



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 06:40 pm GMT

PDB ID : 1VQM
Title : The structure of the transition state analogue "DAN" bound to the large ribosomal subunit of haloarcula marismortui
Authors : Schmeing, T.M.; Steitz, T.A.
Deposited on : 2004-12-16
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

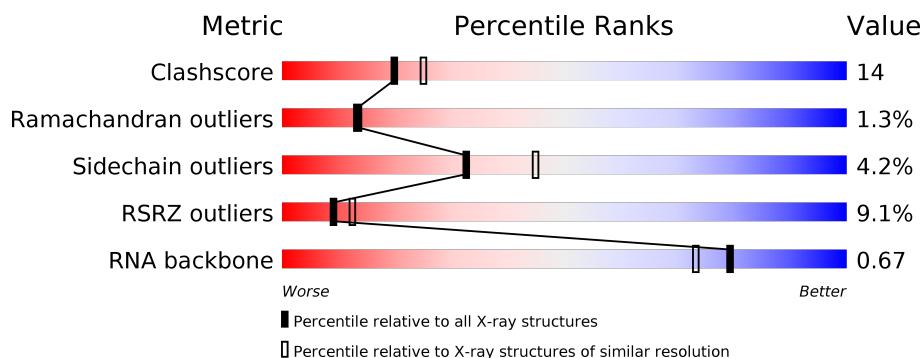
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	122126	5072 (2.30-2.30)
Ramachandran outliers	120053	5022 (2.30-2.30)
Sidechain outliers	120020	5021 (2.30-2.30)
RSRZ outliers	108989	4374 (2.30-2.30)
RNA backbone	2636	1004 (2.76-1.84)

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

Mol	Chain	Length	Quality of chain
1	0	2922	<div> <div>3%</div> <div> <div></div> <div>64%</div> <div>25%</div> <div>5%</div> <div>6%</div> </div> </div>
2	9	122	<div> <div>4%</div> <div> <div></div> <div>61%</div> <div>29%</div> <div>10%</div> <div>•</div> </div> </div>
3	4	7	<div> <div></div> <div> <div></div> <div>57%</div> <div>43%</div> </div> </div>
4	A	240	<div> <div>8%</div> <div> <div></div> <div>59%</div> <div>36%</div> <div>•</div> <div>•</div> </div> </div>
5	B	338	<div> <div>4%</div> <div> <div></div> <div>56%</div> <div>41%</div> <div>•</div> </div> </div>
6	C	246	<div> <div>2%</div> <div> <div></div> <div>68%</div> <div>27%</div> <div>•</div> </div> </div>

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Mol	Chain	Length	Quality of chain
7	D	177	
8	E	178	
9	F	120	
10	G	348	
11	H	171	
12	J	145	
13	K	132	
14	L	165	
15	M	195	
16	N	187	
17	O	116	
18	P	149	
19	Q	96	
20	R	155	
21	S	85	
22	T	120	
23	U	66	
24	V	71	
25	W	154	
26	X	92	
27	Y	241	
28	Z	83	
29	1	57	
30	2	50	
31	3	92	

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Mol	Chain	Length	Quality of chain
32	I	162	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	MG	0	8014	-	-	-	X
33	MG	0	8022	-	-	-	X
33	MG	0	8040	-	-	-	X
33	MG	0	8047	-	-	-	X
33	MG	0	8052	-	-	-	X
33	MG	0	8065	-	-	-	X
33	MG	0	8094	-	-	-	X
35	NA	0	9140	-	-	-	X
35	NA	0	9179	-	-	-	X
35	NA	0	9185	-	-	-	X
37	SR	0	9500	-	-	-	X

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 99045 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

There are 5 discrepancies between the modelled and reference sequences:

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

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

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

- Molecule 3 is a RNA chain called 5'-R(*CP*CP*(PPU)P*(PO2)P*(DA)P*C*C')-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	4	7	Total	C	N	O	P	0	0	0
			135	68	24	38	5			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	87	Total	Mg	0	0
			87	87		
33	Y	1	Total	Mg	0	0
			1	1		
33	K	1	Total	Mg	0	0
			1	1		
33	B	1	Total	Mg	0	0
			1	1		
33	A	1	Total	Mg	0	0
			1	1		
33	T	1	Total	Mg	0	0
			1	1		
33	2	1	Total	Mg	0	0
			1	1		
33	9	1	Total	Mg	0	0
			1	1		

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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	62	Total Na 62 62	0	0
35	J	1	Total Na 1 1	0	0
35	Q	1	Total Na 1 1	0	0
35	H	1	Total Na 1 1	0	0
35	C	1	Total Na 1 1	0	0
35	3	1	Total Na 1 1	0	0
35	R	3	Total Na 3 3	0	0
35	9	3	Total Na 3 3	0	0
35	S	1	Total Na 1 1	0	0
35	M	1	Total Na 1 1	0	0

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

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	M	1	Total	Cl	0	0
			1	1		

- Molecule 37 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	0	98	Total	Sr	0	0
			98	98		
37	1	2	Total	Sr	0	0
			2	2		
37	H	1	Total	Sr	0	0
			1	1		
37	B	2	Total	Sr	0	0
			2	2		
37	3	1	Total	Sr	0	0
			1	1		
37	A	3	Total	Sr	0	0
			3	3		
37	R	1	Total	Sr	0	0
			1	1		
37	9	3	Total	Sr	0	0
			3	3		
37	L	1	Total	Sr	0	0
			1	1		
37	S	1	Total	Sr	0	0
			1	1		
37	F	1	Total	Sr	0	0
			1	1		

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

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

- Molecule 39 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	0	5739	Total 5739	O 5739	0	0
39	9	132	Total 132	O 132	0	0
39	4	8	Total 8	O 8	0	0
39	A	123	Total 123	O 123	0	0
39	B	139	Total 139	O 139	0	0
39	C	177	Total 177	O 177	0	0
39	D	50	Total 50	O 50	0	0
39	E	43	Total 43	O 43	0	0
39	F	28	Total 28	O 28	0	0
39	G	16	Total 16	O 16	0	0
39	H	71	Total 71	O 71	0	0
39	J	53	Total 53	O 53	0	0
39	K	57	Total 57	O 57	0	0
39	L	82	Total 82	O 82	0	0
39	M	125	Total 125	O 125	0	0
39	N	59	Total 59	O 59	0	0
39	O	35	Total 35	O 35	0	0
39	P	59	Total 59	O 59	0	0
39	Q	48	Total 48	O 48	0	0
39	R	86	Total 86	O 86	0	0
39	S	31	Total 31	O 31	0	0

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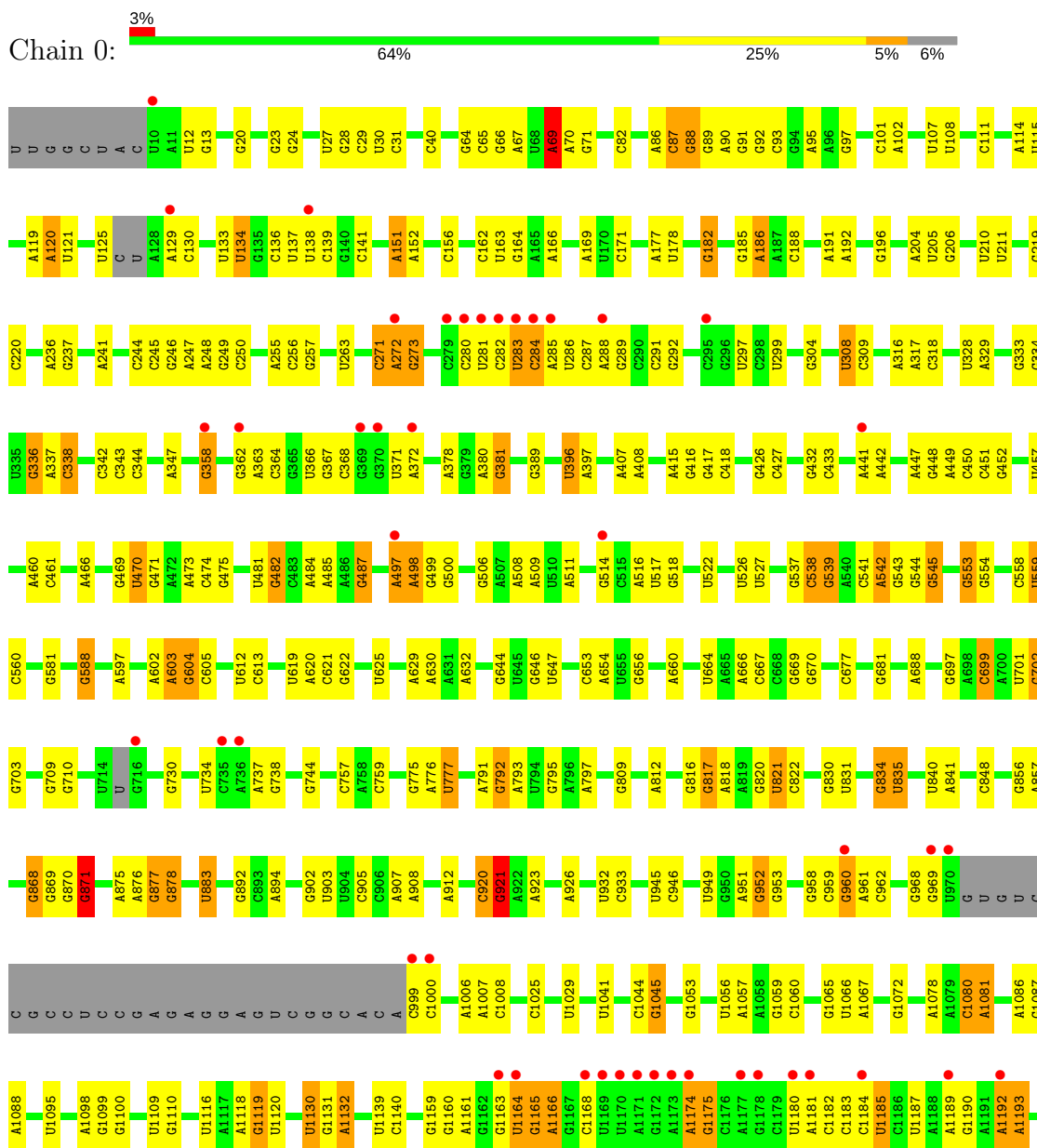
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	T	36	Total 36	O 36	0	0
39	U	26	Total 26	O 26	0	0
39	V	11	Total 11	O 11	0	0
39	W	68	Total 68	O 68	0	0
39	X	23	Total 23	O 23	0	0
39	Y	93	Total 93	O 93	0	0
39	Z	28	Total 28	O 28	0	0
39	1	51	Total 51	O 51	0	0
39	2	41	Total 41	O 41	0	0
39	3	67	Total 67	O 67	0	0
39	I	9	Total 9	O 9	0	0

3 Residue-property plots

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

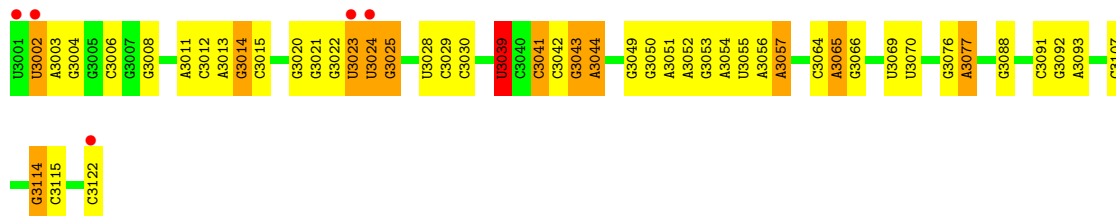
- Molecule 1: 23S ribosomal rna



A2812	A2813	A2814	G2815	G2816	G2817	G2818	G2819	G2820	G2821	G2822	G2823	G2824	G2825	G2826	G2827	G2828	G2829	G2830	G2831	G2832	G2833	G2834	G2835	G2836	G2837	G2838	G2839	G2840	G2841	G2842	G2843	G2844	G2845	G2846	G2847	G2848	G2849	G2850	G2851	G2852	G2853	G2854	G2855	G2856	G2857	G2858	G2859	G2860	G2861	G2862	G2863	G2864	G2865	G2866	G2867	G2868	G2869	G2870	G2871	G2872	G2873	G2874	G2875	G2876	G2877	G2878	G2879	G2880	G2881	G2882	G2883	G2884	G2885	G2886	G2887	G2888	G2889	G2890	G2891	G2892	G2893	G2894	G2895	G2896	G2897	G2898	G2899	G2900	G2901	G2902	G2903	G2904	G2905	G2906	G2907	G2908	G2909	G2910	G2911	G2912	G2913	G2914	G2915	G2916	G2917	G2918	G2919	G2920	G2921	G2922	G2923	G2924	G2925	G2926	G2927	G2928	G2929	G2930	G2931	G2932	G2933	G2934	G2935	G2936	G2937	G2938	G2939	G2940	G2941	G2942	G2943	G2944	G2945	G2946	G2947	G2948	G2949	G2950	G2951	G2952	G2953	G2954	G2955	G2956	G2957	G2958	G2959	G2960	G2961	G2962	G2963	G2964	G2965	G2966	G2967	G2968	G2969	G2970	G2971	G2972	G2973	G2974	G2975	G2976	G2977	G2978	G2979	G2980	G2981	G2982	G2983	G2984	G2985	G2986	G2987	G2988	G2989	G2990	G2991	G2992	G2993	G2994	G2995	G2996	G2997	G2998	G2999	G3000	G3001	G3002	G3003	G3004	G3005	G3006	G3007	G3008	G3009	G3010	G3011	G3012	G3013	G3014	G3015	G3016	G3017	G3018	G3019	G3020	G3021	G3022	G3023	G3024	G3025	G3026	G3027	G3028	G3029	G3030	G3031	G3032	G3033	G3034	G3035	G3036	G3037	G3038	G3039	G3040	G3041	G3042	G3043	G3044	G3045	G3046	G3047	G3048	G3049	G3050	G3051	G3052	G3053	G3054	G3055	G3056	G3057	G3058	G3059	G3060	G3061	G3062	G3063	G3064	G3065	G3066	G3067	G3068	G3069	G3070	G3071	G3072	G3073	G3074	G3075	G3076	G3077	G3078	G3079	G3080	G3081	G3082	G3083	G3084	G3085	G3086	G3087	G3088	G3089	G3090	G3091	G3092	G3093	G3094	G3095	G3096	G3097	G3098	G3099	G3100	G3101	G3102	G3103	G3104	G3105	G3106	G3107	G3108	G3109	G3110	G3111	G3112	G3113	G3114	G3115	G3116	G3117	G3118	G3119	G3120	G3121	G3122	G3123	G3124	G3125	G3126	G3127	G3128	G3129	G3130	G3131	G3132	G3133	G3134	G3135	G3136	G3137	G3138	G3139	G3140	G3141	G3142	G3143	G3144	G3145	G3146	G3147	G3148	G3149	G3150	G3151	G3152	G3153	G3154	G3155	G3156	G3157	G3158	G3159	G3160	G3161	G3162	G3163	G3164	G3165	G3166	G3167	G3168	G3169	G3170	G3171	G3172	G3173	G3174	G3175	G3176	G3177	G3178	G3179	G3180	G3181	G3182	G3183	G3184	G3185	G3186	G3187	G3188	G3189	G3190	G3191	G3192	G3193	G3194	G3195	G3196	G3197	G3198	G3199	G3200	G3201	G3202	G3203	G3204	G3205	G3206	G3207	G3208	G3209	G3210	G3211	G3212	G3213	G3214	G3215	G3216	G3217	G3218	G3219	G3220	G3221	G3222	G3223	G3224	G3225	G3226	G3227	G3228	G3229	G3230	G3231	G3232	G3233	G3234	G3235	G3236	G3237	G3238	G3239	G3240	G3241	G3242	G3243	G3244	G3245	G3246	G3247	G3248	G3249	G3250	G3251	G3252	G3253	G3254	G3255	G3256	G3257	G3258	G3259	G3260	G3261	G3262	G3263	G3264	G3265	G3266
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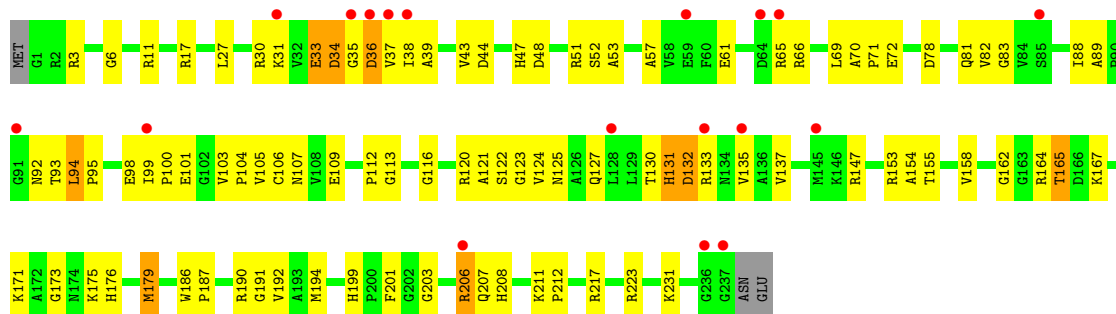
- Molecule 2: 5S ribosomal RNA



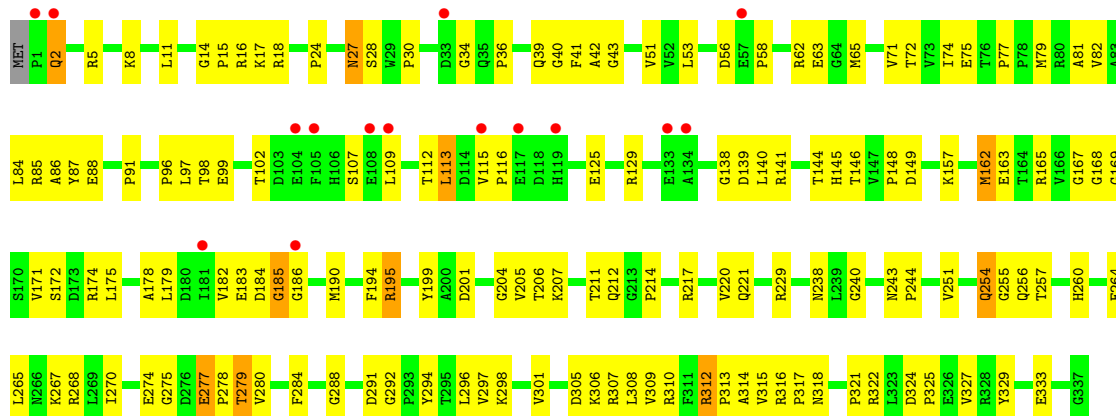
- Molecule 3: 5'-R(*CP*CP*(PPU)P*(PO2)P*(DA)P*C*C)-3')



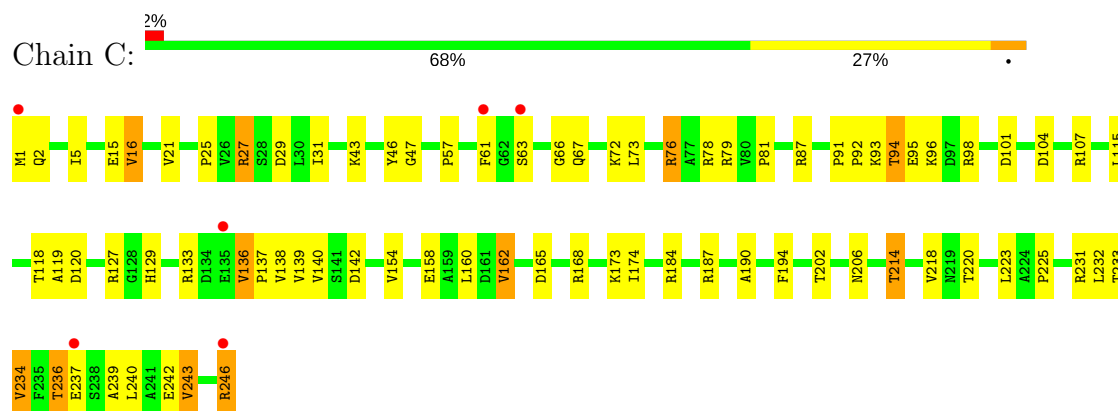
- Molecule 4: 50S ribosomal protein L2P



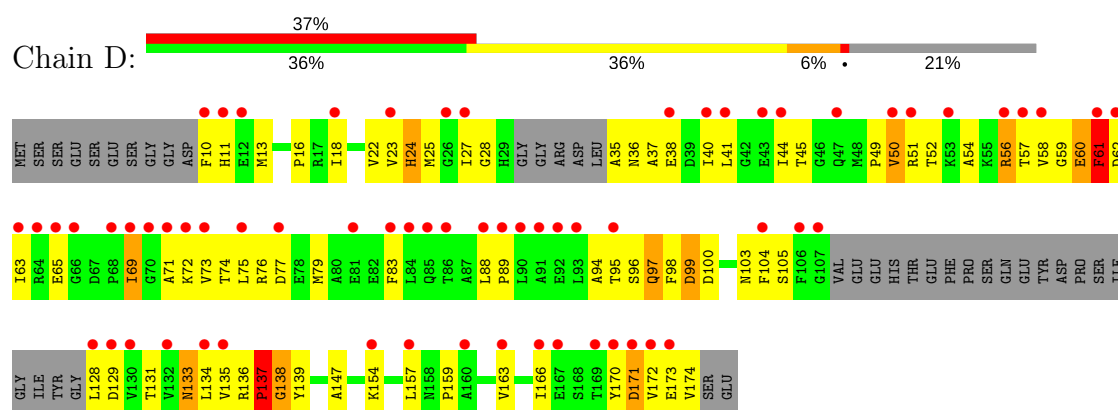
- Molecule 5: 50S ribosomal protein L3P



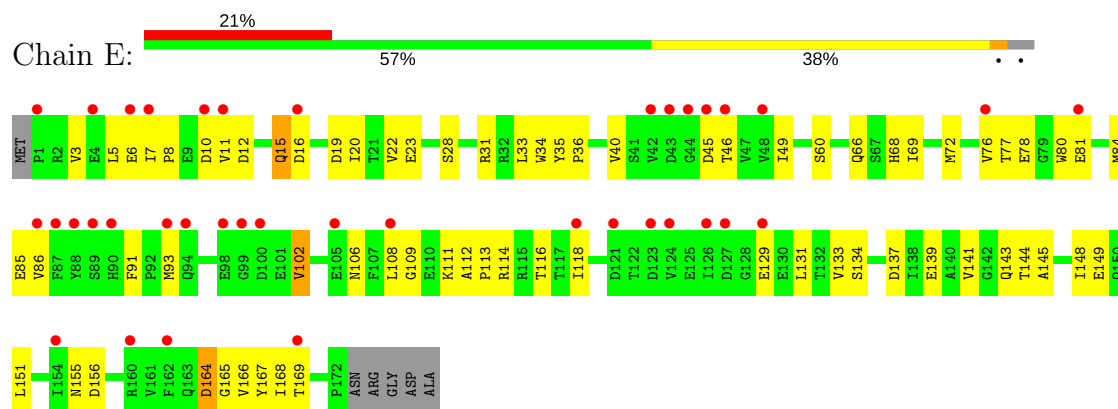
• Molecule 6: 50S ribosomal protein L4E



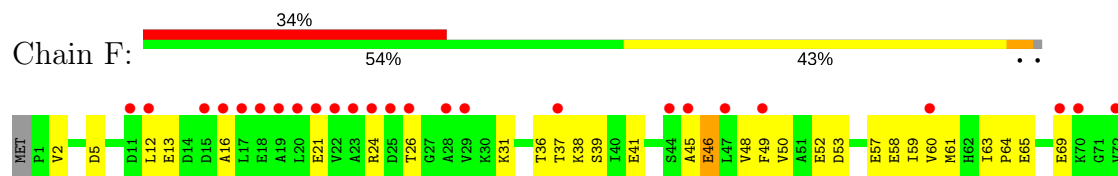
• Molecule 7: 50S ribosomal protein L5P

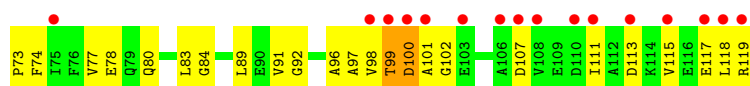


• Molecule 8: 50S ribosomal protein L6P

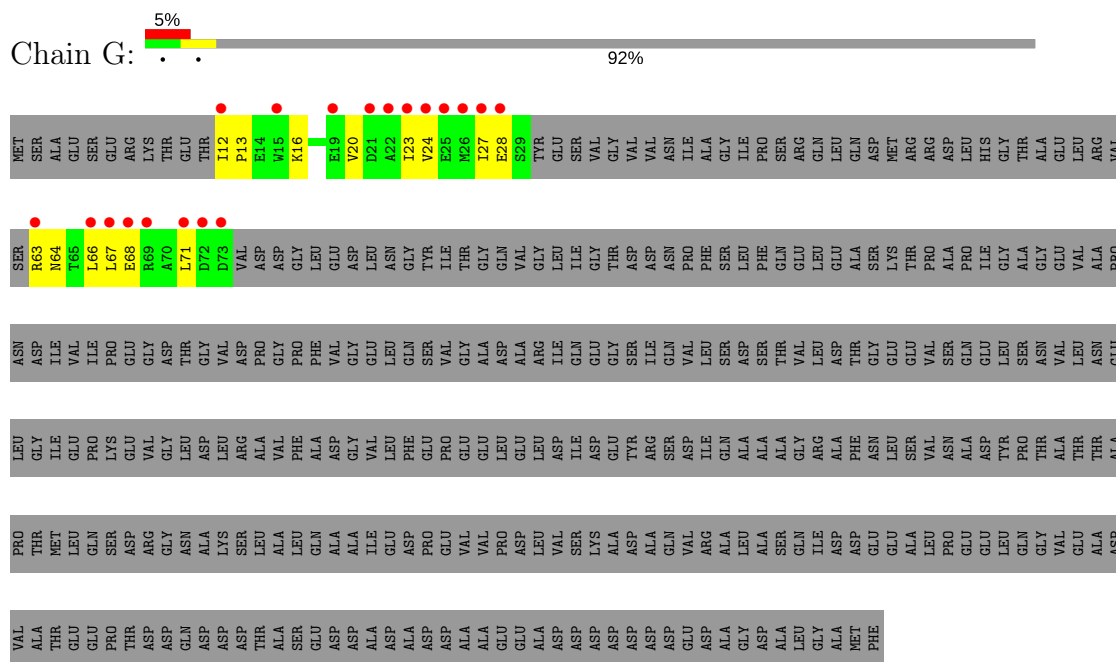


• Molecule 9: 50S ribosomal protein L7AE

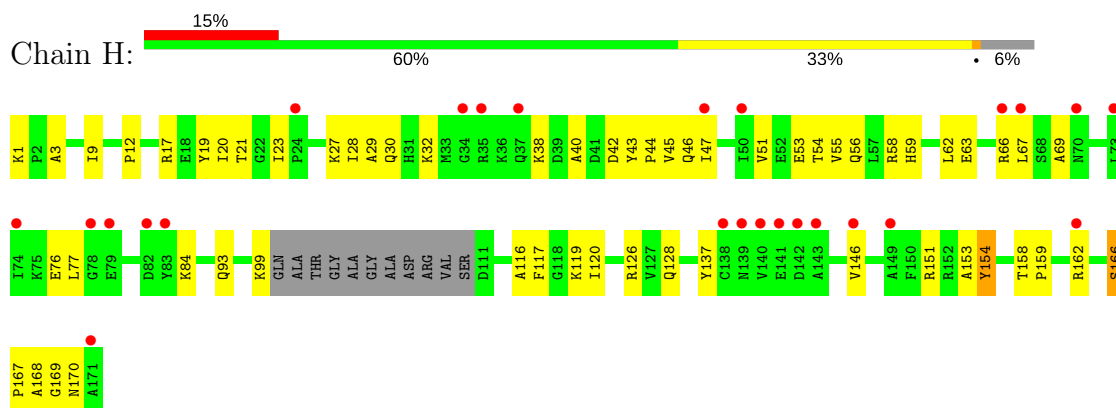




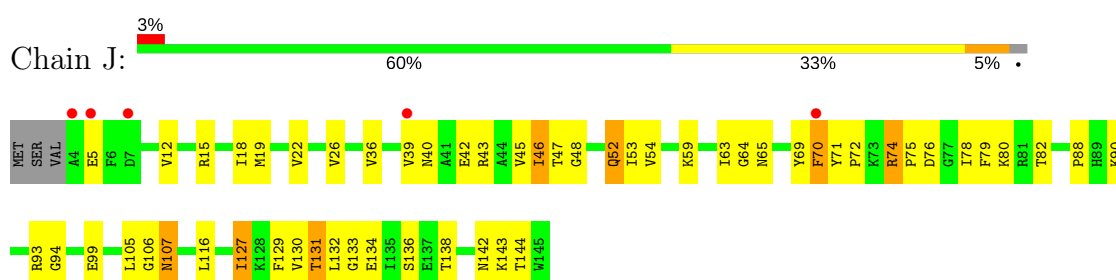
• Molecule 10: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG



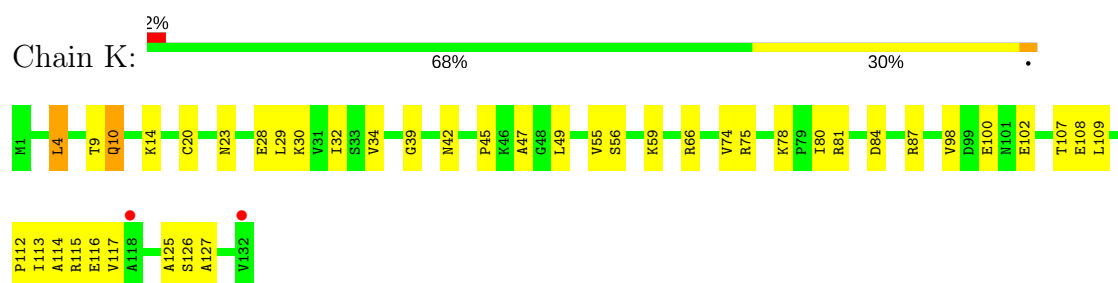
• Molecule 11: 50S RIBOSOMAL PROTEIN L10E



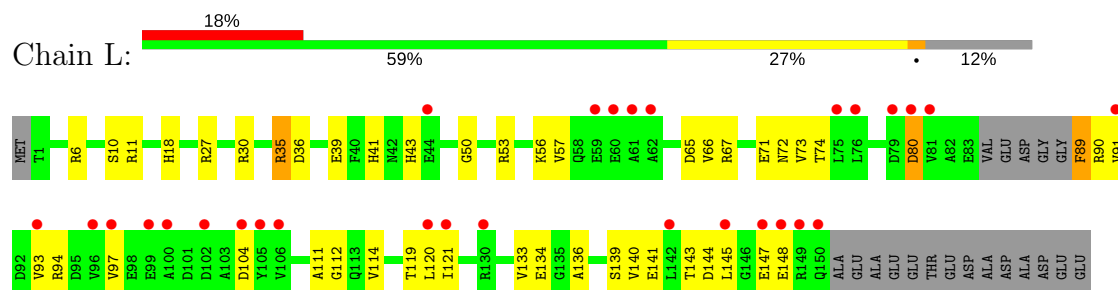
• Molecule 12: 50S ribosomal protein L13P



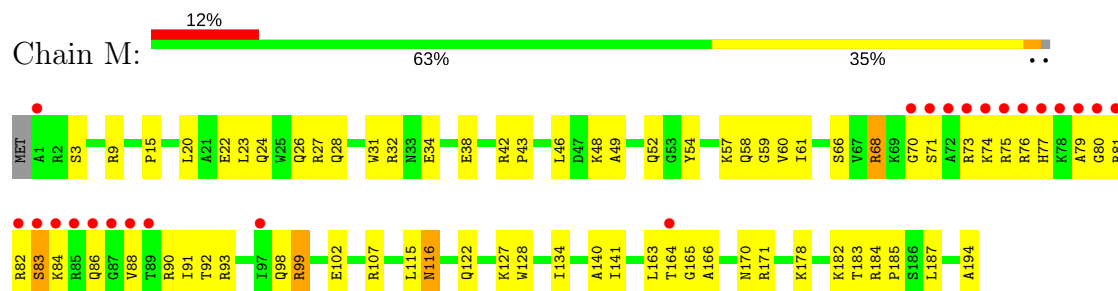
• Molecule 13: 50S ribosomal protein L14P



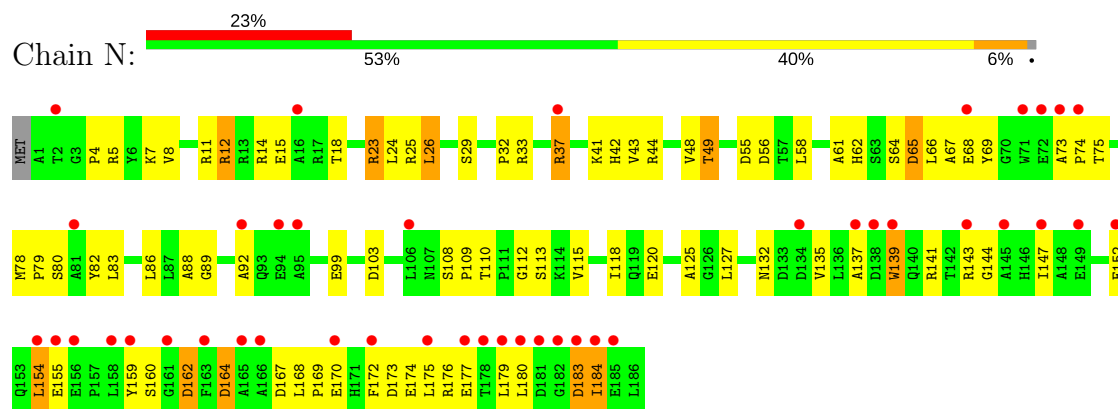
• Molecule 14: 50S ribosomal protein L15P



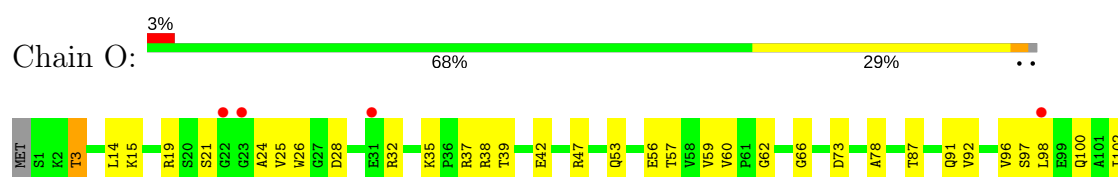
• Molecule 15: 50S Ribosomal Protein L15E



• Molecule 16: 50S ribosomal protein L18P



• Molecule 17: 50S ribosomal protein L18e

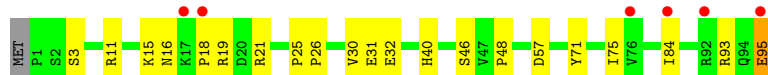
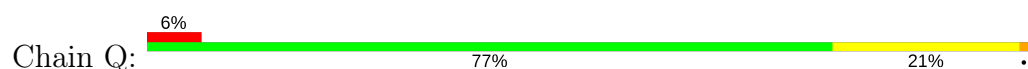




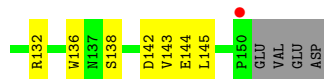
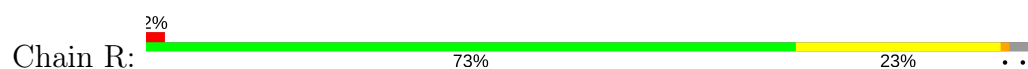
- Molecule 18: 50S ribosomal protein L19E



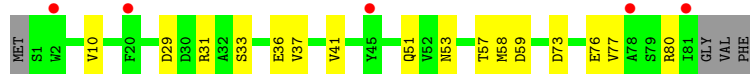
- Molecule 19: 50S ribosomal protein L21e



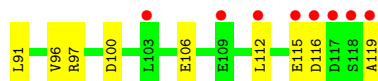
- Molecule 20: 50S ribosomal protein L22P



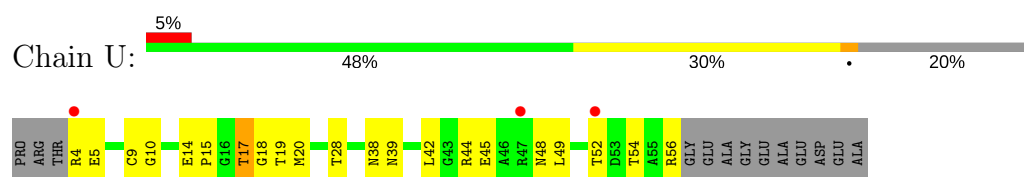
- Molecule 21: 50S ribosomal protein L23P



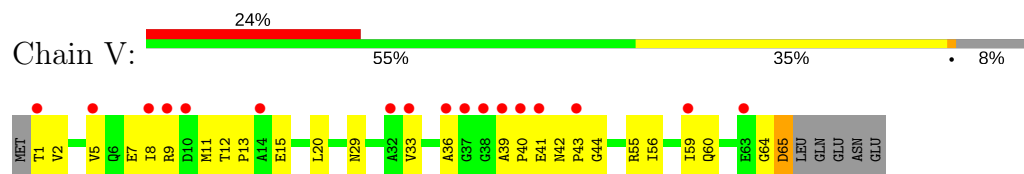
- Molecule 22: 50S ribosomal protein L24P



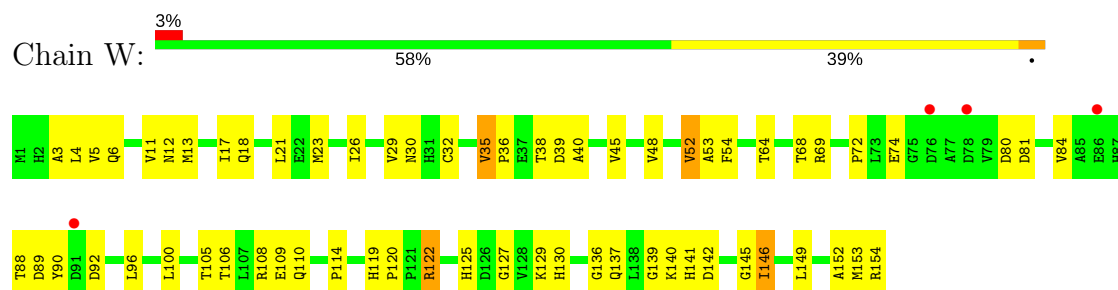
- Molecule 23: 50S ribosomal protein L24E



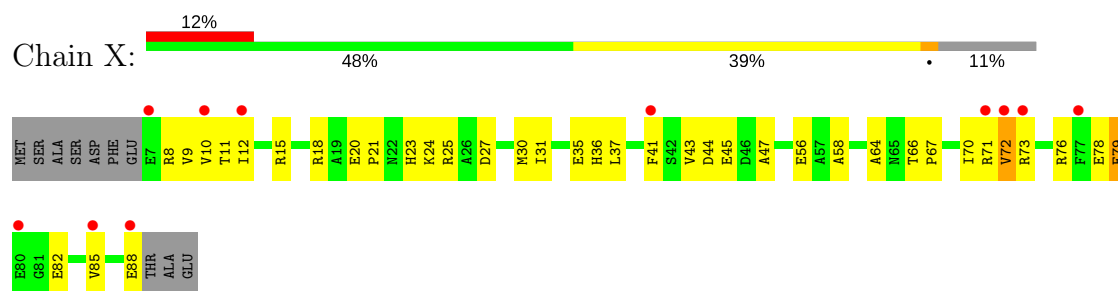
- Molecule 24: 50S ribosomal protein L29P



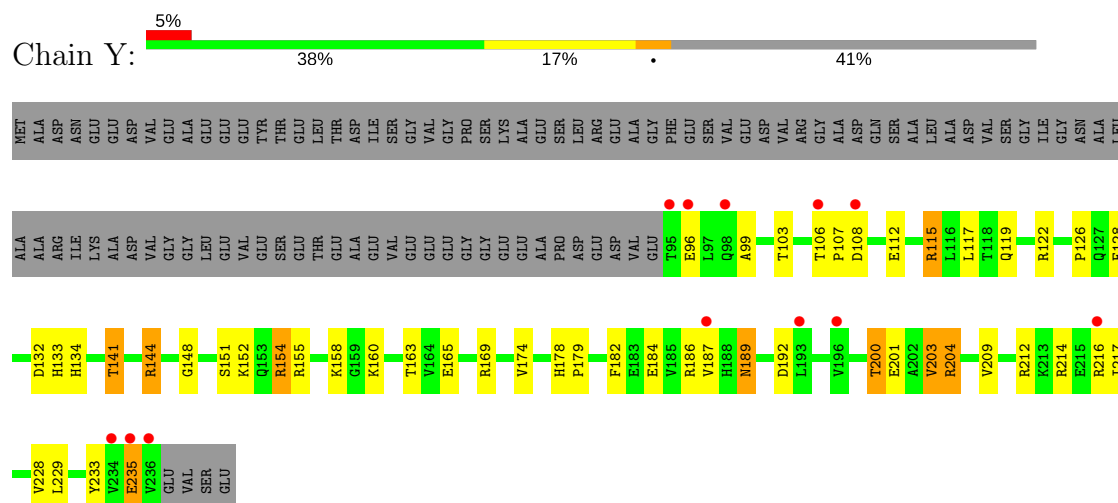
- Molecule 25: 50S ribosomal protein L30P



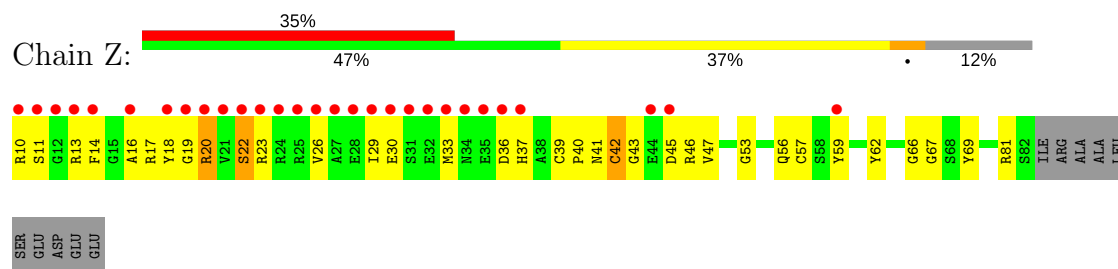
- Molecule 26: 50S ribosomal protein L31e



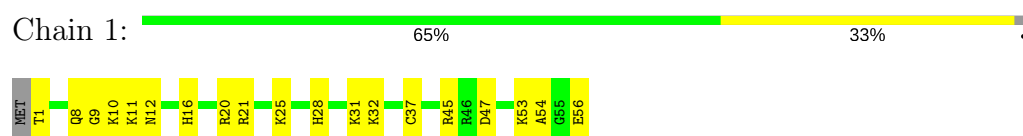
- Molecule 27: 50S ribosomal protein L32E



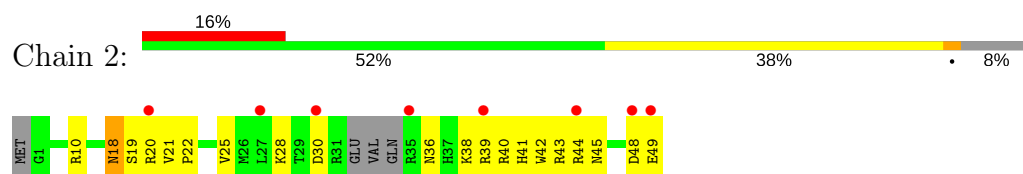
- Molecule 28: 50S ribosomal protein L37Ae



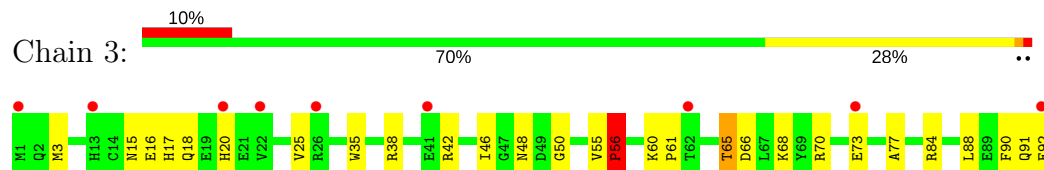
- Molecule 29: 50S ribosomal protein L37e



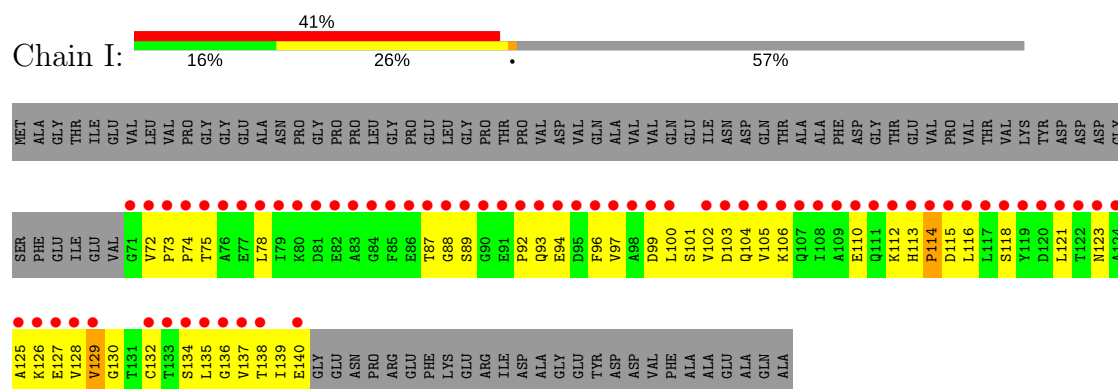
- Molecule 30: 50S ribosomal protein L39e



- Molecule 31: 50S ribosomal protein L44E



- Molecule 32: 50S RIBOSOMAL PROTEIN L11P



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.44Å 298.56Å 574.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 49.61 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.00-2.30) 89.8 (49.61-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.214 , 0.247 0.206 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	47.8	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 61.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	99045	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMG, PPU, CL, SR, NA, K, PO2, CD, OMU, UR3, IMA, 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	24/102870 (0.0%)
2	9	0.32	0/2905	0.70	1/4528 (0.0%)
3	4	0.48	0/102	0.75	0/149
4	A	0.33	0/1786	0.65	0/2408
5	B	0.32	0/2690	0.64	0/3652
6	C	0.37	0/1884	0.65	0/2551
7	D	0.29	0/1111	0.53	0/1498
8	E	0.31	0/1382	0.56	0/1880
9	F	0.30	0/901	0.53	0/1224
10	G	0.27	0/241	0.46	0/324
11	H	0.33	0/1287	0.64	0/1725
12	J	0.34	0/1136	0.60	0/1530
13	K	0.35	0/1001	0.66	0/1347
14	L	0.32	0/1130	0.63	0/1509
15	M	0.35	0/1584	0.60	0/2119
16	N	0.28	0/1474	0.60	0/1999
17	O	0.32	0/874	0.58	1/1181 (0.1%)
18	P	0.34	0/1147	0.55	0/1528
19	Q	0.35	0/749	0.68	0/1005
20	R	0.35	0/1172	0.66	1/1578 (0.1%)
21	S	0.32	0/648	0.58	0/875
22	T	0.30	0/958	0.62	0/1289
23	U	0.34	0/417	0.56	0/562
24	V	0.26	0/502	0.50	0/675
25	W	0.33	0/1219	0.59	0/1655
26	X	0.32	0/664	0.59	0/895
27	Y	0.35	0/1146	0.65	0/1536
28	Z	0.33	0/589	0.59	0/787
29	1	0.44	0/438	0.66	0/578
30	2	0.34	0/401	0.58	0/529
31	3	0.35	0/771	0.58	0/1024
32	I	0.28	0/526	0.50	0/716

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.36	0/98794	0.67	27/147726 (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	44
2	9	0	1
All	All	0	45

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1819	G	C5'-C4'-C3'	7.74	128.38	116.00
1	0	871	G	C5'-C4'-O4'	-7.70	99.86	109.10
1	0	1942	A	C5'-C4'-C3'	7.40	127.83	116.00
2	9	3039	U	N1-C1'-C2'	6.97	123.06	114.00
1	0	1979	G	C2'-C3'-O3'	6.95	124.81	113.70
1	0	1592	G	N9-C1'-C2'	6.57	122.55	114.00
1	0	777	U	O4'-C1'-N1	6.41	113.33	108.20
1	0	1819	G	C4'-C3'-C2'	-6.14	96.46	102.60
1	0	1819	G	C1'-O4'-C4'	-6.12	105.01	109.90
1	0	1504	A	C1'-O4'-C4'	-6.09	105.03	109.90
1	0	389	G	C5'-C4'-C3'	-5.79	106.74	116.00
1	0	883	U	N1-C1'-C2'	5.75	121.47	114.00
1	0	2467	A	C1'-O4'-C4'	-5.66	105.37	109.90
1	0	2291	A	N9-C1'-C2'	5.62	121.31	114.00
1	0	206	G	C5'-C4'-C3'	-5.50	107.19	116.00
1	0	2726	U	N1-C1'-C2'	5.31	120.90	114.00
1	0	1261	A	N9-C1'-C2'	5.26	120.84	114.00
1	0	2313	C	C5'-C4'-O4'	5.21	115.36	109.10
1	0	1504	A	N9-C1'-C2'	5.17	120.73	114.00
17	O	66	GLY	N-CA-C	5.17	126.03	113.10
1	0	1615	A	C5'-C4'-C3'	5.12	124.18	116.00
1	0	841	A	C1'-O4'-C4'	-5.11	105.81	109.90
1	0	921	G	N9-C1'-C2'	5.09	120.62	114.00
1	0	1120	U	C5'-C4'-C3'	-5.09	107.85	116.00
1	0	69	A	C5'-C4'-O4'	-5.06	103.03	109.10
1	0	1452	G	C5'-C4'-C3'	-5.03	107.96	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	R	128	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

All (45) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1078	A	Sidechain
1	0	1132	A	Sidechain
1	0	1327	G	Sidechain
1	0	1340	G	Sidechain
1	0	1342	C	Sidechain
1	0	1361	C	Sidechain
1	0	1458	A	Sidechain
1	0	1777	G	Sidechain
1	0	1809	G	Sidechain
1	0	1819	G	Sidechain
1	0	182	G	Sidechain
1	0	1829	A	Sidechain
1	0	1845	A	Sidechain
1	0	1863	G	Sidechain
1	0	1867	G	Sidechain
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	1970	G	Sidechain
1	0	1979	G	Sidechain
1	0	2036	C	Sidechain
1	0	2412	G	Sidechain
1	0	2465	A	Sidechain
1	0	2493	C	Sidechain
1	0	2503	A	Sidechain
1	0	2506	A	Sidechain
1	0	2552	C	Sidechain
1	0	2599	A	Sidechain
1	0	2607	U	Sidechain
1	0	2632	G	Sidechain
1	0	2842	G	Sidechain
1	0	396	U	Sidechain
1	0	460	A	Sidechain
1	0	469	G	Sidechain
1	0	470	U	Sidechain
1	0	471	G	Sidechain
1	0	482	G	Sidechain

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Mol	Chain	Res	Type	Group
1	0	518	G	Sidechain
1	0	554	G	Sidechain
1	0	619	U	Sidechain
1	0	792	G	Sidechain
1	0	795	G	Sidechain
1	0	817	G	Sidechain
1	0	868	G	Sidechain
1	0	952	G	Sidechain
2	9	3039	U	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59021	0	29813	714	0
2	9	2600	0	1326	52	0
3	4	135	0	83	3	0
4	A	1753	0	1766	108	0
5	B	2625	0	2532	133	0
6	C	1859	0	1816	89	0
7	D	1094	0	1085	77	0
8	E	1357	0	1266	55	0
9	F	890	0	843	47	0
10	G	240	0	231	14	0
11	H	1266	0	1268	57	0
12	J	1120	0	1098	78	0
13	K	992	0	1031	46	0
14	L	1118	0	1076	50	0
15	M	1560	0	1568	72	0
16	N	1445	0	1401	86	0
17	O	865	0	873	37	0
18	P	1136	0	1123	38	0
19	Q	735	0	729	17	0
20	R	1149	0	1122	36	0
21	S	641	0	605	16	0
22	T	950	0	924	49	0
23	U	410	0	364	21	0
24	V	499	0	511	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	W	1196	0	1137	91	0
26	X	654	0	653	38	0
27	Y	1130	0	1133	61	0
28	Z	578	0	539	39	0
29	1	431	0	426	26	0
30	2	396	0	413	28	0
31	3	755	0	728	28	0
32	I	519	0	500	50	0
33	0	87	0	0	0	0
33	2	1	0	0	0	0
33	9	1	0	0	0	0
33	A	1	0	0	0	0
33	B	1	0	0	0	0
33	K	1	0	0	0	0
33	T	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	2	0	0	0	0
35	0	62	0	0	0	0
35	3	1	0	0	0	0
35	9	3	0	0	0	0
35	C	1	0	0	0	0
35	H	1	0	0	0	0
35	J	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	3	0	0	0	0
35	S	1	0	0	0	0
36	0	10	0	0	0	0
36	3	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	J	3	0	0	1	0
36	L	1	0	0	0	0
36	M	1	0	0	0	0
36	N	1	0	0	1	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
36	Y	1	0	0	0	0
37	0	98	0	0	0	0
37	1	2	0	0	0	0
37	3	1	0	0	0	0
37	9	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	A	3	0	0	0	0
37	B	2	0	0	0	0
37	F	1	0	0	0	0
37	H	1	0	0	0	0
37	L	1	0	0	0	0
37	R	1	0	0	0	0
37	S	1	0	0	0	0
38	1	1	0	0	0	0
38	3	1	0	0	0	0
38	O	1	0	0	0	0
38	U	1	0	0	0	0
38	Z	1	0	0	0	0
39	0	5739	0	0	94	0
39	1	51	0	0	1	0
39	2	41	0	0	1	0
39	3	67	0	0	3	0
39	4	8	0	0	0	0
39	9	132	0	0	8	0
39	A	123	0	0	14	0
39	B	139	0	0	19	0
39	C	177	0	0	16	0
39	D	50	0	0	5	0
39	E	43	0	0	2	0
39	F	28	0	0	2	0
39	G	16	0	0	2	0
39	H	71	0	0	8	0
39	I	9	0	0	1	0
39	J	53	0	0	3	0
39	K	57	0	0	4	0
39	L	82	0	0	11	0
39	M	125	0	0	7	0
39	N	59	0	0	7	0
39	O	35	0	0	3	0
39	P	59	0	0	0	0
39	Q	48	0	0	5	0
39	R	86	0	0	2	0
39	S	31	0	0	1	0
39	T	36	0	0	1	0
39	U	26	0	0	1	0
39	V	11	0	0	1	0
39	W	68	0	0	3	0
39	X	23	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	Y	93	0	0	9	0
39	Z	28	0	0	3	0
All	All	99045	0	59983	2061	0

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

All (2061) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:21:LEU:HD21	25:W:48:VAL:HG11	1.23	1.17
26:X:37:LEU:HD13	26:X:85:VAL:HG21	1.31	1.10
2:9:3076:G:H3'	2:9:3077:A:H5''	1.35	1.08
6:C:236:THR:HG22	6:C:239:ALA:H	1.14	1.06
1:0:133:U:H2'	1:0:134:U:H5''	1.37	1.02
13:K:29:LEU:HB3	13:K:55:VAL:HG11	1.42	0.99
22:T:9:LYS:HE3	22:T:13:ARG:NH1	1.78	0.99
7:D:25:MET:HE2	7:D:41:LEU:HG	1.45	0.98
21:S:51:GLN:HE21	21:S:53:ASN:HD21	1.07	0.98
13:K:81:ARG:HB2	13:K:87:ARG:HH11	1.29	0.98
1:0:156:C:H5''	15:M:171:ARG:HD3	1.44	0.97
6:C:104:ASP:HA	6:C:107:ARG:HH12	1.29	0.97
11:H:46:GLN:HB3	11:H:167:PRO:HD2	1.46	0.97
13:K:74:VAL:HG11	13:K:113:ILE:HG12	1.45	0.97
28:Z:11:SER:HB3	28:Z:23:ARG:HB2	1.47	0.96
6:C:127:ARG:NH2	6:C:225:PRO:HG2	1.80	0.96
30:2:18:ASN:HD21	30:2:40:ARG:H	1.05	0.96
7:D:28:GLY:HA2	7:D:69:ILE:HG23	1.48	0.96
15:M:99:ARG:HH21	15:M:170:ASN:HD22	1.13	0.95
9:F:91:VAL:HG12	9:F:92:GLY:H	1.27	0.95
1:0:2812:A:H2	1:0:2814:A:H62	1.11	0.95
29:1:25:LYS:HD2	30:2:49:GLU:H	1.29	0.94
22:T:71:VAL:HG11	22:T:90:PRO:HB3	1.46	0.94
13:K:10:GLN:H	13:K:10:GLN:NE2	1.64	0.93
1:0:542:A:H5'	1:0:542:A:H8	1.34	0.93
1:0:1242:A:H5'	12:J:82:THR:HG23	1.50	0.93
28:Z:36:ASP:HB3	28:Z:45:ASP:HB3	1.48	0.92
1:0:1160:G:H5'	1:0:1161:A:H5'	1.51	0.91
24:V:12:THR:HG22	24:V:15:GLU:HG3	1.53	0.91
15:M:107:ARG:HH11	15:M:107:ARG:HG3	1.36	0.91
30:2:41:HIS:H	30:2:45:ASN:HD22	1.13	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:10:GLN:N	13:K:10:GLN:HE21	1.69	0.90
1:0:2717:C:H2'	1:0:2718:C:H5''	1.53	0.90
16:N:83:LEU:HD13	16:N:175:LEU:HD23	1.52	0.89
1:0:1372:A:H3'	39:0:7657:HOH:O	1.71	0.89
28:Z:46:ARG:HD2	28:Z:59:TYR:HB2	1.53	0.89
13:K:74:VAL:HG13	13:K:113:ILE:HG23	1.55	0.89
8:E:20:ILE:HD11	8:E:40:VAL:HG11	1.53	0.89
25:W:6:GLN:HB2	25:W:26:ILE:HD12	1.56	0.88
12:J:19:MET:HE1	12:J:132:LEU:HD21	1.54	0.88
6:C:1:MET:HG2	6:C:2:GLN:H	1.39	0.88
6:C:5:ILE:HD11	6:C:16:VAL:HG22	1.56	0.88
1:0:1466:C:H42	1:0:1476:A:H61	1.18	0.87
2:9:3056:A:H2'	2:9:3057:A:H5''	1.55	0.87
13:K:10:GLN:H	13:K:10:GLN:HE21	0.87	0.87
20:R:99:ALA:HB1	20:R:109:MET:HE1	1.57	0.86
1:0:2506:A:HO2'	1:0:2507:G:H8	0.87	0.86
1:0:541:C:H2'	1:0:542:A:H5''	1.57	0.86
1:0:1835:U:H5	1:0:1840:A:N7	1.74	0.86
13:K:39:GLY:HA2	39:K:4183:HOH:O	1.74	0.86
5:B:238:ASN:HD22	5:B:240:GLY:H	1.20	0.86
7:D:58:VAL:HB	7:D:62:ASP:HB3	1.57	0.86
1:0:2840:A:OP1	5:B:211:THR:HG23	1.77	0.84
15:M:102:GLU:OE1	15:M:164:THR:HG21	1.77	0.84
1:0:2717:C:C2'	1:0:2718:C:H5''	2.06	0.84
22:T:112:LEU:HD23	22:T:119:ALA:HB3	1.59	0.84
6:C:236:THR:HG22	6:C:239:ALA:N	1.91	0.84
20:R:25:PHE:CE2	20:R:29:LYS:HE2	2.12	0.84
5:B:36:PRO:HA	5:B:168:GLY:HA3	1.59	0.84
5:B:264:GLU:HG2	5:B:267:LYS:HE2	1.59	0.84
1:0:1593:C:OP1	18:P:117:SER:HB3	1.78	0.84
12:J:93:ARG:HH11	12:J:93:ARG:HB3	1.43	0.84
1:0:289:G:H22	1:0:363:A:H2	1.25	0.83
25:W:21:LEU:HD13	25:W:26:ILE:HD11	1.60	0.83
13:K:81:ARG:HB2	13:K:87:ARG:NH1	1.91	0.83
25:W:13:MET:HE1	25:W:18:GLN:HA	1.60	0.83
4:A:206:ARG:HD3	4:A:206:ARG:H	1.41	0.83
1:0:2073:G:H5''	39:0:4402:HOH:O	1.77	0.82
22:T:41:ARG:HG2	22:T:41:ARG:HH11	1.44	0.82
25:W:122:ARG:NH2	25:W:154:ARG:HG2	1.94	0.82
13:K:109:LEU:HD13	13:K:113:ILE:HD11	1.61	0.82
1:0:871:G:C8	1:0:871:G:H5'	2.15	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:81:GLN:HB2	4:A:92:ASN:ND2	1.94	0.82
4:A:191:GLY:HA2	4:A:194:MET:CE	2.09	0.82
6:C:115:LEU:HD21	6:C:243:VAL:HG13	1.62	0.82
25:W:88:THR:HB	39:W:6679:HOH:O	1.80	0.82
13:K:14:LYS:HB2	13:K:45:PRO:HG2	1.62	0.81
16:N:7:LYS:HE3	19:Q:21:ARG:O	1.80	0.81
17:O:32:ARG:HE	17:O:35:LYS:HD2	1.45	0.81
7:D:172:VAL:HG12	7:D:173:GLU:H	1.43	0.81
24:V:1:THR:HG23	24:V:2:VAL:H	1.46	0.81
16:N:144:GLY:O	16:N:147:ILE:HG22	1.79	0.81
4:A:69:LEU:HD23	4:A:107:ASN:HB2	1.62	0.81
6:C:104:ASP:HA	6:C:107:ARG:NH1	1.96	0.81
1:O:1116:U:O2'	1:O:1118:A:H2	1.64	0.81
1:O:2851:G:C2'	1:O:2852:A:H5'	2.11	0.81
8:E:81:GLU:HG2	8:E:134:SER:HB3	1.63	0.81
1:O:1603:A:H5'	1:O:1605:G:O4'	1.82	0.80
4:A:192:VAL:HG22	39:A:9620:HOH:O	1.79	0.80
1:O:133:U:C2'	1:O:134:U:H5''	2.11	0.80
8:E:36:PRO:HD3	12:J:127:ILE:HD12	1.63	0.80
1:O:1474:C:H6	1:O:1474:C:H5'	1.47	0.80
1:O:560:C:H42	1:O:597:A:H61	1.27	0.80
1:O:1159:G:H21	1:O:1189:A:H8	1.30	0.80
27:Y:200:THR:HG22	27:Y:201:GLU:HG3	1.62	0.80
22:T:9:LYS:HE3	22:T:13:ARG:CZ	2.12	0.80
13:K:4:LEU:HD22	13:K:116:GLU:HB3	1.63	0.80
17:O:32:ARG:HD3	17:O:32:ARG:O	1.82	0.80
18:P:115:SER:H	18:P:118:GLN:HE21	1.30	0.80
1:O:541:C:C2'	1:O:542:A:H5''	2.12	0.79
8:E:15:GLN:HG3	8:E:20:ILE:HG12	1.63	0.79
16:N:113:SER:HB2	39:N:9354:HOH:O	1.82	0.79
4:A:192:VAL:HB	39:A:9583:HOH:O	1.81	0.79
39:O:5382:HOH:O	12:J:47:THR:HB	1.80	0.79
15:M:79:ALA:HB3	15:M:81:ARG:HH12	1.45	0.79
1:O:2506:A:O2'	1:O:2507:G:H8	1.64	0.79
7:D:154:LYS:HD2	7:D:154:LYS:H	1.47	0.79
15:M:28:GLN:O	15:M:32:ARG:HG3	1.83	0.79
20:R:99:ALA:HB1	20:R:109:MET:CE	2.13	0.79
1:O:2054:A:N3	20:R:128:ARG:NH2	2.31	0.79
1:O:1041:U:H5'	39:L:9490:HOH:O	1.82	0.79
1:O:1701:A:H4'	1:O:1702:U:H5''	1.65	0.79
1:O:1838:U:H1'	1:O:2644:C:H5'	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:1:25:LYS:HD2	30:2:49:GLU:N	1.98	0.79
1:0:1118:A:H62	1:0:1244:U:H3	1.30	0.79
27:Y:154:ARG:HH12	27:Y:155:ARG:HG3	1.48	0.79
32:I:78:LEU:HD12	32:I:112:LYS:HZ2	1.49	0.78
4:A:191:GLY:HA2	4:A:194:MET:HE2	1.64	0.78
22:T:63:ILE:HD11	22:T:75:GLU:HB2	1.66	0.78
16:N:11:ARG:HG3	16:N:14:ARG:HH12	1.49	0.78
5:B:212:GLN:HB2	5:B:257:THR:HG21	1.65	0.77
15:M:79:ALA:HB3	15:M:81:ARG:NH1	1.99	0.77
25:W:21:LEU:CD2	25:W:48:VAL:HG11	2.10	0.77
26:X:30:MET:HE1	26:X:58:ALA:HB3	1.66	0.77
5:B:307:ARG:HH11	5:B:307:ARG:HG3	1.46	0.77
14:L:91:VAL:HG13	14:L:120:LEU:HD23	1.67	0.77
27:Y:235:GLU:H	27:Y:235:GLU:CD	1.85	0.77
9:F:50:VAL:HG13	9:F:60:VAL:HG11	1.66	0.77
20:R:18:LEU:HB2	20:R:143:VAL:HG12	1.67	0.77
1:0:870:G:H2'	1:0:871:G:H5''	1.67	0.77
11:H:56:GLN:HE21	11:H:126:ARG:HE	1.32	0.77
1:0:1667:A:H8	1:0:1667:A:H5'	1.50	0.77
6:C:246:ARG:HH11	6:C:246:ARG:HB3	1.49	0.76
1:0:1116:U:HO2'	1:0:1118:A:H2	0.80	0.76
1:0:1751:G:H2'	1:0:1752:G:H5''	1.67	0.76
1:0:1973:A:H5'	1:0:1973:A:H8	1.50	0.76
2:9:3039:U:H1'	2:9:3044:A:H61	1.50	0.76
5:B:18:ARG:HG3	5:B:256:GLN:HG3	1.66	0.76
1:0:1119:G:H2'	12:J:52:GLN:NE2	2.01	0.76
5:B:162:MET:HE2	5:B:310:ARG:HD3	1.68	0.76
8:E:15:GLN:HG2	8:E:19:ASP:O	1.84	0.76
1:0:1165:G:H4'	1:0:1174:A:O2'	1.86	0.76
1:0:2851:G:H2'	1:0:2852:A:H5'	1.68	0.76
4:A:192:VAL:CG1	4:A:207:GLN:HB3	2.15	0.76
1:0:1119:G:N2	1:0:1246:A:C2	2.53	0.76
32:I:132:CYS:HB3	32:I:137:VAL:HB	1.66	0.76
6:C:107:ARG:NH1	6:C:107:ARG:HB3	2.02	0.75
1:0:544:G:H2'	1:0:545:G:H5''	1.68	0.75
11:H:27:LYS:H	11:H:59:HIS:HD2	1.30	0.75
21:S:10:VAL:HG11	24:V:36:ALA:HA	1.68	0.75
1:0:559:U:H5'	1:0:559:U:H6	1.51	0.75
14:L:143:THR:HG22	14:L:144:ASP:H	1.49	0.75
1:0:288:A:H61	1:0:364:C:H42	1.32	0.75
32:I:78:LEU:HD12	32:I:112:LYS:NZ	2.02	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:281:U:H2'	1:0:282:C:O4'	1.86	0.74
1:0:871:G:C8	1:0:871:G:C5'	2.70	0.74
8:E:3:VAL:HG22	8:E:49:ILE:HB	1.68	0.74
18:P:115:SER:OG	18:P:118:GLN:HG3	1.87	0.74
16:N:49:THR:HG22	16:N:56:ASP:HB2	1.68	0.74
4:A:95:PRO:HG2	4:A:98:GLU:HG2	1.69	0.74
21:S:57:THR:HG22	21:S:59:ASP:H	1.52	0.74
16:N:132:ASN:O	16:N:135:VAL:HG12	1.87	0.74
1:0:506:G:H22	1:0:509:A:H5''	1.52	0.74
5:B:217:ARG:HG3	5:B:257:THR:HG22	1.70	0.74
25:W:122:ARG:HH11	25:W:122:ARG:HG2	1.53	0.74
1:0:470:U:O2'	29:1:16:HIS:HD2	1.71	0.73
39:0:7902:HOH:O	5:B:211:THR:HG21	1.87	0.73
4:A:192:VAL:HG12	4:A:207:GLN:HB3	1.71	0.73
9:F:58:GLU:HG3	9:F:61:MET:HE1	1.70	0.73
20:R:18:LEU:HD12	20:R:143:VAL:HG11	1.70	0.73
32:I:102:VAL:HG12	32:I:106:LYS:HE3	1.69	0.73
13:K:74:VAL:CG1	13:K:113:ILE:HG12	2.18	0.73
18:P:80:ARG:HG2	18:P:87:ARG:CZ	2.19	0.73
1:0:1175:G:H1'	1:0:1193:A:H2'	1.69	0.73
1:0:2468:A:H61	31:3:48:ASN:HD21	1.37	0.73
1:0:871:G:H8	1:0:871:G:C5'	2.00	0.73
5:B:51:VAL:HG23	5:B:329:TYR:O	1.89	0.73
1:0:380:A:OP2	15:M:9:ARG:HD2	1.89	0.73
7:D:54:ALA:HB2	7:D:69:ILE:HD12	1.71	0.73
18:P:59:ARG:NH2	18:P:66:GLN:HE22	1.86	0.73
1:0:1878:G:H1'	39:0:6632:HOH:O	1.89	0.73
15:M:134:ILE:HG23	15:M:141:ILE:HD13	1.70	0.73
1:0:1160:G:C5'	1:0:1161:A:H5'	2.19	0.73
1:0:2491:G:H1'	39:0:7349:HOH:O	1.87	0.73
25:W:6:GLN:HB2	25:W:26:ILE:CD1	2.19	0.73
25:W:21:LEU:HD21	25:W:48:VAL:CG1	2.12	0.72
6:C:246:ARG:NH1	6:C:246:ARG:HB3	2.04	0.72
28:Z:30:GLU:HA	28:Z:33:MET:HE3	1.72	0.72
17:O:32:ARG:NE	17:O:35:LYS:HD2	2.03	0.72
9:F:53:ASP:OD1	9:F:80:GLN:HB2	1.90	0.72
1:0:1206:U:H6	1:0:1206:U:H5'	1.53	0.72
16:N:37:ARG:HG3	36:N:9307:CL:CL	2.26	0.72
7:D:58:VAL:HG12	7:D:60:GLU:HG2	1.70	0.72
26:X:71:ARG:HD3	39:X:2171:HOH:O	1.90	0.72
1:0:2765:C:H4'	39:0:6049:HOH:O	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:141:ARG:HD2	5:B:163:GLU:OE2	1.90	0.72
39:O:6049:HOH:O	5:B:298:LYS:HG2	1.88	0.72
1:O:2748:G:H2'	39:O:7984:HOH:O	1.90	0.72
28:Z:11:SER:CB	28:Z:23:ARG:HB2	2.20	0.72
7:D:135:VAL:HG21	7:D:139:TYR:CD1	2.25	0.71
25:W:4:LEU:HD22	25:W:52:VAL:HG21	1.72	0.71
1:O:960:G:H4'	39:O:7878:HOH:O	1.89	0.71
9:F:96:ALA:HA	39:F:3111:HOH:O	1.91	0.71
1:O:481:U:H5''	39:O:6176:HOH:O	1.89	0.71
4:A:100:PRO:HG2	4:A:103:VAL:HG21	1.73	0.71
4:A:88:ILE:HD13	4:A:100:PRO:HD3	1.73	0.71
6:C:236:THR:H	6:C:239:ALA:HB3	1.55	0.71
1:O:2291:A:C8	1:O:2309:C:H5'	2.26	0.71
1:O:2716:G:H5''	5:B:206:THR:HG21	1.72	0.71
25:W:137:GLN:HE21	25:W:141:HIS:CE1	2.09	0.71
21:S:51:GLN:HE21	21:S:53:ASN:ND2	1.85	0.71
2:9:3014:G:H8	2:9:3014:G:H5'	1.56	0.71
13:K:32:ILE:HD11	13:K:56:SER:HB3	1.73	0.71
14:L:143:THR:HG22	14:L:144:ASP:N	2.05	0.71
1:O:506:G:H22	1:O:509:A:C5'	2.04	0.71
15:M:134:ILE:CG2	15:M:141:ILE:HD13	2.21	0.71
21:S:51:GLN:NE2	21:S:53:ASN:HD21	1.86	0.71
27:Y:141:THR:HG23	39:Y:9388:HOH:O	1.90	0.71
1:O:93:C:H5''	24:V:1:THR:HB	1.73	0.70
26:X:25:ARG:HD3	26:X:64:ALA:O	1.90	0.70
27:Y:144:ARG:HH11	27:Y:144:ARG:CG	2.02	0.70
1:O:1118:A:H3'	1:O:1118:A:H8	1.56	0.70
5:B:179:LEU:O	5:B:183:GLU:HG2	1.92	0.70
23:U:14:GLU:O	23:U:17:THR:HB	1.92	0.70
9:F:58:GLU:HA	9:F:61:MET:HE2	1.73	0.70
24:V:12:THR:HG22	24:V:15:GLU:CG	2.20	0.70
1:O:1700:C:H5''	1:O:1701:A:OP2	1.90	0.70
6:C:27:ARG:HG3	6:C:29:ASP:OD1	1.91	0.70
10:G:12:ILE:N	10:G:13:PRO:HD3	2.06	0.70
25:W:88:THR:HG22	25:W:89:ASP:N	2.06	0.70
5:B:16:ARG:NH1	39:B:9609:HOH:O	2.25	0.70
6:C:236:THR:CG2	6:C:239:ALA:H	1.98	0.70
6:C:1:MET:HG2	6:C:2:GLN:N	2.06	0.70
17:O:32:ARG:HH21	17:O:35:LYS:NZ	1.88	0.70
11:H:59:HIS:HA	11:H:62:LEU:HD23	1.72	0.70
15:M:164:THR:HG22	15:M:166:ALA:H	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:80:GLY:O	15:M:81:ARG:HD2	1.91	0.70
1:O:2481:G:H5''	39:O:5097:HOH:O	1.91	0.70
12:J:74:ARG:HB3	12:J:74:ARG:HH11	1.54	0.70
1:O:1206:U:H2'	1:O:1207:A:O4'	1.92	0.70
5:B:190:MET:HE2	5:B:194:PHE:HD1	1.57	0.70
1:O:1474:C:C6	1:O:1474:C:H5'	2.27	0.70
16:N:11:ARG:HA	16:N:14:ARG:NH1	2.07	0.70
1:O:969:G:H1	1:O:999:C:H42	1.40	0.69
1:O:1182:C:H1'	1:O:1192:A:H8	1.56	0.69
4:A:105:VAL:HG11	4:A:154:ALA:HB1	1.75	0.69
1:O:1118:A:H3'	1:O:1118:A:C8	2.27	0.69
1:O:2073:G:OP2	1:O:2490:A:H5'	1.92	0.69
2:9:3039:U:H1'	2:9:3044:A:N6	2.06	0.69
6:C:2:GLN:HB3	39:C:9192:HOH:O	1.92	0.69
9:F:37:THR:O	9:F:41:GLU:HG3	1.93	0.69
25:W:80:ASP:O	25:W:84:VAL:HG23	1.90	0.69
13:K:98:VAL:HG13	13:K:102:GLU:HA	1.74	0.69
25:W:81:ASP:OD1	25:W:92:ASP:HB2	1.92	0.69
27:Y:144:ARG:HH11	27:Y:144:ARG:HG3	1.58	0.69
1:O:1184:C:H4'	32:I:126:LYS:HB3	1.75	0.69
20:R:39:THR:HB	20:R:42:GLU:HG3	1.74	0.69
1:O:1184:C:H1'	39:O:7912:HOH:O	1.93	0.69
1:O:1187:U:HO2'	1:O:1189:A:H2	1.41	0.69
1:O:545:G:H8	1:O:545:G:H5'	1.57	0.69
5:B:275:GLY:O	5:B:291:ASP:HA	1.92	0.69
11:H:56:GLN:NE2	11:H:126:ARG:HE	1.89	0.69
20:R:8:ALA:HB1	20:R:13:THR:HG21	1.75	0.69
25:W:137:GLN:HE21	25:W:141:HIS:HE1	1.41	0.69
26:X:72:VAL:HG22	26:X:85:VAL:HG12	1.73	0.69
1:O:541:C:H2'	1:O:542:A:C5'	2.23	0.69
16:N:164:ASP:CG	16:N:167:ASP:HA	2.13	0.69
1:O:1166:A:H1'	1:O:1192:A:C2	2.28	0.69
5:B:140:LEU:HA	39:B:9575:HOH:O	1.92	0.69
25:W:68:THR:HG23	25:W:69:ARG:HG2	1.73	0.69
1:O:542:A:C8	1:O:542:A:H5'	2.23	0.68
9:F:77:VAL:HG21	9:F:83:LEU:HD13	1.76	0.68
12:J:19:MET:CE	12:J:132:LEU:HD11	2.23	0.68
1:O:2534:C:H1'	39:O:4086:HOH:O	1.93	0.68
25:W:137:GLN:NE2	25:W:141:HIS:HE1	1.91	0.68
25:W:4:LEU:HD11	25:W:45:VAL:HG12	1.76	0.68
6:C:47:GLY:HA2	6:C:92:PRO:HB2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:V:39:ALA:N	24:V:40:PRO:HD2	2.07	0.68
11:H:166:SER:HB3	11:H:167:PRO:HD3	1.73	0.68
1:O:381:G:H5''	39:M:9376:HOH:O	1.93	0.68
1:O:1730:G:H5'	1:O:1731:C:C5	2.29	0.68
22:T:115:GLU:HG3	22:T:116:ASP:N	2.08	0.68
23:U:39:ASN:ND2	23:U:44:ARG:HH11	1.90	0.68
1:O:2005:G:H3'	1:O:2005:G:OP2	1.94	0.68
7:D:170:TYR:O	7:D:171:ASP:HB3	1.94	0.68
25:W:108:ARG:HG3	25:W:114:PRO:HG3	1.76	0.68
2:9:3051:A:H5'	16:N:160:SER:HB3	1.76	0.68
25:W:48:VAL:HG12	25:W:48:VAL:O	1.93	0.68
4:A:199:HIS:HD2	4:A:201:PHE:H	1.39	0.67
1:O:2480:G:H3'	39:O:4754:HOH:O	1.94	0.67
5:B:201:ASP:HB2	5:B:312:ARG:HD2	1.77	0.67
22:T:49:GLU:HB3	22:T:59:GLU:HG2	1.76	0.67
1:O:1299:G:O6	14:L:6:ARG:HD3	1.95	0.67
28:Z:37:HIS:HB2	28:Z:47:VAL:HB	1.76	0.67
1:O:1528:A:H2'	1:O:1529:G:O4'	1.95	0.67
1:O:1244:U:OP1	12:J:18:ILE:HD13	1.94	0.67
31:3:35:TRP:HB2	39:3:9488:HOH:O	1.93	0.67
17:O:96:VAL:HG13	17:O:100:GLN:HB2	1.76	0.67
15:M:24:GLN:O	15:M:28:GLN:HG3	1.94	0.67
31:3:70:ARG:HG2	31:3:77:ALA:HB2	1.76	0.67
25:W:88:THR:HG22	25:W:89:ASP:H	1.58	0.67
1:O:280:C:H2'	1:O:281:U:O4'	1.95	0.67
4:A:48:ASP:HB3	39:A:9595:HOH:O	1.94	0.67
8:E:31:ARG:HH12	8:E:68:HIS:CG	2.13	0.67
20:R:18:LEU:HB2	20:R:143:VAL:CG1	2.24	0.67
1:O:1116:U:H3	1:O:1246:A:H62	1.41	0.66
1:O:1377:C:H6	1:O:1377:C:H5'	1.59	0.66
1:O:2780:C:H1'	8:E:143:GLN:HE21	1.60	0.66
1:O:1666:C:H2'	1:O:1667:A:H5'	1.76	0.66
1:O:1681:G:H5''	1:O:1682:A:H5'	1.77	0.66
1:O:2003:U:H4'	1:O:2004:U:H5	1.61	0.66
4:A:51:ARG:HB2	39:A:9595:HOH:O	1.94	0.66
11:H:27:LYS:N	11:H:59:HIS:HD2	1.93	0.66
20:R:18:LEU:HD12	20:R:143:VAL:CG1	2.26	0.66
1:O:338:C:H4'	6:C:174:ILE:CD1	2.26	0.66
28:Z:17:ARG:HD3	39:Z:9218:HOH:O	1.95	0.66
16:N:62:HIS:HB3	16:N:65:ASP:OD1	1.96	0.66
7:D:172:VAL:HG12	7:D:173:GLU:N	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:112:LEU:CD2	22:T:119:ALA:HB3	2.26	0.66
12:J:74:ARG:NH1	12:J:76:ASP:HB2	2.11	0.66
25:W:88:THR:HG23	25:W:110:GLN:NE2	2.11	0.66
1:O:1209:C:H2'	1:O:1210:G:H8	1.59	0.66
1:O:709:G:O2'	17:O:25:VAL:HG12	1.94	0.66
4:A:105:VAL:CG1	4:A:154:ALA:HB1	2.25	0.66
14:L:121:ILE:HG12	14:L:141:GLU:HB2	1.77	0.66
9:F:58:GLU:OE1	15:M:27:ARG:NH2	2.28	0.66
15:M:77:HIS:HD2	15:M:79:ALA:O	1.79	0.66
39:O:4937:HOH:O	15:M:83:SER:HB3	1.96	0.66
1:O:871:G:H8	1:O:871:G:H5'	1.60	0.65
30:2:22:PRO:HG2	30:2:25:VAL:CG2	2.26	0.65
11:H:166:SER:CB	11:H:167:PRO:CD	2.74	0.65
25:W:52:VAL:HG22	25:W:53:ALA:H	1.61	0.65
14:L:35:ARG:HB2	14:L:35:ARG:NH1	2.11	0.65
1:O:134:U:H6	1:O:134:U:C5'	2.09	0.65
30:2:18:ASN:ND2	30:2:40:ARG:H	1.86	0.65
5:B:109:LEU:HG	5:B:113:LEU:HD11	1.78	0.65
6:C:107:ARG:NE	39:C:9263:HOH:O	2.29	0.65
32:I:93:GLN:HA	32:I:96:PHE:HE2	1.60	0.65
39:O:9737:HOH:O	15:M:82:ARG:HD2	1.95	0.65
27:Y:144:ARG:CZ	39:Y:9409:HOH:O	2.44	0.65
18:P:115:SER:H	18:P:118:GLN:NE2	1.93	0.65
20:R:44:VAL:O	20:R:48:GLU:HG3	1.95	0.65
1:O:553:G:P	27:Y:204:ARG:HH22	2.19	0.65
1:O:2676:C:H4'	12:J:70:PHE:CE1	2.32	0.65
13:K:49:LEU:HD12	13:K:80:ILE:HG21	1.79	0.65
1:O:1119:G:H22	1:O:1246:A:H2	1.38	0.65
1:O:1166:A:H61	1:O:1180:U:H3	1.44	0.65
1:O:2676:C:H4'	12:J:70:PHE:CD1	2.32	0.65
26:X:37:LEU:CD1	26:X:85:VAL:HG21	2.20	0.65
24:V:20:LEU:HD22	24:V:60:GLN:HE22	1.62	0.65
1:O:1201:C:H5''	39:O:6742:HOH:O	1.97	0.65
1:O:282:C:O2'	1:O:283:U:H5'	1.96	0.65
28:Z:22:SER:O	28:Z:26:VAL:HG23	1.97	0.65
28:Z:37:HIS:O	28:Z:45:ASP:HA	1.97	0.65
1:O:544:G:C2'	1:O:545:G:H5''	2.26	0.65
9:F:2:VAL:HG22	9:F:57:GLU:OE1	1.97	0.65
21:S:57:THR:HG22	21:S:59:ASP:N	2.11	0.65
1:O:1426:C:H2'	39:O:3204:HOH:O	1.95	0.64
14:L:73:VAL:HG23	14:L:74:THR:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:99:ARG:NH2	15:M:170:ASN:HD22	1.89	0.64
1:O:263:U:O4'	9:F:59:ILE:HD13	1.98	0.64
16:N:80:SER:HB2	39:N:9333:HOH:O	1.95	0.64
22:T:71:VAL:HG11	22:T:90:PRO:CB	2.23	0.64
4:A:125:ASN:HB3	4:A:158:VAL:HG12	1.80	0.64
18:P:91:LYS:O	18:P:95:GLU:HG3	1.97	0.64
27:Y:154:ARG:NH1	27:Y:155:ARG:HG3	2.12	0.64
1:O:2749:U:H5'	39:O:8438:HOH:O	1.96	0.64
15:M:183:THR:HG22	15:M:194:ALA:HB1	1.78	0.64
23:U:52:THR:HG22	23:U:54:THR:N	2.13	0.64
2:9:3029:C:O3'	7:D:138:GLY:HA2	1.97	0.64
27:Y:126:PRO:HG2	27:Y:128:PHE:CE1	2.32	0.64
1:O:1201:C:H2'	1:O:1202:A:H5'	1.79	0.64
4:A:153:ARG:HH11	4:A:153:ARG:HB2	1.62	0.64
12:J:75:PRO:HD3	12:J:136:SER:OG	1.97	0.64
13:K:81:ARG:HD3	13:K:87:ARG:NH1	2.13	0.64
17:O:32:ARG:HH21	17:O:35:LYS:HZ2	1.43	0.64
24:V:56:ILE:O	24:V:60:GLN:HG3	1.97	0.64
7:D:159:PRO:O	7:D:163:VAL:HG23	1.97	0.64
5:B:329:TYR:CE2	23:U:15:PRO:HG2	2.32	0.64
1:O:1771:U:H5'	28:Z:20:ARG:HH21	1.63	0.64
1:O:2908:A:H2'	1:O:2909:G:O4'	1.98	0.64
2:9:3056:A:C2'	2:9:3057:A:H5''	2.27	0.64
16:N:48:VAL:CG1	16:N:55:ASP:HB3	2.27	0.64
1:O:134:U:H5'	1:O:134:U:H6	1.63	0.64
2:9:3029:C:H2'	2:9:3030:C:H5'	1.80	0.64
4:A:107:ASN:OD1	4:A:120:ARG:HD2	1.97	0.64
1:O:1943:C:H4'	4:A:211:LYS:O	1.98	0.64
1:O:1119:G:H2'	12:J:52:GLN:HE22	1.61	0.64
1:O:1183:C:N4	1:O:1184:C:H41	1.96	0.63
5:B:53:LEU:HD11	5:B:327:VAL:HG22	1.78	0.63
1:O:1641:A:H2'	1:O:1642:A:H5'	1.79	0.63
31:3:65:THR:HG22	31:3:88:LEU:HD22	1.78	0.63
12:J:75:PRO:HG2	12:J:105:LEU:HD21	1.81	0.63
15:M:187:LEU:CD2	15:M:194:ALA:HB3	2.28	0.63
5:B:53:LEU:HD21	5:B:270:ILE:HD12	1.80	0.63
17:O:57:THR:HB	17:O:111:VAL:HG23	1.78	0.63
1:O:2426:G:H1'	39:O:6603:HOH:O	1.97	0.63
1:O:2541:U:H5'	39:O:3025:HOH:O	1.96	0.63
6:C:242:GLU:HG3	39:C:9189:HOH:O	1.99	0.63
7:D:105:SER:HB2	7:D:131:THR:HG23	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:34:VAL:HG22	13:K:47:ALA:HB2	1.80	0.63
19:Q:25:PRO:HB2	39:Q:4350:HOH:O	1.98	0.63
27:Y:165:GLU:HB3	39:Y:9393:HOH:O	1.98	0.63
1:O:834:G:H4'	1:O:835:U:OP2	1.99	0.63
5:B:51:VAL:CG2	5:B:327:VAL:HG13	2.28	0.63
1:O:282:C:H1'	1:O:368:C:N4	2.13	0.63
4:A:113:GLY:HA2	4:A:153:ARG:NH2	2.14	0.63
4:A:190:ARG:NH2	4:A:207:GLN:OE1	2.32	0.63
13:K:29:LEU:HB3	13:K:55:VAL:CG1	2.26	0.63
25:W:84:VAL:HG12	39:W:6679:HOH:O	1.98	0.63
29:1:28:HIS:CD2	29:1:31:LYS:HG3	2.34	0.63
2:9:3013:A:O2'	2:9:3014:G:H5''	1.98	0.63
7:D:57:THR:HG23	7:D:63:ILE:HA	1.80	0.63
8:E:34:TRP:O	12:J:127:ILE:HD11	1.99	0.63
9:F:91:VAL:HG12	9:F:92:GLY:N	2.05	0.63
1:O:1328:A:OP1	27:Y:169:ARG:HD2	1.98	0.63
1:O:2578:G:H5'	1:O:2578:G:H8	1.63	0.63
7:D:136:ARG:HH12	7:D:157:LEU:HA	1.63	0.63
25:W:13:MET:HE3	25:W:17:ILE:HG22	1.80	0.63
5:B:305:ASP:O	5:B:306:LYS:HB2	1.99	0.63
9:F:63:ILE:HB	9:F:64:PRO:HD3	1.81	0.63
32:I:99:ASP:OD1	32:I:138:THR:HB	1.98	0.63
27:Y:189:ASN:HA	27:Y:217:ILE:HD11	1.79	0.63
5:B:141:ARG:HG2	5:B:165:ARG:HA	1.81	0.62
6:C:5:ILE:HD11	6:C:16:VAL:CG2	2.27	0.62
8:E:23:GLU:HG2	8:E:28:SER:HB3	1.80	0.62
9:F:21:GLU:O	9:F:24:ARG:HG3	1.99	0.62
1:O:2346:C:O2'	7:D:52:THR:HG21	1.98	0.62
1:O:2896:A:N3	1:O:2896:A:H2'	2.13	0.62
12:J:19:MET:HE1	12:J:132:LEU:HD11	1.81	0.62
1:O:902:G:N7	14:L:18:HIS:HD2	1.98	0.62
17:O:21:SER:OG	17:O:106:PRO:HB2	2.00	0.62
20:R:111:ILE:HG23	20:R:145:LEU:HD11	1.82	0.62
22:T:85:GLU:HG2	22:T:86:GLU:N	2.14	0.62
26:X:76:ARG:HH11	26:X:76:ARG:HG3	1.62	0.62
1:O:1160:G:H5'	1:O:1161:A:C5'	2.28	0.62
8:E:81:GLU:HG2	8:E:134:SER:CB	2.29	0.62
14:L:133:VAL:HA	39:L:9469:HOH:O	1.99	0.62
1:O:538:C:OP2	27:Y:134:HIS:HE1	1.82	0.62
5:B:254:GLN:HG2	5:B:255:GLY:N	2.12	0.62
6:C:129:HIS:CE1	6:C:231:ARG:HA	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:13:GLU:OE2	9:F:78:GLU:HG2	1.99	0.62
27:Y:154:ARG:HH12	27:Y:155:ARG:CG	2.12	0.62
1:O:2064:U:H5'	1:O:2652:U:H4'	1.81	0.62
1:O:877:G:H5'	1:O:878:G:OP1	1.98	0.62
29:1:10:LYS:HG3	39:1:9489:HOH:O	1.99	0.62
5:B:238:ASN:ND2	5:B:240:GLY:H	1.96	0.62
17:O:87:THR:O	17:O:91:GLN:HG3	1.99	0.62
22:T:115:GLU:HG3	22:T:116:ASP:H	1.63	0.62
1:O:1555:G:H4'	1:O:1630:A:H2	1.65	0.62
11:H:63:GLU:HA	39:H:9544:HOH:O	1.98	0.62
32:I:110:GLU:HA	32:I:113:HIS:CE1	2.35	0.62
1:O:1666:C:O2'	1:O:1667:A:H5''	1.99	0.62
4:A:131:HIS:O	4:A:132:ASP:HB2	1.98	0.62
4:A:57:ALA:HB1	4:A:65:ARG:HE	1.64	0.62
9:F:50:VAL:CG1	9:F:60:VAL:HG11	2.29	0.62
32:I:110:GLU:HA	32:I:113:HIS:NE2	2.15	0.62
13:K:55:VAL:HG12	13:K:56:SER:N	2.15	0.62
16:N:11:ARG:HG3	16:N:14:ARG:NH1	2.14	0.62
22:T:41:ARG:NH1	22:T:41:ARG:HG2	2.15	0.62
27:Y:189:ASN:HD22	27:Y:189:ASN:C	2.03	0.62
1:O:625:U:H5''	1:O:1044:C:N4	2.14	0.62
11:H:20:ILE:HG23	11:H:120:ILE:HD11	1.82	0.62
22:T:47:THR:HB	22:T:100:ASP:HB3	1.82	0.62
1:O:2541:U:H4'	1:O:2542:C:OP1	1.99	0.61
4:A:179:MET:HG2	4:A:186:TRP:CB	2.30	0.61
7:D:58:VAL:CG1	7:D:60:GLU:HG2	2.29	0.61
11:H:30:GLN:H	11:H:66:ARG:NH1	1.98	0.61
22:T:38:ARG:NH1	39:T:6217:HOH:O	2.33	0.61
4:A:33:GLU:O	4:A:34:ASP:HB2	1.99	0.61
10:G:20:VAL:O	10:G:24:VAL:HG23	2.00	0.61
13:K:34:VAL:CG2	13:K:47:ALA:HB2	2.31	0.61
1:O:2505:G:O2'	1:O:2506:A:H5'	2.00	0.61
1:O:558:C:C2'	1:O:559:U:H5''	2.30	0.61
1:O:111:C:O2'	29:1:20:ARG:HG2	2.01	0.61
16:N:176:ARG:HG3	16:N:180:LEU:HD13	1.82	0.61
29:1:25:LYS:CD	30:2:49:GLU:H	2.09	0.61
5:B:175:LEU:O	5:B:175:LEU:HD23	2.01	0.61
7:D:25:MET:CE	7:D:41:LEU:HG	2.26	0.61
1:O:1116:U:O2'	1:O:1118:A:C2	2.45	0.61
1:O:244:C:OP2	9:F:38:LYS:HE3	2.00	0.61
12:J:39:VAL:HG13	12:J:106:GLY:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:74:ARG:O	12:J:78:ILE:HG12	2.00	0.61
15:M:76:ARG:HG3	15:M:88:VAL:HG21	1.83	0.61
4:A:33:GLU:CD	4:A:33:GLU:H	2.03	0.61
4:A:35:GLY:O	4:A:36:ASP:HB3	1.99	0.61
4:A:82:VAL:HG13	4:A:93:THR:HB	1.80	0.61
15:M:107:ARG:NH1	15:M:107:ARG:HG3	2.10	0.61
1:0:681:G:N3	1:0:681:G:H5'	2.16	0.61
5:B:307:ARG:NH1	5:B:307:ARG:HG3	2.16	0.61
12:J:74:ARG:HH12	12:J:76:ASP:HB2	1.65	0.61
1:0:1701:A:H4'	1:0:1702:U:C5'	2.30	0.61
1:0:2032:U:H2'	1:0:2033:G:C5'	2.31	0.61
1:0:2032:U:H2'	1:0:2033:G:H5''	1.83	0.61
1:0:2661:U:H3	1:0:2812:A:H62	1.48	0.61
15:M:164:THR:HG22	15:M:166:ALA:N	2.14	0.61
1:0:2890:A:H1'	23:U:56:ARG:NH2	2.15	0.61
25:W:13:MET:CE	25:W:17:ILE:HG22	2.31	0.61
1:0:2524:G:H21	1:0:2526:C:N4	1.99	0.61
1:0:2533:C:H5'	1:0:2533:C:H6	1.65	0.61
16:N:139:TRP:HA	16:N:139:TRP:HE3	1.66	0.61
25:W:38:THR:HG22	25:W:39:ASP:N	2.15	0.61
2:9:3020:G:O2'	2:9:3021:G:H5'	2.00	0.61
8:E:116:THR:HG22	8:E:151:LEU:HD22	1.82	0.61
8:E:68:HIS:O	8:E:72:MET:HG3	2.00	0.61
16:N:139:TRP:HA	16:N:139:TRP:CE3	2.34	0.61
21:S:77:VAL:O	21:S:80:ARG:HG2	2.00	0.61
4:A:105:VAL:HG11	4:A:154:ALA:CB	2.31	0.60
14:L:80:ASP:HB2	14:L:90:ARG:O	2.01	0.60
1:0:447:A:P	22:T:1:SER:HB2	2.40	0.60
1:0:1406:A:H4'	1:0:1407:A:H5''	1.83	0.60
1:0:2748:G:H1'	39:0:8415:HOH:O	2.01	0.60
4:A:153:ARG:NH1	4:A:153:ARG:HB2	2.16	0.60
8:E:108:LEU:HD11	8:E:164:ASP:HB2	1.82	0.60
14:L:67:ARG:O	14:L:71:GLU:HG3	2.01	0.60
16:N:164:ASP:OD1	16:N:167:ASP:HA	2.00	0.60
26:X:71:ARG:HB3	26:X:88:GLU:OE1	2.01	0.60
30:2:22:PRO:HG2	30:2:25:VAL:HG23	1.83	0.60
1:0:558:C:H2'	1:0:559:U:C5'	2.31	0.60
5:B:221:GLN:HE22	13:K:42:ASN:HD22	1.49	0.60
7:D:94:ALA:HA	7:D:174:VAL:HA	1.84	0.60
7:D:25:MET:HE1	7:D:37:ALA:HB1	1.82	0.60
14:L:35:ARG:HB2	14:L:35:ARG:HH11	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:O:6281:HOH:O	22:T:106:GLU:HG3	2.00	0.60
5:B:41:PHE:CD1	5:B:79:MET:HE2	2.35	0.60
9:F:60:VAL:HG12	9:F:60:VAL:O	2.02	0.60
1:O:1168:C:H5''	32:I:87:THR:CG2	2.32	0.60
25:W:130:HIS:O	25:W:136:GLY:HA3	2.02	0.60
1:O:137:U:H2'	1:O:139:C:C5	2.37	0.60
1:O:2420:G:O2'	1:O:2421:G:H5'	2.02	0.60
10:G:23:ILE:HD13	10:G:67:LEU:HD23	1.82	0.60
2:9:3008:G:O6	16:N:11:ARG:NH1	2.34	0.60
25:W:141:HIS:HB2	25:W:146:ILE:HG12	1.84	0.60
1:O:1687:C:O2	29:1:9:GLY:HA2	2.02	0.60
7:D:23:VAL:HG21	7:D:45:THR:HG21	1.83	0.60
7:D:50:VAL:O	7:D:71:ALA:HA	2.02	0.60
15:M:99:ARG:HH21	15:M:170:ASN:ND2	1.93	0.60
27:Y:115:ARG:HH11	27:Y:115:ARG:HB3	1.66	0.60
1:O:1183:C:H2'	39:O:6752:HOH:O	2.01	0.60
4:A:165:THR:HG22	39:A:9608:HOH:O	2.02	0.60
6:C:107:ARG:HH11	6:C:107:ARG:HB3	1.66	0.60
11:H:58:ARG:HG3	11:H:58:ARG:HH11	1.66	0.60
13:K:107:THR:HG22	13:K:108:GLU:HG3	1.84	0.60
13:K:98:VAL:CG1	13:K:102:GLU:HA	2.31	0.60
15:M:68:ARG:HD3	15:M:68:ARG:O	2.02	0.60
16:N:115:VAL:HG22	39:N:9354:HOH:O	2.00	0.60
2:9:3014:G:C8	2:9:3014:G:H5'	2.36	0.60
6:C:127:ARG:HD3	6:C:129:HIS:HE1	1.67	0.60
1:O:271:C:H41	1:O:378:A:H2	1.46	0.59
1:O:316:A:N3	1:O:336:G:O2'	2.33	0.59
2:9:3076:G:H3'	2:9:3077:A:C5'	2.24	0.59
4:A:121:ALA:O	4:A:124:VAL:HG22	2.02	0.59
32:I:102:VAL:O	32:I:106:LYS:HG3	2.02	0.59
15:M:24:GLN:NE2	15:M:27:ARG:HH11	2.00	0.59
1:O:1838:U:O2'	1:O:2644:C:H5'	2.03	0.59
1:O:289:G:N2	1:O:363:A:H2	1.97	0.59
1:O:1168:C:H5''	32:I:87:THR:HG23	1.83	0.59
27:Y:187:VAL:HG23	27:Y:192:ASP:CB	2.32	0.59
1:O:1159:G:H1	1:O:1208:C:H42	1.51	0.59
12:J:45:VAL:HG23	12:J:130:VAL:O	2.01	0.59
17:O:39:THR:O	17:O:115:ARG:NH2	2.36	0.59
22:T:19:ARG:HD3	22:T:67:LEU:O	2.03	0.59
32:I:92:PRO:C	32:I:94:GLU:H	2.05	0.59
1:O:2081:A:H4'	12:J:69:TYR:CE1	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:O:3151:HOH:O	18:P:81:LYS:HG2	2.01	0.59
25:W:5:VAL:HG22	25:W:32:CYS:HB2	1.84	0.59
1:O:797:A:H4'	28:Z:10:ARG:N	2.18	0.59
10:G:24:VAL:O	10:G:28:GLU:HB2	2.02	0.59
24:V:1:THR:HG23	24:V:2:VAL:N	2.17	0.59
25:W:122:ARG:HG2	25:W:152:ALA:O	2.02	0.59
1:O:328:U:O4'	6:C:202:THR:HG22	2.03	0.59
4:A:105:VAL:HG12	4:A:106:CYS:N	2.18	0.59
1:O:2812:A:C2	1:O:2814:A:N6	2.66	0.59
6:C:236:THR:HG21	39:C:9181:HOH:O	2.03	0.59
12:J:54:VAL:HG11	12:J:138:THR:HG21	1.84	0.59
16:N:154:LEU:O	16:N:155:GLU:HB3	2.02	0.59
22:T:71:VAL:HG12	22:T:72:ILE:N	2.18	0.59
1:O:121:U:OP2	30:2:10:ARG:NH2	2.33	0.59
8:E:85:GLU:HG3	8:E:169:THR:OG1	2.03	0.59
12:J:75:PRO:HB3	12:J:132:LEU:HB3	1.85	0.59
17:O:47:ARG:HG3	17:O:47:ARG:HH11	1.68	0.59
5:B:190:MET:HE2	5:B:194:PHE:CD1	2.36	0.58
25:W:119:HIS:HD2	25:W:120:PRO:O	1.86	0.58
1:O:797:A:C4'	28:Z:10:ARG:N	2.66	0.58
1:O:1626:A:H2'	1:O:1627:G:O4'	2.03	0.58
1:O:2878:U:H2'	1:O:2879:A:O4'	2.03	0.58
1:O:775:G:OP1	29:1:16:HIS:HE1	1.85	0.58
4:A:199:HIS:CD2	4:A:201:PHE:H	2.19	0.58
1:O:1119:G:H8	12:J:52:GLN:HE22	1.52	0.58
1:O:1878:G:O2'	1:O:1879:U:OP2	2.20	0.58
4:A:206:ARG:N	4:A:206:ARG:HD3	2.14	0.58
5:B:125:GLU:O	5:B:129:ARG:HG3	2.03	0.58
1:O:2270:G:H4'	4:A:223:ARG:HH12	1.68	0.58
1:O:256:C:H2'	1:O:257:G:O4'	2.03	0.58
1:O:272:A:H5'	1:O:273:G:OP2	2.04	0.58
5:B:72:THR:HB	39:B:9598:HOH:O	2.02	0.58
25:W:149:LEU:HG	25:W:153:MET:CE	2.33	0.58
1:O:1745:G:H22	1:O:2033:G:H5'	1.68	0.58
1:O:558:C:O2'	1:O:559:U:H5''	2.04	0.58
12:J:93:ARG:HH11	12:J:93:ARG:CB	2.17	0.58
22:T:78:THR:HB	22:T:87:VAL:O	2.04	0.58
1:O:2526:C:O2'	1:O:2527:U:H5'	2.03	0.58
39:O:9972:HOH:O	29:1:1:THR:HA	2.02	0.58
4:A:125:ASN:CB	4:A:158:VAL:HG12	2.34	0.58
8:E:20:ILE:CD1	8:E:40:VAL:HG11	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:49:ILE:HD11	8:E:69:ILE:HD12	1.86	0.58
11:H:154:TYR:HB2	39:H:9557:HOH:O	2.04	0.58
32:I:113:HIS:N	32:I:114:PRO:HD2	2.19	0.58
1:O:2721:U:H4'	13:K:87:ARG:HG3	1.85	0.58
1:O:1973:A:H5'	1:O:1973:A:C8	2.37	0.58
1:O:396:U:O2'	1:O:418:C:H4'	2.04	0.58
8:E:31:ARG:NH1	8:E:68:HIS:CG	2.72	0.58
18:P:16:VAL:HG12	18:P:17:GLY:N	2.18	0.58
27:Y:117:LEU:HA	27:Y:174:VAL:HG11	1.86	0.58
1:O:1333:U:H2'	1:O:1334:C:C6	2.40	0.57
1:O:1736:A:H1'	39:O:8095:HOH:O	2.03	0.57
1:O:871:G:H8	1:O:871:G:H5''	1.68	0.57
4:A:191:GLY:HA2	4:A:194:MET:HE3	1.85	0.57
15:M:182:LYS:O	15:M:194:ALA:HB2	2.04	0.57
25:W:88:THR:HG23	25:W:110:GLN:HB3	1.86	0.57
1:O:2502:C:H2'	1:O:2503:A:H5'	1.86	0.57
8:E:102:VAL:HG11	8:E:148:ILE:HG12	1.86	0.57
25:W:106:THR:OG1	25:W:109:GLU:HG3	2.03	0.57
1:O:1080:C:H4'	1:O:1081:A:OP1	2.03	0.57
1:O:516:A:H5'	39:O:6176:HOH:O	2.05	0.57
18:P:40:VAL:O	18:P:44:VAL:HG23	2.04	0.57
8:E:8:PRO:HB2	8:E:11:VAL:HG23	1.86	0.57
15:M:57:LYS:HE2	15:M:140:ALA:O	2.04	0.57
15:M:71:SER:HB2	15:M:92:THR:HG22	1.85	0.57
1:O:138:U:H5''	1:O:139:C:OP2	2.04	0.57
1:O:2769:C:O2'	1:O:2770:G:H5'	2.05	0.57
1:O:447:A:OP1	22:T:2:LYS:HG2	2.05	0.57
13:K:114:ALA:HB3	13:K:117:VAL:HG23	1.85	0.57
25:W:88:THR:HG23	25:W:110:GLN:HE21	1.70	0.57
1:O:2502:C:C2'	1:O:2503:A:H5'	2.35	0.57
1:O:2769:C:C2'	1:O:2770:G:H5'	2.35	0.57
6:C:139:VAL:HG13	39:C:9253:HOH:O	2.05	0.57
32:I:125:ALA:O	32:I:129:VAL:HG23	2.04	0.57
12:J:71:TYR:CD1	12:J:72:PRO:HD2	2.39	0.57
15:M:74:LYS:HG2	15:M:75:ARG:N	2.20	0.57
16:N:23:ARG:HD3	39:N:9344:HOH:O	2.03	0.57
25:W:125:HIS:CD2	25:W:127:GLY:H	2.23	0.57
25:W:21:LEU:HB3	25:W:26:ILE:HG12	1.87	0.57
1:O:1119:G:H8	12:J:52:GLN:NE2	2.02	0.57
5:B:297:VAL:HB	39:B:9598:HOH:O	2.03	0.57
7:D:54:ALA:CB	7:D:69:ILE:HD12	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:485:A:N3	1:0:487:G:H5''	2.20	0.57
1:0:69:A:H5'	1:0:69:A:C8	2.39	0.57
1:0:474:C:O3'	6:C:73:LEU:HD21	2.04	0.57
32:I:134:SER:O	32:I:135:LEU:HD23	2.04	0.57
25:W:4:LEU:HD23	25:W:54:PHE:HB3	1.87	0.57
1:0:450:C:OP1	6:C:184:ARG:NH2	2.37	0.57
15:M:68:ARG:NH2	15:M:73:ARG:HD3	2.18	0.57
39:O:7990:HOH:O	15:M:91:ILE:HG23	2.04	0.57
25:W:21:LEU:HD22	25:W:26:ILE:CD1	2.34	0.57
1:0:1205:U:H2'	1:0:1206:U:C5'	2.35	0.56
1:0:475:G:OP1	6:C:73:LEU:HD22	2.05	0.56
6:C:25:PRO:HG2	39:C:9125:HOH:O	2.05	0.56
6:C:93:LYS:O	6:C:98:ARG:NH2	2.38	0.56
1:0:1786:C:OP1	18:P:74:GLN:HG2	2.05	0.56
15:M:107:ARG:CG	15:M:107:ARG:HH11	2.14	0.56
1:0:2883:A:H2'	1:0:2884:G:O4'	2.06	0.56
4:A:94:LEU:HG	4:A:99:ILE:HD11	1.86	0.56
5:B:62:ARG:HA	5:B:65:MET:CE	2.36	0.56
1:0:2524:G:H21	1:0:2526:C:H41	1.54	0.56
2:9:3024:U:H3'	2:9:3025:G:H5'	1.87	0.56
7:D:44:ILE:HG12	7:D:83:PHE:HE1	1.71	0.56
1:0:1185:U:H4'	32:I:123:ASN:HB3	1.87	0.56
16:N:169:PRO:O	16:N:172:PHE:HB3	2.05	0.56
22:T:26:THR:HA	22:T:39:ASN:HB3	1.87	0.56
28:Z:42:CYS:SG	28:Z:43:GLY:N	2.77	0.56
6:C:194:PHE:CD2	6:C:234:VAL:HG11	2.39	0.56
18:P:16:VAL:HG13	18:P:20:ARG:NH1	2.20	0.56
1:0:2586:U:H3	1:0:2592:G:H22	1.54	0.56
1:0:291:C:H2'	1:0:292:G:O4'	2.05	0.56
29:1:25:LYS:HE2	39:2:7213:HOH:O	2.04	0.56
29:1:8:GLN:HE22	29:1:11:LYS:NZ	2.03	0.56
9:F:84:GLY:O	9:F:89:LEU:HB2	2.05	0.56
13:K:28:GLU:HB3	13:K:59:LYS:HB2	1.87	0.56
15:M:15:PRO:HA	15:M:20:LEU:HD23	1.87	0.56
1:0:1189:A:H3'	39:0:8201:HOH:O	2.06	0.56
1:0:2421:G:H1'	39:0:4283:HOH:O	2.05	0.56
1:0:2670:G:O2'	1:0:2671:U:H5'	2.05	0.56
5:B:85:ARG:NH1	39:B:9628:HOH:O	2.37	0.56
11:H:99:LYS:HD3	11:H:119:LYS:HD3	1.87	0.56
16:N:61:ALA:HB3	16:N:88:ALA:HB2	1.87	0.56
1:0:710:G:H5'	17:O:25:VAL:CG1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2419:U:H5''	1:0:2420:G:H5'	1.87	0.56
24:V:5:VAL:HG23	39:V:2271:HOH:O	2.06	0.56
1:0:151:A:H2'	1:0:152:A:O4'	2.06	0.56
1:0:1979:G:O2'	1:0:1980:U:OP1	2.21	0.56
1:0:316:A:H5'	22:T:54:ASP:OD2	2.05	0.56
6:C:118:THR:HG22	6:C:137:PRO:HB3	1.88	0.56
11:H:166:SER:CB	11:H:167:PRO:HD3	2.36	0.56
12:J:90:LYS:HB2	36:J:9302:CL:CL	2.43	0.56
16:N:86:LEU:HD12	16:N:125:ALA:HB2	1.88	0.56
1:0:1118:A:H8	1:0:1119:G:H5''	1.71	0.56
1:0:1819:G:H2'	1:0:1820:G:H4'	1.87	0.56
1:0:2718:C:H6	1:0:2718:C:H5'	1.70	0.56
1:0:2866:U:H4'	1:0:2867:G:H5'	1.86	0.56
7:D:59:GLY:O	7:D:61:PHE:N	2.39	0.56
7:D:23:VAL:HG22	7:D:73:VAL:HB	1.87	0.56
23:U:17:THR:CG2	23:U:18:GLY:N	2.68	0.56
1:0:1979:G:H2'	39:0:3887:HOH:O	2.05	0.55
6:C:162:VAL:HG22	6:C:232:LEU:HD21	1.86	0.55
7:D:138:GLY:N	39:D:7597:HOH:O	2.37	0.55
7:D:136:ARG:NH1	7:D:157:LEU:HA	2.21	0.55
8:E:35:TYR:HA	12:J:127:ILE:HD12	1.88	0.55
8:E:7:ILE:HG22	8:E:45:ASP:O	2.07	0.55
18:P:9:LEU:O	18:P:13:VAL:HG12	2.05	0.55
1:0:1753:C:O2	5:B:229:ARG:NH2	2.39	0.55
5:B:71:VAL:HG11	5:B:296:LEU:HD22	1.88	0.55
16:N:110:THR:HB	16:N:113:SER:OG	2.06	0.55
1:0:2320:U:H4'	1:0:2321:A:O4'	2.06	0.55
1:0:2769:C:H2'	1:0:2770:G:O4'	2.06	0.55
1:0:2807:U:P	5:B:27:ASN:HD21	2.29	0.55
30:2:20:ARG:HD2	30:2:39:ARG:NH2	2.21	0.55
4:A:94:LEU:HD12	4:A:98:GLU:HB2	1.88	0.55
1:0:1189:A:O2'	1:0:1208:C:H2'	2.06	0.55
10:G:12:ILE:N	10:G:13:PRO:CD	2.70	0.55
18:P:10:ALA:HA	18:P:13:VAL:HG12	1.88	0.55
20:R:106:GLY:HA2	20:R:109:MET:HE3	1.88	0.55
25:W:26:ILE:O	25:W:26:ILE:HG13	2.06	0.55
1:0:2904:U:H4'	26:X:8:ARG:NH1	2.22	0.55
1:0:1634:G:H3'	39:0:4470:HOH:O	2.07	0.55
1:0:558:C:H2'	1:0:559:U:H5'	1.88	0.55
5:B:238:ASN:HD22	5:B:240:GLY:N	1.99	0.55
6:C:136:VAL:HG22	6:C:137:PRO:HA	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:69:ALA:HB2	11:H:153:ALA:HB2	1.89	0.55
32:I:105:VAL:HG11	32:I:129:VAL:HG22	1.89	0.55
26:X:43:VAL:HG12	26:X:44:ASP:N	2.22	0.55
1:0:241:A:C2	1:0:378:A:H4'	2.42	0.55
1:0:1684:A:H1'	30:2:43:ARG:HH22	1.72	0.55
31:3:55:VAL:HB	31:3:56:PRO:HD2	1.89	0.55
24:V:29:ASN:O	24:V:33:VAL:HG23	2.07	0.55
24:V:64:GLY:O	24:V:65:ASP:HB2	2.05	0.55
1:0:441:A:H1'	1:0:442:A:N7	2.21	0.55
17:O:59:VAL:HG23	17:O:111:VAL:HG22	1.88	0.55
27:Y:151:SER:HB3	27:Y:154:ARG:HB3	1.89	0.55
1:0:236:A:H8	1:0:236:A:OP1	1.90	0.55
1:0:2563:U:H2'	1:0:2565:C:O5'	2.07	0.55
1:0:2645:U:OP2	1:0:2645:U:C6	2.60	0.55
12:J:39:VAL:HG11	12:J:107:ASN:CG	2.27	0.55
39:0:7355:HOH:O	15:M:178:LYS:HB2	2.05	0.55
16:N:162:ASP:HA	39:N:9328:HOH:O	2.06	0.55
26:X:12:ILE:HD12	26:X:36:HIS:ND1	2.22	0.55
5:B:268:ARG:NH2	5:B:325:PRO:HG3	2.20	0.55
12:J:19:MET:HE1	12:J:132:LEU:CD2	2.33	0.55
1:0:380:A:H2'	39:0:7695:HOH:O	2.06	0.55
1:0:90:A:H2'	1:0:91:G:O4'	2.07	0.55
1:0:1187:U:O2'	1:0:1189:A:H2	1.89	0.54
8:E:3:VAL:CG2	8:E:49:ILE:HB	2.37	0.54
10:G:12:ILE:HD12	39:G:692:HOH:O	2.06	0.54
1:0:1595:G:O2'	1:0:1596:U:H5'	2.08	0.54
1:0:848:C:H5'	39:0:7735:HOH:O	2.08	0.54
10:G:64:ASN:N	10:G:64:ASN:HD22	2.04	0.54
11:H:17:ARG:HD3	11:H:23:ILE:HD12	1.88	0.54
4:A:36:ASP:C	4:A:38:ILE:H	2.10	0.54
8:E:137:ASP:OD1	8:E:139:GLU:HB2	2.08	0.54
9:F:36:THR:HG23	9:F:97:ALA:HB2	1.90	0.54
11:H:170:ASN:N	11:H:170:ASN:HD22	2.03	0.54
11:H:27:LYS:H	11:H:59:HIS:CD2	2.18	0.54
11:H:76:GLU:O	11:H:77:LEU:HD23	2.07	0.54
39:9:1361:HOH:O	16:N:41:LYS:HE3	2.08	0.54
20:R:113:HIS:HE1	20:R:144:GLU:CD	2.10	0.54
6:C:142:ASP:OD1	6:C:236:THR:HG23	2.06	0.54
39:9:4707:HOH:O	16:N:147:ILE:HD12	2.05	0.54
2:9:3051:A:H5'	16:N:160:SER:CB	2.37	0.54
22:T:79:LEU:HG	22:T:89:ARG:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:2453:G:H5''	39:L:9439:HOH:O	2.07	0.54
7:D:135:VAL:HG22	7:D:136:ARG:N	2.23	0.54
30:2:36:ASN:HB3	30:2:39:ARG:HG3	1.89	0.54
16:N:183:ASP:O	16:N:184:ILE:O	2.25	0.54
25:W:6:GLN:CB	25:W:26:ILE:HD12	2.35	0.54
9:F:46:GLU:OE1	9:F:100:ASP:HA	2.07	0.54
12:J:131:THR:HG22	12:J:134:GLU:H	1.71	0.54
17:O:25:VAL:HG23	17:O:26:TRP:N	2.22	0.54
18:P:59:ARG:HH22	18:P:66:GLN:HE22	1.55	0.54
1:O:20:G:H21	20:R:117:HIS:HD2	1.56	0.54
22:T:40:VAL:HG22	22:T:41:ARG:N	2.23	0.54
1:O:1189:A:H1'	1:O:1209:C:O4'	2.07	0.54
1:O:185:G:H4'	1:O:186:A:H4'	1.89	0.54
1:O:2032:U:C2'	1:O:2033:G:H5''	2.37	0.54
31:3:38:ARG:HB3	31:3:42:ARG:HH12	1.73	0.54
4:A:33:GLU:CD	4:A:33:GLU:N	2.61	0.54
14:L:136:ALA:HB3	39:L:9469:HOH:O	2.07	0.54
1:O:2827:A:H2'	1:O:2828:G:O4'	2.08	0.54
1:O:2851:G:O2'	1:O:2852:A:H5'	2.07	0.54
16:N:42:HIS:CE1	16:N:75:THR:HG1	2.26	0.54
17:O:98:LEU:O	17:O:102:ILE:HG13	2.08	0.54
28:Z:29:ILE:O	28:Z:33:MET:HB2	2.08	0.54
1:O:1477:C:H5'	1:O:1868:G:H5'	1.90	0.54
19:Q:26:PRO:O	19:Q:30:VAL:HG23	2.06	0.54
1:O:1730:G:H5'	1:O:1731:C:C6	2.43	0.53
1:O:949:U:H4'	19:Q:95:GLU:HA	1.89	0.53
39:O:4794:HOH:O	30:2:38:LYS:HE3	2.08	0.53
27:Y:187:VAL:HG23	27:Y:192:ASP:HB3	1.90	0.53
1:O:621:C:H5'	27:Y:132:ASP:OD2	2.07	0.53
18:P:10:ALA:HA	18:P:13:VAL:CG1	2.37	0.53
18:P:13:VAL:HG11	18:P:40:VAL:CG1	2.37	0.53
28:Z:10:ARG:HA	39:Z:9215:HOH:O	2.07	0.53
1:O:1384:C:H5'	26:X:30:MET:HG2	1.88	0.53
11:H:38:LYS:HE2	11:H:42:ASP:HB2	1.90	0.53
1:O:1164:U:OP1	32:I:74:PRO:HA	2.08	0.53
1:O:1724:U:H5''	39:O:4314:HOH:O	2.08	0.53
39:O:9697:HOH:O	5:B:214:PRO:HD2	2.08	0.53
32:I:129:VAL:O	32:I:129:VAL:HG12	2.08	0.53
32:I:138:THR:HG22	32:I:139:ILE:N	2.23	0.53
1:O:1835:U:C5	1:O:1840:A:N7	2.66	0.53
1:O:466:A:OP1	30:2:38:LYS:HE2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:34:ASP:OD1	4:A:35:GLY:N	2.38	0.53
12:J:47:THR:HG22	12:J:48:GLY:N	2.24	0.53
13:K:109:LEU:CD1	13:K:113:ILE:HD11	2.36	0.53
1:O:1189:A:H1'	1:O:1209:C:C1'	2.37	0.53
1:O:12:U:H2'	1:O:13:G:H5'	1.91	0.53
1:O:182:G:H5'	39:M:9399:HOH:O	2.08	0.53
1:O:500:G:H21	20:R:98:ASN:HD21	1.57	0.53
1:O:2364:A:H5''	19:Q:15:LYS:HD3	1.90	0.53
25:W:4:LEU:O	25:W:32:CYS:HA	2.08	0.53
6:C:107:ARG:HH11	6:C:107:ARG:CB	2.21	0.53
21:S:10:VAL:HG11	24:V:36:ALA:CA	2.38	0.53
24:V:55:ARG:O	24:V:59:ILE:HG12	2.08	0.53
25:W:122:ARG:HH11	25:W:122:ARG:CG	2.21	0.53
26:X:9:VAL:HG22	26:X:88:GLU:OE2	2.09	0.53
1:O:1209:C:H2'	1:O:1210:G:C8	2.43	0.53
1:O:1766:U:O2	1:O:1778:A:H5'	2.09	0.53
12:J:75:PRO:HG2	12:J:105:LEU:CD2	2.39	0.53
16:N:32:PRO:HD2	16:N:99:GLU:O	2.09	0.53
28:Z:19:GLY:O	28:Z:23:ARG:HG2	2.09	0.53
1:O:1730:G:C5'	1:O:1731:C:C6	2.92	0.53
1:O:288:A:H2'	1:O:289:G:C8	2.43	0.53
9:F:46:GLU:O	9:F:73:PRO:HD2	2.08	0.53
9:F:58:GLU:HA	9:F:61:MET:CE	2.37	0.53
16:N:11:ARG:O	16:N:15:GLU:HG3	2.08	0.53
16:N:12:ARG:HD3	16:N:18:THR:OG1	2.08	0.53
16:N:74:PRO:HG2	16:N:159:TYR:CE1	2.44	0.53
22:T:49:GLU:CB	22:T:59:GLU:HG2	2.38	0.53
25:W:139:GLY:O	25:W:141:HIS:HD2	1.91	0.53
1:O:2815:G:OP2	12:J:99:GLU:HG2	2.09	0.53
7:D:104:PHE:CE2	7:D:166:ILE:HD13	2.44	0.53
7:D:24:HIS:HB2	7:D:72:LYS:HB3	1.91	0.53
7:D:99:ASP:HB2	7:D:103:ASN:O	2.08	0.53
25:W:11:VAL:O	25:W:12:ASN:HB2	2.09	0.53
1:O:1406:A:H4'	1:O:1407:A:C5'	2.39	0.52
1:O:1741:U:H3'	39:O:3367:HOH:O	2.07	0.52
1:O:2795:C:O2'	1:O:2796:U:H5'	2.09	0.52
1:O:603:A:H5''	1:O:604:G:OP1	2.08	0.52
1:O:757:C:OP1	14:L:27:ARG:HD2	2.09	0.52
29:1:8:GLN:HE22	29:1:11:LYS:HZ2	1.56	0.52
2:9:3076:G:C3'	2:9:3077:A:H5''	2.24	0.52
7:D:24:HIS:HB2	7:D:72:LYS:CB	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:35:TYR:HA	12:J:127:ILE:CD1	2.39	0.52
18:P:105:LEU:CD2	18:P:137:LEU:HD21	2.39	0.52
1:O:2265:U:H2'	1:O:2266:A:C8	2.44	0.52
1:O:2591:C:H2'	1:O:2592:G:O4'	2.08	0.52
1:O:95:A:H5''	1:O:97:G:O4'	2.09	0.52
3:4:176:DA:O4'	3:4:175:C:H2'	2.09	0.52
5:B:102:THR:CG2	5:B:182:VAL:HG12	2.39	0.52
39:O:5513:HOH:O	11:H:58:ARG:HG3	2.08	0.52
16:N:179:LEU:HD23	16:N:184:ILE:HD12	1.91	0.52
1:O:447:A:OP1	22:T:1:SER:HB2	2.10	0.52
27:Y:178:HIS:CG	27:Y:179:PRO:HD2	2.45	0.52
27:Y:212:ARG:HD2	39:Y:9400:HOH:O	2.08	0.52
6:C:236:THR:HG22	6:C:239:ALA:CB	2.39	0.52
1:O:475:G:C5'	6:C:73:LEU:HD23	2.39	0.52
13:K:115:ARG:HG3	13:K:116:GLU:N	2.25	0.52
17:O:59:VAL:HG23	17:O:111:VAL:CG2	2.39	0.52
1:O:1119:G:N2	1:O:1246:A:N1	2.57	0.52
1:O:1252:A:H2'	1:O:1253:C:O4'	2.10	0.52
1:O:248:A:H5'	1:O:249:G:OP2	2.10	0.52
1:O:2894:C:O2'	1:O:2895:C:H5'	2.09	0.52
1:O:920:C:H5''	1:O:921:G:O5'	2.10	0.52
5:B:171:VAL:HG23	5:B:172:SER:N	2.25	0.52
12:J:15:ARG:CZ	12:J:43:ARG:NH1	2.72	0.52
16:N:152:GLU:C	16:N:154:LEU:H	2.13	0.52
18:P:103:THR:O	18:P:107:GLU:HG3	2.09	0.52
1:O:793:A:H5''	18:P:83:LYS:HG2	1.91	0.52
21:S:57:THR:CG2	21:S:58:MET:N	2.73	0.52
1:O:1972:U:H2'	1:O:1973:A:H5'	1.92	0.52
1:O:2443:C:O3'	14:L:56:LYS:HE3	2.10	0.52
6:C:246:ARG:NE	39:C:9230:HOH:O	2.42	0.52
17:O:14:LEU:HG	17:O:102:ILE:HD11	1.91	0.52
19:Q:11:ARG:HD3	39:Q:5620:HOH:O	2.10	0.52
25:W:88:THR:HG22	25:W:90:TYR:HD1	1.74	0.52
32:I:72:VAL:CG1	32:I:73:PRO:HD2	2.39	0.52
15:M:31:TRP:HA	15:M:34:GLU:HG3	1.92	0.52
22:T:38:ARG:HG3	22:T:38:ARG:HH11	1.74	0.52
1:O:1751:G:C2'	1:O:1752:G:H5''	2.39	0.52
1:O:1926:G:H2'	1:O:1927:A:C8	2.44	0.52
1:O:870:G:C2'	1:O:871:G:H5''	2.37	0.52
4:A:192:VAL:HG11	4:A:207:GLN:HB3	1.90	0.52
16:N:43:VAL:HG13	16:N:118:ILE:HD11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:5:GLU:HG2	23:U:10:GLY:O	2.10	0.52
25:W:64:THR:O	25:W:68:THR:HG22	2.09	0.52
1:O:2587:OMU:H6	1:O:2587:OMU:O5'	2.09	0.52
2:9:3069:U:OP1	16:N:4:PRO:HG3	2.10	0.52
39:O:5938:HOH:O	4:A:164:ARG:CZ	2.57	0.52
6:C:233:THR:HG22	6:C:234:VAL:N	2.24	0.52
7:D:41:LEU:HA	7:D:44:ILE:HG22	1.92	0.52
11:H:40:ALA:HB1	11:H:137:TYR:CE2	2.45	0.52
20:R:18:LEU:HG	20:R:91:LEU:HD13	1.92	0.52
27:Y:112:GLU:OE2	27:Y:115:ARG:NH1	2.43	0.52
1:O:156:C:H5''	15:M:171:ARG:CD	2.28	0.52
1:O:2781:U:H1'	8:E:139:GLU:OE2	2.10	0.52
6:C:246:ARG:CB	6:C:246:ARG:HH11	2.20	0.52
7:D:36:ASN:HA	39:D:7500:HOH:O	2.10	0.52
1:O:1981:A:H1'	1:O:1983:C:N4	2.25	0.51
29:1:21:ARG:HD2	29:1:37:CYS:SG	2.50	0.51
6:C:140:VAL:HB	39:C:9256:HOH:O	2.09	0.51
1:O:545:G:C8	1:O:545:G:H5'	2.41	0.51
29:1:56:GLU:OXT	29:1:56:GLU:HG2	2.10	0.51
6:C:57:PRO:HG2	6:C:73:LEU:HD13	1.92	0.51
11:H:166:SER:HB2	11:H:167:PRO:CD	2.41	0.51
12:J:99:GLU:HA	39:J:7377:HOH:O	2.11	0.51
13:K:75:ARG:HD3	13:K:112:PRO:O	2.10	0.51
1:O:164:G:H4'	14:L:30:ARG:HD3	1.93	0.51
16:N:37:ARG:NH2	39:N:9316:HOH:O	2.29	0.51
20:R:96:VAL:HG13	20:R:106:GLY:HA3	1.92	0.51
23:U:45:GLU:HB2	23:U:48:ASN:ND2	2.24	0.51
27:Y:112:GLU:OE1	27:Y:112:GLU:HA	2.11	0.51
5:B:199:TYR:CE2	5:B:268:ARG:HB2	2.45	0.51
6:C:142:ASP:CG	6:C:237:GLU:HB3	2.30	0.51
15:M:86:GLN:O	15:M:88:VAL:HG23	2.11	0.51
18:P:135:ALA:HB1	18:P:139:ARG:NH1	2.26	0.51
25:W:88:THR:CG2	25:W:89:ASP:H	2.23	0.51
27:Y:126:PRO:HG2	27:Y:128:PHE:CZ	2.46	0.51
27:Y:189:ASN:ND2	27:Y:192:ASP:H	2.08	0.51
1:O:969:G:H1	1:O:999:C:N4	2.08	0.51
31:3:16:GLU:HG3	31:3:18:GLN:HE21	1.75	0.51
4:A:66:ARG:HH11	4:A:66:ARG:HB2	1.75	0.51
14:L:120:LEU:HD12	14:L:133:VAL:HG21	1.92	0.51
19:Q:32:GLU:HA	19:Q:71:TYR:OH	2.09	0.51
39:K:7438:HOH:O	23:U:20:MET:HE1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:119:A:H2'	1:0:120:A:H5''	1.92	0.51
7:D:173:GLU:HG3	7:D:174:VAL:N	2.25	0.51
8:E:5:LEU:HD21	8:E:66:GLN:HG3	1.93	0.51
13:K:81:ARG:HD3	13:K:87:ARG:CZ	2.40	0.51
18:P:16:VAL:HG13	18:P:20:ARG:CZ	2.40	0.51
25:W:29:VAL:O	25:W:30:ASN:HB2	2.11	0.51
28:Z:33:MET:HG3	28:Z:69:TYR:O	2.11	0.51
1:0:204:A:C2'	1:0:205:U:H5'	2.41	0.51
39:9:6497:HOH:O	16:N:23:ARG:HD2	2.09	0.51
1:0:2456:A:H2'	1:0:2457:U:C6	2.46	0.51
1:0:2649:A:H5'	1:0:2649:A:H8	1.76	0.51
8:E:84:MET:HE1	8:E:148:ILE:HD12	1.92	0.51
8:E:15:GLN:NE2	8:E:40:VAL:O	2.43	0.51
11:H:45:VAL:HA	11:H:167:PRO:O	2.10	0.51
13:K:125:ALA:C	13:K:127:ALA:H	2.13	0.51
1:0:1205:U:H2'	1:0:1206:U:H5'	1.93	0.51
30:2:20:ARG:HG3	30:2:21:VAL:N	2.26	0.51
5:B:81:ALA:O	5:B:186:GLY:HA3	2.11	0.51
5:B:212:GLN:HB2	5:B:257:THR:CG2	2.40	0.51
12:J:12:VAL:HG21	12:J:116:LEU:HD11	1.92	0.51
1:0:432:G:O2'	1:0:433:C:H5'	2.11	0.51
31:3:55:VAL:HG22	39:3:9444:HOH:O	2.10	0.51
5:B:42:ALA:HB1	5:B:308:LEU:HD11	1.92	0.51
12:J:93:ARG:NH1	12:J:93:ARG:HB3	2.19	0.51
13:K:30:LYS:O	13:K:55:VAL:HG13	2.10	0.51
25:W:21:LEU:HD22	25:W:26:ILE:HD11	1.92	0.51
25:W:88:THR:CG2	25:W:89:ASP:N	2.74	0.51
1:0:625:U:H5'	39:0:3777:HOH:O	2.11	0.51
1:0:776:A:OP1	29:1:28:HIS:HE1	1.94	0.51
4:A:153:ARG:CB	4:A:153:ARG:HH11	2.23	0.51
6:C:133:ARG:NE	6:C:138:VAL:HG22	2.26	0.51
1:0:1946:C:H2'	1:0:1971:G:C8	2.46	0.50
2:9:3003:A:H2'	39:9:2430:HOH:O	2.11	0.50
5:B:62:ARG:HA	5:B:65:MET:HE2	1.93	0.50
7:D:25:MET:HE1	7:D:37:ALA:O	2.11	0.50
1:0:2521:A:OP2	11:H:3:ALA:HB3	2.11	0.50
25:W:149:LEU:HG	25:W:153:MET:HE2	1.93	0.50
5:B:5:ARG:NH1	5:B:8:LYS:HE2	2.26	0.50
11:H:63:GLU:O	11:H:67:LEU:HB2	2.11	0.50
12:J:15:ARG:CZ	12:J:43:ARG:HH11	2.24	0.50
12:J:63:ILE:HG22	12:J:64:GLY:N	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3004:G:H21	16:N:44:ARG:NH1	2.09	0.50
26:X:31:ILE:O	26:X:35:GLU:HG3	2.11	0.50
1:0:653:C:H2'	1:0:654:A:C8	2.45	0.50
1:0:734:U:H1'	1:0:737:A:N6	2.26	0.50
1:0:968:G:H1'	11:H:32:LYS:HD2	1.92	0.50
30:2:20:ARG:HD2	30:2:39:ARG:HH21	1.76	0.50
4:A:39:ALA:O	4:A:61:GLU:HG3	2.11	0.50
1:0:171:C:OP2	15:M:84:LYS:HG3	2.10	0.50
26:X:20:GLU:HG3	26:X:21:PRO:HD2	1.91	0.50
39:0:5240:HOH:O	28:Z:13:ARG:HD3	2.12	0.50
1:0:2064:U:H5'	1:0:2652:U:O3'	2.11	0.50
4:A:109:GLU:HG2	4:A:116:GLY:N	2.25	0.50
4:A:123:GLY:HA3	4:A:162:GLY:HA2	1.93	0.50
5:B:41:PHE:CG	5:B:79:MET:HE2	2.47	0.50
7:D:134:LEU:HD11	7:D:166:ILE:HD11	1.94	0.50
32:I:75:THR:OG1	32:I:112:LYS:HE2	2.11	0.50
25:W:108:ARG:HE	25:W:114:PRO:CG	2.24	0.50
26:X:21:PRO:HG2	26:X:24:LYS:HD3	1.93	0.50
1:0:1268:C:O2'	27:Y:169:ARG:HB2	2.12	0.50
4:A:105:VAL:HG12	4:A:106:CYS:H	1.77	0.50
4:A:81:GLN:HB2	4:A:92:ASN:HD21	1.75	0.50
1:0:1180:U:H2'	1:0:1181:A:C8	2.46	0.50
1:0:1234:U:N3	5:B:244:PRO:HB3	2.27	0.50
1:0:284:C:H4'	1:0:285:A:H8	1.76	0.50
1:0:69:A:H5'	1:0:69:A:H8	1.77	0.50
8:E:149:GLU:OE1	8:E:167:TYR:HA	2.12	0.50
9:F:57:GLU:O	9:F:61:MET:HG3	2.12	0.50
11:H:116:ALA:O	11:H:117:PHE:C	2.50	0.50
17:O:78:ALA:C	17:O:98:LEU:HD13	2.32	0.50
1:0:2472:C:O2'	1:0:2634:G:H4'	2.11	0.50
5:B:41:PHE:CD2	5:B:190:MET:HE3	2.47	0.50
5:B:96:PRO:HG3	39:B:9628:HOH:O	2.11	0.50
8:E:11:VAL:HG12	8:E:12:ASP:N	2.27	0.50
15:M:66:SER:HB3	15:M:128:TRP:CD1	2.46	0.50
1:0:1118:A:C8	1:0:1118:A:C3'	2.90	0.50
1:0:2649:A:H5'	1:0:2649:A:C8	2.47	0.50
1:0:558:C:H2'	1:0:559:U:H5''	1.92	0.50
2:9:3028:U:H2'	2:9:3029:C:C6	2.46	0.50
4:A:192:VAL:HG12	4:A:207:GLN:CB	2.41	0.50
5:B:87:TYR:O	5:B:138:GLY:N	2.38	0.50
6:C:79:ARG:O	6:C:87:ARG:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1342:C:C2'	1:0:1343:C:H5'	2.42	0.50
1:0:1730:G:H5'	1:0:1731:C:H5	1.76	0.50
1:0:299:U:H5'	39:0:7794:HOH:O	2.11	0.50
2:9:3012:C:H5'	2:9:3070:U:O4'	2.12	0.50
5:B:145:HIS:HD2	5:B:146:THR:O	1.95	0.50
5:B:312:ARG:HD3	5:B:315:VAL:HG13	1.93	0.50
9:F:50:VAL:HG21	9:F:63:ILE:HG21	1.93	0.50
32:I:128:VAL:C	32:I:130:GLY:H	2.15	0.50
25:W:105:THR:HA	25:W:109:GLU:OE1	2.11	0.50
27:Y:154:ARG:HB3	27:Y:154:ARG:HH11	1.77	0.50
30:2:22:PRO:HG2	30:2:25:VAL:HG21	1.93	0.49
1:0:1363:G:OP1	6:C:76:ARG:NH2	2.44	0.49
14:L:145:LEU:O	14:L:145:LEU:HD23	2.12	0.49
14:L:36:ASP:HB2	39:L:9433:HOH:O	2.12	0.49
20:R:111:ILE:HG23	20:R:145:LEU:CD1	2.41	0.49
24:V:8:ILE:HA	24:V:11:MET:CE	2.42	0.49
25:W:125:HIS:HD2	25:W:127:GLY:H	1.59	0.49
28:Z:11:SER:O	28:Z:14:PHE:HB2	2.12	0.49
1:0:951:A:C2'	1:0:952:G:H5'	2.41	0.49
39:0:8006:HOH:O	31:3:60:LYS:HG3	2.12	0.49
2:9:3039:U:O2'	2:9:3042:C:C5	2.63	0.49
5:B:17:LYS:O	5:B:260:HIS:HD2	1.95	0.49
7:D:154:LYS:H	7:D:154:LYS:CD	2.22	0.49
9:F:49:PHE:HE1	9:F:98:VAL:HG23	1.77	0.49
11:H:54:THR:O	11:H:55:VAL:HG13	2.13	0.49
32:I:113:HIS:N	32:I:114:PRO:CD	2.75	0.49
14:L:89:PHE:CD1	14:L:89:PHE:N	2.80	0.49
24:V:56:ILE:HG22	24:V:60:GLN:HE21	1.77	0.49
1:0:1666:C:H2'	1:0:1667:A:C5'	2.41	0.49
1:0:1730:G:C5'	1:0:1731:C:H6	2.24	0.49
18:P:105:LEU:HD21	18:P:137:LEU:HD21	1.94	0.49
22:T:96:VAL:CG1	22:T:97:ARG:N	2.75	0.49
27:Y:106:THR:HG23	27:Y:107:PRO:HD2	1.94	0.49
27:Y:96:GLU:O	27:Y:235:GLU:HA	2.12	0.49
1:0:1189:A:H1'	1:0:1209:C:H1'	1.95	0.49
1:0:1462:C:H2'	1:0:1463:A:C8	2.48	0.49
1:0:1972:U:H2'	1:0:1973:A:C5'	2.43	0.49
4:A:104:PRO:HG3	4:A:127:GLN:OE1	2.12	0.49
12:J:39:VAL:CG1	12:J:40:ASN:N	2.75	0.49
17:O:96:VAL:CG1	17:O:100:GLN:HB2	2.41	0.49
18:P:98:ILE:HD12	18:P:102:ARG:NE	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:X:41:PHE:O	26:X:43:VAL:HG23	2.13	0.49
4:A:167:LYS:HB2	28:Z:29:ILE:HD13	1.94	0.49
1:0:2326:U:H4'	1:0:2412:G:C4'	2.42	0.49
1:0:949:U:O2'	19:Q:40:HIS:HE1	1.95	0.49
5:B:74:ILE:HD13	5:B:309:VAL:HG21	1.95	0.49
1:0:2548:C:OP2	5:B:5:ARG:NH2	2.45	0.49
8:E:22:VAL:O	8:E:28:SER:HA	2.12	0.49
11:H:28:ILE:HG23	39:H:9544:HOH:O	2.12	0.49
11:H:58:ARG:O	11:H:62:LEU:HD22	2.12	0.49
12:J:74:ARG:HH12	12:J:76:ASP:CB	2.25	0.49
14:L:104:ASP:HB2	39:L:9458:HOH:O	2.12	0.49
14:L:143:THR:CG2	14:L:144:ASP:N	2.75	0.49
14:L:148:GLU:HB2	39:L:9485:HOH:O	2.12	0.49
30:2:41:HIS:HD2	30:2:44:ARG:H	1.60	0.49
30:2:48:ASP:O	30:2:49:GLU:HB2	2.13	0.49
5:B:139:ASP:HB3	39:B:9547:HOH:O	2.12	0.49
9:F:39:SER:HB3	9:F:45:ALA:HB2	1.93	0.49
32:I:113:HIS:HE1	32:I:121:LEU:HD22	1.75	0.49
32:I:118:SER:HB2	32:I:123:ASN:HB2	1.94	0.49
12:J:15:ARG:NH1	12:J:43:ARG:NH1	2.61	0.49
13:K:55:VAL:CG1	13:K:56:SER:N	2.75	0.49
14:L:145:LEU:O	14:L:148:GLU:HG3	2.11	0.49
16:N:164:ASP:OD2	16:N:167:ASP:HA	2.12	0.49
1:0:2852:A:H5''	39:0:5766:HOH:O	2.11	0.49
1:0:449:A:N7	6:C:43:LYS:HG2	2.27	0.49
7:D:103:ASN:ND2	7:D:134:LEU:H	2.10	0.49
32:I:138:THR:HG22	32:I:139:ILE:H	1.77	0.49
1:0:2815:G:N7	12:J:80:LYS:NZ	2.60	0.49
24:V:39:ALA:N	24:V:40:PRO:CD	2.73	0.49
1:0:1466:C:H42	1:0:1476:A:N6	1.98	0.49
1:0:558:C:C2'	1:0:559:U:C5'	2.91	0.49
1:0:816:G:H5'	1:0:1598:A:H4'	1.94	0.49
12:J:52:GLN:HG3	12:J:53:ILE:N	2.27	0.49
14:L:65:ASP:CG	14:L:111:ALA:HB3	2.33	0.49
20:R:122:GLN:HB3	20:R:138:SER:HB2	1.93	0.49
27:Y:148:GLY:O	27:Y:154:ARG:HD3	2.12	0.49
1:0:1477:C:H2'	1:0:1478:U:C6	2.48	0.49
1:0:603:A:H4'	1:0:604:G:O5'	2.12	0.49
2:9:3049:G:O2'	2:9:3050:G:H5'	2.12	0.49
4:A:36:ASP:O	4:A:38:ILE:N	2.46	0.49
5:B:53:LEU:CD1	5:B:327:VAL:HG22	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:29:LYS:NZ	39:R:9453:HOH:O	2.46	0.49
1:O:2712:G:H5'	39:K:4183:HOH:O	2.13	0.49
4:A:65:ARG:C	4:A:66:ARG:HG3	2.32	0.49
6:C:168:ARG:NH2	6:C:190:ALA:O	2.46	0.49
1:O:1056:U:H2'	1:O:1057:A:O4'	2.13	0.48
1:O:1175:G:H1'	1:O:1193:A:C2'	2.41	0.48
1:O:1466:C:N4	1:O:1476:A:H61	1.98	0.48
1:O:1503:U:H2'	1:O:1504:A:O4'	2.13	0.48
1:O:247:A:H2'	39:O:4499:HOH:O	2.12	0.48
1:O:542:A:H2'	1:O:543:G:O4'	2.13	0.48
1:O:666:A:H2'	1:O:667:C:O4'	2.13	0.48
1:O:883:U:H2'	1:O:883:U:O2	2.12	0.48
4:A:105:VAL:HG13	4:A:155:THR:O	2.13	0.48
1:O:2453:G:H4'	14:L:50:GLY:C	2.33	0.48
16:N:78:MET:HB2	16:N:79:PRO:HD3	1.95	0.48
16:N:86:LEU:HD21	16:N:180:LEU:CD1	2.43	0.48
24:V:64:GLY:O	24:V:65:ASP:CB	2.61	0.48
1:O:2779:G:H21	8:E:143:GLN:NE2	2.11	0.48
1:O:2906:A:H5'	1:O:2907:C:O4'	2.13	0.48
2:9:3054:A:O2'	2:9:3055:U:H5'	2.13	0.48
6:C:154:VAL:O	6:C:158:GLU:HG3	2.13	0.48
1:O:2090:G:H2'	1:O:2091:G:C8	2.48	0.48
1:O:2237:G:H1'	1:O:2238:A:C8	2.48	0.48
30:2:36:ASN:HB3	30:2:39:ARG:NE	2.28	0.48
5:B:75:GLU:C	5:B:77:PRO:HD3	2.32	0.48
7:D:154:LYS:HD2	7:D:154:LYS:N	2.22	0.48
8:E:81:GLU:HA	8:E:133:VAL:O	2.13	0.48
11:H:170:ASN:N	11:H:170:ASN:ND2	2.60	0.48
12:J:19:MET:HE3	12:J:132:LEU:HD11	1.94	0.48
18:P:115:SER:N	18:P:118:GLN:HE21	2.04	0.48
27:Y:203:VAL:CG1	27:Y:228:VAL:HG22	2.43	0.48
1:O:1878:G:O2'	1:O:1879:U:C5	2.62	0.48
1:O:2414:A:H2'	1:O:2415:A:C8	2.49	0.48
29:1:28:HIS:CE1	29:1:31:LYS:HE2	2.48	0.48
2:9:3044:A:O4'	7:D:76:ARG:NE	2.46	0.48
1:O:2545:U:OP2	5:B:2:GLN:NE2	2.47	0.48
9:F:57:GLU:HB2	15:M:23:LEU:HD11	1.94	0.48
12:J:45:VAL:HG21	12:J:129:PHE:CD1	2.49	0.48
13:K:49:LEU:HD12	13:K:80:ILE:HD13	1.94	0.48
39:O:7257:HOH:O	16:N:4:PRO:HD2	2.13	0.48
1:O:1506:U:H6	1:O:1506:U:H5'	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1552:G:N2	1:0:1634:G:H1'	2.29	0.48
1:0:185:G:O3'	1:0:186:A:H4'	2.14	0.48
6:C:236:THR:HA	39:C:9256:HOH:O	2.13	0.48
9:F:91:VAL:CG1	9:F:92:GLY:H	2.11	0.48
18:P:89:ASN:OD1	18:P:92:GLU:HB2	2.13	0.48
1:0:1249:U:H2'	1:0:1250:C:C6	2.49	0.48
1:0:1667:A:C8	1:0:1667:A:H5'	2.39	0.48
4:A:88:ILE:HG22	4:A:88:ILE:O	2.13	0.48
17:O:32:ARG:HB2	39:O:4656:HOH:O	2.14	0.48
28:Z:36:ASP:HB3	28:Z:45:ASP:O	2.14	0.48
1:0:1205:U:H2'	1:0:1206:U:H5''	1.96	0.48
1:0:1377:C:H5'	1:0:1377:C:C6	2.45	0.48
1:0:602:A:O2'	1:0:605:C:H4'	2.14	0.48
1:0:120:A:H5'	29:1:20:ARG:HH21	1.79	0.48
31:3:16:GLU:HG3	31:3:18:GLN:NE2	2.29	0.48
16:N:58:LEU:N	16:N:58:LEU:HD12	2.28	0.48
24:V:39:ALA:O	24:V:41:GLU:N	2.42	0.48
25:W:21:LEU:HB3	25:W:26:ILE:CG1	2.44	0.48
1:0:1878:G:C1'	39:O:6632:HOH:O	2.56	0.48
1:0:2072:G:C6	1:0:2533:C:H1'	2.49	0.48
1:0:2365:G:H5''	39:Q:6597:HOH:O	2.12	0.48
31:3:65:THR:CG2	31:3:88:LEU:HD22	2.44	0.48
5:B:321:PRO:HA	39:B:9650:HOH:O	2.12	0.48
7:D:60:GLU:O	7:D:60:GLU:HG3	2.13	0.48
14:L:53:ARG:NH2	14:L:57:VAL:HG12	2.28	0.48
25:W:108:ARG:CG	25:W:114:PRO:HG3	2.42	0.48
28:Z:40:PRO:C	28:Z:42:CYS:H	2.17	0.48
1:0:834:G:H3'	1:0:835:U:H4'	1.96	0.48
31:3:18:GLN:OE1	31:3:73:GLU:HB3	2.13	0.48
5:B:5:ARG:HH11	5:B:8:LYS:HE2	1.77	0.48
7:D:25:MET:SD	7:D:40:ILE:HD11	2.54	0.48
15:M:187:LEU:HD23	15:M:194:ALA:HB3	1.95	0.48
21:S:33:SER:O	21:S:37:VAL:HG23	2.13	0.48
21:S:37:VAL:O	21:S:41:VAL:HG23	2.13	0.48
24:V:39:ALA:H	24:V:40:PRO:HD2	1.75	0.48
1:0:2415:A:O2'	16:N:29:SER:HB3	2.13	0.48
1:0:88:G:H2'	1:0:89:G:C8	2.49	0.48
12:J:80:LYS:NZ	39:J:7377:HOH:O	2.46	0.48
1:0:1163:G:H1	1:0:1184:C:N4	2.12	0.47
1:0:1789:G:O6	18:P:73:HIS:HE1	1.97	0.47
1:0:2851:G:H4'	5:B:157:LYS:NZ	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:396:U:OP2	31:3:38:ARG:HD2	2.13	0.47
1:0:830:G:O2'	1:0:831:U:H5'	2.14	0.47
31:3:3:MET:O	31:3:90:PHE:HA	2.14	0.47
5:B:254:GLN:HG3	39:B:9530:HOH:O	2.13	0.47
1:0:2338:G:OP1	7:D:97:GLN:HG2	2.14	0.47
32:I:116:LEU:HD22	32:I:127:GLU:OE1	2.13	0.47
32:I:139:ILE:HG22	32:I:140:GLU:N	2.29	0.47
5:B:91:PRO:O	12:J:144:THR:HG21	2.14	0.47
17:O:73:ASP:HA	17:O:92:VAL:O	2.14	0.47
23:U:52:THR:HG22	23:U:54:THR:H	1.78	0.47
24:V:1:THR:CG2	24:V:2:VAL:H	2.15	0.47
25:W:110:GLN:NE2	25:W:110:GLN:HA	2.29	0.47
1:0:1787:C:OP1	18:P:68:LYS:HE2	2.13	0.47
1:0:2421:G:H4'	39:0:5325:HOH:O	2.13	0.47
1:0:343:C:O2'	1:0:344:C:H5'	2.13	0.47
1:0:484:A:N1	1:0:506:G:H4'	2.28	0.47
2:9:3064:C:C2'	2:9:3065:A:H5'	2.44	0.47
5:B:58:PRO:HA	5:B:63:GLU:OE2	2.14	0.47
6:C:214:THR:HG23	39:C:9243:HOH:O	2.14	0.47
16:N:69:TYR:HE2	16:N:184:ILE:HG13	1.79	0.47
19:Q:75:ILE:HD13	19:Q:84:ILE:HD11	1.95	0.47
1:0:2856:A:P	26:X:15:ARG:HH22	2.36	0.47
1:0:482:G:H4'	1:0:508:A:N1	2.29	0.47
4:A:207:GLN:O	4:A:208:HIS:HB3	2.14	0.47
6:C:246:ARG:NH1	39:C:9177:HOH:O	2.46	0.47
12:J:142:ASN:O	12:J:144:THR:N	2.48	0.47
13:K:87:ARG:NH1	39:K:4066:HOH:O	2.48	0.47
15:M:77:HIS:CD2	15:M:79:ALA:O	2.65	0.47
17:O:42:GLU:HB2	39:O:2176:HOH:O	2.14	0.47
18:P:141:ILE:C	18:P:143:ALA:H	2.17	0.47
27:Y:186:ARG:HH11	27:Y:186:ARG:HG2	1.78	0.47
1:0:1236:A:H2'	1:0:1237:U:O4'	2.14	0.47
1:0:920:C:H4'	1:0:921:G:C2	2.50	0.47
1:0:952:G:N3	1:0:2302:A:H2'	2.29	0.47
4:A:203:GLY:HA2	39:A:9535:HOH:O	2.14	0.47
39:0:5171:HOH:O	4:A:6:GLY:HA3	2.14	0.47
5:B:205:VAL:O	5:B:307:ARG:NE	2.40	0.47
11:H:58:ARG:HG3	11:H:58:ARG:NH1	2.29	0.47
17:O:15:LYS:HD3	17:O:19:ARG:NH2	2.29	0.47
20:R:132:ARG:NH2	39:R:9495:HOH:O	2.47	0.47
1:0:1086:A:C6	25:W:11:VAL:HG11	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:155:ARG:NH1	39:Y:9357:HOH:O	2.46	0.47
2:9:3042:C:H5'	2:9:3043:G:OP2	2.14	0.47
4:A:223:ARG:NE	39:A:9563:HOH:O	2.47	0.47
4:A:53:ALA:HB3	39:A:9595:HOH:O	2.13	0.47
4:A:89:ALA:HB3	39:A:9614:HOH:O	2.14	0.47
5:B:41:PHE:CG	5:B:190:MET:HE3	2.50	0.47
18:P:13:VAL:HG11	18:P:40:VAL:HG11	1.96	0.47
1:0:1211:G:O2'	1:0:1212:C:H5'	2.14	0.47
1:0:622:G:P	27:Y:148:GLY:HA3	2.54	0.47
1:0:697:G:H4'	1:0:730:G:O3'	2.15	0.47
1:0:1853:C:OP1	4:A:231:LYS:HG3	2.15	0.47
1:0:2670:G:H5'	5:B:112:THR:O	2.15	0.47
12:J:22:VAL:O	12:J:26:VAL:HG23	2.15	0.47
12:J:59:LYS:O	12:J:63:ILE:HG13	2.14	0.47
17:O:14:LEU:CD2	17:O:102:ILE:HD11	2.44	0.47
17:O:53:GLN:HG2	17:O:56:GLU:OE1	2.15	0.47
22:T:71:VAL:HG13	22:T:91:LEU:O	2.14	0.47
1:0:2747:C:H4'	39:O:8438:HOH:O	2.14	0.47
5:B:277:GLU:N	5:B:278:PRO:HD2	2.29	0.47
8:E:86:VAL:HG12	8:E:129:GLU:O	2.15	0.47
14:L:57:VAL:HG12	14:L:57:VAL:O	2.14	0.47
17:O:47:ARG:HG3	17:O:47:ARG:NH1	2.29	0.47
24:V:11:MET:HB3	24:V:15:GLU:HB2	1.96	0.47
26:X:20:GLU:HG3	26:X:21:PRO:CD	2.45	0.47
27:Y:187:VAL:HG23	27:Y:192:ASP:HB2	1.94	0.47
1:0:1066:U:H2'	1:0:1067:A:C8	2.50	0.47
1:0:204:A:H2'	1:0:205:U:H5'	1.96	0.47
1:0:2820:A:H2'	1:0:2821:C:C6	2.50	0.47
1:0:475:G:H5'	6:C:73:LEU:HD23	1.95	0.47
31:3:42:ARG:HH11	31:3:42:ARG:HG3	1.78	0.47
1:0:2694:A:H4'	8:E:91:PHE:CE1	2.49	0.47
10:G:63:ARG:HB2	10:G:66:LEU:HG	1.96	0.47
12:J:63:ILE:CG2	12:J:64:GLY:N	2.77	0.47
1:0:1992:U:OP2	13:K:66:ARG:HD2	2.14	0.47
14:L:119:THR:HG23	14:L:139:SER:OG	2.15	0.47
14:L:143:THR:CG2	14:L:144:ASP:H	2.22	0.47
25:W:48:VAL:CG1	25:W:48:VAL:O	2.62	0.47
1:0:196:G:H2'	39:O:7143:HOH:O	2.14	0.47
1:0:2503:A:OP1	11:H:151:ARG:NH2	2.47	0.47
1:0:447:A:O2'	1:0:448:G:H5'	2.15	0.47
4:A:69:LEU:HD23	4:A:107:ASN:CB	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:22:VAL:HG22	7:D:74:THR:HG22	1.97	0.47
1:O:1242:A:C5'	12:J:82:THR:HG23	2.34	0.47
15:M:107:ARG:CG	15:M:107:ARG:NH1	2.73	0.47
15:M:60:VAL:C	15:M:61:ILE:HD12	2.35	0.47
20:R:119:VAL:HG21	20:R:142:ASP:CG	2.35	0.47
22:T:78:THR:HG22	22:T:88:PRO:HA	1.96	0.47
24:V:8:ILE:HG21	24:V:59:ILE:HG13	1.96	0.47
27:Y:144:ARG:CG	27:Y:144:ARG:NH1	2.67	0.47
28:Z:57:CYS:SG	28:Z:59:TYR:HB3	2.55	0.47
1:O:1624:A:H4'	1:O:1625:U:H5'	1.96	0.47
1:O:2587:OMU:H2'	1:O:2589:U:H5''	1.96	0.47
1:O:2717:C:O2'	1:O:2718:C:H5''	2.14	0.47
1:O:677:C:H4'	6:C:246:ARG:NH2	2.30	0.47
1:O:2333:G:P	7:D:56:ARG:HH22	2.38	0.47
9:F:5:ASP:O	9:F:119:ARG:NH1	2.48	0.47
1:O:1118:A:C8	1:O:1119:G:H5''	2.49	0.47
1:O:1236:A:C8	12:J:63:ILE:HD11	2.50	0.47
1:O:1328:A:C8	27:Y:169:ARG:HD3	2.49	0.47
1:O:2296:C:H2'	1:O:2297:U:H6	1.80	0.47
1:O:2456:A:H2'	1:O:2457:U:H6	1.80	0.47
1:O:737:A:H2'	1:O:738:G:O4'	2.15	0.47
1:O:820:G:O2'	1:O:856:G:H4'	2.15	0.47
8:E:77:THR:OG1	8:E:78:GLU:N	2.47	0.47
9:F:52:GLU:HG3	9:F:77:VAL:O	2.15	0.47
32:I:87:THR:HG22	32:I:88:GLY:N	2.30	0.47
21:S:73:ASP:OD1	21:S:76:GLU:HG3	2.15	0.47
22:T:89:ARG:HG3	22:T:89:ARG:O	2.15	0.47
22:T:71:VAL:CG1	22:T:90:PRO:HB3	2.31	0.47
27:Y:235:GLU:CD	27:Y:235:GLU:N	2.58	0.47
1:O:1422:U:H2'	1:O:1423:C:C6	2.50	0.46
1:O:1755:A:H2'	1:O:1756:G:O4'	2.15	0.46
1:O:2112:A:H2'	1:O:2113:G:C8	2.50	0.46
1:O:2784:A:H1'	8:E:60:SER:OG	2.15	0.46
1:O:664:U:O4	1:O:681:G:H5''	2.15	0.46
2:9:3049:G:H5''	39:9:4707:HOH:O	2.14	0.46
6:C:127:ARG:HD3	6:C:129:HIS:CE1	2.48	0.46
14:L:93:VAL:HG12	14:L:97:VAL:HG23	1.97	0.46
23:U:39:ASN:ND2	23:U:44:ARG:NH1	2.63	0.46
24:V:5:VAL:CG1	24:V:9:ARG:NH1	2.78	0.46
26:X:23:HIS:CD2	26:X:24:LYS:HG3	2.49	0.46
26:X:30:MET:CE	26:X:58:ALA:HB3	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2372:A:H2'	1:0:2373:U:C6	2.51	0.46
1:0:2326:U:H4'	1:0:2412:G:H4'	1.98	0.46
1:0:812:A:H1'	39:0:4533:HOH:O	2.15	0.46
5:B:30:PRO:HB2	5:B:39:GLN:NE2	2.30	0.46
1:0:1180:U:O2'	32:I:92:PRO:HD2	2.15	0.46
12:J:42:GLU:O	12:J:131:THR:HG23	2.15	0.46
16:N:48:VAL:HG11	16:N:55:ASP:HB3	1.98	0.46
26:X:43:VAL:HG12	26:X:47:ALA:HB3	1.97	0.46
1:0:1192:A:H3'	1:0:1193:A:H5'	1.97	0.46
1:0:177:A:H2'	1:0:178:U:O4'	2.15	0.46
2:9:3029:C:C2'	2:9:3030:C:H5'	2.45	0.46
5:B:36:PRO:CA	5:B:168:GLY:HA3	2.40	0.46
5:B:88:GLU:HB3	5:B:97:LEU:HD12	1.98	0.46
16:N:11:ARG:CG	16:N:14:ARG:HH12	2.25	0.46
16:N:89:GLY:O	16:N:92:ALA:HB3	2.15	0.46
18:P:135:ALA:HB1	18:P:139:ARG:HH12	1.79	0.46
20:R:99:ALA:HB1	20:R:109:MET:HE3	1.95	0.46
1:0:304:G:H1'	1:0:347:A:N6	2.31	0.46
2:9:3049:G:H2'	2:9:3050:G:O4'	2.16	0.46
2:9:3114:G:O6	16:N:11:ARG:HD3	2.15	0.46
9:F:48:VAL:HG12	9:F:97:ALA:CB	2.46	0.46
11:H:66:ARG:HD3	39:H:9544:HOH:O	2.15	0.46
14:L:10:SER:O	14:L:11:ARG:HB3	2.15	0.46
39:0:5491:HOH:O	15:M:82:ARG:HD3	2.15	0.46
4:A:101:GLU:OE2	4:A:131:HIS:HB2	2.16	0.46
12:J:76:ASP:HA	39:J:5907:HOH:O	2.16	0.46
1:0:903:U:O4	14:L:18:HIS:HB2	2.15	0.46
15:M:59:GLY:HA3	15:M:141:ILE:HD12	1.96	0.46
25:W:35:VAL:HA	25:W:36:PRO:HD3	1.86	0.46
1:0:1044:C:H5''	39:0:9648:HOH:O	2.15	0.46
1:0:107:U:H2'	1:0:108:U:H5'	1.98	0.46
7:D:172:VAL:CG1	7:D:173:GLU:H	2.20	0.46
11:H:29:ALA:C	11:H:30:GLN:HG3	2.35	0.46
15:M:122:GLN:OE1	15:M:127:LYS:HE2	2.15	0.46
19:Q:25:PRO:HA	19:Q:26:PRO:HD3	1.80	0.46
21:S:29:ASP:OD1	21:S:31:ARG:NH1	2.49	0.46
26:X:9:VAL:HG13	26:X:88:GLU:OE2	2.16	0.46
1:0:1829:A:H61	28:Z:18:TYR:H	1.64	0.46
1:0:2346:C:O5'	1:0:2346:C:H6	1.97	0.46
31:3:25:VAL:HG22	31:3:68:LYS:HG3	1.96	0.46
5:B:185:GLY:HA2	39:B:9627:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:254:GLN:HG2	5:B:255:GLY:H	1.81	0.46
6:C:118:THR:CG2	6:C:137:PRO:HB3	2.45	0.46
1:O:894:A:N1	6:C:87:ARG:NH2	2.63	0.46
7:D:18:ILE:HG12	7:D:134:LEU:HD23	1.97	0.46
7:D:49:PRO:HB3	39:D:5828:HOH:O	2.16	0.46
9:F:50:VAL:CG2	9:F:63:ILE:HG21	2.46	0.46
9:F:65:GLU:O	9:F:69:GLU:HG2	2.15	0.46
13:K:20:CYS:HB2	13:K:29:LEU:HG	1.98	0.46
15:M:22:GLU:HG2	15:M:26:GLN:NE2	2.31	0.46
1:O:1441:G:O2'	1:O:1442:A:H5'	2.16	0.46
1:O:1942:A:H3'	39:O:7801:HOH:O	2.16	0.46
1:O:2642:G:H2'	1:O:2643:G:O4'	2.16	0.46
39:O:8006:HOH:O	31:3:61:PRO:HG2	2.16	0.46
2:9:3024:U:H3'	2:9:3025:G:C5'	2.46	0.46
2:9:3091:C:H2'	2:9:3092:G:O4'	2.16	0.46
39:O:4967:HOH:O	4:A:11:ARG:CZ	2.64	0.46
4:A:171:LYS:NZ	39:A:9513:HOH:O	2.48	0.46
5:B:321:PRO:HG3	39:B:9593:HOH:O	2.15	0.46
10:G:64:ASN:N	10:G:64:ASN:ND2	2.63	0.46
32:I:75:THR:HA	32:I:112:LYS:NZ	2.31	0.46
16:N:154:LEU:O	16:N:155:GLU:CB	2.64	0.46
26:X:78:GLU:HG2	26:X:79:GLU:OE2	2.15	0.46
4:A:130:THR:HG22	4:A:131:HIS:O	2.15	0.46
5:B:301:VAL:HG11	5:B:309:VAL:HG11	1.97	0.46
6:C:218:VAL:HG12	39:C:9230:HOH:O	2.15	0.46
8:E:106:ASN:ND2	8:E:109:GLY:HA2	2.30	0.46
8:E:118:ILE:HG23	8:E:144:THR:HG21	1.98	0.46
8:E:114:ARG:HB3	8:E:151:LEU:HD11	1.97	0.46
11:H:9:ILE:HD12	11:H:54:THR:HG22	1.98	0.46
14:L:80:ASP:HB2	14:L:90:ARG:HB3	1.98	0.46
16:N:8:VAL:CG1	16:N:14:ARG:HE	2.29	0.46
17:O:38:ARG:NH1	39:O:7674:HOH:O	2.49	0.46
26:X:76:ARG:NH1	26:X:76:ARG:HG3	2.30	0.46
27:Y:99:ALA:HB2	27:Y:233:TYR:CZ	2.51	0.46
1:O:136:C:H2'	1:O:137:U:O4'	2.15	0.46
1:O:1574:C:H2'	1:O:1575:C:C6	2.52	0.46
1:O:1666:C:C2'	1:O:1667:A:C5'	2.94	0.46
1:O:1902:G:H2'	1:O:1903:U:O4'	2.16	0.46
1:O:2825:C:H4'	1:O:2826:G:O5'	2.17	0.46
39:O:7688:HOH:O	4:A:11:ARG:HA	2.16	0.46
1:O:1311:G:O6	6:C:173:LYS:HE3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:10:PHE:CE1	7:D:11:HIS:HB3	2.51	0.46
17:O:24:ALA:O	17:O:28:ASP:HB2	2.16	0.46
22:T:71:VAL:CG1	22:T:72:ILE:N	2.78	0.46
1:O:2904:U:H4'	26:X:8:ARG:HH12	1.80	0.46
27:Y:152:LYS:HB3	27:Y:160:LYS:HG3	1.98	0.46
1:O:2824:C:H5''	1:O:2825:C:H5'	1.98	0.45
5:B:36:PRO:HB3	5:B:174:ARG:CB	2.46	0.45
5:B:190:MET:CE	5:B:194:PHE:CD1	3.00	0.45
9:F:48:VAL:HG12	9:F:97:ALA:HB2	1.98	0.45
11:H:158:THR:HB	11:H:159:PRO:HD3	1.99	0.45
1:O:926:A:H5'	14:L:39:GLU:OE2	2.16	0.45
19:Q:31:GLU:CD	19:Q:93:ARG:HH12	2.19	0.45
21:S:33:SER:OG	21:S:36:GLU:HG3	2.17	0.45
25:W:72:PRO:HB2	25:W:74:GLU:O	2.15	0.45
27:Y:209:VAL:HG12	27:Y:214:ARG:HG3	1.97	0.45
1:O:2270:G:H4'	4:A:223:ARG:NH1	2.31	0.45
1:O:2821:C:H4'	5:B:116:PRO:HG3	1.97	0.45
6:C:115:LEU:O	6:C:118:THR:HB	2.16	0.45
10:G:16:LYS:O	10:G:20:VAL:HG23	2.15	0.45
11:H:54:THR:HG23	11:H:128:GLN:HA	1.97	0.45
11:H:146:VAL:HG22	39:H:9541:HOH:O	2.16	0.45
1:O:1163:G:H5'	32:I:115:ASP:O	2.17	0.45
32:I:92:PRO:C	32:I:94:GLU:N	2.70	0.45
15:M:74:LYS:HG3	39:M:9384:HOH:O	2.16	0.45
19:Q:3:SER:HB3	39:Q:5998:HOH:O	2.17	0.45
25:W:38:THR:CG2	25:W:39:ASP:N	2.78	0.45
25:W:88:THR:CG2	25:W:90:TYR:HD1	2.28	0.45
28:Z:56:GLN:HA	28:Z:62:TYR:O	2.16	0.45
1:O:1741:U:O2'	1:O:2723:G:H4'	2.17	0.45
1:O:2769:C:H2'	1:O:2770:G:C5'	2.45	0.45
39:O:7612:HOH:O	29:1:1:THR:HB	2.16	0.45
32:I:75:THR:HA	32:I:112:LYS:HZ3	1.81	0.45
17:O:60:VAL:C	17:O:62:GLY:H	2.20	0.45
19:Q:75:ILE:HD13	19:Q:84:ILE:CD1	2.46	0.45
25:W:96:LEU:O	25:W:100:LEU:HG	2.16	0.45
1:O:1165:G:H1'	1:O:1174:A:H1'	1.98	0.45
1:O:1714:C:O2'	1:O:1715:C:H5'	2.17	0.45
1:O:292:G:H2'	1:O:358:G:N2	2.32	0.45
5:B:24:PRO:HG3	5:B:204:GLY:HA2	1.97	0.45
14:L:134:GLU:HG3	39:L:9453:HOH:O	2.17	0.45
16:N:154:LEU:HG	16:N:155:GLU:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1771:U:H5'	28:Z:20:ARG:NH2	2.31	0.45
1:0:2508:C:H2'	39:0:7239:HOH:O	2.17	0.45
1:0:286:U:H2'	1:0:287:C:C6	2.52	0.45
1:0:396:U:H1'	39:0:8151:HOH:O	2.17	0.45
1:0:1881:A:OP1	4:A:199:HIS:HE1	1.99	0.45
1:0:1654:U:H2'	4:A:47:HIS:CD2	2.51	0.45
4:A:88:ILE:HD13	4:A:100:PRO:CD	2.45	0.45
4:A:94:LEU:N	4:A:94:LEU:HD23	2.32	0.45
5:B:58:PRO:HA	5:B:63:GLU:CD	2.36	0.45
6:C:133:ARG:NH1	39:C:9218:HOH:O	2.49	0.45
39:0:8228:HOH:O	6:C:94:THR:HG21	2.16	0.45
32:I:99:ASP:O	32:I:100:LEU:HD23	2.17	0.45
23:U:9:CYS:HA	23:U:52:THR:HG23	1.99	0.45
1:0:1025:C:H5'	25:W:23:MET:O	2.17	0.45
1:0:1299:G:N2	39:0:5228:HOH:O	2.49	0.45
1:0:1419:U:H2'	1:0:1685:A:C2	2.52	0.45
1:0:1878:G:O2'	1:0:1879:U:P	2.74	0.45
1:0:2072:G:H3'	1:0:2073:G:C5'	2.47	0.45
1:0:2312:G:H2'	1:0:2313:C:H5'	1.98	0.45
1:0:945:U:H2'	1:0:946:C:C6	2.51	0.45
4:A:70:ALA:HA	4:A:71:PRO:HD3	1.78	0.45
5:B:14:GLY:HA2	5:B:15:PRO:C	2.36	0.45
9:F:60:VAL:O	9:F:60:VAL:CG1	2.64	0.45
10:G:64:ASN:O	10:G:68:GLU:HG3	2.17	0.45
12:J:26:VAL:HG13	12:J:36:VAL:HG11	1.99	0.45
15:M:107:ARG:NH2	39:M:9399:HOH:O	2.48	0.45
1:0:818:A:O2'	28:Z:13:ARG:HD2	2.16	0.45
1:0:1717:A:H5''	18:P:54:LYS:HB2	1.97	0.45
1:0:2361:A:H2'	1:0:2362:A:C8	2.51	0.45
1:0:2626:C:H2'	1:0:2627:G:C8	2.52	0.45
31:3:91:GLN:O	31:3:92:GLU:HB2	2.17	0.45
7:D:49:PRO:HA	7:D:73:VAL:HG22	1.98	0.45
7:D:95:THR:OG1	7:D:174:VAL:HG22	2.16	0.45
11:H:3:ALA:HA	11:H:58:ARG:NH1	2.32	0.45
12:J:88:PRO:O	12:J:94:GLY:HA3	2.17	0.45
9:F:38:LYS:NZ	15:M:3:SER:HA	2.32	0.45
22:T:38:ARG:HG3	22:T:38:ARG:NH1	2.32	0.45
25:W:13:MET:CE	25:W:18:GLN:HA	2.37	0.45
25:W:80:ASP:HB2	39:W:3312:HOH:O	2.15	0.45
1:0:1200:A:H3'	39:0:6280:HOH:O	2.17	0.45
1:0:2504:A:H2'	1:0:2505:G:O4'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2568:A:C2'	1:0:2569:A:H5'	2.47	0.45
30:2:10:ARG:HH11	30:2:49:GLU:CD	2.20	0.45
6:C:5:ILE:HG13	6:C:15:GLU:HA	1.99	0.45
7:D:25:MET:CE	7:D:37:ALA:HB1	2.45	0.45
11:H:151:ARG:HA	11:H:154:TYR:CE2	2.51	0.45
25:W:122:ARG:HH22	25:W:154:ARG:HG2	1.75	0.45
25:W:88:THR:HG22	25:W:90:TYR:CD1	2.52	0.45
27:Y:112:GLU:CD	27:Y:115:ARG:NH1	2.70	0.45
1:0:1773:G:C8	28:Z:16:ALA:HA	2.52	0.45
1:0:1351:G:OP1	6:C:96:LYS:NZ	2.38	0.45
1:0:1847:A:OP1	4:A:175:LYS:HG3	2.17	0.45
1:0:371:U:H2'	1:0:372:A:H8	1.82	0.45
1:0:702:G:O2'	1:0:703:G:H5'	2.17	0.45
1:0:958:G:H2'	1:0:959:C:C6	2.52	0.45
1:0:2250:G:OP1	4:A:31:LYS:HD3	2.16	0.45
5:B:305:ASP:O	5:B:306:LYS:CB	2.63	0.45
8:E:22:VAL:HG12	8:E:76:VAL:HG11	1.99	0.45
12:J:39:VAL:HG21	12:J:107:ASN:ND2	2.32	0.45
20:R:106:GLY:HA2	20:R:109:MET:CE	2.47	0.45
22:T:69:LYS:O	22:T:71:VAL:HG23	2.17	0.45
26:X:43:VAL:CG1	26:X:47:ALA:HB3	2.47	0.45
27:Y:107:PRO:HB3	27:Y:182:PHE:CE2	2.52	0.45
1:0:2511:A:H2'	1:0:2512:U:O4'	2.17	0.45
1:0:526:U:H2'	1:0:527:U:C6	2.52	0.45
29:1:28:HIS:HD2	29:1:31:LYS:H	1.63	0.45
5:B:265:LEU:CD2	5:B:316:ARG:HD3	2.47	0.45
32:I:96:PHE:HD2	32:I:136:GLY:HA2	1.82	0.45
14:L:72:ASN:HB2	39:L:9477:HOH:O	2.16	0.45
2:9:3006:C:H5''	16:N:37:ARG:HE	1.82	0.45
24:V:7:GLU:O	24:V:11:MET:HG3	2.17	0.45
28:Z:53:GLY:HA2	28:Z:67:GLY:O	2.17	0.45
1:0:1369:A:H4'	20:R:64:SER:OG	2.17	0.44
1:0:162:C:H2'	1:0:163:U:H5'	1.99	0.44
1:0:2011:A:H4'	1:0:2012:U:O5'	2.17	0.44
30:2:41:HIS:N	30:2:45:ASN:HD22	1.97	0.44
31:3:60:LYS:HG3	31:3:61:PRO:HD2	1.97	0.44
6:C:57:PRO:HG2	6:C:73:LEU:CD1	2.46	0.44
15:M:164:THR:CG2	15:M:166:ALA:H	2.29	0.44
1:0:317:A:OP1	22:T:52:ARG:O	2.35	0.44
1:0:1266:U:O2'	27:Y:119:GLN:NE2	2.41	0.44
1:0:1730:G:H5''	1:0:1731:C:H6	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:61:PHE:HB3	39:C:9250:HOH:O	2.17	0.44
7:D:128:LEU:HD23	7:D:128:LEU:C	2.38	0.44
12:J:70:PHE:CG	12:J:70:PHE:O	2.70	0.44
12:J:71:TYR:CG	12:J:72:PRO:HD2	2.53	0.44
15:M:98:GLN:O	15:M:102:GLU:HG3	2.17	0.44
15:M:61:ILE:N	15:M:61:ILE:HD12	2.31	0.44
21:S:57:THR:HG22	21:S:58:MET:N	2.32	0.44
22:T:48:VAL:CG2	22:T:96:VAL:CG1	2.94	0.44
1:0:1181:A:N1	1:0:1192:A:O2'	2.49	0.44
1:0:1198:U:H2'	1:0:1200:A:OP2	2.17	0.44
1:0:1592:G:O2'	1:0:1593:C:O4'	2.34	0.44
1:0:1919:A:H4'	39:0:5395:HOH:O	2.17	0.44
1:0:2720:C:O2	13:K:87:ARG:NH2	2.49	0.44
1:0:470:U:O2'	29:1:16:HIS:CD2	2.60	0.44
7:D:135:VAL:HG22	7:D:136:ARG:H	1.80	0.44
11:H:1:LYS:N	39:H:9530:HOH:O	2.49	0.44
32:I:89:SER:HB3	32:I:97:VAL:CG2	2.48	0.44
12:J:131:THR:HB	12:J:134:GLU:OE1	2.17	0.44
14:L:145:LEU:C	14:L:145:LEU:HD23	2.37	0.44
17:O:26:TRP:HA	17:O:26:TRP:CE3	2.52	0.44
25:W:149:LEU:HG	25:W:153:MET:HE1	1.99	0.44
1:0:1007:A:H2'	11:H:19:TYR:CZ	2.52	0.44
1:0:1086:A:N6	25:W:11:VAL:HG11	2.33	0.44
1:0:1218:U:H2'	1:0:1219:U:C6	2.53	0.44
1:0:133:U:C3'	1:0:134:U:H5''	2.48	0.44
1:0:2102:G:H5''	1:0:2538:A:C2	2.52	0.44
1:0:2542:C:H5''	1:0:2608:C:N4	2.33	0.44
1:0:92:G:H4'	24:V:44:GLY:HA3	2.00	0.44
1:0:2427:C:OP2	31:3:84:ARG:HD2	2.17	0.44
2:9:3042:C:O2	7:D:76:ARG:NH1	2.50	0.44
7:D:13:MET:HA	7:D:137:PRO:HG2	1.98	0.44
27:Y:154:ARG:HH11	27:Y:154:ARG:CG	2.30	0.44
28:Z:36:ASP:CB	28:Z:45:ASP:HB3	2.34	0.44
1:0:2251:G:H2'	1:0:2252:A:C8	2.53	0.44
1:0:2518:C:H2'	1:0:2519:C:O4'	2.17	0.44
1:0:2531:U:O2'	1:0:2532:A:H5'	2.17	0.44
3:4:176:DA:H5''	3:4:175:C:H3'	2.00	0.44
6:C:194:PHE:HA	6:C:234:VAL:HG13	2.00	0.44
6:C:31:ILE:HG23	6:C:220:THR:CG2	2.47	0.44
7:D:172:VAL:CG1	7:D:173:GLU:N	2.80	0.44
39:9:5851:HOH:O	16:N:115:VAL:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:64:SER:C	16:N:66:LEU:H	2.20	0.44
27:Y:99:ALA:HB2	27:Y:233:TYR:CE2	2.52	0.44
1:0:1181:A:H2'	1:0:1182:C:H5'	2.00	0.44
1:0:125:U:H2'	39:0:4346:HOH:O	2.17	0.44
1:0:2314:G:C2'	1:0:2315:C:H5'	2.48	0.44
1:0:2353:A:H4'	1:0:2354:A:O5'	2.17	0.44
1:0:2831:C:O3'	20:R:71:LYS:HE2	2.18	0.44
1:0:2857:C:H2'	1:0:2858:U:C6	2.53	0.44
1:0:821:U:H2'	1:0:822:C:H6	1.82	0.44
4:A:36:ASP:HA	4:A:83:GLY:HA3	1.99	0.44
5:B:178:ALA:O	5:B:182:VAL:HG23	2.18	0.44
5:B:254:GLN:NE2	39:B:9585:HOH:O	2.48	0.44
5:B:8:LYS:HG3	5:B:220:VAL:HG12	1.99	0.44
7:D:60:GLU:O	7:D:61:PHE:C	2.55	0.44
9:F:31:LYS:HE3	39:F:2623:HOH:O	2.17	0.44
10:G:67:LEU:O	10:G:71:LEU:HG	2.18	0.44
11:H:169:GLY:C	11:H:170:ASN:HD22	2.21	0.44
11:H:21:THR:O	11:H:120:ILE:HD12	2.18	0.44
39:0:6242:HOH:O	13:K:87:ARG:CZ	2.64	0.44
16:N:24:LEU:HD13	19:Q:26:PRO:HB3	1.98	0.44
1:0:134:U:H5'	1:0:134:U:C6	2.47	0.44
1:0:1921:A:O2'	1:0:1922:A:H5'	2.18	0.44
1:0:2533:C:C6	1:0:2533:C:H5'	2.49	0.44
1:0:333:G:O2'	1:0:334:G:H5'	2.18	0.44
1:0:497:A:H2'	1:0:498:A:C5'	2.48	0.44
8:E:20:ILE:HD11	8:E:40:VAL:CG1	2.38	0.44
9:F:99:THR:O	9:F:100:ASP:HB2	2.17	0.44
10:G:27:ILE:HD13	10:G:71:LEU:HD23	1.99	0.44
11:H:56:GLN:HE22	11:H:93:GLN:HG2	1.83	0.44
2:9:3011:A:P	19:Q:19:ARG:HH21	2.40	0.44
1:0:249:G:O2'	1:0:250:C:H5'	2.18	0.44
1:0:2767:C:OP1	5:B:318:ASN:ND2	2.51	0.44
1:0:629:A:H2'	1:0:630:A:O4'	2.18	0.44
1:0:2101:A:H2'	6:C:63:SER:OG	2.18	0.44
1:0:1181:A:H5'	32:I:94:GLU:OE2	2.18	0.44
13:K:49:LEU:CD1	13:K:80:ILE:HD13	2.48	0.44
20:R:119:VAL:CG1	20:R:119:VAL:O	2.65	0.44
27:Y:133:HIS:HD2	39:Y:9381:HOH:O	2.00	0.44
27:Y:189:ASN:HD22	27:Y:192:ASP:H	1.66	0.44
1:0:1299:G:N7	14:L:6:ARG:NH1	2.65	0.44
1:0:1418:U:OP1	30:2:42:TRP:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2362:A:H2'	1:0:2363:G:C8	2.53	0.44
1:0:603:A:H1'	1:0:605:C:C2	2.52	0.44
1:0:951:A:O2'	1:0:952:G:H5'	2.18	0.44
2:9:3002:U:OP2	2:9:3003:A:H5'	2.18	0.44
5:B:274:GLU:HA	5:B:292:GLY:O	2.18	0.44
6:C:129:HIS:HE1	6:C:231:ARG:HA	1.83	0.44
6:C:194:PHE:CE2	6:C:234:VAL:HG11	2.53	0.44
9:F:107:ASP:O	9:F:111:ILE:HG13	2.17	0.44
22:T:9:LYS:CE	22:T:13:ARG:NH1	2.67	0.44
1:0:656:G:OP2	17:O:37:ARG:HD2	2.17	0.43
30:2:41:HIS:CD2	30:2:44:ARG:H	2.36	0.43
4:A:201:PHE:HB3	39:A:9620:HOH:O	2.16	0.43
8:E:93:MET:HE1	8:E:165:GLY:N	2.33	0.43
25:W:122:ARG:CG	25:W:122:ARG:NH1	2.80	0.43
1:0:1205:U:C2'	1:0:1206:U:H5''	2.49	0.43
1:0:1435:U:H5'	39:0:3204:HOH:O	2.16	0.43
1:0:2568:A:H2'	1:0:2569:A:O4'	2.18	0.43
1:0:2809:G:H2'	1:0:2810:G:O4'	2.19	0.43
1:0:907:A:H2'	1:0:908:A:C8	2.52	0.43
5:B:87:TYR:HD1	39:B:9575:HOH:O	2.01	0.43
6:C:21:VAL:HG13	39:C:9202:HOH:O	2.16	0.43
12:J:131:THR:HG22	12:J:133:GLY:N	2.34	0.43
14:L:94:ARG:NH1	14:L:143:THR:HG21	2.33	0.43
22:T:52:ARG:O	22:T:53:GLY:O	2.36	0.43
1:0:1657:A:H2'	1:0:1658:A:C8	2.54	0.43
1:0:2016:U:H2'	1:0:2017:U:O4'	2.17	0.43
1:0:2416:G:O2'	16:N:25:ARG:HG2	2.18	0.43
1:0:283:U:H5''	1:0:284:C:OP2	2.19	0.43
4:A:132:ASP:OD1	4:A:133:ARG:N	2.42	0.43
5:B:175:LEU:C	5:B:175:LEU:HD23	2.38	0.43
1:0:2898:G:H4'	5:B:288:GLY:HA2	2.00	0.43
8:E:112:ALA:HA	8:E:113:PRO:HD3	1.83	0.43
22:T:32:ARG:NH1	22:T:38:ARG:HH12	2.15	0.43
23:U:38:ASN:O	23:U:42:LEU:HG	2.18	0.43
24:V:12:THR:OG1	24:V:13:PRO:HD2	2.18	0.43
1:0:1829:A:N6	28:Z:18:TYR:HA	2.33	0.43
1:0:1132:A:N6	1:0:1229:C:H2'	2.34	0.43
1:0:1641:A:C2'	1:0:1642:A:H5'	2.47	0.43
1:0:245:C:H2'	1:0:246:G:H5'	2.01	0.43
1:0:2568:A:H2'	1:0:2569:A:H5'	2.01	0.43
1:0:506:G:H22	1:0:509:A:H5'	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:2:41:HIS:HB3	30:2:44:ARG:HB2	2.00	0.43
4:A:211:LYS:HB2	39:A:9576:HOH:O	2.18	0.43
5:B:40:GLY:HA3	39:B:9640:HOH:O	2.17	0.43
25:W:122:ARG:CG	25:W:152:ALA:O	2.66	0.43
1:0:1067:A:H5'	39:0:4907:HOH:O	2.17	0.43
1:0:1160:G:HO2'	1:0:1190:G:H8	1.62	0.43
1:0:338:C:H4'	6:C:174:ILE:HD11	2.00	0.43
5:B:24:PRO:CG	5:B:204:GLY:HA2	2.48	0.43
5:B:307:ARG:HD2	39:B:9645:HOH:O	2.18	0.43
5:B:314:ALA:HB3	5:B:317:PRO:HG3	1.99	0.43
5:B:280:VAL:HG13	5:B:333:GLU:O	2.18	0.43
5:B:84:LEU:HD13	5:B:84:LEU:C	2.39	0.43
6:C:72:LYS:HA	6:C:76:ARG:O	2.19	0.43
7:D:173:GLU:HG3	7:D:174:VAL:H	1.82	0.43
32:I:92:PRO:O	32:I:94:GLU:HG3	2.19	0.43
12:J:74:ARG:NH1	12:J:76:ASP:CB	2.80	0.43
16:N:110:THR:HB	16:N:113:SER:HG	1.84	0.43
20:R:82:GLU:O	20:R:86:LYS:HG3	2.19	0.43
24:V:56:ILE:HG22	24:V:60:GLN:NE2	2.33	0.43
1:0:699:C:H2'	1:0:744:G:O4'	2.18	0.43
1:0:1415:G:H5'	29:1:12:ASN:O	2.19	0.43
5:B:102:THR:HG21	5:B:182:VAL:O	2.19	0.43
7:D:103:ASN:OD1	7:D:133:ASN:ND2	2.52	0.43
13:K:14:LYS:HG3	13:K:32:ILE:O	2.18	0.43
16:N:170:GLU:O	16:N:174:GLU:HG3	2.18	0.43
17:O:26:TRP:HA	17:O:26:TRP:HE3	1.82	0.43
23:U:9:CYS:O	23:U:52:THR:HG23	2.18	0.43
24:V:8:ILE:HA	24:V:11:MET:HE2	2.00	0.43
25:W:142:ASP:O	25:W:145:GLY:N	2.52	0.43
1:0:1119:G:C8	12:J:52:GLN:NE2	2.83	0.43
1:0:1667:A:H2'	1:0:1668:U:C6	2.53	0.43
1:0:2421:G:H2'	39:0:4649:HOH:O	2.18	0.43
1:0:2039:A:H4'	1:0:2760:C:O2'	2.18	0.43
1:0:297:U:H1'	39:0:4511:HOH:O	2.17	0.43
1:0:816:G:C6	1:0:817:G:N1	2.87	0.43
1:0:962:C:H1'	16:N:5:ARG:NH1	2.34	0.43
4:A:65:ARG:HH11	4:A:65:ARG:HG2	1.84	0.43
1:0:2717:C:OP1	5:B:207:LYS:HG3	2.18	0.43
5:B:85:ARG:HB2	5:B:99:GLU:HG2	2.00	0.43
12:J:130:VAL:HG12	12:J:131:THR:H	1.84	0.43
19:Q:46:SER:O	19:Q:48:PRO:HD3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:75:GLU:O	22:T:76:ASP:HB2	2.18	0.43
1:0:1573:A:H2'	1:0:1574:C:O4'	2.18	0.43
1:0:1759:A:N3	1:0:1818:C:H2'	2.34	0.43
1:0:2506:A:O2'	1:0:2507:G:P	2.77	0.43
1:0:820:G:C6	4:A:171:LYS:HB2	2.54	0.43
5:B:243:ASN:HA	5:B:244:PRO:C	2.38	0.43
5:B:56:ASP:CG	5:B:322:ARG:HB3	2.38	0.43
6:C:138:VAL:HG11	6:C:160:LEU:HD13	2.01	0.43
7:D:96:SER:C	7:D:98:PHE:H	2.22	0.43
16:N:86:LEU:HD21	16:N:180:LEU:HD12	2.01	0.43
26:X:73:ARG:HB2	26:X:88:GLU:OE2	2.18	0.43
27:Y:216:ARG:HD2	39:Y:9369:HOH:O	2.19	0.43
1:0:1130:U:H2'	1:0:1131:G:O4'	2.19	0.43
1:0:1456:C:H2'	1:0:1457:U:C6	2.54	0.43
1:0:2506:A:O2'	1:0:2507:G:O5'	2.37	0.43
21:S:53:ASN:ND2	39:S:9480:HOH:O	2.51	0.43
22:T:23:VAL:HG23	22:T:41:ARG:HG3	2.00	0.43
23:U:14:GLU:OE1	23:U:15:PRO:HD2	2.19	0.43
25:W:108:ARG:HE	25:W:114:PRO:HG3	1.83	0.43
25:W:54:PHE:CZ	25:W:140:LYS:HB2	2.53	0.43
25:W:3:ALA:O	25:W:54:PHE:HA	2.19	0.43
27:Y:184:GLU:HG2	27:Y:229:LEU:HD11	2.00	0.43
1:0:2356:A:H2'	1:0:2357:G:O4'	2.18	0.43
1:0:2699:A:H2'	1:0:2700:G:O4'	2.18	0.43
1:0:2726:U:O2	1:0:2749:U:O5'	2.37	0.43
1:0:2831:C:H2'	1:0:2832:C:H5'	2.01	0.43
1:0:64:G:H2'	1:0:65:C:O4'	2.19	0.43
2:9:3050:G:H5''	16:N:159:TYR:HE1	1.83	0.43
5:B:18:ARG:HE	5:B:256:GLN:NE2	2.17	0.43
5:B:279:THR:HA	5:B:284:PHE:HE1	1.84	0.43
7:D:135:VAL:HG21	7:D:139:TYR:CG	2.54	0.43
13:K:80:ILE:O	13:K:87:ARG:HA	2.19	0.43
18:P:13:VAL:HG11	18:P:40:VAL:HG12	2.00	0.43
22:T:40:VAL:HG22	22:T:41:ARG:H	1.82	0.43
28:Z:39:CYS:HB3	28:Z:42:CYS:SG	2.59	0.43
1:0:1095:U:O2	25:W:120:PRO:HG2	2.19	0.42
1:0:1298:U:H2'	1:0:1299:G:C8	2.52	0.42
1:0:2088:C:H1'	1:0:2841:A:N1	2.35	0.42
1:0:2064:U:H4'	1:0:2653:A:OP1	2.18	0.42
1:0:65:C:O2'	1:0:66:G:H5'	2.18	0.42
7:D:51:ARG:HD3	39:D:7636:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:I:102:VAL:CG1	32:I:106:LYS:HE3	2.44	0.42
32:I:113:HIS:CE1	32:I:121:LEU:HD22	2.53	0.42
32:I:132:CYS:C	32:I:134:SER:N	2.72	0.42
13:K:4:LEU:HD23	13:K:4:LEU:HA	1.85	0.42
15:M:115:LEU:HD13	15:M:116:ASN:HB2	2.01	0.42
16:N:137:ALA:HB1	16:N:141:ARG:HD3	2.00	0.42
17:O:97:SER:OG	17:O:100:GLN:HG3	2.19	0.42
22:T:55:PHE:CE1	22:T:89:ARG:HG2	2.54	0.42
23:U:4:ARG:HH11	23:U:4:ARG:HG2	1.84	0.42
28:Z:41:ASN:O	28:Z:42:CYS:HB3	2.19	0.42
1:0:553:G:O4'	1:0:1325:G:H5'	2.19	0.42
1:0:2239:C:H2'	1:0:2240:U:C6	2.54	0.42
1:0:2724:U:H2'	1:0:2725:G:O4'	2.19	0.42
1:0:27:U:H2'	1:0:28:G:O4'	2.19	0.42
1:0:366:U:H2'	1:0:367:G:O4'	2.19	0.42
29:1:21:ARG:HD3	29:1:45:ARG:NE	2.34	0.42
31:3:70:ARG:HB3	39:3:9502:HOH:O	2.18	0.42
4:A:36:ASP:CG	4:A:36:ASP:O	2.57	0.42
5:B:146:THR:C	5:B:148:PRO:HD3	2.40	0.42
8:E:6:GLU:HA	8:E:46:THR:HG22	2.01	0.42
15:M:184:ARG:HG3	15:M:185:PRO:HA	2.01	0.42
15:M:82:ARG:O	15:M:83:SER:C	2.57	0.42
16:N:152:GLU:HA	16:N:152:GLU:OE1	2.19	0.42
20:R:114:VAL:HG13	20:R:114:VAL:O	2.19	0.42
20:R:84:ALA:O	20:R:88:PHE:HD1	2.02	0.42
25:W:52:VAL:HG13	25:W:53:ALA:N	2.33	0.42
26:X:20:GLU:CG	26:X:21:PRO:HD2	2.48	0.42
27:Y:106:THR:CG2	27:Y:107:PRO:HD2	2.49	0.42
1:0:1099:G:H2'	1:0:1100:G:O4'	2.19	0.42
1:0:912:A:C4	1:0:1294:A:C2	3.06	0.42
1:0:1603:A:H5''	1:0:1604:G:H3'	2.00	0.42
1:0:188:C:H5''	15:M:163:LEU:HD21	2.02	0.42
1:0:1940:C:H4'	39:0:7801:HOH:O	2.18	0.42
1:0:2541:U:O2	3:4:76:PPU:HA	2.20	0.42
1:0:2676:C:H4'	12:J:70:PHE:HE1	1.84	0.42
1:0:2807:U:OP2	5:B:27:ASN:ND2	2.50	0.42
1:0:2911:C:O2'	1:0:2912:C:H5'	2.19	0.42
1:0:308:U:C4	1:0:342:C:H1'	2.54	0.42
1:0:415:A:O2'	1:0:416:G:H5'	2.19	0.42
5:B:62:ARG:CB	5:B:65:MET:HE3	2.49	0.42
6:C:46:TYR:CE1	6:C:92:PRO:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:7:ILE:HD11	8:E:11:VAL:C	2.39	0.42
8:E:166:VAL:HG12	39:E:3134:HOH:O	2.18	0.42
15:M:34:GLU:HB3	15:M:38:GLU:HG3	2.01	0.42
27:Y:187:VAL:HB	27:Y:203:VAL:CG2	2.50	0.42
28:Z:26:VAL:HG12	28:Z:30:GLU:OE1	2.18	0.42
1:O:1159:G:H1	1:O:1208:C:N4	2.15	0.42
1:O:1342:C:O2'	1:O:1343:C:H5'	2.19	0.42
2:9:3039:U:HO2'	2:9:3042:C:H5	1.57	0.42
2:9:3107:C:H5	39:9:3167:HOH:O	2.01	0.42
7:D:76:ARG:O	7:D:77:ASP:HB2	2.20	0.42
12:J:132:LEU:HA	12:J:132:LEU:HD23	1.84	0.42
16:N:173:ASP:O	16:N:177:GLU:HB2	2.19	0.42
39:O:5821:HOH:O	25:W:122:ARG:NH2	2.51	0.42
26:X:66:THR:HG23	26:X:67:PRO:HD2	2.01	0.42
1:O:1181:A:C2'	1:O:1182:C:H5'	2.49	0.42
1:O:1226:G:H5'	39:O:5084:HOH:O	2.19	0.42
1:O:2263:G:O2'	15:M:70:GLY:HA2	2.20	0.42
1:O:793:A:C5'	18:P:83:LYS:HG2	2.49	0.42
1:O:87:C:H2'	30:2:28:LYS:O	2.19	0.42
2:9:3039:U:O2'	2:9:3042:C:H5	2.02	0.42
4:A:130:THR:HB	4:A:137:VAL:HB	2.02	0.42
5:B:294:TYR:HE2	39:B:9642:HOH:O	2.01	0.42
7:D:136:ARG:HB3	7:D:137:PRO:HD2	2.01	0.42
9:F:111:ILE:O	9:F:115:VAL:HG23	2.20	0.42
9:F:48:VAL:CG2	9:F:74:PHE:HB3	2.48	0.42
11:H:154:TYR:C	11:H:154:TYR:CD1	2.93	0.42
12:J:39:VAL:HG11	12:J:107:ASN:CB	2.50	0.42
16:N:108:SER:HA	16:N:109:PRO:HD3	1.80	0.42
1:O:497:A:H2'	1:O:498:A:H5'	2.01	0.42
1:O:588:G:O6	25:W:154:ARG:NH1	2.53	0.42
1:O:945:U:H2'	1:O:946:C:H6	1.84	0.42
5:B:41:PHE:HA	5:B:79:MET:CE	2.49	0.42
6:C:119:ALA:HA	6:C:137:PRO:HD3	2.01	0.42
7:D:99:ASP:N	7:D:103:ASN:O	2.47	0.42
26:X:45:GLU:HG3	39:X:6178:HOH:O	2.19	0.42
27:Y:154:ARG:HH11	27:Y:154:ARG:CB	2.33	0.42
1:O:1314:U:H2'	39:O:6398:HOH:O	2.20	0.42
1:O:1616:A:H5''	1:O:1617:C:OP1	2.20	0.42
1:O:2449:G:H2'	1:O:2450:C:O4'	2.19	0.42
1:O:2436:U:H5'	31:3:68:LYS:HE2	2.01	0.42
4:A:93:THR:C	4:A:94:LEU:HD23	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:62:ARG:HA	5:B:65:MET:HE3	2.02	0.42
5:B:41:PHE:HA	5:B:79:MET:HE2	2.02	0.42
5:B:86:ALA:HA	39:B:9575:HOH:O	2.19	0.42
7:D:88:LEU:N	7:D:89:PRO:CD	2.82	0.42
11:H:43:TYR:HA	11:H:44:PRO:HD3	1.79	0.42
15:M:59:GLY:HA3	15:M:141:ILE:CD1	2.49	0.42
16:N:167:ASP:C	16:N:168:LEU:HG	2.39	0.42
18:P:18:LYS:O	18:P:21:VAL:HG13	2.20	0.42
20:R:39:THR:CG2	20:R:107:GLU:O	2.68	0.42
22:T:85:GLU:CG	22:T:86:GLU:N	2.80	0.42
23:U:20:MET:CG	23:U:28:THR:HG23	2.50	0.42
1:0:1065:G:H5'	39:0:4138:HOH:O	2.19	0.42
1:0:1218:U:H2'	1:0:1219:U:H6	1.84	0.42
1:0:1119:G:N2	1:0:1246:A:H2	2.08	0.42
1:0:1778:A:H2'	1:0:1779:A:H5'	2.01	0.42
1:0:220:C:H1'	39:0:6282:HOH:O	2.18	0.42
1:0:2649:A:O4'	1:0:2650:U:H5	2.02	0.42
1:0:2769:C:H2'	1:0:2770:G:H5'	2.01	0.42
1:0:2787:C:H5	39:0:5181:HOH:O	2.02	0.42
1:0:362:G:H2'	1:0:363:A:C8	2.54	0.42
1:0:426:G:H2'	1:0:427:C:O4'	2.20	0.42
1:0:612:U:H2'	1:0:613:C:C6	2.55	0.42
1:0:820:G:C5	4:A:171:LYS:HB2	2.55	0.42
1:0:835:U:P	5:B:229:ARG:HH12	2.43	0.42
1:0:932:U:H2'	1:0:933:C:C6	2.55	0.42
1:0:960:G:N3	1:0:960:G:H2'	2.34	0.42
4:A:100:PRO:HG2	4:A:103:VAL:CG2	2.45	0.42
8:E:145:ALA:HB1	8:E:168:ILE:CD1	2.49	0.42
10:G:12:ILE:HG13	39:G:6833:HOH:O	2.19	0.42
11:H:51:VAL:CG1	11:H:53:GLU:O	2.67	0.42
12:J:74:ARG:HH11	12:J:74:ARG:CB	2.28	0.42
15:M:48:LYS:O	15:M:52:GLN:HG3	2.20	0.42
16:N:43:VAL:CG1	16:N:118:ILE:HD11	2.49	0.42
23:U:17:THR:HG23	23:U:18:GLY:N	2.34	0.42
39:0:3167:HOH:O	25:W:119:HIS:HE1	2.03	0.42
1:0:2269:C:H2'	1:0:2270:G:O4'	2.19	0.42
31:3:17:HIS:O	31:3:18:GLN:HG3	2.20	0.42
4:A:122:SER:O	4:A:124:VAL:HG13	2.19	0.42
4:A:52:SER:HB2	4:A:164:ARG:HH11	1.85	0.42
5:B:51:VAL:HG23	5:B:327:VAL:HG13	2.01	0.42
6:C:129:HIS:HD2	6:C:165:ASP:OD2	2.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:162:VAL:CG2	6:C:232:LEU:HD21	2.50	0.42
32:I:92:PRO:HB3	39:I:6825:HOH:O	2.19	0.42
14:L:91:VAL:CG1	14:L:120:LEU:HD23	2.43	0.42
14:L:144:ASP:O	14:L:147:GLU:HB2	2.19	0.42
15:M:164:THR:CG2	15:M:165:GLY:N	2.81	0.42
16:N:82:TYR:HE1	16:N:120:GLU:HG2	1.84	0.42
1:0:1398:G:H5'	18:P:23:PHE:O	2.19	0.42
1:0:1849:G:H1'	1:0:2011:A:N1	2.34	0.42
1:0:2015:A:H2'	1:0:2016:U:O4'	2.20	0.42
1:0:2296:C:H2'	1:0:2297:U:C6	2.55	0.42
1:0:2338:G:H2'	7:D:129:ASP:OD1	2.20	0.42
1:0:2837:U:H2'	39:0:7320:HOH:O	2.20	0.42
1:0:40:C:H6	1:0:40:C:O5'	2.03	0.42
2:9:3003:A:H2	2:9:3021:G:N3	2.18	0.42
8:E:10:ASP:HA	39:E:3707:HOH:O	2.20	0.42
8:E:20:ILE:HD12	8:E:33:LEU:HD12	2.02	0.42
9:F:16:ALA:HA	9:F:111:ILE:HD13	2.02	0.42
9:F:113:ASP:O	9:F:117:GLU:HG3	2.19	0.42
18:P:14:LEU:O	18:P:16:VAL:HG23	2.19	0.42
24:V:42:ASN:O	24:V:44:GLY:N	2.53	0.42
1:0:1400:C:H4'	26:X:56:GLU:HG2	2.01	0.42
27:Y:115:ARG:NE	39:Y:9355:HOH:O	2.52	0.42
1:0:2505:G:C2'	1:0:2506:A:H5'	2.50	0.41
1:0:2819:C:H2'	1:0:2820:A:C8	2.55	0.41
1:0:449:A:C8	6:C:43:LYS:HG2	2.55	0.41
2:9:3041:C:C6	7:D:50:VAL:HG21	2.54	0.41
4:A:43:VAL:O	4:A:44:ASP:HB2	2.20	0.41
22:T:48:VAL:O	22:T:59:GLU:HA	2.20	0.41
25:W:108:ARG:HE	25:W:114:PRO:HG2	1.85	0.41
26:X:8:ARG:HE	26:X:8:ARG:HB3	1.63	0.41
39:0:6789:HOH:O	27:Y:158:LYS:HD3	2.19	0.41
1:0:1203:G:O2'	1:0:1204:C:H5'	2.20	0.41
1:0:907:A:H2'	1:0:908:A:H8	1.85	0.41
5:B:115:VAL:HA	5:B:116:PRO:HD3	1.94	0.41
5:B:41:PHE:CD1	5:B:79:MET:CE	3.03	0.41
39:0:3827:HOH:O	32:I:92:PRO:HD3	2.19	0.41
16:N:24:LEU:HD22	39:Q:2847:HOH:O	2.19	0.41
1:0:1603:A:H5''	1:0:1605:G:H5'	2.01	0.41
1:0:451:C:O2'	1:0:452:G:H5'	2.20	0.41
1:0:522:U:O2'	1:0:1366:C:H5'	2.20	0.41
1:0:538:C:H5''	1:0:539:G:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:926:A:O2'	14:L:41:HIS:HD2	2.03	0.41
6:C:120:ASP:C	6:C:120:ASP:OD1	2.58	0.41
32:I:112:LYS:C	32:I:114:PRO:HD2	2.40	0.41
14:L:6:ARG:NH2	39:L:9445:HOH:O	2.53	0.41
14:L:80:ASP:CB	14:L:90:ARG:HB3	2.50	0.41
15:M:82:ARG:HA	39:M:9339:HOH:O	2.19	0.41
23:U:4:ARG:NH1	23:U:4:ARG:HG2	2.35	0.41
1:0:2323:G:H5'	39:0:7497:HOH:O	2.19	0.41
1:0:2886:C:O2'	1:0:2887:G:H5'	2.20	0.41
1:0:407:A:H2'	1:0:408:A:C8	2.55	0.41
1:0:82:C:OP1	22:T:67:LEU:HB2	2.20	0.41
2:9:3050:G:H5''	16:N:159:TYR:CE1	2.55	0.41
4:A:192:VAL:HG13	39:A:9546:HOH:O	2.20	0.41
4:A:30:ARG:HB3	4:A:30:ARG:HE	1.72	0.41
6:C:133:ARG:HG3	6:C:133:ARG:HH11	1.84	0.41
11:H:76:GLU:C	11:H:77:LEU:HD23	2.41	0.41
32:I:103:ASP:HA	32:I:106:LYS:HD2	2.02	0.41
16:N:33:ARG:NH1	16:N:103:ASP:OD2	2.51	0.41
26:X:18:ARG:NH1	39:X:4132:HOH:O	2.41	0.41
28:Z:41:ASN:O	28:Z:41:ASN:ND2	2.53	0.41
1:0:1098:A:O3'	25:W:129:LYS:HE2	2.20	0.41
1:0:1131:G:C6	1:0:1230:A:C4	3.08	0.41
1:0:1139:U:H2'	1:0:1140:C:C6	2.56	0.41
1:0:1797:A:H2'	1:0:1799:G:O5'	2.21	0.41
1:0:2415:A:N3	16:N:26:LEU:HD13	2.35	0.41
1:0:2676:C:H4'	12:J:70:PHE:HD1	1.82	0.41
1:0:2748:G:H4'	1:0:2749:U:H5'	2.02	0.41
4:A:186:TRP:CG	4:A:187:PRO:HA	2.56	0.41
4:A:192:VAL:HG12	4:A:192:VAL:O	2.19	0.41
5:B:16:ARG:NH2	39:B:9552:HOH:O	2.44	0.41
5:B:183:GLU:O	5:B:184:ASP:C	2.58	0.41
7:D:88:LEU:HB2	7:D:89:PRO:HD3	2.02	0.41
11:H:47:ILE:HG21	39:H:9541:HOH:O	2.19	0.41
12:J:15:ARG:NH1	12:J:43:ARG:HH11	2.17	0.41
14:L:66:VAL:HG23	14:L:67:ARG:N	2.35	0.41
39:C:9165:HOH:O	17:O:3:THR:HG21	2.19	0.41
1:0:1335:C:H2'	1:0:1336:U:C6	2.56	0.41
1:0:1552:G:H2'	1:0:1553:C:C6	2.56	0.41
1:0:1829:A:H2'	1:0:1830:C:H5'	2.03	0.41
1:0:2717:C:H2'	1:0:2718:C:C5'	2.37	0.41
1:0:29:C:C2'	1:0:30:U:H5'	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:517:U:H1'	39:0:8071:HOH:O	2.19	0.41
29:1:28:HIS:O	29:1:32:LYS:N	2.47	0.41
2:9:3088:G:OP1	25:W:130:HIS:NE2	2.47	0.41
13:K:23:ASN:HD21	13:K:107:THR:HB	1.84	0.41
24:V:8:ILE:CG2	24:V:59:ILE:HG13	2.50	0.41
25:W:122:ARG:NH1	25:W:152:ALA:O	2.54	0.41
1:0:1044:C:H3'	1:0:1045:G:H5''	2.02	0.41
1:0:1182:C:H1'	1:0:1192:A:C8	2.45	0.41
1:0:1183:C:H5	1:0:1192:A:OP1	2.03	0.41
1:0:2379:G:N3	1:0:2418:G:H2'	2.35	0.41
1:0:255:A:H2'	1:0:256:C:C6	2.55	0.41
1:0:329:A:OP2	6:C:206:ASN:HB2	2.20	0.41
1:0:892:G:H5''	29:1:54:ALA:HB2	2.02	0.41
8:E:133:VAL:HG12	8:E:141:VAL:HG13	2.03	0.41
32:I:102:VAL:HG23	32:I:140:GLU:O	2.20	0.41
15:M:49:ALA:C	15:M:54:TYR:HB3	2.40	0.41
1:0:1495:C:H2'	1:0:1496:G:C8	2.56	0.41
1:0:1795:G:H2'	1:0:1796:A:O4'	2.20	0.41
1:0:1867:G:O2'	1:0:1868:G:H5'	2.21	0.41
1:0:1943:C:O4'	4:A:212:PRO:HA	2.20	0.41
1:0:2346:C:H4'	7:D:52:THR:CG2	2.51	0.41
1:0:2690:U:H4'	8:E:111:LYS:HE3	2.03	0.41
1:0:441:A:H8	1:0:441:A:O5'	2.03	0.41
30:2:19:SER:O	30:2:36:ASN:ND2	2.53	0.41
5:B:43:GLY:O	5:B:308:LEU:HD12	2.20	0.41
5:B:312:ARG:HG2	5:B:313:PRO:N	2.35	0.41
7:D:75:LEU:HD22	7:D:79:MET:HB3	2.02	0.41
39:0:7990:HOH:O	15:M:91:ILE:HG12	2.19	0.41
27:Y:122:ARG:NH2	39:Y:9335:HOH:O	2.53	0.41
28:Z:30:GLU:HB2	39:Z:9215:HOH:O	2.20	0.41
1:0:2053:G:H4'	20:R:136:TRP:CE2	2.56	0.41
1:0:2134:G:C6	1:0:2258:A:C8	3.09	0.41
2:9:3092:G:H2'	2:9:3093:A:C8	2.56	0.41
8:E:80:TRP:O	8:E:134:SER:HA	2.19	0.41
8:E:7:ILE:HA	8:E:8:PRO:HD3	1.95	0.41
32:I:101:SER:OG	32:I:104:GLN:HG3	2.21	0.41
13:K:9:THR:HG21	13:K:78:LYS:HE2	2.03	0.41
14:L:67:ARG:HB2	14:L:112:GLY:HA3	2.02	0.41
15:M:90:ARG:HB2	31:3:46:ILE:HD11	2.03	0.41
18:P:16:VAL:HG12	18:P:17:GLY:H	1.84	0.41
20:R:9:ASP:O	20:R:13:THR:HB	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:189:ASN:ND2	27:Y:189:ASN:C	2.73	0.41
1:O:101:C:H2'	1:O:102:A:C8	2.56	0.41
1:O:1268:C:O2'	1:O:1269:G:H5'	2.20	0.41
1:O:2032:U:H2'	1:O:2033:G:H5'	2.02	0.41
1:O:210:U:H2'	1:O:211:U:C6	2.55	0.41
1:O:2453:G:H5'	39:O:5235:HOH:O	2.21	0.41
1:O:2456:A:H5'	39:O:6223:HOH:O	2.21	0.41
1:O:499:G:O2'	1:O:500:G:H5'	2.20	0.41
2:9:3052:A:H2'	2:9:3053:G:O4'	2.21	0.41
6:C:236:THR:HG22	6:C:239:ALA:HB2	2.03	0.41
14:L:73:VAL:HG23	14:L:74:THR:N	2.31	0.41
16:N:73:ALA:HB1	16:N:74:PRO:CD	2.50	0.41
23:U:19:THR:HG22	23:U:20:MET:N	2.35	0.41
25:W:26:ILE:O	25:W:26:ILE:CG1	2.68	0.41
26:X:43:VAL:CG1	26:X:44:ASP:N	2.83	0.41
1:O:1555:G:H4'	1:O:1630:A:C2	2.50	0.41
1:O:1929:G:H1'	39:O:5691:HOH:O	2.20	0.41
1:O:2044:G:OP1	26:X:23:HIS:HE1	2.04	0.41
1:O:2115:U:H2'	1:O:2116:U:C6	2.56	0.41
1:O:2597:U:H2'	1:O:2598:U:H5'	2.02	0.41
1:O:2698:G:H2'	1:O:2699:A:C8	2.56	0.41
2:9:3054:A:H2	39:9:3535:HOH:O	2.04	0.41
4:A:130:THR:HG22	4:A:131:HIS:N	2.36	0.41
7:D:37:ALA:O	7:D:40:ILE:HG12	2.21	0.41
11:H:20:ILE:HG23	11:H:120:ILE:CD1	2.50	0.41
1:O:1235:G:O4'	12:J:63:ILE:HG23	2.20	0.41
14:L:145:LEU:C	14:L:147:GLU:N	2.74	0.41
15:M:74:LYS:HA	39:M:9375:HOH:O	2.20	0.41
16:N:69:TYR:CE2	16:N:184:ILE:HG13	2.55	0.41
1:O:1098:A:H2'	1:O:1099:G:O4'	2.21	0.40
1:O:2523:U:O2'	1:O:2524:G:H5'	2.21	0.40
1:O:646:G:H2'	1:O:647:U:C6	2.56	0.40
2:9:3023:U:O2'	2:9:3024:U:H4'	2.21	0.40
4:A:103:VAL:O	4:A:105:VAL:HG23	2.21	0.40
4:A:179:MET:HG2	4:A:186:TRP:HB2	2.02	0.40
4:A:72:GLU:HG3	28:Z:66:GLY:HA2	2.02	0.40
5:B:195:ARG:NH1	5:B:324:ASP:OD1	2.55	0.40
39:O:4099:HOH:O	6:C:81:PRO:HD3	2.21	0.40
11:H:162:ARG:HD3	39:H:9548:HOH:O	2.20	0.40
11:H:29:ALA:H	11:H:66:ARG:HH12	1.69	0.40
12:J:45:VAL:HG22	12:J:46:ILE:N	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:112:GLY:HA2	16:N:137:ALA:N	2.36	0.40
27:Y:108:ASP:N	27:Y:108:ASP:OD1	2.53	0.40
1:0:1333:U:H2'	1:0:1334:C:H6	1.85	0.40
1:0:2032:U:C2'	1:0:2033:G:C5'	2.97	0.40
1:0:2101:A:OP2	6:C:66:GLY:HA2	2.21	0.40
1:0:2442:G:H3'	39:0:7117:HOH:O	2.20	0.40
1:0:23:G:C6	1:0:24:G:N1	2.89	0.40
1:0:2672:C:H1'	39:B:9628:HOH:O	2.20	0.40
1:0:2782:G:O6	1:0:2790:C:H5''	2.21	0.40
31:3:20:HIS:HA	31:3:70:ARG:O	2.21	0.40
2:9:3014:G:H2'	2:9:3015:C:H5'	2.03	0.40
5:B:144:THR:HG22	5:B:145:HIS:N	2.36	0.40
9:F:99:THR:HG23	9:F:99:THR:O	2.22	0.40
15:M:58:GLN:HG3	39:M:9408:HOH:O	2.21	0.40
16:N:167:ASP:O	16:N:168:LEU:HG	2.21	0.40
16:N:67:ALA:C	16:N:69:TYR:H	2.24	0.40
20:R:39:THR:HG22	20:R:107:GLU:O	2.21	0.40
20:R:25:PHE:CZ	20:R:29:LYS:HE2	2.55	0.40
1:0:1304:U:H2'	1:0:1305:C:C6	2.56	0.40
1:0:1314:U:H5''	1:0:1316:G:O4'	2.21	0.40
1:0:1462:C:H2'	1:0:1463:A:H8	1.85	0.40
1:0:2072:G:H3'	1:0:2073:G:H5''	2.03	0.40
1:0:669:G:O2'	1:0:670:G:H5'	2.21	0.40
1:0:791:A:H2'	1:0:792:G:O4'	2.22	0.40
1:0:999:C:H2'	1:0:1000:C:O4'	2.21	0.40
1:0:87:C:C2	30:2:30:ASP:OD2	2.74	0.40
4:A:17:ARG:HD2	39:A:9532:HOH:O	2.20	0.40
7:D:35:ALA:O	7:D:38:GLU:HG3	2.21	0.40
14:L:114:VAL:HB	39:L:9469:HOH:O	2.21	0.40
15:M:82:ARG:O	15:M:84:LYS:N	2.55	0.40
23:U:49:LEU:HG	39:U:3805:HOH:O	2.22	0.40
26:X:10:VAL:HG12	26:X:11:THR:N	2.36	0.40
28:Z:39:CYS:O	28:Z:42:CYS:O	2.39	0.40
1:0:1525:G:H5'	1:0:1526:A:OP2	2.21	0.40
1:0:1636:G:O2'	1:0:1637:A:H5'	2.20	0.40
1:0:2238:A:O2'	1:0:2239:C:H5'	2.21	0.40
1:0:2912:C:H2'	1:0:2913:A:O4'	2.21	0.40
1:0:710:G:H5'	17:O:25:VAL:HG13	2.04	0.40
1:0:876:A:H2'	1:0:876:A:N3	2.37	0.40
29:1:53:LYS:HD3	29:1:53:LYS:HA	1.89	0.40
31:3:25:VAL:HB	31:3:66:ASP:OD2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3114:G:H2'	2:9:3115:C:C6	2.57	0.40
4:A:135:VAL:HG21	4:A:147:ARG:NH1	2.37	0.40
4:A:173:GLY:O	4:A:176:HIS:HB3	2.22	0.40
5:B:217:ARG:CG	5:B:257:THR:HG22	2.43	0.40
5:B:36:PRO:HA	5:B:167:GLY:O	2.22	0.40
7:D:57:THR:HA	39:D:5728:HOH:O	2.22	0.40
9:F:118:LEU:O	9:F:119:ARG:HB3	2.21	0.40
15:M:42:ARG:HA	15:M:43:PRO:HD3	1.90	0.40
16:N:110:THR:HG22	39:N:9349:HOH:O	2.20	0.40
16:N:143:ARG:HE	16:N:143:ARG:HB3	1.70	0.40
17:O:32:ARG:HD3	17:O:32:ARG:C	2.41	0.40
1:O:949:U:C4'	19:Q:95:GLU:HA	2.52	0.40
22:T:20:HIS:HB3	22:T:41:ARG:HD2	2.03	0.40
26:X:70:ILE:O	26:X:70:ILE:HG23	2.22	0.40
1:O:1602:C:OP2	28:Z:46:ARG:NH2	2.54	0.40
1:O:1834:C:H2'	1:O:1840:A:N6	2.37	0.40
1:O:2408:A:H4'	31:3:15:ASN:O	2.22	0.40
31:3:48:ASN:ND2	31:3:50:GLY:H	2.20	0.40
9:F:26:THR:HG21	9:F:102:GLY:C	2.42	0.40
1:O:1053:G:OP1	11:H:12:PRO:HG3	2.21	0.40
25:W:38:THR:HG22	25:W:40:ALA:H	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	235/240 (98%)	213 (91%)	17 (7%)	5 (2%)	8	6
5	B	335/338 (99%)	312 (93%)	18 (5%)	5 (2%)	11	11
6	C	244/246 (99%)	226 (93%)	18 (7%)	0	100	100
7	D	134/177 (76%)	104 (78%)	18 (13%)	12 (9%)	1	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	E	170/178 (96%)	164 (96%)	6 (4%)	0	100	100
9	F	117/120 (98%)	104 (89%)	11 (9%)	2 (2%)	10	9
10	G	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
11	H	156/171 (91%)	141 (90%)	13 (8%)	2 (1%)	13	13
12	J	140/145 (97%)	132 (94%)	5 (4%)	3 (2%)	8	6
13	K	130/132 (98%)	121 (93%)	8 (6%)	1 (1%)	21	25
14	L	141/165 (86%)	120 (85%)	20 (14%)	1 (1%)	24	29
15	M	192/195 (98%)	180 (94%)	11 (6%)	1 (0%)	31	38
16	N	184/187 (98%)	162 (88%)	15 (8%)	7 (4%)	3	2
17	O	113/116 (97%)	107 (95%)	6 (5%)	0	100	100
18	P	141/149 (95%)	137 (97%)	4 (3%)	0	100	100
19	Q	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
20	R	148/155 (96%)	142 (96%)	6 (4%)	0	100	100
21	S	79/85 (93%)	74 (94%)	5 (6%)	0	100	100
22	T	117/120 (98%)	108 (92%)	8 (7%)	1 (1%)	19	22
23	U	51/66 (77%)	47 (92%)	4 (8%)	0	100	100
24	V	63/71 (89%)	55 (87%)	7 (11%)	1 (2%)	11	10
25	W	152/154 (99%)	149 (98%)	3 (2%)	0	100	100
26	X	80/92 (87%)	71 (89%)	9 (11%)	0	100	100
27	Y	140/241 (58%)	139 (99%)	1 (1%)	0	100	100
28	Z	71/83 (86%)	58 (82%)	10 (14%)	3 (4%)	3	1
29	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
30	2	42/50 (84%)	40 (95%)	2 (5%)	0	100	100
31	3	90/92 (98%)	87 (97%)	2 (2%)	1 (1%)	16	17
32	I	68/162 (42%)	52 (76%)	14 (21%)	2 (3%)	5	3
All	All	3705/4431 (84%)	3409 (92%)	249 (7%)	47 (1%)	13	13

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	37	VAL
7	D	137	PRO
9	F	101	ALA

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Mol	Chain	Res	Type
11	H	166	SER
12	J	143	LYS
14	L	80	ASP
16	N	154	LEU
16	N	183	ASP
16	N	184	ILE
28	Z	42	CYS
28	Z	81	ARG
4	A	34	ASP
5	B	169	GLY
7	D	60	GLU
7	D	171	ASP
11	H	168	ALA
22	T	53	GLY
28	Z	20	ARG
32	I	129	VAL
4	A	132	ASP
5	B	34	GLY
7	D	16	PRO
7	D	56	ARG
7	D	138	GLY
7	D	147	ALA
12	J	65	ASN
15	M	83	SER
16	N	162	ASP
4	A	27	LEU
5	B	185	GLY
7	D	61	PHE
12	J	5	GLU
13	K	126	SER
16	N	68	GLU
24	V	43	PRO
31	3	56	PRO
7	D	65	GLU
7	D	97	GLN
16	N	65	ASP
16	N	164	ASP
5	B	107	SER
9	F	100	ASP
4	A	112	PRO
7	D	27	ILE
7	D	69	ILE

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Mol	Chain	Res	Type
32	I	114	PRO
5	B	2	GLN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	179/182 (98%)	169 (94%)	10 (6%)	23	32
5	B	282/283 (100%)	268 (95%)	14 (5%)	27	37
6	C	193/193 (100%)	174 (90%)	19 (10%)	9	10
7	D	117/148 (79%)	110 (94%)	7 (6%)	21	28
8	E	152/156 (97%)	145 (95%)	7 (5%)	29	41
9	F	93/94 (99%)	90 (97%)	3 (3%)	42	58
10	G	27/283 (10%)	27 (100%)	0	100	100
11	H	132/138 (96%)	130 (98%)	2 (2%)	67	82
12	J	118/121 (98%)	110 (93%)	8 (7%)	17	22
13	K	106/106 (100%)	102 (96%)	4 (4%)	36	50
14	L	113/127 (89%)	109 (96%)	4 (4%)	39	53
15	M	158/159 (99%)	153 (97%)	5 (3%)	42	58
16	N	149/150 (99%)	142 (95%)	7 (5%)	29	40
17	O	93/94 (99%)	91 (98%)	2 (2%)	55	72
18	P	113/117 (97%)	110 (97%)	3 (3%)	48	65
19	Q	79/80 (99%)	75 (95%)	4 (5%)	26	36
20	R	117/122 (96%)	117 (100%)	0	100	100
21	S	71/74 (96%)	71 (100%)	0	100	100
22	T	105/106 (99%)	101 (96%)	4 (4%)	36	50
23	U	44/52 (85%)	43 (98%)	1 (2%)	53	71
24	V	51/57 (90%)	50 (98%)	1 (2%)	58	75
25	W	130/130 (100%)	126 (97%)	4 (3%)	43	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	X	66/74 (89%)	62 (94%)	4 (6%)	20	28
27	Y	120/196 (61%)	109 (91%)	11 (9%)	10	12
28	Z	60/68 (88%)	59 (98%)	1 (2%)	63	79
29	1	46/47 (98%)	45 (98%)	1 (2%)	55	72
30	2	42/46 (91%)	41 (98%)	1 (2%)	52	69
31	3	79/79 (100%)	77 (98%)	2 (2%)	50	68
32	I	58/130 (45%)	58 (100%)	0	100	100
All	All	3093/3612 (86%)	2964 (96%)	129 (4%)	32	45

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	3	ARG
4	A	33	GLU
4	A	36	ASP
4	A	78	ASP
4	A	94	LEU
4	A	131	HIS
4	A	165	THR
4	A	179	MET
4	A	206	ARG
4	A	217	ARG
5	B	11	LEU
5	B	27	ASN
5	B	28	SER
5	B	82	VAL
5	B	98	THR
5	B	113	LEU
5	B	149	ASP
5	B	162	MET
5	B	195	ARG
5	B	251	VAL
5	B	254	GLN
5	B	277	GLU
5	B	279	THR
5	B	312	ARG
6	C	16	VAL
6	C	27	ARG
6	C	67	GLN
6	C	76	ARG

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Mol	Chain	Res	Type
6	C	78	ARG
6	C	91	PRO
6	C	94	THR
6	C	95	GLU
6	C	101	ASP
6	C	136	VAL
6	C	162	VAL
6	C	187	ARG
6	C	214	THR
6	C	223	LEU
6	C	234	VAL
6	C	236	THR
6	C	240	LEU
6	C	243	VAL
6	C	246	ARG
7	D	24	HIS
7	D	50	VAL
7	D	61	PHE
7	D	99	ASP
7	D	100	ASP
7	D	133	ASN
7	D	137	PRO
8	E	15	GLN
8	E	16	ASP
8	E	102	VAL
8	E	131	LEU
8	E	155	ASN
8	E	156	ASP
8	E	164	ASP
9	F	12	LEU
9	F	46	GLU
9	F	99	THR
11	H	84	LYS
11	H	154	TYR
12	J	46	ILE
12	J	52	GLN
12	J	70	PHE
12	J	74	ARG
12	J	79	PHE
12	J	107	ASN
12	J	127	ILE
12	J	131	THR

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Mol	Chain	Res	Type
13	K	4	LEU
13	K	10	GLN
13	K	84	ASP
13	K	100	GLU
14	L	35	ARG
14	L	43	HIS
14	L	89	PHE
14	L	140	VAL
15	M	46	LEU
15	M	68	ARG
15	M	93	ARG
15	M	99	ARG
15	M	116	ASN
16	N	12	ARG
16	N	23	ARG
16	N	26	LEU
16	N	37	ARG
16	N	49	THR
16	N	127	LEU
16	N	139	TRP
17	O	3	THR
17	O	111	VAL
18	P	81	LYS
18	P	98	ILE
18	P	117	SER
19	Q	16	ASN
19	Q	18	PRO
19	Q	57	ASP
19	Q	95	GLU
22	T	26	THR
22	T	39	ASN
22	T	48	VAL
22	T	89	ARG
23	U	17	THR
24	V	65	ASP
25	W	35	VAL
25	W	52	VAL
25	W	122	ARG
25	W	146	ILE
26	X	27	ASP
26	X	72	VAL
26	X	79	GLU

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Mol	Chain	Res	Type
26	X	82	GLU
27	Y	103	THR
27	Y	115	ARG
27	Y	141	THR
27	Y	144	ARG
27	Y	154	ARG
27	Y	163	THR
27	Y	189	ASN
27	Y	200	THR
27	Y	203	VAL
27	Y	204	ARG
27	Y	235	GLU
28	Z	22	SER
29	1	47	ASP
30	2	18	ASN
31	3	56	PRO
31	3	65	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	29	HIS
4	A	199	HIS
5	B	27	ASN
5	B	145	HIS
5	B	221	GLN
5	B	238	ASN
5	B	256	GLN
5	B	260	HIS
5	B	320	GLN
5	B	332	ASN
6	C	39	GLN
6	C	129	HIS
7	D	47	GLN
7	D	103	ASN
7	D	133	ASN
8	E	106	ASN
8	E	143	GLN
10	G	64	ASN
11	H	31	HIS
11	H	56	GLN
11	H	59	HIS

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Mol	Chain	Res	Type
11	H	70	ASN
11	H	170	ASN
12	J	52	GLN
12	J	107	ASN
13	K	10	GLN
14	L	18	HIS
14	L	41	HIS
14	L	42	ASN
14	L	43	HIS
14	L	116	HIS
15	M	24	GLN
15	M	26	GLN
15	M	58	GLN
15	M	77	HIS
15	M	143	ASN
15	M	170	ASN
16	N	93	GLN
16	N	107	ASN
16	N	153	GLN
17	O	53	GLN
17	O	100	GLN
18	P	50	GLN
18	P	66	GLN
18	P	73	HIS
18	P	88	GLN
18	P	118	GLN
19	Q	16	ASN
19	Q	40	HIS
20	R	61	GLN
20	R	94	ASN
20	R	98	ASN
20	R	113	HIS
20	R	117	HIS
21	S	53	ASN
22	T	37	GLN
22	T	39	ASN
23	U	39	ASN
23	U	48	ASN
24	V	29	ASN
24	V	60	GLN
25	W	27	HIS
25	W	110	GLN

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Mol	Chain	Res	Type
25	W	119	HIS
25	W	125	HIS
25	W	141	HIS
26	X	22	ASN
27	Y	119	GLN
27	Y	134	HIS
27	Y	149	GLN
27	Y	189	ASN
28	Z	41	ASN
29	1	8	GLN
29	1	16	HIS
29	1	28	HIS
30	2	16	ASN
30	2	18	ASN
30	2	41	HIS
30	2	45	ASN
31	3	30	GLN
31	3	48	ASN
32	I	113	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	235 (8%)	36 (1%)
2	9	121/122 (99%)	14 (11%)	1 (0%)
3	4	1/7 (14%)	0	0
All	All	2867/3051 (93%)	249 (8%)	37 (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

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Mol	Chain	Res	Type
1	0	120	A
1	0	130	C
1	0	134	U
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
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	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

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Mol	Chain	Res	Type
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	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	868	G
1	0	869	G
1	0	871	G
1	0	875	A
1	0	877	G
1	0	878	G
1	0	905	C
1	0	920	C
1	0	921	G
1	0	923	A
1	0	953	G
1	0	960	G
1	0	961	A
1	0	1006	A
1	0	1008	C
1	0	1029	U
1	0	1045	G
1	0	1059	G
1	0	1060	C
1	0	1072	G
1	0	1081	A
1	0	1087	G
1	0	1088	A
1	0	1109	U
1	0	1110	G
1	0	1119	G
1	0	1130	U
1	0	1164	U

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Mol	Chain	Res	Type
1	0	1165	G
1	0	1166	A
1	0	1174	A
1	0	1175	G
1	0	1185	U
1	0	1192	A
1	0	1193	A
1	0	1206	U
1	0	1216	G
1	0	1237	U
1	0	1238	C
1	0	1239	G
1	0	1279	U
1	0	1289	C
1	0	1331	A
1	0	1342	C
1	0	1353	C
1	0	1360	C
1	0	1377	C
1	0	1378	G
1	0	1407	A
1	0	1409	G
1	0	1474	C
1	0	1505	U
1	0	1506	U
1	0	1524	U
1	0	1525	G
1	0	1526	A
1	0	1528	A
1	0	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

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Mol	Chain	Res	Type
1	0	1723	G
1	0	1725	C
1	0	1731	C
1	0	1732	A
1	0	1752	G
1	0	1778	A
1	0	1798	C
1	0	1820	G
1	0	1829	A
1	0	1856	C
1	0	1873	G
1	0	1879	U
1	0	1919	A
1	0	1942	A
1	0	1967	U
1	0	1971	G
1	0	1973	A
1	0	1979	G
1	0	1980	U
1	0	1996	U
1	0	2004	U
1	0	2006	C
1	0	2008	U
1	0	2011	A
1	0	2012	U
1	0	2013	G
1	0	2033	G
1	0	2034	U
1	0	2064	U
1	0	2072	G
1	0	2073	G
1	0	2074	A
1	0	2096	A
1	0	2101	A
1	0	2102	G
1	0	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

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Mol	Chain	Res	Type
1	0	2291	A
1	0	2317	C
1	0	2321	A
1	0	2354	A
1	0	2361	A
1	0	2369	A
1	0	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
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	2727	A
1	0	2747	C
1	0	2748	G
1	0	2749	U

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Mol	Chain	Res	Type
1	0	2750	G
1	0	2762	C
1	0	2768	A
1	0	2786	G
1	0	2792	A
1	0	2800	A
1	0	2811	A
1	0	2812	A
1	0	2825	C
1	0	2852	A
1	0	2876	G
1	0	2890	A
1	0	2896	A
1	0	2903	C
1	0	2914	A
2	9	3002	U
2	9	3014	G
2	9	3022	G
2	9	3023	U
2	9	3024	U
2	9	3025	G
2	9	3041	C
2	9	3043	G
2	9	3044	A
2	9	3057	A
2	9	3066	G
2	9	3077	A
2	9	3114	G
2	9	3122	C

All (37) RNA pucker outliers are listed below:

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

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Mol	Chain	Res	Type
1	0	871	G
1	0	877	G
1	0	1080	C
1	0	1232	A
1	0	1237	U
1	0	1246	A
1	0	1352	A
1	0	1506	U
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1730	G
1	0	1819	G
1	0	1856	C
1	0	1942	A
1	0	1979	G
1	0	2011	A
1	0	2313	C
1	0	2467	A
1	0	2536	C
1	0	2541	U
1	0	2649	A
1	0	2718	C
1	0	2726	U
1	0	2761	A
1	0	2791	U
1	0	2852	A
2	9	3065	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMU	0	2587	1	14,22,23	0.96	1 (7%)	18,31,34	3.65	2 (11%)
1	OMG	0	2588	1,3	19,26,27	1.03	1 (5%)	22,38,41	2.48	5 (22%)
1	UR3	0	2619	1	13,22,23	0.89	1 (7%)	15,32,35	0.68	0
1	PSU	0	2621	1	16,21,22	1.70	3 (18%)	20,30,33	5.38	4 (20%)
1	1MA	0	628	1	16,25,26	1.00	1 (6%)	12,37,40	1.24	1 (8%)
3	PPU	4	76	1,3	31,40,41	1.17	1 (3%)	33,57,60	0.97	3 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	0	2587	1	-	0/5/27/28	0/2/2/2
1	OMG	0	2588	1,3	-	0/5/27/28	0/3/3/3
1	UR3	0	2619	1	-	0/3/25/26	0/2/2/2
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	1MA	0	628	1	-	0/3/25/26	0/3/3/3
3	PPU	4	76	1,3	-	0/21/43/44	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	4	76	PPU	OC-CM	-5.44	1.26	1.42
1	0	2621	PSU	C5-C1'	-4.88	1.48	1.52
1	0	2619	UR3	C6-C5	-2.18	1.33	1.38
1	0	2587	OMU	C4-N3	2.53	1.37	1.33
1	0	2621	PSU	C2-N1	2.79	1.43	1.38
1	0	2621	PSU	C4-N3	2.93	1.38	1.33
1	0	628	1MA	C6-N6	2.96	1.34	1.27
1	0	2588	OMG	C6-N1	3.18	1.38	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	N1-C2-N3	-17.03	114.72	128.41
1	0	2588	OMG	C5-C6-N1	-8.31	111.65	123.47
1	0	2621	PSU	C5-C4-N3	-8.22	114.76	125.36
1	0	628	1MA	C2-N3-C4	-3.74	110.79	116.51
1	0	2587	OMU	C5-C4-N3	-3.58	114.84	123.17
1	0	2588	OMG	C2-N3-C4	-2.79	111.90	115.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2588	OMG	N3-C2-N1	-2.34	123.97	127.41
3	4	76	PPU	C3'-N3'-C	-2.18	119.92	123.21
1	0	2588	OMG	C6-C5-C4	-2.04	118.85	120.85
3	4	76	PPU	CM-OC-CZ	2.07	122.00	117.51
1	0	2621	PSU	C6-N1-C2	2.60	119.51	115.36
3	4	76	PPU	C2-N1-C6	2.90	118.86	111.81
1	0	2588	OMG	C6-N1-C2	6.37	125.22	116.06
1	0	2621	PSU	C4-N3-C2	14.20	127.23	115.14
1	0	2587	OMU	C4-N3-C2	14.90	126.96	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	2	0
3	4	76	PPU	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	4	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	4	176:DA	O3'	175:C	P	8.63

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%)	-0.12	75 (2%) 54 62	26, 50, 94, 154	0
2	9	122/122 (100%)	0.14	5 (4%) 37 44	45, 70, 97, 154	0
3	4	5/7 (71%)	-0.62	0 100 100	46, 48, 54, 54	0
4	A	237/240 (98%)	0.54	18 (7%) 14 18	31, 55, 88, 108	0
5	B	337/338 (99%)	0.41	15 (4%) 33 40	32, 57, 83, 94	0
6	C	246/246 (100%)	0.19	6 (2%) 59 66	29, 51, 76, 90	0
7	D	140/177 (79%)	2.40	65 (46%) 0 0	64, 100, 128, 135	0
8	E	172/178 (96%)	1.14	38 (22%) 0 1	47, 71, 89, 96	0
9	F	119/120 (99%)	1.46	41 (34%) 0 0	51, 77, 106, 112	0
10	G	29/348 (8%)	2.78	19 (65%) 0 0	75, 97, 105, 106	0
11	H	160/171 (93%)	0.89	25 (15%) 2 3	49, 66, 97, 105	0
12	J	142/145 (97%)	0.28	5 (3%) 44 51	40, 55, 76, 95	0
13	K	132/132 (100%)	0.08	2 (1%) 73 78	36, 52, 74, 83	0
14	L	145/165 (87%)	1.00	29 (20%) 1 1	29, 70, 114, 125	0
15	M	194/195 (99%)	0.99	23 (11%) 4 6	36, 49, 90, 98	0
16	N	186/187 (99%)	1.27	43 (23%) 0 1	48, 70, 117, 121	0
17	O	115/116 (99%)	0.39	4 (3%) 44 51	42, 60, 75, 81	0
18	P	143/149 (95%)	0.30	4 (2%) 53 60	41, 56, 69, 81	0
19	Q	95/96 (98%)	0.38	6 (6%) 20 26	42, 54, 70, 78	0
20	R	150/155 (96%)	0.12	3 (2%) 65 71	33, 49, 69, 77	0
21	S	81/85 (95%)	0.43	5 (6%) 20 27	42, 60, 81, 98	0
22	T	119/120 (99%)	0.89	15 (12%) 3 5	46, 59, 89, 113	0
23	U	53/66 (80%)	0.38	3 (5%) 24 30	46, 57, 77, 84	0
24	V	65/71 (91%)	1.83	17 (26%) 0 0	55, 80, 116, 121	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	154/154 (100%)	0.34	4 (2%) 56 63	42, 56, 79, 88	0
26	X	82/92 (89%)	0.91	11 (13%) 3 4	46, 60, 88, 105	0
27	Y	142/241 (58%)	0.40	12 (8%) 11 15	32, 49, 70, 90	0
28	Z	73/83 (87%)	2.19	29 (39%) 0 0	51, 83, 99, 106	0
29	1	56/57 (98%)	-0.28	0 100 100	30, 36, 45, 54	0
30	2	46/50 (92%)	1.06	8 (17%) 1 1	39, 63, 88, 100	0
31	3	92/92 (100%)	0.62	9 (9%) 7 10	39, 61, 76, 90	0
32	I	70/162 (43%)	6.05	66 (94%) 0 0	114, 127, 144, 146	0
All	All	6651/7482 (88%)	0.43	605 (9%) 9 12	26, 56, 102, 154	0

All (605) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	I	71	GLY	20.6
24	V	1	THR	16.1
7	D	63	ILE	14.8
15	M	70	GLY	13.7
32	I	133	THR	13.6
16	N	166	ALA	12.8
7	D	57	THR	12.6
32	I	79	ILE	11.6
24	V	39	ALA	11.5
15	M	80	GLY	11.4
22	T	119	ALA	11.2
28	Z	22	SER	11.2
32	I	109	ALA	11.1
28	Z	11	SER	11.0
32	I	75	THR	10.5
32	I	105	VAL	10.5
15	M	79	ALA	10.4
32	I	137	VAL	10.3
32	I	76	ALA	10.2
24	V	40	PRO	10.1
32	I	96	PHE	9.8
32	I	121	LEU	9.4
32	I	102	VAL	9.3
32	I	118	SER	9.1
26	X	88	GLU	8.9
15	M	74	LYS	8.7

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Mol	Chain	Res	Type	RSRZ
32	I	85	PHE	8.6
2	9	3001	U	8.5
32	I	116	LEU	8.5
30	2	49	GLU	8.4
32	I	125	ALA	8.1
32	I	81	ASP	8.0
32	I	107	GLN	7.8
15	M	87	GLY	7.8
32	I	126	LYS	7.8
32	I	111	GLN	7.8
32	I	77	GLU	7.8
28	Z	21	VAL	7.7
28	Z	20	ARG	7.7
32	I	108	ILE	7.7
32	I	129	VAL	7.7
32	I	114	PRO	7.6
32	I	113	HIS	7.5
15	M	86	GLN	7.4
32	I	93	GLN	7.4
32	I	104	GLN	7.4
15	M	71	SER	7.3
32	I	132	CYS	7.2
32	I	78	LEU	7.2
15	M	77	HIS	7.2
28	Z	19	GLY	7.1
7	D	61	PHE	7.1
24	V	38	GLY	7.0
32	I	91	GLU	6.9
10	G	26	MET	6.9
10	G	23	ILE	6.9
1	0	1951	G	6.7
4	A	37	VAL	6.7
32	I	87	THR	6.7
1	0	282	C	6.6
32	I	88	GLY	6.6
15	M	78	LYS	6.6
7	D	88	LEU	6.6
32	I	138	THR	6.6
8	E	45	ASP	6.5
28	Z	29	ILE	6.5
32	I	83	ALA	6.4
4	A	237	GLY	6.3

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Mol	Chain	Res	Type	RSRZ
28	Z	18	TYR	6.3
15	M	76	ARG	6.2
7	D	166	ILE	6.2
7	D	90	LEU	6.1
28	Z	24	ARG	6.0
32	I	97	VAL	6.0
28	Z	25	ARG	6.0
16	N	175	LEU	6.0
30	2	35	ARG	6.0
32	I	117	LEU	6.0
7	D	170	TYR	5.9
10	G	27	ILE	5.9
1	0	1199	A	5.9
7	D	134	LEU	5.9
28	Z	23	ARG	5.9
15	M	83	SER	5.8
7	D	64	ARG	5.8
32	I	136	GLY	5.7
32	I	74	PRO	5.6
16	N	165	ALA	5.6
16	N	147	ILE	5.6
28	Z	12	GLY	5.5
7	D	27	ILE	5.5
21	S	81	ILE	5.5
28	Z	31	SER	5.5
9	F	16	ALA	5.5
1	0	2004	U	5.4
1	0	497	A	5.4
28	Z	45	ASP	5.4
28	Z	34	ASN	5.4
32	I	89	SER	5.4
2	9	3024	U	5.3
15	M	75	ARG	5.3
7	D	104	PHE	5.3
16	N	163	PHE	5.3
7	D	44	ILE	5.3
24	V	36	ALA	5.2
1	0	1177	A	5.1
32	I	86	GLU	5.1
7	D	135	VAL	5.1
15	M	73	ARG	5.1
7	D	69	ILE	5.1

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Mol	Chain	Res	Type	RSRZ
14	L	93	VAL	5.0
1	0	1173	A	5.0
28	Z	33	MET	5.0
9	F	119	ARG	5.0
32	I	103	ASP	4.9
9	F	106	ALA	4.9
28	Z	32	GLU	4.9
1	0	1172	G	4.9
22	T	118	SER	4.9
14	L	75	LEU	4.8
4	A	133	ARG	4.8
16	N	155	GLU	4.8
1	0	1198	U	4.8
2	9	3023	U	4.8
1	0	272	A	4.8
15	M	81	ARG	4.7
8	E	86	VAL	4.7
7	D	10	PHE	4.7
7	D	62	ASP	4.7
1	0	970	U	4.7
16	N	68	GLU	4.7
32	I	123	ASN	4.6
16	N	95	ALA	4.6
7	D	81	GLU	4.6
9	F	22	VAL	4.6
14	L	91	VAL	4.6
7	D	40	ILE	4.6
22	T	116	ASP	4.6
11	H	171	ALA	4.6
7	D	92	GLU	4.6
11	H	73	LEU	4.6
1	0	280	C	4.5
1	0	960	G	4.5
7	D	73	VAL	4.5
14	L	106	VAL	4.5
14	L	76	LEU	4.5
24	V	41	GLU	4.5
7	D	26	GLY	4.5
8	E	4	GLU	4.5
9	F	118	LEU	4.4
32	I	99	ASP	4.4
1	0	285	A	4.4

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Mol	Chain	Res	Type	RSRZ
26	X	80	GLU	4.4
7	D	93	LEU	4.4
9	F	110	ASP	4.4
1	0	735	C	4.4
24	V	37	GLY	4.3
25	W	86	GLU	4.3
28	Z	30	GLU	4.3
13	K	132	VAL	4.3
11	H	74	ILE	4.3
1	0	999	C	4.3
6	C	61	PHE	4.3
9	F	49	PHE	4.3
12	J	70	PHE	4.3
7	D	85	GLN	4.3
32	I	122	THR	4.3
17	O	22	GLY	4.3
15	M	84	LYS	4.2
1	0	1202	A	4.2
14	L	105	TYR	4.2
30	2	39	ARG	4.2
7	D	18	ILE	4.2
1	0	1525	G	4.1
28	Z	14	PHE	4.1
9	F	28	ALA	4.1
4	A	36	ASP	4.1
15	M	82	ARG	4.1
16	N	159	TYR	4.1
9	F	117	GLU	4.1
1	0	2645	U	4.1
8	E	108	LEU	4.1
1	0	2238	A	4.0
32	I	112	LYS	4.0
32	I	72	VAL	4.0
10	G	24	VAL	4.0
14	L	102	ASP	4.0
31	3	92	GLU	4.0
10	G	73	ASP	4.0
7	D	11	HIS	4.0
1	0	1965	C	4.0
7	D	56	ARG	3.9
8	E	10	ASP	3.9
1	0	514	G	3.9

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Mol	Chain	Res	Type	RSRZ
1	0	2237	G	3.9
8	E	6	GLU	3.9
15	M	88	VAL	3.9
16	N	184	ILE	3.9
27	Y	235	GLU	3.9
14	L	80	ASP	3.9
1	0	1948	G	3.9
2	9	3002	U	3.9
9	F	17	LEU	3.9
7	D	172	VAL	3.9
8	E	87	PHE	3.9
32	I	134	SER	3.9
11	H	37	GLN	3.8
9	F	25	ASP	3.7
31	3	62	THR	3.7
28	Z	36	ASP	3.7
10	G	69	ARG	3.7
27	Y	216	ARG	3.7
26	X	85	VAL	3.7
7	D	41	LEU	3.7
10	G	71	LEU	3.7
24	V	8	ILE	3.7
28	Z	26	VAL	3.7
7	D	89	PRO	3.7
22	T	117	ASP	3.7
24	V	43	PRO	3.7
1	0	288	A	3.7
9	F	100	ASP	3.7
16	N	161	GLY	3.7
11	H	146	VAL	3.7
32	I	110	GLU	3.6
7	D	130	VAL	3.6
1	0	1169	U	3.6
1	0	284	C	3.6
32	I	98	ALA	3.6
32	I	115	ASP	3.6
9	F	108	VAL	3.6
16	N	152	GLU	3.6
32	I	80	LYS	3.6
32	I	106	LYS	3.6
24	V	63	GLU	3.6
1	0	2769	C	3.6

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Mol	Chain	Res	Type	RSRZ
15	M	85	ARG	3.6
10	G	67	LEU	3.6
10	G	25	GLU	3.6
19	Q	95	GLU	3.6
1	O	1200	A	3.6
11	H	78	GLY	3.6
16	N	158	LEU	3.6
28	Z	37	HIS	3.5
9	F	99	THR	3.5
22	T	82	THR	3.5
1	O	2508	C	3.5
16	N	181	ASP	3.5
16	N	154	LEU	3.5
26	X	10	VAL	3.5
7	D	167	GLU	3.5
14	L	60	GLU	3.5
7	D	84	LEU	3.5
1	O	1163	G	3.5
4	A	145	MET	3.5
14	L	104	ASP	3.5
14	L	120	LEU	3.5
28	Z	28	GLU	3.5
30	2	27	LEU	3.5
10	G	22	ALA	3.5
14	L	62	ALA	3.5
15	M	72	ALA	3.5
11	H	35	ARG	3.5
1	O	10	U	3.5
26	X	7	GLU	3.5
7	D	23	VAL	3.4
14	L	81	VAL	3.4
32	I	95	ASP	3.4
14	L	148	GLU	3.4
32	I	120	ASP	3.4
8	E	88	TYR	3.4
9	F	19	ALA	3.4
13	K	118	ALA	3.4
14	L	145	LEU	3.4
26	X	77	PHE	3.4
9	F	98	VAL	3.4
16	N	178	THR	3.4
8	E	42	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
32	I	119	TYR	3.4
23	U	47	ARG	3.4
8	E	76	VAL	3.3
26	X	71	ARG	3.3
1	0	969	G	3.3
7	D	68	PRO	3.3
1	0	1171	A	3.3
1	0	2748	G	3.3
27	Y	96	GLU	3.3
27	Y	108	ASP	3.3
8	E	11	VAL	3.3
16	N	185	GLU	3.3
27	Y	236	VAL	3.3
1	0	1168	C	3.3
8	E	160	ARG	3.3
7	D	157	LEU	3.3
14	L	97	VAL	3.3
1	0	1000	C	3.3
7	D	106	PHE	3.3
14	L	121	ILE	3.3
5	B	108	GLU	3.3
1	0	2511	A	3.2
8	E	94	GLN	3.2
9	F	21	GLU	3.2
28	Z	10	ARG	3.2
6	C	1	MET	3.2
9	F	12	LEU	3.2
9	F	107	ASP	3.2
14	L	79	ASP	3.2
16	N	183	ASP	3.2
30	2	48	ASP	3.2
28	Z	16	ALA	3.2
4	A	35	GLY	3.2
8	E	100	ASP	3.2
16	N	180	LEU	3.2
32	I	94	GLU	3.1
4	A	85	SER	3.1
12	J	4	ALA	3.1
16	N	134	ASP	3.1
5	B	57	GLU	3.1
7	D	66	GLY	3.1
10	G	66	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
9	F	15	ASP	3.1
1	0	1966	U	3.1
14	L	99	GLU	3.1
9	F	11	ASP	3.1
4	A	31	LYS	3.1
8	E	1	PRO	3.1
1	0	138	U	3.1
1	0	281	U	3.1
9	F	101	ALA	3.1
26	X	72	VAL	3.0
8	E	43	ASP	3.0
27	Y	95	THR	3.0
30	2	44	ARG	3.0
16	N	71	TRP	3.0
8	E	118	ILE	3.0
21	S	45	TYR	3.0
32	I	124	ALA	3.0
9	F	72	VAL	3.0
11	H	143	ALA	3.0
7	D	65	GLU	3.0
8	E	127	ASP	3.0
11	H	138	CYS	2.9
16	N	137	ALA	2.9
7	D	58	VAL	2.9
1	0	1950	G	2.9
8	E	98	GLU	2.9
9	F	69	GLU	2.9
16	N	139	TRP	2.9
14	L	142	LEU	2.9
14	L	44	GLU	2.9
14	L	100	ALA	2.9
16	N	143	ARG	2.9
16	N	156	GLU	2.9
1	0	1178	G	2.9
19	Q	76	VAL	2.9
11	H	82	ASP	2.9
7	D	53	LYS	2.9
22	T	115	GLU	2.9
16	N	172	PHE	2.9
7	D	160	ALA	2.9
31	3	41	GLU	2.9
32	I	92	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
8	E	7	ILE	2.8
8	E	89	SER	2.8
11	H	141	GLU	2.8
7	D	75	LEU	2.8
24	V	10	ASP	2.8
4	A	91	GLY	2.8
9	F	44	SER	2.8
22	T	112	LEU	2.8
25	W	76	ASP	2.8
28	Z	59	TYR	2.8
1	0	1170	U	2.8
7	D	154	LYS	2.8
2	9	3122	C	2.8
21	S	20	PHE	2.8
1	0	2344	G	2.8
14	L	130	ARG	2.8
32	I	127	GLU	2.8
5	B	104	GLU	2.8
9	F	18	GLU	2.8
4	A	38	ILE	2.8
8	E	154	ILE	2.8
7	D	51	ARG	2.8
15	M	1	ALA	2.7
22	T	42	VAL	2.7
16	N	94	GLU	2.7
8	E	93	MET	2.7
16	N	138	ASP	2.7
5	B	2	GLN	2.7
11	H	149	ALA	2.7
16	N	179	LEU	2.7
7	D	77	ASP	2.7
10	G	21	ASP	2.7
16	N	72	GLU	2.7
18	P	111	GLU	2.7
24	V	5	VAL	2.7
31	3	1	MET	2.7
11	H	79	GLU	2.7
16	N	16	ALA	2.7
10	G	72	ASP	2.7
12	J	7	ASP	2.7
18	P	108	LEU	2.7
27	Y	196	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
11	H	83	TYR	2.7
22	T	35	TYR	2.7
25	W	91	ASP	2.6
16	N	2	THR	2.6
16	N	106	LEU	2.6
1	0	1279	U	2.6
14	L	61	ALA	2.6
24	V	59	ILE	2.6
31	3	20	HIS	2.6
1	0	1929	G	2.6
27	Y	234	VAL	2.6
32	I	100	LEU	2.6
32	I	135	LEU	2.6
1	0	283	U	2.6
7	D	91	ALA	2.6
8	E	90	HIS	2.6
26	X	73	ARG	2.6
7	D	129	ASP	2.6
18	P	114	LEU	2.6
1	0	362	G	2.6
32	I	73	PRO	2.6
4	A	236	GLY	2.6
11	H	139	ASN	2.6
14	L	149	ARG	2.6
28	Z	13	ARG	2.6
32	I	82	GLU	2.6
7	D	107	GLY	2.6
9	F	45	ALA	2.6
21	S	78	ALA	2.6
24	V	32	ALA	2.6
7	D	171	ASP	2.6
8	E	121	ASP	2.6
1	0	372	A	2.6
7	D	173	GLU	2.6
4	A	99	ILE	2.6
9	F	75	ILE	2.6
15	M	89	THR	2.5
5	B	105	PHE	2.5
32	I	128	VAL	2.5
8	E	44	GLY	2.5
8	E	99	GLY	2.5
12	J	5	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
30	2	20	ARG	2.5
5	B	109	LEU	2.5
7	D	38	GLU	2.5
1	0	1181	A	2.5
18	P	141	ILE	2.5
19	Q	18	PRO	2.5
27	Y	98	GLN	2.5
11	H	34	GLY	2.5
7	D	132	VAL	2.5
8	E	162	PHE	2.5
1	0	736	A	2.5
8	E	123	ASP	2.5
7	D	12	GLU	2.5
8	E	124	VAL	2.5
10	G	28	GLU	2.5
1	0	1208	C	2.5
1	0	1625	U	2.5
1	0	1967	U	2.5
6	C	246	ARG	2.5
9	F	111	ILE	2.5
4	A	59	GLU	2.5
5	B	117	GLU	2.5
27	Y	187	VAL	2.5
28	Z	27	ALA	2.5
4	A	65	ARG	2.4
16	N	92	ALA	2.4
1	0	279	C	2.4
10	G	15	TRP	2.4
1	0	370	G	2.4
4	A	64	ASP	2.4
8	E	126	ILE	2.4
22	T	59	GLU	2.4
1	0	358	G	2.4
27	Y	193	LEU	2.4
20	R	96	VAL	2.4
7	D	70	GLY	2.4
16	N	37	ARG	2.4
16	N	149	GLU	2.4
11	H	67	LEU	2.4
9	F	24	ARG	2.4
9	F	29	VAL	2.4
31	3	22	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
11	H	47	ILE	2.4
6	C	135	GLU	2.4
7	D	43	GLU	2.4
16	N	177	GLU	2.4
28	Z	44	GLU	2.4
5	B	1	PRO	2.4
5	B	134	ALA	2.4
20	R	150	PRO	2.4
1	0	369	G	2.4
11	H	140	VAL	2.4
8	E	105	GLU	2.4
5	B	119	HIS	2.4
1	0	1189	A	2.3
19	Q	92	ARG	2.3
8	E	129	GLU	2.3
10	G	12	ILE	2.3
11	H	24	PRO	2.3
7	D	128	LEU	2.3
7	D	50	VAL	2.3
1	0	295	C	2.3
16	N	73	ALA	2.3
9	F	37	THR	2.3
15	M	164	THR	2.3
1	0	1192	A	2.3
1	0	716	G	2.3
5	B	33	ASP	2.3
7	D	95	THR	2.3
4	A	206	ARG	2.3
16	N	170	GLU	2.3
16	N	145	ALA	2.3
16	N	182	GLY	2.3
22	T	36	GLY	2.3
10	G	63	ARG	2.3
22	T	13	ARG	2.3
8	E	46	THR	2.2
1	0	441	A	2.2
6	C	237	GLU	2.2
9	F	23	ALA	2.2
19	Q	84	ILE	2.2
1	0	1164	U	2.2
23	U	52	THR	2.2
1	0	1947	G	2.2

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Mol	Chain	Res	Type	RSRZ
11	H	66	ARG	2.2
1	0	1180	U	2.2
9	F	70	LYS	2.2
1	0	1196	C	2.2
8	E	169	THR	2.2
17	O	23	GLY	2.2
32	I	84	GLY	2.2
17	O	98	LEU	2.2
28	Z	35	GLU	2.2
22	T	77	VAL	2.2
24	V	33	VAL	2.2
32	I	90	GLY	2.2
7	D	86	THR	2.2
9	F	47	LEU	2.2
8	E	48	VAL	2.2
9	F	115	VAL	2.2
32	I	140	GLU	2.2
26	X	41	PHE	2.2
7	D	71	ALA	2.2
1	0	1981	A	2.2
11	H	162	ARG	2.2
22	T	103	LEU	2.2
22	T	109	GLU	2.2
1	0	1203	G	2.1
4	A	135	VAL	2.1
31	3	26	ARG	2.1
1	0	1206	U	2.1
1	0	1174	A	2.1
1	0	2345	A	2.1
10	G	68	GLU	2.1
9	F	20	LEU	2.1
19	Q	17	LYS	2.1
21	S	2	TRP	2.1
5	B	115	VAL	2.1
5	B	133	GLU	2.1
8	E	81	GLU	2.1
1	0	129	A	2.1
11	H	50	ILE	2.1
26	X	12	ILE	2.1
9	F	60	VAL	2.1
9	F	113	ASP	2.1
4	A	128	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
5	B	186	GLY	2.1
10	G	19	GLU	2.1
31	3	73	GLU	2.1
1	0	1184	C	2.1
17	O	31	GLU	2.1
20	R	104	PHE	2.1
8	E	16	ASP	2.1
30	2	30	ASP	2.1
14	L	59	GLU	2.1
9	F	26	THR	2.1
11	H	70	ASN	2.1
7	D	163	VAL	2.1
14	L	96	VAL	2.1
5	B	181	ILE	2.1
7	D	47	GLN	2.1
9	F	103	GLU	2.1
14	L	147	GLU	2.1
27	Y	106	THR	2.1
24	V	14	ALA	2.1
14	L	150	GLN	2.0
15	M	97	ILE	2.0
7	D	72	LYS	2.0
7	D	169	THR	2.0
16	N	74	PRO	2.0
7	D	83	PHE	2.0
23	U	4	ARG	2.0
16	N	81	ALA	2.0
11	H	142	ASP	2.0
12	J	39	VAL	2.0
31	3	13	HIS	2.0
6	C	63	SER	2.0
24	V	9	ARG	2.0
25	W	78	ASP	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	OMG	0	2588	24/25	0.97	0.12	34,37,42,43	0
3	PPU	4	76	37/38	0.98	0.12	38,43,49,54	0
1	UR3	0	2619	21/22	0.98	0.14	39,40,43,47	0
1	PSU	0	2621	20/21	0.98	0.13	35,39,43,44	0
1	1MA	0	628	23/24	0.98	0.15	35,37,40,44	0
1	OMU	0	2587	21/22	0.98	0.12	35,40,43,43	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
37	SR	0	9537	1/1	0.14	0.21	159,159,159,159	0
33	MG	0	8047	1/1	0.18	1.13	111,111,111,111	0
35	NA	0	9129	1/1	0.29	0.32	82,82,82,82	0
37	SR	0	9547	1/1	0.38	0.28	184,184,184,184	0
33	MG	0	8102	1/1	0.43	0.16	76,76,76,76	0
33	MG	0	8108	1/1	0.47	0.13	107,107,107,107	0
38	CD	Z	9203	1/1	0.48	0.19	93,93,93,93	0
33	MG	0	8094	1/1	0.51	0.68	93,93,93,93	0
35	NA	0	9184	1/1	0.56	0.21	83,83,83,83	0
35	NA	0	9111	1/1	0.67	0.27	70,70,70,70	0
35	NA	0	9185	1/1	0.67	0.47	62,62,62,62	0
35	NA	0	9179	1/1	0.69	1.23	96,96,96,96	0
35	NA	9	9151	1/1	0.71	0.23	83,83,83,83	0
33	MG	0	8050	1/1	0.72	0.18	86,86,86,86	0
35	NA	S	9112	1/1	0.72	0.31	85,85,85,85	0
33	MG	0	8059	1/1	0.72	0.40	71,71,71,71	0
33	MG	0	8065	1/1	0.74	0.47	90,90,90,90	0
35	NA	0	9178	1/1	0.75	0.26	57,57,57,57	0
33	MG	0	8042	1/1	0.76	0.09	58,58,58,58	0
33	MG	0	8052	1/1	0.76	0.41	87,87,87,87	0
33	MG	0	8022	1/1	0.76	1.07	123,123,123,123	0
36	CL	0	9316	1/1	0.77	0.24	86,86,86,86	0
33	MG	0	8091	1/1	0.77	0.08	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	MG	0	8014	1/1	0.77	0.86	94,94,94,94	0
37	SR	0	9484	1/1	0.77	0.08	139,139,139,139	0
37	SR	9	9588	1/1	0.78	0.14	141,141,141,141	0
33	MG	0	8032	1/1	0.78	0.10	47,47,47,47	0
33	MG	0	8040	1/1	0.78	0.44	100,100,100,100	0
33	MG	0	8072	1/1	0.79	0.33	78,78,78,78	0
37	SR	0	9500	1/1	0.79	1.25	200,200,200,200	0
35	NA	0	9140	1/1	0.79	0.55	67,67,67,67	0
35	NA	0	9171	1/1	0.81	0.25	66,66,66,66	0
35	NA	H	9122	1/1	0.81	0.19	78,78,78,78	0
33	MG	0	8089	1/1	0.81	0.23	64,64,64,64	0
35	NA	0	9168	1/1	0.82	0.15	68,68,68,68	0
33	MG	0	8107	1/1	0.82	0.16	67,67,67,67	0
35	NA	0	9182	1/1	0.82	0.14	81,81,81,81	0
33	MG	0	8084	1/1	0.83	0.33	84,84,84,84	0
35	NA	0	9102	1/1	0.83	0.24	64,64,64,64	0
35	NA	0	9174	1/1	0.83	0.51	71,71,71,71	0
35	NA	0	9163	1/1	0.83	0.19	65,65,65,65	0
35	NA	0	9170	1/1	0.84	0.38	87,87,87,87	0
33	MG	0	8041	1/1	0.84	0.12	56,56,56,56	0
35	NA	0	9158	1/1	0.84	0.23	62,62,62,62	0
33	MG	0	8099	1/1	0.84	0.19	74,74,74,74	0
33	MG	0	8116	1/1	0.84	0.08	59,59,59,59	0
33	MG	0	8092	1/1	0.84	0.49	79,79,79,79	0
35	NA	0	9164	1/1	0.84	0.34	62,62,62,62	0
35	NA	0	9125	1/1	0.85	0.56	87,87,87,87	0
33	MG	0	8054	1/1	0.85	0.14	60,60,60,60	0
33	MG	0	8101	1/1	0.85	0.15	68,68,68,68	0
33	MG	0	8114	1/1	0.86	0.39	79,79,79,79	0
33	MG	0	8093	1/1	0.86	0.18	52,52,52,52	0
35	NA	0	9157	1/1	0.86	0.17	52,52,52,52	0
35	NA	9	9152	1/1	0.87	0.48	76,76,76,76	0
33	MG	0	8113	1/1	0.87	0.13	49,49,49,49	0
35	NA	0	9161	1/1	0.88	0.20	61,61,61,61	0
37	SR	0	9504	1/1	0.88	0.12	107,107,107,107	0
37	SR	0	9626	1/1	0.88	0.38	147,147,147,147	0
34	K	0	9001	1/1	0.88	0.71	92,92,92,92	0
35	NA	9	9183	1/1	0.88	0.13	80,80,80,80	0
35	NA	0	9118	1/1	0.88	0.30	71,71,71,71	0
35	NA	0	9172	1/1	0.88	0.36	78,78,78,78	0
35	NA	0	9107	1/1	0.89	0.25	59,59,59,59	0
33	MG	0	8063	1/1	0.89	0.12	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	NA	3	9169	1/1	0.89	0.40	98,98,98,98	0
33	MG	0	8117	1/1	0.89	0.15	48,48,48,48	0
38	CD	O	9205	1/1	0.89	0.04	138,138,138,138	0
37	SR	B	9521	1/1	0.89	0.40	184,184,184,184	0
35	NA	R	9137	1/1	0.89	0.11	43,43,43,43	0
33	MG	0	8090	1/1	0.89	0.18	67,67,67,67	0
35	NA	0	9173	1/1	0.89	0.37	69,69,69,69	0
34	K	0	9002	1/1	0.89	0.12	90,90,90,90	0
33	MG	0	8046	1/1	0.90	0.10	47,47,47,47	0
35	NA	0	9126	1/1	0.90	0.11	64,64,64,64	0
35	NA	0	9110	1/1	0.90	0.15	49,49,49,49	0
33	MG	0	8045	1/1	0.90	0.32	82,82,82,82	0
35	NA	0	9156	1/1	0.90	0.34	59,59,59,59	0
33	MG	0	8024	1/1	0.90	0.42	76,76,76,76	0
35	NA	0	9130	1/1	0.90	0.14	53,53,53,53	0
35	NA	0	9167	1/1	0.91	0.16	57,57,57,57	0
35	NA	0	9149	1/1	0.91	0.21	52,52,52,52	0
37	SR	0	9459	1/1	0.91	0.07	107,107,107,107	0
35	NA	0	9175	1/1	0.91	0.19	55,55,55,55	0
33	MG	B	8055	1/1	0.91	0.27	94,94,94,94	0
33	MG	0	8079	1/1	0.91	0.14	33,33,33,33	0
33	MG	9	8095	1/1	0.91	0.26	61,61,61,61	0
36	CL	B	9319	1/1	0.91	0.23	62,62,62,62	0
35	NA	0	9131	1/1	0.91	0.21	52,52,52,52	0
35	NA	0	9113	1/1	0.91	0.11	74,74,74,74	0
33	MG	0	8051	1/1	0.91	0.29	33,33,33,33	0
37	SR	0	9467	1/1	0.92	0.10	91,91,91,91	0
35	NA	0	9154	1/1	0.92	0.26	57,57,57,57	0
37	SR	0	9517	1/1	0.92	0.04	117,117,117,117	0
37	SR	0	9529	1/1	0.92	0.09	120,120,120,120	0
33	MG	0	8082	1/1	0.92	0.41	89,89,89,89	0
33	MG	0	8115	1/1	0.92	0.17	61,61,61,61	0
33	MG	0	8021	1/1	0.92	0.18	58,58,58,58	0
33	MG	0	8080	1/1	0.92	0.20	58,58,58,58	0
33	MG	0	8085	1/1	0.93	0.32	68,68,68,68	0
35	NA	C	9104	1/1	0.93	0.11	33,33,33,33	0
35	NA	0	9155	1/1	0.93	0.29	62,62,62,62	0
35	NA	0	9177	1/1	0.93	0.35	78,78,78,78	0
35	NA	0	9132	1/1	0.93	0.15	57,57,57,57	0
33	MG	0	8103	1/1	0.93	0.20	74,74,74,74	0
33	MG	0	8075	1/1	0.93	0.05	41,41,41,41	0
33	MG	T	8073	1/1	0.93	0.12	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	MG	0	8039	1/1	0.93	0.09	66,66,66,66	0
35	NA	J	9146	1/1	0.93	0.12	58,58,58,58	0
33	MG	0	8043	1/1	0.93	0.06	57,57,57,57	0
37	SR	0	9539	1/1	0.93	0.50	162,162,162,162	0
37	SR	0	9532	1/1	0.93	0.05	127,127,127,127	0
37	SR	0	9475	1/1	0.94	0.12	84,84,84,84	0
36	CL	0	9322	1/1	0.94	0.20	58,58,58,58	0
33	MG	Y	8109	1/1	0.94	0.12	47,47,47,47	0
37	SR	0	9581	1/1	0.94	0.10	136,136,136,136	0
35	NA	0	9159	1/1	0.94	0.21	54,54,54,54	0
33	MG	0	8096	1/1	0.94	0.12	51,51,51,51	0
35	NA	0	9141	1/1	0.94	0.08	64,64,64,64	0
33	MG	2	8076	1/1	0.94	0.20	64,64,64,64	0
33	MG	0	8097	1/1	0.94	0.23	63,63,63,63	0
35	NA	0	9124	1/1	0.94	0.12	54,54,54,54	0
35	NA	0	9181	1/1	0.94	0.20	55,55,55,55	0
37	SR	0	9590	1/1	0.94	0.10	98,98,98,98	0
35	NA	0	9127	1/1	0.94	0.19	71,71,71,71	0
33	MG	0	8060	1/1	0.94	0.17	97,97,97,97	0
33	MG	0	8106	1/1	0.94	0.08	50,50,50,50	0
33	MG	0	8083	1/1	0.94	0.08	59,59,59,59	0
36	CL	N	9307	1/1	0.95	0.14	65,65,65,65	0
33	MG	0	8002	1/1	0.95	0.10	37,37,37,37	0
33	MG	0	8027	1/1	0.95	0.25	40,40,40,40	0
36	CL	J	9302	1/1	0.95	0.08	63,63,63,63	0
37	SR	0	9560	1/1	0.95	0.08	98,98,98,98	0
35	NA	0	9128	1/1	0.95	0.09	48,48,48,48	0
35	NA	Q	9148	1/1	0.95	0.12	48,48,48,48	0
33	MG	0	8058	1/1	0.95	0.56	92,92,92,92	0
33	MG	0	8015	1/1	0.95	0.10	33,33,33,33	0
35	NA	0	9116	1/1	0.95	0.45	55,55,55,55	0
37	SR	0	9468	1/1	0.95	0.03	120,120,120,120	0
36	CL	J	9321	1/1	0.95	0.13	68,68,68,68	0
36	CL	0	9315	1/1	0.95	0.10	59,59,59,59	0
35	NA	0	9134	1/1	0.95	0.06	52,52,52,52	0
35	NA	0	9162	1/1	0.95	0.18	50,50,50,50	0
33	MG	0	8088	1/1	0.95	0.08	39,39,39,39	0
37	SR	0	9505	1/1	0.95	0.08	91,91,91,91	0
35	NA	0	9160	1/1	0.95	0.16	45,45,45,45	0
33	MG	0	8104	1/1	0.95	0.10	59,59,59,59	0
37	SR	0	9465	1/1	0.96	0.09	101,101,101,101	0
36	CL	0	9317	1/1	0.96	0.07	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	MG	0	8098	1/1	0.96	0.07	47,47,47,47	0
35	NA	0	9166	1/1	0.96	0.08	68,68,68,68	0
33	MG	0	8013	1/1	0.96	0.37	24,24,24,24	0
33	MG	0	8028	1/1	0.96	0.12	37,37,37,37	0
33	MG	0	8074	1/1	0.96	0.19	32,32,32,32	0
33	MG	0	8019	1/1	0.96	0.05	51,51,51,51	0
37	SR	0	9489	1/1	0.96	0.08	92,92,92,92	0
33	MG	0	8067	1/1	0.96	0.10	44,44,44,44	0
37	SR	0	9515	1/1	0.96	0.16	94,94,94,94	0
33	MG	A	8066	1/1	0.96	0.13	53,53,53,53	0
33	MG	0	8057	1/1	0.96	0.34	68,68,68,68	0
33	MG	0	8012	1/1	0.96	0.22	46,46,46,46	0
35	NA	0	9165	1/1	0.96	0.23	46,46,46,46	0
36	CL	A	9309	1/1	0.96	0.11	60,60,60,60	0
36	CL	J	9301	1/1	0.96	0.10	59,59,59,59	0
35	NA	0	9120	1/1	0.96	0.26	61,61,61,61	0
37	SR	F	9595	1/1	0.96	0.15	104,104,104,104	0
35	NA	R	9186	1/1	0.96	0.19	71,71,71,71	0
35	NA	0	9150	1/1	0.96	0.16	52,52,52,52	0
37	SR	9	9503	1/1	0.96	0.04	116,116,116,116	0
35	NA	R	9138	1/1	0.96	0.11	76,76,76,76	0
37	SR	0	9522	1/1	0.96	0.07	118,118,118,118	0
33	MG	0	8061	1/1	0.96	0.12	81,81,81,81	0
33	MG	0	8068	1/1	0.96	0.13	55,55,55,55	0
35	NA	0	9139	1/1	0.96	0.08	50,50,50,50	0
35	NA	M	9147	1/1	0.96	0.18	45,45,45,45	0
36	CL	0	9311	1/1	0.96	0.10	64,64,64,64	0
37	SR	0	9585	1/1	0.96	0.10	94,94,94,94	0
37	SR	0	9452	1/1	0.96	0.11	107,107,107,107	0
35	NA	0	9106	1/1	0.97	0.37	44,44,44,44	0
37	SR	0	9566	1/1	0.97	0.07	80,80,80,80	0
35	NA	0	9136	1/1	0.97	0.14	38,38,38,38	0
37	SR	0	9455	1/1	0.97	0.07	77,77,77,77	0
37	SR	0	9508	1/1	0.97	0.07	91,91,91,91	0
37	SR	0	9417	1/1	0.97	0.13	61,61,61,61	0
36	CL	Y	9320	1/1	0.97	0.10	49,49,49,49	0
33	MG	0	8017	1/1	0.97	0.12	30,30,30,30	0
37	SR	0	9482	1/1	0.97	0.26	122,122,122,122	0
37	SR	0	9534	1/1	0.97	0.17	108,108,108,108	0
37	SR	0	9473	1/1	0.97	0.02	79,79,79,79	0
36	CL	L	9310	1/1	0.97	0.09	58,58,58,58	0
36	CL	0	9314	1/1	0.97	0.09	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
37	SR	0	9442	1/1	0.97	0.11	65,65,65,65	0
37	SR	0	9429	1/1	0.97	0.11	71,71,71,71	0
37	SR	0	9464	1/1	0.97	0.05	83,83,83,83	0
35	NA	0	9115	1/1	0.97	0.17	47,47,47,47	0
37	SR	A	9437	1/1	0.97	0.12	73,73,73,73	0
35	NA	0	9135	1/1	0.97	0.18	54,54,54,54	0
35	NA	0	9114	1/1	0.97	0.13	46,46,46,46	0
37	SR	0	9530	1/1	0.97	0.14	73,73,73,73	0
37	SR	H	9486	1/1	0.97	0.22	114,114,114,114	0
33	MG	0	8030	1/1	0.97	0.05	37,37,37,37	0
37	SR	0	9477	1/1	0.97	0.07	83,83,83,83	0
37	SR	0	9629	1/1	0.97	0.08	77,77,77,77	0
33	MG	0	8031	1/1	0.97	0.09	55,55,55,55	0
37	SR	0	9469	1/1	0.97	0.03	91,91,91,91	0
37	SR	0	9509	1/1	0.97	0.12	91,91,91,91	0
35	NA	0	9108	1/1	0.98	0.15	35,35,35,35	0
33	MG	0	8008	1/1	0.98	0.19	22,22,22,22	0
37	SR	0	9433	1/1	0.98	0.13	75,75,75,75	0
37	SR	0	9435	1/1	0.98	0.08	75,75,75,75	0
37	SR	0	9488	1/1	0.98	0.12	84,84,84,84	0
33	MG	0	8037	1/1	0.98	0.07	42,42,42,42	0
37	SR	0	9427	1/1	0.98	0.13	58,58,58,58	0
33	MG	0	8029	1/1	0.98	0.31	37,37,37,37	0
37	SR	0	9466	1/1	0.98	0.04	101,101,101,101	0
36	CL	O	9308	1/1	0.98	0.08	66,66,66,66	0
33	MG	0	8025	1/1	0.98	0.40	33,33,33,33	0
33	MG	0	8003	1/1	0.98	0.16	38,38,38,38	0
33	MG	K	8069	1/1	0.98	0.19	26,26,26,26	0
37	SR	0	9446	1/1	0.98	0.11	93,93,93,93	0
36	CL	0	9305	1/1	0.98	0.07	58,58,58,58	0
37	SR	0	9490	1/1	0.98	0.09	108,108,108,108	0
37	SR	S	9470	1/1	0.98	0.12	99,99,99,99	0
37	SR	0	9450	1/1	0.98	0.07	76,76,76,76	0
37	SR	0	9405	1/1	0.98	0.15	59,59,59,59	0
33	MG	0	8020	1/1	0.98	0.19	38,38,38,38	0
35	NA	0	9105	1/1	0.98	0.10	45,45,45,45	0
33	MG	0	8118	1/1	0.98	0.15	30,30,30,30	0
37	SR	0	9495	1/1	0.98	0.10	102,102,102,102	0
37	SR	0	9420	1/1	0.98	0.14	73,73,73,73	0
37	SR	0	9483	1/1	0.98	0.07	80,80,80,80	0
37	SR	B	9458	1/1	0.98	0.08	83,83,83,83	0
35	NA	0	9117	1/1	0.98	0.12	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	MG	0	8056	1/1	0.98	0.18	47,47,47,47	0
35	NA	0	9143	1/1	0.98	0.08	46,46,46,46	0
33	MG	0	8026	1/1	0.98	0.18	35,35,35,35	0
35	NA	0	9123	1/1	0.98	0.09	42,42,42,42	0
37	SR	0	9447	1/1	0.98	0.11	69,69,69,69	0
37	SR	0	9570	1/1	0.98	0.04	105,105,105,105	0
37	SR	0	9414	1/1	0.98	0.11	58,58,58,58	0
37	SR	0	9431	1/1	0.98	0.15	66,66,66,66	0
37	SR	0	9568	1/1	0.98	0.07	77,77,77,77	0
33	MG	0	8044	1/1	0.98	0.06	44,44,44,44	0
33	MG	0	8036	1/1	0.98	0.10	60,60,60,60	0
33	MG	0	8070	1/1	0.98	0.16	28,28,28,28	0
37	SR	0	9426	1/1	0.98	0.08	72,72,72,72	0
37	SR	0	9449	1/1	0.98	0.07	66,66,66,66	0
36	CL	3	9304	1/1	0.99	0.10	65,65,65,65	0
37	SR	0	9441	1/1	0.99	0.07	68,68,68,68	0
36	CL	0	9303	1/1	0.99	0.10	50,50,50,50	0
37	SR	0	9474	1/1	0.99	0.11	61,61,61,61	0
37	SR	0	9423	1/1	0.99	0.09	58,58,58,58	0
37	SR	0	9422	1/1	0.99	0.12	59,59,59,59	0
37	SR	0	9545	1/1	0.99	0.05	79,79,79,79	0
37	SR	A	9497	1/1	0.99	0.10	91,91,91,91	0
37	SR	0	9415	1/1	0.99	0.11	58,58,58,58	0
37	SR	0	9506	1/1	0.99	0.04	71,71,71,71	0
33	MG	0	8004	1/1	0.99	0.11	36,36,36,36	0
38	CD	3	9204	1/1	0.99	0.05	63,63,63,63	0
37	SR	0	9448	1/1	0.99	0.06	63,63,63,63	0
35	NA	0	9101	1/1	0.99	0.17	50,50,50,50	0
37	SR	1	9460	1/1	0.99	0.11	53,53,53,53	0
36	CL	M	9318	1/1	0.99	0.18	43,43,43,43	0
37	SR	0	9407	1/1	0.99	0.15	46,46,46,46	0
37	SR	0	9601	1/1	0.99	0.04	95,95,95,95	0
37	SR	0	9413	1/1	0.99	0.12	50,50,50,50	0
33	MG	0	8038	1/1	0.99	0.26	27,27,27,27	0
36	CL	0	9312	1/1	0.99	0.09	60,60,60,60	0
37	SR	0	9440	1/1	0.99	0.04	73,73,73,73	0
33	MG	0	8112	1/1	0.99	0.07	43,43,43,43	0
37	SR	0	9432	1/1	0.99	0.13	67,67,67,67	0
36	CL	R	9306	1/1	0.99	0.07	48,48,48,48	0
33	MG	0	8001	1/1	0.99	0.24	19,19,19,19	0
38	CD	U	9201	1/1	0.99	0.09	60,60,60,60	0
37	SR	0	9438	1/1	0.99	0.10	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
37	SR	0	9462	1/1	0.99	0.12	73,73,73,73	0
37	SR	0	9445	1/1	0.99	0.10	59,59,59,59	0
37	SR	0	9411	1/1	0.99	0.18	46,46,46,46	0
33	MG	0	8005	1/1	0.99	0.10	34,34,34,34	0
37	SR	0	9416	1/1	0.99	0.10	47,47,47,47	0
37	SR	3	9439	1/1	0.99	0.03	74,74,74,74	0
37	SR	0	9456	1/1	0.99	0.09	64,64,64,64	0
33	MG	0	8110	1/1	0.99	0.10	46,46,46,46	0
37	SR	0	9425	1/1	0.99	0.12	59,59,59,59	0
37	SR	0	9434	1/1	0.99	0.13	68,68,68,68	0
33	MG	0	8009	1/1	0.99	0.13	26,26,26,26	0
37	SR	0	9501	1/1	0.99	0.11	76,76,76,76	0
37	SR	0	9457	1/1	0.99	0.10	54,54,54,54	0
37	SR	1	9419	1/1	0.99	0.11	42,42,42,42	0
37	SR	0	9498	1/1	0.99	0.05	66,66,66,66	0
37	SR	A	9436	1/1	0.99	0.07	57,57,57,57	0
37	SR	R	9418	1/1	0.99	0.14	59,59,59,59	0
37	SR	0	9412	1/1	0.99	0.12	46,46,46,46	0
36	CL	0	9313	1/1	0.99	0.07	57,57,57,57	0
37	SR	0	9454	1/1	0.99	0.07	83,83,83,83	0
37	SR	0	9443	1/1	0.99	0.09	59,59,59,59	0
37	SR	0	9480	1/1	0.99	0.05	95,95,95,95	0
37	SR	0	9461	1/1	0.99	0.04	80,80,80,80	0
37	SR	0	9453	1/1	0.99	0.07	71,71,71,71	0
37	SR	0	9410	1/1	0.99	0.12	41,41,41,41	0
37	SR	0	9478	1/1	1.00	0.06	76,76,76,76	0
37	SR	0	9430	1/1	1.00	0.10	50,50,50,50	0
37	SR	0	9428	1/1	1.00	0.07	55,55,55,55	0
37	SR	0	9408	1/1	1.00	0.16	41,41,41,41	0
37	SR	0	9406	1/1	1.00	0.17	36,36,36,36	0
37	SR	L	9409	1/1	1.00	0.13	44,44,44,44	0
37	SR	0	9451	1/1	1.00	0.11	60,60,60,60	0
37	SR	9	9481	1/1	1.00	0.06	88,88,88,88	0
37	SR	0	9424	1/1	1.00	0.14	47,47,47,47	0
38	CD	1	9202	1/1	1.00	0.04	55,55,55,55	0
37	SR	0	9421	1/1	1.00	0.11	74,74,74,74	0
37	SR	0	9444	1/1	1.00	0.09	56,56,56,56	0

6.5 Other polymers ⓘ

There are no such residues in this entry.