	0.10	-	23,23,23,23	0
35	NA	R	8532	1/1	0.93	0.09	-	37,37,37,37	0
37	SR	9	9003	1/1	0.90	0.08	-	141,141,141,141	0
35	NA	0	8541	1/1	0.88	0.15	-	41,41,41,41	0
37	SR	0	8934	1/1	0.96	0.12	-	116,116,116,116	0
37	SR	0	8974	1/1	0.56	0.20	-	159,159,159,159	0
37	SR	0	8954	1/1	0.95	0.11	-	88,88,88,88	0

6.5 Other polymers ⓘ

There are no such residues in this entry.