



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:08 PM GMT

PDB ID : 1VQN
Title : The structure of CC-HPMN AND CCA-PHE-CAP-BIO bound to the large ribosomal subunit of haloarcula marismortui
Authors : Schmeing, T.M.; Steitz, T.A.
Deposited on : 2004-12-16
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

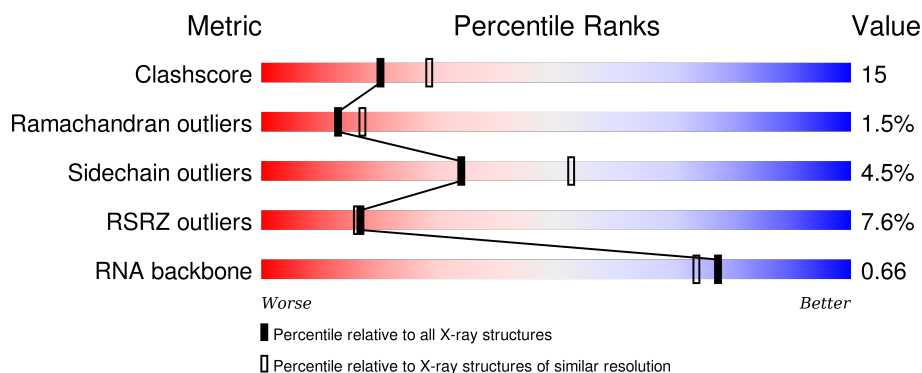
1 Overall quality at a glance ⓘ

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))
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>2%</div> <div>62%</div> <div>27%</div> <div>5%</div> <div>6%</div> </div>
2	9	122	<div> <div>5%</div> <div>57%</div> <div>32%</div> <div>11%</div> <div>•</div> </div>
3	4	4	<div> <div>50%</div> <div>50%</div> </div>
4	5	6	<div> <div>17%</div> <div>17%</div> <div>67%</div> <div>17%</div> </div>
5	A	240	<div> <div>6%</div> <div>61%</div> <div>33%</div> <div>5%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
6	B	338	
7	C	246	
8	D	177	
9	E	178	
10	F	120	
11	G	348	
12	H	171	
13	J	145	
14	K	132	
15	L	165	
16	M	194	
17	N	187	
18	O	116	
19	P	149	
20	Q	96	
21	R	155	
22	S	85	
23	T	120	
24	U	66	
25	V	71	
26	W	154	
27	X	92	
28	Y	241	
29	Z	83	
30	1	57	

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Mol	Chain	Length	Quality of chain
31	2	50	
32	3	92	
33	I	162	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	MG	0	8001	-	-	-	X
34	MG	0	8008	-	-	-	X
34	MG	0	8012	-	-	-	X
34	MG	0	8013	-	-	-	X
34	MG	0	8021	-	-	-	X
34	MG	0	8038	-	-	-	X
34	MG	0	8052	-	-	-	X
34	MG	0	8054	-	-	-	X
34	MG	0	8056	-	-	-	X
34	MG	0	8065	-	-	-	X
34	MG	0	8080	-	-	-	X
34	MG	0	8091	-	-	-	X
34	MG	0	8101	-	-	-	X
34	MG	5	8118	-	-	-	X
35	K	0	9001	-	-	-	X
36	NA	0	9114	-	-	-	X
36	NA	0	9115	-	-	-	X
36	NA	0	9120	-	-	-	X
36	NA	0	9125	-	-	-	X
36	NA	0	9131	-	-	-	X
36	NA	0	9132	-	-	-	X
36	NA	0	9135	-	-	-	X
36	NA	0	9150	-	-	-	X
36	NA	0	9156	-	-	-	X
36	NA	0	9159	-	-	-	X
36	NA	0	9161	-	-	-	X
36	NA	0	9164	-	-	-	X
36	NA	0	9165	-	-	-	X
36	NA	0	9168	-	-	-	X
36	NA	0	9171	-	-	-	X
36	NA	0	9172	-	-	-	X
36	NA	0	9173	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	NA	0	9174	-	-	-	X
36	NA	0	9177	-	-	-	X
36	NA	0	9178	-	-	-	X
36	NA	0	9182	-	-	-	X
36	NA	9	9183	-	-	-	X
36	NA	R	9186	-	-	-	X
37	CL	0	9316	-	-	-	X
38	SR	0	9482	-	-	-	X
38	SR	B	9521	-	-	-	X

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 99077 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

- Molecule 3 is a RNA chain called 5'-R(*CP*CP*(PPU)*(LOF))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	4	4	Total	C	N	O	P	0	0	0
			72	39	12	19	2			

- Molecule 4 is a RNA chain called 5'-R(*CP*CP*AP*(PHE)*(ACA)*(BTN))-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	5	6	Total	C	N	O	P	S	0	0	0
			93	53	15	22	2	1			

- Molecule 5 is a protein called 50S ribosomal protein L2P.

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

- Molecule 6 is a protein called 50S ribosomal protein L3P.

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

- Molecule 7 is a protein called 50S ribosomal protein L4E.

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

- Molecule 8 is a protein called 50S ribosomal protein L5P.

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

- Molecule 9 is a protein called 50S ribosomal protein L6P.

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

- Molecule 10 is a protein called 50S ribosomal protein L7AE.

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

- Molecule 11 is a protein called ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG.

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

- Molecule 12 is a protein called 50S RIBOSOMAL PROTEIN L10E.

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

- Molecule 13 is a protein called 50S ribosomal protein L13P.

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

- Molecule 14 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	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 15 is a protein called 50S ribosomal protein L15P.

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

- Molecule 16 is a protein called 50S Ribosomal Protein L15E.

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 17 is a protein called 50S ribosomal protein L18P.

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

- Molecule 18 is a protein called 50S ribosomal protein L18e.

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

- Molecule 19 is a protein called 50S ribosomal protein L19E.

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

- Molecule 20 is a protein called 50S ribosomal protein L21e.

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

- Molecule 21 is a protein called 50S ribosomal protein L22P.

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

- Molecule 22 is a protein called 50S ribosomal protein L23P.

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

- Molecule 23 is a protein called 50S ribosomal protein L24P.

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

- Molecule 24 is a protein called 50S ribosomal protein L24E.

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

- Molecule 25 is a protein called 50S ribosomal protein L29P.

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

- Molecule 26 is a protein called 50S ribosomal protein L30P.

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

- Molecule 27 is a protein called 50S ribosomal protein L31e.

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

- Molecule 28 is a protein called 50S ribosomal protein L32E.

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

- Molecule 29 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	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 30 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 31 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 32 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L11P.

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

- Molecule 34 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	87	Total	Mg	0	0
			87	87		
34	Y	1	Total	Mg	0	0
			1	1		
34	K	1	Total	Mg	0	0
			1	1		
34	A	1	Total	Mg	0	0
			1	1		
34	T	1	Total	Mg	0	0
			1	1		
34	5	1	Total	Mg	0	0
			1	1		
34	2	1	Total	Mg	0	0
			1	1		
34	9	1	Total	Mg	0	0
			1	1		

- Molecule 35 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	2	Total	K	0	0
			2	2		

- Molecule 36 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	66	Total	Na	0	0
			66	66		
36	J	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	Q	1	Total 1	Na 1	0	0
36	D	1	Total 1	Na 1	0	0
36	C	1	Total 1	Na 1	0	0
36	R	2	Total 2	Na 2	0	0
36	9	1	Total 1	Na 1	0	0
36	S	1	Total 1	Na 1	0	0
36	M	1	Total 1	Na 1	0	0

- Molecule 37 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	0	10	Total 10	Cl 10	0	0
37	J	3	Total 3	Cl 3	0	0
37	B	1	Total 1	Cl 1	0	0
37	A	1	Total 1	Cl 1	0	0
37	N	1	Total 1	Cl 1	0	0
37	O	1	Total 1	Cl 1	0	0
37	R	1	Total 1	Cl 1	0	0
37	Y	1	Total 1	Cl 1	0	0
37	L	1	Total 1	Cl 1	0	0
37	3	1	Total 1	Cl 1	0	0
37	M	1	Total 1	Cl 1	0	0

- Molecule 38 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	0	98	Total 98	Sr 98	0	0
38	1	2	Total 2	Sr 2	0	0
38	H	1	Total 1	Sr 1	0	0
38	B	2	Total 2	Sr 2	0	0
38	3	1	Total 1	Sr 1	0	0
38	A	3	Total 3	Sr 3	0	0
38	R	1	Total 1	Sr 1	0	0
38	9	3	Total 3	Sr 3	0	0
38	L	1	Total 1	Sr 1	0	0
38	S	1	Total 1	Sr 1	0	0
38	F	1	Total 1	Sr 1	0	0

- Molecule 39 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	O	1	Total 1	Cd 1	0	0
39	Z	1	Total 1	Cd 1	0	0
39	1	1	Total 1	Cd 1	0	0
39	3	1	Total 1	Cd 1	0	0
39	U	1	Total 1	Cd 1	0	0

- Molecule 40 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	0	5727	Total 5727	O 5727	0	0
40	9	137	Total 137	O 137	0	0

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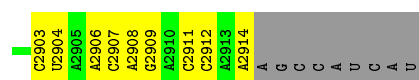
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	4	1	Total 1	O 1	0	0
40	5	2	Total 2	O 2	0	0
40	A	120	Total 120	O 120	0	0
40	B	138	Total 138	O 138	0	0
40	C	180	Total 180	O 180	0	0
40	D	48	Total 48	O 48	0	0
40	E	44	Total 44	O 44	0	0
40	F	24	Total 24	O 24	0	0
40	G	14	Total 14	O 14	0	0
40	H	72	Total 72	O 72	0	0
40	J	54	Total 54	O 54	0	0
40	K	61	Total 61	O 61	0	0
40	L	83	Total 83	O 83	0	0
40	M	128	Total 128	O 128	0	0
40	N	58	Total 58	O 58	0	0
40	O	39	Total 39	O 39	0	0
40	P	61	Total 61	O 61	0	0
40	Q	51	Total 51	O 51	0	0
40	R	78	Total 78	O 78	0	0
40	S	31	Total 31	O 31	0	0
40	T	35	Total 35	O 35	0	0

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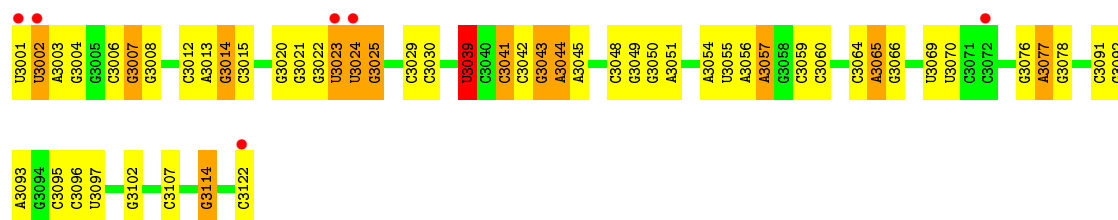
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	U	28	Total 28	O 28	0	0
40	V	12	Total 12	O 12	0	0
40	W	62	Total 62	O 62	0	0
40	X	21	Total 21	O 21	0	0
40	Y	93	Total 93	O 93	0	0
40	Z	34	Total 34	O 34	0	0
40	1	59	Total 59	O 59	0	0
40	2	40	Total 40	O 40	0	0
40	3	71	Total 71	O 71	0	0
40	I	10	Total 10	O 10	0	0

C2795	C2824	C2825	C2826	C2827	C2828	C2829	U2837	A2840	A2841	A2842	G2851	A2852	U2853	A2856	U2857	U2858	G2862	U2866	G2867	G2876	G2877	G2878	U2879	A2883	G2884	A2890	C2894	C2895	A2896																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
G2670	U2607	U2608	G2613	U2619	U2620	U2627	U2636	U2637	U2638	U2639	U2640	U2641	U2642	U2643	U2644	U2645	U2646	U2647	U2648	U2649	U2650	U2651	U2652	U2653	U2654	U2655	U2656	U2657	U2658																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
G2466	G2472	G2476	G2477	G2478	G2479	G2480	G2481	G2482	G2483	G2487	A2490	G2491	U2492	C2493	C2502	A2503	A2504	G2505	A2506	G2507	C2508	A2509	C2510	U2512	G2515	G2516	A2521	G2524	G2525	C2526	U2531	C2532	C2533	U2534	U2535	C2536	G2537	U2541	C2542	C2548	C2552	A2553																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
C2346	C2351	C2352	A2353	A2354	G2355	G2356	G2357	A2361	A2362	A2363	A2364	G2365	A2369	A2372	U2373	A2374	G2375	U2376	A2401	A2402	G2412	A2413	A2414	A2415	A2416	C2417	G2418	U2419	G2420	G2421	U2422	G2426	C2427	A2434	C2443	U2444	U2445	G2446	G2453	A2456	U2457	G2462	A2465																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
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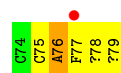
- Molecule 2: 5S ribosomal RNA



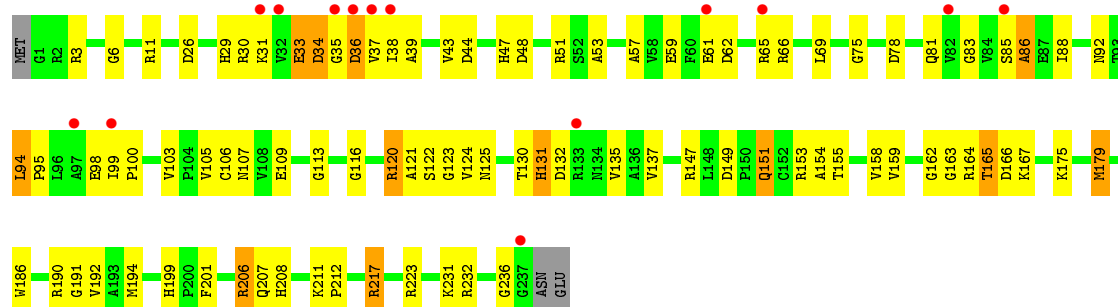
- Molecule 3: 5'-R(*CP*CP*(PPU)*(LOF))-3'



- Molecule 4: 5'-R(*CP*CP*AP*(PHE)*(ACA)*(BTN))-3'

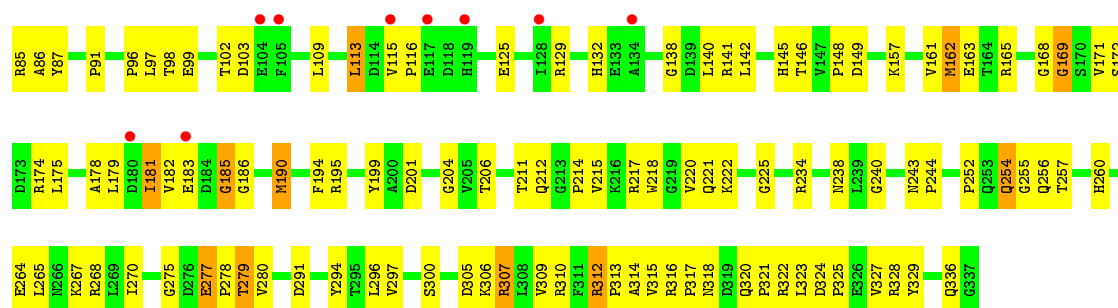


- Molecule 5: 50S ribosomal protein L2P

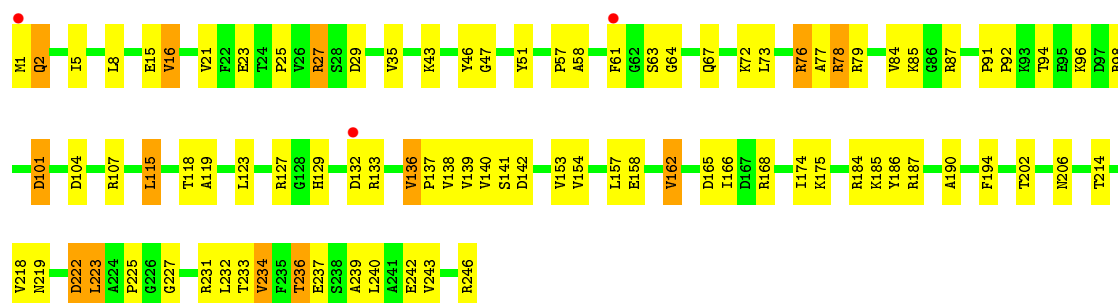


- Molecule 6: 50S ribosomal protein L3P

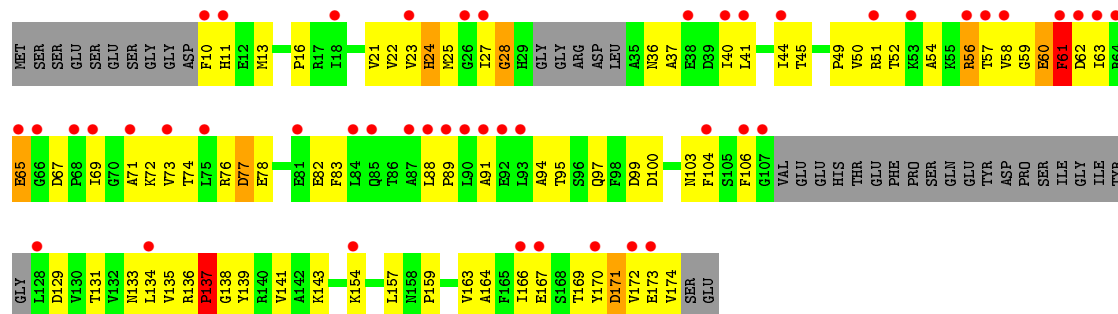




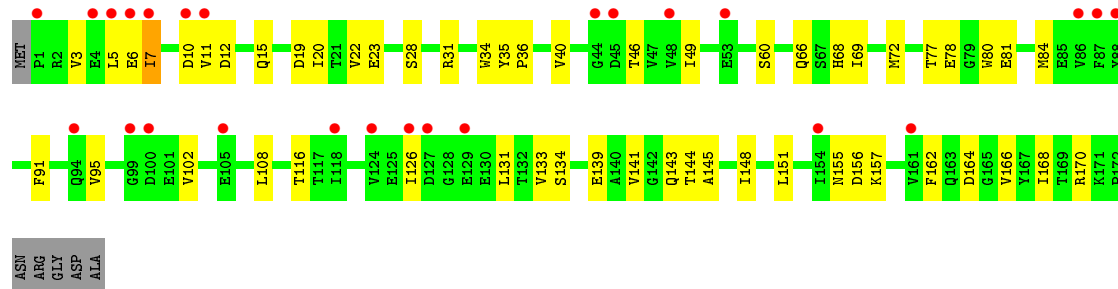
• Molecule 7: 50S ribosomal protein L4E



• Molecule 8: 50S ribosomal protein L5P

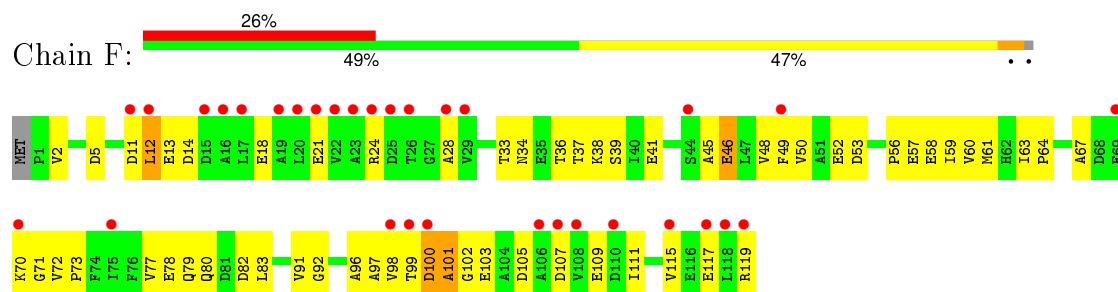


• Molecule 9: 50S ribosomal protein L6P

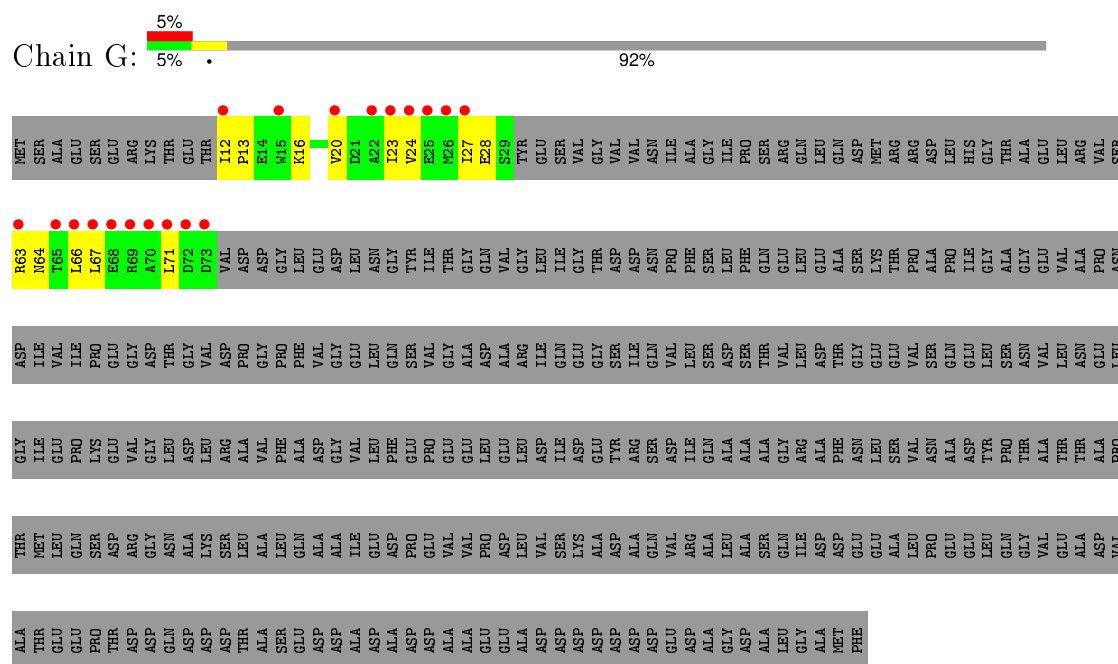


ASN
ARG
GLY
ASP
ALA

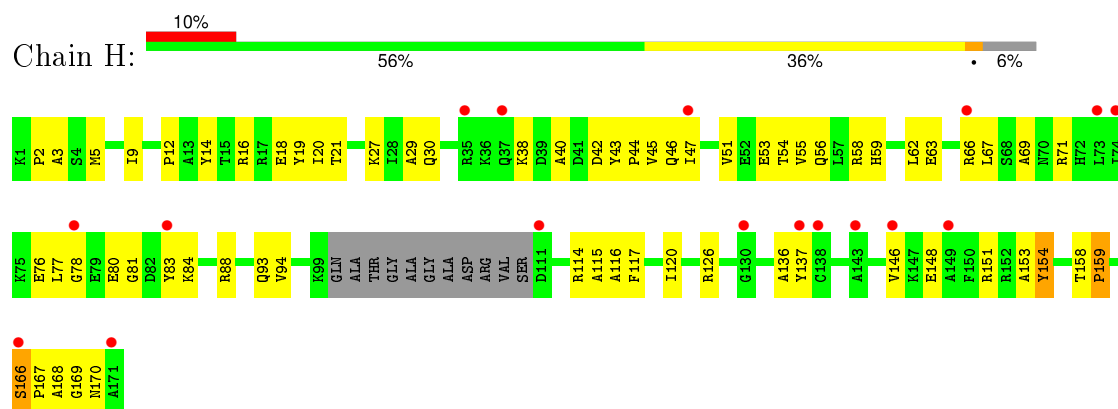
- Molecule 10: 50S ribosomal protein L7AE



- Molecule 11: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG

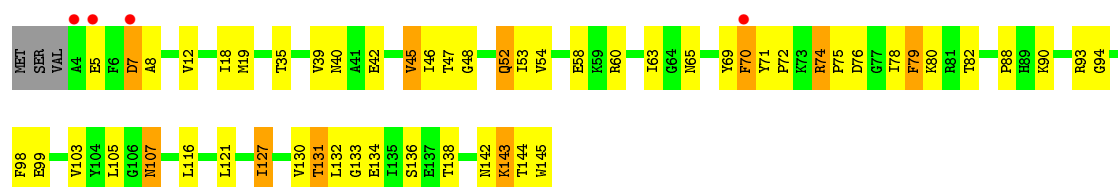


- Molecule 12: 50S RIBOSOMAL PROTEIN L10E

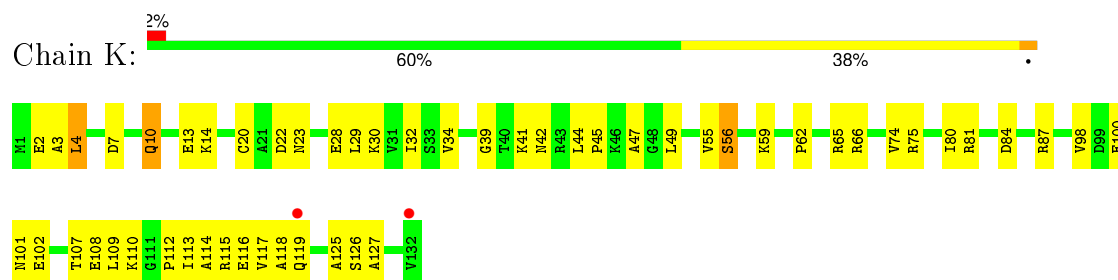


- Molecule 13: 50S ribosomal protein L13P

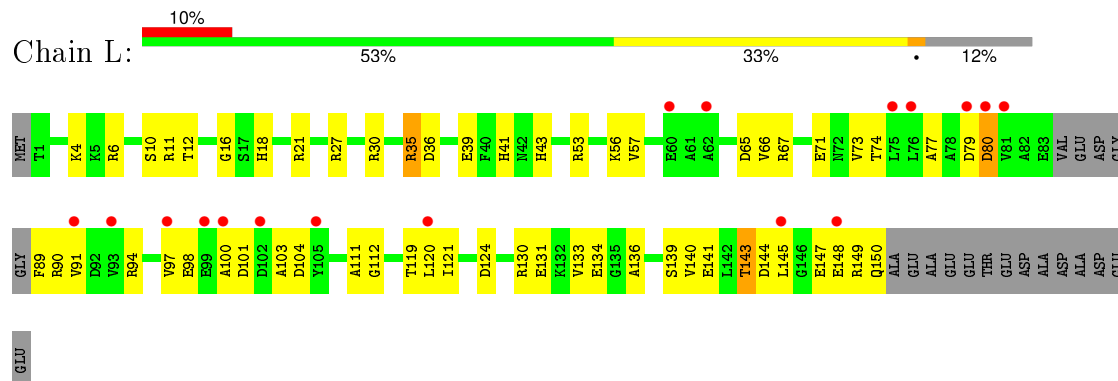




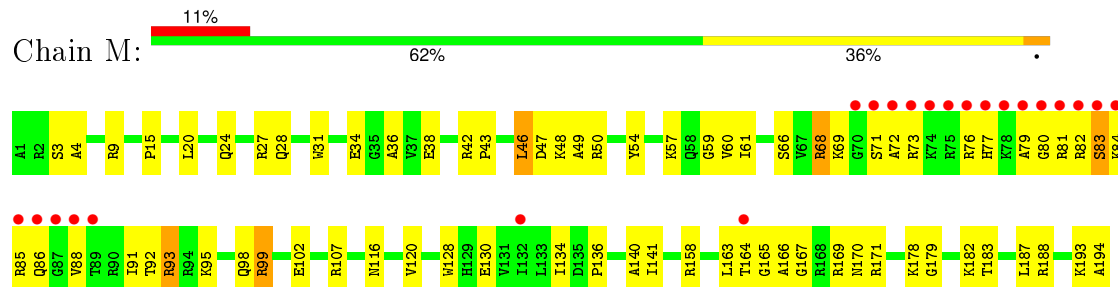
• Molecule 14: 50S ribosomal protein L14P



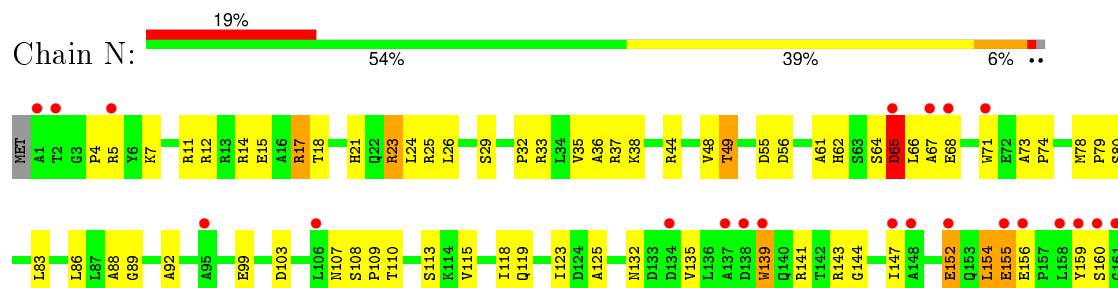
• Molecule 15: 50S ribosomal protein L15P

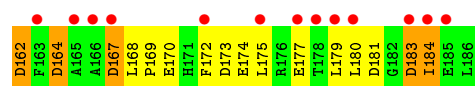


• Molecule 16: 50S Ribosomal Protein L15E

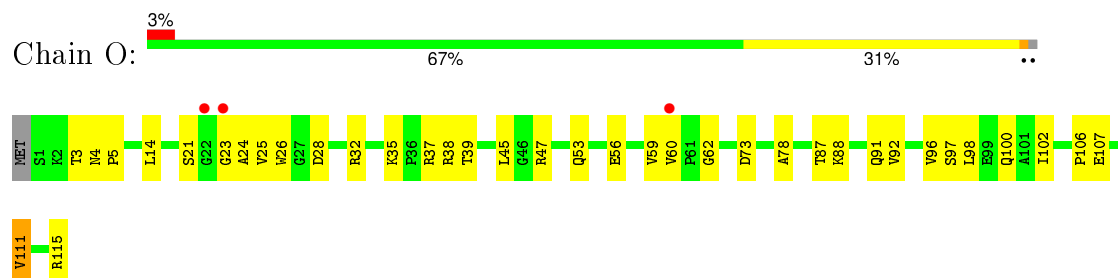


• Molecule 17: 50S ribosomal protein L18P

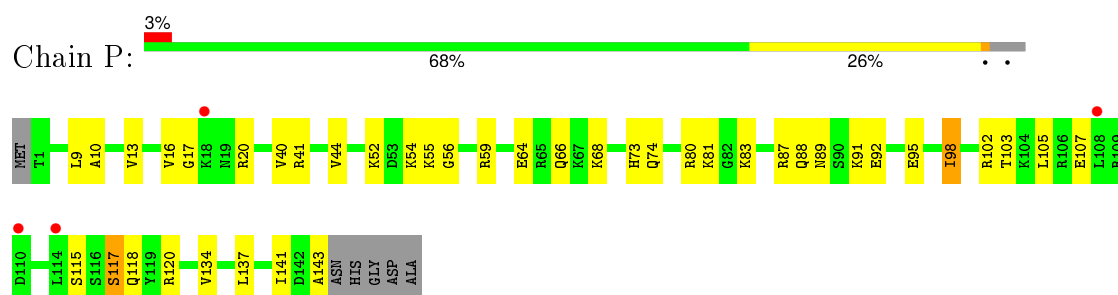




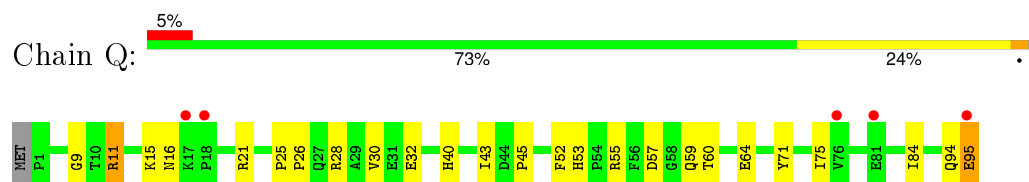
- Molecule 18: 50S ribosomal protein L18e



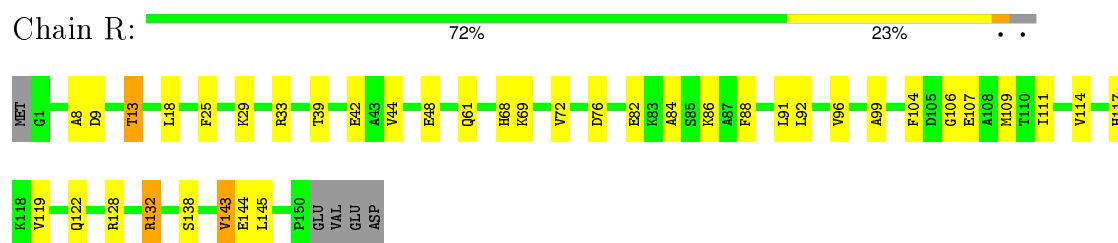
- Molecule 19: 50S ribosomal protein L19E



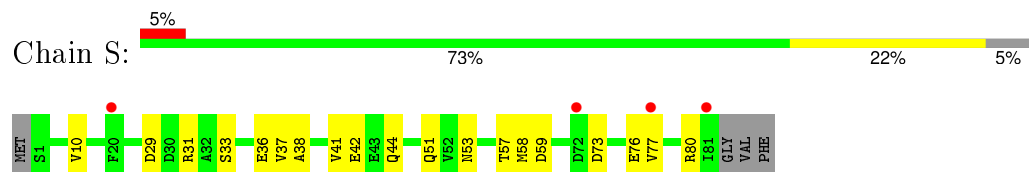
- Molecule 20: 50S ribosomal protein L21e



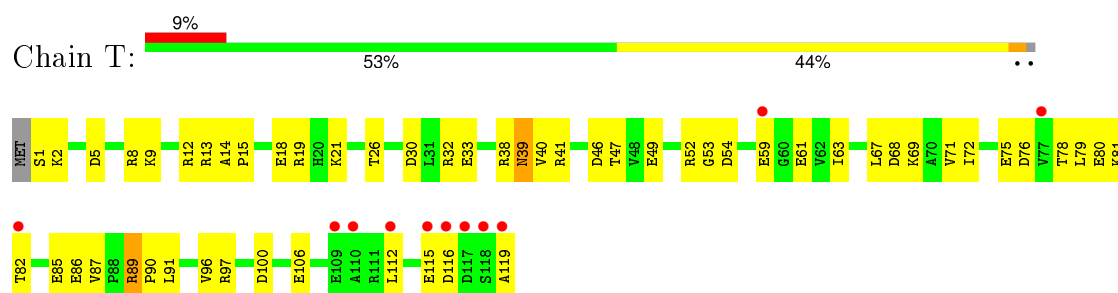
- Molecule 21: 50S ribosomal protein L22P



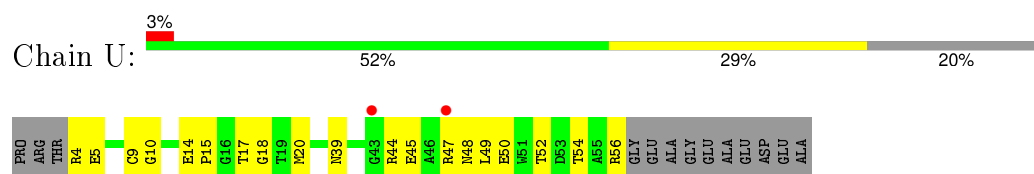
- Molecule 22: 50S ribosomal protein L23P



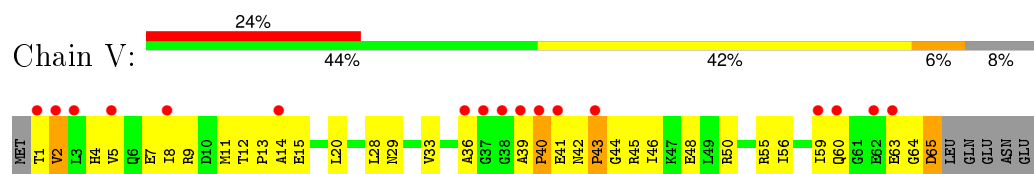
- Molecule 23: 50S ribosomal protein L24P



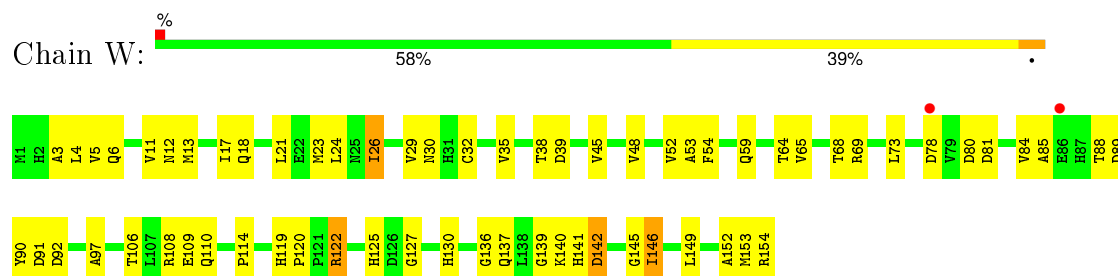
- Molecule 24: 50S ribosomal protein L24E



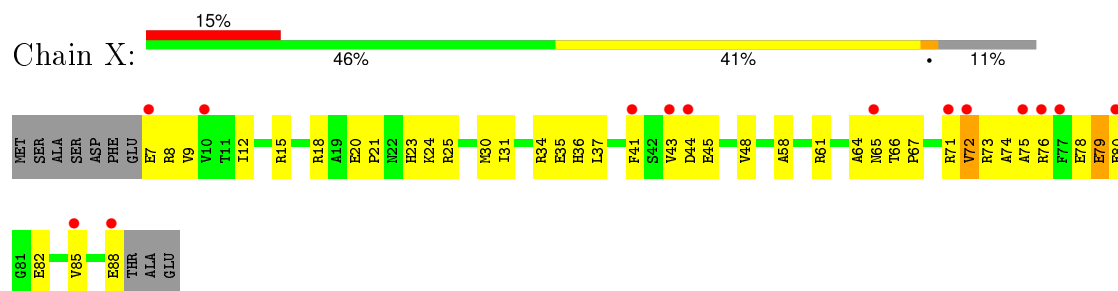
- Molecule 25: 50S ribosomal protein L29P



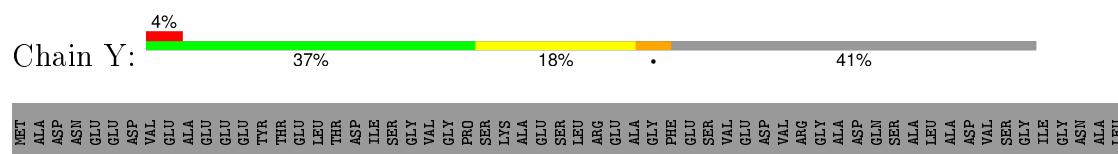
- Molecule 26: 50S ribosomal protein L30P

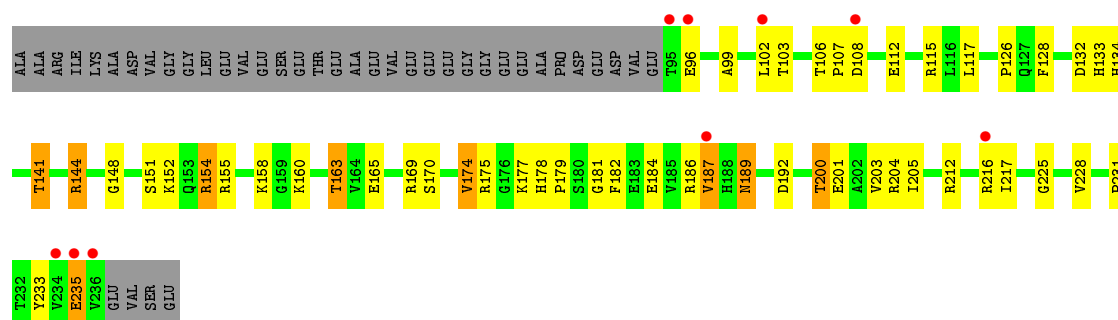


- Molecule 27: 50S ribosomal protein L31e

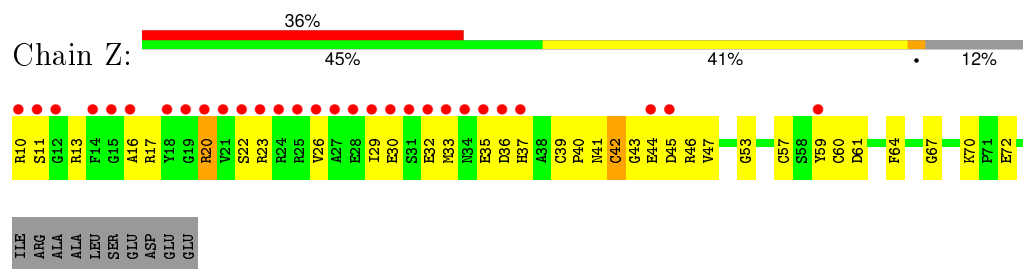


- Molecule 28: 50S ribosomal protein L32E

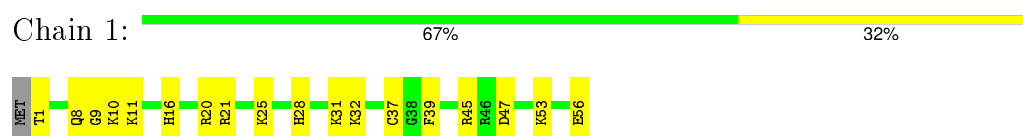




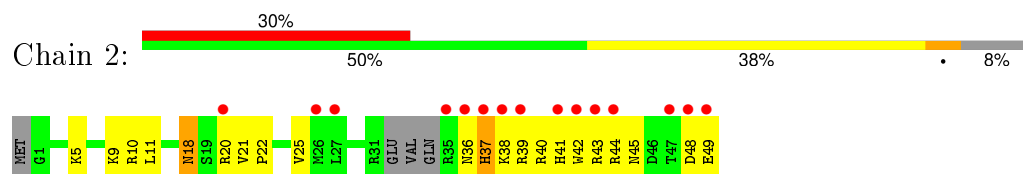
- Molecule 29: 50S ribosomal protein L37Ae



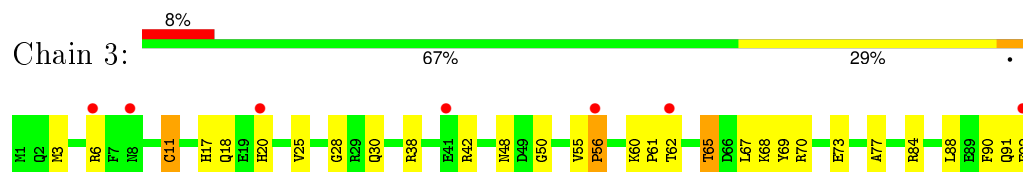
- Molecule 30: 50S ribosomal protein L37e



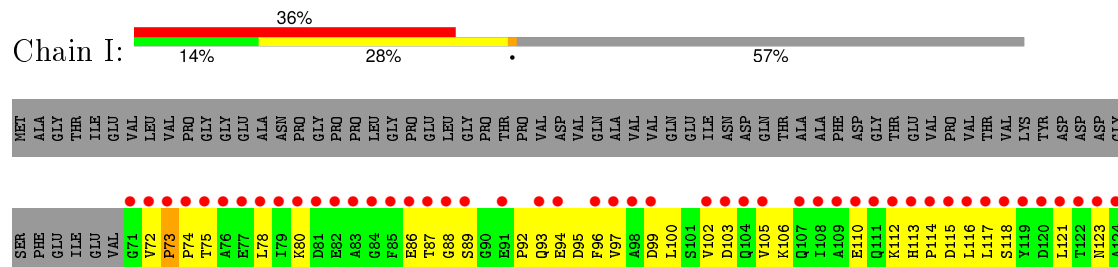
- Molecule 31: 50S ribosomal protein L39e



- Molecule 32: 50S ribosomal protein L44E



- Molecule 33: 50S RIBOSOMAL PROTEIN L11P



A125	K126	E127	V128	V129	G130	T131	C132	T133	S134	L135	G136	V137	T138	I139	E140	GLY	GLU	ASN	PRO	ARG	GLU	PHE	LYS	GLU	ARG	ILE	ASP	ALA	GLY	GLU	TYR	ASP	ASP	VAL	PHE	ALA	ALA	GLU	ALA	GLN	ALA
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.72Å 298.78Å 575.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 49.32 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.00-2.40) 89.2 (49.32-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.212 , 0.248 0.210 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	45.1	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 64.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 697789 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	99077	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.44% 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: ACA, OMG, PPU, CL, SR, NA, K, MG, CD, HFA, OMU, UR3, 1MA, BTN, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.38	0/65959	0.70	25/102870 (0.0%)
2	9	0.33	0/2905	0.70	1/4528 (0.0%)
3	4	0.47	0/40	0.68	0/60
4	5	0.51	0/76	0.79	0/112
5	A	0.33	0/1786	0.65	0/2408
6	B	0.34	0/2690	0.65	0/3652
7	C	0.38	0/1884	0.65	0/2551
8	D	0.29	0/1111	0.54	0/1498
9	E	0.32	0/1382	0.58	0/1880
10	F	0.33	0/901	0.54	0/1224
11	G	0.28	0/241	0.48	0/324
12	H	0.34	0/1287	0.64	0/1725
13	J	0.35	0/1136	0.62	0/1530
14	K	0.36	0/1001	0.68	0/1347
15	L	0.32	0/1130	0.64	0/1509
16	M	0.34	0/1584	0.59	0/2119
17	N	0.29	0/1474	0.61	0/1999
18	O	0.32	0/874	0.58	0/1181
19	P	0.35	0/1147	0.55	0/1528
20	Q	0.34	0/749	0.69	0/1005
21	R	0.37	0/1172	0.67	0/1578
22	S	0.32	0/648	0.56	0/875
23	T	0.31	0/958	0.63	0/1289
24	U	0.35	0/417	0.58	0/562
25	V	0.27	0/502	0.52	0/675
26	W	0.35	0/1219	0.60	0/1655
27	X	0.34	0/664	0.61	0/895
28	Y	0.37	0/1146	0.66	0/1536
29	Z	0.32	0/589	0.57	0/787
30	1	0.43	0/438	0.63	0/578
31	2	0.32	0/401	0.57	0/529
32	3	0.35	0/771	0.57	0/1024

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	I	0.29	0/526	0.51	0/716
All	All	0.37	0/98808	0.67	26/147749 (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	55
2	9	0	1
All	All	0	56

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	871	G	C5'-C4'-O4'	-7.44	100.17	109.10
1	0	1942	A	C5'-C4'-C3'	7.11	127.37	116.00
1	0	1592	G	N9-C1'-C2'	6.67	122.67	114.00
1	0	1819	G	C5'-C4'-C3'	6.40	126.24	116.00
1	0	883	U	N1-C1'-C2'	6.20	122.06	114.00
1	0	2726	U	N1-C1'-C2'	6.13	121.97	114.00
1	0	1504	A	C1'-O4'-C4'	-6.08	105.03	109.90
1	0	777	U	O4'-C1'-N1	5.98	112.98	108.20
2	9	3039	U	N1-C1'-C2'	5.95	121.73	114.00
1	0	1120	U	C5'-C4'-C3'	-5.79	106.73	116.00
1	0	2467	A	C1'-O4'-C4'	-5.79	105.27	109.90
1	0	2541	U	C2'-C3'-O3'	5.76	122.91	113.70
1	0	1819	G	C1'-O4'-C4'	-5.69	105.35	109.90
1	0	1504	A	N9-C1'-C2'	5.65	121.34	114.00
1	0	1979	G	C2'-C3'-O3'	5.55	122.58	113.70
1	0	2291	A	N9-C1'-C2'	5.45	121.09	114.00
1	0	206	G	C5'-C4'-C3'	-5.26	107.58	116.00
1	0	2313	C	C5'-C4'-O4'	5.26	115.42	109.10
1	0	841	A	C1'-O4'-C4'	-5.24	105.70	109.90
1	0	1615	A	C5'-C4'-C3'	5.20	124.33	116.00
1	0	2301	A	N9-C1'-C2'	5.12	120.66	114.00
1	0	1352	A	OP1-P-O3'	5.07	116.36	105.20
1	0	921	G	N9-C1'-C2'	5.05	120.57	114.00
1	0	1261	A	N9-C1'-C2'	5.05	120.57	114.00
1	0	457	U	C1'-O4'-C4'	-5.04	105.86	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	389	G	C5'-C4'-C3'	-5.00	108.00	116.00

There are no chirality outliers.

All (56) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1039	G	Sidechain
1	0	1078	A	Sidechain
1	0	1080	C	Sidechain
1	0	1132	A	Sidechain
1	0	1340	G	Sidechain
1	0	1458	A	Sidechain
1	0	1491	G	Sidechain
1	0	1592	G	Sidechain
1	0	1718	G	Sidechain
1	0	1744	G	Sidechain
1	0	1777	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	1885	A	Sidechain
1	0	191	A	Sidechain
1	0	1970	G	Sidechain
1	0	2115	U	Sidechain
1	0	22	U	Sidechain
1	0	2465	A	Sidechain
1	0	2493	C	Sidechain
1	0	2503	A	Sidechain
1	0	2506	A	Sidechain
1	0	2552	C	Sidechain
1	0	2599	A	Sidechain
1	0	2607	U	Sidechain
1	0	2620	U	Sidechain
1	0	2630	G	Sidechain
1	0	2632	G	Sidechain
1	0	2645	U	Sidechain
1	0	2681	A	Sidechain
1	0	270	U	Sidechain

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Mol	Chain	Res	Type	Group
1	0	2726	U	Sidechain
1	0	2842	G	Sidechain
1	0	333	G	Sidechain
1	0	396	U	Sidechain
1	0	458	G	Sidechain
1	0	469	G	Sidechain
1	0	470	U	Sidechain
1	0	471	G	Sidechain
1	0	482	G	Sidechain
1	0	507	A	Sidechain
1	0	518	G	Sidechain
1	0	619	U	Sidechain
1	0	722	G	Sidechain
1	0	771	G	Sidechain
1	0	795	G	Sidechain
1	0	817	G	Sidechain
1	0	868	G	Sidechain
1	0	888	U	Sidechain
1	0	952	G	Sidechain
2	9	3039	U	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59021	0	29812	769	0
2	9	2600	0	1326	58	0
3	4	72	0	47	1	0
4	5	93	0	68	4	0
5	A	1753	0	1765	111	0
6	B	2625	0	2532	151	0
7	C	1859	0	1816	97	0
8	D	1094	0	1085	92	0
9	E	1357	0	1266	50	0
10	F	890	0	843	55	0
11	G	240	0	231	12	0
12	H	1266	0	1268	63	0
13	J	1120	0	1098	69	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	K	992	0	1031	58	0
15	L	1118	0	1076	61	0
16	M	1560	0	1568	75	0
17	N	1445	0	1401	87	0
18	O	865	0	873	42	0
19	P	1136	0	1123	42	0
20	Q	735	0	728	22	0
21	R	1149	0	1122	39	0
22	S	641	0	605	17	0
23	T	950	0	923	52	0
24	U	410	0	364	22	0
25	V	499	0	511	43	0
26	W	1196	0	1137	83	0
27	X	654	0	653	41	0
28	Y	1130	0	1133	60	0
29	Z	578	0	539	39	0
30	1	431	0	426	29	0
31	2	396	0	413	30	0
32	3	755	0	728	30	0
33	I	519	0	500	60	0
34	0	87	0	0	0	0
34	2	1	0	0	0	0
34	5	1	0	0	0	0
34	9	1	0	0	0	0
34	A	1	0	0	0	0
34	K	1	0	0	0	0
34	T	1	0	0	0	0
34	Y	1	0	0	0	0
35	0	2	0	0	0	0
36	0	66	0	0	0	0
36	9	1	0	0	0	0
36	C	1	0	0	0	0
36	D	1	0	0	0	0
36	J	1	0	0	0	0
36	M	1	0	0	0	0
36	Q	1	0	0	0	0
36	R	2	0	0	0	0
36	S	1	0	0	0	0
37	0	10	0	0	0	0
37	3	1	0	0	0	0
37	A	1	0	0	0	0
37	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	J	3	0	0	1	0
37	L	1	0	0	0	0
37	M	1	0	0	0	0
37	N	1	0	0	0	0
37	O	1	0	0	0	0
37	R	1	0	0	0	0
37	Y	1	0	0	0	0
38	0	98	0	0	0	0
38	1	2	0	0	0	0
38	3	1	0	0	0	0
38	9	3	0	0	0	0
38	A	3	0	0	0	0
38	B	2	0	0	0	0
38	F	1	0	0	0	0
38	H	1	0	0	0	0
38	L	1	0	0	0	0
38	R	1	0	0	0	0
38	S	1	0	0	0	0
39	1	1	0	0	0	0
39	3	1	0	0	0	0
39	O	1	0	0	0	0
39	U	1	0	0	0	0
39	Z	1	0	0	0	0
40	0	5727	0	0	102	0
40	1	59	0	0	3	0
40	2	40	0	0	1	0
40	3	71	0	0	5	0
40	4	1	0	0	0	0
40	5	2	0	0	0	0
40	9	137	0	0	5	0
40	A	120	0	0	8	0
40	B	138	0	0	18	0
40	C	180	0	0	19	0
40	D	48	0	0	11	0
40	E	44	0	0	4	0
40	F	24	0	0	2	0
40	G	14	0	0	0	0
40	H	72	0	0	6	0
40	I	10	0	0	2	0
40	J	54	0	0	3	0
40	K	61	0	0	4	0
40	L	83	0	0	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	M	128	0	0	3	0
40	N	58	0	0	4	0
40	O	39	0	0	3	0
40	P	61	0	0	2	0
40	Q	51	0	0	5	0
40	R	78	0	0	4	0
40	S	31	0	0	1	0
40	T	35	0	0	4	0
40	U	28	0	0	3	0
40	V	12	0	0	2	0
40	W	62	0	0	6	0
40	X	21	0	0	5	0
40	Y	93	0	0	10	0
40	Z	34	0	0	2	0
All	All	99077	0	60011	2220	0

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

All (2220) 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)
26:W:21:LEU:HD21	26:W:48:VAL:HG11	1.35	1.08
14:K:29:LEU:HB3	14:K:55:VAL:HG11	1.33	1.07
1:0:1160:G:H5'	1:0:1161:A:H5'	1.36	1.07
27:X:37:LEU:HD13	27:X:85:VAL:HG21	1.39	1.04
2:9:3076:G:H3'	2:9:3077:A:H5''	1.36	1.04
23:T:9:LYS:HE3	23:T:13:ARG:NH1	1.73	1.04
13:J:93:ARG:HH11	13:J:93:ARG:HB3	1.21	1.02
25:V:12:THR:HG22	25:V:15:GLU:HG3	1.38	1.02
8:D:25:MET:HE2	8:D:41:LEU:HG	1.41	1.00
6:B:162:MET:HE2	6:B:310:ARG:HD3	1.44	0.99
1:0:871:G:C8	1:0:871:G:H5'	1.96	0.99
22:S:51:GLN:HE21	22:S:53:ASN:HD21	1.05	0.99
9:E:20:ILE:HD11	9:E:40:VAL:HG11	1.46	0.98
7:C:236:THR:HG22	7:C:239:ALA:H	1.24	0.98
1:0:156:C:H5''	16:M:171:ARG:HD3	1.46	0.97
7:C:127:ARG:NH2	7:C:225:PRO:HG2	1.80	0.96
5:A:211:LYS:HG2	5:A:212:PRO:HD2	1.45	0.96
10:F:91:VAL:HG12	10:F:92:GLY:H	1.26	0.96
23:T:71:VAL:HG11	23:T:90:PRO:HB3	1.46	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:78:ARG:HG3	7:C:78:ARG:HH11	1.30	0.96
1:0:1771:U:H5'	29:Z:20:ARG:HH21	1.31	0.95
1:0:871:G:H8	1:0:871:G:H5'	1.28	0.95
1:0:870:G:H2'	1:0:871:G:H5''	1.48	0.95
1:0:542:A:H5'	1:0:542:A:H8	1.34	0.93
14:K:10:GLN:H	14:K:10:GLN:HE21	0.93	0.92
1:0:1242:A:H5'	13:J:82:THR:HG23	1.50	0.92
17:N:11:ARG:HG3	17:N:14:ARG:HH12	1.34	0.92
14:K:10:GLN:H	14:K:10:GLN:NE2	1.66	0.91
8:D:28:GLY:HA2	8:D:69:ILE:HG23	1.52	0.91
1:0:1372:A:H3'	40:0:7638:HOH:O	1.70	0.91
5:A:192:VAL:HG12	5:A:207:GLN:HB3	1.53	0.91
5:A:81:GLN:HB2	5:A:92:ASN:ND2	1.86	0.90
26:W:6:GLN:HB2	26:W:26:ILE:HD12	1.53	0.90
1:0:2812:A:H2	1:0:2814:A:H62	1.19	0.90
17:N:144:GLY:O	17:N:147:ILE:HG22	1.70	0.90
28:Y:235:GLU:H	28:Y:235:GLU:CD	1.75	0.90
6:B:238:ASN:HD22	6:B:240:GLY:H	1.18	0.90
31:2:18:ASN:HD21	31:2:40:ARG:H	1.17	0.89
14:K:74:VAL:HG13	14:K:113:ILE:HG23	1.54	0.89
6:B:307:ARG:HH11	6:B:307:ARG:HG3	1.36	0.89
12:H:29:ALA:HB3	12:H:66:ARG:HH12	1.37	0.89
7:C:1:MET:HG2	7:C:2:GLN:H	1.38	0.89
8:D:58:VAL:HB	8:D:62:ASP:HB3	1.54	0.89
6:B:36:PRO:HA	6:B:168:GLY:HA3	1.55	0.89
18:O:32:ARG:HE	18:O:35:LYS:HD2	1.36	0.88
14:K:81:ARG:HB2	14:K:87:ARG:HH11	1.37	0.88
1:0:2717:C:H2'	1:0:2718:C:H5''	1.53	0.88
14:K:74:VAL:HG11	14:K:113:ILE:HG12	1.54	0.88
1:0:289:G:H22	1:0:363:A:H2	1.21	0.87
16:M:102:GLU:OE1	16:M:164:THR:HG21	1.73	0.87
19:P:115:SER:H	19:P:118:GLN:HE21	1.20	0.87
21:R:25:PHE:CE2	21:R:29:LYS:HE2	2.09	0.87
1:0:541:C:H2'	1:0:542:A:H5''	1.57	0.86
17:N:49:THR:HG22	17:N:56:ASP:HB2	1.55	0.86
29:Z:11:SER:HB3	29:Z:23:ARG:HB2	1.55	0.86
17:N:113:SER:HB2	40:N:9354:HOH:O	1.75	0.86
17:N:83:LEU:HD13	17:N:175:LEU:HD23	1.56	0.85
7:C:5:ILE:HD11	7:C:16:VAL:HG22	1.57	0.85
5:A:192:VAL:CG1	5:A:207:GLN:HB3	2.07	0.85
2:9:3056:A:H2'	2:9:3057:A:H5''	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1835:U:H5	1:0:1840:A:N7	1.75	0.85
26:W:137:GLN:HE21	26:W:141:HIS:HE1	1.25	0.85
9:E:15:GLN:HG2	9:E:19:ASP:O	1.77	0.85
8:D:172:VAL:HG12	8:D:173:GLU:H	1.40	0.85
29:Z:37:HIS:HB2	29:Z:47:VAL:HB	1.59	0.84
16:M:99:ARG:HH21	16:M:170:ASN:HD22	1.25	0.84
21:R:8:ALA:HB1	21:R:13:THR:HG21	1.58	0.84
28:Y:200:THR:HG22	28:Y:201:GLU:HG3	1.58	0.84
14:K:10:GLN:N	14:K:10:GLN:HE21	1.74	0.84
15:L:80:ASP:HB2	15:L:90:ARG:O	1.78	0.83
2:9:3006:C:H5''	17:N:37:ARG:NH1	1.94	0.83
19:P:115:SER:OG	19:P:118:GLN:HG3	1.78	0.83
1:0:1116:U:HO2'	1:0:1118:A:H2	0.85	0.83
5:A:192:VAL:HG22	40:A:9617:HOH:O	1.78	0.83
1:0:2506:A:O2'	1:0:2507:G:H8	1.62	0.83
26:W:122:ARG:HH11	26:W:122:ARG:HG2	1.43	0.83
1:0:2717:C:C2'	1:0:2718:C:H5''	2.08	0.83
1:0:1474:C:H6	1:0:1474:C:H5'	1.43	0.82
1:0:2506:A:HO2'	1:0:2507:G:H8	0.87	0.82
29:Z:36:ASP:HB3	29:Z:45:ASP:HB3	1.62	0.82
1:0:2840:A:OP1	6:B:211:THR:HG23	1.77	0.82
14:K:39:GLY:HA2	40:K:4183:HOH:O	1.80	0.82
12:H:56:GLN:HE22	12:H:93:GLN:HG2	1.45	0.82
6:B:162:MET:CE	6:B:310:ARG:HD3	2.10	0.82
2:9:3006:C:H5''	17:N:37:ARG:HH12	1.45	0.81
21:R:99:ALA:HB1	21:R:109:MET:HE1	1.61	0.81
1:0:871:G:H8	1:0:871:G:C5'	1.94	0.81
16:M:134:ILE:HG23	16:M:141:ILE:HD13	1.63	0.81
31:2:41:HIS:H	31:2:45:ASN:HD22	1.26	0.81
1:0:288:A:H61	1:0:364:C:H42	1.29	0.80
5:A:191:GLY:HA2	5:A:194:MET:CE	2.11	0.80
8:D:134:LEU:HD11	8:D:166:ILE:HD11	1.63	0.80
14:K:107:THR:HG22	14:K:108:GLU:HG3	1.64	0.80
1:0:2851:G:C2'	1:0:2852:A:H5'	2.12	0.80
8:D:136:ARG:HH12	8:D:157:LEU:HA	1.46	0.79
26:W:6:GLN:HB2	26:W:26:ILE:CD1	2.13	0.79
26:W:88:THR:HB	40:W:6679:HOH:O	1.82	0.79
6:B:179:LEU:O	6:B:183:GLU:HG2	1.81	0.79
1:0:1160:G:C5'	1:0:1161:A:H5'	2.13	0.79
1:0:2716:G:H5''	6:B:206:THR:HG21	1.65	0.79
14:K:4:LEU:HD22	14:K:116:GLU:HB3	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:12:ILE:N	11:G:13:PRO:HD3	1.97	0.79
27:X:72:VAL:HG22	27:X:85:VAL:HG12	1.64	0.79
1:0:1119:G:H2'	13:J:52:GLN:NE2	1.98	0.79
1:0:1603:A:H5'	1:0:1605:G:O4'	1.83	0.79
14:K:98:VAL:HG13	14:K:102:GLU:HA	1.63	0.79
9:E:81:GLU:HG2	9:E:134:SER:HB3	1.64	0.79
17:N:11:ARG:HA	17:N:14:ARG:NH1	1.97	0.79
26:W:4:LEU:HD22	26:W:52:VAL:HG21	1.63	0.79
1:0:2534:C:H1'	40:0:4081:HOH:O	1.80	0.78
21:R:99:ALA:HB1	21:R:109:MET:CE	2.12	0.78
1:0:541:C:C2'	1:0:542:A:H5''	2.11	0.78
33:I:102:VAL:HG12	33:I:106:LYS:HE3	1.62	0.78
16:M:107:ARG:HH11	16:M:107:ARG:HG3	1.47	0.78
1:0:969:G:H1	1:0:999:C:H42	1.32	0.78
26:W:88:THR:HG23	26:W:110:GLN:NE2	1.99	0.78
1:0:2054:A:N3	21:R:128:ARG:NH2	2.31	0.78
1:0:1973:A:H5'	1:0:1973:A:H8	1.49	0.77
17:N:12:ARG:HD3	17:N:18:THR:OG1	1.85	0.77
31:2:22:PRO:HG2	31:2:25:VAL:HG23	1.67	0.77
12:H:27:LYS:H	12:H:59:HIS:HD2	1.30	0.77
1:0:2073:G:H5''	40:0:4400:HOH:O	1.83	0.77
1:0:1118:A:H3'	1:0:1118:A:H8	1.50	0.77
6:B:212:GLN:HB2	6:B:257:THR:HG21	1.66	0.77
21:R:18:LEU:HD12	21:R:143:VAL:HG11	1.68	0.76
5:A:199:HIS:HD2	5:A:201:PHE:H	1.32	0.76
13:J:93:ARG:NH1	13:J:93:ARG:HB3	1.99	0.76
10:F:91:VAL:HG12	10:F:92:GLY:N	2.01	0.76
40:0:5371:HOH:O	13:J:47:THR:HB	1.83	0.76
26:W:122:ARG:HH11	26:W:122:ARG:CG	1.97	0.76
26:W:125:HIS:HD2	26:W:127:GLY:H	1.30	0.76
14:K:98:VAL:CG1	14:K:102:GLU:HA	2.15	0.76
1:0:559:U:H5'	1:0:559:U:H6	1.50	0.76
1:0:560:C:H42	1:0:597:A:H61	1.33	0.76
17:N:11:ARG:HG3	17:N:14:ARG:NH1	2.01	0.76
8:D:57:THR:HG23	8:D:63:ILE:HA	1.67	0.76
1:0:1041:U:H5'	40:L:9491:HOH:O	1.85	0.76
16:M:79:ALA:HB3	16:M:81:ARG:NH1	2.00	0.76
1:0:1667:A:H8	1:0:1667:A:H5'	1.51	0.75
1:0:960:G:H4'	40:0:7866:HOH:O	1.84	0.75
21:R:111:ILE:HG23	21:R:145:LEU:HD11	1.67	0.75
2:9:3014:G:H8	2:9:3014:G:H5'	1.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:J:93:ARG:HH11	13:J:93:ARG:CB	2.00	0.75
7:C:104:ASP:HA	7:C:107:ARG:HH12	1.50	0.75
1:0:1119:G:N2	1:0:1246:A:C2	2.53	0.75
1:0:2533:C:H5'	1:0:2533:C:H6	1.51	0.75
6:B:195:ARG:HG2	6:B:323:LEU:HD22	1.68	0.75
9:E:15:GLN:HG3	9:E:20:ILE:HG12	1.68	0.75
1:0:506:G:H22	1:0:509:A:C5'	2.00	0.75
5:A:153:ARG:HH11	5:A:153:ARG:HB2	1.50	0.75
13:J:19:MET:HE1	13:J:132:LEU:HD21	1.69	0.75
25:V:39:ALA:N	25:V:40:PRO:HD2	2.02	0.75
26:W:13:MET:HE1	26:W:18:GLN:HA	1.67	0.75
8:D:25:MET:HE1	8:D:37:ALA:HB1	1.67	0.74
1:0:1116:U:O2'	1:0:1118:A:H2	1.67	0.74
13:J:19:MET:HE3	13:J:132:LEU:HD11	1.68	0.74
14:K:14:LYS:HB2	14:K:45:PRO:HG2	1.70	0.74
32:3:70:ARG:HG2	32:3:77:ALA:HB2	1.69	0.74
5:A:206:ARG:HD3	5:A:206:ARG:H	1.51	0.74
1:0:1244:U:OP1	13:J:18:ILE:HD13	1.87	0.74
9:E:3:VAL:HG22	9:E:49:ILE:HB	1.69	0.74
6:B:51:VAL:CG2	6:B:327:VAL:HG13	2.18	0.74
1:0:1118:A:C8	1:0:1118:A:H3'	2.22	0.74
29:Z:46:ARG:HD2	29:Z:59:TYR:HB2	1.68	0.74
9:E:84:MET:HE1	9:E:148:ILE:HD12	1.69	0.74
1:0:281:U:H2'	1:0:282:C:O4'	1.86	0.74
33:I:78:LEU:HD12	33:I:112:LYS:HZ2	1.53	0.74
17:N:80:SER:HB2	40:N:9333:HOH:O	1.85	0.74
5:A:35:GLY:O	5:A:36:ASP:HB3	1.88	0.74
8:D:54:ALA:HB2	8:D:69:ILE:HD12	1.70	0.74
21:R:39:THR:HB	21:R:42:GLU:HG3	1.69	0.74
28:Y:154:ARG:HH12	28:Y:155:ARG:HG3	1.53	0.73
1:0:1377:C:H6	1:0:1377:C:H5'	1.52	0.73
26:W:88:THR:HG22	26:W:89:ASP:N	2.03	0.73
13:J:74:ARG:HB3	13:J:74:ARG:HH11	1.51	0.73
1:0:1751:G:H2'	1:0:1752:G:H5''	1.70	0.73
15:L:143:THR:HG22	15:L:144:ASP:H	1.52	0.73
9:E:36:PRO:HD3	13:J:127:ILE:HD12	1.68	0.73
33:I:99:ASP:OD1	33:I:138:THR:HB	1.89	0.73
1:0:1206:U:H6	1:0:1206:U:H5'	1.52	0.73
22:S:57:THR:HG22	22:S:59:ASP:H	1.54	0.73
32:3:65:THR:HG22	32:3:67:LEU:HG	1.69	0.73
7:C:236:THR:HG22	7:C:239:ALA:N	2.00	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:W:137:GLN:HE21	26:W:141:HIS:CE1	2.07	0.73
1:O:567:U:H5''	40:W:5817:HOH:O	1.88	0.73
25:V:1:THR:HG23	25:V:2:VAL:H	1.54	0.73
1:O:111:C:O2'	30:1:20:ARG:HG2	1.88	0.73
1:O:1165:G:H4'	1:O:1174:A:O2'	1.89	0.73
23:T:49:GLU:HB3	23:T:59:GLU:HG2	1.71	0.73
18:O:32:ARG:HD3	18:O:32:ARG:O	1.87	0.72
16:M:69:LYS:O	16:M:73:ARG:NH2	2.22	0.72
1:O:506:G:H22	1:O:509:A:H5''	1.53	0.72
1:O:870:G:C2'	1:O:871:G:H5''	2.18	0.72
1:O:1118:A:H62	1:O:1244:U:H3	1.35	0.72
1:O:656:G:H5'	18:O:3:THR:HB	1.71	0.72
1:O:2890:A:H1'	24:U:56:ARG:NH2	2.04	0.72
15:L:143:THR:HG22	15:L:144:ASP:N	2.05	0.72
7:C:104:ASP:HA	7:C:107:ARG:NH1	2.05	0.72
2:9:3039:U:H1'	2:9:3044:A:H61	1.55	0.72
19:P:115:SER:H	19:P:118:GLN:NE2	1.88	0.71
1:O:545:G:H8	1:O:545:G:H5'	1.55	0.71
14:K:74:VAL:CG1	14:K:113:ILE:HG12	2.19	0.71
14:K:81:ARG:HB2	14:K:87:ARG:NH1	2.04	0.71
1:O:1700:C:H5''	1:O:1701:A:OP2	1.90	0.71
1:O:2851:G:H2'	1:O:2852:A:H5'	1.72	0.71
5:A:88:ILE:HD13	5:A:100:PRO:HD3	1.71	0.71
8:D:58:VAL:HG12	8:D:60:GLU:HG2	1.72	0.71
33:I:110:GLU:HA	33:I:113:HIS:NE2	2.06	0.71
1:O:2005:G:H3'	1:O:2005:G:OP2	1.91	0.71
10:F:58:GLU:OE1	16:M:27:ARG:NH2	2.23	0.71
14:K:29:LEU:HB3	14:K:55:VAL:CG1	2.19	0.71
13:J:74:ARG:NH1	13:J:76:ASP:HB2	2.06	0.71
10:F:50:VAL:HG13	10:F:60:VAL:HG11	1.71	0.71
5:A:191:GLY:HA2	5:A:194:MET:HE2	1.72	0.71
1:O:544:G:H2'	1:O:545:G:H5''	1.72	0.71
28:Y:165:GLU:HB3	40:Y:9390:HOH:O	1.90	0.71
1:O:1299:G:O6	15:L:6:ARG:HD3	1.91	0.71
40:O:7889:HOH:O	6:B:211:THR:HG21	1.91	0.70
1:O:1701:A:H4'	1:O:1702:U:H5''	1.73	0.70
8:D:135:VAL:HG21	8:D:139:TYR:CD1	2.26	0.70
16:M:31:TRP:HA	16:M:34:GLU:HG3	1.72	0.70
7:C:236:THR:CG2	7:C:239:ALA:H	2.04	0.70
1:O:2364:A:H5''	20:Q:15:LYS:HD3	1.73	0.70
26:W:80:ASP:O	26:W:84:VAL:HG23	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:962:C:H1'	17:N:5:ARG:NH1	2.06	0.70
10:F:77:VAL:HG21	10:F:83:LEU:HD13	1.74	0.70
27:X:74:ALA:HB2	27:X:85:VAL:HG13	1.72	0.70
19:P:115:SER:N	19:P:118:GLN:HE21	1.89	0.70
12:H:21:THR:O	12:H:120:ILE:HD12	1.92	0.70
10:F:96:ALA:HA	40:F:3111:HOH:O	1.91	0.70
16:M:79:ALA:HB3	16:M:81:ARG:HH12	1.57	0.70
33:I:132:CYS:HB3	33:I:137:VAL:HB	1.74	0.70
7:C:132:ASP:HB3	40:C:9172:HOH:O	1.91	0.70
7:C:78:ARG:HG3	7:C:78:ARG:NH1	2.04	0.70
19:P:59:ARG:NH2	19:P:66:GLN:HE22	1.89	0.70
17:N:17:ARG:HB3	17:N:17:ARG:HH11	1.57	0.70
5:A:33:GLU:CD	5:A:33:GLU:H	1.93	0.70
30:1:25:LYS:HD2	31:2:48:ASP:HA	1.72	0.70
6:B:275:GLY:O	6:B:291:ASP:HA	1.91	0.70
23:T:71:VAL:HG11	23:T:90:PRO:CB	2.21	0.70
26:W:52:VAL:HG22	26:W:53:ALA:H	1.57	0.69
33:I:78:LEU:HD12	33:I:112:LYS:NZ	2.07	0.69
1:0:1160:G:H5'	1:0:1161:A:C5'	2.18	0.69
31:2:18:ASN:HD21	31:2:40:ARG:N	1.89	0.69
10:F:37:THR:O	10:F:41:GLU:HG3	1.93	0.69
30:1:28:HIS:CD2	30:1:31:LYS:HG3	2.27	0.69
1:0:1771:U:H5'	29:Z:20:ARG:NH2	2.07	0.69
1:0:542:A:H5'	1:0:542:A:C8	2.22	0.69
1:0:481:U:H5''	40:0:6167:HOH:O	1.92	0.69
6:B:125:GLU:O	6:B:129:ARG:HG3	1.93	0.69
12:H:56:GLN:NE2	12:H:126:ARG:HE	1.90	0.69
26:W:88:THR:HG22	26:W:89:ASP:H	1.57	0.69
1:0:2491:G:H1'	40:0:7335:HOH:O	1.93	0.69
26:W:13:MET:HE3	26:W:17:ILE:HG22	1.74	0.69
22:S:77:VAL:O	22:S:80:ARG:HG2	1.92	0.69
28:Y:212:ARG:HD2	40:Y:9398:HOH:O	1.92	0.69
7:C:47:GLY:HA2	7:C:92:PRO:HB2	1.74	0.69
5:A:51:ARG:HB2	40:A:9591:HOH:O	1.93	0.69
8:D:172:VAL:HG12	8:D:173:GLU:N	2.07	0.69
1:0:380:A:OP2	16:M:9:ARG:HD2	1.93	0.69
18:O:32:ARG:NE	18:O:35:LYS:HD2	2.08	0.69
1:0:1474:C:C6	1:0:1474:C:H5'	2.26	0.69
1:0:1641:A:H2'	1:0:1642:A:H5'	1.74	0.69
26:W:122:ARG:NH2	26:W:154:ARG:HG2	2.07	0.68
1:0:2749:U:H5'	40:0:8429:HOH:O	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:76:ARG:HH11	27:X:76:ARG:HG3	1.57	0.68
1:O:871:G:C8	1:O:871:G:C5'	2.70	0.68
26:W:130:HIS:O	26:W:136:GLY:HA3	1.93	0.68
16:M:107:ARG:NH1	16:M:107:ARG:HG3	2.05	0.68
6:B:238:ASN:HD22	6:B:240:GLY:N	1.92	0.68
14:K:23:ASN:HD21	14:K:107:THR:HB	1.58	0.68
15:L:67:ARG:O	15:L:71:GLU:HG3	1.93	0.68
33:I:134:SER:O	33:I:135:LEU:HD23	1.93	0.68
26:W:137:GLN:NE2	26:W:141:HIS:HE1	1.90	0.68
21:R:18:LEU:HD12	21:R:143:VAL:CG1	2.23	0.68
26:W:81:ASP:OD1	26:W:92:ASP:HB2	1.94	0.68
7:C:2:GLN:HB3	40:C:9195:HOH:O	1.94	0.68
9:E:6:GLU:HA	9:E:46:THR:HG22	1.74	0.68
13:J:131:THR:HG22	13:J:134:GLU:H	1.56	0.68
14:K:81:ARG:HD3	14:K:87:ARG:NH1	2.08	0.68
12:H:56:GLN:NE2	12:H:93:GLN:HG2	2.08	0.68
1:O:1201:C:H2'	1:O:1202:A:H5'	1.74	0.68
19:P:91:LYS:O	19:P:95:GLU:HG3	1.93	0.68
1:O:1116:U:O2'	1:O:1118:A:C2	2.46	0.67
13:J:74:ARG:HH12	13:J:76:ASP:HB2	1.60	0.67
17:N:62:HIS:HB3	17:N:65:ASP:OD1	1.95	0.67
1:O:1182:C:H1'	1:O:1192:A:H8	1.58	0.67
12:H:30:GLN:H	12:H:66:ARG:NH1	1.93	0.67
12:H:59:HIS:HA	12:H:62:LEU:HD23	1.76	0.67
21:R:18:LEU:HB2	21:R:143:VAL:CG1	2.24	0.67
6:B:62:ARG:HA	6:B:65:MET:CE	2.24	0.67
18:O:96:VAL:HG13	18:O:100:GLN:HB2	1.75	0.67
1:O:2908:A:H2'	1:O:2909:G:O4'	1.95	0.67
8:D:159:PRO:O	8:D:163:VAL:HG23	1.94	0.67
1:O:1166:A:H1'	1:O:1192:A:C2	2.29	0.67
27:X:71:ARG:HD3	40:X:2171:HOH:O	1.95	0.67
1:O:1184:C:H1'	40:O:7899:HOH:O	1.93	0.67
23:T:115:GLU:HG3	23:T:116:ASP:N	2.09	0.67
24:U:5:GLU:HG2	24:U:10:GLY:O	1.95	0.67
1:O:2676:C:H4'	13:J:70:PHE:CE1	2.30	0.67
1:O:2676:C:H4'	13:J:70:PHE:CD1	2.30	0.67
5:A:199:HIS:CD2	5:A:201:PHE:H	2.11	0.67
1:O:2468:A:H61	32:3:48:ASN:HD21	1.43	0.67
1:O:883:U:H2'	1:O:883:U:O2	1.95	0.67
12:H:27:LYS:N	12:H:59:HIS:HD2	1.92	0.67
5:A:100:PRO:HG2	5:A:103:VAL:HG21	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:797:A:C4'	29:Z:10:ARG:N	2.57	0.67
26:W:21:LEU:CD2	26:W:48:VAL:HG11	2.19	0.66
1:0:2420:G:O2'	1:0:2421:G:H5'	1.96	0.66
1:0:1183:C:H2'	40:0:6739:HOH:O	1.94	0.66
10:F:13:GLU:OE2	10:F:78:GLU:HG2	1.95	0.66
27:X:71:ARG:HB3	27:X:88:GLU:OE1	1.95	0.66
1:0:877:G:H5'	1:0:878:G:OP1	1.95	0.66
1:0:2073:G:OP2	1:0:2490:A:H5'	1.94	0.66
5:A:153:ARG:NH1	5:A:153:ARG:HB2	2.10	0.66
19:P:59:ARG:HH22	19:P:66:GLN:HE22	1.42	0.66
1:0:1838:U:O2'	1:0:2644:C:H5'	1.95	0.66
1:0:541:C:H2'	1:0:542:A:C5'	2.26	0.66
1:0:2578:G:H5'	1:0:2578:G:H8	1.59	0.66
8:D:41:LEU:HA	8:D:44:ILE:HG22	1.76	0.66
28:Y:189:ASN:HA	28:Y:217:ILE:HD11	1.78	0.66
1:0:1666:C:H2'	1:0:1667:A:H5'	1.77	0.66
28:Y:144:ARG:HH11	28:Y:144:ARG:CG	2.09	0.66
6:B:140:LEU:HA	40:B:9575:HOH:O	1.95	0.66
1:0:2505:G:O2'	1:0:2506:A:H5'	1.96	0.66
29:Z:22:SER:O	29:Z:26:VAL:HG23	1.94	0.66
6:B:51:VAL:HG23	6:B:329:TYR:O	1.96	0.66
26:W:68:THR:HG23	26:W:69:ARG:HG2	1.78	0.66
10:F:58:GLU:CD	16:M:27:ARG:HH22	1.97	0.66
1:0:1116:U:H3	1:0:1246:A:H62	1.44	0.65
1:0:1159:G:H21	1:0:1189:A:H8	1.44	0.65
6:B:254:GLN:HG2	6:B:255:GLY:N	2.10	0.65
22:S:10:VAL:HG11	25:V:36:ALA:HA	1.78	0.65
18:O:32:ARG:HH21	18:O:35:LYS:NZ	1.94	0.65
6:B:53:LEU:HD11	6:B:327:VAL:HG22	1.77	0.65
13:J:45:VAL:HG11	13:J:121:LEU:HD22	1.79	0.65
23:T:41:ARG:HG2	23:T:41:ARG:HH11	1.59	0.65
19:P:9:LEU:O	19:P:13:VAL:HG12	1.97	0.65
1:0:1687:C:O2	30:I:9:GLY:HA2	1.97	0.65
6:B:16:ARG:NH1	40:B:9612:HOH:O	2.28	0.65
7:C:162:VAL:HG22	7:C:232:LEU:HD21	1.77	0.65
15:L:73:VAL:HG23	15:L:74:THR:H	1.62	0.65
23:T:49:GLU:OE2	23:T:97:ARG:HD2	1.95	0.65
28:Y:144:ARG:CZ	40:Y:9409:HOH:O	2.44	0.65
18:O:32:ARG:HH21	18:O:35:LYS:HZ2	1.44	0.65
23:T:32:ARG:NH1	23:T:38:ARG:HH12	1.94	0.65
5:A:48:ASP:HB3	40:A:9591:HOH:O	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1162:G:H1'	33:I:117:LEU:HD11	1.79	0.65
12:H:166:SER:HB3	12:H:167:PRO:HD3	1.78	0.65
1:0:2661:U:H3	1:0:2812:A:H62	1.43	0.65
1:0:2521:A:OP2	12:H:3:ALA:HB3	1.96	0.65
28:Y:144:ARG:HG3	28:Y:144:ARG:HH11	1.60	0.65
6:B:201:ASP:HB2	6:B:312:ARG:HD2	1.79	0.65
17:N:48:VAL:CG1	17:N:55:ASP:HB3	2.27	0.65
6:B:307:ARG:NH1	6:B:307:ARG:HG3	2.05	0.65
1:0:1175:G:H1'	1:0:1193:A:H2'	1.78	0.65
1:0:1119:G:H22	1:0:1246:A:H2	1.41	0.64
16:M:134:ILE:CG2	16:M:141:ILE:HD13	2.26	0.64
1:0:282:C:O2'	1:0:283:U:H5'	1.96	0.64
1:0:1730:G:H5'	1:0:1731:C:C5	2.31	0.64
26:W:48:VAL:HG12	26:W:48:VAL:O	1.97	0.64
26:W:88:THR:HG23	26:W:110:GLN:HE21	1.61	0.64
10:F:2:VAL:HG22	10:F:57:GLU:OE1	1.97	0.64
6:B:74:ILE:HD13	6:B:309:VAL:HG21	1.78	0.64
1:0:2896:A:H5''	40:0:6599:HOH:O	1.96	0.64
10:F:53:ASP:OD1	10:F:80:GLN:HB2	1.96	0.64
17:N:139:TRP:HA	17:N:139:TRP:CE3	2.33	0.64
16:M:68:ARG:NH2	16:M:73:ARG:HD3	2.13	0.64
1:0:1209:C:H2'	1:0:1210:G:H8	1.61	0.64
18:O:21:SER:OG	18:O:106:PRO:HB2	1.98	0.64
23:T:112:LEU:HD23	23:T:119:ALA:HB3	1.79	0.64
29:Z:42:CYS:SG	29:Z:43:GLY:N	2.70	0.64
1:0:272:A:H5'	1:0:273:G:OP2	1.97	0.64
1:0:544:G:C2'	1:0:545:G:H5''	2.27	0.64
6:B:18:ARG:HG3	6:B:256:GLN:HG3	1.78	0.64
6:B:41:PHE:CD2	6:B:190:MET:HE3	2.32	0.64
13:J:75:PRO:HG2	13:J:105:LEU:HD21	1.79	0.64
10:F:63:ILE:HB	10:F:64:PRO:HD3	1.80	0.64
12:H:46:GLN:HB3	12:H:167:PRO:HD2	1.78	0.64
1:0:1878:G:H1'	40:0:6620:HOH:O	1.97	0.64
1:0:381:G:H5''	40:M:9373:HOH:O	1.97	0.64
24:U:45:GLU:HB2	24:U:48:ASN:ND2	2.12	0.64
31:2:18:ASN:ND2	31:2:40:ARG:H	1.93	0.64
14:K:49:LEU:HD12	14:K:80:ILE:HG21	1.80	0.64
6:B:190:MET:HE2	6:B:194:PHE:HD1	1.61	0.64
16:M:187:LEU:CD2	16:M:194:ALA:HB3	2.28	0.64
20:Q:75:ILE:HD13	20:Q:84:ILE:HD11	1.78	0.64
23:T:9:LYS:HE3	23:T:13:ARG:HH12	1.58	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:W:108:ARG:HG3	26:W:114:PRO:HG3	1.80	0.64
1:O:709:G:O2'	18:O:25:VAL:HG12	1.97	0.64
33:I:125:ALA:O	33:I:129:VAL:HG23	1.97	0.64
9:E:20:ILE:CD1	9:E:40:VAL:HG11	2.26	0.64
21:R:111:ILE:HG23	21:R:145:LEU:CD1	2.28	0.64
14:K:75:ARG:HD3	14:K:112:PRO:O	1.98	0.64
1:O:2064:U:H5'	1:O:2652:U:H4'	1.80	0.64
33:I:110:GLU:HA	33:I:113:HIS:CE1	2.33	0.63
12:H:166:SER:CB	12:H:167:PRO:CD	2.75	0.63
7:C:157:LEU:HD13	7:C:166:ILE:HD11	1.81	0.63
7:C:77:ALA:O	7:C:78:ARG:HG3	1.97	0.63
2:9:3056:A:C2'	2:9:3057:A:H5''	2.26	0.63
2:9:3039:U:HO2'	2:9:3042:C:H5	1.44	0.63
28:Y:126:PRO:HG2	28:Y:128:PHE:CE1	2.33	0.63
5:A:36:ASP:OD2	5:A:85:SER:HB2	1.98	0.63
17:N:164:ASP:CG	17:N:167:ASP:HA	2.18	0.63
1:O:1427:A:H61	1:O:1440:U:H1'	1.62	0.63
1:O:263:U:O4'	10:F:59:ILE:HD13	1.99	0.63
33:I:113:HIS:N	33:I:114:PRO:HD2	2.14	0.63
16:M:80:GLY:O	16:M:81:ARG:HD2	1.99	0.63
1:O:447:A:P	23:T:1:SER:HB2	2.38	0.63
1:O:88:G:H2'	1:O:89:G:C8	2.34	0.63
1:O:2587:OMU:H5	40:O:7918:HOH:O	1.97	0.63
25:V:20:LEU:HD22	25:V:60:GLN:HE22	1.63	0.63
1:O:2541:U:H4'	1:O:2542:C:OP1	1.97	0.63
14:K:55:VAL:HG12	14:K:56:SER:N	2.13	0.63
40:O:9739:HOH:O	16:M:82:ARG:HD2	1.98	0.63
2:9:3014:G:C8	2:9:3014:G:H5'	2.33	0.63
5:A:94:LEU:HG	5:A:99:ILE:HD11	1.80	0.63
1:O:2533:C:C6	1:O:2533:C:H5'	2.32	0.62
13:J:90:LYS:HB2	37:J:9302:CL:CL	2.35	0.62
30:1:25:LYS:HD2	31:2:49:GLU:H	1.64	0.62
32:3:38:ARG:HB3	32:3:42:ARG:HH12	1.64	0.62
1:O:2896:A:N3	1:O:2896:A:H2'	2.15	0.62
30:1:45:ARG:NH2	40:1:9488:HOH:O	2.31	0.62
12:H:27:LYS:H	12:H:59:HIS:CD2	2.17	0.62
1:O:1206:U:H2'	1:O:1207:A:O4'	2.00	0.62
12:H:40:ALA:HB1	12:H:137:TYR:CE2	2.34	0.62
1:O:1528:A:H2'	1:O:1529:G:O4'	1.98	0.62
16:M:164:THR:HG22	16:M:166:ALA:N	2.14	0.62
26:W:4:LEU:HD11	26:W:45:VAL:HG12	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:2:22:PRO:HG2	31:2:25:VAL:CG2	2.29	0.62
23:T:71:VAL:HG12	23:T:72:ILE:N	2.15	0.62
1:0:524:A:H5"	21:R:29:LYS:HD3	1.82	0.62
26:W:141:HIS:HB2	26:W:146:ILE:HG12	1.80	0.62
21:R:18:LEU:HB2	21:R:143:VAL:HG13	1.82	0.62
17:N:139:TRP:HA	17:N:139:TRP:HE3	1.65	0.62
1:0:2780:C:H1'	9:E:143:GLN:HE21	1.64	0.62
9:E:23:GLU:HG2	9:E:28:SER:HB3	1.80	0.62
27:X:25:ARG:HD3	27:X:64:ALA:O	1.99	0.62
17:N:154:LEU:HG	17:N:155:GLU:H	1.63	0.62
21:R:44:VAL:O	21:R:48:GLU:HG3	2.00	0.62
30:1:10:LYS:HG3	40:1:9492:HOH:O	1.98	0.62
2:9:3029:C:O3'	8:D:138:GLY:HA2	2.00	0.62
40:9:4707:HOH:O	17:N:147:ILE:HD12	1.99	0.62
1:0:1183:C:N4	1:0:1184:C:H41	1.98	0.62
2:9:3051:A:H5'	17:N:160:SER:HB3	1.82	0.62
19:P:80:ARG:HG2	19:P:87:ARG:CZ	2.30	0.62
2:9:3020:G:O2'	2:9:3021:G:H5'	1.99	0.62
16:M:164:THR:HG22	16:M:167:GLY:H	1.65	0.62
1:0:1118:A:H8	1:0:1119:G:H5"	1.64	0.62
12:H:20:ILE:HG23	12:H:120:ILE:HD11	1.81	0.62
5:A:135:VAL:HG21	5:A:147:ARG:NH1	2.15	0.62
1:0:1328:A:OP1	28:Y:169:ARG:HD2	2.00	0.62
11:G:12:ILE:N	11:G:13:PRO:CD	2.63	0.62
2:9:3029:C:H2'	2:9:3030:C:H5'	1.81	0.62
19:P:64:GLU:HG2	40:P:165:HOH:O	2.00	0.62
1:0:470:U:O2'	30:1:16:HIS:HD2	1.83	0.62
29:Z:72:GLU:OE1	29:Z:77:LYS:HE2	1.99	0.62
14:K:109:LEU:HD13	14:K:113:ILE:HD11	1.81	0.61
13:J:19:MET:CE	13:J:132:LEU:HD11	2.29	0.61
6:B:141:ARG:HD2	6:B:163:GLU:OE2	1.99	0.61
30:1:8:GLN:HE22	30:1:11:LYS:NZ	1.97	0.61
7:C:118:THR:HG22	7:C:137:PRO:HB3	1.81	0.61
24:U:14:GLU:O	24:U:17:THR:HB	2.01	0.61
6:B:225:GLY:HA3	40:B:9562:HOH:O	2.00	0.61
28:Y:187:VAL:HG12	28:Y:205:ILE:HA	1.81	0.61
28:Y:112:GLU:OE1	28:Y:112:GLU:HA	2.00	0.61
1:0:2586:U:H3	1:0:2592:G:H22	1.47	0.61
17:N:11:ARG:CG	17:N:14:ARG:HH12	2.09	0.61
30:1:25:LYS:HD2	31:2:49:GLU:N	2.15	0.61
1:0:485:A:N3	1:0:487:G:H5"	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2807:U:P	6:B:27:ASN:HD21	2.24	0.61
24:U:52:THR:HG22	24:U:54:THR:N	2.16	0.61
8:D:59:GLY:O	8:D:61:PHE:N	2.33	0.61
1:0:289:G:N2	1:0:363:A:H2	1.94	0.61
2:9:3039:U:H1'	2:9:3044:A:N6	2.15	0.61
5:A:105:VAL:CG1	5:A:154:ALA:HB1	2.31	0.61
5:A:107:ASN:OD1	5:A:120:ARG:HD2	2.00	0.61
25:V:56:ILE:HG22	25:V:60:GLN:HE21	1.66	0.61
6:B:175:LEU:O	6:B:175:LEU:HD23	2.00	0.61
6:B:217:ARG:HG3	6:B:257:THR:HG22	1.80	0.61
27:X:43:VAL:HG12	27:X:44:ASP:N	2.16	0.61
8:D:136:ARG:NH1	8:D:157:LEU:HA	2.15	0.61
1:0:282:C:H1'	1:0:368:C:N4	2.15	0.61
9:E:35:TYR:HA	13:J:127:ILE:HD12	1.82	0.61
18:O:25:VAL:HG23	18:O:26:TRP:N	2.16	0.61
1:0:553:G:P	28:Y:204:ARG:HH22	2.23	0.61
5:A:191:GLY:HA2	5:A:194:MET:HE3	1.81	0.61
6:B:329:TYR:CE2	24:U:15:PRO:HG2	2.35	0.61
1:0:280:C:H2'	1:0:281:U:O4'	2.01	0.61
17:N:164:ASP:OD1	17:N:167:ASP:HA	2.01	0.61
20:Q:25:PRO:HB2	40:Q:4350:HOH:O	2.00	0.61
27:X:66:THR:HG23	27:X:67:PRO:HD2	1.83	0.61
5:A:69:LEU:HD23	5:A:107:ASN:HB2	1.81	0.61
1:0:263:U:O2	16:M:42:ARG:HD2	2.01	0.61
8:D:13:MET:HA	8:D:137:PRO:HG2	1.83	0.61
32:3:65:THR:HG23	32:3:88:LEU:HD22	1.83	0.61
17:N:132:ASN:O	17:N:135:VAL:HG12	2.00	0.61
1:0:2563:U:H2'	1:0:2565:C:O5'	2.00	0.61
6:B:102:THR:CG2	6:B:182:VAL:HG12	2.31	0.61
7:C:129:HIS:CE1	7:C:231:ARG:HA	2.36	0.60
5:A:81:GLN:HB2	5:A:92:ASN:HD21	1.62	0.60
8:D:58:VAL:CG1	8:D:60:GLU:HG2	2.30	0.60
17:N:61:ALA:HB3	17:N:88:ALA:HB2	1.83	0.60
1:0:475:G:OP1	7:C:73:LEU:HD22	2.01	0.60
26:W:21:LEU:HD22	26:W:26:ILE:CD1	2.31	0.60
9:E:68:HIS:O	9:E:72:MET:HG3	2.00	0.60
7:C:136:VAL:HG22	7:C:137:PRO:HA	1.83	0.60
5:A:123:GLY:HA3	5:A:162:GLY:HA2	1.83	0.60
1:0:902:G:N7	15:L:18:HIS:HD2	1.99	0.60
1:0:2769:C:C2'	1:0:2770:G:H5'	2.32	0.60
33:I:92:PRO:C	33:I:94:GLU:H	2.05	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:I:129:VAL:O	33:I:129:VAL:HG12	2.01	0.60
16:M:71:SER:HB2	16:M:92:THR:HG22	1.83	0.60
7:C:139:VAL:HG13	40:C:9254:HOH:O	2.00	0.60
25:V:39:ALA:N	25:V:40:PRO:CD	2.64	0.60
16:M:183:THR:HG22	16:M:194:ALA:HB1	1.82	0.60
28:Y:187:VAL:HB	28:Y:203:VAL:HG22	1.83	0.60
1:0:2426:G:H1'	40:0:6592:HOH:O	2.00	0.60
1:0:2291:A:C8	1:0:2309:C:H5'	2.36	0.60
1:0:338:C:H4'	7:C:174:ILE:CD1	2.32	0.60
8:D:94:ALA:HA	8:D:174:VAL:HA	1.83	0.60
5:A:105:VAL:HG11	5:A:154:ALA:HB1	1.83	0.60
1:0:848:C:H5'	40:0:7714:HOH:O	2.02	0.60
1:0:2365:G:H5''	40:Q:6597:HOH:O	2.01	0.60
7:C:27:ARG:HG3	7:C:29:ASP:OD1	2.02	0.60
1:0:156:C:H5''	16:M:171:ARG:CD	2.28	0.60
1:0:1943:C:H4'	5:A:211:LYS:O	2.02	0.60
2:9:3013:A:O2'	2:9:3014:G:H5''	2.01	0.60
1:0:1201:C:H5''	40:0:6728:HOH:O	2.01	0.60
10:F:58:GLU:HA	10:F:61:MET:HE2	1.82	0.60
2:9:3076:G:C3'	2:9:3077:A:H5''	2.24	0.60
22:S:57:THR:HG22	22:S:59:ASP:N	2.16	0.60
1:0:2346:C:O2'	8:D:52:THR:HG21	2.00	0.60
26:W:21:LEU:HB3	26:W:26:ILE:HG12	1.83	0.60
1:0:796:A:HO2'	29:Z:10:ARG:N	1.98	0.60
1:0:2427:C:OP2	32:3:84:ARG:HD2	2.00	0.60
2:9:3004:G:H21	17:N:44:ARG:NH1	2.00	0.60
8:D:23:VAL:HG21	8:D:45:THR:HG21	1.83	0.60
1:0:2507:G:H2'	1:0:2510:C:H42	1.66	0.60
8:D:135:VAL:HG22	8:D:136:ARG:N	2.17	0.60
26:W:125:HIS:CD2	26:W:127:GLY:H	2.16	0.60
10:F:46:GLU:O	10:F:73:PRO:HD2	2.02	0.60
14:K:113:ILE:HG22	14:K:114:ALA:N	2.16	0.60
33:I:113:HIS:CE1	33:I:121:LEU:HD22	2.36	0.60
1:0:1164:U:OP1	33:I:74:PRO:HA	2.01	0.60
1:0:236:A:H8	1:0:236:A:OP1	1.84	0.60
8:D:23:VAL:HG22	8:D:73:VAL:HB	1.82	0.59
13:J:75:PRO:HD3	13:J:136:SER:OG	2.01	0.59
19:P:16:VAL:HG12	19:P:17:GLY:N	2.17	0.59
25:V:39:ALA:C	25:V:41:GLU:H	2.06	0.59
25:V:56:ILE:O	25:V:60:GLN:HG3	2.02	0.59
12:H:170:ASN:HD22	12:H:170:ASN:N	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:264:GLU:HG2	6:B:267:LYS:HE2	1.84	0.59
6:B:71:VAL:HG11	6:B:296:LEU:HD22	1.83	0.59
25:V:11:MET:HB3	25:V:15:GLU:HB2	1.84	0.59
28:Y:154:ARG:NH1	28:Y:155:ARG:HG3	2.16	0.59
10:F:50:VAL:HG21	10:F:63:ILE:HG21	1.83	0.59
40:O:4936:HOH:O	16:M:83:SER:HB3	2.01	0.59
1:O:396:U:O2'	1:O:418:C:H4'	2.02	0.59
5:A:153:ARG:CB	5:A:153:ARG:HH11	2.15	0.59
17:N:162:ASP:HA	40:N:9328:HOH:O	2.03	0.59
26:W:119:HIS:HD2	26:W:120:PRO:O	1.86	0.59
33:I:106:LYS:O	33:I:110:GLU:HG3	2.02	0.59
6:B:62:ARG:HA	6:B:65:MET:HE3	1.83	0.59
10:F:91:VAL:CG1	10:F:92:GLY:H	2.10	0.59
23:T:38:ARG:NH1	40:T:6217:HOH:O	2.35	0.59
1:O:1878:G:O2'	1:O:1879:U:C6	2.55	0.59
33:I:105:VAL:HG11	33:I:129:VAL:HG22	1.84	0.59
1:O:1555:G:H4'	1:O:1630:A:H2	1.68	0.59
1:O:462:A:N3	31:2:37:HIS:HB3	2.18	0.59
31:2:36:ASN:HB3	31:2:39:ARG:NE	2.17	0.59
7:C:236:THR:H	7:C:239:ALA:HB3	1.68	0.59
5:A:33:GLU:O	5:A:34:ASP:HB2	2.02	0.59
1:O:1946:C:H2'	1:O:1971:G:C8	2.37	0.59
17:N:23:ARG:HH11	17:N:23:ARG:HG2	1.67	0.59
7:C:233:THR:HG22	7:C:234:VAL:N	2.17	0.59
5:A:36:ASP:C	5:A:38:ILE:H	2.06	0.58
1:O:1187:U:HO2'	1:O:1189:A:H2	1.51	0.58
1:O:316:A:H5'	23:T:54:ASP:OD2	2.02	0.58
1:O:1418:U:OP1	31:2:42:TRP:HB3	2.02	0.58
1:O:1819:G:H2'	1:O:1820:G:H4'	1.85	0.58
1:O:2649:A:H5'	1:O:2649:A:H8	1.67	0.58
25:V:12:THR:HG22	25:V:15:GLU:CG	2.21	0.58
1:O:558:C:C2'	1:O:559:U:H5"	2.33	0.58
1:O:797:A:H4'	29:Z:10:ARG:N	2.18	0.58
12:H:46:GLN:HE21	12:H:137:TYR:HE2	1.51	0.58
6:B:265:LEU:HD21	6:B:316:ARG:HD3	1.85	0.58
14:K:62:PRO:HG3	14:K:65:ARG:HH21	1.66	0.58
6:B:254:GLN:HG2	6:B:255:GLY:H	1.68	0.58
1:O:343:C:O2'	1:O:344:C:H5'	2.02	0.58
29:Z:11:SER:CB	29:Z:23:ARG:HB2	2.28	0.58
16:M:24:GLN:NE2	16:M:27:ARG:HH11	2.02	0.58
32:3:55:VAL:HG22	40:3:9444:HOH:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:164:THR:HG22	16:M:166:ALA:H	1.68	0.58
14:K:109:LEU:CD1	14:K:113:ILE:HD11	2.32	0.58
1:0:1163:G:H5'	33:I:115:ASP:O	2.04	0.58
1:0:1973:A:H5'	1:0:1973:A:C8	2.37	0.58
15:L:148:GLU:HB2	40:L:9486:HOH:O	2.03	0.58
17:N:78:MET:HB2	17:N:79:PRO:HD3	1.85	0.58
6:B:145:HIS:HD2	6:B:146:THR:O	1.85	0.58
17:N:143:ARG:HH21	17:N:169:PRO:HB2	1.68	0.58
9:E:116:THR:HG22	9:E:151:LEU:HD22	1.85	0.58
14:K:32:ILE:HD11	14:K:56:SER:HB3	1.86	0.58
8:D:54:ALA:CB	8:D:69:ILE:HD12	2.32	0.58
6:B:87:TYR:O	6:B:138:GLY:N	2.27	0.58
1:0:2769:C:O2'	1:0:2770:G:H5'	2.04	0.58
1:0:316:A:N3	1:0:336:G:O2'	2.35	0.58
24:U:47:ARG:HG3	40:U:4381:HOH:O	2.03	0.58
8:D:50:VAL:O	8:D:71:ALA:HA	2.04	0.58
1:0:2081:A:H4'	13:J:69:TYR:CE1	2.39	0.58
15:L:133:VAL:HA	40:L:9470:HOH:O	2.04	0.58
12:H:58:ARG:HG3	12:H:58:ARG:HH11	1.68	0.58
1:0:558:C:O2'	1:0:559:U:H5''	2.04	0.58
1:0:1701:A:H4'	1:0:1702:U:C5'	2.32	0.58
1:0:1187:U:O2'	1:0:1189:A:H2	1.86	0.58
7:C:168:ARG:NH2	7:C:190:ALA:O	2.36	0.58
13:J:47:THR:HG22	13:J:48:GLY:N	2.17	0.58
1:0:969:G:H1	1:0:999:C:N4	2.01	0.58
1:0:119:A:H2'	1:0:120:A:H5''	1.86	0.58
26:W:38:THR:HG22	26:W:39:ASP:N	2.19	0.58
6:B:85:ARG:NH1	40:B:9629:HOH:O	2.37	0.58
1:0:69:A:H5'	1:0:69:A:C8	2.39	0.58
17:N:115:VAL:HG22	40:N:9354:HOH:O	2.04	0.58
7:C:242:GLU:HB2	40:C:9192:HOH:O	2.04	0.58
8:D:25:MET:CE	8:D:37:ALA:HB1	2.33	0.57
12:H:30:GLN:H	12:H:66:ARG:HH11	1.51	0.57
9:E:81:GLU:HG2	9:E:134:SER:CB	2.33	0.57
10:F:60:VAL:HG12	10:F:60:VAL:O	2.04	0.57
7:C:115:LEU:HD13	7:C:223:LEU:HD21	1.86	0.57
1:0:474:C:O3'	7:C:73:LEU:HD21	2.03	0.57
1:0:681:G:N3	1:0:681:G:H5'	2.19	0.57
6:B:5:ARG:HH11	6:B:8:LYS:HE2	1.69	0.57
13:J:54:VAL:HG11	13:J:138:THR:HG21	1.86	0.57
1:0:2443:C:O3'	15:L:56:LYS:HE3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:3:60:LYS:HG3	32:3:61:PRO:HD2	1.85	0.57
17:N:110:THR:HB	17:N:113:SER:OG	2.04	0.57
1:0:558:C:H2'	1:0:559:U:C5'	2.33	0.57
1:0:1835:U:C5	1:0:1840:A:N7	2.65	0.57
18:O:25:VAL:HG23	18:O:26:TRP:H	1.69	0.57
25:V:64:GLY:O	25:V:65:ASP:HB2	2.03	0.57
11:G:24:VAL:O	11:G:28:GLU:HB2	2.04	0.57
5:A:88:ILE:HG22	5:A:88:ILE:O	2.03	0.57
8:D:138:GLY:N	40:D:7597:HOH:O	2.36	0.57
5:A:179:MET:HG2	5:A:186:TRP:CB	2.35	0.57
13:J:74:ARG:O	13:J:78:ILE:HG12	2.03	0.57
1:0:1205:U:H2'	1:0:1206:U:C5'	2.35	0.57
1:0:1878:G:HO2'	1:0:1879:U:H6	1.49	0.57
1:0:2541:U:H3'	1:0:2541:U:H6	1.70	0.57
6:B:321:PRO:HA	40:B:9650:HOH:O	2.03	0.57
27:X:37:LEU:CD1	27:X:85:VAL:HG21	2.25	0.57
1:0:1666:C:O2'	1:0:1667:A:H5''	2.04	0.57
9:E:126:ILE:HB	9:E:131:LEU:HD23	1.86	0.57
25:V:55:ARG:O	25:V:59:ILE:HG12	2.04	0.57
26:W:139:GLY:O	26:W:141:HIS:HD2	1.87	0.57
29:Z:30:GLU:HA	29:Z:33:MET:HE3	1.87	0.57
8:D:170:TYR:O	8:D:171:ASP:HB3	2.03	0.57
6:B:17:LYS:O	6:B:260:HIS:HD2	1.87	0.57
5:A:165:THR:HG22	40:A:9604:HOH:O	2.05	0.57
1:0:1352:A:O2'	1:0:1353:C:OP1	2.22	0.57
2:9:3008:G:O6	17:N:11:ARG:NH1	2.33	0.57
16:M:77:HIS:HD2	16:M:79:ALA:O	1.88	0.57
1:0:462:A:C2	31:2:37:HIS:HB3	2.39	0.57
1:0:2795:C:O2'	1:0:2796:U:H5'	2.05	0.57
1:0:1625:U:H4'	40:0:5209:HOH:O	2.05	0.57
1:0:1351:G:OP1	7:C:96:LYS:NZ	2.36	0.57
1:0:1919:A:H4'	40:0:5385:HOH:O	2.05	0.57
26:W:88:THR:CG2	26:W:89:ASP:H	2.18	0.56
9:E:126:ILE:HB	9:E:131:LEU:CD2	2.35	0.56
10:F:21:GLU:O	10:F:24:ARG:HG3	2.05	0.56
33:I:128:VAL:C	33:I:130:GLY:H	2.08	0.56
11:G:23:ILE:HD13	11:G:67:LEU:HD23	1.86	0.56
1:0:20:G:H21	21:R:117:HIS:HD2	1.53	0.56
1:0:1684:A:H1'	31:2:43:ARG:HH22	1.70	0.56
28:Y:235:GLU:CD	28:Y:235:GLU:N	2.52	0.56
14:K:114:ALA:HB3	14:K:117:VAL:HG23	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2718:C:H6	1:0:2718:C:H5'	1.69	0.56
21:R:9:ASP:O	21:R:13:THR:HB	2.05	0.56
26:W:84:VAL:HG12	40:W:6679:HOH:O	2.04	0.56
6:B:195:ARG:HD2	6:B:324:ASP:OD1	2.04	0.56
24:U:17:THR:CG2	24:U:18:GLY:N	2.67	0.56
1:0:1189:A:H1'	1:0:1209:C:O4'	2.05	0.56
6:B:190:MET:HE2	6:B:194:PHE:CD1	2.39	0.56
1:0:2815:G:N7	13:J:80:LYS:NZ	2.53	0.56
1:0:2824:C:H5''	1:0:2825:C:H5'	1.86	0.56
16:M:60:VAL:C	16:M:61:ILE:HD12	2.25	0.56
1:0:820:G:O2'	1:0:856:G:H4'	2.05	0.56
13:J:99:GLU:HA	40:J:7377:HOH:O	2.05	0.56
1:0:2878:U:H2'	1:0:2879:A:O4'	2.04	0.56
8:D:49:PRO:HA	8:D:73:VAL:HG22	1.87	0.56
26:W:4:LEU:O	26:W:32:CYS:HA	2.05	0.56
24:U:17:THR:HG22	24:U:18:GLY:N	2.19	0.56
28:Y:187:VAL:HB	28:Y:203:VAL:CG2	2.35	0.56
1:0:2032:U:H2'	1:0:2033:G:C5'	2.35	0.56
1:0:1426:C:H2'	40:0:3203:HOH:O	2.05	0.56
26:W:122:ARG:CG	26:W:122:ARG:NH1	2.64	0.56
29:Z:29:ILE:O	29:Z:33:MET:HB2	2.06	0.56
19:P:10:ALA:HA	19:P:13:VAL:CG1	2.35	0.56
17:N:169:PRO:O	17:N:172:PHE:HB3	2.06	0.56
1:0:757:C:OP1	15:L:27:ARG:HD2	2.05	0.56
8:D:22:VAL:HG22	8:D:74:THR:HG22	1.87	0.56
1:0:2090:G:H2'	1:0:2091:G:C8	2.41	0.56
15:L:121:ILE:HG12	15:L:141:GLU:HB2	1.87	0.56
1:0:93:C:H5''	25:V:1:THR:HB	1.88	0.56
19:P:40:VAL:O	19:P:44:VAL:HG23	2.05	0.56
1:0:2346:C:H6	1:0:2346:C:O5'	1.87	0.56
40:0:9699:HOH:O	6:B:214:PRO:HD2	2.04	0.56
1:0:2721:U:H4'	14:K:87:ARG:HG3	1.87	0.56
1:0:1118:A:C8	1:0:1119:G:H5''	2.40	0.56
1:0:506:G:H22	1:0:509:A:H5'	1.71	0.56
5:A:105:VAL:HG11	5:A:154:ALA:CB	2.35	0.56
1:0:2649:A:C8	1:0:2649:A:H5'	2.41	0.56
40:0:3149:HOH:O	19:P:81:LYS:HG2	2.06	0.56
1:0:538:C:OP2	28:Y:134:HIS:HE1	1.89	0.56
1:0:1441:G:O2'	1:0:1442:A:H5'	2.05	0.56
8:D:103:ASN:ND2	8:D:134:LEU:H	2.03	0.56
15:L:136:ALA:HB3	40:L:9470:HOH:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:244:C:OP2	10:F:38:LYS:HE3	2.05	0.56
40:0:8433:HOH:O	12:H:154:TYR:HB2	2.06	0.56
1:0:920:C:H4'	1:0:921:G:C2	2.40	0.56
1:0:2866:U:H4'	1:0:2867:G:H5'	1.88	0.56
5:A:57:ALA:HB1	5:A:65:ARG:HE	1.69	0.56
21:R:18:LEU:HG	21:R:91:LEU:HD13	1.88	0.56
1:0:2421:G:H1'	40:0:4280:HOH:O	2.06	0.56
1:0:1594:C:OP2	19:P:120:ARG:HD2	2.06	0.56
27:X:30:MET:HE1	27:X:58:ALA:HB3	1.88	0.56
26:W:149:LEU:HG	26:W:153:MET:CE	2.36	0.56
8:D:135:VAL:HG21	8:D:139:TYR:CG	2.41	0.56
8:D:76:ARG:O	8:D:77:ASP:HB2	2.06	0.56
1:0:949:U:H4'	20:Q:95:GLU:HA	1.86	0.56
1:0:90:A:H2'	1:0:91:G:O4'	2.05	0.56
1:0:120:A:H5'	30:1:20:ARG:HH21	1.71	0.55
1:0:2032:U:H2'	1:0:2033:G:H5''	1.88	0.55
14:K:34:VAL:HG22	14:K:47:ALA:HB2	1.86	0.55
6:B:297:VAL:HB	40:B:9600:HOH:O	2.05	0.55
8:D:135:VAL:HG22	8:D:136:ARG:H	1.71	0.55
1:0:558:C:H2'	1:0:559:U:H5'	1.88	0.55
1:0:625:U:H5''	1:0:1044:C:N4	2.21	0.55
1:0:138:U:H5''	1:0:139:C:OP2	2.06	0.55
8:D:24:HIS:HB2	8:D:72:LYS:CB	2.35	0.55
1:0:1060:C:H6	1:0:1060:C:H5'	1.72	0.55
1:0:621:C:H5'	28:Y:132:ASP:OD2	2.07	0.55
2:9:3024:U:H3'	2:9:3025:G:H5'	1.88	0.55
25:V:1:THR:HG23	25:V:2:VAL:N	2.20	0.55
6:B:305:ASP:O	6:B:306:LYS:HB2	2.07	0.55
1:0:1748:U:H4'	40:0:7953:HOH:O	2.04	0.55
5:A:125:ASN:HB3	5:A:158:VAL:HG12	1.88	0.55
1:0:2481:G:H5''	40:0:5094:HOH:O	2.05	0.55
1:0:1180:U:O2'	33:I:92:PRO:HD2	2.05	0.55
1:0:2502:C:C2'	1:0:2503:A:H5'	2.37	0.55
1:0:2416:G:O2'	17:N:25:ARG:HG2	2.05	0.55
17:N:86:LEU:HD12	17:N:125:ALA:HB2	1.88	0.55
1:0:164:G:H4'	15:L:30:ARG:HD3	1.89	0.55
1:0:1205:U:H2'	1:0:1206:U:H5'	1.89	0.55
12:H:166:SER:HB3	12:H:167:PRO:CD	2.35	0.55
1:0:2587:OMU:H2'	1:0:2589:U:H5''	1.88	0.55
1:0:407:A:H2'	1:0:408:A:C8	2.41	0.55
16:M:57:LYS:HE2	16:M:140:ALA:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:834:G:H4'	1:0:835:U:OP2	2.07	0.55
1:0:2851:G:O2'	1:0:2852:A:H5'	2.05	0.55
16:M:34:GLU:HB3	16:M:38:GLU:HG3	1.89	0.55
6:B:132:HIS:CE1	6:B:171:VAL:HG21	2.42	0.55
29:Z:37:HIS:O	29:Z:45:ASP:HA	2.07	0.55
9:E:31:ARG:NH1	9:E:68:HIS:CG	2.75	0.55
10:F:50:VAL:CG2	10:F:63:ILE:HG21	2.37	0.55
1:0:1168:C:H5''	33:I:87:THR:CG2	2.37	0.55
1:0:137:U:H2'	1:0:139:C:C5	2.42	0.55
1:0:121:U:OP2	31:2:10:ARG:NH2	2.35	0.55
16:M:120:VAL:HG11	16:M:130:GLU:HG3	1.88	0.55
13:J:76:ASP:HA	40:J:5907:HOH:O	2.06	0.55
13:J:130:VAL:HG12	13:J:131:THR:N	2.22	0.55
27:X:9:VAL:HG22	27:X:88:GLU:OE2	2.07	0.55
1:0:2591:C:H2'	1:0:2592:G:O4'	2.06	0.55
10:F:46:GLU:OE1	10:F:100:ASP:HA	2.07	0.55
6:B:5:ARG:NH1	6:B:8:LYS:HE2	2.22	0.55
15:L:10:SER:O	15:L:11:ARG:HB3	2.06	0.55
27:X:78:GLU:HG2	27:X:79:GLU:OE2	2.07	0.55
23:T:63:ILE:HD11	23:T:75:GLU:HB2	1.89	0.55
14:K:30:LYS:O	14:K:55:VAL:HG13	2.06	0.54
28:Y:154:ARG:HH12	28:Y:155:ARG:CG	2.20	0.54
1:0:2270:G:H4'	5:A:223:ARG:HH12	1.72	0.54
1:0:1595:G:O2'	1:0:1596:U:H5'	2.06	0.54
17:N:32:PRO:HD2	17:N:99:GLU:O	2.06	0.54
6:B:40:GLY:HA3	40:B:9641:HOH:O	2.06	0.54
28:Y:108:ASP:N	28:Y:108:ASP:OD1	2.36	0.54
6:B:221:GLN:HE22	14:K:42:ASN:HD22	1.55	0.54
29:Z:53:GLY:HA2	29:Z:67:GLY:O	2.06	0.54
14:K:4:LEU:CD2	14:K:116:GLU:HB3	2.36	0.54
8:D:24:HIS:HB2	8:D:72:LYS:HB3	1.89	0.54
28:Y:133:HIS:HD2	40:Y:9381:HOH:O	1.90	0.54
1:0:2670:G:O2'	1:0:2671:U:H5'	2.07	0.54
1:0:1202:A:H2'	1:0:1203:G:O4'	2.08	0.54
5:A:65:ARG:C	5:A:66:ARG:HG3	2.26	0.54
5:A:192:VAL:HB	40:A:9580:HOH:O	2.06	0.54
7:C:1:MET:HG2	7:C:2:GLN:N	2.16	0.54
6:B:321:PRO:HG3	40:B:9595:HOH:O	2.06	0.54
5:A:66:ARG:HH11	5:A:66:ARG:HB2	1.72	0.54
1:0:2414:A:H2'	1:0:2415:A:C8	2.43	0.54
1:0:1451:C:H5'	1:0:1505:U:C5	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:O:87:THR:O	18:O:91:GLN:HG3	2.07	0.54
16:M:164:THR:CG2	16:M:165:GLY:N	2.70	0.54
9:E:144:THR:O	9:E:148:ILE:HG13	2.08	0.54
10:F:50:VAL:CG1	10:F:60:VAL:HG11	2.36	0.54
1:O:1189:A:O2'	1:O:1208:C:H2'	2.07	0.54
15:L:53:ARG:NH2	15:L:57:VAL:HG12	2.22	0.54
1:O:1853:C:OP1	5:A:231:LYS:HG3	2.08	0.54
2:9:3107:C:H5	40:9:3167:HOH:O	1.90	0.54
1:O:291:C:H2'	1:O:292:G:O4'	2.08	0.54
9:E:145:ALA:HB1	9:E:168:ILE:HD11	1.88	0.54
29:Z:57:CYS:SG	29:Z:59:TYR:HB3	2.48	0.54
1:O:2748:G:H2'	40:0:7972:HOH:O	2.07	0.54
40:0:7978:HOH:O	16:M:91:ILE:HG12	2.07	0.54
1:O:1773:G:C8	29:Z:16:ALA:HA	2.43	0.54
1:O:95:A:H5''	1:O:97:G:O4'	2.08	0.54
18:O:47:ARG:HG3	18:O:47:ARG:HH11	1.73	0.54
8:D:44:ILE:HG12	8:D:83:PHE:HE1	1.73	0.54
18:O:97:SER:H	18:O:100:GLN:NE2	2.05	0.54
28:Y:189:ASN:HD22	28:Y:189:ASN:C	2.11	0.54
1:O:482:G:H4'	1:O:508:A:N1	2.23	0.54
1:O:441:A:H1'	1:O:442:A:N7	2.22	0.54
33:I:113:HIS:HE1	33:I:121:LEU:HD22	1.70	0.54
1:O:1377:C:H5'	1:O:1377:C:C6	2.38	0.54
23:T:32:ARG:NH1	23:T:38:ARG:NH1	2.54	0.54
16:M:187:LEU:HD23	16:M:194:ALA:HB3	1.89	0.54
1:O:69:A:H5'	1:O:69:A:H8	1.73	0.54
1:O:328:U:O4'	7:C:202:THR:HG22	2.08	0.54
1:O:603:A:H5''	1:O:604:G:OP1	2.08	0.54
8:D:154:LYS:HD2	8:D:154:LYS:H	1.73	0.54
5:A:105:VAL:HG12	5:A:106:CYS:N	2.24	0.53
16:M:61:ILE:N	16:M:61:ILE:HD12	2.23	0.53
1:O:1847:A:OP1	5:A:175:LYS:HG3	2.08	0.53
28:Y:170:SER:OG	28:Y:175:ARG:HG3	2.08	0.53
1:O:2837:U:H2'	40:0:7305:HOH:O	2.09	0.53
1:O:1730:G:C5'	1:O:1731:C:C6	2.91	0.53
16:M:182:LYS:O	16:M:194:ALA:HB2	2.07	0.53
1:O:1477:C:O2'	1:O:1478:U:H5'	2.08	0.53
5:A:217:ARG:HH11	5:A:217:ARG:CG	2.20	0.53
1:O:1184:C:H4'	33:I:126:LYS:HB3	1.89	0.53
1:O:475:G:H5'	7:C:73:LEU:HD23	1.90	0.53
1:O:1766:U:O2	1:O:1778:A:H5'	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:P:103:THR:O	19:P:107:GLU:HG3	2.08	0.53
33:I:93:GLN:HA	33:I:96:PHE:HE2	1.73	0.53
1:0:1172:G:H1'	40:0:5505:HOH:O	2.09	0.53
8:D:95:THR:OG1	8:D:174:VAL:HG22	2.08	0.53
6:B:102:THR:HG21	6:B:182:VAL:O	2.07	0.53
31:2:36:ASN:HB3	31:2:39:ARG:HG3	1.90	0.53
32:3:56:PRO:HA	40:3:9486:HOH:O	2.09	0.53
6:B:320:GLN:HE21	6:B:321:PRO:HD2	1.73	0.53
18:O:53:GLN:HG2	18:O:56:GLU:OE1	2.08	0.53
8:D:36:ASN:HA	40:D:7500:HOH:O	2.07	0.53
1:0:653:C:H2'	1:0:654:A:C8	2.43	0.53
1:0:12:U:H2'	1:0:13:G:H5'	1.91	0.53
18:O:14:LEU:CD2	18:O:102:ILE:HD11	2.38	0.53
1:0:1626:A:H2'	1:0:1627:G:O4'	2.08	0.53
30:1:25:LYS:HD2	31:2:48:ASP:CA	2.38	0.53
1:0:1838:U:H1'	1:0:2644:C:H5'	1.91	0.53
6:B:312:ARG:HD3	6:B:315:VAL:HG13	1.89	0.53
1:0:2769:C:H2'	1:0:2770:G:C5'	2.39	0.53
1:0:1066:U:H2'	1:0:1067:A:C8	2.44	0.53
7:C:25:PRO:HG2	40:C:9126:HOH:O	2.09	0.53
15:L:119:THR:HG23	15:L:139:SER:OG	2.08	0.53
23:T:47:THR:HB	23:T:100:ASP:HB3	1.90	0.53
1:0:1972:U:H2'	1:0:1973:A:H5'	1.91	0.53
9:E:3:VAL:CG2	9:E:49:ILE:HB	2.38	0.53
1:0:2694:A:H4'	9:E:91:PHE:CE1	2.44	0.53
1:0:2883:A:H2'	1:0:2884:G:O4'	2.09	0.53
1:0:1077:G:H2'	1:0:1080:C:H42	1.73	0.53
1:0:2812:A:C2	1:0:2814:A:N6	2.70	0.53
1:0:516:A:H5'	40:0:6167:HOH:O	2.09	0.53
1:0:775:G:OP1	30:1:16:HIS:HE1	1.91	0.53
1:0:151:A:H2'	1:0:152:A:O4'	2.08	0.53
26:W:88:THR:HG22	26:W:90:TYR:HD1	1.72	0.53
1:0:447:A:OP2	23:T:1:SER:HB2	2.08	0.53
28:Y:112:GLU:CD	28:Y:115:ARG:NH1	2.63	0.53
7:C:233:THR:HG22	7:C:234:VAL:H	1.73	0.53
14:K:49:LEU:HD12	14:K:80:ILE:HD13	1.90	0.53
1:0:545:G:C8	1:0:545:G:H5'	2.42	0.53
18:O:97:SER:OG	18:O:100:GLN:HG3	2.09	0.53
6:B:41:PHE:CD1	6:B:79:MET:HE2	2.44	0.53
1:0:1786:C:OP1	19:P:74:GLN:HG2	2.09	0.53
5:A:121:ALA:O	5:A:124:VAL:HG22	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1667:A:H2'	1:0:1668:U:C6	2.44	0.53
19:P:16:VAL:HG13	19:P:20:ARG:NH1	2.24	0.53
1:0:1741:U:H3'	40:0:3363:HOH:O	2.09	0.53
40:0:4793:HOH:O	31:2:38:LYS:HE3	2.08	0.53
30:1:1:THR:HA	40:1:9468:HOH:O	2.08	0.53
1:0:1552:G:N2	1:0:1634:G:H1'	2.24	0.53
8:D:62:ASP:HA	40:D:4233:HOH:O	2.08	0.52
1:0:362:G:H2'	1:0:363:A:C8	2.44	0.52
33:I:113:HIS:N	33:I:114:PRO:CD	2.72	0.52
5:A:95:PRO:HG2	5:A:98:GLU:HG2	1.91	0.52
1:0:1836:A:H1'	30:1:1:THR:O	2.09	0.52
1:0:204:A:C2'	1:0:205:U:H5'	2.39	0.52
32:3:30:GLN:HG3	40:3:9452:HOH:O	2.09	0.52
10:F:48:VAL:HG12	10:F:97:ALA:CB	2.39	0.52
1:0:1252:A:H2'	1:0:1253:C:O4'	2.09	0.52
33:I:138:THR:HG22	33:I:139:ILE:N	2.24	0.52
7:C:107:ARG:NH1	7:C:107:ARG:HB3	2.24	0.52
1:0:1730:G:H5''	1:0:1731:C:H6	1.74	0.52
7:C:194:PHE:CD2	7:C:234:VAL:HG11	2.43	0.52
27:X:12:ILE:HD12	27:X:36:HIS:ND1	2.24	0.52
1:0:2817:G:P	40:0:8435:HOH:O	2.67	0.52
1:0:2361:A:H2'	1:0:2362:A:C8	2.44	0.52
22:S:73:ASP:OD1	22:S:76:GLU:HG3	2.09	0.52
6:B:36:PRO:HB3	6:B:174:ARG:CB	2.40	0.52
26:W:88:THR:CG2	26:W:89:ASP:N	2.69	0.52
17:N:86:LEU:HD21	17:N:180:LEU:CD1	2.40	0.52
21:R:114:VAL:HA	21:R:144:GLU:O	2.09	0.52
40:0:5237:HOH:O	29:Z:13:ARG:HD3	2.09	0.52
9:E:10:ASP:HA	40:E:3707:HOH:O	2.08	0.52
7:C:236:THR:HG22	7:C:239:ALA:CB	2.40	0.52
26:W:13:MET:CE	26:W:17:ILE:HG22	2.39	0.52
15:L:134:GLU:HG3	40:L:9452:HOH:O	2.09	0.52
26:W:29:VAL:O	26:W:30:ASN:HB2	2.10	0.52
4:5:77:PHE:CE1	4:5:79:BTN:H62	2.43	0.52
19:P:98:ILE:HD12	19:P:102:ARG:NE	2.25	0.52
7:C:246:ARG:NH1	40:C:9180:HOH:O	2.43	0.52
5:A:43:VAL:HG21	5:A:59:GLU:HG3	1.90	0.52
12:H:63:GLU:HA	40:H:9546:HOH:O	2.08	0.52
25:V:12:THR:HG23	25:V:14:ALA:H	1.73	0.52
26:W:52:VAL:HG22	26:W:53:ALA:N	2.23	0.52
30:1:28:HIS:HD2	30:1:31:LYS:H	1.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:2644:C:O2'	1:O:2645:U:H5'	2.08	0.52
6:B:141:ARG:HG2	6:B:165:ARG:HA	1.90	0.52
6:B:41:PHE:CG	6:B:79:MET:HE2	2.45	0.52
18:O:78:ALA:C	18:O:98:LEU:HD13	2.30	0.52
1:O:2326:U:H4'	1:O:2412:G:C4'	2.40	0.52
1:O:1562:C:H42	1:O:2738:G:H1	1.58	0.52
32:3:70:ARG:HB3	40:3:9508:HOH:O	2.09	0.52
17:N:24:LEU:HD22	40:Q:2847:HOH:O	2.10	0.52
1:O:2502:C:H2'	1:O:2503:A:H5'	1.91	0.52
23:T:40:VAL:HG22	23:T:41:ARG:N	2.25	0.52
1:O:1462:C:H2'	1:O:1463:A:C8	2.45	0.52
5:A:109:GLU:HG2	5:A:116:GLY:N	2.25	0.52
8:D:136:ARG:HB3	8:D:137:PRO:HD2	1.91	0.52
16:M:31:TRP:CA	16:M:34:GLU:HG3	2.40	0.52
14:K:34:VAL:CG2	14:K:47:ALA:HB2	2.39	0.52
1:O:497:A:H2'	1:O:498:A:C5'	2.40	0.52
12:H:38:LYS:HE2	12:H:42:ASP:HB2	1.92	0.52
16:M:107:ARG:NH1	40:M:9378:HOH:O	2.43	0.52
1:O:2419:U:H5''	1:O:2420:G:H5'	1.91	0.52
28:Y:184:GLU:OE1	28:Y:204:ARG:NH1	2.43	0.52
12:H:76:GLU:O	12:H:77:LEU:HD23	2.09	0.52
23:T:19:ARG:HD3	23:T:67:LEU:O	2.10	0.52
40:K:7438:HOH:O	24:U:20:MET:HE1	2.09	0.52
2:9:3069:U:OP1	17:N:4:PRO:HG3	2.10	0.52
1:O:1119:G:H2'	13:J:52:GLN:HE22	1.73	0.51
13:J:130:VAL:HG12	13:J:131:THR:H	1.74	0.51
6:B:254:GLN:HG3	40:B:9531:HOH:O	2.10	0.51
6:B:41:PHE:HB3	6:B:190:MET:CE	2.40	0.51
28:Y:187:VAL:HG23	40:Y:9369:HOH:O	2.10	0.51
8:D:65:GLU:HA	40:D:6752:HOH:O	2.08	0.51
15:L:36:ASP:HB2	40:L:9431:HOH:O	2.09	0.51
23:T:49:GLU:CB	23:T:59:GLU:HG2	2.39	0.51
1:O:2645:U:OP2	1:O:2645:U:C6	2.63	0.51
2:9:3051:A:H5'	17:N:160:SER:CB	2.40	0.51
12:H:63:GLU:O	12:H:67:LEU:HB2	2.09	0.51
1:O:497:A:H2'	1:O:498:A:H5'	1.91	0.51
1:O:2320:U:H4'	1:O:2321:A:O4'	2.10	0.51
13:J:71:TYR:CD1	13:J:72:PRO:HD2	2.45	0.51
1:O:899:C:H5'	40:O:3792:HOH:O	2.09	0.51
6:B:58:PRO:HA	6:B:63:GLU:OE2	2.11	0.51
11:G:64:ASN:N	11:G:64:ASN:HD22	2.07	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:236:THR:HA	40:C:9257:HOH:O	2.10	0.51
7:C:127:ARG:CZ	7:C:225:PRO:HG2	2.40	0.51
1:0:1118:A:C8	1:0:1118:A:C3'	2.86	0.51
7:C:118:THR:CG2	7:C:137:PRO:HB3	2.40	0.51
1:0:2415:A:H2'	1:0:2416:G:H5'	1.91	0.51
5:A:149:ASP:OD1	5:A:151:GLN:HB2	2.10	0.51
30:1:21:ARG:HD2	30:1:37:CYS:SG	2.51	0.51
5:A:94:LEU:HD12	5:A:98:GLU:HB2	1.91	0.51
5:A:36:ASP:O	5:A:38:ILE:N	2.44	0.51
27:X:76:ARG:NH1	27:X:76:ARG:HG3	2.24	0.51
1:0:1159:G:H1	1:0:1208:C:H42	1.57	0.51
24:U:9:CYS:O	24:U:52:THR:HG23	2.10	0.51
33:I:89:SER:HB3	33:I:97:VAL:CG2	2.40	0.51
8:D:49:PRO:HB3	40:D:5828:HOH:O	2.10	0.51
7:C:129:HIS:HD2	7:C:165:ASP:OD2	1.94	0.51
17:N:67:ALA:HA	17:N:71:TRP:HB3	1.93	0.51
16:M:99:ARG:NH2	16:M:170:ASN:HD22	2.00	0.51
9:E:34:TRP:O	13:J:127:ILE:HD11	2.11	0.51
1:0:1234:U:N3	6:B:244:PRO:HB3	2.25	0.51
6:B:41:PHE:HB3	6:B:190:MET:HE3	1.93	0.51
1:0:1384:C:H5'	27:X:30:MET:HG2	1.92	0.51
1:0:926:A:H5'	15:L:39:GLU:OE2	2.09	0.51
6:B:199:TYR:CE2	6:B:268:ARG:HB2	2.46	0.51
1:0:1189:A:H3'	40:0:8193:HOH:O	2.10	0.51
18:O:106:PRO:HG2	18:O:107:GLU:OE1	2.10	0.51
23:T:112:LEU:CD2	23:T:119:ALA:HB3	2.39	0.51
1:0:1211:G:O2'	1:0:1212:C:H5'	2.10	0.51
1:0:317:A:H5''	23:T:52:ARG:HD2	1.92	0.51
40:0:5933:HOH:O	5:A:164:ARG:CZ	2.59	0.51
5:A:211:LYS:CG	5:A:212:PRO:HD2	2.30	0.51
21:R:106:GLY:HA2	21:R:109:MET:HE3	1.92	0.51
33:I:78:LEU:CD1	33:I:112:LYS:HZ2	2.24	0.51
21:R:39:THR:HG22	21:R:107:GLU:O	2.10	0.51
1:0:1209:C:H2'	1:0:1210:G:C8	2.45	0.51
10:F:36:THR:HG23	10:F:97:ALA:HB2	1.93	0.51
18:O:73:ASP:HA	18:O:92:VAL:O	2.11	0.51
1:0:2619:UR3:H6	1:0:2619:UR3:O5'	2.11	0.51
1:0:1886:A:O2'	29:Z:20:ARG:HB2	2.11	0.51
11:G:67:LEU:O	11:G:71:LEU:HG	2.11	0.51
1:0:1484:G:H2'	40:0:9725:HOH:O	2.11	0.51
1:0:1669:A:H2'	1:0:1670:G:C8	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:248:A:H5'	1:0:249:G:OP2	2.11	0.51
15:L:35:ARG:HB2	15:L:35:ARG:NH1	2.25	0.51
1:0:1160:G:HO2'	1:0:1190:G:H8	1.59	0.51
17:N:66:LEU:HD11	17:N:175:LEU:HD21	1.92	0.51
12:H:56:GLN:HE21	12:H:126:ARG:HE	1.56	0.51
1:0:308:U:H5'	23:T:97:ARG:NH2	2.26	0.51
1:0:475:G:C5'	7:C:73:LEU:HD23	2.40	0.51
1:0:2694:A:H4'	9:E:91:PHE:HE1	1.76	0.51
40:0:7340:HOH:O	16:M:178:LYS:HB2	2.11	0.51
14:K:115:ARG:HG3	14:K:116:GLU:N	2.27	0.50
6:B:53:LEU:HD21	6:B:270:ILE:HD12	1.92	0.50
15:L:145:LEU:O	15:L:145:LEU:HD23	2.11	0.50
1:0:2421:G:H2'	40:0:4646:HOH:O	2.10	0.50
29:Z:30:GLU:HG2	29:Z:33:MET:HE3	1.94	0.50
13:J:45:VAL:HG11	13:J:121:LEU:CD2	2.40	0.50
6:B:72:THR:HB	40:B:9600:HOH:O	2.11	0.50
1:0:1077:G:H2'	1:0:1080:C:N4	2.25	0.50
1:0:1306:U:OP1	7:C:184:ARG:HD2	2.11	0.50
1:0:2894:C:O2'	1:0:2895:C:H5'	2.10	0.50
1:0:1218:U:H2'	1:0:1219:U:C6	2.46	0.50
2:9:3054:A:H2	40:9:3535:HOH:O	1.93	0.50
2:9:3054:A:O2'	2:9:3055:U:H5'	2.11	0.50
22:S:29:ASP:OD1	22:S:31:ARG:NH1	2.44	0.50
1:0:1717:A:H5''	19:P:54:LYS:HB2	1.92	0.50
26:W:21:LEU:HD22	26:W:26:ILE:HD13	1.92	0.50
7:C:236:THR:HG21	40:C:9184:HOH:O	2.10	0.50
8:D:104:PHE:CE2	8:D:166:ILE:HD13	2.46	0.50
33:I:87:THR:HG22	33:I:88:GLY:N	2.25	0.50
20:Q:75:ILE:HD13	20:Q:84:ILE:CD1	2.41	0.50
6:B:265:LEU:CD2	6:B:316:ARG:HD3	2.41	0.50
1:0:2825:C:H4'	1:0:2826:G:O5'	2.12	0.50
1:0:432:G:O2'	1:0:433:C:H5'	2.11	0.50
1:0:299:U:H5'	40:0:7775:HOH:O	2.11	0.50
1:0:2016:U:H2'	1:0:2017:U:O4'	2.10	0.50
19:P:115:SER:HG	19:P:118:GLN:HG3	1.76	0.50
31:2:20:ARG:HG3	31:2:39:ARG:HH21	1.76	0.50
40:0:7989:HOH:O	32:3:61:PRO:HG2	2.10	0.50
40:0:6777:HOH:O	28:Y:158:LYS:HD3	2.12	0.50
17:N:179:LEU:HD23	17:N:184:ILE:HD12	1.94	0.50
1:0:2296:C:H2'	1:0:2297:U:H6	1.77	0.50
1:0:285:A:H2'	1:0:286:U:O4'	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:25:MET:HE1	8:D:37:ALA:O	2.11	0.50
9:E:133:VAL:HG12	9:E:141:VAL:HG13	1.94	0.50
21:R:92:LEU:HD23	21:R:145:LEU:HD21	1.94	0.50
1:0:1198:U:H2'	1:0:1200:A:OP2	2.11	0.50
1:0:2906:A:H5'	1:0:2907:C:O4'	2.12	0.50
1:0:1333:U:H2'	1:0:1334:C:C6	2.47	0.50
26:W:122:ARG:CZ	40:W:5817:HOH:O	2.58	0.50
1:0:1972:U:H2'	1:0:1973:A:C5'	2.42	0.50
13:J:75:PRO:HG2	13:J:105:LEU:CD2	2.41	0.50
1:0:2816:A:H2'	40:0:8435:HOH:O	2.12	0.50
1:0:2326:U:H4'	1:0:2412:G:H4'	1.94	0.50
6:B:268:ARG:NH2	6:B:325:PRO:HG3	2.25	0.50
5:A:163:GLY:HA2	5:A:166:ASP:OD2	2.12	0.50
1:0:177:A:H2'	1:0:178:U:O4'	2.11	0.50
13:J:74:ARG:NH1	13:J:105:LEU:HD11	2.27	0.50
16:M:82:ARG:O	16:M:84:LYS:N	2.44	0.50
9:E:145:ALA:HB1	9:E:168:ILE:CD1	2.42	0.50
6:B:314:ALA:HB3	6:B:317:PRO:HG3	1.92	0.50
2:9:3059:C:H2'	2:9:3060:C:C6	2.46	0.50
12:H:158:THR:HB	12:H:159:PRO:HD3	1.94	0.50
1:0:1992:U:OP2	14:K:66:ARG:HD2	2.11	0.50
21:R:69:LYS:HB2	21:R:72:VAL:HG23	1.92	0.50
26:W:110:GLN:NE2	26:W:110:GLN:HA	2.27	0.50
26:W:5:VAL:HG22	26:W:32:CYS:HB2	1.93	0.50
10:F:48:VAL:HG12	10:F:97:ALA:HB2	1.94	0.50
28:Y:107:PRO:HD3	28:Y:182:PHE:CE1	2.46	0.50
1:0:155:C:OP2	16:M:188:ARG:HD3	2.11	0.50
1:0:2338:G:OP1	8:D:97:GLN:HG2	2.11	0.50
1:0:1714:C:O2'	1:0:1715:C:H5'	2.11	0.50
29:Z:10:ARG:HA	40:Z:9215:HOH:O	2.11	0.50
1:0:2769:C:H2'	1:0:2770:G:H5'	1.92	0.50
1:0:123:U:H5'	40:0:7132:HOH:O	2.12	0.50
7:C:154:VAL:O	7:C:158:GLU:HG3	2.12	0.50
8:D:28:GLY:CA	8:D:69:ILE:HG23	2.35	0.50
1:0:1751:G:C2'	1:0:1752:G:H5''	2.40	0.50
2:9:3042:C:O2	8:D:76:ARG:NH1	2.45	0.50
1:0:962:C:H1'	17:N:5:ARG:HH12	1.75	0.50
2:9:3007:G:H4'	17:N:55:ASP:OD2	2.12	0.50
28:Y:126:PRO:HG2	28:Y:128:PHE:CZ	2.47	0.50
6:B:58:PRO:HA	6:B:63:GLU:CD	2.32	0.50
1:0:247:A:H2'	40:0:4495:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2827:A:H2'	1:0:2828:G:O4'	2.12	0.50
8:D:25:MET:SD	8:D:40:ILE:HD11	2.51	0.49
10:F:13:GLU:OE1	10:F:77:VAL:HG13	2.12	0.49
18:O:96:VAL:CG1	18:O:100:GLN:HB2	2.40	0.49
19:P:13:VAL:HG11	19:P:40:VAL:CG1	2.42	0.49
7:C:57:PRO:HG2	7:C:73:LEU:HD13	1.93	0.49
1:0:1745:G:H22	1:0:2033:G:H5'	1.77	0.49
2:9:3049:G:O2'	2:9:3050:G:H5'	2.11	0.49
6:B:310:ARG:HD2	40:B:9586:HOH:O	2.10	0.49
13:J:19:MET:HE2	13:J:79:PHE:HA	1.92	0.49
6:B:51:VAL:HG23	6:B:327:VAL:HG13	1.94	0.49
33:I:131:THR:O	33:I:135:LEU:HG	2.12	0.49
1:0:2748:G:H1'	40:0:8408:HOH:O	2.11	0.49
25:V:59:ILE:O	25:V:63:GLU:HG2	2.11	0.49
1:0:204:A:H2'	1:0:205:U:H5'	1.93	0.49
1:0:926:A:O2'	15:L:41:HIS:HD2	1.95	0.49
7:C:185:LYS:HD3	7:C:186:TYR:CE1	2.47	0.49
1:0:951:A:C2'	1:0:952:G:H5'	2.41	0.49
7:C:127:ARG:HD3	7:C:129:HIS:HE1	1.76	0.49
15:L:143:THR:CG2	15:L:144:ASP:N	2.75	0.49
1:0:820:G:H5'	1:0:821:U:H5'	1.94	0.49
1:0:920:C:H5''	1:0:921:G:O5'	2.13	0.49
17:N:119:GLN:O	17:N:123:ILE:HG13	2.12	0.49
17:N:89:GLY:O	17:N:92:ALA:HB3	2.12	0.49
28:Y:177:LYS:HD3	28:Y:181:GLY:O	2.12	0.49
13:J:88:PRO:O	13:J:94:GLY:HA3	2.12	0.49
14:K:55:VAL:CG1	14:K:56:SER:N	2.74	0.49
23:T:38:ARG:HG3	23:T:38:ARG:HH11	1.77	0.49
11:G:20:VAL:O	11:G:24:VAL:HG23	2.13	0.49
30:1:21:ARG:HD2	30:1:39:PHE:HB2	1.95	0.49
14:K:22:ASP:O	14:K:110:LYS:HE3	2.12	0.49
32:3:3:MET:O	32:3:90:PHE:HA	2.12	0.49
27:X:61:ARG:HH11	27:X:61:ARG:HG3	1.77	0.49
2:9:3095:C:O2'	2:9:3096:C:H5'	2.12	0.49
13:J:12:VAL:HG21	13:J:116:LEU:HD11	1.94	0.49
23:T:106:GLU:HG3	40:T:4913:HOH:O	2.11	0.49
1:0:1506:U:H5'	1:0:1506:U:H6	1.78	0.49
9:E:81:GLU:HA	9:E:133:VAL:O	2.12	0.49
10:F:38:LYS:NZ	16:M:3:SER:HA	2.27	0.49
1:0:2333:G:P	8:D:56:ARG:HH22	2.36	0.49
8:D:56:ARG:N	40:D:6752:HOH:O	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1503:U:H2'	1:0:1504:A:O4'	2.12	0.49
1:0:1056:U:H2'	1:0:1057:A:O4'	2.11	0.49
32:3:25:VAL:HG22	32:3:68:LYS:HG3	1.94	0.49
14:K:125:ALA:C	14:K:127:ALA:H	2.14	0.49
8:D:10:PHE:CE1	8:D:11:HIS:HB3	2.47	0.49
1:0:734:U:H1'	1:0:737:A:N6	2.27	0.49
6:B:84:LEU:HD13	6:B:84:LEU:O	2.13	0.49
1:0:288:A:H2'	1:0:289:G:C8	2.47	0.49
25:V:1:THR:CG2	25:V:2:VAL:H	2.19	0.49
5:A:125:ASN:CB	5:A:158:VAL:HG12	2.42	0.49
1:0:1755:A:H2'	1:0:1756:G:O4'	2.12	0.49
1:0:333:G:O2'	1:0:334:G:H5'	2.13	0.49
24:U:39:ASN:ND2	24:U:44:ARG:HH11	2.10	0.49
25:V:12:THR:HG23	25:V:14:ALA:N	2.27	0.49
8:D:41:LEU:HA	8:D:44:ILE:CG2	2.43	0.49
1:0:1119:G:H8	13:J:52:GLN:NE2	2.10	0.49
21:R:18:LEU:HB2	21:R:143:VAL:HG12	1.94	0.49
1:0:960:G:H2'	1:0:960:G:N3	2.28	0.49
5:A:94:LEU:HG	5:A:99:ILE:CD1	2.43	0.49
25:V:1:THR:HG22	25:V:48:GLU:OE1	2.13	0.49
1:0:1878:G:O2'	1:0:1879:U:OP2	2.30	0.49
17:N:152:GLU:C	17:N:154:LEU:H	2.16	0.49
19:P:16:VAL:HG13	19:P:20:ARG:CZ	2.43	0.49
1:0:830:G:O2'	1:0:831:U:H5'	2.13	0.49
1:0:2531:U:O2'	1:0:2532:A:H5'	2.12	0.49
10:F:34:ASN:HA	16:M:4:ALA:HB2	1.93	0.49
1:0:2453:G:H5''	40:L:9438:HOH:O	2.12	0.49
1:0:793:A:H5''	19:P:83:LYS:HG2	1.95	0.49
1:0:2735:U:H2'	1:0:2736:U:C6	2.47	0.49
3:4:75:C:N4	3:4:76:PPU:H102	2.28	0.49
2:9:3078:G:N2	2:9:3102:G:H2'	2.28	0.49
23:T:69:LYS:O	23:T:71:VAL:HG23	2.13	0.49
21:R:99:ALA:HB1	21:R:109:MET:HE3	1.92	0.49
1:0:1666:C:H2'	1:0:1667:A:C5'	2.42	0.49
5:A:94:LEU:N	5:A:94:LEU:HD23	2.28	0.49
23:T:41:ARG:NH1	23:T:41:ARG:HG2	2.27	0.49
1:0:2032:U:C2'	1:0:2033:G:H5''	2.42	0.49
1:0:669:G:O2'	1:0:670:G:H5'	2.12	0.49
1:0:2781:U:H1'	9:E:139:GLU:OE2	2.12	0.49
12:H:148:GLU:HA	12:H:148:GLU:OE1	2.11	0.49
8:D:37:ALA:O	8:D:40:ILE:HG12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:190:ARG:NH2	5:A:207:GLN:OE1	2.46	0.49
8:D:172:VAL:CG1	8:D:173:GLU:H	2.18	0.49
26:W:122:ARG:HG3	26:W:152:ALA:O	2.13	0.49
9:E:80:TRP:O	9:E:134:SER:HA	2.13	0.49
6:B:41:PHE:CG	6:B:190:MET:HE3	2.47	0.49
20:Q:32:GLU:HA	20:Q:71:TYR:OH	2.13	0.49
1:O:2252:A:H2'	1:O:2253:G:O4'	2.13	0.49
21:R:84:ALA:O	21:R:88:PHE:HD1	1.96	0.49
9:E:11:VAL:HG12	9:E:12:ASP:N	2.26	0.49
6:B:62:ARG:HA	6:B:65:MET:HE2	1.93	0.49
18:O:97:SER:H	18:O:100:GLN:HE21	1.59	0.49
17:N:164:ASP:OD2	17:N:167:ASP:HA	2.12	0.49
17:N:155:GLU:O	17:N:156:GLU:HG3	2.12	0.49
1:O:65:C:O2'	1:O:66:G:H5'	2.12	0.49
8:D:51:ARG:HD3	40:D:7636:HOH:O	2.13	0.49
1:O:2445:U:H2'	1:O:2446:G:C8	2.47	0.49
12:H:69:ALA:HB2	12:H:153:ALA:HB2	1.94	0.49
28:Y:186:ARG:HH11	28:Y:186:ARG:HG2	1.76	0.49
30:1:25:LYS:HG3	31:2:49:GLU:H	1.77	0.48
1:O:1730:G:H5'	1:O:1731:C:H5	1.77	0.48
12:H:170:ASN:N	12:H:170:ASN:ND2	2.61	0.48
1:O:2265:U:H2'	1:O:2266:A:C8	2.48	0.48
16:M:99:ARG:HH21	16:M:170:ASN:ND2	2.02	0.48
31:2:41:HIS:HD2	31:2:44:ARG:H	1.61	0.48
33:I:138:THR:HG22	33:I:139:ILE:H	1.78	0.48
5:A:167:LYS:HB2	29:Z:29:ILE:HD13	1.95	0.48
14:K:28:GLU:HB3	14:K:59:LYS:HB2	1.94	0.48
1:O:750:A:O3'	7:C:101:ASP:HB2	2.12	0.48
1:O:2784:A:H1'	9:E:60:SER:OG	2.13	0.48
7:C:142:ASP:OD1	7:C:236:THR:HG23	2.14	0.48
8:D:99:ASP:HB3	8:D:103:ASN:H	1.77	0.48
2:9:3024:U:H3'	2:9:3025:G:C5'	2.43	0.48
1:O:2809:G:H2'	1:O:2810:G:O4'	2.13	0.48
15:L:97:VAL:HG12	15:L:98:GLU:O	2.13	0.48
1:O:1242:A:C5'	13:J:82:THR:HG23	2.34	0.48
40:O:6232:HOH:O	14:K:87:ARG:CZ	2.60	0.48
8:D:103:ASN:HD21	8:D:134:LEU:H	1.60	0.48
28:Y:144:ARG:NH1	40:Y:9374:HOH:O	2.46	0.48
26:W:65:VAL:HA	26:W:68:THR:HG22	1.95	0.48
20:Q:75:ILE:CD1	20:Q:84:ILE:HD11	2.42	0.48
1:O:2064:U:H5'	1:O:2652:U:O3'	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:399:C:H5'	16:M:179:GLY:O	2.13	0.48
20:Q:40:HIS:CD2	20:Q:60:THR:HG23	2.49	0.48
1:0:426:G:H2'	1:0:427:C:O4'	2.13	0.48
16:M:36:ALA:HB1	40:M:9352:HOH:O	2.13	0.48
40:0:5270:HOH:O	17:N:21:HIS:HD2	1.94	0.48
1:0:1654:U:H2'	5:A:47:HIS:HD2	1.77	0.48
22:S:44:GLN:HE21	25:V:28:LEU:CD2	2.27	0.48
21:R:96:VAL:HG13	21:R:106:GLY:HA3	1.96	0.48
8:D:134:LEU:CD1	8:D:166:ILE:HD11	2.41	0.48
1:0:2541:U:H3'	1:0:2541:U:C6	2.47	0.48
6:B:146:THR:C	6:B:148:PRO:HD3	2.34	0.48
10:F:117:GLU:C	10:F:119:ARG:H	2.17	0.48
25:V:7:GLU:O	25:V:11:MET:HG3	2.13	0.48
12:H:3:ALA:HA	12:H:58:ARG:NH1	2.28	0.48
1:0:2779:G:H21	9:E:143:GLN:NE2	2.12	0.48
1:0:1171:A:H2'	1:0:1172:G:H5'	1.94	0.48
27:X:61:ARG:HB2	27:X:65:ASN:O	2.14	0.48
10:F:39:SER:HB3	10:F:45:ALA:HB2	1.96	0.48
1:0:2456:A:H2'	1:0:2457:U:C6	2.48	0.48
30:1:28:HIS:CE1	30:1:31:LYS:HE2	2.49	0.48
32:3:42:ARG:HH11	32:3:42:ARG:HG3	1.79	0.48
17:N:154:LEU:O	17:N:155:GLU:HB3	2.14	0.48
27:X:61:ARG:HD2	27:X:65:ASN:O	2.14	0.48
13:J:39:VAL:HG11	13:J:107:ASN:CG	2.34	0.48
1:0:31:C:OP2	23:T:8:ARG:NH1	2.44	0.48
1:0:1736:A:H1'	40:0:8069:HOH:O	2.13	0.48
12:H:58:ARG:O	12:H:62:LEU:HD22	2.14	0.48
6:B:212:GLN:HB2	6:B:257:THR:CG2	2.38	0.48
25:V:39:ALA:O	25:V:41:GLU:N	2.47	0.48
12:H:116:ALA:O	12:H:117:PHE:C	2.52	0.48
2:9:3064:C:C2'	2:9:3065:A:H5'	2.42	0.48
23:T:61:GLU:HG3	40:T:3851:HOH:O	2.14	0.48
13:J:47:THR:CG2	13:J:48:GLY:N	2.77	0.48
16:M:134:ILE:O	16:M:136:PRO:HD3	2.13	0.48
26:W:88:THR:HG22	26:W:90:TYR:CD1	2.49	0.48
1:0:656:G:OP2	18:O:37:ARG:HD2	2.13	0.48
1:0:776:A:OP1	30:1:28:HIS:HE1	1.97	0.48
1:0:1730:G:C5'	1:0:1731:C:H6	2.26	0.48
1:0:241:A:C2	1:0:378:A:H4'	2.49	0.48
1:0:1044:C:H3'	1:0:1045:G:H5''	1.96	0.48
1:0:602:A:O2'	1:0:605:C:H4'	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:O:7242:HOH:O	17:N:4:PRO:HD2	2.12	0.48
1:O:2480:G:H3'	40:O:4750:HOH:O	2.14	0.48
6:B:277:GLU:N	6:B:278:PRO:HD2	2.29	0.48
9:E:166:VAL:HG12	40:E:3134:HOH:O	2.13	0.48
21:R:29:LYS:NZ	40:R:9449:HOH:O	2.47	0.48
16:M:59:GLY:HA3	16:M:141:ILE:HD12	1.96	0.48
22:S:57:THR:HG22	22:S:58:MET:N	2.28	0.48
27:X:9:VAL:HG13	27:X:88:GLU:OE1	2.14	0.48
1:O:666:A:H2'	1:O:667:C:O4'	2.14	0.48
1:O:1236:A:C8	13:J:63:ILE:HD11	2.49	0.48
4:5:75:C:H2'	4:5:76:A:O4'	2.14	0.48
14:K:10:GLN:N	14:K:10:GLN:NE2	2.48	0.47
1:O:558:C:C2'	1:O:559:U:C5'	2.92	0.47
15:L:145:LEU:O	15:L:148:GLU:HG3	2.13	0.47
10:F:49:PHE:HE1	10:F:98:VAL:HG23	1.79	0.47
1:O:1189:A:H1'	1:O:1209:C:C1'	2.44	0.47
1:O:2504:A:H4'	12:H:71:ARG:HH11	1.80	0.47
1:O:2862:G:H4'	6:B:336:GLN:O	2.14	0.47
6:B:91:PRO:O	13:J:144:THR:HG21	2.14	0.47
1:O:1098:A:H2'	1:O:1099:G:O4'	2.14	0.47
24:U:4:ARG:HH11	24:U:4:ARG:HG2	1.79	0.47
23:T:96:VAL:CG1	23:T:97:ARG:N	2.78	0.47
12:H:46:GLN:NE2	12:H:137:TYR:HE2	2.11	0.47
1:O:2253:G:O2'	1:O:2254:G:H5'	2.15	0.47
1:O:2719:A:C2	6:B:70:PRO:HG3	2.49	0.47
23:T:26:THR:HA	23:T:39:ASN:HB3	1.96	0.47
33:I:139:ILE:C	33:I:140:GLU:HG3	2.34	0.47
1:O:308:U:C4	1:O:342:C:H1'	2.49	0.47
30:1:25:LYS:CD	31:2:49:GLU:H	2.27	0.47
13:J:54:VAL:O	13:J:58:GLU:HG3	2.14	0.47
12:H:38:LYS:HE2	12:H:42:ASP:CB	2.45	0.47
1:O:392:U:C5'	16:M:193:LYS:HB3	2.45	0.47
25:V:5:VAL:CG1	25:V:9:ARG:NH1	2.77	0.47
7:C:133:ARG:NH1	40:C:9220:HOH:O	2.47	0.47
21:R:82:GLU:O	21:R:86:LYS:HG3	2.14	0.47
2:9:3076:G:H3'	2:9:3077:A:C5'	2.26	0.47
32:3:11:CYS:HB2	32:3:20:HIS:CE1	2.49	0.47
9:E:31:ARG:HH12	9:E:68:HIS:CG	2.31	0.47
9:E:49:ILE:HD11	9:E:69:ILE:HD12	1.96	0.47
22:S:57:THR:CG2	22:S:58:MET:N	2.77	0.47
6:B:254:GLN:NE2	40:B:9587:HOH:O	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1058:A:H2'	1:0:1060:C:H5''	1.96	0.47
12:H:77:LEU:HD12	12:H:83:TYR:CD2	2.49	0.47
1:0:210:U:H2'	1:0:211:U:C6	2.49	0.47
1:0:2626:C:H2'	1:0:2627:G:C8	2.50	0.47
1:0:347:A:H2'	1:0:348:C:O4'	2.14	0.47
1:0:1149:U:H5''	1:0:1151:G:O4'	2.14	0.47
18:O:39:THR:O	18:O:115:ARG:NH2	2.47	0.47
21:R:119:VAL:HG12	21:R:119:VAL:O	2.13	0.47
17:N:15:GLU:HB3	17:N:17:ARG:HD2	1.97	0.47
26:W:64:THR:O	26:W:68:THR:HG22	2.15	0.47
1:0:1878:G:O2'	1:0:1879:U:P	2.72	0.47
7:C:157:LEU:CD1	7:C:166:ILE:HD11	2.44	0.47
6:B:178:ALA:O	6:B:182:VAL:HG23	2.15	0.47
5:A:123:GLY:HA3	5:A:162:GLY:CA	2.44	0.47
1:0:912:A:C4	1:0:1294:A:C2	3.02	0.47
32:3:17:HIS:O	32:3:18:GLN:HG3	2.15	0.47
1:0:1167:G:H4'	33:I:135:LEU:HD22	1.96	0.47
6:B:87:TYR:OH	6:B:163:GLU:OE2	2.30	0.47
17:N:154:LEU:O	17:N:155:GLU:CB	2.63	0.47
1:0:329:A:OP2	7:C:206:ASN:HB2	2.15	0.47
19:P:141:ILE:C	19:P:143:ALA:H	2.17	0.47
29:Z:32:GLU:CD	29:Z:70:LYS:HZ2	2.18	0.47
1:0:29:C:C2'	1:0:30:U:H5'	2.44	0.47
2:9:3003:A:H2'	40:9:2430:HOH:O	2.15	0.47
27:X:7:GLU:HA	27:X:74:ALA:O	2.15	0.47
7:C:140:VAL:HB	40:C:9257:HOH:O	2.14	0.47
16:M:165:GLY:O	16:M:169:ARG:HG3	2.15	0.47
14:K:113:ILE:CG2	14:K:114:ALA:N	2.77	0.47
8:D:173:GLU:HG3	8:D:174:VAL:N	2.30	0.47
1:0:999:C:H2'	1:0:1000:C:O4'	2.15	0.47
1:0:1667:A:C8	1:0:1667:A:H5'	2.40	0.47
32:3:20:HIS:HA	32:3:70:ARG:O	2.15	0.47
10:F:60:VAL:O	10:F:60:VAL:CG1	2.62	0.47
15:L:53:ARG:HH22	15:L:57:VAL:HG12	1.80	0.47
25:V:64:GLY:O	25:V:65:ASP:CB	2.62	0.47
1:0:834:G:H3'	1:0:835:U:H4'	1.97	0.47
13:J:142:ASN:O	13:J:144:THR:N	2.48	0.47
1:0:2434:A:O3'	32:3:28:GLY:HA3	2.15	0.47
17:N:7:LYS:HE3	20:Q:21:ARG:O	2.13	0.47
6:B:75:GLU:C	6:B:77:PRO:HD3	2.35	0.47
10:F:14:ASP:O	10:F:18:GLU:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3048:C:H4'	17:N:141:ARG:HH21	1.79	0.47
22:S:38:ALA:O	22:S:42:GLU:HG3	2.15	0.47
1:0:2379:G:N3	1:0:2418:G:H2'	2.30	0.47
1:0:635:A:H2'	1:0:636:G:H5''	1.96	0.47
21:R:132:ARG:NH2	40:R:9489:HOH:O	2.46	0.47
32:3:91:GLN:O	32:3:92:GLU:HB2	2.15	0.47
16:M:86:GLN:O	16:M:88:VAL:HG23	2.15	0.47
24:U:49:LEU:HG	40:U:3805:HOH:O	2.14	0.47
1:0:2133:U:H4'	1:0:2134:G:H5'	1.97	0.47
17:N:64:SER:C	17:N:66:LEU:H	2.18	0.47
33:I:102:VAL:O	33:I:106:LYS:HG3	2.14	0.47
33:I:75:THR:HA	33:I:112:LYS:NZ	2.29	0.47
13:J:19:MET:CE	13:J:132:LEU:HD21	2.44	0.47
17:N:17:ARG:NH1	17:N:17:ARG:HB3	2.27	0.47
1:0:1158:G:O2'	1:0:1159:G:H5'	2.15	0.47
17:N:167:ASP:C	17:N:168:LEU:HG	2.35	0.47
1:0:171:C:OP2	16:M:84:LYS:HG3	2.14	0.47
2:9:3029:C:C2'	2:9:3030:C:H5'	2.44	0.47
6:B:215:VAL:HA	6:B:220:VAL:HG22	1.97	0.47
26:W:149:LEU:HG	26:W:153:MET:HE2	1.96	0.47
6:B:294:TYR:HE2	40:B:9643:HOH:O	1.97	0.47
1:0:764:C:H2'	1:0:765:G:O4'	2.15	0.47
1:0:1787:C:OP1	19:P:68:LYS:HE2	2.14	0.47
1:0:1921:A:O2'	1:0:1922:A:H5'	2.15	0.47
14:K:7:ASP:OD2	14:K:81:ARG:NH2	2.48	0.47
5:A:69:LEU:HD23	5:A:107:ASN:CB	2.45	0.47
1:0:447:A:O2'	1:0:448:G:H5'	2.15	0.47
24:U:52:THR:HG22	24:U:54:THR:H	1.79	0.47
15:L:97:VAL:HB	15:L:100:ALA:HB2	1.97	0.47
40:0:5212:HOH:O	6:B:300:SER:HB3	2.15	0.47
1:0:1681:G:H5''	1:0:1682:A:H5'	1.97	0.47
15:L:21:ARG:N	40:L:9425:HOH:O	2.47	0.47
9:E:5:LEU:HD21	9:E:66:GLN:HG3	1.95	0.47
9:E:77:THR:OG1	9:E:78:GLU:N	2.47	0.47
27:X:80:GLU:HG2	27:X:80:GLU:O	2.15	0.47
22:S:53:ASN:ND2	40:S:9479:HOH:O	2.49	0.47
13:J:52:GLN:HG3	13:J:53:ILE:N	2.30	0.47
1:0:2506:A:O2'	1:0:2507:G:O5'	2.33	0.47
10:F:58:GLU:HA	10:F:61:MET:HG3	1.97	0.47
1:0:1299:G:N7	15:L:6:ARG:NH1	2.63	0.47
1:0:1641:A:C2'	1:0:1642:A:H5'	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1268:C:O2'	28:Y:169:ARG:HB2	2.15	0.47
1:0:1634:G:H3'	40:0:4467:HOH:O	2.14	0.47
9:E:157:LYS:HD2	9:E:162:PHE:CZ	2.50	0.47
33:I:72:VAL:CG1	33:I:73:PRO:HD2	2.45	0.47
1:0:1783:A:O2'	1:0:1784:U:H5'	2.15	0.47
1:0:1192:A:H3'	1:0:1193:A:H5'	1.96	0.46
33:I:100:LEU:O	33:I:139:ILE:HG23	2.15	0.46
28:Y:155:ARG:NH1	40:Y:9355:HOH:O	2.49	0.46
7:C:153:VAL:O	7:C:157:LEU:HG	2.15	0.46
1:0:657:G:OP1	7:C:27:ARG:NH2	2.30	0.46
8:D:154:LYS:HD2	8:D:154:LYS:N	2.30	0.46
8:D:65:GLU:HG3	40:D:6752:HOH:O	2.14	0.46
1:0:1794:G:N2	1:0:1796:A:H3'	2.30	0.46
1:0:894:A:N1	7:C:87:ARG:NH2	2.63	0.46
1:0:2374:A:H2'	1:0:2375:G:C8	2.51	0.46
17:N:38:LYS:HD3	17:N:107:ASN:ND2	2.29	0.46
1:0:451:C:O2'	1:0:452:G:H5'	2.15	0.46
14:K:81:ARG:HD3	14:K:87:ARG:CZ	2.44	0.46
40:0:5814:HOH:O	26:W:122:ARG:NH2	2.47	0.46
8:D:166:ILE:HB	40:D:6326:HOH:O	2.14	0.46
1:0:1180:U:H1'	40:I:1549:HOH:O	2.14	0.46
33:I:112:LYS:C	33:I:114:PRO:HD2	2.35	0.46
32:3:65:THR:HG22	32:3:67:LEU:CG	2.42	0.46
1:0:136:C:H2'	1:0:137:U:O4'	2.14	0.46
23:T:75:GLU:O	23:T:76:ASP:HB2	2.16	0.46
1:0:2270:G:H4'	5:A:223:ARG:NH1	2.30	0.46
1:0:603:A:H1'	1:0:605:C:C2	2.50	0.46
1:0:56:G:H5''	25:V:50:ARG:NH1	2.31	0.46
1:0:1406:A:H5'	1:0:1407:A:C8	2.51	0.46
1:0:2256:G:H2'	1:0:2257:G:C5'	2.46	0.46
7:C:35:VAL:HG21	7:C:227:GLY:HA2	1.96	0.46
8:D:88:LEU:HB2	8:D:89:PRO:HD3	1.97	0.46
10:F:102:GLY:O	10:F:103:GLU:HB2	2.15	0.46
1:0:449:A:N7	7:C:43:LYS:HG2	2.31	0.46
8:D:60:GLU:O	8:D:60:GLU:HG3	2.15	0.46
26:W:88:THR:HG23	26:W:110:GLN:HB3	1.97	0.46
10:F:56:PRO:HB2	10:F:58:GLU:OE1	2.16	0.46
15:L:57:VAL:HG12	15:L:57:VAL:O	2.15	0.46
5:A:65:ARG:HH11	5:A:65:ARG:HG2	1.80	0.46
1:0:1679:C:H5'	40:0:9938:HOH:O	2.16	0.46
1:0:1307:A:H2'	1:0:1308:A:C8	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:105:ASP:O	10:F:109:GLU:HB2	2.16	0.46
8:D:172:VAL:CG1	8:D:173:GLU:N	2.78	0.46
13:J:131:THR:HG22	13:J:133:GLY:N	2.30	0.46
6:B:62:ARG:HG2	6:B:65:MET:HE3	1.97	0.46
25:V:4:HIS:O	25:V:8:ILE:HG13	2.15	0.46
1:0:2453:G:H5'	40:0:5233:HOH:O	2.16	0.46
40:0:3854:HOH:O	6:B:222:LYS:HE2	2.16	0.46
7:C:218:VAL:HG12	40:C:9232:HOH:O	2.16	0.46
1:0:1799:G:H21	19:P:88:GLN:NE2	2.14	0.46
25:V:29:ASN:O	25:V:33:VAL:HG23	2.16	0.46
27:X:72:VAL:CG2	27:X:85:VAL:HG12	2.42	0.46
8:D:58:VAL:N	8:D:62:ASP:O	2.45	0.46
1:0:2072:G:H3'	1:0:2073:G:C5'	2.45	0.46
10:F:57:GLU:O	10:F:61:MET:HG3	2.15	0.46
6:B:41:PHE:HA	6:B:79:MET:CE	2.45	0.46
24:U:45:GLU:HB2	24:U:48:ASN:HD22	1.78	0.46
1:0:1435:U:H5'	40:0:3203:HOH:O	2.15	0.46
4:5:78:ACA:H61	4:5:79:BTN:H101	1.60	0.46
28:Y:102:LEU:HD11	28:Y:225:GLY:HA2	1.97	0.46
26:W:4:LEU:CD2	26:W:52:VAL:HG21	2.39	0.46
18:O:26:TRP:N	40:O:3062:HOH:O	2.49	0.46
1:0:2587:OMU:H6	1:0:2587:OMU:O5'	2.16	0.46
1:0:1014:A:H2'	1:0:1015:C:H5'	1.97	0.46
30:1:56:GLU:HG2	30:1:56:GLU:OXT	2.16	0.46
6:B:14:GLY:HA2	6:B:15:PRO:C	2.36	0.46
1:0:702:G:O2'	1:0:703:G:H5'	2.16	0.46
7:C:236:THR:O	7:C:237:GLU:C	2.53	0.46
23:T:71:VAL:HG13	23:T:91:LEU:O	2.16	0.46
33:I:103:ASP:HA	33:I:106:LYS:HD2	1.97	0.46
12:H:58:ARG:HG3	12:H:58:ARG:NH1	2.30	0.46
21:R:39:THR:CG2	21:R:107:GLU:O	2.63	0.46
12:H:45:VAL:HA	12:H:167:PRO:O	2.15	0.46
1:0:319:A:H4'	1:0:338:C:C5	2.49	0.46
6:B:215:VAL:HB	6:B:234:ARG:HH12	1.81	0.46
8:D:10:PHE:CG	8:D:11:HIS:N	2.84	0.46
28:Y:99:ALA:HB2	28:Y:233:TYR:CZ	2.51	0.46
1:0:2511:A:H2'	1:0:2512:U:O4'	2.15	0.46
1:0:1789:G:O6	19:P:73:HIS:HE1	1.99	0.46
29:Z:17:ARG:HD3	40:Z:9220:HOH:O	2.15	0.46
29:Z:39:CYS:SG	29:Z:41:ASN:HB3	2.55	0.46
1:0:1636:G:O2'	1:0:1637:A:H5'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:236:THR:O	7:C:239:ALA:N	2.49	0.46
2:9:3057:A:H8	8:D:141:VAL:HG21	1.80	0.46
33:I:99:ASP:O	33:I:100:LEU:HD23	2.16	0.46
6:B:87:TYR:HD1	40:B:9575:HOH:O	1.99	0.46
27:X:43:VAL:CG1	27:X:44:ASP:N	2.79	0.46
1:0:1778:A:H2'	1:0:1779:A:H5'	1.97	0.46
21:R:114:VAL:HG13	21:R:114:VAL:O	2.15	0.46
13:J:71:TYR:CG	13:J:72:PRO:HD2	2.51	0.46
17:N:183:ASP:O	17:N:184:ILE:O	2.34	0.46
1:0:894:A:C2	7:C:87:ARG:NH2	2.83	0.46
1:0:2524:G:H21	1:0:2526:C:N4	2.13	0.46
27:X:34:ARG:NH1	27:X:48:VAL:O	2.48	0.46
15:L:79:ASP:HB3	40:L:9453:HOH:O	2.15	0.46
26:W:142:ASP:HB2	40:W:6373:HOH:O	2.15	0.46
14:K:87:ARG:NH1	40:K:4066:HOH:O	2.49	0.46
6:B:51:VAL:HG21	6:B:327:VAL:HG13	1.94	0.46
15:L:91:VAL:CG1	15:L:120:LEU:HD23	2.46	0.46
1:0:1015:C:H2'	1:0:1016:U:C6	2.51	0.46
27:X:20:GLU:HG3	27:X:21:PRO:HD2	1.98	0.46
1:0:2011:A:H4'	1:0:2012:U:O5'	2.16	0.46
1:0:2487:C:H5	40:0:5422:HOH:O	1.98	0.46
12:H:9:ILE:HD12	12:H:54:THR:HG22	1.97	0.46
1:0:2505:G:C2'	1:0:2506:A:H5'	2.46	0.46
6:B:217:ARG:HG3	6:B:257:THR:CG2	2.46	0.46
7:C:107:ARG:NE	40:C:9266:HOH:O	2.32	0.46
25:V:45:ARG:HA	25:V:48:GLU:HB2	1.98	0.46
1:0:1200:A:H3'	40:0:6272:HOH:O	2.15	0.46
1:0:1298:U:H2'	1:0:1299:G:C8	2.50	0.46
1:0:1730:G:H5'	1:0:1731:C:C6	2.51	0.46
1:0:951:A:O2'	1:0:952:G:H5'	2.16	0.46
1:0:1654:U:H2'	5:A:47:HIS:CD2	2.51	0.46
2:9:3064:C:H2'	2:9:3065:A:H5'	1.97	0.46
1:0:1799:G:H21	19:P:88:GLN:HE22	1.64	0.46
28:Y:152:LYS:HB3	28:Y:160:LYS:HG3	1.98	0.46
1:0:2904:U:H4'	27:X:8:ARG:NH1	2.31	0.46
1:0:2372:A:H2'	1:0:2373:U:C6	2.51	0.46
1:0:802:G:H2'	1:0:803:C:C6	2.50	0.46
2:9:3092:G:H2'	2:9:3093:A:C8	2.51	0.46
10:F:107:ASP:O	10:F:111:ILE:HG13	2.16	0.46
26:W:21:LEU:HD13	26:W:26:ILE:HD11	1.99	0.45
14:K:101:ASN:O	14:K:102:GLU:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:W:3:ALA:O	26:W:54:PHE:HA	2.16	0.45
32:3:6:ARG:HA	32:3:20:HIS:O	2.16	0.45
1:0:1878:G:O2'	1:0:1879:U:C5	2.61	0.45
1:0:2346:C:H4'	8:D:52:THR:CG2	2.47	0.45
5:A:217:ARG:NH1	5:A:217:ARG:CG	2.78	0.45
12:H:54:THR:O	12:H:55:VAL:HG13	2.16	0.45
5:A:232:ARG:NH2	5:A:236:GLY:O	2.45	0.45
1:0:1250:C:O2'	1:0:1251:C:H5'	2.16	0.45
5:A:39:ALA:HB3	5:A:61:GLU:OE2	2.16	0.45
7:C:78:ARG:CG	7:C:78:ARG:NH1	2.76	0.45
7:C:5:ILE:HG13	7:C:15:GLU:HA	1.99	0.45
6:B:86:ALA:HA	40:B:9575:HOH:O	2.15	0.45
6:B:42:ALA:H	6:B:79:MET:HE2	1.81	0.45
1:0:1067:A:H5'	40:0:4906:HOH:O	2.15	0.45
1:0:2338:G:H2'	8:D:129:ASP:OD1	2.16	0.45
13:J:8:ALA:HA	13:J:35:THR:HG22	1.98	0.45
28:Y:117:LEU:HA	28:Y:174:VAL:HG11	1.98	0.45
26:W:11:VAL:O	26:W:12:ASN:HB2	2.15	0.45
26:W:59:GLN:NE2	26:W:97:ALA:HB3	2.32	0.45
17:N:110:THR:HB	17:N:113:SER:HG	1.80	0.45
19:P:10:ALA:HA	19:P:13:VAL:HG12	1.98	0.45
1:0:1980:U:H5'	1:0:2626:C:H1'	1.98	0.45
5:A:130:THR:HB	5:A:137:VAL:HB	1.97	0.45
1:0:1942:A:H3'	40:0:7785:HOH:O	2.16	0.45
1:0:2356:A:H2'	1:0:2357:G:O4'	2.16	0.45
12:H:43:TYR:HA	12:H:44:PRO:HD3	1.77	0.45
6:B:168:GLY:O	6:B:169:GLY:O	2.35	0.45
8:D:167:GLU:C	8:D:169:THR:H	2.20	0.45
1:0:1603:A:H5''	1:0:1605:G:H5'	1.98	0.45
1:0:1182:C:H1'	1:0:1192:A:C8	2.45	0.45
1:0:2072:G:C6	1:0:2533:C:H1'	2.52	0.45
1:0:558:C:H2'	1:0:559:U:H5''	1.97	0.45
1:0:1205:U:H2'	1:0:1206:U:H5''	1.99	0.45
1:0:1441:G:H1'	40:0:8275:HOH:O	2.16	0.45
28:Y:107:PRO:HB3	28:Y:182:PHE:CE2	2.51	0.45
1:0:737:A:H2'	1:0:738:G:O4'	2.16	0.45
16:M:66:SER:HB3	16:M:128:TRP:CD1	2.51	0.45
33:I:116:LEU:HD22	33:I:127:GLU:OE1	2.17	0.45
1:0:2003:U:H4'	1:0:2004:U:H5	1.80	0.45
15:L:90:ARG:NH2	15:L:121:ILE:HD11	2.32	0.45
16:M:68:ARG:HD3	16:M:68:ARG:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2747:C:H4'	40:0:8429:HOH:O	2.16	0.45
1:0:447:A:OP1	23:T:2:LYS:HG2	2.16	0.45
17:N:154:LEU:CG	17:N:155:GLU:H	2.25	0.45
17:N:73:ALA:HB1	17:N:74:PRO:CD	2.46	0.45
1:0:2101:A:H2'	7:C:63:SER:OG	2.16	0.45
6:B:97:LEU:HD21	40:B:9637:HOH:O	2.17	0.45
1:0:27:U:H2'	1:0:28:G:O4'	2.17	0.45
1:0:2672:C:O2'	1:0:2673:U:H5'	2.16	0.45
1:0:1180:U:H2'	1:0:1181:A:C8	2.51	0.45
9:E:31:ARG:HH12	9:E:68:HIS:CE1	2.35	0.45
9:E:69:ILE:HA	9:E:72:MET:CE	2.47	0.45
9:E:95:VAL:HG11	9:E:131:LEU:HD11	1.97	0.45
15:L:143:THR:CG2	15:L:144:ASP:H	2.23	0.45
13:J:131:THR:HB	13:J:134:GLU:OE1	2.16	0.45
22:S:10:VAL:HG11	25:V:36:ALA:CA	2.45	0.45
2:9:3041:C:C6	8:D:50:VAL:HG21	2.51	0.45
25:V:8:ILE:HG21	25:V:59:ILE:HG13	1.98	0.45
33:I:89:SER:HB2	33:I:95:ASP:HB2	1.99	0.45
15:L:77:ALA:C	15:L:79:ASP:H	2.20	0.45
23:T:78:THR:HB	23:T:87:VAL:O	2.17	0.45
12:H:136:ALA:HB3	12:H:146:VAL:HG21	1.97	0.45
2:9:3045:A:H4'	8:D:143:LYS:O	2.16	0.45
26:W:88:THR:CG2	26:W:90:TYR:HD1	2.29	0.45
1:0:1163:G:H2'	1:0:1164:U:C5	2.52	0.45
33:I:75:THR:OG1	33:I:112:LYS:HE2	2.17	0.45
24:U:14:GLU:OE1	24:U:15:PRO:HD2	2.17	0.45
26:W:108:ARG:CG	26:W:114:PRO:HG3	2.44	0.45
5:A:223:ARG:CZ	40:A:9562:HOH:O	2.64	0.45
23:T:85:GLU:CG	23:T:86:GLU:N	2.79	0.45
40:0:6180:HOH:O	23:T:68:ASP:HB2	2.16	0.45
15:L:101:ASP:C	15:L:103:ALA:H	2.20	0.45
26:W:85:ALA:HB2	26:W:91:ASP:O	2.17	0.45
20:Q:30:VAL:HG12	20:Q:30:VAL:O	2.17	0.45
8:D:44:ILE:HG23	8:D:45:THR:HG23	1.99	0.45
23:T:71:VAL:HG12	23:T:72:ILE:H	1.82	0.45
1:0:1201:C:C2'	1:0:1202:A:H5'	2.43	0.45
1:0:962:C:H5'	40:0:7430:HOH:O	2.16	0.45
1:0:1167:G:H2'	1:0:1168:C:O4'	2.17	0.45
5:A:131:HIS:O	5:A:132:ASP:HB2	2.17	0.45
7:C:119:ALA:HA	7:C:137:PRO:HD3	1.99	0.45
7:C:133:ARG:NE	7:C:138:VAL:HG22	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2256:G:H2'	1:0:2257:G:H5'	1.99	0.45
1:0:1574:C:H2'	1:0:1575:C:C6	2.52	0.45
20:Q:53:HIS:CE1	20:Q:55:ARG:HB2	2.52	0.45
14:K:80:ILE:O	14:K:87:ARG:HA	2.16	0.45
1:0:1168:C:H5''	33:I:87:THR:HG23	1.99	0.45
28:Y:187:VAL:HG23	28:Y:192:ASP:HB3	1.98	0.45
1:0:1477:C:H5'	1:0:1868:G:C5'	2.47	0.45
20:Q:40:HIS:HD2	20:Q:60:THR:HG23	1.82	0.45
21:R:119:VAL:O	21:R:119:VAL:CG1	2.64	0.45
1:0:2250:G:OP1	5:A:31:LYS:HD3	2.17	0.45
15:L:149:ARG:O	15:L:150:GLN:HB2	2.16	0.45
1:0:790:A:H1'	1:0:1710:A:H2'	1.99	0.45
16:M:46:LEU:HD22	16:M:50:ARG:HG3	1.98	0.45
1:0:1180:U:H2'	1:0:1181:A:O4'	2.17	0.45
5:A:206:ARG:N	5:A:206:ARG:HD3	2.27	0.45
28:Y:144:ARG:CG	28:Y:144:ARG:NH1	2.71	0.45
5:A:167:LYS:HE3	29:Z:26:VAL:HG13	1.99	0.45
1:0:2541:U:C6	1:0:2541:U:C3'	3.00	0.45
19:P:16:VAL:HG12	19:P:17:GLY:H	1.80	0.45
16:M:120:VAL:CG1	16:M:130:GLU:HG3	2.46	0.45
18:O:47:ARG:HG3	18:O:47:ARG:NH1	2.32	0.45
24:U:4:ARG:NH1	24:U:4:ARG:HG2	2.32	0.45
1:0:2256:G:C2'	1:0:2257:G:H5'	2.47	0.45
1:0:1015:C:H2'	1:0:1016:U:H6	1.81	0.45
12:H:146:VAL:HG22	40:H:9543:HOH:O	2.17	0.45
1:0:622:G:P	28:Y:148:GLY:HA3	2.57	0.45
16:M:158:ARG:HB2	16:M:163:LEU:HB2	1.97	0.45
1:0:907:A:H2'	1:0:908:A:C8	2.51	0.45
1:0:816:G:H5'	1:0:1598:A:H4'	1.97	0.45
17:N:49:THR:HG22	17:N:56:ASP:CB	2.39	0.44
5:A:105:VAL:HG12	5:A:106:CYS:H	1.82	0.44
6:B:41:PHE:CB	6:B:190:MET:HE3	2.47	0.44
10:F:33:THR:HG21	10:F:59:ILE:O	2.17	0.44
6:B:175:LEU:C	6:B:175:LEU:HD23	2.37	0.44
1:0:2769:C:H2'	1:0:2770:G:O4'	2.17	0.44
1:0:2365:G:H4'	20:Q:45:PRO:O	2.17	0.44
1:0:1350:U:H2'	1:0:1351:G:O4'	2.17	0.44
4:5:76:A:H4'	4:5:76:A:OP1	2.17	0.44
27:X:21:PRO:HG2	27:X:24:LYS:HD3	1.98	0.44
28:Y:163:THR:HB	40:Y:9397:HOH:O	2.16	0.44
1:0:2724:U:H2'	1:0:2725:G:O4'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:O:24:ALA:O	18:O:28:ASP:HB2	2.17	0.44
9:E:170:ARG:HE	9:E:170:ARG:HB2	1.67	0.44
15:L:89:PHE:CD1	15:L:89:PHE:N	2.85	0.44
2:9:3056:A:C3'	2:9:3057:A:H5''	2.47	0.44
14:K:115:ARG:O	14:K:118:ALA:HB3	2.16	0.44
1:0:1163:G:H1	1:0:1184:C:N4	2.15	0.44
12:H:58:ARG:HG3	40:H:9520:HOH:O	2.18	0.44
9:E:31:ARG:NH1	40:E:5919:HOH:O	2.49	0.44
15:L:145:LEU:C	15:L:145:LEU:HD23	2.38	0.44
1:0:2443:C:H5'	15:L:57:VAL:HG21	1.99	0.44
1:0:603:A:H4'	1:0:604:G:O5'	2.16	0.44
2:9:3049:G:H2'	2:9:3050:G:O4'	2.17	0.44
2:9:3001:U:H5''	2:9:3003:A:OP1	2.17	0.44
25:V:42:ASN:O	25:V:44:GLY:N	2.50	0.44
1:0:1593:C:OP1	19:P:117:SER:HB3	2.17	0.44
10:F:28:ALA:HB3	10:F:99:THR:O	2.18	0.44
7:C:107:ARG:NH1	40:C:9238:HOH:O	2.50	0.44
1:0:656:G:H1'	40:C:9267:HOH:O	2.17	0.44
1:0:2726:U:O2	1:0:2749:U:O5'	2.34	0.44
27:X:73:ARG:HB2	27:X:88:GLU:OE2	2.17	0.44
6:B:41:PHE:HA	6:B:79:MET:HE1	1.99	0.44
9:E:22:VAL:O	9:E:28:SER:HA	2.17	0.44
7:C:115:LEU:O	7:C:118:THR:HB	2.17	0.44
27:X:41:PHE:O	27:X:43:VAL:HG23	2.16	0.44
6:B:8:LYS:HG3	6:B:220:VAL:HG12	1.99	0.44
33:I:97:VAL:N	33:I:136:GLY:O	2.51	0.44
13:J:39:VAL:CG1	13:J:40:ASN:N	2.81	0.44
1:0:794:U:H3	1:0:819:A:H61	1.64	0.44
6:B:113:LEU:HD21	6:B:161:VAL:HG21	1.98	0.44
6:B:185:GLY:HA2	40:B:9628:HOH:O	2.16	0.44
1:0:1380:U:O4	1:0:2043:U:H4'	2.17	0.44
13:J:42:GLU:O	13:J:131:THR:HG23	2.18	0.44
5:A:179:MET:HG2	5:A:186:TRP:CG	2.52	0.44
15:L:35:ARG:HB2	15:L:35:ARG:HH11	1.82	0.44
1:0:154:C:P	16:M:188:ARG:HH12	2.40	0.44
10:F:5:ASP:O	10:F:119:ARG:NH1	2.50	0.44
19:P:143:ALA:HA	40:P:164:HOH:O	2.17	0.44
8:D:78:GLU:O	8:D:82:GLU:HG3	2.18	0.44
2:9:3114:G:O6	17:N:11:ARG:HD3	2.17	0.44
12:H:29:ALA:C	12:H:30:GLN:HG3	2.38	0.44
1:0:2541:U:C2	1:0:2620:U:O4	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:407:A:H5'	40:0:6529:HOH:O	2.18	0.44
1:0:82:C:OP1	23:T:67:LEU:HB2	2.18	0.44
1:0:2100:A:H4'	7:C:64:GLY:O	2.16	0.44
1:0:2857:C:H2'	1:0:2858:U:C6	2.52	0.44
23:T:71:VAL:CG1	23:T:72:ILE:N	2.80	0.44
1:0:1185:U:H5'	40:0:7899:HOH:O	2.18	0.44
33:I:92:PRO:O	33:I:94:GLU:N	2.50	0.44
6:B:53:LEU:CD1	6:B:327:VAL:HG22	2.46	0.44
25:V:56:ILE:HG22	25:V:60:GLN:NE2	2.32	0.44
1:0:1266:U:H4'	28:Y:115:ARG:HH21	1.82	0.44
40:0:3165:HOH:O	26:W:119:HIS:HE1	2.01	0.44
6:B:85:ARG:HB2	6:B:99:GLU:HG2	1.99	0.44
1:0:1552:G:H2'	1:0:1553:C:C6	2.52	0.44
1:0:1104:C:H4'	13:J:88:PRO:HD3	1.99	0.44
18:O:60:VAL:HG12	18:O:62:GLY:H	1.81	0.44
1:0:256:C:H2'	1:0:257:G:O4'	2.17	0.44
1:0:2019:A:H5'	40:0:5087:HOH:O	2.17	0.44
1:0:1278:A:H4'	1:0:1279:U:C4	2.52	0.44
16:M:98:GLN:O	16:M:102:GLU:HG3	2.17	0.44
7:C:1:MET:HG2	7:C:2:GLN:NE2	2.33	0.44
8:D:60:GLU:O	8:D:61:PHE:C	2.55	0.44
26:W:122:ARG:NE	40:W:5817:HOH:O	2.50	0.44
33:I:139:ILE:HG22	33:I:140:GLU:N	2.32	0.44
1:0:2533:C:H6	1:0:2533:C:C5'	2.25	0.44
6:B:217:ARG:HD3	6:B:218:TRP:NE1	2.33	0.44
1:0:1666:C:C2'	1:0:1667:A:C5'	2.96	0.44
1:0:2748:G:H4'	1:0:2749:U:C5'	2.47	0.44
27:X:9:VAL:HG13	27:X:88:GLU:OE2	2.17	0.44
1:0:1162:G:H1'	33:I:117:LEU:CD1	2.47	0.44
16:M:82:ARG:O	16:M:83:SER:C	2.56	0.44
28:Y:203:VAL:CG1	28:Y:228:VAL:HG22	2.48	0.44
6:B:96:PRO:HG3	40:B:9629:HOH:O	2.17	0.44
27:X:18:ARG:NH1	40:X:4132:HOH:O	2.50	0.44
1:0:2296:C:H2'	1:0:2297:U:C6	2.52	0.44
25:V:5:VAL:HG23	40:V:2271:HOH:O	2.18	0.44
31:2:5:LYS:O	31:2:9:LYS:HG3	2.17	0.44
1:0:645:U:OP2	15:L:4:LYS:HE2	2.18	0.44
1:0:371:U:H2'	1:0:372:A:H8	1.82	0.44
6:B:66:GLU:OE1	6:B:328:ARG:HD2	2.18	0.44
2:9:3012:C:H5'	2:9:3070:U:O4'	2.18	0.44
1:0:1771:U:C4'	29:Z:20:ARG:HE	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1119:G:H8	13:J:52:GLN:HE22	1.66	0.44
1:0:2712:G:H5'	40:K:4183:HOH:O	2.17	0.44
1:0:656:G:H4'	40:C:9167:HOH:O	2.18	0.44
5:A:103:VAL:O	5:A:105:VAL:HG23	2.18	0.44
1:0:1350:U:H1'	40:0:3273:HOH:O	2.17	0.44
1:0:1044:C:H5''	40:0:9648:HOH:O	2.18	0.44
1:0:2895:C:H4'	40:X:4132:HOH:O	2.18	0.44
1:0:29:C:O2'	1:0:30:U:H5'	2.18	0.44
1:0:2335:C:H2'	1:0:2336:G:H8	1.83	0.44
1:0:1244:U:H2'	13:J:47:THR:HG21	1.99	0.44
1:0:960:G:N3	1:0:960:G:C2'	2.81	0.44
18:O:4:ASN:HA	18:O:5:PRO:HD3	1.90	0.44
6:B:71:VAL:CG1	6:B:296:LEU:HD22	2.48	0.44
12:H:55:VAL:HG12	40:H:9540:HOH:O	2.18	0.44
1:0:1592:G:O2'	1:0:1593:C:O4'	2.34	0.44
40:0:4557:HOH:O	23:T:82:THR:HA	2.17	0.44
27:X:31:ILE:O	27:X:35:GLU:HG3	2.16	0.44
1:0:1139:U:H2'	1:0:1140:C:C6	2.53	0.44
1:0:2472:C:O2'	1:0:2634:G:H4'	2.18	0.44
21:R:61:GLN:NE2	40:R:9449:HOH:O	2.50	0.43
13:J:75:PRO:HB3	13:J:132:LEU:HB3	2.00	0.43
15:L:144:ASP:O	15:L:147:GLU:HB2	2.18	0.43
29:Z:30:GLU:HA	29:Z:33:MET:HB3	1.99	0.43
23:T:38:ARG:NH1	23:T:38:ARG:HG3	2.32	0.43
5:A:132:ASP:HB3	5:A:135:VAL:H	1.83	0.43
27:X:61:ARG:HG3	27:X:61:ARG:NH1	2.33	0.43
1:0:1086:A:C6	26:W:11:VAL:HG11	2.52	0.43
1:0:2044:G:OP1	27:X:23:HIS:HE1	2.01	0.43
1:0:213:G:N2	1:0:225:G:H2'	2.33	0.43
7:C:219:ASN:N	7:C:222:ASP:OD1	2.44	0.43
1:0:1053:G:OP1	12:H:12:PRO:HG3	2.18	0.43
1:0:556:C:H2'	1:0:557:C:C6	2.53	0.43
5:A:29:HIS:CD2	5:A:153:ARG:NH1	2.86	0.43
28:Y:151:SER:HB3	28:Y:154:ARG:HB3	2.00	0.43
23:T:96:VAL:HG13	23:T:97:ARG:N	2.32	0.43
5:A:105:VAL:HG13	5:A:155:THR:O	2.18	0.43
20:Q:25:PRO:HA	20:Q:26:PRO:HD3	1.85	0.43
1:0:338:C:H5''	40:C:9230:HOH:O	2.16	0.43
1:0:2548:C:OP2	6:B:5:ARG:NH2	2.51	0.43
1:0:2503:A:OP1	12:H:151:ARG:NH2	2.42	0.43
28:Y:106:THR:HG23	28:Y:107:PRO:HD2	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:P:55:LYS:CG	19:P:56:GLY:N	2.80	0.43
1:0:157:G:H4'	16:M:95:LYS:HE2	1.99	0.43
23:T:30:ASP:O	23:T:33:GLU:HB3	2.18	0.43
1:0:2401:A:H2'	1:0:2402:A:C8	2.53	0.43
6:B:279:THR:CG2	6:B:280:VAL:N	2.80	0.43
2:9:3057:A:C8	8:D:141:VAL:HG21	2.52	0.43
31:2:41:HIS:CD2	31:2:44:ARG:H	2.35	0.43
12:H:169:GLY:C	12:H:170:ASN:HD22	2.20	0.43
6:B:243:ASN:HA	6:B:244:PRO:C	2.37	0.43
8:D:88:LEU:N	8:D:89:PRO:CD	2.81	0.43
6:B:181:ILE:HG22	6:B:186:GLY:HA2	1.98	0.43
28:Y:216:ARG:HD2	40:Y:9368:HOH:O	2.16	0.43
29:Z:60:CYS:O	29:Z:61:ASP:HB2	2.18	0.43
40:0:5154:HOH:O	5:A:206:ARG:HD3	2.18	0.43
1:0:1174:A:H62	1:0:1200:A:H2'	1.83	0.43
5:A:123:GLY:HA2	5:A:159:VAL:O	2.18	0.43
1:0:2787:C:H5	40:0:5178:HOH:O	2.01	0.43
1:0:661:G:C5	1:0:686:A:C2	3.06	0.43
16:M:49:ALA:C	16:M:54:TYR:HB3	2.39	0.43
1:0:2568:A:H2'	1:0:2569:A:O4'	2.18	0.43
15:L:130:ARG:O	15:L:131:GLU:C	2.57	0.43
16:M:72:ALA:HB2	16:M:93:ARG:HG2	2.01	0.43
7:C:142:ASP:CG	7:C:237:GLU:HB3	2.39	0.43
17:N:11:ARG:CG	17:N:14:ARG:NH1	2.73	0.43
1:0:1884:G:O6	5:A:190:ARG:HD2	2.16	0.43
6:B:36:PRO:HB3	6:B:174:ARG:HB2	1.99	0.43
17:N:71:TRP:CE3	17:N:175:LEU:HD22	2.53	0.43
9:E:84:MET:CE	9:E:148:ILE:HD12	2.45	0.43
2:9:3042:C:H5'	2:9:3043:G:OP2	2.17	0.43
2:9:3044:A:O4'	8:D:76:ARG:NE	2.51	0.43
7:C:79:ARG:O	7:C:87:ARG:HG2	2.18	0.43
1:0:1482:A:O2'	1:0:1483:C:H5'	2.19	0.43
1:0:1928:C:C2'	1:0:1929:G:H5'	2.47	0.43
20:Q:59:GLN:HB3	40:Q:6286:HOH:O	2.17	0.43
26:W:106:THR:OG1	26:W:109:GLU:HG3	2.18	0.43
1:0:1289:C:O2'	1:0:1290:G:H5'	2.19	0.43
7:C:123:LEU:HA	7:C:123:LEU:HD23	1.86	0.43
20:Q:64:GLU:OE1	20:Q:64:GLU:HA	2.18	0.43
1:0:588:G:O6	26:W:154:ARG:NH1	2.52	0.43
21:R:104:PHE:HB3	21:R:109:MET:CE	2.49	0.43
26:W:110:GLN:HE21	26:W:110:GLN:HA	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1181:A:N1	1:0:1192:A:O2'	2.51	0.43
9:E:35:TYR:HB2	40:E:5715:HOH:O	2.18	0.43
1:0:903:U:O4	15:L:18:HIS:HB2	2.17	0.43
1:0:2363:G:O3'	20:Q:11:ARG:NH1	2.51	0.43
10:F:11:ASP:O	10:F:14:ASP:HB2	2.17	0.43
7:C:51:TYR:CD1	30:1:56:GLU:HB2	2.54	0.43
12:H:47:ILE:HG21	40:H:9543:HOH:O	2.18	0.43
40:0:6985:HOH:O	28:Y:141:THR:HG23	2.19	0.43
1:0:2776:A:H2'	1:0:2777:G:O4'	2.18	0.43
1:0:1657:A:H2'	1:0:1658:A:C8	2.54	0.43
1:0:415:A:O2'	1:0:416:G:H5'	2.19	0.43
1:0:1511:U:O2'	1:0:1512:G:H5'	2.18	0.43
1:0:2478:U:O2'	1:0:2479:A:H5'	2.19	0.43
1:0:542:A:H2'	1:0:543:G:O4'	2.19	0.43
26:W:146:ILE:HA	26:W:146:ILE:HD13	1.92	0.43
12:H:56:GLN:HG2	12:H:126:ARG:HG2	2.00	0.43
16:M:107:ARG:CG	16:M:107:ARG:NH1	2.77	0.43
16:M:24:GLN:O	16:M:28:GLN:HG3	2.19	0.43
10:F:60:VAL:HG13	10:F:63:ILE:HG13	2.01	0.43
33:I:132:CYS:C	33:I:134:SER:H	2.21	0.43
19:P:13:VAL:HG21	19:P:41:ARG:HG2	2.01	0.43
1:0:1878:G:O2'	1:0:1879:U:H6	1.98	0.43
7:C:27:ARG:HD2	18:O:5:PRO:HD2	2.01	0.43
7:C:194:PHE:HA	7:C:234:VAL:HG13	2.01	0.43
12:H:83:TYR:C	12:H:83:TYR:CD1	2.92	0.43
1:0:1218:U:H2'	1:0:1219:U:H6	1.83	0.43
23:T:79:LEU:HG	23:T:89:ARG:HB2	2.01	0.43
1:0:2856:A:P	27:X:15:ARG:HH22	2.42	0.43
15:L:12:THR:HG21	15:L:16:GLY:O	2.18	0.43
30:1:53:LYS:HA	30:1:53:LYS:HD3	1.84	0.43
40:C:9167:HOH:O	18:O:3:THR:HG21	2.18	0.43
10:F:49:PHE:CB	10:F:83:LEU:HD11	2.49	0.43
10:F:52:GLU:HG3	10:F:77:VAL:O	2.19	0.43
33:I:132:CYS:C	33:I:134:SER:N	2.71	0.43
28:Y:112:GLU:OE2	28:Y:115:ARG:NH1	2.52	0.43
1:0:2015:A:O2'	1:0:2016:U:H5'	2.19	0.43
1:0:830:G:H2'	1:0:831:U:C6	2.54	0.43
1:0:1236:A:H2'	1:0:1237:U:O4'	2.19	0.43
6:B:109:LEU:HD11	6:B:113:LEU:HD11	2.00	0.43
1:0:2001:G:O2'	1:0:2002:C:H5'	2.19	0.43
1:0:1185:U:H4'	33:I:123:ASN:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2676:C:H4'	13:J:70:PHE:HD1	1.83	0.43
12:H:166:SER:HB2	12:H:167:PRO:CD	2.48	0.43
17:N:48:VAL:HG11	17:N:55:ASP:HB3	1.99	0.43
26:W:108:ARG:HE	26:W:114:PRO:CG	2.32	0.43
1:0:710:G:N2	1:0:719:C:C2	2.87	0.43
24:U:52:THR:CG2	24:U:54:THR:HB	2.49	0.43
5:A:217:ARG:HH11	5:A:217:ARG:HG3	1.84	0.43
1:0:1979:G:HO2'	1:0:1980:U:P	2.41	0.43
17:N:74:PRO:HG2	17:N:159:TYR:CE1	2.54	0.43
1:0:907:A:H2'	1:0:908:A:H8	1.84	0.43
1:0:660:A:H4'	1:0:661:G:O5'	2.19	0.43
40:0:4966:HOH:O	5:A:11:ARG:CZ	2.67	0.43
1:0:883:U:C2'	1:0:883:U:O2	2.65	0.43
1:0:821:U:H2'	1:0:822:C:H6	1.84	0.43
1:0:818:A:O2'	29:Z:13:ARG:HD2	2.19	0.43
28:Y:107:PRO:HB3	28:Y:182:PHE:CD2	2.54	0.43
13:J:39:VAL:HG21	13:J:107:ASN:ND2	2.34	0.43
25:V:5:VAL:HG11	25:V:9:ARG:NH1	2.33	0.43
19:P:55:LYS:HG2	19:P:56:GLY:N	2.33	0.43
1:0:2515:C:H2'	1:0:2516:G:O4'	2.19	0.43
19:P:105:LEU:CD2	19:P:137:LEU:HD21	2.49	0.43
7:C:46:TYR:CE2	7:C:98:ARG:NH1	2.87	0.43
10:F:101:ALA:HA	40:F:5413:HOH:O	2.19	0.43
14:K:13:GLU:OE1	14:K:44:LEU:HD12	2.19	0.43
12:H:2:PRO:HD2	12:H:5:MET:SD	2.58	0.43
25:V:12:THR:OG1	25:V:13:PRO:HD2	2.19	0.42
5:A:207:GLN:O	5:A:208:HIS:HB3	2.19	0.42
1:0:2851:G:H4'	6:B:157:LYS:NZ	2.34	0.42
1:0:2072:G:N2	40:0:7335:HOH:O	2.50	0.42
1:0:797:A:O4'	29:Z:10:ARG:N	2.51	0.42
6:B:190:MET:CE	6:B:194:PHE:CD1	3.01	0.42
6:B:102:THR:HG23	6:B:182:VAL:HG12	1.99	0.42
1:0:292:G:H2'	1:0:358:G:N2	2.33	0.42
7:C:246:ARG:HB3	7:C:246:ARG:NH1	2.33	0.42
1:0:1008:C:H2'	1:0:1009:U:C6	2.54	0.42
22:S:37:VAL:O	22:S:41:VAL:HG23	2.18	0.42
1:0:2088:C:H1'	1:0:2841:A:N1	2.34	0.42
1:0:185:G:H4'	1:0:186:A:H4'	2.00	0.42
40:9:5851:HOH:O	17:N:115:VAL:HG13	2.19	0.42
31:2:44:ARG:HA	31:2:44:ARG:HD3	1.78	0.42
33:I:102:VAL:HG23	33:I:140:GLU:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2748:G:H5'	40:0:7972:HOH:O	2.19	0.42
16:M:42:ARG:HA	16:M:43:PRO:HD3	1.87	0.42
15:L:91:VAL:HG12	15:L:120:LEU:HD23	2.01	0.42
1:0:920:C:H5'	1:0:921:G:C4	2.54	0.42
1:0:2866:U:C4	24:U:50:GLU:HB3	2.55	0.42
1:0:1151:G:OP1	11:G:63:ARG:NH1	2.52	0.42
26:W:142:ASP:HB3	26:W:145:GLY:H	1.84	0.42
1:0:1926:G:H2'	1:0:1927:A:C8	2.54	0.42
1:0:958:G:H2'	1:0:959:C:C6	2.53	0.42
1:0:461:C:N3	1:0:479:G:H5'	2.34	0.42
1:0:1182:C:C1'	1:0:1192:A:H8	2.30	0.42
31:2:48:ASP:O	31:2:49:GLU:HB2	2.19	0.42
1:0:1315:G:C4	28:Y:212:ARG:HB2	2.55	0.42
1:0:709:G:O2'	18:O:25:VAL:CG1	2.67	0.42
12:H:154:TYR:C	12:H:154:TYR:CD1	2.92	0.42
1:0:2663:U:O2	40:0:8435:HOH:O	2.22	0.42
1:0:952:G:N3	1:0:2302:A:H2'	2.34	0.42
1:0:2134:G:C6	1:0:2258:A:C8	3.08	0.42
10:F:111:ILE:O	10:F:115:VAL:HG23	2.19	0.42
1:0:816:G:C6	1:0:817:G:N1	2.87	0.42
1:0:1947:G:H2'	1:0:1948:G:H8	1.84	0.42
1:0:1363:G:OP1	7:C:76:ARG:NH2	2.48	0.42
1:0:37:A:H2'	1:0:38:G:C8	2.54	0.42
7:C:127:ARG:HG2	7:C:127:ARG:HH11	1.85	0.42
1:0:1819:G:H2'	1:0:1820:G:C4'	2.50	0.42
1:0:2415:A:O2'	17:N:29:SER:HB3	2.19	0.42
18:O:98:LEU:O	18:O:102:ILE:HG13	2.19	0.42
11:G:64:ASN:N	11:G:64:ASN:ND2	2.67	0.42
17:N:181:ASP:O	17:N:184:ILE:HG22	2.19	0.42
6:B:69:VAL:HA	6:B:70:PRO:HD3	1.84	0.42
32:3:18:GLN:OE1	32:3:73:GLU:HB3	2.19	0.42
1:0:483:C:C4	1:0:484:A:C6	3.07	0.42
1:0:945:U:H2'	1:0:946:C:C6	2.55	0.42
22:S:51:GLN:HE21	22:S:53:ASN:ND2	1.90	0.42
16:M:167:GLY:O	16:M:171:ARG:HG3	2.20	0.42
13:J:132:LEU:HA	13:J:132:LEU:HD23	1.82	0.42
19:P:13:VAL:HG11	19:P:40:VAL:HG12	2.01	0.42
1:0:2064:U:H4'	1:0:2653:A:OP1	2.19	0.42
29:Z:32:GLU:HA	29:Z:35:GLU:HG3	2.01	0.42
27:X:20:GLU:CG	27:X:21:PRO:HD2	2.49	0.42
18:O:59:VAL:HG21	18:O:111:VAL:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:T:14:ALA:HA	23:T:15:PRO:HD3	1.95	0.42
22:S:33:SER:OG	22:S:36:GLU:HG3	2.19	0.42
1:0:1257:C:H2'	1:0:1258:G:O4'	2.19	0.42
21:R:122:GLN:HB3	21:R:138:SER:HB2	2.00	0.42
40:O:7289:HOH:O	7:C:175:LYS:HE3	2.19	0.42
14:K:49:LEU:CD1	14:K:80:ILE:HD13	2.49	0.42
1:0:2506:A:O2'	1:0:2507:G:P	2.77	0.42
5:A:113:GLY:HA2	5:A:153:ARG:NH2	2.34	0.42
1:0:710:G:H5'	18:O:25:VAL:CG1	2.49	0.42
2:9:3004:G:O2'	17:N:44:ARG:NH2	2.53	0.42
5:A:109:GLU:HG2	5:A:116:GLY:H	1.85	0.42
1:0:1574:C:H6	1:0:1574:C:O5'	2.02	0.42
1:0:2793:A:H2'	1:0:2794:G:H5'	2.00	0.42
1:0:2248:C:H3'	40:O:5967:HOH:O	2.18	0.42
1:0:2713:G:O2'	1:0:2714:U:H5'	2.20	0.42
1:0:325:U:H2'	1:0:326:G:H8	1.84	0.42
16:M:15:PRO:HA	16:M:20:LEU:HD23	2.02	0.42
1:0:1342:C:O2'	1:0:1343:C:H5'	2.20	0.42
13:J:74:ARG:HH12	13:J:76:ASP:CB	2.30	0.42
25:V:1:THR:CG2	25:V:2:VAL:N	2.82	0.42
1:0:1298:U:H2'	1:0:1299:G:H8	1.85	0.42
1:0:470:U:O2'	30:1:16:HIS:CD2	2.70	0.42
2:9:3023:U:O2'	2:9:3024:U:H4'	2.19	0.42
7:C:133:ARG:HE	7:C:138:VAL:HG22	1.85	0.42
1:0:107:U:H2'	1:0:108:U:H5'	2.02	0.42
1:0:564:G:H1'	40:O:6803:HOH:O	2.18	0.42
23:T:12:ARG:NH1	40:T:3035:HOH:O	2.47	0.42
1:0:1422:U:H2'	1:0:1423:C:C6	2.55	0.42
1:0:2911:C:O2'	1:0:2912:C:H5'	2.20	0.42
17:N:36:ALA:HB1	17:N:118:ILE:HD12	2.02	0.42
18:O:38:ARG:NH1	40:O:7674:HOH:O	2.53	0.42
26:W:73:LEU:HA	26:W:73:LEU:HD12	1.83	0.42
27:X:7:GLU:HA	27:X:75:ALA:HA	2.00	0.42
33:I:118:SER:HB2	33:I:123:ASN:HB2	2.02	0.42
1:0:1205:U:C2'	1:0:1206:U:H5''	2.50	0.42
15:L:6:ARG:NH2	40:L:9444:HOH:O	2.53	0.42
5:A:51:ARG:NH1	5:A:120:ARG:O	2.53	0.42
1:0:271:C:C2	1:0:273:G:O4'	2.73	0.42
10:F:67:ALA:HB1	10:F:72:VAL:O	2.19	0.42
1:0:2821:C:H4'	6:B:116:PRO:HG3	2.01	0.42
6:B:17:LYS:O	6:B:260:HIS:CD2	2.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Q:94:GLN:O	20:Q:95:GLU:HB2	2.20	0.42
2:9:3096:C:H2'	2:9:3097:U:C6	2.55	0.42
1:0:64:G:H2'	1:0:65:C:O4'	2.20	0.42
7:C:218:VAL:N	40:C:9232:HOH:O	2.52	0.42
12:H:14:TYR:CD2	12:H:94:VAL:HB	2.54	0.42
14:K:20:CYS:HB2	14:K:29:LEU:HG	2.01	0.42
22:S:51:GLN:NE2	22:S:53:ASN:HD21	1.90	0.42
2:9:3006:C:H4'	17:N:35:VAL:HG11	2.02	0.42
1:0:2716:G:H5''	6:B:206:THR:CG2	2.45	0.42
1:0:1733:A:H4'	6:B:212:GLN:HA	2.02	0.42
29:Z:46:ARG:O	29:Z:57:CYS:HA	2.19	0.42
5:A:33:GLU:OE1	5:A:33:GLU:N	2.36	0.42
1:0:380:A:H2'	40:0:7673:HOH:O	2.19	0.42
17:N:61:ALA:CB	17:N:88:ALA:HB2	2.48	0.42
15:L:133:VAL:HB	40:L:9452:HOH:O	2.19	0.42
11:G:23:ILE:O	11:G:27:ILE:HG13	2.20	0.42
6:B:277:GLU:N	6:B:278:PRO:CD	2.82	0.42
10:F:99:THR:HG23	10:F:99:THR:O	2.19	0.42
1:0:695:C:H2'	1:0:696:C:C6	2.54	0.42
17:N:173:ASP:O	17:N:177:GLU:HB2	2.20	0.42
16:M:47:ASP:CG	16:M:48:LYS:N	2.73	0.42
12:H:51:VAL:CG1	12:H:53:GLU:O	2.67	0.42
33:I:92:PRO:HD3	40:I:1549:HOH:O	2.19	0.42
1:0:1739:G:H1'	1:0:2726:U:O4	2.20	0.42
32:3:48:ASN:ND2	32:3:50:GLY:H	2.18	0.42
1:0:2089:A:O2'	1:0:2090:G:H5'	2.20	0.42
8:D:10:PHE:CD1	8:D:11:HIS:N	2.88	0.42
1:0:2456:A:H2'	1:0:2457:U:H6	1.85	0.42
11:G:63:ARG:HB2	11:G:66:LEU:HG	2.02	0.42
27:X:80:GLU:HB3	40:X:5564:HOH:O	2.19	0.42
1:0:1940:C:H4'	40:0:7785:HOH:O	2.19	0.42
1:0:1363:G:P	7:C:76:ARG:HH22	2.43	0.42
1:0:1314:U:H2'	40:0:6383:HOH:O	2.20	0.42
1:0:2642:G:H2'	1:0:2643:G:O4'	2.20	0.42
15:L:104:ASP:HB2	40:L:9460:HOH:O	2.19	0.42
1:0:1367:A:H2'	1:0:1368:U:O4'	2.19	0.42
8:D:167:GLU:OE2	8:D:173:GLU:HB3	2.20	0.41
1:0:1473:U:O2'	1:0:1474:C:H5''	2.20	0.41
33:I:74:PRO:C	33:I:112:LYS:HZ1	2.23	0.41
32:3:69:TYR:O	32:3:77:ALA:HA	2.19	0.41
6:B:62:ARG:CA	6:B:65:MET:HE3	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:3:55:VAL:HB	32:3:56:PRO:HD2	2.02	0.41
5:A:122:SER:O	5:A:124:VAL:HG13	2.20	0.41
1:0:1311:G:O2'	1:0:1312:G:H5'	2.20	0.41
1:0:226:A:H1'	1:0:393:G:C5	2.54	0.41
1:0:629:A:H2'	1:0:630:A:O4'	2.20	0.41
7:C:21:VAL:C	7:C:23:GLU:H	2.23	0.41
1:0:1242:A:OP2	13:J:60:ARG:NH2	2.46	0.41
5:A:36:ASP:O	5:A:36:ASP:CG	2.59	0.41
25:V:45:ARG:O	25:V:48:GLU:N	2.53	0.41
1:0:1380:U:O4	1:0:2748:G:O2'	2.28	0.41
1:0:396:U:OP2	32:3:38:ARG:HD2	2.19	0.41
10:F:70:LYS:C	10:F:72:VAL:H	2.22	0.41
40:0:7470:HOH:O	6:B:264:GLU:HG3	2.19	0.41
6:B:115:VAL:HA	6:B:116:PRO:HD3	1.93	0.41
1:0:2445:U:H2'	1:0:2446:G:H8	1.85	0.41
1:0:1406:A:H4'	1:0:1407:A:H5''	2.01	0.41
1:0:2256:G:O2'	1:0:2257:G:H5'	2.21	0.41
40:0:7460:HOH:O	20:Q:9:GLY:HA2	2.20	0.41
32:3:62:THR:HB	40:3:9487:HOH:O	2.20	0.41
1:0:1902:G:H2'	1:0:1903:U:O4'	2.20	0.41
5:A:75:GLY:HA2	29:Z:64:PHE:HA	2.02	0.41
8:D:173:GLU:O	8:D:174:VAL:C	2.59	0.41
8:D:163:VAL:HA	40:D:6326:HOH:O	2.20	0.41
1:0:553:G:O4'	1:0:1325:G:H5'	2.20	0.41
19:P:16:VAL:CG1	19:P:17:GLY:N	2.83	0.41
12:H:169:GLY:HA3	40:H:9557:HOH:O	2.20	0.41
26:W:38:THR:HG22	26:W:39:ASP:H	1.85	0.41
8:D:170:TYR:CD1	8:D:170:TYR:N	2.89	0.41
6:B:171:VAL:HG23	6:B:172:SER:N	2.35	0.41
6:B:56:ASP:OD1	6:B:322:ARG:HB3	2.21	0.41
33:I:80:LYS:HD3	33:I:86:GLU:O	2.20	0.41
1:0:1826:C:O2'	1:0:1827:G:H5'	2.20	0.41
1:0:195:C:H2'	1:0:196:G:H5'	2.01	0.41
16:M:81:ARG:HG2	16:M:85:ARG:O	2.19	0.41
28:Y:154:ARG:HH11	28:Y:154:ARG:CG	2.34	0.41
1:0:1174:A:C6	1:0:1201:C:H4'	2.55	0.41
24:U:47:ARG:HG2	24:U:54:THR:HG21	2.03	0.41
20:Q:28:ARG:HG2	40:Q:4350:HOH:O	2.20	0.41
1:0:1451:C:H5'	1:0:1505:U:C4	2.56	0.41
18:O:14:LEU:HG	18:O:102:ILE:HD11	2.03	0.41
1:0:2362:A:H2'	1:0:2363:G:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2015:A:H2'	1:0:2016:U:O4'	2.19	0.41
1:0:1086:A:N6	26:W:11:VAL:HG11	2.35	0.41
1:0:1120:U:H5'	1:0:1121:G:OP2	2.20	0.41
19:P:89:ASN:HB3	19:P:92:GLU:HB2	2.01	0.41
21:R:96:VAL:O	21:R:99:ALA:HB3	2.20	0.41
26:W:5:VAL:O	26:W:52:VAL:CG2	2.68	0.41
1:0:1181:A:H2'	1:0:1182:C:H5'	2.03	0.41
1:0:1183:C:H5	1:0:1192:A:OP1	2.04	0.41
5:A:29:HIS:CD2	5:A:153:ARG:HH12	2.37	0.41
15:L:145:LEU:C	15:L:147:GLU:H	2.23	0.41
5:A:53:ALA:HB3	40:A:9591:HOH:O	2.20	0.41
15:L:73:VAL:HG23	15:L:74:THR:N	2.32	0.41
1:0:1730:G:H5''	1:0:1731:C:C6	2.55	0.41
1:0:20:G:H5''	1:0:510:U:O4	2.21	0.41
1:0:790:A:H1'	1:0:1710:A:O2'	2.21	0.41
1:0:162:C:H2'	1:0:163:U:H5'	2.02	0.41
26:W:21:LEU:HD22	26:W:26:ILE:HD11	2.02	0.41
33:I:110:GLU:HA	33:I:113:HIS:CD2	2.55	0.41
5:A:36:ASP:HA	5:A:83:GLY:HA3	2.02	0.41
6:B:305:ASP:O	6:B:306:LYS:CB	2.67	0.41
1:0:407:A:H8	40:0:5010:HOH:O	2.03	0.41
14:K:41:LYS:O	14:K:42:ASN:HB2	2.20	0.41
6:B:294:TYR:CD1	6:B:294:TYR:C	2.93	0.41
1:0:1979:G:O2'	1:0:1980:U:OP1	2.30	0.41
6:B:81:ALA:HB1	6:B:142:LEU:HD13	2.03	0.41
1:0:2324:G:N2	1:0:2377:U:H1'	2.36	0.41
14:K:2:GLU:O	14:K:3:ALA:C	2.58	0.41
17:N:170:GLU:O	17:N:174:GLU:HG3	2.21	0.41
1:0:1524:U:HO2'	1:0:1525:G:P	2.44	0.41
5:A:6:GLY:HA3	40:A:9557:HOH:O	2.20	0.41
16:M:164:THR:CG2	16:M:166:ALA:H	2.32	0.41
5:A:95:PRO:HA	5:A:153:ARG:HA	2.03	0.41
2:9:3039:U:O2'	2:9:3042:C:H5	2.03	0.41
15:L:66:VAL:HG23	15:L:67:ARG:N	2.35	0.41
29:Z:30:GLU:HG2	29:Z:33:MET:CE	2.51	0.41
1:0:447:A:OP1	23:T:1:SER:HB2	2.21	0.41
30:1:8:GLN:HE22	30:1:11:LYS:HZ2	1.65	0.41
1:0:440:C:H2'	1:0:441:A:C8	2.54	0.41
15:L:35:ARG:HD3	15:L:35:ARG:C	2.41	0.41
18:O:45:LEU:CD1	18:O:88:LYS:HD2	2.51	0.41
1:0:2351:C:H2'	1:0:2352:G:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1535:G:H2'	1:0:1536:C:C6	2.56	0.41
17:N:108:SER:HA	17:N:109:PRO:HD3	1.80	0.41
5:A:30:ARG:HB3	5:A:30:ARG:HE	1.64	0.41
40:0:4333:HOH:O	23:T:9:LYS:HD2	2.20	0.41
26:W:5:VAL:O	26:W:52:VAL:HG23	2.20	0.41
9:E:69:ILE:HA	9:E:72:MET:HE3	2.01	0.41
15:L:94:ARG:NH1	15:L:143:THR:HG21	2.36	0.41
40:0:3646:HOH:O	19:P:91:LYS:HA	2.21	0.41
6:B:18:ARG:HE	6:B:256:GLN:NE2	2.19	0.41
1:0:1427:A:N6	1:0:1440:U:H1'	2.33	0.41
31:2:39:ARG:HG2	40:2:3143:HOH:O	2.21	0.41
1:0:1594:C:O2'	1:0:1607:A:H4'	2.21	0.41
16:M:76:ARG:HG3	16:M:88:VAL:HG21	2.03	0.41
29:Z:39:CYS:HA	29:Z:40:PRO:HD3	1.97	0.41
1:0:1849:G:H1'	1:0:2011:A:N1	2.35	0.41
15:L:124:ASP:OD1	15:L:149:ARG:NH2	2.54	0.41
1:0:2335:C:H2'	1:0:2336:G:C8	2.56	0.41
25:V:43:PRO:O	25:V:46:ILE:HG22	2.19	0.41
1:0:1025:C:H5'	26:W:23:MET:O	2.21	0.41
7:C:61:PHE:HB3	40:C:9251:HOH:O	2.20	0.41
21:R:33:ARG:NH1	40:R:9452:HOH:O	2.51	0.41
1:0:1076:G:C2	1:0:1084:C:C2	3.09	0.41
13:J:143:LYS:HA	13:J:145:TRP:CZ3	2.55	0.41
31:2:11:LEU:HA	31:2:11:LEU:HD23	1.91	0.41
10:F:12:LEU:HD23	10:F:12:LEU:O	2.21	0.41
8:D:23:VAL:O	8:D:23:VAL:HG23	2.21	0.41
1:0:1882:C:OP1	5:A:192:VAL:HG23	2.21	0.41
29:Z:36:ASP:HB3	29:Z:45:ASP:O	2.21	0.41
1:0:875:A:C2	5:A:194:MET:SD	3.14	0.41
14:K:107:THR:HG22	14:K:108:GLU:CG	2.44	0.41
14:K:118:ALA:O	14:K:119:GLN:C	2.59	0.41
14:K:98:VAL:HG11	14:K:102:GLU:HA	1.99	0.41
26:W:54:PHE:CZ	26:W:140:LYS:HB2	2.55	0.41
33:I:92:PRO:C	33:I:94:GLU:N	2.72	0.41
1:0:1181:A:H4'	33:I:92:PRO:HG2	2.03	0.41
9:E:84:MET:HB2	9:E:131:LEU:HB2	2.03	0.41
1:0:2748:G:H4'	1:0:2749:U:H5'	2.02	0.41
6:B:312:ARG:HG2	6:B:313:PRO:N	2.34	0.41
1:0:271:C:H41	1:0:378:A:H2	1.68	0.41
6:B:41:PHE:CD1	6:B:79:MET:CE	3.04	0.41
6:B:27:ASN:H	6:B:27:ASN:HD22	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:24:LEU:HD13	20:Q:26:PRO:HB3	2.02	0.41
1:0:2819:C:O4'	6:B:96:PRO:HB2	2.21	0.41
1:0:2820:A:H2'	1:0:2821:C:C6	2.56	0.41
5:A:65:ARG:NH1	5:A:65:ARG:HG2	2.36	0.41
5:A:66:ARG:HH11	5:A:66:ARG:CB	2.33	0.41
27:X:30:MET:CE	27:X:58:ALA:HB3	2.50	0.41
33:I:93:GLN:HA	33:I:96:PHE:CE2	2.54	0.41
1:0:284:C:H4'	1:0:285:A:H8	1.86	0.41
1:0:737:A:H3'	1:0:737:A:C8	2.56	0.41
1:0:392:U:H5''	16:M:193:LYS:HB3	2.01	0.41
23:T:81:LYS:HD2	23:T:87:VAL:HG11	2.03	0.41
1:0:2336:G:H1'	40:D:5675:HOH:O	2.20	0.41
19:P:134:VAL:O	19:P:137:LEU:HB3	2.21	0.41
27:X:45:GLU:HG3	40:X:6178:HOH:O	2.21	0.41
40:0:3421:HOH:O	6:B:252:PRO:HD3	2.21	0.41
10:F:79:GLN:HB2	10:F:82:ASP:OD2	2.21	0.41
1:0:1821:A:O2'	1:0:1822:A:H5'	2.21	0.41
1:0:1414:A:H2'	1:0:1415:G:O4'	2.20	0.41
17:N:33:ARG:NH1	17:N:103:ASP:OD2	2.47	0.41
1:0:1834:C:H2'	1:0:1840:A:N6	2.36	0.41
26:W:4:LEU:HD23	26:W:54:PHE:HB3	2.03	0.41
2:9:3014:G:H2'	2:9:3015:C:H5'	2.03	0.41
24:U:17:THR:HG21	40:U:3194:HOH:O	2.21	0.41
30:1:28:HIS:O	30:1:32:LYS:N	2.49	0.41
31:2:20:ARG:HG3	31:2:21:VAL:H	1.86	0.41
15:L:120:LEU:HD12	15:L:133:VAL:HG21	2.02	0.41
18:O:14:LEU:HD23	18:O:102:ILE:HD11	2.02	0.41
1:0:2828:G:H2'	1:0:2829:G:O4'	2.21	0.41
18:O:60:VAL:C	18:O:62:GLY:H	2.24	0.41
28:Y:178:HIS:CG	28:Y:179:PRO:HD2	2.56	0.41
1:0:791:A:H2'	1:0:792:G:O4'	2.21	0.41
21:R:68:HIS:CD2	21:R:76:ASP:HB2	2.56	0.41
1:0:1453:G:H2'	1:0:1454:U:O4'	2.21	0.41
1:0:2767:C:OP1	6:B:318:ASN:ND2	2.54	0.41
7:C:140:VAL:HG12	7:C:141:SER:N	2.36	0.40
7:C:72:LYS:HG2	7:C:77:ALA:HA	2.02	0.40
1:0:2720:C:O2	14:K:87:ARG:NH2	2.54	0.40
25:V:1:THR:OG1	25:V:2:VAL:N	2.53	0.40
5:A:135:VAL:HG13	5:A:135:VAL:O	2.21	0.40
40:0:9644:HOH:O	15:L:30:ARG:HD2	2.20	0.40
9:E:7:ILE:HD11	9:E:11:VAL:C	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Y:186:ARG:HG2	28:Y:186:ARG:NH1	2.36	0.40
1:0:556:C:H2'	1:0:557:C:H6	1.86	0.40
1:0:185:G:O3'	1:0:186:A:H4'	2.21	0.40
1:0:1816:C:H2'	1:0:1817:U:O4'	2.21	0.40
1:0:1724:U:H5''	40:0:4311:HOH:O	2.19	0.40
12:H:114:ARG:O	12:H:115:ALA:C	2.60	0.40
1:0:932:U:H2'	1:0:933:C:C6	2.56	0.40
8:D:23:VAL:CG2	8:D:73:VAL:HB	2.51	0.40
17:N:37:ARG:HA	17:N:37:ARG:HD3	1.69	0.40
1:0:1119:G:C6	1:0:1244:U:C5	3.09	0.40
26:W:4:LEU:CD1	26:W:24:LEU:HD13	2.51	0.40
5:A:38:ILE:HA	5:A:38:ILE:HD13	1.92	0.40
25:V:1:THR:O	25:V:2:VAL:C	2.59	0.40
1:0:2748:G:C5'	40:0:7972:HOH:O	2.69	0.40
10:F:72:VAL:HA	10:F:73:PRO:HD3	1.92	0.40
1:0:2361:A:H2'	1:0:2362:A:O4'	2.21	0.40
6:B:278:PRO:HD3	6:B:294:TYR:CE2	2.56	0.40
1:0:2329:C:O2'	1:0:2330:U:H5'	2.21	0.40
20:Q:43:ILE:HG13	20:Q:52:PHE:CZ	2.56	0.40
8:D:21:VAL:HA	8:D:131:THR:O	2.21	0.40
8:D:67:ASP:O	8:D:69:ILE:HG13	2.21	0.40
5:A:81:GLN:H	5:A:92:ASN:CG	2.24	0.40
28:Y:96:GLU:O	28:Y:235:GLU:HA	2.21	0.40
1:0:1589:G:N2	1:0:1605:G:H1'	2.35	0.40
5:A:85:SER:O	5:A:86:ALA:C	2.60	0.40
1:0:120:A:H2'	1:0:120:A:N3	2.37	0.40
28:Y:187:VAL:CG1	28:Y:205:ILE:HG12	2.51	0.40
28:Y:115:ARG:NE	40:Y:9353:HOH:O	2.55	0.40
25:V:8:ILE:CG2	25:V:59:ILE:HG13	2.51	0.40
1:0:2824:C:C5'	1:0:2825:C:H5'	2.51	0.40
5:A:43:VAL:O	5:A:44:ASP:HB2	2.21	0.40
1:0:2101:A:H5'	7:C:63:SER:HB3	2.04	0.40
25:V:42:ASN:HB3	40:V:7247:HOH:O	2.21	0.40
6:B:279:THR:HG23	6:B:280:VAL:N	2.35	0.40
6:B:81:ALA:O	6:B:186:GLY:HA3	2.22	0.40
17:N:103:ASP:OD1	17:N:103:ASP:C	2.60	0.40
12:H:78:GLY:C	12:H:80:GLU:H	2.25	0.40
8:D:91:ALA:HB2	8:D:106:PHE:CD2	2.56	0.40
7:C:84:VAL:HG12	7:C:85:LYS:HG2	2.04	0.40
1:0:1829:A:C8	1:0:1885:A:C8	3.09	0.40
23:T:18:GLU:O	23:T:21:LYS:HG2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:60:SER:HA	6:B:61:PRO:HD3	1.92	0.40
1:0:2070:G:H2'	1:0:2072:G:OP1	2.21	0.40
1:0:1299:G:N2	40:0:5226:HOH:O	2.53	0.40
40:0:7989:HOH:O	32:3:60:LYS:HG3	2.21	0.40
1:0:1462:C:H2'	1:0:1463:A:H8	1.85	0.40
1:0:1235:G:C1'	13:J:63:ILE:HG23	2.51	0.40
18:O:59:VAL:HG23	18:O:111:VAL:HG23	2.02	0.40
1:0:294:C:H2'	1:0:295:C:O4'	2.21	0.40
15:L:65:ASP:CG	15:L:111:ALA:HB3	2.42	0.40
2:9:3008:G:OP1	17:N:23:ARG:NH1	2.51	0.40
1:0:1881:A:OP1	5:A:199:HIS:HE1	2.04	0.40
13:J:103:VAL:HG12	40:J:5907:HOH:O	2.21	0.40
30:1:25:LYS:CG	31:2:49:GLU:H	2.35	0.40
15:L:67:ARG:HB2	15:L:112:GLY:HA3	2.03	0.40
18:O:23:GLY:C	40:O:3062:HOH:O	2.59	0.40
7:C:57:PRO:HG2	7:C:73:LEU:CD1	2.51	0.40
1:0:2819:C:H2'	1:0:2820:A:C8	2.56	0.40
11:G:16:LYS:O	11:G:20:VAL:HG23	2.22	0.40
13:J:80:LYS:HE2	13:J:98:PHE:CZ	2.56	0.40
1:0:1626:A:H2'	1:0:1627:G:C5'	2.52	0.40
32:3:30:GLN:HE21	32:3:30:GLN:HB3	1.61	0.40
2:9:3002:U:OP2	2:9:3003:A:H5'	2.22	0.40
2:9:3091:C:H2'	2:9:3092:G:O4'	2.22	0.40
6:B:24:PRO:CG	6:B:204:GLY:HA2	2.52	0.40
1:0:1007:A:H2'	12:H:19:TYR:CZ	2.56	0.40
1:0:565:A:OP2	1:0:592:G:N1	2.49	0.40
1:0:423:A:O2'	1:0:424:C:H5'	2.21	0.40
1:0:1081:A:H5''	40:0:3742:HOH:O	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	
5	A	235/240 (98%)	207 (88%)	25 (11%)	3 (1%)	15	21
6	B	335/338 (99%)	309 (92%)	21 (6%)	5 (2%)	13	17
7	C	244/246 (99%)	223 (91%)	19 (8%)	2 (1%)	24	35
8	D	134/177 (76%)	104 (78%)	19 (14%)	11 (8%)	1	0
9	E	170/178 (96%)	162 (95%)	8 (5%)	0	100	100
10	F	117/120 (98%)	103 (88%)	11 (9%)	3 (3%)	7	6
11	G	25/348 (7%)	25 (100%)	0	0	100	100
12	H	156/171 (91%)	136 (87%)	16 (10%)	4 (3%)	7	6
13	J	140/145 (97%)	130 (93%)	6 (4%)	4 (3%)	6	5
14	K	130/132 (98%)	120 (92%)	9 (7%)	1 (1%)	24	35
15	L	141/165 (86%)	118 (84%)	21 (15%)	2 (1%)	14	19
16	M	192/194 (99%)	178 (93%)	13 (7%)	1 (0%)	34	48
17	N	184/187 (98%)	161 (88%)	14 (8%)	9 (5%)	3	1
18	O	113/116 (97%)	107 (95%)	6 (5%)	0	100	100
19	P	141/149 (95%)	137 (97%)	4 (3%)	0	100	100
20	Q	93/96 (97%)	87 (94%)	6 (6%)	0	100	100
21	R	148/155 (96%)	142 (96%)	6 (4%)	0	100	100
22	S	79/85 (93%)	73 (92%)	6 (8%)	0	100	100
23	T	117/120 (98%)	107 (92%)	8 (7%)	2 (2%)	11	14
24	U	51/66 (77%)	47 (92%)	4 (8%)	0	100	100
25	V	63/71 (89%)	59 (94%)	1 (2%)	3 (5%)	3	1
26	W	152/154 (99%)	148 (97%)	4 (3%)	0	100	100
27	X	80/92 (87%)	72 (90%)	8 (10%)	0	100	100
28	Y	140/241 (58%)	138 (99%)	2 (1%)	0	100	100
29	Z	71/83 (86%)	58 (82%)	10 (14%)	3 (4%)	3	2
30	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
31	2	42/50 (84%)	41 (98%)	0	1 (2%)	7	7
32	3	90/92 (98%)	87 (97%)	2 (2%)	1 (1%)	17	25
33	I	68/162 (42%)	54 (79%)	12 (18%)	2 (3%)	6	5
All	All	3705/4430 (84%)	3385 (91%)	263 (7%)	57 (2%)	13	17

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	B	169	GLY
8	D	60	GLU
8	D	137	PRO
10	F	101	ALA
12	H	166	SER
13	J	143	LYS
15	L	80	ASP
17	N	154	LEU
17	N	184	ILE
29	Z	81	ARG
5	A	37	VAL
6	B	34	GLY
8	D	27	ILE
8	D	61	PHE
8	D	65	GLU
12	H	168	ALA
15	L	143	THR
16	M	83	SER
23	T	53	GLY
25	V	43	PRO
29	Z	20	ARG
31	2	37	HIS
33	I	129	VAL
5	A	86	ALA
6	B	185	GLY
8	D	28	GLY
8	D	56	ARG
8	D	164	ALA
10	F	71	GLY
17	N	183	ASP
23	T	46	ASP
5	A	34	ASP
7	C	8	LEU
7	C	58	ALA
8	D	171	ASP
12	H	16	ARG
12	H	81	GLY
13	J	5	GLU
13	J	7	ASP
17	N	65	ASP
17	N	155	GLU
17	N	162	ASP
8	D	77	ASP

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Mol	Chain	Res	Type
10	F	100	ASP
14	K	126	SER
17	N	164	ASP
17	N	167	ASP
29	Z	42	CYS
32	3	56	PRO
6	B	2	GLN
8	D	16	PRO
13	J	65	ASN
17	N	68	GLU
25	V	40	PRO
25	V	2	VAL
6	B	181	ILE
33	I	73	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	A	179/182 (98%)	165 (92%)	14 (8%)	16	24
6	B	282/283 (100%)	267 (95%)	15 (5%)	28	44
7	C	193/193 (100%)	173 (90%)	20 (10%)	9	12
8	D	117/148 (79%)	112 (96%)	5 (4%)	35	55
9	E	152/156 (97%)	146 (96%)	6 (4%)	39	59
10	F	93/94 (99%)	91 (98%)	2 (2%)	60	79
11	G	27/283 (10%)	27 (100%)	0	100	100
12	H	132/138 (96%)	127 (96%)	5 (4%)	40	60
13	J	118/121 (98%)	108 (92%)	10 (8%)	13	20
14	K	106/106 (100%)	101 (95%)	5 (5%)	32	50
15	L	113/127 (89%)	110 (97%)	3 (3%)	52	73
16	M	158/158 (100%)	153 (97%)	5 (3%)	46	68
17	N	149/150 (99%)	142 (95%)	7 (5%)	32	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	O	93/94 (99%)	92 (99%)	1 (1%)	80	92
19	P	113/117 (97%)	110 (97%)	3 (3%)	52	73
20	Q	79/80 (99%)	75 (95%)	4 (5%)	29	46
21	R	117/122 (96%)	114 (97%)	3 (3%)	54	74
22	S	71/74 (96%)	71 (100%)	0	100	100
23	T	105/106 (99%)	101 (96%)	4 (4%)	40	60
24	U	44/52 (85%)	44 (100%)	0	100	100
25	V	51/57 (90%)	50 (98%)	1 (2%)	63	81
26	W	130/130 (100%)	124 (95%)	6 (5%)	33	51
27	X	66/74 (89%)	63 (96%)	3 (4%)	34	52
28	Y	120/196 (61%)	109 (91%)	11 (9%)	11	16
29	Z	60/68 (88%)	59 (98%)	1 (2%)	68	85
30	1	46/47 (98%)	45 (98%)	1 (2%)	60	79
31	2	42/46 (91%)	41 (98%)	1 (2%)	57	76
32	3	79/79 (100%)	77 (98%)	2 (2%)	55	76
33	I	58/130 (45%)	58 (100%)	0	100	100
All	All	3093/3611 (86%)	2955 (96%)	138 (4%)	34	52

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	A	3	ARG
5	A	26	ASP
5	A	33	GLU
5	A	36	ASP
5	A	62	ASP
5	A	78	ASP
5	A	94	LEU
5	A	120	ARG
5	A	131	HIS
5	A	151	GLN
5	A	165	THR
5	A	179	MET
5	A	206	ARG
5	A	217	ARG
6	B	11	LEU

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Mol	Chain	Res	Type
6	B	27	ASN
6	B	82	VAL
6	B	84	LEU
6	B	98	THR
6	B	103	ASP
6	B	113	LEU
6	B	149	ASP
6	B	162	MET
6	B	190	MET
6	B	254	GLN
6	B	277	GLU
6	B	279	THR
6	B	307	ARG
6	B	312	ARG
7	C	2	GLN
7	C	16	VAL
7	C	27	ARG
7	C	67	GLN
7	C	76	ARG
7	C	78	ARG
7	C	91	PRO
7	C	94	THR
7	C	101	ASP
7	C	115	LEU
7	C	136	VAL
7	C	162	VAL
7	C	187	ARG
7	C	214	THR
7	C	222	ASP
7	C	223	LEU
7	C	234	VAL
7	C	236	THR
7	C	240	LEU
7	C	243	VAL
8	D	24	HIS
8	D	61	PHE
8	D	100	ASP
8	D	133	ASN
8	D	137	PRO
9	E	7	ILE
9	E	102	VAL
9	E	108	LEU

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Mol	Chain	Res	Type
9	E	155	ASN
9	E	156	ASP
9	E	164	ASP
10	F	12	LEU
10	F	46	GLU
12	H	18	GLU
12	H	84	LYS
12	H	88	ARG
12	H	154	TYR
12	H	159	PRO
13	J	7	ASP
13	J	45	VAL
13	J	46	ILE
13	J	52	GLN
13	J	70	PHE
13	J	74	ARG
13	J	79	PHE
13	J	107	ASN
13	J	127	ILE
13	J	131	THR
14	K	4	LEU
14	K	10	GLN
14	K	56	SER
14	K	84	ASP
14	K	100	GLU
15	L	35	ARG
15	L	43	HIS
15	L	140	VAL
16	M	46	LEU
16	M	68	ARG
16	M	93	ARG
16	M	99	ARG
16	M	116	ASN
17	N	17	ARG
17	N	23	ARG
17	N	26	LEU
17	N	49	THR
17	N	65	ASP
17	N	139	TRP
17	N	152	GLU
18	O	111	VAL
19	P	52	LYS

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Mol	Chain	Res	Type
19	P	98	ILE
19	P	117	SER
20	Q	11	ARG
20	Q	16	ASN
20	Q	57	ASP
20	Q	95	GLU
21	R	13	THR
21	R	132	ARG
21	R	143	VAL
23	T	5	ASP
23	T	39	ASN
23	T	80	GLU
23	T	89	ARG
25	V	65	ASP
26	W	26	ILE
26	W	35	VAL
26	W	78	ASP
26	W	122	ARG
26	W	142	ASP
26	W	146	ILE
27	X	72	VAL
27	X	79	GLU
27	X	82	GLU
28	Y	103	THR
28	Y	141	THR
28	Y	144	ARG
28	Y	154	ARG
28	Y	163	THR
28	Y	174	VAL
28	Y	187	VAL
28	Y	189	ASN
28	Y	200	THR
28	Y	231	PRO
28	Y	235	GLU
29	Z	44	GLU
30	1	47	ASP
31	2	18	ASN
32	3	11	CYS
32	3	65	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
5	A	29	HIS
5	A	199	HIS
6	B	27	ASN
6	B	145	HIS
6	B	221	GLN
6	B	238	ASN
6	B	256	GLN
6	B	260	HIS
6	B	320	GLN
6	B	332	ASN
7	C	2	GLN
7	C	39	GLN
7	C	129	HIS
8	D	47	GLN
8	D	103	ASN
8	D	133	ASN
9	E	106	ASN
9	E	143	GLN
11	G	64	ASN
12	H	56	GLN
12	H	59	HIS
12	H	70	ASN
12	H	170	ASN
13	J	52	GLN
13	J	107	ASN
14	K	10	GLN
15	L	18	HIS
15	L	41	HIS
15	L	42	ASN
16	M	24	GLN
16	M	77	HIS
16	M	170	ASN
17	N	93	GLN
17	N	107	ASN
17	N	153	GLN
18	O	100	GLN
19	P	50	GLN
19	P	66	GLN
19	P	73	HIS
19	P	88	GLN
19	P	89	ASN
19	P	118	GLN
20	Q	16	ASN

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Mol	Chain	Res	Type
20	Q	40	HIS
21	R	61	GLN
21	R	94	ASN
21	R	98	ASN
21	R	113	HIS
21	R	117	HIS
22	S	44	GLN
22	S	53	ASN
22	S	55	GLN
23	T	37	GLN
23	T	39	ASN
24	U	39	ASN
24	U	48	ASN
25	V	60	GLN
26	W	2	HIS
26	W	28	HIS
26	W	110	GLN
26	W	119	HIS
26	W	125	HIS
26	W	141	HIS
27	X	22	ASN
27	X	23	HIS
28	Y	119	GLN
28	Y	134	HIS
28	Y	149	GLN
28	Y	189	ASN
29	Z	41	ASN
30	1	8	GLN
30	1	16	HIS
30	1	28	HIS
31	2	16	ASN
31	2	18	ASN
31	2	41	HIS
31	2	45	ASN
32	3	30	GLN
32	3	48	ASN
33	I	113	HIS

5.3.3 RNA ⓘ

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	233 (8%)	32 (1%)
2	9	121/122 (99%)	15 (12%)	1 (0%)
3	4	1/4 (25%)	0	0
4	5	2/6 (33%)	1 (50%)	0
All	All	2869/3054 (93%)	249 (8%)	33 (1%)

All (249) 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	186	A
1	0	191	A
1	0	192	A
1	0	219	G
1	0	237	G
1	0	271	C
1	0	272	A
1	0	273	G
1	0	283	U
1	0	284	C
1	0	308	U
1	0	309	C
1	0	318	C
1	0	336	G
1	0	337	A
1	0	358	G
1	0	381	G
1	0	397	A

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Mol	Chain	Res	Type
1	0	417	G
1	0	457	U
1	0	461	C
1	0	473	A
1	0	487	G
1	0	497	A
1	0	498	A
1	0	510	U
1	0	511	A
1	0	514	G
1	0	537	G
1	0	538	C
1	0	539	G
1	0	542	A
1	0	545	G
1	0	553	G
1	0	559	U
1	0	581	G
1	0	588	G
1	0	604	G
1	0	620	A
1	0	632	A
1	0	644	G
1	0	660	A
1	0	688	A
1	0	698	A
1	0	701	U
1	0	702	G
1	0	759	C
1	0	777	U
1	0	809	G
1	0	821	U
1	0	835	U
1	0	840	U
1	0	857	A
1	0	858	U
1	0	868	G
1	0	869	G
1	0	871	G
1	0	875	A
1	0	877	G
1	0	878	G

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Mol	Chain	Res	Type
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	1087	G
1	0	1088	A
1	0	1100	G
1	0	1109	U
1	0	1110	G
1	0	1119	G
1	0	1130	U
1	0	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	1208	C
1	0	1216	G
1	0	1237	U
1	0	1238	C
1	0	1239	G
1	0	1279	U
1	0	1289	C
1	0	1342	C
1	0	1353	C
1	0	1360	C
1	0	1377	C

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Mol	Chain	Res	Type
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	1528	A
1	0	1592	G
1	0	1625	U
1	0	1626	A
1	0	1633	C
1	0	1634	G
1	0	1656	A
1	0	1667	A
1	0	1682	A
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1701	A
1	0	1722	U
1	0	1723	G
1	0	1725	C
1	0	1731	C
1	0	1752	G
1	0	1778	A
1	0	1798	C
1	0	1819	G
1	0	1820	G
1	0	1829	A
1	0	1856	C
1	0	1879	U
1	0	1919	A
1	0	1942	A
1	0	1971	G
1	0	1973	A
1	0	1979	G
1	0	1980	U
1	0	1996	U
1	0	2006	C
1	0	2008	U

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Mol	Chain	Res	Type
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	2110	G
1	0	2238	A
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	2467	A
1	0	2469	A
1	0	2476	C
1	0	2480	G
1	0	2483	A
1	0	2507	G
1	0	2509	A
1	0	2511	A
1	0	2533	C
1	0	2537	G
1	0	2541	U
1	0	2542	C
1	0	2553	A
1	0	2564	G
1	0	2589	U

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Mol	Chain	Res	Type
1	0	2601	A
1	0	2602	G
1	0	2608	C
1	0	2613	G
1	0	2634	G
1	0	2637	A
1	0	2644	C
1	0	2645	U
1	0	2648	U
1	0	2649	A
1	0	2664	A
1	0	2681	A
1	0	2682	C
1	0	2726	U
1	0	2747	C
1	0	2748	G
1	0	2749	U
1	0	2750	G
1	0	2762	C
1	0	2768	A
1	0	2783	A
1	0	2786	G
1	0	2800	A
1	0	2811	A
1	0	2812	A
1	0	2825	C
1	0	2852	A
1	0	2853	U
1	0	2876	G
1	0	2890	A
1	0	2896	A
1	0	2903	C
1	0	2914	A
2	9	3002	U
2	9	3007	G
2	9	3014	G
2	9	3022	G
2	9	3023	U
2	9	3024	U
2	9	3025	G
2	9	3041	C
2	9	3043	G

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Mol	Chain	Res	Type
2	9	3044	A
2	9	3057	A
2	9	3066	G
2	9	3077	A
2	9	3114	G
2	9	3122	C
4	5	76	A

All (33) 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	1232	A
1	0	1237	U
1	0	1246	A
1	0	1352	A
1	0	1506	U
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1730	G
1	0	1942	A
1	0	1979	G
1	0	2011	A
1	0	2313	C
1	0	2467	A
1	0	2536	C
1	0	2541	U
1	0	2637	A
1	0	2649	A
1	0	2718	C
1	0	2726	U
1	0	2761	A

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Mol	Chain	Res	Type
1	0	2852	A
2	9	3065	A

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

7 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	1.05	2 (16%)	19,31,34	3.08	2 (10%)
1	OMG	0	2588	1,3	17,26,27	1.08	2 (11%)	21,38,41	2.53	3 (14%)
1	UR3	0	2619	1,38	12,22,23	0.98	0	16,32,35	0.74	0
1	PSU	0	2621	1	13,21,22	1.64	2 (15%)	18,30,33	6.14	3 (16%)
1	1MA	0	628	1,36	14,25,26	0.99	1 (7%)	15,37,40	1.17	1 (6%)
3	PPU	4	76	1,3	16,26,41	0.72	0	15,38,60	1.16	1 (6%)
3	HFA	4	77	3	11,11,12	0.84	1 (9%)	13,13,15	0.75	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	0	2587	1	-	0/5/27/28	0/2/2/2
1	OMG	0	2588	1,3	-	0/5/27/28	0/3/3/3
1	UR3	0	2619	1,38	-	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	1,36	-	0/3/25/26	0/3/3/3
3	PPU	4	76	1,3	-	0/7/29/44	0/3/3/4
3	HFA	4	77	3	-	0/4/6/8	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C5-C1'	-4.68	1.48	1.52
1	0	2587	OMU	C6-C5	-2.10	1.33	1.38
1	0	2588	OMG	C8-N7	-2.04	1.30	1.34
3	4	77	HFA	OA-CA	2.05	1.48	1.43
1	0	2587	OMU	C4-N3	2.53	1.37	1.33
1	0	628	1MA	C6-N6	2.77	1.34	1.29
1	0	2621	PSU	C4-N3	3.03	1.38	1.33
1	0	2588	OMG	C6-N1	3.17	1.39	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	N1-C2-N3	-21.59	114.56	128.33
1	0	2588	OMG	C5-C6-N1	-8.71	111.69	123.59
1	0	628	1MA	C2-N3-C4	-3.60	110.83	116.40
1	0	2587	OMU	C5-C4-N3	-3.24	114.82	123.12
1	0	2588	OMG	N3-C2-N1	-2.32	123.91	127.44
3	4	77	HFA	CB-CA-C	-2.06	107.83	111.70
1	0	2621	PSU	C6-N1-C2	2.69	119.80	115.47
3	4	76	PPU	C2-N1-C6	3.50	118.88	111.43
1	0	2588	OMG	C6-N1-C2	6.63	125.14	115.94
1	0	2587	OMU	C4-N3-C2	12.79	126.81	114.14
1	0	2621	PSU	C4-N3-C2	13.88	127.24	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 312 ligands modelled in this entry, 312 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	0	2749/2922 (94%)	-0.44	67 (2%) 62 61	24, 49, 93, 153	0
2	9	122/122 (100%)	-0.07	6 (4%) 33 34	41, 69, 93, 152	0
3	4	2/4 (50%)	-0.89	0 100 100	43, 43, 43, 52	0
4	5	4/6 (66%)	0.09	1 (25%) 1 1	55, 57, 58, 66	0
5	A	237/240 (98%)	0.40	14 (5%) 26 26	31, 54, 86, 106	0
6	B	337/338 (99%)	0.19	12 (3%) 46 47	31, 55, 79, 93	0
7	C	246/246 (100%)	-0.01	3 (1%) 81 81	27, 49, 70, 87	0
8	D	140/177 (79%)	1.82	47 (33%) 0 0	64, 96, 125, 132	0
9	E	172/178 (96%)	0.82	25 (14%) 3 3	44, 66, 86, 92	0
10	F	119/120 (99%)	1.09	31 (26%) 1 1	49, 74, 100, 112	0
11	G	29/348 (8%)	2.52	19 (65%) 0 0	74, 92, 103, 105	0
12	H	160/171 (93%)	0.68	17 (10%) 8 8	47, 65, 96, 103	0
13	J	142/145 (97%)	0.05	4 (2%) 56 55	37, 52, 72, 93	0
14	K	132/132 (100%)	-0.10	2 (1%) 76 75	37, 48, 71, 84	0
15	L	145/165 (87%)	0.68	17 (11%) 6 6	29, 69, 112, 121	0
16	M	194/194 (100%)	0.59	22 (11%) 7 7	37, 48, 85, 93	0
17	N	186/187 (99%)	0.98	35 (18%) 2 1	49, 68, 112, 119	0
18	O	115/116 (99%)	0.21	3 (2%) 59 58	40, 59, 73, 81	0
19	P	143/149 (95%)	0.30	4 (2%) 56 55	39, 55, 66, 79	0
20	Q	95/96 (98%)	0.11	5 (5%) 30 30	42, 52, 67, 76	0
21	R	150/155 (96%)	-0.10	0 100 100	33, 47, 66, 75	0
22	S	81/85 (95%)	0.37	4 (4%) 33 34	43, 61, 84, 97	0
23	T	119/120 (99%)	0.75	11 (9%) 11 11	41, 59, 85, 110	0
24	U	53/66 (80%)	0.33	2 (3%) 44 45	42, 56, 73, 82	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	V	65/71 (91%)	1.72	17 (26%) 1 1	56, 78, 115, 120	0
26	W	154/154 (100%)	0.07	2 (1%) 79 79	40, 53, 74, 82	0
27	X	82/92 (89%)	0.74	14 (17%) 2 2	44, 58, 84, 103	0
28	Y	142/241 (58%)	0.16	9 (6%) 23 24	29, 45, 68, 90	0
29	Z	73/83 (87%)	1.85	30 (41%) 0 0	52, 83, 97, 105	0
30	1	56/57 (98%)	-0.38	0 100 100	31, 36, 46, 55	0
31	2	46/50 (92%)	1.54	15 (32%) 1 1	41, 68, 96, 102	0
32	3	92/92 (100%)	0.39	7 (7%) 17 16	41, 61, 73, 86	0
33	I	70/162 (43%)	5.23	58 (82%) 0 0	111, 125, 142, 144	0
All	All	6652/7484 (88%)	0.15	503 (7%) 17 16	24, 54, 100, 153	0

All (503) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
33	I	71	GLY	15.8
25	V	1	THR	14.6
33	I	76	ALA	12.8
33	I	79	ILE	12.7
33	I	133	THR	12.2
8	D	63	ILE	12.0
29	Z	11	SER	11.8
23	T	119	ALA	11.4
33	I	85	PHE	10.3
2	9	3001	U	10.0
17	N	166	ALA	10.0
8	D	57	THR	9.5
16	M	70	GLY	9.5
31	2	49	GLU	9.2
29	Z	22	SER	9.1
25	V	40	PRO	9.0
33	I	88	GLY	8.9
25	V	39	ALA	8.6
33	I	81	ASP	8.5
33	I	121	LEU	8.5
33	I	75	THR	8.4
33	I	137	VAL	8.3
33	I	77	GLU	8.2
33	I	116	LEU	8.2
33	I	91	GLU	8.1

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Mol	Chain	Res	Type	RSRZ
33	I	105	VAL	8.0
16	M	79	ALA	8.0
33	I	129	VAL	7.8
33	I	118	SER	7.7
33	I	109	ALA	7.7
33	I	87	THR	7.5
8	D	90	LEU	7.3
33	I	96	PHE	7.3
33	I	78	LEU	7.2
5	A	37	VAL	7.1
33	I	126	LYS	7.1
31	2	48	ASP	7.0
33	I	113	HIS	6.6
33	I	132	CYS	6.6
5	A	237	GLY	6.5
33	I	89	SER	6.4
2	9	3024	U	6.3
1	0	282	C	6.2
29	Z	20	ARG	6.1
33	I	93	GLN	6.1
33	I	108	ILE	6.1
23	T	118	SER	6.0
31	2	39	ARG	6.0
29	Z	45	ASP	5.9
33	I	74	PRO	5.9
25	V	38	GLY	5.8
8	D	69	ILE	5.7
33	I	111	GLN	5.7
16	M	74	LYS	5.6
33	I	107	GLN	5.6
27	X	88	GLU	5.5
8	D	64	ARG	5.5
33	I	83	ALA	5.4
29	Z	18	TYR	5.3
31	2	41	HIS	5.3
29	Z	12	GLY	5.3
33	I	104	GLN	5.3
14	K	132	VAL	5.2
11	G	26	MET	5.2
33	I	98	ALA	5.2
16	M	75	ARG	5.2
33	I	80	LYS	5.2

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Mol	Chain	Res	Type	RSRZ
27	X	80	GLU	5.2
17	N	155	GLU	5.2
2	9	3023	U	5.2
29	Z	25	ARG	5.1
11	G	69	ARG	5.1
16	M	86	GLN	5.0
29	Z	21	VAL	5.0
29	Z	32	GLU	5.0
25	V	41	GLU	5.0
8	D	61	PHE	5.0
1	0	1199	A	5.0
33	I	125	ALA	5.0
1	0	1951	G	4.9
17	N	68	GLU	4.9
16	M	71	SER	4.9
16	M	87	GLY	4.8
33	I	138	THR	4.8
15	L	81	VAL	4.8
29	Z	14	PHE	4.8
31	2	47	THR	4.8
29	Z	23	ARG	4.8
11	G	23	ILE	4.7
11	G	71	LEU	4.7
31	2	44	ARG	4.7
8	D	66	GLY	4.7
33	I	86	GLU	4.7
33	I	102	VAL	4.6
17	N	175	LEU	4.6
23	T	117	ASP	4.6
17	N	163	PHE	4.5
8	D	170	TYR	4.5
1	0	497	A	4.5
1	0	1172	G	4.5
1	0	2237	G	4.5
1	0	1177	A	4.5
17	N	147	ILE	4.4
11	G	27	ILE	4.4
9	E	10	ASP	4.4
33	I	114	PRO	4.4
12	H	138	CYS	4.4
11	G	66	LEU	4.4
23	T	116	ASP	4.4

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Mol	Chain	Res	Type	RSRZ
2	9	3002	U	4.3
9	E	45	ASP	4.3
8	D	44	ILE	4.3
27	X	77	PHE	4.3
1	0	1169	U	4.3
12	H	74	ILE	4.2
29	Z	37	HIS	4.2
8	D	26	GLY	4.2
12	H	73	LEU	4.2
29	Z	34	ASN	4.2
12	H	78	GLY	4.2
15	L	80	ASP	4.2
1	0	2508	C	4.2
28	Y	216	ARG	4.1
15	L	93	VAL	4.1
1	0	280	C	4.1
1	0	2004	U	4.1
10	F	28	ALA	4.1
33	I	112	LYS	4.0
33	I	122	THR	4.0
8	D	134	LEU	4.0
28	Y	235	GLU	4.0
31	2	38	LYS	4.0
29	Z	24	ARG	4.0
10	F	107	ASP	4.0
15	L	76	LEU	3.9
8	D	92	GLU	3.9
27	X	41	PHE	3.9
29	Z	33	MET	3.9
5	A	31	LYS	3.8
5	A	133	ARG	3.8
1	0	285	A	3.8
8	D	56	ARG	3.8
1	0	2511	A	3.8
8	D	73	VAL	3.8
25	V	59	ILE	3.8
16	M	78	LYS	3.8
25	V	37	GLY	3.7
8	D	154	LYS	3.7
9	E	100	ASP	3.7
12	H	146	VAL	3.7
33	I	119	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
16	M	77	HIS	3.7
29	Z	19	GLY	3.7
29	Z	31	SER	3.7
1	0	1173	A	3.7
31	2	42	TRP	3.6
33	I	134	SER	3.6
25	V	36	ALA	3.6
8	D	40	ILE	3.6
9	E	86	VAL	3.6
10	F	117	GLU	3.6
33	I	84	GLY	3.6
8	D	10	PHE	3.6
9	E	87	PHE	3.6
8	D	166	ILE	3.6
17	N	185	GLU	3.6
17	N	178	THR	3.6
15	L	97	VAL	3.6
33	I	99	ASP	3.6
15	L	100	ALA	3.5
31	2	35	ARG	3.5
27	X	7	GLU	3.5
8	D	128	LEU	3.5
5	A	36	ASP	3.5
1	0	970	U	3.5
1	0	1202	A	3.5
8	D	88	LEU	3.5
23	T	82	THR	3.5
15	L	91	VAL	3.5
1	0	960	G	3.5
1	0	1948	G	3.5
16	M	72	ALA	3.5
22	S	81	ILE	3.5
25	V	63	GLU	3.5
17	N	95	ALA	3.5
32	3	92	GLU	3.5
25	V	8	ILE	3.5
5	A	35	GLY	3.5
1	0	514	G	3.5
8	D	18	ILE	3.4
16	M	81	ARG	3.4
10	F	16	ALA	3.4
8	D	27	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	0	1198	U	3.4
29	Z	29	ILE	3.4
8	D	68	PRO	3.4
1	0	2238	A	3.4
17	N	134	ASP	3.4
1	0	272	A	3.4
1	0	1163	G	3.4
17	N	184	ILE	3.4
8	D	62	ASP	3.4
27	X	85	VAL	3.3
33	I	117	LEU	3.3
1	0	2645	U	3.3
22	S	20	PHE	3.3
8	D	41	LEU	3.3
16	M	80	GLY	3.3
10	F	100	ASP	3.3
33	I	120	ASP	3.3
9	E	124	VAL	3.3
29	Z	30	GLU	3.3
8	D	172	VAL	3.3
33	I	123	ASN	3.3
15	L	120	LEU	3.3
1	0	1965	C	3.3
33	I	73	PRO	3.3
31	2	26	MET	3.3
15	L	145	LEU	3.3
31	2	27	LEU	3.3
17	N	2	THR	3.3
12	H	171	ALA	3.3
6	B	104	GLU	3.2
1	0	1966	U	3.2
15	L	60	GLU	3.2
10	F	17	LEU	3.2
1	0	1950	G	3.2
8	D	53	LYS	3.2
9	E	127	ASP	3.2
13	J	70	PHE	3.2
17	N	180	LEU	3.2
5	A	32	VAL	3.2
16	M	76	ARG	3.2
17	N	139	TRP	3.2
29	Z	10	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
8	D	11	HIS	3.2
1	0	716	G	3.2
20	Q	95	GLU	3.2
5	A	65	ARG	3.2
8	D	107	GLY	3.1
6	B	2	GLN	3.1
1	0	735	C	3.1
11	G	22	ALA	3.1
9	E	88	TYR	3.1
28	Y	95	THR	3.1
33	I	82	GLU	3.1
15	L	102	ASP	3.1
1	0	284	C	3.1
33	I	72	VAL	3.1
1	0	358	G	3.1
10	F	49	PHE	3.1
31	2	37	HIS	3.1
12	H	149	ALA	3.1
10	F	22	VAL	3.1
1	0	1168	C	3.0
10	F	44	SER	3.0
17	N	179	LEU	3.0
33	I	94	GLU	3.0
10	F	106	ALA	3.0
12	H	47	ILE	3.0
8	D	173	GLU	3.0
9	E	6	GLU	3.0
11	G	73	ASP	3.0
1	0	1981	A	3.0
8	D	85	GLN	3.0
29	Z	59	TYR	3.0
1	0	1180	U	3.0
11	G	72	ASP	3.0
25	V	3	LEU	3.0
33	I	115	ASP	3.0
29	Z	26	VAL	3.0
10	F	99	THR	3.0
24	U	47	ARG	3.0
17	N	67	ALA	3.0
29	Z	36	ASP	3.0
10	F	119	ARG	2.9
24	U	43	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
29	Z	16	ALA	2.9
1	0	1200	A	2.9
8	D	89	PRO	2.9
10	F	110	ASP	2.9
17	N	138	ASP	2.9
1	0	1171	A	2.9
8	D	51	ARG	2.9
11	G	63	ARG	2.9
9	E	4	GLU	2.9
32	3	41	GLU	2.9
8	D	93	LEU	2.9
23	T	112	LEU	2.9
16	M	82	ARG	2.9
10	F	12	LEU	2.9
19	P	18	LYS	2.9
8	D	106	PHE	2.9
17	N	156	GLU	2.9
8	D	91	ALA	2.9
17	N	165	ALA	2.9
11	G	12	ILE	2.9
1	0	999	C	2.9
13	J	5	GLU	2.8
10	F	108	VAL	2.8
6	B	180	ASP	2.8
17	N	71	TRP	2.8
12	H	130	GLY	2.8
17	N	1	ALA	2.8
1	0	281	U	2.8
6	B	117	GLU	2.8
11	G	67	LEU	2.8
11	G	24	VAL	2.8
25	V	2	VAL	2.8
27	X	10	VAL	2.8
1	0	138	U	2.8
9	E	11	VAL	2.8
16	M	89	THR	2.8
25	V	14	ALA	2.8
1	0	1192	A	2.8
17	N	160	SER	2.8
1	0	1170	U	2.8
10	F	25	ASP	2.8
27	X	71	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
9	E	99	GLY	2.8
8	D	167	GLU	2.8
12	H	143	ALA	2.8
28	Y	102	LEU	2.7
10	F	98	VAL	2.7
10	F	21	GLU	2.7
12	H	37	GLN	2.7
1	0	1625	U	2.7
16	M	73	ARG	2.7
20	Q	18	PRO	2.7
33	I	97	VAL	2.7
1	0	1164	U	2.7
25	V	43	PRO	2.7
1	0	10	U	2.7
11	G	25	GLU	2.7
28	Y	234	VAL	2.7
1	0	1967	U	2.7
17	N	172	PHE	2.7
17	N	159	TYR	2.7
10	F	70	LYS	2.7
16	M	84	LYS	2.7
9	E	118	ILE	2.7
5	A	85	SER	2.7
7	C	61	PHE	2.7
10	F	75	ILE	2.6
17	N	137	ALA	2.6
8	D	65	GLU	2.6
19	P	114	LEU	2.6
6	B	1	PRO	2.6
1	0	1525	G	2.6
1	0	2769	C	2.6
9	E	44	GLY	2.6
1	0	370	G	2.6
13	J	4	ALA	2.6
20	Q	76	VAL	2.6
6	B	183	GLU	2.6
23	T	77	VAL	2.6
27	X	43	VAL	2.6
33	I	135	LEU	2.6
5	A	97	ALA	2.6
8	D	104	PHE	2.6
10	F	29	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	0	288	A	2.5
15	L	79	ASP	2.5
9	E	126	ILE	2.5
11	G	70	ALA	2.5
17	N	65	ASP	2.5
1	0	2748	G	2.5
9	E	48	VAL	2.5
6	B	128	ILE	2.5
33	I	103	ASP	2.5
11	G	15	TRP	2.5
1	0	1947	G	2.5
12	H	66	ARG	2.5
23	T	109	GLU	2.5
28	Y	96	GLU	2.5
9	E	5	LEU	2.5
2	9	3072	C	2.5
5	A	99	ILE	2.5
9	E	154	ILE	2.5
32	3	62	THR	2.5
1	0	1929	G	2.5
8	D	84	LEU	2.5
1	0	283	U	2.5
33	I	124	ALA	2.5
10	F	15	ASP	2.4
1	0	1203	G	2.4
29	Z	35	GLU	2.4
8	D	81	GLU	2.4
27	X	72	VAL	2.4
29	Z	28	GLU	2.4
31	2	36	ASN	2.4
1	0	362	G	2.4
31	2	43	ARG	2.4
20	Q	17	LYS	2.4
16	M	85	ARG	2.4
31	2	20	ARG	2.4
17	N	158	LEU	2.4
17	N	167	ASP	2.4
22	S	72	ASP	2.4
17	N	161	GLY	2.4
28	Y	236	VAL	2.4
28	Y	108	ASP	2.4
9	E	94	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
6	B	134	ALA	2.4
9	E	1	PRO	2.4
6	B	105	PHE	2.4
12	H	35	ARG	2.4
12	H	111	ASP	2.4
16	M	132	ILE	2.4
23	T	115	GLU	2.4
8	D	87	ALA	2.4
27	X	65	ASN	2.3
9	E	161	VAL	2.3
17	N	106	LEU	2.3
11	G	68	GLU	2.3
23	T	110	ALA	2.3
27	X	76	ARG	2.3
17	N	183	ASP	2.3
12	H	83	TYR	2.3
6	B	57	GLU	2.3
5	A	82	VAL	2.3
1	0	2344	G	2.3
10	F	19	ALA	2.3
18	O	23	GLY	2.3
14	K	119	GLN	2.3
2	9	3122	C	2.3
29	Z	15	GLY	2.3
29	Z	27	ALA	2.3
10	F	24	ARG	2.3
15	L	75	LEU	2.3
15	L	105	TYR	2.3
25	V	5	VAL	2.3
27	X	44	ASP	2.3
4	5	77	PHE	2.3
32	3	6	ARG	2.3
17	N	152	GLU	2.3
26	W	86	GLU	2.3
6	B	119	HIS	2.3
8	D	58	VAL	2.3
10	F	11	ASP	2.3
10	F	118	LEU	2.3
18	O	22	GLY	2.3
1	0	1181	A	2.3
1	0	2345	A	2.3
1	0	359	U	2.2

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Mol	Chain	Res	Type	RSRZ
25	V	60	GLN	2.2
9	E	7	ILE	2.2
15	L	148	GLU	2.2
1	0	371	U	2.2
1	0	2747	C	2.2
19	P	110	ASP	2.2
9	E	105	GLU	2.2
17	N	177	GLU	2.2
23	T	59	GLU	2.2
8	D	71	ALA	2.2
10	F	23	ALA	2.2
1	0	2239	C	2.2
32	3	56	PRO	2.2
8	D	23	VAL	2.2
26	W	78	ASP	2.2
1	0	293	A	2.2
29	Z	44	GLU	2.2
33	I	110	GLU	2.2
11	G	20	VAL	2.1
16	M	88	VAL	2.1
32	3	20	HIS	2.1
9	E	53	GLU	2.1
1	0	1161	A	2.1
22	S	77	VAL	2.1
13	J	7	ASP	2.1
12	H	137	TYR	2.1
5	A	38	ILE	2.1
8	D	38	GLU	2.1
16	M	164	THR	2.1
29	Z	80	ARG	2.1
5	A	61	GLU	2.1
10	F	69	GLU	2.1
12	H	166	SER	2.1
32	3	8	ASN	2.1
8	D	75	LEU	2.1
11	G	65	THR	2.1
15	L	62	ALA	2.0
27	X	75	ALA	2.0
1	0	441	A	2.0
7	C	1	MET	2.0
15	L	99	GLU	2.0
18	O	60	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
10	F	20	LEU	2.0
10	F	26	THR	2.0
16	M	83	SER	2.0
9	E	129	GLU	2.0
17	N	5	ARG	2.0
25	V	62	GLU	2.0
17	N	148	ALA	2.0
10	F	115	VAL	2.0
1	0	1189	A	2.0
33	I	130	GLY	2.0
7	C	132	ASP	2.0
1	0	1178	G	2.0
6	B	115	VAL	2.0
28	Y	187	VAL	2.0
20	Q	81	GLU	2.0
19	P	108	LEU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	PSU	0	2621	20/21	0.98	0.14	-	36,38,43,43	0
1	1MA	0	628	23/24	0.98	0.12	-	32,35,37,38	0
1	OMG	0	2588	24/25	0.98	0.13	-	31,34,39,41	0
3	PPU	4	76	24/38	0.98	0.13	-	41,44,45,49	0
1	OMU	0	2587	21/22	0.98	0.13	-	32,37,40,40	0
3	HFA	4	77	11/12	0.95	0.19	-	42,44,47,48	0
1	UR3	0	2619	21/22	0.97	0.15	-	39,42,45,48	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
36	NA	0	9125	1/1	0.95	0.82	77.79	92,92,92,92	0
36	NA	0	9164	1/1	0.87	0.56	60.98	61,61,61,61	0
36	NA	0	9161	1/1	0.85	0.72	43.33	68,68,68,68	0
36	NA	0	9135	1/1	0.72	0.30	35.12	55,55,55,55	0
36	NA	0	9171	1/1	0.93	0.31	20.63	61,61,61,61	0
38	SR	B	9521	1/1	0.59	0.63	18.92	200,200,200,200	0
34	MG	0	8013	1/1	0.84	0.34	18.68	25,25,25,25	0
34	MG	0	8052	1/1	0.83	0.25	18.55	99,99,99,99	0
36	NA	0	9178	1/1	0.96	0.46	16.82	54,54,54,54	0
38	SR	0	9482	1/1	0.90	0.35	15.85	135,135,135,135	0
36	NA	0	9177	1/1	0.91	0.35	13.20	77,77,77,77	0
35	K	0	9001	1/1	0.88	0.31	13.00	74,74,74,74	0
36	NA	9	9183	1/1	0.76	0.38	12.87	75,75,75,75	0
36	NA	0	9182	1/1	0.62	0.40	12.50	90,90,90,90	0
36	NA	R	9186	1/1	0.83	0.39	12.42	80,80,80,80	0
34	MG	5	8118	1/1	0.88	0.34	11.85	45,45,45,45	0
36	NA	0	9173	1/1	0.93	0.34	10.94	69,69,69,69	0
36	NA	0	9159	1/1	0.93	0.35	10.57	58,58,58,58	0
36	NA	0	9174	1/1	0.91	0.38	10.49	65,65,65,65	0
34	MG	0	8038	1/1	0.99	0.25	10.45	25,25,25,25	0
34	MG	0	8101	1/1	0.62	0.28	10.41	80,80,80,80	0
36	NA	0	9150	1/1	0.94	0.21	9.56	47,47,47,47	0
36	NA	0	9172	1/1	0.83	0.35	9.54	76,76,76,76	0
36	NA	0	9168	1/1	0.90	0.17	9.19	69,69,69,69	0
34	MG	0	8012	1/1	0.97	0.22	7.62	39,39,39,39	0
36	NA	0	9120	1/1	0.93	0.21	7.11	61,61,61,61	0
36	NA	0	9132	1/1	0.86	0.23	5.52	68,68,68,68	0
34	MG	0	8001	1/1	0.97	0.19	4.99	22,22,22,22	0
34	MG	0	8008	1/1	0.99	0.19	4.76	16,16,16,16	0
36	NA	0	9165	1/1	0.89	0.30	4.41	45,45,45,45	0
34	MG	0	8065	1/1	0.81	0.35	4.36	107,107,107,107	0
36	NA	0	9115	1/1	0.96	0.18	4.21	41,41,41,41	0
34	MG	0	8054	1/1	0.93	0.16	4.16	63,63,63,63	0
34	MG	0	8056	1/1	0.98	0.23	3.85	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	MG	0	8091	1/1	0.89	0.15	3.78	64,64,64,64	0
36	NA	0	9114	1/1	0.75	0.20	3.64	65,65,65,65	0
37	CL	0	9316	1/1	0.97	0.26	3.56	78,78,78,78	0
34	MG	0	8080	1/1	0.98	0.17	2.85	57,57,57,57	0
36	NA	0	9131	1/1	0.90	0.14	2.58	47,47,47,47	0
36	NA	0	9156	1/1	0.96	0.16	2.35	57,57,57,57	0
34	MG	0	8021	1/1	0.95	0.17	2.28	56,56,56,56	0
37	CL	B	9319	1/1	0.99	0.16	1.43	54,54,54,54	0
36	NA	0	9162	1/1	0.96	0.15	1.40	52,52,52,52	0
34	MG	0	8107	1/1	0.84	0.17	1.24	65,65,65,65	0
34	MG	0	8017	1/1	0.98	0.14	1.07	31,31,31,31	0
36	NA	0	9124	1/1	0.93	0.19	1.03	50,50,50,50	0
38	SR	0	9475	1/1	0.98	0.13	1.01	83,83,83,83	0
38	SR	0	9410	1/1	0.99	0.14	1.00	41,41,41,41	0
34	MG	0	8074	1/1	0.99	0.18	0.89	27,27,27,27	0
34	MG	0	8020	1/1	0.98	0.16	0.87	36,36,36,36	0
38	SR	0	9515	1/1	0.99	0.14	0.86	100,100,100,100	0
38	SR	0	9406	1/1	1.00	0.13	0.66	35,35,35,35	0
34	MG	0	8057	1/1	0.94	0.20	0.62	77,77,77,77	0
36	NA	M	9147	1/1	0.93	0.18	0.52	42,42,42,42	0
38	SR	0	9407	1/1	1.00	0.13	0.50	47,47,47,47	0
38	SR	0	9509	1/1	0.92	0.15	0.38	95,95,95,95	0
38	SR	0	9490	1/1	0.96	0.13	0.37	116,116,116,116	0
34	MG	0	8070	1/1	0.96	0.14	0.31	24,24,24,24	0
38	SR	0	9451	1/1	0.99	0.12	0.30	60,60,60,60	0
38	SR	0	9534	1/1	0.97	0.14	0.16	111,111,111,111	0
35	K	0	9002	1/1	0.76	0.18	0.13	88,88,88,88	0
38	SR	H	9486	1/1	0.95	0.15	0.08	125,125,125,125	0
38	SR	F	9595	1/1	0.96	0.16	-0.02	109,109,109,109	0
34	MG	0	8097	1/1	0.94	0.13	-0.04	57,57,57,57	0
36	NA	C	9104	1/1	0.95	0.16	-0.36	33,33,33,33	0
38	SR	0	9424	1/1	1.00	0.16	-0.56	49,49,49,49	0
37	CL	M	9318	1/1	0.95	0.17	-0.57	41,41,41,41	0
36	NA	0	9143	1/1	0.89	0.14	-0.62	40,40,40,40	0
36	NA	0	9139	1/1	0.95	0.10	-0.80	43,43,43,43	0
38	SR	0	9455	1/1	0.98	0.09	-0.87	88,88,88,88	0
39	CD	Z	9203	1/1	0.75	0.13	-0.90	84,84,84,84	0
36	NA	J	9146	1/1	0.79	0.11	-1.01	55,55,55,55	0
37	CL	J	9321	1/1	0.96	0.11	-1.04	66,66,66,66	0
38	SR	0	9504	1/1	0.91	0.11	-1.25	108,108,108,108	0
37	CL	0	9312	1/1	0.99	0.10	-1.32	57,57,57,57	0
34	MG	A	8066	1/1	0.97	0.11	-1.33	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	NA	0	9166	1/1	0.89	0.09	-1.37	74,74,74,74	0
34	MG	0	8004	1/1	0.95	0.10	-1.42	35,35,35,35	0
39	CD	U	9201	1/1	1.00	0.09	-1.45	53,53,53,53	0
36	NA	0	9117	1/1	0.93	0.07	-1.45	51,51,51,51	0
34	MG	Y	8109	1/1	0.96	0.12	-1.58	45,45,45,45	0
37	CL	O	9308	1/1	0.98	0.09	-1.61	67,67,67,67	0
34	MG	0	8028	1/1	0.99	0.13	-1.63	37,37,37,37	0
38	SR	0	9450	1/1	0.99	0.07	-1.71	72,72,72,72	0
34	MG	T	8073	1/1	0.94	0.11	-1.76	43,43,43,43	0
36	NA	Q	9148	1/1	0.98	0.09	-1.84	49,49,49,49	0
34	MG	0	8015	1/1	0.99	0.09	-1.89	35,35,35,35	0
36	NA	0	9127	1/1	0.96	0.10	-2.14	60,60,60,60	0
39	CD	3	9204	1/1	0.99	0.04	-2.19	64,64,64,64	0
36	NA	0	9138	1/1	0.97	0.07	-2.20	62,62,62,62	0
36	NA	R	9137	1/1	0.96	0.08	-2.25	36,36,36,36	0
38	SR	1	9419	1/1	0.99	0.09	-2.38	40,40,40,40	0
38	SR	0	9428	1/1	0.99	0.07	-2.38	55,55,55,55	0
34	MG	0	8003	1/1	0.95	0.13	-2.52	35,35,35,35	0
38	SR	3	9439	1/1	0.99	0.05	-2.54	72,72,72,72	0
38	SR	0	9456	1/1	0.98	0.10	-2.54	67,67,67,67	0
38	SR	0	9468	1/1	0.91	0.05	-2.75	128,128,128,128	0
37	CL	3	9304	1/1	0.96	0.07	-2.79	61,61,61,61	0
34	MG	0	8067	1/1	0.95	0.11	-2.80	40,40,40,40	0
34	MG	0	8002	1/1	0.97	0.09	-3.00	34,34,34,34	0
38	SR	A	9436	1/1	0.97	0.06	-3.02	60,60,60,60	0
34	MG	0	8060	1/1	0.96	0.08	-3.10	82,82,82,82	0
34	MG	0	8096	1/1	0.98	0.06	-3.40	41,41,41,41	0
34	MG	0	8032	1/1	0.92	0.10	-3.48	48,48,48,48	0
38	SR	L	9409	1/1	0.99	0.07	-3.52	37,37,37,37	0
38	SR	0	9532	1/1	0.90	0.05	-3.54	120,120,120,120	0
37	CL	0	9305	1/1	0.97	0.07	-3.55	61,61,61,61	0
34	MG	0	8110	1/1	0.97	0.11	-3.71	45,45,45,45	0
39	CD	1	9202	1/1	0.99	0.05	-3.76	54,54,54,54	0
38	SR	0	9457	1/1	0.98	0.08	-4.14	51,51,51,51	0
36	NA	0	9105	1/1	0.96	0.09	-4.22	44,44,44,44	0
34	MG	0	8044	1/1	0.97	0.07	-4.61	35,35,35,35	0
38	SR	0	9416	1/1	1.00	0.08	-4.74	43,43,43,43	0
34	MG	0	8112	1/1	0.96	0.06	-4.79	46,46,46,46	0
38	SR	0	9444	1/1	0.99	0.05	-5.06	55,55,55,55	0
34	MG	0	8019	1/1	0.92	0.06	-5.38	51,51,51,51	0
38	SR	0	9483	1/1	0.94	0.06	-5.71	77,77,77,77	0
37	CL	0	9315	1/1	0.97	0.09	-5.89	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
38	SR	0	9442	1/1	0.97	0.10	-6.28	66,66,66,66	0
36	NA	0	9123	1/1	0.99	0.09	-6.29	52,52,52,52	0
38	SR	0	9473	1/1	0.99	0.03	-6.47	82,82,82,82	0
38	SR	0	9453	1/1	0.99	0.06	-6.87	72,72,72,72	0
38	SR	0	9498	1/1	0.99	0.05	-7.61	63,63,63,63	0
38	SR	0	9506	1/1	0.98	0.04	-9.14	68,68,68,68	0
38	SR	0	9425	1/1	0.99	0.15	-	56,56,56,56	0
34	MG	0	8039	1/1	0.98	0.17	-	49,49,49,49	0
36	NA	0	9155	1/1	0.95	0.18	-	60,60,60,60	0
34	MG	0	8037	1/1	0.84	0.10	-	46,46,46,46	0
38	SR	0	9405	1/1	0.97	0.16	-	59,59,59,59	0
36	NA	0	9107	1/1	0.95	0.39	-	71,71,71,71	0
38	SR	B	9458	1/1	0.99	0.05	-	82,82,82,82	0
34	MG	0	8058	1/1	0.90	0.21	-	41,41,41,41	0
38	SR	0	9477	1/1	0.98	0.10	-	86,86,86,86	0
38	SR	0	9421	1/1	0.98	0.10	-	78,78,78,78	0
34	MG	0	8014	1/1	0.90	0.39	-	73,73,73,73	0
38	SR	R	9418	1/1	0.99	0.15	-	57,57,57,57	0
34	MG	0	8061	1/1	0.86	0.19	-	87,87,87,87	0
38	SR	0	9466	1/1	0.97	0.06	-	96,96,96,96	0
36	NA	0	9154	1/1	0.98	0.14	-	54,54,54,54	0
34	MG	0	8092	1/1	0.82	0.34	-	77,77,77,77	0
34	MG	9	8095	1/1	0.92	0.35	-	55,55,55,55	0
36	NA	0	9170	1/1	0.89	0.29	-	77,77,77,77	0
38	SR	0	9501	1/1	0.65	0.20	-	159,159,159,159	0
38	SR	0	9547	1/1	0.52	0.39	-	194,194,194,194	0
34	MG	0	8043	1/1	0.91	0.06	-	52,52,52,52	0
38	SR	0	9415	1/1	1.00	0.10	-	56,56,56,56	0
34	MG	0	8083	1/1	0.95	0.11	-	53,53,53,53	0
34	MG	2	8076	1/1	0.95	0.17	-	64,64,64,64	0
36	NA	0	9157	1/1	0.94	0.18	-	47,47,47,47	0
36	NA	0	9179	1/1	0.91	0.59	-	121,121,121,121	0
34	MG	K	8069	1/1	0.97	0.17	-	25,25,25,25	0
38	SR	0	9448	1/1	1.00	0.07	-	63,63,63,63	0
38	SR	0	9469	1/1	0.98	0.05	-	85,85,85,85	0
38	SR	0	9413	1/1	0.99	0.12	-	49,49,49,49	0
38	SR	0	9522	1/1	0.96	0.04	-	114,114,114,114	0
36	NA	0	9136	1/1	0.98	0.12	-	34,34,34,34	0
37	CL	N	9307	1/1	0.96	0.16	-	65,65,65,65	0
34	MG	0	8084	1/1	0.97	0.40	-	89,89,89,89	0
34	MG	0	8108	1/1	0.68	0.14	-	103,103,103,103	0
38	SR	0	9440	1/1	0.96	0.05	-	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	NA	0	9175	1/1	0.93	0.34	-	55,55,55,55	0
38	SR	0	9464	1/1	0.98	0.05	-	81,81,81,81	0
36	NA	0	9102	1/1	0.87	0.22	-	63,63,63,63	0
34	MG	0	8114	1/1	0.97	0.47	-	83,83,83,83	0
34	MG	0	8094	1/1	0.92	0.50	-	72,72,72,72	0
36	NA	0	9169	1/1	0.86	0.39	-	116,116,116,116	0
38	SR	0	9517	1/1	0.95	0.06	-	110,110,110,110	0
37	CL	J	9301	1/1	0.93	0.18	-	60,60,60,60	0
38	SR	0	9626	1/1	0.91	0.25	-	154,154,154,154	0
38	SR	0	9435	1/1	0.98	0.08	-	76,76,76,76	0
34	MG	0	8031	1/1	0.98	0.12	-	49,49,49,49	0
38	SR	0	9443	1/1	0.98	0.10	-	63,63,63,63	0
36	NA	0	9128	1/1	0.90	0.15	-	49,49,49,49	0
38	SR	0	9478	1/1	0.99	0.06	-	77,77,77,77	0
38	SR	0	9454	1/1	0.98	0.10	-	82,82,82,82	0
34	MG	0	8099	1/1	0.91	0.14	-	75,75,75,75	0
34	MG	0	8116	1/1	0.95	0.10	-	64,64,64,64	0
36	NA	0	9122	1/1	0.58	0.40	-	90,90,90,90	0
38	SR	0	9484	1/1	0.32	0.14	-	149,149,149,149	0
38	SR	0	9430	1/1	0.99	0.10	-	49,49,49,49	0
34	MG	0	8042	1/1	0.96	0.11	-	48,48,48,48	0
38	SR	0	9568	1/1	0.97	0.07	-	80,80,80,80	0
34	MG	0	8102	1/1	0.85	0.12	-	68,68,68,68	0
36	NA	0	9163	1/1	0.94	0.16	-	73,73,73,73	0
34	MG	0	8025	1/1	0.90	0.42	-	27,27,27,27	0
38	SR	0	9417	1/1	0.99	0.08	-	63,63,63,63	0
38	SR	0	9441	1/1	0.98	0.07	-	68,68,68,68	0
36	NA	0	9181	1/1	0.72	0.16	-	54,54,54,54	0
37	CL	0	9303	1/1	0.99	0.13	-	53,53,53,53	0
38	SR	0	9462	1/1	0.98	0.10	-	74,74,74,74	0
34	MG	0	8090	1/1	0.80	0.36	-	68,68,68,68	0
38	SR	9	9503	1/1	0.91	0.05	-	122,122,122,122	0
36	NA	0	9167	1/1	0.91	0.10	-	65,65,65,65	0
38	SR	0	9500	1/1	0.88	1.54	-	200,200,200,200	0
34	MG	0	8103	1/1	0.89	0.17	-	67,67,67,67	0
34	MG	0	8050	1/1	0.88	0.22	-	89,89,89,89	0
38	SR	0	9474	1/1	0.99	0.08	-	73,73,73,73	0
36	NA	0	9149	1/1	0.94	0.29	-	49,49,49,49	0
38	SR	0	9629	1/1	0.98	0.08	-	75,75,75,75	0
38	SR	0	9459	1/1	0.91	0.10	-	103,103,103,103	0
38	SR	0	9449	1/1	0.99	0.09	-	67,67,67,67	0
36	NA	0	9152	1/1	0.77	1.03	-	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	MG	0	8046	1/1	0.97	0.06	-	39,39,39,39	0
34	MG	0	8117	1/1	0.97	0.12	-	46,46,46,46	0
38	SR	0	9461	1/1	0.98	0.06	-	82,82,82,82	0
38	SR	0	9411	1/1	0.99	0.14	-	43,43,43,43	0
38	SR	0	9480	1/1	0.98	0.05	-	93,93,93,93	0
38	SR	0	9429	1/1	0.99	0.10	-	72,72,72,72	0
34	MG	0	8051	1/1	0.90	0.21	-	36,36,36,36	0
38	SR	0	9495	1/1	0.95	0.14	-	111,111,111,111	0
36	NA	0	9129	1/1	0.79	0.13	-	72,72,72,72	0
38	SR	0	9422	1/1	0.99	0.10	-	58,58,58,58	0
34	MG	0	8072	1/1	0.89	0.65	-	89,89,89,89	0
36	NA	0	9158	1/1	0.85	0.43	-	66,66,66,66	0
36	NA	0	9116	1/1	0.77	0.36	-	52,52,52,52	0
36	NA	0	9118	1/1	0.98	0.21	-	66,66,66,66	0
38	SR	0	9570	1/1	0.94	0.07	-	111,111,111,111	0
34	MG	0	8026	1/1	0.99	0.14	-	30,30,30,30	0
37	CL	0	9313	1/1	0.99	0.10	-	59,59,59,59	0
34	MG	0	8079	1/1	0.95	0.13	-	33,33,33,33	0
36	NA	0	9108	1/1	0.97	0.10	-	34,34,34,34	0
36	NA	0	9141	1/1	0.75	0.13	-	73,73,73,73	0
38	SR	0	9423	1/1	1.00	0.05	-	64,64,64,64	0
34	MG	0	8106	1/1	0.88	0.09	-	51,51,51,51	0
38	SR	0	9412	1/1	0.99	0.13	-	45,45,45,45	0
34	MG	0	8055	1/1	0.91	0.31	-	97,97,97,97	0
38	SR	A	9497	1/1	0.98	0.09	-	96,96,96,96	0
34	MG	0	8085	1/1	0.93	0.21	-	63,63,63,63	0
34	MG	0	8059	1/1	0.83	0.42	-	84,84,84,84	0
34	MG	0	8045	1/1	0.95	0.26	-	72,72,72,72	0
34	MG	0	8104	1/1	0.84	0.13	-	57,57,57,57	0
36	NA	0	9101	1/1	0.92	0.13	-	46,46,46,46	0
34	MG	0	8041	1/1	0.97	0.09	-	55,55,55,55	0
38	SR	0	9447	1/1	0.97	0.07	-	73,73,73,73	0
36	NA	D	9151	1/1	0.70	0.23	-	68,68,68,68	0
37	CL	0	9311	1/1	0.97	0.15	-	71,71,71,71	0
38	SR	0	9590	1/1	0.90	0.12	-	131,131,131,131	0
38	SR	0	9426	1/1	0.97	0.08	-	71,71,71,71	0
38	SR	0	9434	1/1	0.99	0.14	-	64,64,64,64	0
34	MG	0	8009	1/1	0.97	0.10	-	21,21,21,21	0
37	CL	Y	9320	1/1	0.96	0.08	-	47,47,47,47	0
38	SR	0	9431	1/1	0.98	0.13	-	65,65,65,65	0
38	SR	0	9585	1/1	0.96	0.08	-	94,94,94,94	0
34	MG	0	8047	1/1	0.55	0.55	-	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	NA	0	9110	1/1	0.94	0.32	-	46,46,46,46	0
34	MG	0	8082	1/1	0.95	0.20	-	82,82,82,82	0
38	SR	0	9438	1/1	0.97	0.09	-	70,70,70,70	0
38	SR	0	9505	1/1	0.95	0.07	-	106,106,106,106	0
34	MG	0	8040	1/1	0.90	0.21	-	92,92,92,92	0
38	SR	A	9437	1/1	0.97	0.10	-	70,70,70,70	0
37	CL	L	9310	1/1	0.92	0.12	-	58,58,58,58	0
38	SR	0	9539	1/1	0.88	0.38	-	157,157,157,157	0
38	SR	0	9445	1/1	0.98	0.09	-	57,57,57,57	0
38	SR	0	9488	1/1	0.99	0.11	-	86,86,86,86	0
34	MG	0	8036	1/1	0.94	0.11	-	65,65,65,65	0
36	NA	0	9184	1/1	0.41	0.41	-	87,87,87,87	0
38	SR	9	9588	1/1	0.59	0.15	-	143,143,143,143	0
34	MG	0	8005	1/1	0.98	0.06	-	29,29,29,29	0
34	MG	0	8093	1/1	0.79	0.13	-	49,49,49,49	0
36	NA	0	9111	1/1	0.91	0.31	-	63,63,63,63	0
36	NA	0	9113	1/1	0.94	0.12	-	60,60,60,60	0
34	MG	0	8022	1/1	0.85	0.93	-	112,112,112,112	0
38	SR	0	9432	1/1	0.97	0.14	-	68,68,68,68	0
38	SR	0	9581	1/1	0.87	0.08	-	130,130,130,130	0
38	SR	0	9529	1/1	-0.08	0.27	-	131,131,131,131	0
38	SR	0	9414	1/1	0.98	0.12	-	57,57,57,57	0
38	SR	0	9452	1/1	0.94	0.16	-	106,106,106,106	0
38	SR	1	9460	1/1	1.00	0.10	-	52,52,52,52	0
34	MG	0	8024	1/1	0.88	0.41	-	86,86,86,86	0
37	CL	0	9314	1/1	0.99	0.06	-	51,51,51,51	0
34	MG	0	8113	1/1	0.88	0.12	-	52,52,52,52	0
38	SR	S	9470	1/1	0.99	0.16	-	101,101,101,101	0
38	SR	0	9489	1/1	0.98	0.11	-	94,94,94,94	0
34	MG	0	8075	1/1	0.98	0.07	-	47,47,47,47	0
38	SR	0	9465	1/1	0.92	0.10	-	107,107,107,107	0
38	SR	9	9481	1/1	0.98	0.08	-	89,89,89,89	0
37	CL	0	9322	1/1	0.95	0.38	-	61,61,61,61	0
34	MG	0	8068	1/1	0.95	0.14	-	48,48,48,48	0
37	CL	0	9317	1/1	0.95	0.06	-	52,52,52,52	0
34	MG	0	8027	1/1	0.97	0.24	-	36,36,36,36	0
38	SR	0	9537	1/1	0.50	0.23	-	157,157,157,157	0
39	CD	O	9205	1/1	0.94	0.05	-	132,132,132,132	0
37	CL	J	9302	1/1	0.96	0.07	-	53,53,53,53	0
38	SR	0	9467	1/1	0.99	0.10	-	86,86,86,86	0
36	NA	0	9185	1/1	0.85	0.61	-	54,54,54,54	0
38	SR	0	9601	1/1	0.98	0.05	-	119,119,119,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
38	SR	0	9560	1/1	0.95	0.08	-	101,101,101,101	0
38	SR	0	9427	1/1	0.98	0.13	-	56,56,56,56	0
34	MG	0	8089	1/1	0.88	0.17	-	61,61,61,61	0
38	SR	0	9530	1/1	0.96	0.11	-	72,72,72,72	0
36	NA	0	9126	1/1	0.78	0.12	-	63,63,63,63	0
34	MG	0	8063	1/1	0.92	0.10	-	65,65,65,65	0
36	NA	0	9106	1/1	0.93	0.44	-	44,44,44,44	0
34	MG	0	8115	1/1	0.93	0.09	-	59,59,59,59	0
38	SR	0	9446	1/1	0.97	0.07	-	88,88,88,88	0
36	NA	0	9130	1/1	0.98	0.15	-	50,50,50,50	0
34	MG	0	8088	1/1	0.97	0.11	-	28,28,28,28	0
36	NA	S	9112	1/1	0.87	0.25	-	80,80,80,80	0
38	SR	0	9420	1/1	1.00	0.17	-	70,70,70,70	0
36	NA	0	9160	1/1	0.97	0.17	-	46,46,46,46	0
38	SR	0	9433	1/1	0.96	0.12	-	75,75,75,75	0
34	MG	0	8098	1/1	0.95	0.07	-	45,45,45,45	0
37	CL	A	9309	1/1	0.92	0.19	-	66,66,66,66	0
34	MG	0	8030	1/1	0.87	0.08	-	37,37,37,37	0
34	MG	0	8029	1/1	0.95	0.22	-	35,35,35,35	0
38	SR	0	9545	1/1	0.97	0.06	-	85,85,85,85	0
36	NA	0	9134	1/1	0.97	0.10	-	47,47,47,47	0
36	NA	0	9140	1/1	0.89	0.15	-	57,57,57,57	0
38	SR	0	9566	1/1	0.98	0.04	-	80,80,80,80	0
37	CL	R	9306	1/1	0.97	0.10	-	45,45,45,45	0
38	SR	0	9508	1/1	0.94	0.08	-	97,97,97,97	0
38	SR	0	9408	1/1	0.99	0.12	-	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.