



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Sep 6, 2017 – 04:30 AM EDT

PDB ID : 5L3P
EMDB ID: : EMD-4001
Title : Cryo-EM structure of stringent response factor RelA bound to ErmCL-stalled ribosome complex
Authors : Arenz, S.; Wilson, D.N.
Deposited on : unknown
Resolution : 3.70 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

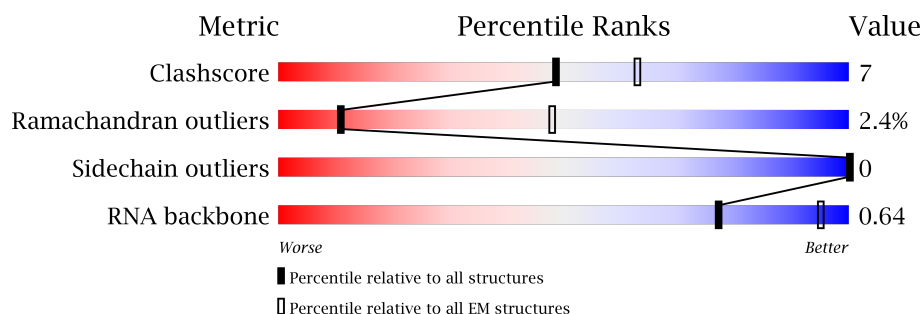
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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.
















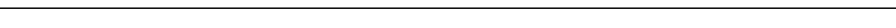











Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	2903	63% 32% 5%
2	B	120	69% 26% 5%
3	D	273	73% 26% .
4	E	209	78% 22%
5	F	201	76% 24%
6	G	179	75% 24% .
7	H	177	83% 16% .
8	I	149	79% 19% .


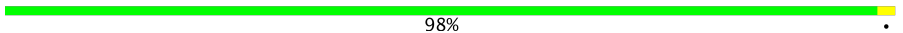



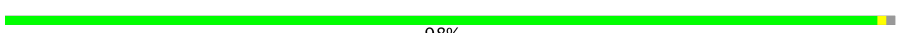










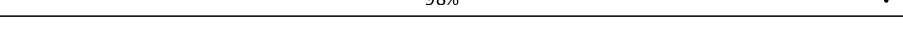

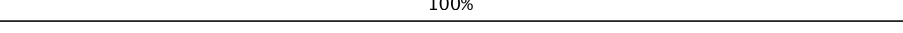



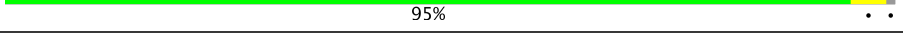


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Mol	Chain	Length	Quality of chain
9	N	142	
10	O	123	
11	P	144	
12	Q	136	
13	R	127	
14	S	117	
15	T	115	
16	U	118	
17	V	103	
18	W	110	
19	X	100	
20	Y	104	
21	Z	94	
22	0	85	
23	1	78	
24	2	63	
25	3	59	
26	4	70	
27	5	57	
28	6	55	
29	7	46	
30	8	65	
31	9	38	
32	a	1539	
33	b	240	

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Mol	Chain	Length	Quality of chain
34	c	233	
35	d	206	
36	e	167	
37	f	135	
38	g	179	
39	h	130	
40	i	130	
41	j	103	
42	k	129	
43	l	124	
44	m	118	
45	o	89	
46	p	82	
47	q	84	
48	r	75	
49	t	87	
50	u	71	
51	v	6	
52	x	77	
53	J	165	
54	K	142	
55	n	102	
56	s	92	
57	z	819	
58	y	73	

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
1	2MG	A	1835	X	-	-	-
1	PSU	A	1911	X	-	-	-
1	3TD	A	1915	X	-	-	-
1	PSU	A	1917	X	-	-	-
1	5MU	A	1939	X	-	-	-
1	7MG	A	2069	X	-	-	-
1	OMG	A	2251	X	-	-	-
1	2MG	A	2445	X	-	-	-
1	H2U	A	2449	X	-	-	-
1	PSU	A	2457	X	-	-	-
1	OMC	A	2498	X	-	-	-
1	2MA	A	2503	X	-	-	-
1	PSU	A	2504	X	-	-	-
1	OMU	A	2552	X	-	-	-
1	PSU	A	2580	X	-	-	-
1	PSU	A	2604	X	-	-	-
1	PSU	A	2605	X	-	-	-
1	PSU	A	746	X	-	-	-
1	PSU	A	955	X	-	-	-
32	2MG	a	1207	X	-	-	-
32	4OC	a	1402	X	-	-	-
32	UR3	a	1498	X	-	-	-
32	2MG	a	1516	X	-	-	-
32	MA6	a	1518	X	-	-	-
32	MA6	a	1519	X	-	-	-
32	PSU	a	516	X	-	-	-
32	7MG	a	527	X	-	-	-
32	2MG	a	966	X	-	-	-
52	H2U	x	20	X	-	-	-
52	5MU	x	54	X	-	-	-
52	PSU	x	55	X	-	-	-
52	4SU	x	8	X	-	-	-
58	H2U	y	16	X	-	-	-
58	H2U	y	17	X	-	-	-
58	H2U	y	20	X	-	-	-
58	7MG	y	46	X	-	-	-
58	5MU	y	54	X	-	-	-
58	PSU	y	55	X	-	-	-

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 149606 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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					AltConf	Trace
1	A	2890	Total	C	N	O	P	0	0
			62057	27688	11422	20057	2890		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1847	G	A	conflict	GB 802133627

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	120	Total	C	N	O	P	0	0
			2572	1145	471	836	120		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	120	A	U	conflict	GB 999944586

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	N	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	O	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	P	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Q	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	R	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	S	116	Total	C	N	O	S	0	0
			892	552	178	162			

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	U	117	Total	C	N	O	S	0	0
			947	604	192	151			

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	V	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	X	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Y	102	Total	C	N	O	S	0	0
			779	492	146	141			

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Z	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	0	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	1	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	2	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	3	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	4	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	5	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	6	50	Total	C	N	O	S	0	0
			409	263	75	71			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	7	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	8	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	9	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 32 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	1539	Total	C	N	O	P	0	0
			33029	14738	6052	10700	1539		

- Molecule 33 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 34 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	c	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 35 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	d	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 36 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	e	157	Total	C	N	O	S	0	0
			1141	709	218	208	6		

- Molecule 37 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	f	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 38 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	g	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 39 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	h	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 40 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	i	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 41 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	j	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 42 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	k	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 43 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	l	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 44 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	m	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 45 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	o	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 46 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	p	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 47 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 48 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	r	65	Total	C	N	O	0	0
			504	317	96	91		

- Molecule 49 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	t	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 50 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	u	65	Total	C	N	O	S	0	0
			495	307	100	87	1		

- Molecule 51 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	v	6	Total	C	N	O	P	0	0
			129	58	24	41	6		

- Molecule 52 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	x	77	Total	C	N	O	P	S	0	0
			1644	733	297	536	77	1		

- Molecule 53 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	J	131	Total	C	N	O	S	0	0
			988	625	175	183	5		

- Molecule 54 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	K	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 55 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	n	101	Total	C	N	O	S	0	0
			799	498	165	133	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	35	ALA	-	insertion	UNP P0AG59

- Molecule 56 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	s	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 57 is a protein called GTP pyrophosphokinase,GTP pyrophosphokinase,GTP pyrophosphokinase.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	z	545	Total	C	N	O		0	0
			2255	1165	545	545			

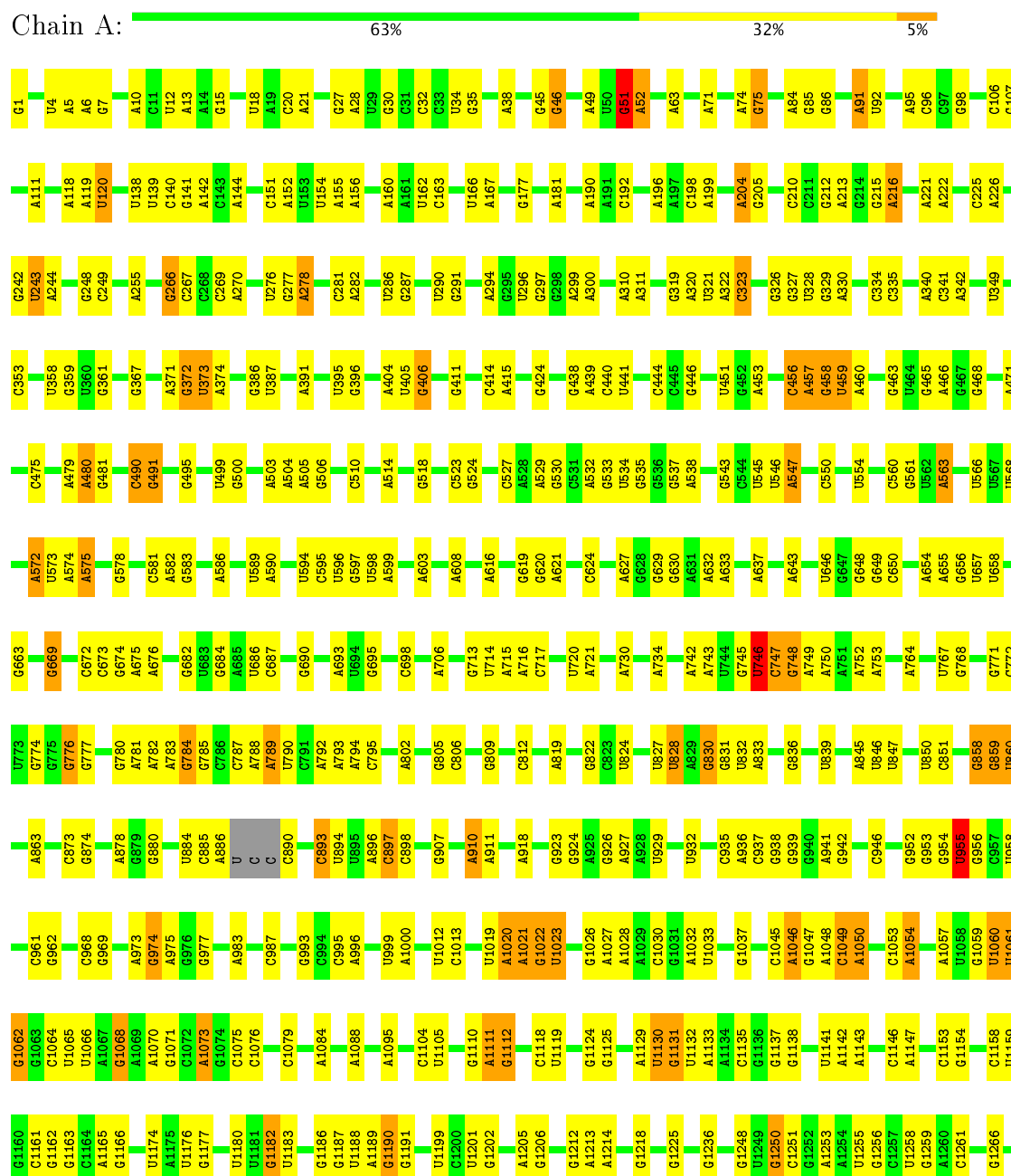
- Molecule 58 is a RNA chain called deacylated A/R-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	y	73	Total	C	N	O	P	0	0
			1581	709	280	519	73		

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. 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. 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



A2778	A2779	G2780	C2781	G2782	C2783	G2784	C2785	G2786	C2787	G2788	C2789	G2790	C2791	G2792	C2793	G2794	C2795	G2796	C2797	G2798	C2799	G2800	C2801	G2802	C2803	G2804	C2805	G2806	C2807	G2808	C2809	G2810	C2811	G2812	C2813	G2814	C2815	G2816	C2817	G2818	C2819	G2820	C2821	G2822	C2823	G2824	C2825	G2826	C2827	G2828	C2829	G2830	C2831	G2832	C2833	G2834	C2835	G2836	C2837	G2838	C2839	G2840	C2841	G2842	C2843	G2844	C2845	G2846	C2847	G2848	C2849	G2850	C2851	G2852	C2853	G2854	C2855	G2856	C2857	G2858	C2859	G2860	C2861	G2862	C2863	G2864	C2865	G2866	C2867	G2868	C2869	G2870	C2871	G2872	C2873	G2874	C2875	G2876	C2877	G2878	C2879	G2880	C2881	G2882	C2883	G2884	C2885	A2886	C2887	G2888	C2889	A2890	C2891	G2892	C2893	A2894	C2895	G2896	C2897	A2898	C2899	G2900	C2901	A2902	C2903	G2904	C2905	A2906	C2907	G2908	C2909	A2910	C2911	G2912	C2913	A2914	C2915	G2916	C2917	A2918	C2919	G2920	C2921	A2922	C2923	G2924	C2925	A2926	C2927	G2928	C2929	A2930	C2931	G2932	C2933	A2934	C2935	G2936	C2937	A2938	C2939	G2940	C2941	A2942	C2943	G2944	C2945	A2946	C2947	G2948	C2949	A2950	C2951	G2952	C2953	A2954	C2955	G2956	C2957	A2958	C2959	G2960	C2961	A2962	C2963	G2964	C2965	A2966	C2967	G2968	C2969	A2970	C2971	G2972	C2973	A2974	C2975	G2976	C2977	A2978	C2979	G2980	C2981	A2982	C2983	G2984	C2985	A2986	C2987	G2988	C2989	A2990	C2991	G2992	C2993	A2994	C2995	G2996	C2997	A2998	C2999	G3000	C3001	A3002	C3003	G3004	C3005	A3006	C3007	G3008	C3009	A3010	C3011	G3012	C3013	A3014	C3015	G3016	C3017	A3018	C3019	G3020	C3021	A3022	C3023	G3024	C3025	A3026	C3027	G3028	C3029	A3030	C3031	G3032	C3033	A3034	C3035	G3036	C3037	A3038	C3039	G3040	C3041	A3042	C3043	G3044	C3045	A3046	C3047	G3048	C3049	A3050	C3051	G3052	C3053	A3054	C3055	G3056	C3057	A3058	C3059	G3060	C3061	A3062	C3063	G3064	C3065	A3066	C3067	G3068	C3069	A3070	C3071	G3072	C3073	A3074	C3075	G3076	C3077	A3078	C3079	G3080	C3081	A3082	C3083	G3084	C3085	A3086	C3087	G3088	C3089	A3090	C3091	G3092	C3093	A3094	C3095	G3096	C3097	A3098	C3099	G3100	C3101	A3102	C3103	G3104	C3105	A3106	C3107	G3108	C3109	A3110	C3111	G3112	C3113	A3114	C3115	G3116	C3117	A3118	C3119	G3120	C3121	A3122	C3123	G3124	C3125	A3126	C3127	G3128	C3129	A3130	C3131	G3132	C3133	A3134	C3135	G3136	C3137	A3138	C3139	G3140	C3141	A3142	C3143	G3144	C3145	A3146	C3147	G3148	C3149	A3150	C3151	G3152	C3153	A3154	C3155	G3156	C3157	A3158	C3159	G3160	C3161	A3162	C3163	G3164	C3165	A3166	C3167	G3168	C3169	A3170	C3171	G3172	C3173	A3174	C3175	G3176	C3177	A3178	C3179	G3180	C3181	A3182	C3183	G3184	C3185	A3186	C3187	G3188	C3189	A3190	C3191	G3192	C3193	A3194	C3195	G3196	C3197	A3198	C3199	G3200	C3201	A3202	C3203	G3204	C3205	A3206	C3207	G3208	C3209	A3210	C3211	G3212	C3213	A3214	C3215	G3216	C3217	A3218	C3219	G3220	C3221	A3222	C3223	G3224	C3225	A3226	C3227	G3228	C3229	A3230	C3231	G3232	C3233	A3234	C3235	G3236	C3237	A3238	C3239	G3240	C3241	A3242	C3243	G3244	C3245	A3246	C3247	G3248	C3249	A3250	C3251	G3252	C3253	A3254	C3255	G3256	C3257	A3258	C3259	G3260	C3261	A3262	C3263	G3264	C3265	A3266	C3267	G3268	C3269	A3270	C3271	G3272	C3273	A3274	C3275	G3276	C3277	A3278	C3279	G3280	C3281	A3282	C3283	G3284	C3285	A3286	C3287	G3288	C3289	A3290	C3291	G3292	C3293	A3294	C3295	G3296	C3297	A3298	C3299	G3300	C3301	A3302	C3303	G3304	C3305	A3306	C3307	G3308	C3309	A3310	C3311	G3312	C3313	A3314	C3315	G3316	C3317	A3318	C3319	G3320	C3321	A3322	C3323	G3324	C3325	A3326	C3327	G3328	C3329	A3330	C3331	G3332	C3333	A3334	C3335	G3336	C3337	A3338	C3339	G3340	C3341	A3342	C3343	G3344	C3345	A3346	C3347	G3348	C3349	A3350	C3351	G3352	C3353	A3354	C3355	G3356	C3357	A3358	C3359	G3360	C3361	A3362	C3363	G3364	C3365	A3366	C3367	G3368	C3369	A3370	C3371	G3372	C3373	A3374	C3375	G3376	C3377	A3378	C3379	G3380	C3381	A3382	C3383	G3384	C3385	A3386	C3387	G3388	C3389	A3390	C3391	G3392	C3393	A3394	C3395	G3396	C3397	A3398	C3399	G3400	C3401	A3402	C3403	G3404	C3405	A3406	C3407	G3408	C3409	A3410	C3411	G3412	C3413	A3414	C3415	G3416	C3417	A3418	C3419	G3420	C3421	A3422	C3423	G3424	C3425	A3426	C3427	G3428	C3429	A3430	C3431	G3432	C3433	A3434	C3435	G3436	C3437	A3438	C3439	G3440	C3441	A3442	C3443	G3444	C3445	A3446	C3447	G3448	C3449	A3450	C3451	G3452	C3453	A3454	C3455	G3456	C3457	A3458	C3459	G3460	C3461	A3462	C3463	G3464	C3465	A3466	C3467	G3468	C3469	A3470	C3471	G3472	C3473	A3474	C3475	G3476	C3477	A3478	C3479	G3480	C3481	A3482	C3483	G3484	C3485	A3486	C3487	G3488	C3489	A3490	C3491	G3492	C3493	A3494	C3495	G3496	C3497	A3498	C3499	G3500	C3501	A3502	C3503	G3504	C3505	A3506	C3507	G3508	C3509	A3510	C3511	G3512	C3513	A3514	C3515	G3516	C3517	A3518	C3519	G3520	C3521	A3522	C3523	G3524	C3525	A3526	C3527	G3528	C3529	A3530	C3531	G3532	C3533	A3534	C3535	G3536	C3537	A3538	C3539	G3540	C3541	A3542	C3543	G3544	C3545	A3546	C3547	G3548	C3549	A3550	C3551	G3552	C3553	A3554	C3555	G3556	C3557	A3558	C3559	G3560	C3561	A3562	C3563	G3564	C3565	A3566	C3567	G3568	C3569	A3570	C3571	G3572	C3573	A3574	C3575	G3576	C3577	A3578	C3579	G3580	C3581	A3582	C3583	G3584	C3585	A3586	C3587	G3588	C3589	A3590	C3591	G3592	C3593	A3594	C3595	G3596	C3597	A3598	C3599	G3600	C3601	A3602	C3603	G3604	C3605	A3606	C3607	G3608	C3609	A3610	C3611	G3612	C3613	A3614	C3615	G3616	C3617	A3618	C3619	G3620	C3621	A3622	C3623	G3624	C3625	A3626	C3627	G3628	C3629	A3630	C3631	G3632	C3633	A3634	C3635	G3636	C3637	A3638	C3639	G3640	C3641	A3642	C3643	G3644	C3645	A3646	C3647	G3648	C3649	A3650	C3651	G3652	C3653	A3654	C3655	G3656	C3657	A3658	C3659	G3660	C3661	A3662	C3663	G3664	C3665	A3666	C3667	G3668	C3669	A3670	C3671	G3672	C3673	A3674	C3675	G3676	C3677	A3678	C3679	G3680	C3681	A3682	C3683	G3684	C3685	A3686	C3687	G3688	C3689	A3690	C3691	G3692	C3693	A3694	C3695	G3696	C3697	A3698	C3699	G3700	C3701	A3702	C3703	G3704	C3705	A3706	C3707	G3708	C3709	A3710	C3711	G3712	C3713	A3714	C3715	G3716	C3717	A3718	C3719	G3720	C3721	A3722	C3723	G3724	C3725	A3726	C3727	G3728	C3729	A3730	C3731	G3732	C3733	A3734	C3735	G3736	C3737	A3738	C3739	G3740	C3741	A3742	C3743	G3744	C3745	A3746	C3747	G3748	C3749	A3750	C3751	G3752	C3753	A3754	C3755	G3756	C3757	A3758	C3759	G3760	C3761	A3762	C3763	G3764	C3765	A3766	C3767	G3768	C3769	A3770	C3771	G3772	C3773	A3774	C3775	G3776	C3777	A3778	C3779	G3780	C3781	A3782	C3783	G3784	C3785	A3786	C3787	G3788	C3789	A3790	C3791	G3792	C3793	A3794	C3795	G3796	C3797	A3798	C3799	G3800	C3801	A3802	C3803	G3804	C3805	A3806	C3807	G3808	C3809	A3810	C3811	G3812	C3813	A3814	C3815	G3816	C3817	A3818	C3819	G3820	C3821	A3822	C3823	G3824	C3825	A3826	C3827	G3828	C3829	A3830	C3831	G3832	C3833	A3834	C3835	G3836	C3837	A3838	C3839	G3840	C3841	A3842	C3843	G3844	C3845	A3846	C3847	G3848	C3849	A3850	C3851	G3852	C3853	A3854	C3855	G3856	C3857	A3858	C3859	G3860	C3861	A3862	C3863	G3864	C3865	A3866	C3867	G3868	C3869	A3870	C3871	G3872	C3873	A3874	C3875	G3876	C3877	A3878	C3879	G3880	C3881	A3882	C3883	G3884	C3885	A3886	C3887	G3888	C3889	A3890	C3891	G3892	C3893	A3894	C3895	G3896	C3897	A3898	C3899	G3900	C3901	A3902	C3903	G3904	C3905	A3906	C3907	G3908	C3909	A3910	C3911	G3912	C3913	A3914	C3915	G3916	C3917	A3918	C3919	G3920	C3921	A3922	C3923	G3924	C3925	A3926	C3927	G3928	C3929	A3930	C3931	G3932	C3933	A3934	C3935	G3936	C3937	A3938	C3939	G3940	C3941	A3942	C3943	G3944	C3945	A3946	C3947	G3948	C3949	A3950	C3951	G3952	C3953	A3954	C3955	G3956	C3957	A3958	C3959	G3960	C3961	A3962	C3963	G3964	C3965	A3966	C3967	G3968	C3969	A3970	C3971	G3972	C3973	A3974	C3975	G3976	C3977	A3978	C3979	G3980	C3981	A3982	C3983	G3984	C3985	A3986	C3987	G3988	C3989	A3990	C3991	G3992	C3993	A3994	C3995	G3996	C3997	A3998	C3999	G4000	C4001	A4002	C4003	G4004	C4005	A4006	C4007	G4008	C4009	A4010	C4011	G4012	C4013	A4014	C4015	G4016	C4017	A4018	C4019	G4020	C4021	A4022	C4023	G4024	C4025	A4026	C4027	G4028	C4029	A4030	C4031	G4032	C4033	A4034	C4035	G4036	C4037	A4038	C4039	G4040	C4041	A4042	C4043	G4044	C4045	A4046	C4047	G4048	C4049	A4050	C4051	G4052	C4053	A4054	C4055	G4056	C4057	A4058	C4059	G4060	C4061	A4062	C4063	G4064	C4065	A4066	C4067	G4068	C4069	A4070	C4071	G4072	C4073	A4074	C4075	G4076	C4077	A4078	C4079	G4080	C4081	A4082	C4083	G4084	C4085	A4086	C4087	G4088	C4089	A4090	C4091	G4092	C4093	A4094	C4095	G4096	C4097	A4098	C4099	G4100	C4101	A4102	C4103	G4104	C4105	A4106	C4107	G4108	C4109	A4110	C4111	G4112	C4113	A4114	C4115	G4116	C4117	A4118	C4119	G4120	C4121	A4122	C4123	G4124	C4125	A4126	C4127	G4128	C4129	A4130	C4131	G4132	C4133	A4134	C4135	G4136	C4137	A4138
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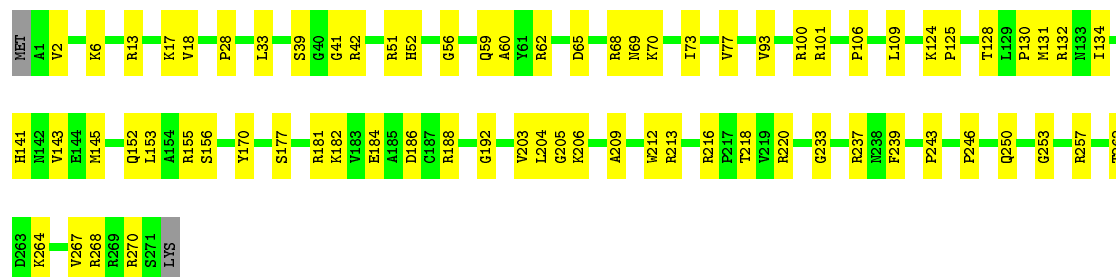
- Molecule 2: 5S ribosomal RNA

Chain B: 




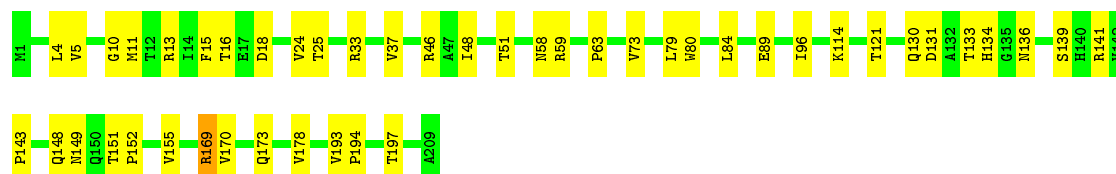
- Molecule 3: 50S ribosomal protein L2

Chain D: 




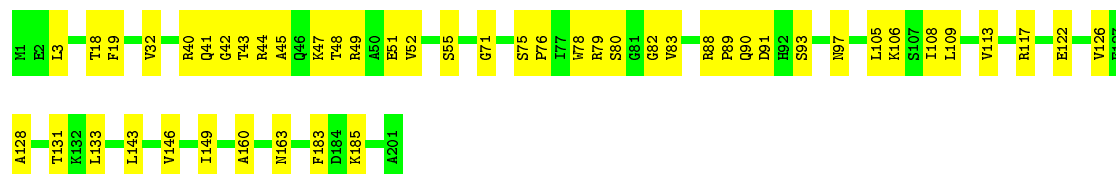
- Molecule 4: 50S ribosomal protein L3

Chain E: 



- Molecule 5: 50S ribosomal protein L4

Chain F: 




- Molecule 6: 50S ribosomal protein L5

Chain G: 




- Molecule 7: 50S ribosomal protein L6

Chain H:  83% 16%



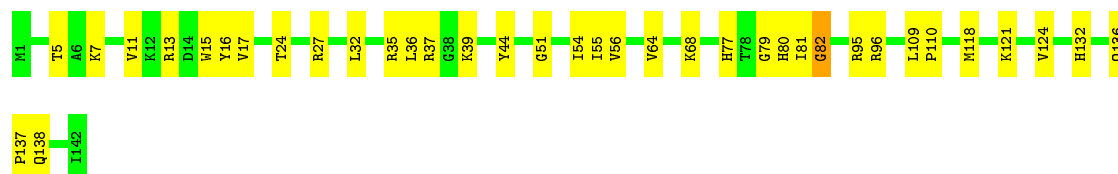
- Molecule 8: 50S ribosomal protein L9

Chain I:  79% 19%



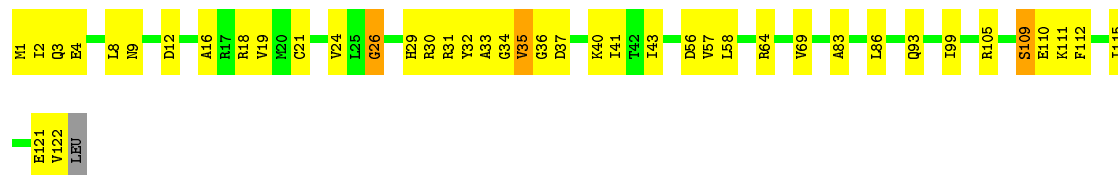
- Molecule 9: 50S ribosomal protein L13

Chain N:  74% 25%



- Molecule 10: 50S ribosomal protein L14

Chain O:  65% 32%




- Molecule 11: 50S ribosomal protein L15

Chain P:  66% 33%

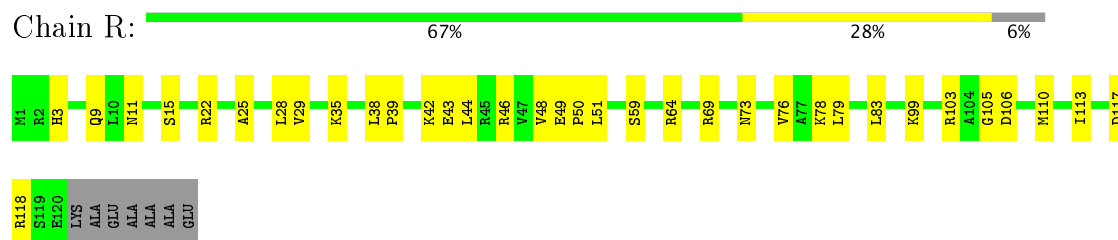


- Molecule 12: 50S ribosomal protein L16

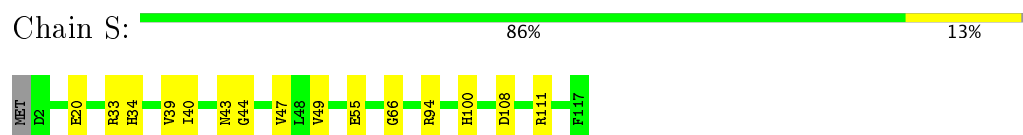
Chain Q:  81% 18%



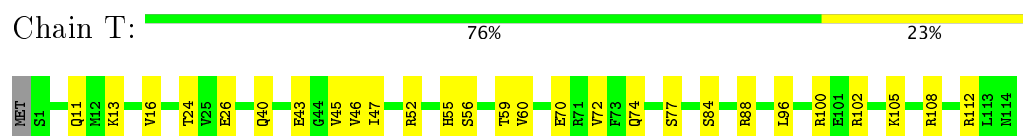
- Molecule 13: 50S ribosomal protein L17



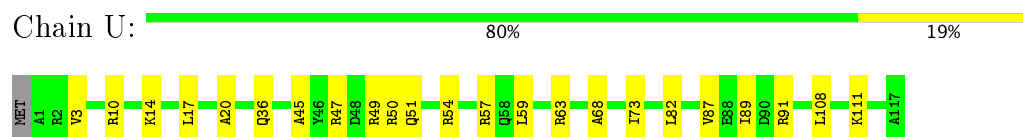
- Molecule 14: 50S ribosomal protein L18



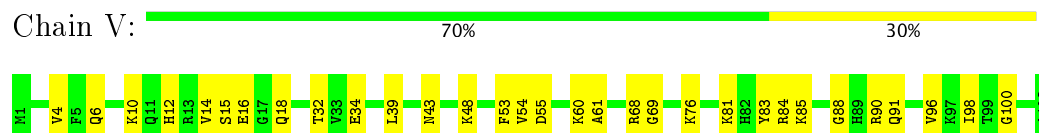
- Molecule 15: 50S ribosomal protein L19



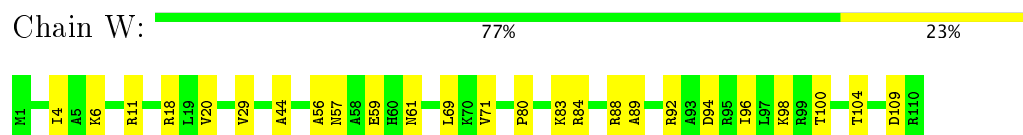
- Molecule 16: 50S ribosomal protein L20



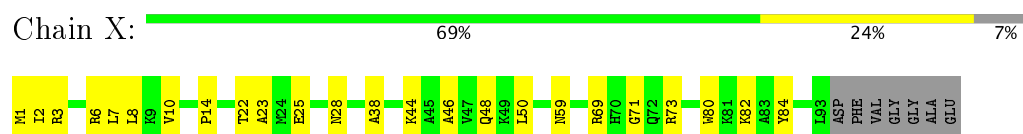
- Molecule 17: 50S ribosomal protein L21



- Molecule 18: 50S ribosomal protein L22

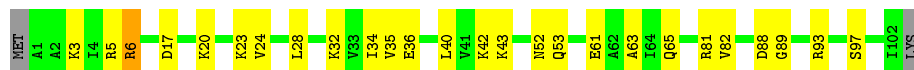


- Molecule 19: 50S ribosomal protein L23



- Molecule 20: 50S ribosomal protein L24

Chain Y:  73% 24% ..



- Molecule 21: 50S ribosomal protein L25

Chain Z:  74% 26%




- Molecule 22: 50S ribosomal protein L27

Chain 0:  65% 22% 12%




- Molecule 23: 50S ribosomal protein L28

Chain 1:  81% 18%



- Molecule 24: 50S ribosomal protein L29

Chain 2:  76% 24%



- Molecule 25: 50S ribosomal protein L30

Chain 3:  69% 29%



- Molecule 26: 50S ribosomal protein L31

Chain 4:  80% 13% 6%



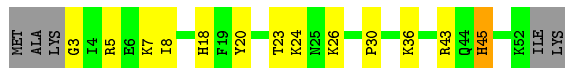
- Molecule 27: 50S ribosomal protein L32

Chain 5:  79% 19%



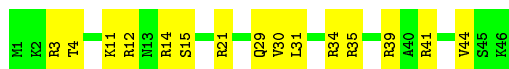
- Molecule 28: 50S ribosomal protein L33

Chain 6: 67% 22% 9%



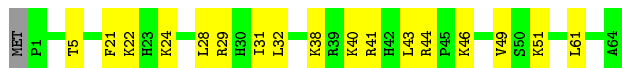
- Molecule 29: 50S ribosomal protein L34

Chain 7: 67% 33%



- Molecule 30: 50S ribosomal protein L35

Chain 8: 72% 26%



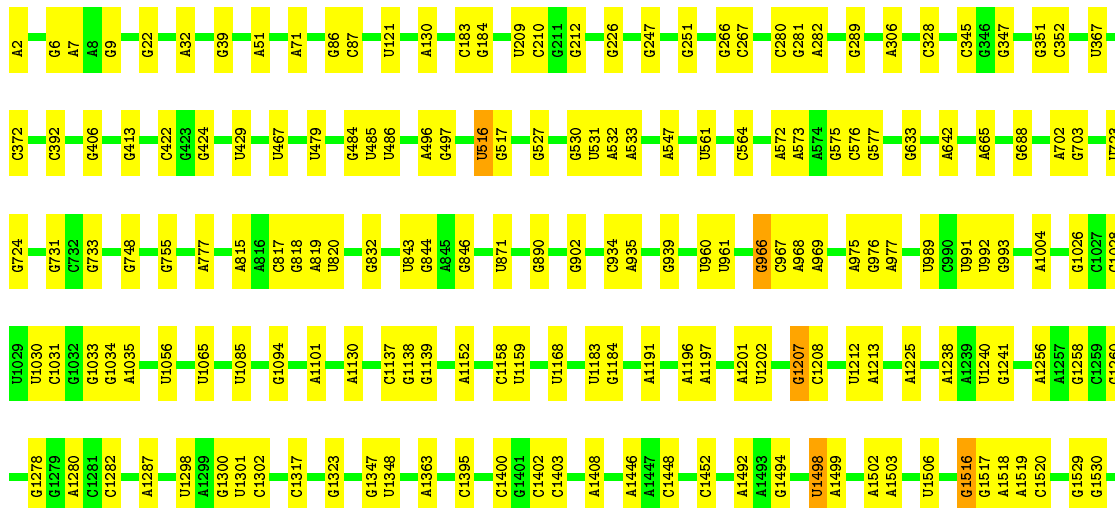
- Molecule 31: 50S ribosomal protein L36

Chain 9: 79% 21%



- Molecule 32: 16S ribosomal RNA

Chain a: 88% 11%





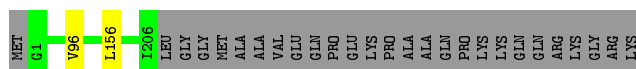
- Molecule 33: 30S ribosomal protein S2

Chain b: 89% 9%



- Molecule 34: 30S ribosomal protein S3

Chain c: 88% 12%



- Molecule 35: 30S ribosomal protein S4

Chain d: 98%



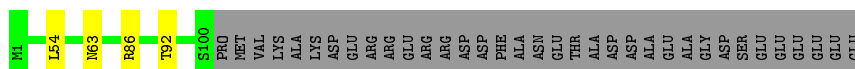
- Molecule 36: 30S ribosomal protein S5

Chain e: 90% 6%



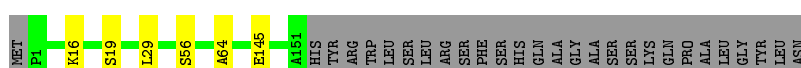
- Molecule 37: 30S ribosomal protein S6

Chain f: 71% 26%



- Molecule 38: 30S ribosomal protein S7

Chain g: 81% 16%



- Molecule 39: 30S ribosomal protein S8

Chain h: 98%




- Molecule 40: 30S ribosomal protein S9

Chain i:  94% . .



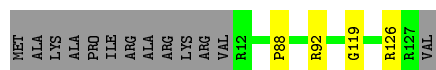
- Molecule 41: 30S ribosomal protein S10

Chain j:  89% 6% 5%



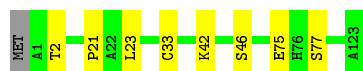
- Molecule 42: 30S ribosomal protein S11

Chain k:  87% . 10%



- Molecule 43: 30S ribosomal protein S12

Chain l:  93% 6% .



- Molecule 44: 30S ribosomal protein S13

Chain m:  95% . .



- Molecule 45: 30S ribosomal protein S15

Chain o:  93% 6% .




- Molecule 46: 30S ribosomal protein S16

Chain p:  98% .




- Molecule 47: 30S ribosomal protein S17

Chain q:  90% 5% 5%



- Molecule 48: 30S ribosomal protein S18

Chain r:  83% 13%




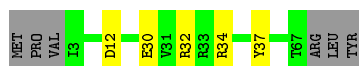
- Molecule 49: 30S ribosomal protein S20

Chain t:  98%



- Molecule 50: 30S ribosomal protein S21

Chain u:  85% 7% 8%




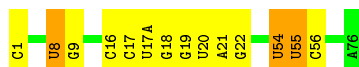
- Molecule 51: mRNA

Chain v:  100%

There are no outlier residues recorded for this chain.

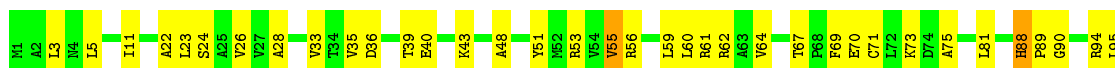
- Molecule 52: P-site tRNA

Chain x:  82% 14%



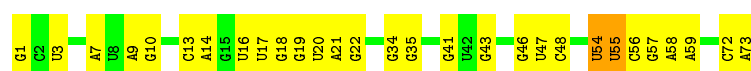
- Molecule 53: 50S ribosomal protein L10

Chain J:  50% 27% 21%



- Molecule 54: 50S ribosomal protein L11

Chain K:  75% 23%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	24749	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 3TD, OMC, OMG, OMU, MA6, H2U, YG, 2MA, 6MZ, 2MG, 5MC, UR3, 4OC, 4SU, 7MG, 5MU, 1MG, 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 > 2	RMSZ	# Z > 2
1	A	0.12	1/68920 (0.0%)	0.67	20/107498 (0.0%)
10	O	0.20	0/947	0.40	0/1268
11	P	0.20	0/1054	0.39	0/1403
12	Q	0.21	0/1093	0.41	0/1460
13	R	0.21	0/973	0.39	0/1301
14	S	0.20	0/902	0.35	0/1209
15	T	0.20	0/929	0.41	0/1242
16	U	0.21	0/960	0.35	0/1278
17	V	0.21	0/829	0.38	0/1107
18	W	0.19	0/864	0.39	0/1156
19	X	0.20	0/744	0.39	0/994
2	B	0.23	1/2876 (0.0%)	0.65	0/4483
20	Y	0.21	0/787	0.37	0/1051
21	Z	0.20	0/766	0.36	0/1025
22	0	0.20	0/582	0.35	0/769
23	1	0.19	0/635	0.36	0/848
24	2	0.21	0/510	0.36	0/677
25	3	0.21	0/453	0.41	0/605
26	4	0.21	0/531	0.40	0/709
27	5	0.19	0/450	0.36	0/599
28	6	0.21	0/416	0.41	0/554
29	7	0.20	0/380	0.36	0/498
3	D	0.20	0/2121	0.39	0/2852
30	8	0.21	0/513	0.42	0/676
31	9	0.19	0/303	0.38	0/397
32	a	0.13	1/36701 (0.0%)	0.66	5/57246 (0.0%)
33	b	0.21	0/1735	0.39	0/2338
34	c	0.21	0/1651	0.41	0/2225
35	d	0.21	0/1665	0.38	0/2227
36	e	0.22	0/1154	0.41	0/1554
37	f	0.21	0/835	0.39	0/1128

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
38	g	0.20	0/1195	0.39	0/1602
39	h	0.21	0/989	0.40	0/1326
4	E	0.21	0/1586	0.38	0/2134
40	i	0.21	0/1034	0.40	0/1375
41	j	0.21	0/796	0.42	0/1077
42	k	0.20	0/885	0.39	0/1195
43	l	0.21	0/969	0.42	0/1300
44	m	0.20	0/892	0.41	0/1193
45	o	0.20	0/722	0.35	0/964
46	p	0.20	0/659	0.35	0/884
47	q	0.22	0/657	0.43	0/881
48	r	0.20	0/511	0.40	0/689
49	t	0.20	0/671	0.34	0/888
5	F	0.20	0/1571	0.37	0/2113
50	u	0.21	0/500	0.38	0/668
51	v	0.10	0/144	0.64	0/222
52	x	0.27	1/1747 (0.1%)	0.64	0/2721
53	J	0.22	0/1001	0.43	0/1350
54	K	0.21	0/1046	0.41	0/1410
55	n	0.20	0/811	0.37	0/1081
56	s	0.20	0/652	0.37	0/877
57	z	0.16	0/1874	0.32	0/2332
58	y	0.29	1/1585 (0.1%)	0.66	0/2469
6	G	0.21	0/1434	0.40	0/1926
7	H	0.20	0/1343	0.37	0/1816
8	I	0.21	0/1122	0.38	0/1515
9	N	0.21	0/1152	0.39	0/1551
All	All	0.16	5/160827 (0.0%)	0.60	25/239936 (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	A	35	0
32	a	17	0
52	x	9	0
58	y	9	0
All	All	70	0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	U	OP3-P	-10.62	1.48	1.61
58	y	1	G	OP3-P	-10.62	1.48	1.61
52	x	1	C	OP3-P	-10.58	1.48	1.61
32	a	2	A	OP3-P	-10.57	1.48	1.61
1	A	1	G	OP3-P	-10.54	1.48	1.61

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1049	C	C2-N3-C4	18.01	128.91	119.90
1	A	1050	A	N1-C2-N3	16.54	137.57	129.30
1	A	1073	A	N1-C2-N3	16.48	137.54	129.30
1	A	1050	A	C2-N3-C4	12.07	116.63	110.60
1	A	1073	A	C2-N3-C4	11.70	116.45	110.60
1	A	1049	C	N3-C4-C5	10.61	126.14	121.90
1	A	1073	A	C6-N1-C2	10.21	124.72	118.60
1	A	1050	A	C6-N1-C2	10.07	124.64	118.60
32	a	1158	C	N1-C2-O2	8.98	124.29	118.90
32	a	1158	C	C2-N1-C1'	8.38	128.02	118.80
1	A	1313	U	C2-N1-C1'	7.96	127.25	117.70
1	A	2884	U	C2-N1-C1'	7.82	127.09	117.70
32	a	1158	C	N3-C2-O2	-7.38	116.73	121.90
1	A	2884	U	N1-C2-O2	7.29	127.90	122.80
1	A	1313	U	N1-C2-O2	7.25	127.88	122.80
1	A	2884	U	N3-C2-O2	-6.77	117.46	122.20
1	A	1313	U	N3-C2-O2	-6.54	117.62	122.20
32	a	1158	C	C6-N1-C2	-5.82	117.97	120.30
1	A	51	G	OP2-P-O3'	5.76	117.88	105.20
1	A	1049	C	N1-C2-N3	5.75	123.22	119.20
32	a	1158	C	C6-N1-C1'	-5.73	113.93	120.80
1	A	893	C	P-O3'-C3'	5.42	126.20	119.70
1	A	1313	U	C6-N1-C1'	-5.19	113.94	121.20
1	A	51	G	P-O3'-C3'	5.14	125.87	119.70
1	A	2884	U	C6-N1-C1'	-5.01	114.19	121.20

All (70) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	746	PSU	C4',C2'
1	A	955	PSU	C4',C2'
1	A	1835	2MG	C2',C3'
1	A	1911	PSU	C4',C2'
1	A	1915	3TD	C4'

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Mol	Chain	Res	Type	Atom
1	A	1917	PSU	C4',C2'
1	A	1939	5MU	C4',C2',C3'
1	A	2069	7MG	C1'
1	A	2251	OMG	C3',C1'
1	A	2445	2MG	C2',C3'
1	A	2449	H2U	C1'
1	A	2457	PSU	C4',C2'
1	A	2498	OMC	C4',C2'
1	A	2503	2MA	C2',C1'
1	A	2504	PSU	C4',C2'
1	A	2552	OMU	C4'
1	A	2580	PSU	C4',C2'
1	A	2604	PSU	C4',C2'
1	A	2605	PSU	C4',C2'
32	a	516	PSU	C4',C2'
32	a	527	7MG	C1'
32	a	966	2MG	C2',C3'
32	a	1207	2MG	C2',C3'
32	a	1402	4OC	C2',C1'
32	a	1498	UR3	C2',C3'
32	a	1516	2MG	C2',C3'
32	a	1518	MA6	C2',C3'
32	a	1519	MA6	C2',C3'
52	x	8	4SU	C4',C2',C3'
52	x	20	H2U	C1'
52	x	54	5MU	C4',C2',C3'
52	x	55	PSU	C4',C2'
58	y	16	H2U	C1'
58	y	17	H2U	C1'
58	y	20	H2U	C1'
58	y	46	7MG	C1'
58	y	54	5MU	C4',C2',C3'
58	y	55	PSU	C4',C2'

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	62057	0	31229	577	0
2	B	2572	0	1302	20	0
3	D	2082	0	2157	57	0
4	E	1565	0	1616	36	0
5	F	1552	0	1619	34	0
6	G	1410	0	1447	27	0
7	H	1323	0	1374	17	0
8	I	1111	0	1148	19	0
9	N	1129	0	1162	28	0
10	O	938	0	1012	26	0
11	P	1045	0	1117	32	0
12	Q	1074	0	1157	18	0
13	R	960	0	1000	25	0
14	S	892	0	923	10	0
15	T	917	0	965	20	0
16	U	947	0	1022	18	0
17	V	816	0	839	20	0
18	W	857	0	922	19	0
19	X	738	0	807	15	0
20	Y	779	0	834	16	0
21	Z	753	0	780	17	0
22	0	575	0	592	16	0
23	1	625	0	655	10	0
24	2	509	0	543	11	0
25	3	449	0	491	13	0
26	4	522	0	522	9	0
27	5	444	0	461	6	0
28	6	409	0	440	10	0
29	7	377	0	418	16	0
30	8	504	0	574	11	0
31	9	302	0	343	6	0
32	a	33029	0	16645	0	0
33	b	1704	0	1732	0	0
34	c	1624	0	1699	0	0
35	d	1643	0	1710	0	0
36	e	1141	0	1170	0	0
37	f	817	0	808	0	0
38	g	1181	0	1240	0	0
39	h	979	0	1034	0	0
40	i	1022	0	1070	0	0
41	j	786	0	828	0	0
42	k	869	0	878	0	0
43	l	955	0	1019	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	m	883	0	944	0	0
45	o	714	0	737	0	0
46	p	649	0	666	0	0
47	q	648	0	691	0	0
48	r	504	0	502	0	0
49	t	665	0	714	0	0
50	u	495	0	486	0	0
51	v	129	0	65	0	0
52	x	1644	0	840	0	0
53	J	988	0	1025	26	0
54	K	1032	0	1088	19	0
55	n	799	0	841	0	0
56	s	637	0	665	0	0
57	z	2255	0	592	0	0
58	y	1581	0	813	0	0
All	All	149606	0	99973	1011	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 7.

All (1011) 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)
6:G:140:ILE:HG22	6:G:142:TYR:H	1.46	0.80
21:Z:9:ARG:HD3	21:Z:39:ALA:HB1	1.65	0.77
1:A:2279:G:HO2'	1:A:2327:A:HO2'	1.31	0.77
17:V:98:ILE:HG22	17:V:100:GLY:H	1.50	0.77
7:H:94:ARG:HB2	7:H:105:SER:HB2	1.68	0.76
5:F:146:VAL:HG12	5:F:185:LYS:HB2	1.69	0.75
22:O:33:ILE:HG22	22:O:34:VAL:HG23	1.69	0.74
11:P:23:ILE:HD13	17:V:84:ARG:HH22	1.52	0.73
53:J:73:LYS:HB3	53:J:117:LEU:HD11	1.69	0.73
1:A:38:A:H4'	5:F:45:ALA:HB3	1.71	0.73
1:A:2746:U:H5''	7:H:137:LYS:HE2	1.71	0.72
1:A:910:A:H62	12:Q:12:MET:HA	1.54	0.72
10:O:121:GLU:HG2	10:O:122:VAL:HG23	1.72	0.72
28:6:36:LYS:HE2	28:6:45:HIS:HD2	1.55	0.71
1:A:1060:U:H5'	1:A:1062:G:H5'	1.72	0.70
1:A:1759:A:HO2'	1:A:2714:G:HO2'	1.37	0.70
22:O:15:LYS:HG3	22:O:37:ARG:HH22	1.56	0.70
25:3:8:GLN:HB2	25:3:28:LEU:HD13	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2417:C:H5''	30:8:44:ARG:HE	1.56	0.70
5:F:75:SER:HB3	5:F:78:TRP:HD1	1.55	0.69
1:A:1046:A:H4'	53:J:61:ARG:HB3	1.74	0.69
1:A:210:C:OP1	29:7:29:GLN:NE2	2.24	0.68
1:A:2478:A:H5'	31:9:32:LYS:HE3	1.75	0.68
2:B:30:C:H1'	2:B:57:A:H61	1.58	0.68
1:A:45:G:H5''	1:A:46:G:H5'	1.75	0.68
13:R:28:LEU:HD23	13:R:48:VAL:HG21	1.75	0.67
3:D:143:VAL:HB	3:D:153:LEU:HB2	1.77	0.67
1:A:776:G:H22	1:A:2072:C:H5'	1.59	0.67
1:A:1363:C:O2'	1:A:1809:A:N3	2.27	0.67
1:A:910:A:N3	1:A:2264:C:O2'	2.28	0.67
1:A:51:G:H4'	1:A:52:A:H5'	1.77	0.67
10:O:105:ARG:NH2	15:T:40:GLN:OE1	2.28	0.66
7:H:104:LEU:HB2	7:H:112:VAL:HB	1.77	0.66
1:A:1320:C:N4	1:A:1330:C:OP2	2.28	0.66
1:A:2394:C:H5''	11:P:63:LYS:HE3	1.76	0.66
6:G:35:LEU:HB2	6:G:88:VAL:HB	1.76	0.66
1:A:747:5MC:O2'	18:W:88:ARG:NH1	2.29	0.65
5:F:117:ARG:NH2	5:F:183:PHE:O	2.27	0.65
15:T:59:THR:HG22	15:T:72:VAL:HG12	1.77	0.65
23:1:39:VAL:HG12	23:1:42:GLU:H	1.61	0.65
1:A:560:C:O2'	16:U:47:ARG:NH2	2.29	0.65
1:A:177:G:N2	1:A:177:G:OP2	2.28	0.65
14:S:108:ASP:OD1	14:S:111:ARG:NH1	2.30	0.65
1:A:1799:G:N2	1:A:1819:A:OP2	2.25	0.65
1:A:673:C:OP1	5:F:49:ARG:NH2	2.30	0.65
54:K:11:GLN:NE2	54:K:54:ILE:O	2.30	0.65
1:A:621:A:OP2	11:P:99:ASN:ND2	2.30	0.64
1:A:2032:G:N2	4:E:151:THR:OG1	2.30	0.64
24:2:16:THR:O	24:2:20:ASN:ND2	2.29	0.64
18:W:57:ASN:OD1	18:W:61:ASN:ND2	2.30	0.64
1:A:1054:A:H61	1:A:1105:U:H3	1.42	0.64
6:G:134:GLN:NE2	6:G:149:ARG:O	2.30	0.64
9:N:80:HIS:O	9:N:82:GLY:N	2.27	0.64
9:N:32:LEU:HD22	9:N:54:ILE:HG21	1.80	0.64
21:Z:77:VAL:HG23	21:Z:89:ILE:HG12	1.77	0.64
1:A:772:C:O2	3:D:42:ARG:NH1	2.31	0.64
6:G:62:GLN:HE22	6:G:90:LEU:HB3	1.62	0.64
11:P:33:ARG:NH2	11:P:39:LYS:O	2.31	0.64
1:A:572:A:H61	1:A:2029:G:H21	1.44	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:W:88:ARG:NH2	18:W:94:ASP:OD2	2.32	0.63
1:A:1992:G:N2	1:A:1996:C:O2'	2.31	0.63
1:A:291:G:H1	1:A:349:U:H3	1.46	0.63
1:A:466:A:OP1	29:7:34:ARG:NH1	2.31	0.63
1:A:444:C:OP2	5:F:44:ARG:NH2	2.32	0.63
1:A:672:C:OP2	11:P:42:SER:OG	2.17	0.63
21:Z:25:LYS:HG2	21:Z:43:ASP:HA	1.80	0.63
53:J:33:VAL:HG12	53:J:35:VAL:H	1.62	0.63
29:7:34:ARG:NH2	29:7:41:ARG:O	2.32	0.63
4:E:15:PHE:H	15:T:11:GLN:HE22	1.46	0.63
4:E:121:THR:HG21	4:E:143:PRO:HB3	1.81	0.63
1:A:684:G:O2'	1:A:788:A:N7	2.32	0.62
1:A:514:A:N3	1:A:581:C:O2'	2.31	0.62
1:A:1798:U:H5''	3:D:257:ARG:HB2	1.82	0.62
11:P:33:ARG:HD2	11:P:40:SER:HA	1.82	0.62
17:V:76:LYS:HB2	17:V:85:LYS:HB3	1.80	0.62
1:A:499:U:H5''	20:Y:42:LYS:HE2	1.82	0.62
26:4:28:VAL:HG11	26:4:32:LEU:HD13	1.82	0.62
1:A:1394:U:H4'	1:A:1603:A:H4'	1.82	0.62
6:G:147:ARG:HG3	6:G:149:ARG:H	1.64	0.62
1:A:144:A:H4'	19:X:2:ILE:HD11	1.82	0.62
1:A:2688:G:N1	1:A:2720:U:OP2	2.31	0.62
1:A:886:A:H2'	1:A:890:C:H42	1.65	0.61
10:O:19:VAL:HG12	10:O:43:ILE:HA	1.81	0.61
10:O:21:CYS:HA	10:O:41:ILE:HG22	1.82	0.61
1:A:2893:A:H5''	1:A:2894:G:H5'	1.81	0.61
11:P:49:GLY:HA3	11:P:58:TYR:HE2	1.64	0.61
1:A:1022:G:N2	1:A:1023:U:O4	2.31	0.61
1:A:563:A:N3	16:U:36:GLN:NE2	2.45	0.61
28:6:36:LYS:HE2	28:6:45:HIS:CD2	2.36	0.61
1:A:468:G:O6	29:7:39:ARG:NH2	2.33	0.61
1:A:574:A:N6	1:A:2034:U:OP1	2.33	0.61
25:3:12:ALA:HB1	25:3:20:LYS:HG2	1.82	0.61
1:A:453:A:N3	1:A:457:A:O2'	2.33	0.61
7:H:8:VAL:HB	7:H:49:LEU:HB2	1.83	0.61
8:I:108:VAL:HG12	8:I:110:VAL:H	1.66	0.61
1:A:1858:A:N6	1:A:1884:G:O2'	2.34	0.60
1:A:828:U:O4	1:A:858:G:N2	40.70	0.60
3:D:51:ARG:HH12	3:D:246:PRO:HG2	1.65	0.60
11:P:62:PRO:HB2	30:8:29:ARG:HH11	1.66	0.60
1:A:297:G:N2	1:A:300:A:OP2	13.06	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:674:G:H5''	5:F:71:GLY:H	1.65	0.60
1:A:1899:A:H4'	1:A:1901:A:H5''	1.82	0.60
1:A:1992:G:O2'	1:A:1997:C:N4	2.34	0.60
3:D:106:PRO:HG2	3:D:109:LEU:HB2	1.83	0.60
5:F:75:SER:HB3	5:F:78:TRP:CD1	2.36	0.60
13:R:38:LEU:HG	13:R:42:LYS:HE2	1.84	0.60
4:E:131:ASP:O	4:E:136:ASN:ND2	2.34	0.60
5:F:41:GLN:NE2	5:F:43:THR:OG1	2.34	0.60
53:J:26:VAL:HG21	53:J:114:GLU:HG2	1.83	0.60
9:N:17:VAL:HG23	9:N:137:PRO:HB2	1.84	0.60
11:P:78:ARG:NH2	11:P:80:SER:OG	2.35	0.60
11:P:101:ILE:HB	11:P:105:ILE:HG13	1.83	0.59
14:S:40:ILE:HG12	14:S:47:VAL:HG12	1.83	0.59
29:7:15:SER:O	29:7:21:ARG:NH2	2.35	0.59
1:A:2743:U:O2'	7:H:152:ARG:NH1	2.35	0.59
10:O:43:ILE:HD12	10:O:56:ASP:HB2	1.84	0.59
12:Q:42:THR:HA	12:Q:93:VAL:HG12	1.84	0.59
21:Z:86:LEU:HD13	21:Z:89:ILE:HD11	1.82	0.59
1:A:2262:U:OP1	22:0:37:ARG:NH2	2.36	0.59
1:A:1801:A:N6	1:A:2201:G:O2'	2.35	0.59
1:A:1416:G:O2'	1:A:1587:G:N2	2.35	0.59
6:G:176:PHE:O	26:4:47:LYS:NZ	2.36	0.59
53:J:88:HIS:HB2	53:J:89:PRO:HD3	1.83	0.59
10:O:29:HIS:CE1	10:O:31:ARG:HH12	2.20	0.59
11:P:93:ASN:O	11:P:95:LEU:N	2.34	0.59
1:A:977:G:H5'	16:U:54:ARG:HH22	1.68	0.59
24:2:25:GLN:HE21	24:2:50:VAL:HG21	1.66	0.59
9:N:35:ARG:HB2	9:N:54:ILE:HD11	1.84	0.59
17:V:34:GLU:HG2	17:V:60:LYS:HG2	1.84	0.59
15:T:52:ARG:H	15:T:56:SER:HB3	1.68	0.58
20:Y:17:ASP:HB3	20:Y:20:LYS:HD2	1.84	0.58
19:X:3:ARG:HH12	19:X:7:LEU:HD21	1.68	0.58
1:A:743:A:O2'	1:A:1659:G:OP1	2.20	0.58
25:3:10:ARG:NH2	25:3:52:PHE:O	2.37	0.58
2:B:3:C:H3'	2:B:4:C:H5''	1.85	0.58
13:R:43:GLU:OE2	13:R:46:ARG:NH2	2.36	0.58
1:A:527:C:N4	1:A:2777:G:O2'	2.37	0.58
19:X:1:MET:HG3	19:X:3:ARG:H	1.66	0.58
1:A:1818:U:H5'	3:D:156:SER:HB2	1.85	0.58
4:E:37:VAL:HG22	4:E:48:ILE:HG22	1.86	0.58
1:A:1199:U:H1'	16:U:3:VAL:HG22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2075:U:OP2	1:A:2238:G:O2'	2.22	0.58
21:Z:64:VAL:HG22	21:Z:69:GLU:HG2	1.85	0.58
1:A:2581:G:N2	1:A:2581:G:OP2	2.36	0.57
1:A:973:A:H5'	1:A:1188:U:H1'	1.85	0.57
1:A:2748:A:H5'	7:H:3:VAL:HG21	1.86	0.57
12:Q:64:TRP:HB2	12:Q:104:GLU:HB2	1.84	0.57
27:5:27:LEU:HD23	27:5:36:LYS:HB3	1.86	0.57
1:A:192:C:O2'	1:A:802:A:N3	2.32	0.57
7:H:32:LEU:HD21	7:H:136:ASP:HB2	1.85	0.57
1:A:2451:A:N6	1:A:2504:PSU:O2	2.38	0.57
1:A:771:G:OP2	29:7:11:LYS:NZ	2.38	0.57
11:P:29:LYS:HG2	11:P:30:THR:HG23	1.85	0.57
1:A:1406:U:O2	1:A:1517:G:N2	33.55	0.57
1:A:955:PSU:HN3	1:A:962:G:H1	1.53	0.57
6:G:104:THR:HA	26:4:38:SER:HB3	1.86	0.57
1:A:880:G:H1	1:A:897:C:H42	1.52	0.57
53:J:53:ARG:HB3	53:J:55:VAL:HG13	1.86	0.57
25:3:10:ARG:HD2	25:3:53:MET:HA	1.85	0.57
1:A:1062:G:N2	54:K:134:SER:OG	2.38	0.57
1:A:1343:G:O6	1:A:1403:A:N6	2.37	0.57
1:A:2291:U:OP1	1:A:2380:C:O2'	2.23	0.57
1:A:2420:C:H5''	28:6:7:LYS:HD2	1.87	0.57
1:A:643:A:N1	1:A:2369:A:O2'	2.38	0.57
1:A:63:A:N6	1:A:91:A:N1	2.47	0.57
54:K:61:TYR:HE2	54:K:67:THR:HG22	1.69	0.57
21:Z:76:ASP:HB3	21:Z:90:ASP:HB2	1.86	0.57
23:1:36:ARG:HA	23:1:47:THR:HA	1.86	0.57
1:A:1250:G:OP2	11:P:21:ARG:NH2	2.37	0.57
11:P:73:ILE:HD12	11:P:106:GLU:HB2	1.87	0.57
20:Y:28:LEU:HD12	20:Y:32:LYS:HB2	1.85	0.57
1:A:698:C:O2'	1:A:734:A:N6	2.37	0.56
5:F:48:THR:OG1	5:F:51:GLU:OE1	2.16	0.56
1:A:1218:G:OP2	16:U:14:LYS:NZ	2.36	0.56
18:W:6:LYS:HA	18:W:104:THR:HA	1.86	0.56
1:A:2331:G:H4'	22:0:39:THR:H	1.69	0.56
1:A:1323:C:OP1	18:W:98:LYS:NZ	2.38	0.56
5:F:45:ALA:HB2	5:F:89:PRO:HD3	1.87	0.56
22:0:15:LYS:HG3	22:0:37:ARG:NH2	2.20	0.56
6:G:59:ILE:O	6:G:101:ARG:NH1	2.38	0.56
53:J:3:LEU:HD12	53:J:5:LEU:H	1.69	0.56
1:A:952:G:OP1	12:Q:18:ARG:NH2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:R:78:LYS:HE2	13:R:83:LEU:HD21	1.86	0.56
1:A:1796:U:H2'	1:A:1797:G:H8	1.71	0.56
1:A:747:5MC:H3'	1:A:748:G:H5'	1.88	0.56
5:F:40:ARG:HG2	5:F:42:GLY:H	1.69	0.56
9:N:64:VAL:HB	9:N:68:LYS:HE3	1.86	0.56
18:W:20:VAL:HG11	18:W:44:ALA:HA	1.87	0.56
1:A:198:C:H1'	1:A:2434:A:H61	1.71	0.56
1:A:962:G:HO2'	1:A:2496:C:HO2'	1.51	0.56
18:W:80:PRO:O	18:W:100:THR:OG1	2.20	0.56
1:A:1187:G:N2	1:A:1188:U:O4	2.39	0.56
1:A:2576:G:O2'	1:A:2579:C:OP2	2.24	0.56
10:O:112:PHE:HD1	10:O:115:ILE:HD12	1.71	0.56
1:A:1528:A:N6	1:A:1543:G:O2'	2.40	0.55
1:A:824:U:O2'	1:A:2358:A:N6	2.37	0.55
1:A:597:G:O2'	11:P:11:GLY:O	2.22	0.55
1:A:911:A:N6	12:Q:11:LYS:O	2.29	0.55
1:A:684:G:OP1	29:7:21:ARG:NH1	2.39	0.55
1:A:2297:A:N7	1:A:2318:G:N2	2.54	0.55
1:A:2618:G:H21	4:E:155:VAL:HG21	1.71	0.55
1:A:1073:A:C6	1:A:1073:A:C4	2.95	0.55
1:A:1323:C:N4	1:A:1324:G:O6	2.39	0.55
2:B:54:G:N2	6:G:25:MET:SD	2.78	0.55
18:W:4:ILE:HD12	18:W:6:LYS:HE3	1.87	0.55
1:A:2061:G:H5''	1:A:2503:2MA:HM22	1.88	0.55
17:V:61:ALA:HB1	17:V:96:VAL:HB	1.89	0.55
1:A:1296:G:OP1	1:A:2709:G:O2'	2.21	0.55
1:A:463:G:N2	1:A:466:A:OP2	2.30	0.55
1:A:2831:G:OP2	4:E:59:ARG:NH1	2.40	0.55
54:K:44:LYS:HE2	54:K:70:THR:HG21	1.89	0.55
1:A:1355:G:H2'	1:A:1356:G:H8	1.72	0.55
1:A:1818:U:C5	3:D:155:ARG:HD3	2.41	0.55
5:F:76:PRO:HA	5:F:82:GLY:HA3	1.87	0.55
1:A:1613:G:H4'	29:7:3:ARG:HE	1.72	0.55
1:A:1154:G:OP2	16:U:57:ARG:NH1	2.34	0.55
1:A:1998:A:OP2	4:E:141:ARG:NH1	2.35	0.55
1:A:2709:G:H5'	13:R:22:ARG:HH22	1.71	0.55
7:H:6:ALA:O	7:H:68:ARG:NE	2.38	0.55
1:A:1050:A:C6	1:A:1050:A:C4	2.95	0.55
1:A:578:G:OP1	1:A:1255:U:O2'	2.21	0.54
1:A:793:A:OP2	1:A:2071:A:O2'	2.20	0.54
53:J:48:ALA:HB3	53:J:51:TYR:HE2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:N:95:ARG:HG2	9:N:96:ARG:HG2	1.88	0.54
22:O:21:ARG:HB2	22:O:33:ILE:HG23	1.89	0.54
19:X:14:PRO:HD3	24:2:30:MET:HG3	1.89	0.54
11:P:127:VAL:HG21	11:P:142:ILE:HG21	1.88	0.54
30:8:32:LEU:HB3	30:8:40:LYS:HD3	1.89	0.54
1:A:1826:G:O2'	1:A:1971:U:OP2	2.20	0.54
14:S:20:GLU:OE2	22:O:58:LYS:NZ	2.41	0.54
16:U:87:VAL:HG12	16:U:89:ILE:H	1.71	0.54
5:F:91:ASP:OD2	5:F:93:SER:OG	2.25	0.54
6:G:1:ALA:N	6:G:100:GLU:OE1	2.39	0.54
17:V:16:GLU:HG3	17:V:100:GLY:HA2	1.89	0.54
1:A:111:A:O2'	24:2:58:ASN:ND2	2.41	0.54
1:A:2069:7MG:H2'	1:A:2070:A:H8	1.73	0.54
1:A:806:C:O2	1:A:2444:G:O2'	2.25	0.54
29:7:12:ARG:HE	29:7:44:VAL:HG21	1.72	0.54
1:A:2857:G:N2	1:A:2860:A:OP2	2.33	0.54
12:Q:34:LYS:HE3	12:Q:131:VAL:HG11	1.90	0.54
30:8:22:LYS:HB2	30:8:46:LYS:HB3	1.89	0.53
1:A:2788:C:O2'	1:A:2809:A:N3	2.38	0.53
1:A:1020:A:H4'	1:A:1021:A:O5'	2.07	0.53
1:A:1824:G:H5''	3:D:51:ARG:HH21	1.72	0.53
1:A:2249:U:N3	1:A:2253:G:OP2	2.39	0.53
1:A:2059:A:N6	1:A:2503:2MA:H1'	2.23	0.53
1:A:321:U:H5''	5:F:131:THR:HG23	1.89	0.53
3:D:69:ASN:HA	3:D:188:ARG:HH12	1.73	0.53
8:I:28:ASN:OD1	23:1:35:HIS:NE2	2.37	0.53
23:1:16:ASN:N	23:1:24:THR:O	2.38	0.53
1:A:2744:G:N2	7:H:142:GLN:OE1	2.34	0.53
18:W:56:ALA:HA	18:W:59:GLU:HG2	1.91	0.53
1:A:1266:G:N2	1:A:1269:A:OP2	13.06	0.53
2:B:95:U:H2'	2:B:96:G:H8	1.74	0.53
1:A:682:G:O6	1:A:794:A:N6	2.42	0.53
1:A:2676:C:OP1	10:O:31:ARG:NH2	2.42	0.53
13:R:76:VAL:HA	13:R:79:LEU:HD12	1.90	0.53
1:A:1182:G:H5'	1:A:1183:U:OP1	5.97	0.52
1:A:575:A:OP2	1:A:2499:C:O2'	2.27	0.52
4:E:46:ARG:NH2	4:E:89:GLU:OE1	2.42	0.52
53:J:94:ARG:HD3	53:J:131:THR:HG22	1.90	0.52
13:R:103:ARG:HG2	13:R:105:GLY:H	1.72	0.52
3:D:184:GLU:HG3	3:D:186:ASP:H	1.74	0.52
1:A:1864:U:OP1	1:A:2410:G:O2'	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:693:A:O2'	1:A:1353:A:N3	2.42	0.52
27:5:39:ARG:O	27:5:41:HIS:ND1	2.35	0.52
1:A:320:A:N3	5:F:163:ASN:ND2	2.57	0.52
1:A:1272:A:O2'	1:A:1274:A:OP1	2.23	0.52
15:T:105:LYS:HB3	15:T:108:ARG:HH22	1.73	0.52
1:A:1905:C:N4	1:A:1969:A:OP2	2.42	0.52
1:A:2267:A:H5''	1:A:2268:A:H5'	1.91	0.52
1:A:2278:A:OP1	12:Q:11:LYS:NZ	2.34	0.52
1:A:538:A:H4'	9:N:7:LYS:HG2	1.90	0.52
1:A:781:A:OP1	3:D:216:ARG:NH2	2.36	0.52
3:D:130:PRO:HA	3:D:188:ARG:HA	1.91	0.52
54:K:91:LYS:HG3	54:K:94:LYS:HE2	1.92	0.52
17:V:68:ARG:HH11	17:V:90:ARG:HB2	1.74	0.52
1:A:1792:G:O2'	1:A:1830:C:OP1	2.27	0.52
1:A:28:A:O2'	1:A:296:U:OP1	48.98	0.52
1:A:767:U:H2'	1:A:768:G:H8	1.75	0.52
9:N:17:VAL:HG22	9:N:55:ILE:HB	1.90	0.52
10:O:8:LEU:HB2	10:O:19:VAL:HG23	1.91	0.52
1:A:328:U:H4'	20:Y:65:GLN:HG3	1.91	0.52
1:A:244:A:H5''	11:P:67:THR:HG21	1.91	0.52
1:A:619:G:H3'	1:A:620:G:H21	1.75	0.52
1:A:2002:G:H5''	13:R:9:GLN:HE21	1.75	0.52
1:A:2258:C:O2'	1:A:2427:C:OP2	2.24	0.52
54:K:107:GLU:O	54:K:110:GLN:NE2	2.43	0.52
1:A:1693:U:O2'	3:D:13:ARG:NH1	2.43	0.51
1:A:2092:U:OP2	8:I:28:ASN:ND2	2.41	0.51
1:A:2440:C:H5''	1:A:2587:A:H4'	1.91	0.51
1:A:568:U:H1'	1:A:2030:6MZ:H9C1	1.92	0.51
26:4:26:SER:OG	26:4:27:THR:N	2.43	0.51
1:A:690:G:H1	1:A:772:C:H42	1.57	0.51
1:A:830:G:H22	1:A:2446:G:H5'	1.76	0.51
1:A:2039:U:H2'	1:A:2040:G:C8	2.45	0.51
3:D:2:VAL:HG22	3:D:18:VAL:HG13	1.92	0.51
20:Y:40:LEU:HD23	20:Y:61:GLU:HG3	1.92	0.51
1:A:676:A:H62	1:A:802:A:H61	1.58	0.51
4:E:24:VAL:HG12	4:E:178:VAL:HG21	1.91	0.51
1:A:518:G:OP2	27:5:12:ARG:NH2	2.40	0.51
1:A:2006:C:O2'	1:A:2823:A:N3	2.44	0.51
1:A:1571:A:H2'	1:A:1572:A:C8	2.46	0.51
27:5:30:ASP:HB3	27:5:34:GLY:H	1.75	0.51
1:A:968:C:H2'	1:A:969:G:C8	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:O:64:ARG:HB2	10:O:83:ALA:HB3	1.93	0.51
7:H:88:LEU:HD23	7:H:93:TYR:HB3	1.93	0.51
12:Q:4:PRO:HG2	12:Q:92:TRP:CZ3	2.46	0.51
1:A:2283:C:OP1	28:6:3:GLY:N	2.44	0.51
1:A:1450:G:H21	1:A:1452:G:H1	1.57	0.51
1:A:2039:U:H2'	1:A:2040:G:H8	1.75	0.51
22:O:42:HIS:CD2	22:O:73:ARG:HD3	2.46	0.50
1:A:1158:C:O2	1:A:1158:C:H2'	2.94	0.50
1:A:2144:G:O2'	1:A:2147:A:N1	2.43	0.50
1:A:2645:G:N2	1:A:2645:G:OP2	2.32	0.50
1:A:2794:C:H42	1:A:2802:G:H1	1.59	0.50
6:G:92:GLY:O	6:G:95:MET:HG2	2.11	0.50
8:I:80:ILE:HG22	8:I:82:SER:H	1.75	0.50
1:A:1187:G:H5''	17:V:83:TYR:CZ	2.46	0.50
1:A:2370:G:H4'	28:6:43:ARG:HH11	1.76	0.50
1:A:714:U:N3	1:A:717:C:OP2	2.40	0.50
1:A:918:A:N3	2:B:80:U:O2'	2.39	0.50
3:D:243:PRO:O	3:D:250:GLN:NE2	2.44	0.50
3:D:77:VAL:HG22	3:D:93:VAL:HG22	1.92	0.50
4:E:130:GLN:OE1	4:E:139:SER:OG	2.24	0.50
15:T:26:GLU:HA	15:T:43:GLU:HA	1.92	0.50
1:A:1261:C:OP2	18:W:83:LYS:NZ	2.34	0.50
15:T:47:ILE:HA	15:T:96:LEU:HD12	1.94	0.50
1:A:1287:A:OP2	13:R:103:ARG:NH1	2.38	0.50
1:A:2595:G:N2	1:A:2598:A:OP2	2.35	0.50
1:A:863:A:OP1	12:Q:22:GLN:NE2	2.44	0.50
1:A:1656:C:P	4:E:141:ARG:HE	2.35	0.50
8:I:30:LEU:HB3	8:I:36:ALA:HB3	1.92	0.50
1:A:1153:C:OP1	16:U:91:ARG:NH2	2.44	0.50
22:O:17:LEU:O	22:O:20:LYS:NZ	2.45	0.50
1:A:1863:G:H4'	1:A:2411:A:H4'	1.94	0.50
1:A:2787:C:H1'	4:E:63:PRO:HG3	1.93	0.50
1:A:790:U:H3	1:A:795:C:H5'	1.76	0.50
4:E:10:GLY:H	4:E:197:THR:HG23	1.77	0.50
1:A:1940:U:H4'	1:A:1941:C:O5'	2.11	0.50
1:A:2598:A:H5''	3:D:233:GLY:HA3	1.94	0.50
1:A:1162:G:H2'	1:A:1163:G:H8	1.77	0.50
1:A:322:A:H5'	1:A:340:A:H1'	1.93	0.50
18:W:29:VAL:HG22	18:W:71:VAL:HG23	1.94	0.50
29:7:39:ARG:HG2	29:7:41:ARG:H	1.76	0.50
1:A:1255:U:O4'	1:A:2502:G:N2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:780:G:O2'	1:A:783:A:N6	2.44	0.50
4:E:48:ILE:HG23	4:E:84:LEU:HD21	1.94	0.50
29:7:30:VAL:O	29:7:34:ARG:HG2	2.11	0.50
1:A:1378:A:OP1	29:7:14:ARG:NH1	2.44	0.50
1:A:299:A:N3	1:A:319:G:O2'	2.38	0.50
1:A:518:G:OP1	18:W:18:ARG:NH1	2.30	0.50
1:A:1283:G:N1	1:A:1286:A:OP2	2.44	0.49
8:I:9:VAL:HB	8:I:13:GLY:HA3	1.94	0.49
1:A:958:U:H5	12:Q:40:ARG:HH21	1.59	0.49
1:A:2680:U:O2'	4:E:11:MET:SD	2.70	0.49
1:A:372:G:O2'	1:A:373:U:O5'	2.28	0.49
6:G:97:GLU:OE2	26:4:25:ARG:N	2.43	0.49
1:A:190:A:H5''	1:A:204:A:H61	1.76	0.49
3:D:106:PRO:HD2	3:D:109:LEU:HD22	1.93	0.49
8:I:115:VAL:HG21	53:J:62:ARG:HB2	190.85	0.49
1:A:495:G:O2'	18:W:61:ASN:ND2	2.45	0.49
1:A:674:G:H5''	5:F:71:GLY:N	2.26	0.49
1:A:746:PSU:H1'	1:A:748:G:H21	1.77	0.49
1:A:747:5MC:H3'	1:A:748:G:C5'	2.43	0.49
3:D:204:LEU:HD21	3:D:213:ARG:HH21	1.77	0.49
3:D:206:LYS:HD3	3:D:212:TRP:HH2	1.76	0.49
53:J:23:LEU:HD21	53:J:96:PHE:HB2	1.94	0.49
1:A:1937:A:H62	1:A:1940:U:H5	1.59	0.49
1:A:471:A:OP1	5:F:79:ARG:NH1	2.42	0.49
6:G:56:LEU:HB2	6:G:64:PRO:HG3	1.94	0.49
10:O:12:ASP:HB3	10:O:99:ILE:HG12	1.94	0.49
1:A:1026:G:H2'	1:A:1027:A:H8	1.77	0.49
1:A:942:G:OP2	11:P:39:LYS:NZ	2.46	0.49
1:A:1798:U:OP2	3:D:270:ARG:NH2	2.40	0.49
1:A:783:A:H2'	1:A:784:G:H4'	1.95	0.49
1:A:774:G:N2	1:A:787:C:O2'	2.46	0.49
9:N:77:HIS:HD1	9:N:79:GLY:H	1.60	0.49
11:P:79:LEU:H	11:P:113:ALA:HB3	1.78	0.49
15:T:74:GLN:HB2	15:T:77:SER:HB2	1.94	0.49
15:T:88:ARG:HH11	15:T:112:ARG:NH1	2.11	0.49
1:A:1048:A:OP2	1:A:1110:G:N2	2.45	0.49
1:A:676:A:HO2'	1:A:2442:C:HO2'	1.56	0.49
1:A:993:G:OP2	16:U:50:ARG:NH2	2.33	0.49
4:E:133:THR:OG1	4:E:134:HIS:N	2.45	0.49
54:K:33:ASN:OD1	54:K:34:ILE:N	2.46	0.49
10:O:2:ILE:HD12	10:O:8:LEU:HD21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:663:G:H5''	11:P:17:LYS:HD3	1.94	0.49
29:7:34:ARG:HH21	29:7:39:ARG:HD2	1.78	0.49
1:A:1509:A:H2'	1:A:1510:G:C8	2.48	0.49
1:A:2069:7MG:H2'	1:A:2070:A:C8	2.48	0.49
1:A:2540:C:O2'	1:A:2740:A:N3	2.45	0.49
16:U:47:ARG:NH2	16:U:51:GLN:OE1	2.46	0.49
1:A:1225:G:H5'	17:V:88:GLY:H	1.77	0.49
1:A:1787:A:OP1	3:D:237:ARG:NH2	2.46	0.48
1:A:1915:3TD:H3'	1:A:1916:A:H8	1.76	0.48
1:A:2081:U:H5''	23:1:16:ASN:HD22	1.78	0.48
53:J:67:THR:HG21	53:J:75:ALA:HB2	1.95	0.48
11:P:95:LEU:HB3	11:P:100:ILE:HD11	1.94	0.48
1:A:1528:A:OP2	1:A:1543:G:N2	2.47	0.48
9:N:24:THR:HB	9:N:27:ARG:HB2	1.95	0.48
19:X:23:ALA:O	19:X:28:ASN:N	2.46	0.48
22:0:55:LEU:HD12	22:0:76:ILE:HD12	1.95	0.48
28:6:3:GLY:O	28:6:5:ARG:N	2.43	0.48
1:A:1447:C:O2'	1:A:1544:A:N3	2.43	0.48
1:A:1818:U:H4'	1:A:1821:A:H1'	1.94	0.48
1:A:2086:U:H2'	1:A:2087:G:C8	2.48	0.48
1:A:2508:G:H1	1:A:2580:PSU:HN3	1.61	0.48
28:6:8:ILE:HD13	28:6:24:LYS:HE3	1.96	0.48
1:A:942:G:O2'	1:A:1189:A:N3	2.44	0.48
22:0:19:VAL:HG13	22:0:34:VAL:HG22	1.95	0.48
1:A:1364:G:N2	1:A:1367:A:OP2	2.42	0.48
1:A:2391:G:O2'	1:A:2392:A:O5'	2.23	0.48
1:A:2771:C:O2'	4:E:173:GLN:NE2	2.45	0.48
1:A:648:G:H2'	1:A:649:G:H8	1.78	0.48
3:D:141:HIS:ND1	3:D:192:GLY:O	2.46	0.48
1:A:2305:U:H5''	6:G:130:GLY:HA3	1.96	0.48
10:O:30:ARG:NH2	10:O:37:ASP:OD2	2.29	0.48
1:A:742:A:H2'	1:A:743:A:C8	2.49	0.48
1:A:953:G:H2'	1:A:954:G:C8	2.49	0.48
2:B:1:U:H2'	2:B:2:G:C8	2.49	0.48
1:A:973:A:H5''	17:V:81:LYS:HD2	1.96	0.48
9:N:56:VAL:HB	9:N:124:VAL:HA	1.96	0.48
10:O:9:ASN:OD1	10:O:18:ARG:NH1	2.47	0.48
1:A:1068:G:N2	1:A:1095:A:O2'	2.46	0.48
1:A:1321:A:O2'	18:W:11:ARG:NH2	2.36	0.48
5:F:18:THR:HG23	5:F:106:LYS:HG2	1.96	0.48
9:N:37:ARG:HH22	9:N:110:PRO:HG3	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:S:33:ARG:HG2	14:S:34:HIS:CD2	2.49	0.48
2:B:116:G:H5'	14:S:55:GLU:HG2	1.96	0.48
1:A:1364:G:H5'	1:A:1809:A:H1'	1.96	0.48
53:J:59:LEU:HB3	53:J:62:ARG:HB3	1.96	0.48
9:N:55:ILE:HD11	9:N:132:HIS:HB2	1.95	0.48
17:V:69:GLY:N	17:V:91:GLN:O	2.39	0.48
1:A:1514:G:O2'	1:A:1557:C:O2'	2.32	0.47
1:A:2271:G:H5'	22:O:16:ARG:HD3	1.95	0.47
2:B:88:C:O2'	2:B:89:U:O5'	2.23	0.47
7:H:97:VAL:HG22	7:H:102:ILE:HG23	1.95	0.47
54:K:108:ILE:O	54:K:111:THR:OG1	2.26	0.47
1:A:1137:G:H2'	1:A:1138:G:H8	1.79	0.47
1:A:1201:U:H2'	1:A:1202:G:H8	1.78	0.47
1:A:2313:C:H2'	1:A:2314:A:C8	2.49	0.47
5:F:18:THR:HA	5:F:106:LYS:HE3	1.95	0.47
1:A:2548:U:O2'	10:O:4:GLU:OE2	2.31	0.47
17:V:14:VAL:HG21	17:V:98:ILE:HG13	1.95	0.47
19:X:59:ASN:OD1	19:X:84:TYR:HB2	2.14	0.47
25:3:16:LEU:HB2	25:3:19:HIS:HD2	1.79	0.47
1:A:1000:A:OP2	1:A:1154:G:N1	2.36	0.47
1:A:830:G:N3	1:A:2448:A:N6	2.63	0.47
1:A:290:U:H2'	1:A:291:G:C8	2.50	0.47
1:A:326:G:H2'	1:A:327:G:H8	1.80	0.47
1:A:395:U:H2'	1:A:396:G:C8	2.49	0.47
1:A:546:U:H2'	1:A:547:A:H4'	1.95	0.47
3:D:56:GLY:HA2	3:D:212:TRP:HA	1.95	0.47
2:B:91:C:OP1	12:Q:38:ARG:NH2	2.47	0.47
1:A:1032:A:H1'	31:9:23:ILE:HD13	1.95	0.47
1:A:2069:7MG:O6	1:A:2443:C:N4	2.48	0.47
1:A:2316:G:H4'	6:G:124:ARG:HH21	1.79	0.47
6:G:129:MET:HG2	6:G:153:ILE:HB	1.96	0.47
53:J:36:ASP:O	53:J:39:THR:OG1	2.23	0.47
1:A:95:A:O2'	24:2:41:HIS:ND1	2.42	0.47
26:4:11:GLU:HA	26:4:25:ARG:HA	1.97	0.47
1:A:1800:C:N4	1:A:1818:U:O2'	2.48	0.47
1:A:2439:A:H61	1:A:2585:U:H4'	1.80	0.47
1:A:500:G:N1	1:A:503:A:OP2	2.47	0.47
9:N:36:LEU:HD22	9:N:121:LYS:HB2	1.95	0.47
1:A:1158:C:H5''	25:3:30:ARG:HD2	1.97	0.47
1:A:2144:G:H1'	1:A:2147:A:H61	1.79	0.47
53:J:103:ASN:HA	53:J:107:GLU:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:J:24:SER:HB2	53:J:116:GLU:HG3	1.96	0.47
15:T:70:GLU:OE2	15:T:100:ARG:NH1	2.47	0.47
17:V:14:VAL:HG22	17:V:15:SER:O	2.14	0.47
1:A:851:C:O2'	25:3:42:ALA:O	2.33	0.47
25:3:53:MET:HG3	25:3:54:VAL:HG13	1.97	0.47
27:5:42:ILE:HG22	27:5:48:TYR:HB2	1.95	0.47
1:A:1019:U:H3	1:A:1142:A:H62	1.63	0.47
1:A:749:A:H5'	1:A:1271:G:H1'	1.97	0.47
3:D:28:PRO:HB2	3:D:33:LEU:HD11	1.96	0.47
53:J:121:SER:OG	53:J:122:GLN:N	2.45	0.47
1:A:2899:A:H4'	9:N:136:GLN:HE22	1.80	0.47
12:Q:14:LYS:O	12:Q:71:LYS:NZ	2.42	0.47
16:U:68:ALA:HB1	16:U:73:ILE:HG23	1.96	0.47
1:A:669:G:N2	1:A:672:C:OP1	2.40	0.47
1:A:676:A:O2'	1:A:2442:C:O2'	2.28	0.47
1:A:1307:A:N6	1:A:1606:C:O2'	2.48	0.47
1:A:1935:G:N2	1:A:1964:G:O4'	2.47	0.47
1:A:2372:U:H2'	1:A:2373:G:H8	1.80	0.47
1:A:581:C:H2'	1:A:582:A:C8	2.50	0.47
1:A:586:A:N1	1:A:809:G:O2'	2.42	0.47
25:3:16:LEU:HB2	25:3:19:HIS:CD2	2.50	0.47
1:A:2339:C:H2'	1:A:2340:A:C8	2.50	0.47
1:A:2830:C:O2'	1:A:2883:A:N1	2.44	0.47
4:E:16:THR:OG1	4:E:18:ASP:OD1	2.33	0.47
11:P:56:PRO:HD2	11:P:59:ARG:HD3	1.96	0.47
1:A:468:G:H5''	5:F:55:SER:HB3	1.97	0.47
1:A:1754:A:N1	1:A:2716:C:O2'	2.46	0.46
1:A:2399:G:H2'	1:A:2400:G:H8	1.80	0.46
1:A:968:C:H2'	1:A:969:G:H8	1.80	0.46
10:O:40:LYS:HE3	10:O:57:VAL:HG12	1.97	0.46
13:R:35:LYS:NZ	13:R:110:MET:SD	2.78	0.46
1:A:1849:G:H2'	1:A:1850:G:H8	1.80	0.46
53:J:39:THR:OG1	53:J:40:GLU:OE1	2.34	0.46
1:A:1022:G:H4'	1:A:1023:U:O5'	2.16	0.46
1:A:2326:C:O2'	1:A:2327:A:OP1	2.30	0.46
1:A:993:G:O6	1:A:1045:C:N4	82.65	0.46
10:O:34:GLY:O	10:O:36:GLY:N	2.48	0.46
16:U:17:LEU:HA	16:U:20:ALA:HB3	1.98	0.46
20:Y:52:ASN:OD1	20:Y:53:GLN:N	2.48	0.46
12:Q:34:LYS:HD3	21:Z:82:TYR:HA	1.97	0.46
13:R:78:LYS:HG2	13:R:83:LEU:HG	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Y:5:ARG:HG2	20:Y:93:ARG:HH22	1.81	0.46
1:A:1037:G:N2	1:A:1118:C:O2	2.39	0.46
3:D:65:ASP:HB2	3:D:101:ARG:HB3	1.97	0.46
7:H:21:GLN:NE2	7:H:37:ASN:O	2.48	0.46
7:H:37:ASN:OD1	7:H:38:ASP:N	2.48	0.46
10:O:1:MET:HG3	10:O:32:TYR:CG	2.50	0.46
25:3:46:MET:O	25:3:50:VAL:HG22	2.16	0.46
1:A:1165:A:H2'	1:A:1166:G:H8	1.79	0.46
1:A:2120:G:H2'	1:A:2121:G:C8	2.50	0.46
1:A:2189:U:H2'	1:A:2190:G:C8	2.51	0.46
1:A:1915:3TD:H3'	1:A:1916:A:C8	2.51	0.46
1:A:266:G:O6	1:A:270:A:N6	13.02	0.46
54:K:4:VAL:HA	54:K:7:TYR:HE2	1.80	0.46
28:6:26:LYS:NZ	28:6:30:PRO:O	2.49	0.46
1:A:1415:U:H2'	1:A:1416:G:H4'	1.98	0.46
1:A:225:C:H2'	1:A:226:A:O4'	2.16	0.46
9:N:15:TRP:HB3	9:N:137:PRO:HB3	1.98	0.46
1:A:1258:U:H2'	1:A:1259:G:C8	2.51	0.46
1:A:2087:G:H2'	1:A:2088:A:C8	2.51	0.46
1:A:2623:G:H2'	1:A:2624:G:C8	2.51	0.46
1:A:953:G:H2'	1:A:954:G:H8	1.80	0.46
2:B:76:G:OP1	21:Z:9:ARG:NH2	2.46	0.46
5:F:131:THR:HG22	5:F:160:ALA:HA	1.97	0.46
15:T:47:ILE:HB	15:T:96:LEU:HB2	1.98	0.46
1:A:1992:G:HO2'	1:A:1997:C:H42	1.64	0.46
6:G:137:PHE:HA	6:G:138:PRO:HD3	1.85	0.46
1:A:2816:G:H5''	13:R:99:LYS:HE2	1.97	0.46
20:Y:34:ILE:HG12	20:Y:63:ALA:HA	1.98	0.46
21:Z:32:GLY:O	21:Z:93:ARG:NH1	2.49	0.46
1:A:1837:C:O2'	1:A:1927:A:N3	2.42	0.45
1:A:2830:C:H3'	4:E:59:ARG:HH11	1.81	0.45
1:A:538:A:H5''	9:N:7:LYS:HE3	1.97	0.45
6:G:1:ALA:N	6:G:97:GLU:OE1	2.46	0.45
54:K:74:PRO:HG2	54:K:77:VAL:HG22	1.97	0.45
1:A:1566:A:O2'	1:A:1568:G:N2	2.49	0.45
1:A:2681:C:OP2	4:E:114:LYS:NZ	2.49	0.45
1:A:534:U:H2'	1:A:535:G:H8	1.81	0.45
8:I:124:THR:O	8:I:128:HIS:NE2	2.45	0.45
9:N:51:GLY:O	9:N:121:LYS:NZ	2.40	0.45
17:V:32:THR:OG1	17:V:61:ALA:O	2.27	0.45
1:A:1213:A:N6	1:A:1236:G:H1'	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:A:O2'	1:A:15:G:N7	2.48	0.45
1:A:106:C:H2'	1:A:107:G:C8	2.66	0.45
1:A:2033:A:O2'	1:A:2035:G:OP1	2.34	0.45
1:A:1129:A:O2'	1:A:2515:C:O2	2.32	0.45
4:E:51:THR:HB	4:E:79:LEU:HD23	1.98	0.45
19:X:80:TRP:HZ3	19:X:82:LYS:HB3	1.80	0.45
1:A:789:A:H5'	29:7:4:THR:HG21	1.98	0.45
1:A:215:G:H4'	1:A:216:A:H4'	1.99	0.45
1:A:2772:C:H5'	4:E:173:GLN:HE21	1.81	0.45
1:A:326:G:H2'	1:A:327:G:C8	2.52	0.45
1:A:405:U:H3'	1:A:406:G:H5'	3.72	0.45
1:A:598:U:H2'	1:A:599:A:C8	2.52	0.45
1:A:1022:G:H1'	1:A:1023:U:OP2	2.16	0.45
1:A:1363:C:H2'	1:A:1364:G:H8	1.81	0.45
1:A:1902:C:H5''	3:D:239:PHE:HE2	1.81	0.45
1:A:2453:A:H2'	1:A:2454:G:C8	2.52	0.45
1:A:334:C:OP1	1:A:335:C:N4	2.47	0.45
11:P:71:ALA:O	11:P:74:THR:HG22	2.17	0.45
1:A:85:G:OP1	20:Y:6:ARG:N	2.50	0.45
22:0:66:GLU:HB2	22:0:75:PHE:HB2	1.98	0.45
23:1:9:LYS:HE3	23:1:53:LYS:HD3	1.99	0.45
28:6:5:ARG:HG2	28:6:23:THR:HB	1.99	0.45
1:A:1130:U:O2'	1:A:1131:G:OP1	2.32	0.45
1:A:154:U:H2'	1:A:155:A:C8	2.52	0.45
1:A:1871:A:H8	1:A:1872:A:C8	2.35	0.45
1:A:2443:C:H2'	1:A:2444:G:C8	2.51	0.45
1:A:2656:U:H2'	1:A:2657:A:H8	1.81	0.45
2:B:114:C:H2'	2:B:115:A:C8	2.52	0.45
4:E:25:THR:HG21	4:E:193:VAL:HG21	1.99	0.45
1:A:1808:A:H3'	1:A:1809:A:C8	2.52	0.45
1:A:2374:C:N4	1:A:2375:G:O6	2.50	0.45
1:A:750:A:OP1	1:A:1615:C:N4	2.33	0.45
3:D:70:LYS:HB3	3:D:73:ILE:HD12	1.98	0.45
11:P:14:LYS:O	11:P:16:GLY:N	2.50	0.45
1:A:2200:C:H2'	1:A:2201:G:H8	1.82	0.45
1:A:414:C:H2'	1:A:415:A:C8	2.52	0.45
2:B:65:U:H3'	2:B:108:A:H61	1.81	0.45
53:J:56:ARG:HD3	53:J:81:LEU:HD11	1.99	0.45
9:N:13:ARG:HE	9:N:121:LYS:HZ1	1.65	0.45
13:R:79:LEU:HD23	13:R:83:LEU:HD12	1.99	0.45
1:A:1059:G:H5'	1:A:1060:U:OP2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2851:A:O3'	13:R:64:ARG:NH2	2.50	0.45
1:A:937:C:OP2	30:8:51:LYS:NZ	2.49	0.45
3:D:204:LEU:HD22	3:D:209:ALA:HB1	1.99	0.45
3:D:60:ALA:HB3	3:D:62:ARG:HH12	1.82	0.45
53:J:69:PHE:CD2	53:J:70:GLU:HG2	2.52	0.45
1:A:2566:A:H4'	1:A:2567:G:O5'	2.16	0.44
1:A:873:C:H2'	1:A:874:G:C8	2.53	0.44
3:D:52:HIS:CE1	3:D:218:THR:HA	2.52	0.44
4:E:5:VAL:HG21	4:E:80:TRP:CD2	2.52	0.44
5:F:128:ALA:HB3	5:F:133:LEU:HD12	1.99	0.44
53:J:11:ILE:HD11	53:J:62:ARG:HG2	1.99	0.44
1:A:582:A:H4'	16:U:10:ARG:HH22	1.81	0.44
1:A:2029:G:N1	1:A:2033:A:OP2	2.37	0.44
1:A:2291:U:H2'	1:A:2292:U:C6	2.51	0.44
1:A:2751:G:OP1	1:A:2751:G:N2	2.31	0.44
54:K:10:LEU:O	54:K:10:LEU:HD12	2.17	0.44
54:K:36:GLU:OE2	54:K:64:ARG:NH2	2.51	0.44
13:R:51:LEU:HD21	13:R:69:ARG:HD2	1.99	0.44
19:X:8:LEU:HD11	24:2:22:LEU:HD12	1.99	0.44
21:Z:2:PHE:O	21:Z:62:THR:OG1	2.26	0.44
1:A:1365:A:P	23:1:27:ARG:HH22	2.40	0.44
1:A:1629:U:O4	1:A:1630:A:N6	2.50	0.44
3:D:257:ARG:NH2	3:D:262:THR:OG1	2.47	0.44
1:A:1813:G:O2'	3:D:41:GLY:O	2.35	0.44
1:A:1046:A:O2'	53:J:61:ARG:O	2.24	0.44
10:O:29:HIS:ND1	10:O:29:HIS:O	2.50	0.44
4:E:13:ARG:HH11	15:T:55:HIS:HA	1.81	0.44
19:X:44:LYS:O	19:X:48:GLN:HG2	2.17	0.44
13:R:118:ARG:NH1	27:5:54:ILE:O	2.44	0.44
1:A:1955:U:C4	1:A:2552:OMU:H6	2.51	0.44
1:A:1965:C:H5''	1:A:1966:A:H2'	1.99	0.44
1:A:2853:C:H2'	1:A:2854:G:C8	2.53	0.44
1:A:935:C:H2'	1:A:936:A:H8	1.82	0.44
4:E:133:THR:HG23	4:E:134:HIS:CD2	2.52	0.44
53:J:118:ILE:HB	53:J:119:PRO:HD3	2.00	0.44
54:K:92:PRO:HB2	54:K:93:ASN:H	1.68	0.44
9:N:44:TYR:O	16:U:63:ARG:NE	2.51	0.44
17:V:68:ARG:NH1	17:V:90:ARG:HB2	2.33	0.44
1:A:456:C:H2'	19:X:73:ARG:HH22	1.82	0.44
1:A:1190:G:H2'	1:A:1191:G:C8	2.53	0.44
1:A:1656:C:OP1	4:E:141:ARG:NE	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:C:H4'	1:A:510:C:H5'	1.99	0.44
3:D:267:VAL:HG12	3:D:268:ARG:HG2	1.98	0.44
6:G:141:ASP:HB2	6:G:144:LYS:HD3	1.99	0.44
10:O:58:LEU:HD11	10:O:86:LEU:HD22	1.99	0.44
21:Z:9:ARG:HG2	21:Z:41:GLU:HB2	2.00	0.44
1:A:106:C:H2'	1:A:107:G:H8	1.97	0.44
1:A:30:G:O2'	1:A:1214:A:N3	2.49	0.44
5:F:47:LYS:HB2	5:F:51:GLU:HB2	2.00	0.44
1:A:2335:A:HO2'	1:A:2336:A:H8	1.65	0.44
1:A:2399:G:H2'	1:A:2400:G:C8	2.53	0.44
1:A:2724:U:H2'	1:A:2725:A:C8	2.53	0.44
1:A:2757:A:OP1	31:9:20:ASP:N	2.49	0.44
1:A:720:U:H2'	1:A:721:A:C8	2.52	0.44
2:B:118:C:H2'	2:B:119:A:H8	1.83	0.44
1:A:566:U:H5''	11:P:29:LYS:HE3	2.00	0.44
30:8:5:THR:HG23	30:8:61:LEU:HA	1.99	0.44
1:A:20:C:H2'	1:A:21:A:C8	2.53	0.44
1:A:2101:A:H2'	1:A:2102:G:H8	1.82	0.44
1:A:534:U:H2'	1:A:535:G:C8	2.53	0.44
3:D:203:VAL:O	3:D:205:GLY:N	2.50	0.44
4:E:33:ARG:HD3	4:E:73:VAL:HB	2.00	0.44
5:F:109:LEU:O	5:F:113:VAL:HG23	2.18	0.44
5:F:32:VAL:HG21	11:P:3:LEU:HD11	1.99	0.44
9:N:16:TYR:HE1	9:N:138:GLN:HE21	1.66	0.44
13:R:25:ALA:O	13:R:29:VAL:HG23	2.18	0.44
30:8:38:LYS:HA	30:8:41:ARG:HE	1.83	0.44
1:A:160:A:N3	1:A:2208:C:O2'	2.40	0.44
1:A:1844:C:H2'	1:A:1845:G:C8	2.52	0.44
1:A:414:C:O3'	1:A:1878:G:N2	2.51	0.44
8:I:121:VAL:HG23	8:I:123:ARG:HG3	2.00	0.44
54:K:4:VAL:HA	54:K:7:TYR:CE2	2.53	0.44
24:2:24:GLU:HB3	24:2:46:VAL:HG21	2.00	0.43
1:A:1248:G:OP1	5:F:44:ARG:NH1	2.51	0.43
1:A:1752:C:H2'	1:A:1753:G:C8	2.53	0.43
1:A:2809:A:H2'	1:A:2810:A:C8	2.53	0.43
1:A:457:A:H2	1:A:458:G:H21	1.66	0.43
1:A:18:U:O2'	1:A:554:U:OP1	2.36	0.43
10:O:26:GLY:HA3	10:O:30:ARG:HH11	1.81	0.43
11:P:62:PRO:HG2	30:8:24:LYS:HB3	1.99	0.43
15:T:24:THR:HA	15:T:45:VAL:HA	1.99	0.43
21:Z:20:LEU:HD11	21:Z:41:GLU:HG3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1915:3TD:O4	1:A:1915:3TD:O4'	2.36	0.43
1:A:2893:A:H4'	1:A:2894:G:C4	2.52	0.43
1:A:839:U:H3	1:A:939:G:H1	1.66	0.43
2:B:80:U:H2'	2:B:81:G:H8	1.83	0.43
3:D:132:ARG:HH12	8:I:93:SER:H	1.66	0.43
7:H:123:GLU:HB2	7:H:131:VAL:HB	2.00	0.43
17:V:4:VAL:HA	17:V:12:HIS:O	2.18	0.43
20:Y:3:LYS:HB3	20:Y:82:VAL:HG21	2.00	0.43
25:3:8:GLN:HA	25:3:54:VAL:HG12	2.00	0.43
1:A:1475:G:O2'	1:A:1732:C:N4	2.51	0.43
1:A:1844:C:H2'	1:A:1845:G:H8	1.82	0.43
1:A:633:A:O2'	1:A:2404:U:OP1	2.32	0.43
3:D:68:ARG:O	3:D:188:ARG:NH1	2.51	0.43
8:I:132:PHE:HB2	8:I:140:ALA:HB3	2.00	0.43
20:Y:24:VAL:HA	20:Y:35:VAL:HG22	1.99	0.43
1:A:1423:G:H2'	1:A:1424:G:H8	1.83	0.43
1:A:2224:G:OP1	3:D:264:LYS:NZ	2.39	0.43
1:A:2464:G:H1	1:A:2486:C:H42	1.65	0.43
1:A:2521:C:O2'	1:A:2564:A:N3	2.48	0.43
1:A:2768:U:O2'	9:N:95:ARG:NH2	2.51	0.43
1:A:2718:G:O2'	1:A:2847:U:OP1	2.25	0.43
54:K:101:SER:HA	54:K:140:GLU:H	1.83	0.43
9:N:37:ARG:HD3	9:N:39:LYS:HD2	2.00	0.43
15:T:13:LYS:HG3	15:T:16:VAL:HG23	2.00	0.43
21:Z:76:ASP:OD1	21:Z:77:VAL:N	2.52	0.43
24:2:44:LYS:HG3	24:2:47:ARG:HH12	1.82	0.43
1:A:119:A:H4'	1:A:120:U:H5'	1.99	0.43
1:A:589:U:H2'	1:A:590:A:C8	2.54	0.43
1:A:624:C:O2'	1:A:657:U:OP1	2.36	0.43
1:A:674:G:H2'	1:A:675:A:C8	4.94	0.43
1:A:1501:G:P	3:D:100:ARG:HH22	2.41	0.43
5:F:88:ARG:O	5:F:90:GLN:N	2.47	0.43
53:J:43:LYS:HE3	53:J:95:LEU:HD22	2.00	0.43
18:W:89:ALA:O	18:W:92:ARG:HG2	2.19	0.43
18:W:88:ARG:HB2	18:W:92:ARG:HG3	2.01	0.43
24:2:10:SER:HA	24:2:13:GLU:HG2	1.99	0.43
1:A:1653:G:O6	13:R:11:ASN:N	2.46	0.43
1:A:2622:U:O2'	1:A:2825:G:N7	2.50	0.43
1:A:269:C:H2'	1:A:270:A:H8	1.84	0.43
1:A:290:U:H2'	1:A:291:G:H8	1.84	0.43
1:A:459:U:H2'	1:A:460:A:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:21:GLN:NE2	7:H:40:VAL:O	2.43	0.43
17:V:6:GLN:HG3	17:V:39:LEU:HD11	2.00	0.43
1:A:2260:C:N4	22:0:10:ARG:HD2	2.34	0.43
1:A:1506:U:H2'	1:A:1507:C:C6	2.54	0.43
1:A:2443:C:H2'	1:A:2444:G:H8	1.83	0.43
1:A:2725:A:H2'	1:A:2726:A:H2'	2.00	0.43
1:A:745:1MG:O2'	1:A:748:G:H1'	2.19	0.43
4:E:170:VAL:HG23	4:E:194:PRO:HB3	2.01	0.43
9:N:109:LEU:HD13	9:N:118:MET:HG3	2.00	0.43
12:Q:77:PRO:HB2	12:Q:80:VAL:HG21	2.00	0.43
30:8:40:LYS:HA	30:8:43:LEU:HD12	2.00	0.43
1:A:2185:U:H2'	1:A:2186:G:C8	2.53	0.43
1:A:2790:U:OP2	1:A:2893:A:N6	2.52	0.43
5:F:105:LEU:HA	5:F:108:ILE:HG12	2.01	0.43
1:A:1165:A:H2'	1:A:1166:G:C8	2.53	0.43
1:A:1418:G:N1	1:A:1579:A:OP2	2.39	0.43
1:A:2818:U:H2'	1:A:2819:G:C8	2.54	0.43
1:A:563:A:H61	1:A:884:U:H3	106.07	0.43
2:B:28:C:H2'	2:B:29:A:C8	2.54	0.43
53:J:28:ALA:H	53:J:110:ALA:HA	1.83	0.43
11:P:110:VAL:HG11	11:P:135:ILE:HD11	2.01	0.43
22:0:23:GLY:HA2	22:0:63:VAL:HB	2.00	0.43
23:1:70:LEU:HD23	23:1:73:ARG:HH21	1.84	0.43
1:A:1124:G:O2'	31:9:37:GLN:OE1	2.26	0.43
1:A:1469:A:H2'	1:A:1470:A:C8	2.54	0.43
1:A:2137:U:H2'	1:A:2138:G:C8	2.54	0.43
1:A:2522:U:O2'	1:A:2647:U:OP1	2.21	0.43
1:A:286:U:H2'	1:A:287:G:C8	2.54	0.43
1:A:373:U:H2'	1:A:374:A:H8	1.83	0.43
1:A:75:G:OP1	24:2:48:ARG:NH2	2.52	0.43
1:A:926:G:H2'	1:A:927:A:C8	2.53	0.43
3:D:145:MET:HG2	3:D:152:GLN:HG3	2.01	0.43
4:E:151:THR:HB	4:E:152:PRO:HD3	2.01	0.43
6:G:138:PRO:HB3	26:4:32:LEU:HD11	2.01	0.43
22:0:42:HIS:CD2	22:0:73:ARG:HB2	2.54	0.42
6:G:139:GLU:HA	26:4:28:VAL:HG22	2.01	0.42
28:6:18:HIS:HE1	28:6:20:TYR:CZ	2.36	0.42
31:9:3:VAL:HG12	31:9:36:ARG:HE	1.84	0.42
1:A:2233:U:H2'	1:A:2234:G:C8	2.54	0.42
1:A:648:G:H2'	1:A:649:G:C8	2.54	0.42
1:A:832:U:H2'	1:A:833:A:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:60:SER:HA	6:G:101:ARG:HH12	1.83	0.42
8:I:58:LEU:HA	8:I:61:VAL:HG22	2.01	0.42
8:I:55:GLU:HA	8:I:58:LEU:HD12	2.01	0.42
25:3:40:THR:OG1	25:3:41:PRO:HD2	2.19	0.42
29:7:31:LEU:HB3	29:7:35:ARG:HH12	1.83	0.42
1:A:1310:G:H1'	1:A:1611:C:H5''	2.01	0.42
1:A:1336:A:H2'	1:A:1337:G:C8	2.54	0.42
1:A:1814:G:OP1	3:D:39:SER:OG	2.33	0.42
1:A:2417:C:H2'	1:A:2418:A:C8	2.54	0.42
1:A:2747:G:H1	1:A:2754:U:H2'	1.84	0.42
1:A:2760:C:H2'	1:A:2761:A:H8	1.83	0.42
1:A:32:C:N4	1:A:446:G:O2'	2.52	0.42
1:A:608:A:N7	1:A:619:G:N2	2.67	0.42
1:A:672:C:H5	11:P:42:SER:HB2	1.84	0.42
2:B:71:C:H42	2:B:105:G:H1	1.68	0.42
10:O:16:ALA:HB3	10:O:86:LEU:HD11	2.01	0.42
21:Z:25:LYS:HD3	21:Z:41:GLU:OE2	2.19	0.42
1:A:2233:U:H2'	1:A:2234:G:H8	1.85	0.42
1:A:2073:C:O2'	1:A:2598:A:O2'	2.33	0.42
1:A:2646:C:N4	1:A:2675:A:N1	2.68	0.42
1:A:2808:G:O2'	1:A:2809:A:H8	2.02	0.42
1:A:323:C:H2'	1:A:1205:A:N1	2.35	0.42
1:A:629:G:H5''	1:A:650:C:O2'	2.20	0.42
1:A:655:A:H4'	1:A:656:G:H5'	2.00	0.42
1:A:918:A:O2'	2:B:96:G:N2	2.52	0.42
2:B:52:A:N6	14:S:33:ARG:HB2	2.33	0.42
3:D:77:VAL:HA	3:D:93:VAL:HA	2.00	0.42
1:A:658:U:O2'	5:F:97:ASN:OD1	2.34	0.42
54:K:113:ALA:HA	54:K:116:MET:HB2	2.00	0.42
15:T:26:GLU:OE1	15:T:84:SER:OG	2.33	0.42
1:A:987:C:O2'	1:A:1000:A:N3	2.48	0.42
1:A:1313:U:H2'	1:A:1313:U:O2	2.17	0.42
1:A:1331:G:O2'	1:A:1332:G:N2	2.51	0.42
1:A:1334:G:H5''	19:X:69:ARG:NH2	2.34	0.42
1:A:1550:C:H2'	1:A:1551:A:H8	1.85	0.42
1:A:1658:C:H2'	1:A:1659:G:H8	1.84	0.42
1:A:1799:G:O5'	1:A:1819:A:N6	2.52	0.42
1:A:2200:C:H2'	1:A:2201:G:C8	2.55	0.42
1:A:440:C:H2'	1:A:441:U:C6	2.55	0.42
1:A:523:C:H2'	1:A:524:G:C8	2.54	0.42
1:A:594:U:H2'	1:A:595:C:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:136:ASP:OD2	7:H:139:VAL:HG23	2.20	0.42
21:Z:10:LYS:HG3	21:Z:11:GLU:HG3	2.01	0.42
1:A:1363:C:H2'	1:A:1364:G:C8	2.54	0.42
1:A:2146:C:H4'	1:A:2147:A:C5	2.54	0.42
4:E:13:ARG:HG2	15:T:55:HIS:CE1	2.55	0.42
8:I:33:GLN:HB2	8:I:35:LYS:HG2	2.01	0.42
8:I:9:VAL:HG12	8:I:11:ASN:H	1.84	0.42
19:X:22:THR:HA	19:X:25:GLU:HG2	2.01	0.42
26:4:44:PHE:CE1	26:4:45:THR:HG23	2.53	0.42
1:A:1137:G:H2'	1:A:1138:G:C8	2.53	0.42
1:A:1190:G:H2'	1:A:1191:G:H8	1.84	0.42
1:A:1434:A:H2'	1:A:1435:G:C8	2.53	0.42
1:A:1491:G:H2'	1:A:1492:G:C8	2.54	0.42
1:A:2580:PSU:H3'	1:A:2581:G:C2	2.55	0.42
1:A:341:C:H2'	1:A:342:A:C8	2.55	0.42
1:A:859:G:H1'	1:A:860:U:H5	1.85	0.42
1:A:935:C:H2'	1:A:936:A:C8	2.54	0.42
4:E:4:LEU:HD21	4:E:96:ILE:HG22	2.00	0.42
12:Q:57:VAL:HA	12:Q:112:LEU:HD21	2.01	0.42
18:W:84:ARG:HB2	18:W:96:ILE:HG13	2.02	0.42
21:Z:56:PHE:CE1	21:Z:61:LEU:HD21	2.55	0.42
1:A:1162:G:H2'	1:A:1163:G:C8	2.53	0.42
1:A:1491:G:H2'	1:A:1492:G:H8	1.84	0.42
1:A:1572:A:H2'	1:A:1573:G:H8	1.85	0.42
1:A:1475:G:H4'	1:A:1689:A:H4'	68.78	0.42
1:A:2139:U:H2'	1:A:2140:G:C8	2.54	0.42
1:A:2183:A:H2'	1:A:2184:A:C8	2.55	0.42
5:F:52:VAL:HG21	5:F:82:GLY:H	1.85	0.42
8:I:3:VAL:HA	8:I:38:PRO:HA	2.00	0.42
11:P:79:LEU:HD12	11:P:114:GLY:H	1.84	0.42
1:A:1429:G:H2'	1:A:1430:G:H8	1.85	0.42
1:A:2197:U:H1'	1:A:2198:A:C8	2.55	0.42
1:A:2853:C:H2'	1:A:2854:G:H8	1.84	0.42
2:B:115:A:H2'	2:B:116:G:C8	2.54	0.42
5:F:143:LEU:HB3	5:F:146:VAL:HG11	2.02	0.42
6:G:73:VAL:HG22	6:G:78:ILE:HD11	2.01	0.42
10:O:109:SER:O	10:O:111:LYS:N	2.51	0.42
13:R:49:GLU:HB2	13:R:50:PRO:HD3	2.01	0.42
1:A:480:A:O3'	20:Y:43:LYS:HG3	2.19	0.42
20:Y:88:ASP:CG	20:Y:89:GLY:H	2.24	0.42
1:A:1030:C:H42	1:A:1124:G:H1	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1429:G:H2'	1:A:1430:G:C8	2.55	0.42
1:A:1666:G:H1	1:A:1994:C:H42	1.68	0.42
1:A:1822:C:H2'	1:A:1823:G:H8	1.84	0.42
1:A:2698:U:H2'	1:A:2699:C:C6	2.55	0.42
1:A:2845:U:O3'	15:T:52:ARG:NH1	2.52	0.42
1:A:537:G:H4'	9:N:5:THR:HG21	2.02	0.42
1:A:767:U:H2'	1:A:768:G:C8	2.55	0.42
20:Y:36:GLU:HA	20:Y:61:GLU:HG2	2.01	0.42
1:A:1481:U:H2'	1:A:1482:G:C8	7.01	0.42
1:A:1651:G:H5'	13:R:39:PRO:HG2	2.02	0.42
1:A:1751:U:H2'	1:A:1752:C:C6	2.55	0.42
1:A:2483:C:N3	12:Q:123:LYS:NZ	2.65	0.42
1:A:2710:C:OP1	13:R:15:SER:OG	2.25	0.42
1:A:690:G:H21	3:D:42:ARG:HH22	1.68	0.42
1:A:715:A:H2'	1:A:716:A:C8	2.92	0.42
3:D:124:LYS:HA	3:D:125:PRO:HD3	1.86	0.42
5:F:3:LEU:HD21	5:F:19:PHE:CZ	2.55	0.42
13:R:73:ASN:HA	13:R:76:VAL:HG12	2.00	0.42
1:A:1614:A:H61	18:W:88:ARG:H	1.68	0.42
1:A:2345:G:H4'	1:A:2346:A:H3'	2.02	0.41
1:A:438:G:H2'	1:A:439:A:C8	2.55	0.41
1:A:674:G:H1	1:A:806:C:H42	1.69	0.41
19:X:6:ARG:O	19:X:10:VAL:HG23	2.19	0.41
1:A:1186:G:H2'	1:A:1187:G:C8	3.03	0.41
1:A:1326:U:H2'	1:A:1327:A:C8	2.54	0.41
1:A:1790:C:H2'	1:A:1791:A:C5	2.54	0.41
1:A:2120:G:H2'	1:A:2121:G:H8	1.85	0.41
1:A:459:U:H2'	1:A:460:A:H8	1.85	0.41
1:A:630:G:N2	1:A:633:A:OP2	2.36	0.41
1:A:836:G:H1	1:A:850:U:H3	29.43	0.41
1:A:923:G:H2'	1:A:924:G:H8	1.84	0.41
1:A:974:G:H1'	1:A:975:A:C8	2.55	0.41
13:R:44:LEU:HD23	13:R:113:ILE:HD13	2.01	0.41
14:S:43:ASN:OD1	14:S:44:GLY:N	2.53	0.41
21:Z:60:VAL:HG11	21:Z:71:LYS:HE3	2.01	0.41
1:A:358:U:H2'	1:A:359:G:C8	3.34	0.41
3:D:177:SER:O	3:D:270:ARG:HG3	2.21	0.41
1:A:1568:G:H5'	3:D:59:GLN:HA	2.03	0.41
2:B:27:C:OP2	14:S:33:ARG:NH1	2.53	0.41
1:A:1061:U:N3	54:K:11:GLN:O	2.53	0.41
1:A:1141:U:H4'	1:A:1142:A:O4'	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1357:C:H2'	1:A:1358:G:O4'	2.20	0.41
1:A:1660:G:H2'	1:A:1661:G:H8	1.85	0.41
1:A:2430:A:H5'	1:A:2431:U:OP2	2.20	0.41
1:A:632:A:H2'	1:A:633:A:C8	2.56	0.41
16:U:59:LEU:O	16:U:63:ARG:HG2	2.20	0.41
1:A:1565:C:H5'	3:D:17:LYS:HE3	2.02	0.41
1:A:1595:C:H2'	1:A:1596:A:C8	2.55	0.41
1:A:1675:C:O2	4:E:133:THR:OG1	2.33	0.41
1:A:1787:A:H5''	3:D:237:ARG:HH21	1.85	0.41
1:A:2101:A:H2'	1:A:2102:G:C8	2.55	0.41
1:A:690:G:H21	3:D:42:ARG:HH12	1.68	0.41
6:G:22:ASN:N	6:G:26:GLN:OE1	2.53	0.41
1:A:7:G:H5'	9:N:132:HIS:HE1	1.86	0.41
1:A:1754:A:HO2'	15:T:102:ARG:HH22	1.64	0.41
17:V:10:LYS:HE2	17:V:12:HIS:CE1	2.55	0.41
1:A:999:U:H2'	1:A:1000:A:H8	1.86	0.41
1:A:1501:G:OP1	3:D:100:ARG:NH2	2.52	0.41
1:A:1783:A:N1	1:A:2587:A:H2'	2.35	0.41
1:A:1962:5MC:O2'	1:A:1964:G:OP2	2.30	0.41
1:A:243:U:H2'	1:A:244:A:H8	1.86	0.41
1:A:2453:A:H2'	1:A:2454:G:H8	1.85	0.41
1:A:2837:A:H2'	1:A:2838:G:C8	2.56	0.41
1:A:2899:A:H2'	1:A:2900:A:C8	2.55	0.41
1:A:490:C:O2'	1:A:491:G:OP2	2.35	0.41
3:D:131:MET:HA	3:D:134:ILE:HD12	2.02	0.41
11:P:109:LYS:HD2	11:P:126:ARG:HH11	1.86	0.41
12:Q:75:GLU:HB3	12:Q:90:GLU:HG3	2.01	0.41
19:X:7:LEU:HD22	19:X:46:ALA:HB2	2.03	0.41
1:A:1530:G:H22	1:A:1542:U:H1'	1.86	0.41
1:A:2051:A:H2'	1:A:2578:G:OP1	2.21	0.41
1:A:2302:U:H2'	1:A:2303:G:H8	1.86	0.41
1:A:372:G:H8	23:1:57:VAL:HG22	1.85	0.41
1:A:5:A:H2'	1:A:6:A:C8	2.55	0.41
1:A:746:PSU:O2'	1:A:2611:C:H4'	2.21	0.41
1:A:774:G:H1'	1:A:777:G:H21	1.86	0.41
6:G:107:VAL:HB	6:G:108:PRO:HD3	2.02	0.41
1:A:2198:A:C2	8:I:29:PHE:HB2	2.55	0.41
54:K:20:SER:HB3	54:K:21:PRO:HD3	2.03	0.41
9:N:36:LEU:O	9:N:51:GLY:HA3	2.21	0.41
14:S:39:VAL:N	14:S:49:VAL:O	2.51	0.41
1:A:929:U:H4'	25:3:37:ARG:NH2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1028:A:N6	1:A:1125:G:H2'	2.36	0.41
1:A:1158:C:H2'	1:A:1159:U:H4'	4.13	0.41
1:A:1365:A:OP1	23:1:2:ARG:NH1	2.41	0.41
1:A:1672:A:C2	1:A:2582:G:H5'	2.55	0.41
1:A:1765:U:H2'	1:A:1766:G:C8	2.56	0.41
1:A:1783:A:H5'	1:A:2608:G:H4'	2.03	0.41
1:A:676:A:N6	1:A:713:G:O6	92.47	0.41
3:D:170:TYR:HB3	3:D:182:LYS:HD3	2.02	0.41
11:P:2:ARG:O	11:P:5:THR:OG1	2.26	0.41
17:V:15:SER:O	17:V:18:GLN:HG2	2.21	0.41
1:A:212:G:H2'	1:A:213:A:C8	2.56	0.41
1:A:2293:G:OP1	14:S:94:ARG:NH1	2.54	0.41
3:D:68:ARG:NH1	3:D:128:THR:OG1	2.54	0.41
6:G:34:THR:HB	6:G:154:THR:HB	2.02	0.41
8:I:25:TYR:O	8:I:29:PHE:HB3	2.21	0.41
13:R:38:LEU:HB3	13:R:39:PRO:HD3	2.02	0.41
15:T:105:LYS:HE3	15:T:108:ARG:NH2	2.35	0.41
19:X:8:LEU:HD23	19:X:50:LEU:HD21	2.03	0.41
30:8:28:LEU:HA	30:8:32:LEU:HD21	2.03	0.41
1:A:1539:U:H2'	1:A:1540:G:C8	2.55	0.41
1:A:1771:C:O2'	1:A:1786:A:O4'	2.38	0.41
1:A:1788:C:OP1	3:D:220:ARG:NH2	2.52	0.41
1:A:2328:A:H2'	1:A:2329:U:C6	2.56	0.41
1:A:2691:C:H2'	1:A:2692:G:C8	2.56	0.41
1:A:2773:C:OP1	4:E:169:ARG:NH2	2.54	0.41
3:D:153:LEU:HD11	3:D:181:ARG:NH2	2.35	0.41
5:F:126:VAL:HG22	5:F:128:ALA:H	1.86	0.41
1:A:2208:C:H2'	1:A:2209:G:C8	2.55	0.41
1:A:2251:OMG:H2'	1:A:2252:G:O5'	2.21	0.41
1:A:2467:C:OP1	31:9:8:LYS:NZ	2.48	0.41
1:A:2569:G:H2'	1:A:2570:G:H8	1.86	0.41
1:A:706:A:OP1	3:D:6:LYS:NZ	2.54	0.41
53:J:60:LEU:O	53:J:64:VAL:HB	2.21	0.41
54:K:131:THR:O	54:K:134:SER:OG	2.28	0.41
9:N:7:LYS:O	9:N:11:VAL:HG23	2.21	0.41
10:O:24:VAL:HG13	10:O:33:ALA:HB2	2.03	0.41
30:8:21:PHE:O	30:8:49:VAL:HG23	2.21	0.40
1:A:1020:A:H1'	1:A:1021:A:OP2	2.21	0.40
1:A:1111:A:H2'	1:A:1112:G:H4'	2.03	0.40
1:A:1255:U:H5'	1:A:2502:G:H22	1.86	0.40
1:A:1351:C:H2'	1:A:1352:U:C6	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1405:U:H2'	1:A:1406:U:C6	2.56	0.40
1:A:4:U:H2'	1:A:5:A:C8	2.55	0.40
6:G:124:ARG:HB3	6:G:126:ASN:HD22	1.86	0.40
15:T:46:VAL:HG22	15:T:60:VAL:HG22	2.02	0.40
16:U:82:LEU:HD21	16:U:108:LEU:HD21	2.03	0.40
20:Y:23:LYS:O	20:Y:35:VAL:HG13	2.21	0.40
1:A:300:A:P	20:Y:81:ARG:HH12	2.43	0.40
1:A:465:G:P	29:7:12:ARG:HH12	2.45	0.40
1:A:1490:A:N6	3:D:73:ILE:HG23	2.37	0.40
1:A:155:A:H2'	1:A:156:A:C8	2.57	0.40
1:A:1666:G:N3	10:O:3:GLN:NE2	2.70	0.40
1:A:1847:G:O2'	1:A:1848:A:H8	2.05	0.40
1:A:1874:C:H2'	1:A:1875:G:O4'	2.21	0.40
1:A:2447:G:H21	1:A:2450:A:P	2.43	0.40
1:A:2572:A:OP2	4:E:149:ASN:HB3	2.21	0.40
1:A:2594:C:N4	1:A:2595:G:O6	2.55	0.40
1:A:923:G:H2'	1:A:924:G:C8	2.56	0.40
1:A:938:G:H2'	1:A:939:G:H8	1.86	0.40
10:O:35:VAL:HA	10:O:69:VAL:HG11	2.03	0.40
1:A:2722:G:O2'	13:R:3:HIS:O	2.35	0.40
1:A:1161:C:H2'	1:A:1162:G:C8	2.57	0.40
1:A:1301:A:H2'	1:A:1301:A:N3	2.37	0.40
1:A:1320:C:O2'	1:A:1321:A:H8	2.04	0.40
1:A:1433:A:H2'	1:A:1434:A:C8	2.56	0.40
1:A:151:C:H2'	1:A:152:A:C8	2.56	0.40
1:A:1889:A:H2'	1:A:1890:A:C8	2.57	0.40
1:A:2333:A:H4'	1:A:2334:U:O5'	2.22	0.40
1:A:277:G:H4'	1:A:278:A:N7	2.37	0.40
1:A:745:1MG:HM11	1:A:745:1MG:HN21	1.63	0.40
16:U:111:LYS:HB2	17:V:48:LYS:HD2	2.04	0.40
1:A:1550:C:H2'	1:A:1551:A:C8	2.56	0.40
1:A:2027:G:H1	1:A:2036:C:H42	1.69	0.40
1:A:2137:U:H2'	1:A:2138:G:H8	1.86	0.40
1:A:2377:A:H2'	1:A:2378:A:C8	2.56	0.40
1:A:281:C:H2'	1:A:282:A:C8	2.56	0.40
1:A:341:C:H2'	1:A:342:A:H8	1.86	0.40
1:A:582:A:H2'	1:A:583:G:C8	2.57	0.40
8:I:90:LEU:HG	8:I:92:GLY:H	1.87	0.40
12:Q:76:LYS:HA	12:Q:77:PRO:HD3	1.92	0.40
1:A:96:C:H4'	24:2:41:HIS:CD2	2.56	0.40
1:A:1049:C:C5	1:A:1049:C:N1	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1146:C:H2'	1:A:1147:A:C8	2.56	0.40
1:A:166:U:H2'	1:A:167:A:C8	2.84	0.40
1:A:2052:A:H2'	1:A:2053:G:H8	1.85	0.40
1:A:2756:U:H1'	1:A:2757:A:H5''	2.04	0.40
1:A:560:C:H2'	1:A:561:G:C8	2.57	0.40
1:A:596:U:H2'	1:A:597:G:C8	2.57	0.40
7:H:51:PHE:CZ	7:H:71:LEU:HD22	2.56	0.40
16:U:45:ALA:O	16:U:49:ARG:HG3	2.20	0.40
18:W:69:LEU:HA	18:W:109:ASP:HA	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	269/273 (98%)	243 (90%)	25 (9%)	1 (0%)	38	77
4	E	207/209 (99%)	187 (90%)	17 (8%)	3 (1%)	13	55
5	F	199/201 (99%)	184 (92%)	11 (6%)	4 (2%)	9	50
6	G	175/179 (98%)	154 (88%)	18 (10%)	3 (2%)	11	53
7	H	174/177 (98%)	149 (86%)	23 (13%)	2 (1%)	17	61
8	I	147/149 (99%)	129 (88%)	14 (10%)	4 (3%)	6	43
9	N	140/142 (99%)	130 (93%)	8 (6%)	2 (1%)	13	55
10	O	120/123 (98%)	108 (90%)	7 (6%)	5 (4%)	3	32
11	P	141/144 (98%)	122 (86%)	13 (9%)	6 (4%)	3	32
12	Q	134/136 (98%)	123 (92%)	8 (6%)	3 (2%)	8	48
13	R	118/127 (93%)	103 (87%)	12 (10%)	3 (2%)	6	45
14	S	114/117 (97%)	106 (93%)	6 (5%)	2 (2%)	10	52
15	T	112/115 (97%)	105 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	U	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
17	V	101/103 (98%)	91 (90%)	6 (6%)	4 (4%)	3	34
18	W	108/110 (98%)	94 (87%)	14 (13%)	0	100	100
19	X	91/100 (91%)	81 (89%)	8 (9%)	2 (2%)	8	48
20	Y	100/104 (96%)	87 (87%)	11 (11%)	2 (2%)	9	50
21	Z	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
22	0	73/85 (86%)	68 (93%)	4 (6%)	1 (1%)	13	55
23	1	75/78 (96%)	71 (95%)	4 (5%)	0	100	100
24	2	61/63 (97%)	59 (97%)	2 (3%)	0	100	100
25	3	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
26	4	64/70 (91%)	56 (88%)	7 (11%)	1 (2%)	11	54
27	5	54/57 (95%)	51 (94%)	2 (4%)	1 (2%)	9	51
28	6	48/55 (87%)	43 (90%)	4 (8%)	1 (2%)	8	49
29	7	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
30	8	62/65 (95%)	58 (94%)	3 (5%)	1 (2%)	11	54
31	9	36/38 (95%)	32 (89%)	3 (8%)	1 (3%)	6	43
33	b	216/240 (90%)	187 (87%)	25 (12%)	4 (2%)	9	51
34	c	204/233 (88%)	188 (92%)	14 (7%)	2 (1%)	18	62
35	d	203/206 (98%)	180 (89%)	19 (9%)	4 (2%)	9	50
36	e	155/167 (93%)	132 (85%)	17 (11%)	6 (4%)	3	34
37	f	98/135 (73%)	85 (87%)	9 (9%)	4 (4%)	3	33
38	g	149/179 (83%)	130 (87%)	13 (9%)	6 (4%)	3	34
39	h	127/130 (98%)	115 (91%)	11 (9%)	1 (1%)	22	66
40	i	125/130 (96%)	107 (86%)	13 (10%)	5 (4%)	3	34
41	j	96/103 (93%)	79 (82%)	11 (12%)	6 (6%)	1	23
42	k	114/129 (88%)	99 (87%)	11 (10%)	4 (4%)	4	38
43	l	121/124 (98%)	104 (86%)	9 (7%)	8 (7%)	1	22
44	m	112/118 (95%)	103 (92%)	7 (6%)	2 (2%)	10	52
45	o	86/89 (97%)	76 (88%)	5 (6%)	5 (6%)	2	24
46	p	80/82 (98%)	71 (89%)	7 (9%)	2 (2%)	6	45
47	q	78/84 (93%)	65 (83%)	9 (12%)	4 (5%)	2	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	r	63/75 (84%)	56 (89%)	4 (6%)	3 (5%)	2	29
49	t	83/87 (95%)	80 (96%)	3 (4%)	0	100	100
50	u	63/71 (89%)	48 (76%)	10 (16%)	5 (8%)	1	16
53	J	129/165 (78%)	102 (79%)	21 (16%)	6 (5%)	3	30
54	K	139/142 (98%)	118 (85%)	14 (10%)	7 (5%)	2	28
55	n	99/102 (97%)	87 (88%)	8 (8%)	4 (4%)	3	34
56	s	77/92 (84%)	71 (92%)	5 (6%)	1 (1%)	14	57
57	z	458/819 (56%)	423 (92%)	24 (5%)	11 (2%)	7	46
All	All	6305/7039 (90%)	5637 (89%)	516 (8%)	152 (2%)	11	46

All (152) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	N	81	ILE
11	P	128	THR
34	c	96	VAL
34	c	156	LEU
36	e	122	VAL
48	r	17	VAL
54	K	22	PRO
54	K	92	PRO
55	n	38	ASP
57	z	50	PRO
57	z	104	VAL
57	z	304	PRO
57	z	316	PRO
57	z	329	PRO
57	z	732	VAL
7	H	108	PHE
8	I	9	VAL
9	N	82	GLY
11	P	85	VAL
11	P	111	ILE
17	V	55	ASP
20	Y	97	SER
28	6	45	HIS
31	9	29	ALA
35	d	26	ALA
35	d	191	SER

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Mol	Chain	Res	Type
37	f	92	THR
38	g	16	LYS
38	g	29	LEU
38	g	56	SER
39	h	74	ILE
40	i	90	ASP
41	j	57	VAL
42	k	88	PRO
43	l	42	LYS
44	m	6	ILE
46	p	8	ARG
50	u	30	GLU
50	u	37	TYR
53	J	55	VAL
53	J	90	GLY
54	K	12	VAL
55	n	54	ASP
57	z	56	LEU
4	E	169	ARG
5	F	122	GLU
6	G	18	GLU
7	H	45	ALA
8	I	15	LEU
11	P	29	LYS
11	P	94	THR
13	R	59	SER
17	V	43	ASN
20	Y	6	ARG
22	0	17	LEU
33	b	11	ALA
35	d	152	SER
36	e	23	THR
36	e	98	ALA
37	f	54	LEU
37	f	63	ASN
37	f	86	ARG
38	g	64	ALA
38	g	145	GLU
40	i	57	VAL
40	i	107	ALA
40	i	125	GLN
42	k	92	ARG

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Mol	Chain	Res	Type
43	l	2	THR
43	l	23	LEU
43	l	33	CYS
44	m	113	LYS
45	o	2	LEU
47	q	17	GLU
47	q	49	ASN
48	r	18	GLN
50	u	12	ASP
54	K	20	SER
54	K	64	ARG
54	K	100	ILE
55	n	2	LYS
4	E	58	ASN
4	E	148	GLN
5	F	80	SER
10	O	109	SER
12	Q	14	LYS
12	Q	70	ASP
14	S	100	HIS
19	X	38	ALA
26	4	26	SER
33	b	71	THR
33	b	153	MET
35	d	166	LYS
36	e	102	THR
41	j	29	ALA
41	j	35	GLN
43	l	46	SER
45	o	13	GLU
45	o	45	HIS
47	q	16	MET
50	u	34	ARG
53	J	22	ALA
53	J	88	HIS
55	n	22	LYS
57	z	134	ASN
57	z	276	VAL
57	z	416	VAL
5	F	83	VAL
8	I	3	VAL
8	I	89	LYS

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Mol	Chain	Res	Type
10	O	35	VAL
10	O	93	GLN
10	O	110	GLU
11	P	36	LYS
13	R	117	ASP
14	S	66	GLY
17	V	53	PHE
27	5	2	VAL
33	b	122	ASP
41	j	33	GLY
41	j	75	ASP
42	k	126	ARG
43	l	75	GLU
43	l	77	SER
45	o	21	THR
45	o	87	ARG
50	u	32	ARG
53	J	71	CYS
53	J	118	ILE
54	K	3	LYS
6	G	61	GLY
13	R	106	ASP
38	g	19	SER
40	i	9	GLY
41	j	41	PRO
47	q	79	GLU
48	r	46	THR
57	z	710	ILE
3	D	253	GLY
19	X	71	GLY
42	k	119	GLY
30	8	31	ILE
43	l	21	PRO
56	s	7	GLY
5	F	149	ILE
6	G	174	PHE
12	Q	69	PRO
46	p	36	VAL
10	O	26	GLY
17	V	54	VAL
36	e	24	VAL
36	e	93	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	216/218 (99%)	216 (100%)	0	100	100
4	E	164/164 (100%)	164 (100%)	0	100	100
5	F	165/165 (100%)	165 (100%)	0	100	100
6	G	148/150 (99%)	148 (100%)	0	100	100
7	H	137/138 (99%)	137 (100%)	0	100	100
8	I	114/114 (100%)	114 (100%)	0	100	100
9	N	116/116 (100%)	116 (100%)	0	100	100
10	O	103/104 (99%)	103 (100%)	0	100	100
11	P	102/103 (99%)	102 (100%)	0	100	100
12	Q	109/109 (100%)	109 (100%)	0	100	100
13	R	100/103 (97%)	100 (100%)	0	100	100
14	S	86/87 (99%)	86 (100%)	0	100	100
15	T	99/100 (99%)	99 (100%)	0	100	100
16	U	89/90 (99%)	89 (100%)	0	100	100
17	V	84/84 (100%)	84 (100%)	0	100	100
18	W	93/93 (100%)	93 (100%)	0	100	100
19	X	80/84 (95%)	80 (100%)	0	100	100
20	Y	83/85 (98%)	83 (100%)	0	100	100
21	Z	78/78 (100%)	78 (100%)	0	100	100
22	0	57/63 (90%)	57 (100%)	0	100	100
23	1	67/68 (98%)	67 (100%)	0	100	100
24	2	55/55 (100%)	55 (100%)	0	100	100
25	3	48/49 (98%)	48 (100%)	0	100	100
26	4	59/62 (95%)	59 (100%)	0	100	100
27	5	47/48 (98%)	47 (100%)	0	100	100
28	6	45/49 (92%)	45 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	7	38/38 (100%)	38 (100%)	0	100	100
30	8	51/52 (98%)	51 (100%)	0	100	100
31	9	34/34 (100%)	34 (100%)	0	100	100
33	b	180/198 (91%)	180 (100%)	0	100	100
34	c	170/190 (90%)	170 (100%)	0	100	100
35	d	172/173 (99%)	172 (100%)	0	100	100
36	e	114/126 (90%)	114 (100%)	0	100	100
37	f	87/116 (75%)	87 (100%)	0	100	100
38	g	124/147 (84%)	124 (100%)	0	100	100
39	h	104/105 (99%)	104 (100%)	0	100	100
40	i	105/107 (98%)	105 (100%)	0	100	100
41	j	86/90 (96%)	86 (100%)	0	100	100
42	k	89/99 (90%)	89 (100%)	0	100	100
43	l	103/104 (99%)	103 (100%)	0	100	100
44	m	92/96 (96%)	92 (100%)	0	100	100
45	o	76/77 (99%)	76 (100%)	0	100	100
46	p	65/65 (100%)	65 (100%)	0	100	100
47	q	74/78 (95%)	74 (100%)	0	100	100
48	r	48/65 (74%)	48 (100%)	0	100	100
49	t	65/66 (98%)	65 (100%)	0	100	100
50	u	44/61 (72%)	44 (100%)	0	100	100
53	J	100/123 (81%)	100 (100%)	0	100	100
54	K	109/110 (99%)	109 (100%)	0	100	100
55	n	79/84 (94%)	79 (100%)	0	100	100
56	s	70/79 (89%)	70 (100%)	0	100	100
All	All	4823/5062 (95%)	4823 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	225	ASN

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Mol	Chain	Res	Type
4	E	32	ASN
4	E	173	GLN
5	F	41	GLN
5	F	165	HIS
6	G	4	HIS
7	H	138	GLN
10	O	3	GLN
11	P	99	ASN
12	Q	13	HIS
13	R	9	GLN
15	T	2	ASN
15	T	11	GLN
17	V	18	GLN
18	W	7	HIS
18	W	40	ASN
18	W	61	ASN
20	Y	73	ASN
21	Z	87	GLN
22	0	42	HIS
23	1	16	ASN
24	2	25	GLN
24	2	58	ASN
25	3	19	HIS
28	6	18	HIS
28	6	45	HIS
31	9	35	GLN
33	b	18	GLN
33	b	41	ASN
35	d	119	HIS
35	d	125	ASN
36	e	145	ASN
37	f	11	HIS
37	f	58	HIS
38	g	141	HIS
39	h	3	GLN
40	i	4	GLN
41	j	70	HIS
42	k	27	ASN
43	l	4	ASN
44	m	11	HIS
44	m	90	HIS
45	o	39	GLN

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Mol	Chain	Res	Type
46	p	9	HIS
46	p	63	GLN
46	p	79	ASN
47	q	30	HIS
49	t	2	ASN
49	t	74	HIS
53	J	4	ASN
53	J	88	HIS
56	s	55	GLN
56	s	68	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2881/2903 (99%)	415 (14%)	43 (1%)
2	B	119/120 (99%)	13 (10%)	2 (1%)
32	a	1535/1539 (99%)	176 (11%)	0
51	v	5/6 (83%)	0	0
52	x	76/77 (98%)	13 (17%)	0
58	y	72/73 (98%)	28 (38%)	0
All	All	4688/4718 (99%)	645 (13%)	45 (0%)

All (645) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	A
1	A	12	U
1	A	27	G
1	A	34	U
1	A	35	G
1	A	46	G
1	A	49	A
1	A	51	G
1	A	52	A
1	A	71	A
1	A	74	A
1	A	75	G
1	A	84	A
1	A	91	A
1	A	92	U
1	A	98	G

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Mol	Chain	Res	Type
1	A	118	A
1	A	120	U
1	A	138	U
1	A	139	U
1	A	140	C
1	A	141	G
1	A	142	A
1	A	162	U
1	A	163	C
1	A	181	A
1	A	196	A
1	A	199	A
1	A	205	G
1	A	216	A
1	A	221	A
1	A	222	A
1	A	242	G
1	A	243	U
1	A	248	G
1	A	249	C
1	A	255	A
1	A	266	G
1	A	267	C
1	A	276	U
1	A	278	A
1	A	294	A
1	A	310	A
1	A	311	A
1	A	323	C
1	A	329	G
1	A	330	A
1	A	353	C
1	A	361	G
1	A	367	G
1	A	371	A
1	A	373	U
1	A	386	G
1	A	387	U
1	A	391	A
1	A	404	A
1	A	406	G
1	A	411	G

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Mol	Chain	Res	Type
1	A	424	G
1	A	451	U
1	A	456	C
1	A	457	A
1	A	458	G
1	A	459	U
1	A	480	A
1	A	481	G
1	A	491	G
1	A	504	A
1	A	505	A
1	A	506	G
1	A	529	A
1	A	530	G
1	A	532	A
1	A	533	G
1	A	543	G
1	A	545	U
1	A	547	A
1	A	550	C
1	A	563	A
1	A	572	A
1	A	573	U
1	A	575	A
1	A	603	A
1	A	616	A
1	A	627	A
1	A	637	A
1	A	646	U
1	A	654	A
1	A	669	G
1	A	686	U
1	A	687	C
1	A	695	G
1	A	730	A
1	A	746	PSU
1	A	747	5MC
1	A	748	G
1	A	752	A
1	A	753	A
1	A	764	A
1	A	776	G

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Mol	Chain	Res	Type
1	A	782	A
1	A	784	G
1	A	785	G
1	A	789	A
1	A	792	A
1	A	805	G
1	A	812	C
1	A	819	A
1	A	822	G
1	A	827	U
1	A	828	U
1	A	830	G
1	A	831	G
1	A	845	A
1	A	846	U
1	A	847	U
1	A	858	G
1	A	859	G
1	A	860	U
1	A	878	A
1	A	885	C
1	A	894	U
1	A	896	A
1	A	897	C
1	A	898	C
1	A	907	G
1	A	910	A
1	A	932	U
1	A	941	A
1	A	946	C
1	A	955	PSU
1	A	956	G
1	A	961	C
1	A	974	G
1	A	983	A
1	A	995	C
1	A	996	A
1	A	1012	U
1	A	1013	C
1	A	1021	A
1	A	1022	G
1	A	1023	U

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Mol	Chain	Res	Type
1	A	1033	U
1	A	1046	A
1	A	1047	G
1	A	1053	C
1	A	1054	A
1	A	1057	A
1	A	1060	U
1	A	1061	U
1	A	1062	G
1	A	1064	C
1	A	1065	U
1	A	1066	U
1	A	1068	G
1	A	1070	A
1	A	1071	G
1	A	1075	C
1	A	1076	C
1	A	1079	C
1	A	1084	A
1	A	1088	A
1	A	1104	C
1	A	1111	A
1	A	1112	G
1	A	1119	U
1	A	1130	U
1	A	1131	G
1	A	1132	U
1	A	1133	A
1	A	1135	C
1	A	1143	A
1	A	1174	U
1	A	1176	U
1	A	1177	G
1	A	1180	U
1	A	1206	G
1	A	1212	G
1	A	1250	G
1	A	1251	C
1	A	1253	A
1	A	1256	G
1	A	1271	G
1	A	1272	A

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Mol	Chain	Res	Type
1	A	1300	G
1	A	1301	A
1	A	1306	C
1	A	1314	C
1	A	1321	A
1	A	1329	U
1	A	1332	G
1	A	1341	G
1	A	1345	C
1	A	1365	A
1	A	1368	G
1	A	1378	A
1	A	1379	U
1	A	1383	A
1	A	1416	G
1	A	1419	A
1	A	1420	A
1	A	1428	C
1	A	1454	C
1	A	1461	C
1	A	1475	G
1	A	1482	G
1	A	1490	A
1	A	1491	G
1	A	1504	A
1	A	1515	A
1	A	1524	G
1	A	1533	C
1	A	1535	A
1	A	1536	C
1	A	1555	G
1	A	1559	U
1	A	1560	G
1	A	1569	A
1	A	1581	G
1	A	1585	C
1	A	1611	C
1	A	1634	A
1	A	1647	U
1	A	1648	U
1	A	1654	A
1	A	1670	C

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Mol	Chain	Res	Type
1	A	1674	G
1	A	1694	C
1	A	1695	G
1	A	1715	G
1	A	1729	U
1	A	1730	C
1	A	1733	G
1	A	1738	G
1	A	1758	U
1	A	1764	C
1	A	1773	A
1	A	1780	A
1	A	1781	U
1	A	1784	A
1	A	1791	A
1	A	1800	C
1	A	1801	A
1	A	1802	A
1	A	1808	A
1	A	1816	C
1	A	1829	A
1	A	1833	C
1	A	1835	2MG
1	A	1836	C
1	A	1871	A
1	A	1901	A
1	A	1906	G
1	A	1911	PSU
1	A	1912	A
1	A	1913	A
1	A	1914	C
1	A	1917	PSU
1	A	1918	A
1	A	1919	A
1	A	1929	G
1	A	1930	G
1	A	1937	A
1	A	1938	A
1	A	1939	5MU
1	A	1940	U
1	A	1941	C
1	A	1944	U

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Mol	Chain	Res	Type
1	A	1955	U
1	A	1967	C
1	A	1970	A
1	A	1971	U
1	A	1972	G
1	A	1991	U
1	A	1993	U
1	A	1997	C
1	A	2021	C
1	A	2022	U
1	A	2023	C
1	A	2031	A
1	A	2033	A
1	A	2043	C
1	A	2049	G
1	A	2052	A
1	A	2055	C
1	A	2056	G
1	A	2060	A
1	A	2061	G
1	A	2062	A
1	A	2069	7MG
1	A	2072	C
1	A	2093	G
1	A	2096	C
1	A	2098	U
1	A	2110	G
1	A	2111	U
1	A	2112	G
1	A	2113	U
1	A	2116	G
1	A	2118	U
1	A	2119	A
1	A	2127	G
1	A	2131	U
1	A	2132	U
1	A	2133	G
1	A	2145	C
1	A	2162	G
1	A	2164	C
1	A	2170	A
1	A	2172	U

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Mol	Chain	Res	Type
1	A	2173	A
1	A	2198	A
1	A	2204	G
1	A	2211	A
1	A	2213	U
1	A	2225	A
1	A	2226	C
1	A	2250	G
1	A	2251	OMG
1	A	2252	G
1	A	2278	A
1	A	2283	C
1	A	2286	G
1	A	2287	A
1	A	2305	U
1	A	2309	A
1	A	2320	U
1	A	2327	A
1	A	2334	U
1	A	2335	A
1	A	2350	C
1	A	2354	C
1	A	2383	G
1	A	2385	C
1	A	2392	A
1	A	2402	U
1	A	2407	A
1	A	2423	U
1	A	2424	C
1	A	2426	A
1	A	2428	G
1	A	2429	G
1	A	2430	A
1	A	2431	U
1	A	2435	A
1	A	2441	U
1	A	2445	2MG
1	A	2446	G
1	A	2448	A
1	A	2449	H2U
1	A	2450	A
1	A	2457	PSU

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Mol	Chain	Res	Type
1	A	2458	G
1	A	2476	A
1	A	2498	OMC
1	A	2499	C
1	A	2502	G
1	A	2504	PSU
1	A	2505	G
1	A	2506	U
1	A	2518	A
1	A	2529	G
1	A	2547	A
1	A	2552	OMU
1	A	2553	G
1	A	2554	U
1	A	2567	G
1	A	2572	A
1	A	2580	PSU
1	A	2581	G
1	A	2585	U
1	A	2586	U
1	A	2602	A
1	A	2604	PSU
1	A	2605	PSU
1	A	2606	C
1	A	2609	U
1	A	2613	U
1	A	2614	A
1	A	2629	U
1	A	2636	C
1	A	2646	C
1	A	2655	G
1	A	2656	U
1	A	2682	A
1	A	2689	U
1	A	2690	U
1	A	2714	G
1	A	2718	G
1	A	2726	A
1	A	2739	U
1	A	2744	G
1	A	2748	A
1	A	2757	A

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Mol	Chain	Res	Type
1	A	2764	A
1	A	2765	A
1	A	2778	A
1	A	2779	U
1	A	2780	G
1	A	2791	G
1	A	2794	C
1	A	2797	U
1	A	2799	A
1	A	2800	A
1	A	2808	G
1	A	2809	A
1	A	2818	U
1	A	2820	A
1	A	2833	U
1	A	2849	U
1	A	2867	G
1	A	2868	A
1	A	2880	C
1	A	2893	A
1	A	2894	G
2	B	4	C
2	B	13	G
2	B	35	C
2	B	44	G
2	B	45	A
2	B	53	A
2	B	67	G
2	B	88	C
2	B	89	U
2	B	90	C
2	B	91	C
2	B	108	A
2	B	109	A
32	a	6	G
32	a	7	A
32	a	9	G
32	a	22	G
32	a	32	A
32	a	39	G
32	a	51	A
32	a	71	A

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Mol	Chain	Res	Type
32	a	86	G
32	a	87	C
32	a	121	U
32	a	130	A
32	a	183	C
32	a	184	G
32	a	209	U
32	a	210	C
32	a	212	G
32	a	226	G
32	a	247	G
32	a	251	G
32	a	266	G
32	a	267	C
32	a	280	C
32	a	281	G
32	a	282	A
32	a	289	G
32	a	306	A
32	a	328	C
32	a	345	C
32	a	347	G
32	a	351	G
32	a	352	C
32	a	367	U
32	a	372	C
32	a	392	C
32	a	406	G
32	a	413	G
32	a	422	C
32	a	424	G
32	a	429	U
32	a	467	U
32	a	479	U
32	a	484	G
32	a	485	U
32	a	486	U
32	a	496	A
32	a	497	G
32	a	516	PSU
32	a	517	G
32	a	527	7MG

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Mol	Chain	Res	Type
32	a	530	G
32	a	531	U
32	a	532	A
32	a	533	A
32	a	547	A
32	a	561	U
32	a	564	C
32	a	572	A
32	a	573	A
32	a	575	G
32	a	576	C
32	a	577	G
32	a	633	G
32	a	642	A
32	a	665	A
32	a	688	G
32	a	702	A
32	a	703	G
32	a	723	U
32	a	724	G
32	a	731	G
32	a	733	G
32	a	748	G
32	a	755	G
32	a	777	A
32	a	815	A
32	a	817	C
32	a	818	G
32	a	819	A
32	a	820	U
32	a	832	G
32	a	843	U
32	a	844	G
32	a	846	G
32	a	871	U
32	a	890	G
32	a	902	G
32	a	934	C
32	a	935	A
32	a	939	G
32	a	960	U
32	a	961	U

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Mol	Chain	Res	Type
32	a	966	2MG
32	a	967	5MC
32	a	968	A
32	a	969	A
32	a	975	A
32	a	976	G
32	a	977	A
32	a	989	U
32	a	991	U
32	a	992	U
32	a	993	G
32	a	1004	A
32	a	1026	G
32	a	1028	C
32	a	1030	U
32	a	1031	C
32	a	1033	G
32	a	1034	G
32	a	1035	A
32	a	1056	U
32	a	1065	U
32	a	1085	U
32	a	1094	G
32	a	1101	A
32	a	1130	A
32	a	1137	C
32	a	1138	G
32	a	1139	G
32	a	1152	A
32	a	1159	U
32	a	1168	U
32	a	1183	U
32	a	1184	G
32	a	1191	A
32	a	1196	A
32	a	1197	A
32	a	1201	A
32	a	1202	U
32	a	1207	2MG
32	a	1208	C
32	a	1212	U
32	a	1213	A

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Mol	Chain	Res	Type
32	a	1225	A
32	a	1238	A
32	a	1240	U
32	a	1241	G
32	a	1256	A
32	a	1258	G
32	a	1260	G
32	a	1278	G
32	a	1280	A
32	a	1282	C
32	a	1287	A
32	a	1298	U
32	a	1300	G
32	a	1301	U
32	a	1302	C
32	a	1317	C
32	a	1323	G
32	a	1347	G
32	a	1348	U
32	a	1363	A
32	a	1395	C
32	a	1400	C
32	a	1403	C
32	a	1408	A
32	a	1446	A
32	a	1448	C
32	a	1452	C
32	a	1492	A
32	a	1494	G
32	a	1498	UR3
32	a	1499	A
32	a	1502	A
32	a	1503	A
32	a	1506	U
32	a	1516	2MG
32	a	1517	G
32	a	1520	C
32	a	1529	G
32	a	1530	G
32	a	1534	A
32	a	1535	C
32	a	1536	C

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Mol	Chain	Res	Type
52	x	8	4SU
52	x	9	G
52	x	16	C
52	x	17	C
52	x	17(A)	U
52	x	18	G
52	x	19	G
52	x	20	H2U
52	x	21	A
52	x	22	G
52	x	54	5MU
52	x	55	PSU
52	x	56	C
58	y	3	U
58	y	7	A
58	y	9	A
58	y	10	G
58	y	13	C
58	y	14	A
58	y	16	H2U
58	y	17	H2U
58	y	18	G
58	y	19	G
58	y	20	H2U
58	y	21	A
58	y	22	G
58	y	34	G
58	y	35	G
58	y	41	G
58	y	43	G
58	y	46	7MG
58	y	47	U
58	y	48	C
58	y	54	5MU
58	y	55	PSU
58	y	56	C
58	y	57	G
58	y	58	A
58	y	59	A
58	y	72	C
58	y	73	A

All (45) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	51	G
1	A	86	G
1	A	204	A
1	A	242	G
1	A	372	G
1	A	458	G
1	A	479	A
1	A	490	C
1	A	746	PSU
1	A	752	A
1	A	858	G
1	A	859	G
1	A	893	C
1	A	955	PSU
1	A	1020	A
1	A	1022	G
1	A	1070	A
1	A	1130	U
1	A	1182	G
1	A	1190	G
1	A	1300	G
1	A	1399	C
1	A	1835	2MG
1	A	1911	PSU
1	A	1917	PSU
1	A	1939	5MU
1	A	1940	U
1	A	2251	OMG
1	A	2286	G
1	A	2326	C
1	A	2333	A
1	A	2391	G
1	A	2445	2MG
1	A	2449	H2U
1	A	2457	PSU
1	A	2498	OMC
1	A	2504	PSU
1	A	2566	A
1	A	2580	PSU
1	A	2605	PSU
1	A	2655	G
1	A	2756	U
1	A	2808	G

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Mol	Chain	Res	Type
2	B	66	A
2	B	88	C

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

46 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	6MZ	A	1618	1	18,25,26	0.80	1 (5%)	16,36,39	3.13	4 (25%)
1	2MG	A	1835	1	19,26,27	3.42	2 (10%)	20,38,41	2.49	9 (45%)
1	PSU	A	1911	1	16,21,22	1.37	3 (18%)	20,30,33	3.07	5 (25%)
1	3TD	A	1915	1	16,22,23	2.17	4 (25%)	19,32,35	1.46	4 (21%)
1	PSU	A	1917	1	16,21,22	1.47	3 (18%)	20,30,33	3.13	5 (25%)
1	5MU	A	1939	1	14,22,23	1.40	1 (7%)	16,32,35	2.77	4 (25%)
1	5MC	A	1962	1	15,22,23	1.31	2 (13%)	17,32,35	1.14	2 (11%)
1	6MZ	A	2030	1	18,25,26	0.79	1 (5%)	16,36,39	3.15	4 (25%)
1	7MG	A	2069	1	20,26,27	2.77	6 (30%)	22,39,42	2.26	6 (27%)
1	OMG	A	2251	1,52	18,26,27	2.41	2 (11%)	22,38,41	1.81	6 (27%)
1	2MG	A	2445	1	19,26,27	3.42	2 (10%)	20,38,41	2.37	9 (45%)
1	H2U	A	2449	1	17,21,22	3.65	5 (29%)	21,30,33	2.71	5 (23%)
1	PSU	A	2457	1	16,21,22	1.40	3 (18%)	20,30,33	3.06	5 (25%)
1	OMC	A	2498	1	15,22,23	1.07	2 (13%)	19,31,34	0.87	1 (5%)
1	2MA	A	2503	1	18,25,26	1.73	1 (5%)	17,37,40	1.88	2 (11%)
1	PSU	A	2504	1	16,21,22	1.36	2 (12%)	20,30,33	3.08	5 (25%)
1	OMU	A	2552	1	14,22,23	2.12	3 (21%)	18,31,34	2.05	1 (5%)
1	PSU	A	2580	1	16,21,22	1.49	3 (18%)	20,30,33	3.16	6 (30%)
1	PSU	A	2604	1	16,21,22	1.34	2 (12%)	20,30,33	3.10	6 (30%)
1	PSU	A	2605	1	16,21,22	1.47	3 (18%)	20,30,33	3.09	5 (25%)
1	1MG	A	745	1	18,26,27	2.41	3 (16%)	18,39,42	1.78	3 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	A	746	1	16,21,22	1.30	2 (12%)	20,30,33	3.17	6 (30%)
1	5MC	A	747	1	15,22,23	1.31	2 (13%)	17,32,35	1.15	2 (11%)
1	PSU	A	955	1	16,21,22	1.42	3 (18%)	20,30,33	3.08	5 (25%)
32	2MG	a	1207	32	19,26,27	3.43	2 (10%)	20,38,41	2.38	9 (45%)
32	4OC	a	1402	32	16,23,24	1.25	2 (12%)	19,32,35	1.30	2 (10%)
32	5MC	a	1407	32	15,22,23	1.32	2 (13%)	17,32,35	1.13	2 (11%)
32	UR3	a	1498	32	14,22,23	1.63	2 (14%)	16,32,35	0.64	0
32	2MG	a	1516	32	19,26,27	3.44	2 (10%)	20,38,41	2.36	9 (45%)
32	MA6	a	1518	32	16,26,27	0.60	0	18,38,41	1.85	4 (22%)
32	MA6	a	1519	32	16,26,27	0.53	0	18,38,41	2.00	4 (22%)
32	PSU	a	516	32	16,21,22	1.38	3 (18%)	20,30,33	3.09	5 (25%)
32	7MG	a	527	32	20,26,27	2.74	5 (25%)	22,39,42	2.07	4 (18%)
32	2MG	a	966	32	19,26,27	3.41	2 (10%)	20,38,41	2.43	9 (45%)
32	5MC	a	967	32	15,22,23	1.37	2 (13%)	17,32,35	1.20	2 (11%)
52	H2U	x	20	52	17,21,22	3.65	5 (29%)	21,30,33	2.69	5 (23%)
52	5MU	x	54	52	14,22,23	1.38	1 (7%)	16,32,35	2.75	4 (25%)
52	PSU	x	55	52	16,21,22	1.45	4 (25%)	20,30,33	3.18	5 (25%)
52	4SU	x	8	52	14,21,22	1.74	3 (21%)	15,30,33	1.38	2 (13%)
58	H2U	y	16	58	17,21,22	3.68	5 (29%)	21,30,33	2.67	5 (23%)
58	H2U	y	17	58	17,21,22	3.65	5 (29%)	21,30,33	2.75	5 (23%)
58	H2U	y	20	58	17,21,22	3.64	5 (29%)	21,30,33	2.69	4 (19%)
58	YG	y	37	1,58	29,42,43	1.46	2 (6%)	29,62,65	1.87	8 (27%)
58	7MG	y	46	58	20,26,27	2.74	5 (25%)	22,39,42	1.89	5 (22%)
58	5MU	y	54	58	14,22,23	1.38	1 (7%)	16,32,35	2.83	4 (25%)
58	PSU	y	55	58	16,21,22	1.48	3 (18%)	20,30,33	3.22	6 (30%)

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	6MZ	A	1618	1	-	0/5/27/28	0/3/3/3
1	2MG	A	1835	1	2/2/5/6	0/5/27/28	0/3/3/3
1	PSU	A	1911	1	2/2/5/5	0/7/25/26	0/2/2/2
1	3TD	A	1915	1	1/1/5/5	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	A	1917	1	2/2/5/5	0/7/25/26	0/2/2/2
1	5MU	A	1939	1	3/3/5/5	0/3/25/26	0/2/2/2
1	5MC	A	1962	1	-	0/3/25/26	0/2/2/2
1	6MZ	A	2030	1	-	0/5/27/28	0/3/3/3
1	7MG	A	2069	1	1/1/7/7	0/7/37/38	0/3/3/3
1	OMG	A	2251	1,52	2/2/5/5	0/5/27/28	0/3/3/3
1	2MG	A	2445	1	2/2/5/6	0/5/27/28	0/3/3/3
1	H2U	A	2449	1	1/1/8/9	0/7/38/39	0/2/2/2
1	PSU	A	2457	1	2/2/5/5	0/7/25/26	0/2/2/2
1	OMC	A	2498	1	2/2/5/5	0/5/27/28	0/2/2/2
1	2MA	A	2503	1	2/2/5/5	0/3/25/26	0/3/3/3
1	PSU	A	2504	1	2/2/5/5	0/7/25/26	0/2/2/2
1	OMU	A	2552	1	1/1/5/5	0/5/27/28	0/2/2/2
1	PSU	A	2580	1	2/2/5/5	0/7/25/26	0/2/2/2
1	PSU	A	2604	1	2/2/5/5	0/7/25/26	0/2/2/2
1	PSU	A	2605	1	2/2/5/5	0/7/25/26	0/2/2/2
1	1MG	A	745	1	-	0/3/25/26	0/3/3/3
1	PSU	A	746	1	2/2/5/5	0/7/25/26	0/2/2/2
1	5MC	A	747	1	-	0/3/25/26	0/2/2/2
1	PSU	A	955	1	2/2/5/5	0/7/25/26	0/2/2/2
32	2MG	a	1207	32	2/2/5/6	0/5/27/28	0/3/3/3
32	4OC	a	1402	32	2/2/5/6	0/7/29/30	0/2/2/2
32	5MC	a	1407	32	-	0/3/25/26	0/2/2/2
32	UR3	a	1498	32	2/2/5/5	0/3/25/26	0/2/2/2
32	2MG	a	1516	32	2/2/5/6	0/5/27/28	0/3/3/3
32	MA6	a	1518	32	2/2/6/6	0/7/29/30	0/3/3/3
32	MA6	a	1519	32	2/2/6/6	0/7/29/30	0/3/3/3
32	PSU	a	516	32	2/2/5/5	0/7/25/26	0/2/2/2
32	7MG	a	527	32	1/1/7/7	0/7/37/38	0/3/3/3
32	2MG	a	966	32	2/2/5/6	0/5/27/28	0/3/3/3
32	5MC	a	967	32	-	0/3/25/26	0/2/2/2
52	H2U	x	20	52	1/1/8/9	0/7/38/39	0/2/2/2
52	5MU	x	54	52	3/3/5/5	0/3/25/26	0/2/2/2
52	PSU	x	55	52	2/2/5/5	0/7/25/26	0/2/2/2
52	4SU	x	8	52	3/3/5/5	0/3/25/26	0/2/2/2
58	H2U	y	16	58	1/1/8/9	0/7/38/39	0/2/2/2
58	H2U	y	17	58	1/1/8/9	0/7/38/39	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	H2U	y	20	58	1/1/8/9	0/7/38/39	0/2/2/2
58	YG	y	37	1,58	-	0/20/42/43	0/4/4/4
58	7MG	y	46	58	1/1/7/7	0/7/37/38	0/3/3/3
58	5MU	y	54	58	3/3/5/5	0/3/25/26	0/2/2/2
58	PSU	y	55	58	2/2/5/5	0/7/25/26	0/2/2/2

All (122) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	y	16	H2U	C6-N1	-9.40	1.35	1.47
1	A	2449	H2U	C6-N1	-9.25	1.35	1.47
52	x	20	H2U	C6-N1	-9.21	1.35	1.47
58	y	17	H2U	C6-N1	-9.21	1.35	1.47
58	y	20	H2U	C6-N1	-9.18	1.35	1.47
58	y	46	7MG	C8-N9	-7.44	1.34	1.45
1	A	2069	7MG	C8-N9	-7.43	1.34	1.45
32	a	527	7MG	C8-N9	-7.41	1.34	1.45
58	y	37	YG	O23-C21	-6.02	1.25	1.34
58	y	20	H2U	C6-C5	-5.43	1.42	1.52
1	A	2449	H2U	C6-C5	-5.43	1.42	1.52
52	x	20	H2U	C6-C5	-5.42	1.42	1.52
58	y	16	H2U	C6-C5	-5.42	1.42	1.52
58	y	17	H2U	C6-C5	-5.39	1.42	1.52
58	y	54	5MU	C2-N3	-4.30	1.29	1.38
1	A	1939	5MU	C2-N3	-4.30	1.29	1.38
52	x	54	5MU	C2-N3	-4.24	1.29	1.38
52	x	20	H2U	C5-C4	-4.10	1.40	1.50
58	y	16	H2U	C5-C4	-4.09	1.40	1.50
58	y	20	H2U	C5-C4	-4.09	1.40	1.50
1	A	2449	H2U	C5-C4	-4.07	1.40	1.50
58	y	17	H2U	C5-C4	-4.06	1.40	1.50
1	A	745	1MG	CM1-N1	-3.66	1.39	1.47
1	A	955	PSU	C2-N1	-3.29	1.31	1.38
32	a	516	PSU	C2-N1	-3.29	1.31	1.38
58	y	55	PSU	C2-N1	-3.27	1.31	1.38
1	A	1911	PSU	C2-N1	-3.26	1.31	1.38
52	x	55	PSU	C2-N1	-3.26	1.31	1.38
1	A	1917	PSU	C2-N1	-3.26	1.31	1.38
1	A	2605	PSU	C2-N1	-3.25	1.31	1.38
1	A	2580	PSU	C2-N1	-3.23	1.31	1.38
1	A	2504	PSU	C2-N1	-3.22	1.31	1.38
1	A	2457	PSU	C2-N1	-3.21	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	746	PSU	C2-N1	-3.20	1.31	1.38
1	A	2604	PSU	C2-N1	-3.18	1.31	1.38
58	y	37	YG	O18-C16	-3.02	1.25	1.33
52	x	20	H2U	C2-N3	-3.00	1.32	1.38
58	y	17	H2U	C2-N3	-2.98	1.32	1.38
58	y	16	H2U	C2-N3	-2.98	1.32	1.38
58	y	20	H2U	C2-N3	-2.97	1.32	1.38
1	A	2449	H2U	C2-N3	-2.95	1.32	1.38
1	A	1917	PSU	O4'-C1'	-2.90	1.40	1.44
1	A	2580	PSU	O4'-C1'	-2.89	1.40	1.44
52	x	8	4SU	C2-N3	-2.81	1.32	1.38
32	a	1402	4OC	C2-N3	-2.80	1.32	1.38
1	A	1915	3TD	C10-N3	-2.71	1.41	1.47
32	a	1407	5MC	C2-N3	-2.63	1.33	1.38
32	a	967	5MC	C2-N3	-2.62	1.33	1.38
1	A	747	5MC	C2-N3	-2.60	1.33	1.38
1	A	1962	5MC	C2-N3	-2.60	1.33	1.38
58	y	55	PSU	O4'-C1'	-2.59	1.40	1.44
1	A	2605	PSU	O4'-C1'	-2.59	1.40	1.44
58	y	55	PSU	C2-N3	-2.48	1.33	1.38
52	x	55	PSU	C2-N3	-2.45	1.33	1.38
1	A	2552	OMU	C2-N3	-2.43	1.33	1.38
1	A	2457	PSU	O4'-C1'	-2.40	1.40	1.44
1	A	955	PSU	O4'-C1'	-2.39	1.40	1.44
1	A	2580	PSU	C2-N3	-2.37	1.33	1.38
1	A	2605	PSU	C2-N3	-2.30	1.33	1.38
1	A	1911	PSU	C2-N3	-2.29	1.33	1.38
1	A	2457	PSU	C2-N3	-2.29	1.33	1.38
1	A	1917	PSU	C2-N3	-2.28	1.33	1.38
1	A	2552	OMU	C6-N1	-2.27	1.32	1.35
1	A	2504	PSU	C2-N3	-2.27	1.33	1.38
1	A	2604	PSU	C2-N3	-2.26	1.33	1.38
32	a	516	PSU	C2-N3	-2.26	1.33	1.38
1	A	955	PSU	C2-N3	-2.24	1.33	1.38
1	A	746	PSU	C2-N3	-2.24	1.33	1.38
52	x	55	PSU	O4'-C1'	-2.23	1.41	1.44
32	a	516	PSU	O4'-C1'	-2.16	1.41	1.44
1	A	1915	3TD	C2-N1	-2.09	1.34	1.38
1	A	1911	PSU	O4'-C1'	-2.09	1.41	1.44
1	A	2498	OMC	C2-N3	-2.03	1.34	1.38
1	A	2069	7MG	C8-N7	-2.01	1.34	1.43
52	x	55	PSU	C6-C5	2.03	1.41	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	x	8	4SU	C4-S4	2.05	1.71	1.67
1	A	2030	6MZ	C6-N6	2.12	1.38	1.35
58	y	46	7MG	C4-N3	2.20	1.37	1.34
32	a	1498	UR3	C6-C5	2.21	1.42	1.38
1	A	1618	6MZ	C6-N6	2.22	1.39	1.35
32	a	527	7MG	C6-C5	2.25	1.44	1.41
1	A	2498	OMC	C4-N4	2.30	1.42	1.35
58	y	46	7MG	C6-C5	2.31	1.44	1.41
1	A	2069	7MG	C6-C5	2.37	1.44	1.41
1	A	2069	7MG	C4-N3	2.38	1.37	1.34
32	a	527	7MG	C4-N3	2.50	1.37	1.34
1	A	1915	3TD	C6-C5	2.89	1.42	1.38
32	a	1402	4OC	C4-N4	3.17	1.43	1.36
1	A	1962	5MC	C4-N4	3.62	1.43	1.34
1	A	747	5MC	C4-N4	3.64	1.43	1.34
32	a	1407	5MC	C4-N4	3.65	1.43	1.34
32	a	967	5MC	C4-N4	3.66	1.43	1.34
32	a	527	7MG	C2-N2	4.99	1.44	1.34
1	A	2069	7MG	C2-N2	5.02	1.44	1.34
58	y	46	7MG	C2-N2	5.03	1.44	1.34
52	x	8	4SU	C5-C4	5.07	1.44	1.38
1	A	745	1MG	C2-N2	5.26	1.44	1.33
32	a	1498	UR3	O4-C4	5.32	1.37	1.24
1	A	2251	OMG	C2-N2	6.01	1.46	1.34
1	A	1835	2MG	O6-C6	6.73	1.41	1.24
1	A	1915	3TD	O4-C4	6.74	1.41	1.24
32	a	527	7MG	O6-C6	6.74	1.41	1.24
1	A	2552	OMU	O4-C4	6.74	1.41	1.24
1	A	2445	2MG	O6-C6	6.77	1.41	1.24
32	a	966	2MG	O6-C6	6.79	1.41	1.24
32	a	1516	2MG	O6-C6	6.80	1.41	1.24
32	a	1207	2MG	O6-C6	6.80	1.41	1.24
58	y	46	7MG	O6-C6	6.85	1.41	1.24
1	A	2069	7MG	O6-C6	6.86	1.41	1.24
1	A	2503	2MA	C6-N6	6.88	1.43	1.27
1	A	745	1MG	O6-C6	7.17	1.42	1.24
1	A	2251	OMG	O6-C6	7.75	1.44	1.24
58	y	16	H2U	O4-C4	9.07	1.42	1.23
52	x	20	H2U	O4-C4	9.08	1.42	1.23
58	y	20	H2U	O4-C4	9.09	1.42	1.23
1	A	2449	H2U	O4-C4	9.10	1.42	1.23
58	y	17	H2U	O4-C4	9.11	1.42	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	a	966	2MG	C2-N2	12.92	1.45	1.34
1	A	1835	2MG	C2-N2	12.94	1.45	1.34
32	a	1207	2MG	C2-N2	12.98	1.45	1.34
1	A	2445	2MG	C2-N2	12.98	1.45	1.34
32	a	1516	2MG	C2-N2	13.01	1.45	1.34

All (213) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1618	6MZ	N3-C2-N1	-9.08	120.95	128.86
1	A	2030	6MZ	N3-C2-N1	-9.02	121.00	128.86
52	x	55	PSU	N1-C2-N3	-8.58	122.23	128.40
58	y	55	PSU	N1-C2-N3	-8.50	122.29	128.40
1	A	2580	PSU	N1-C2-N3	-8.41	122.35	128.40
1	A	2605	PSU	N1-C2-N3	-8.38	122.37	128.40
1	A	1917	PSU	N1-C2-N3	-8.35	122.39	128.40
1	A	746	PSU	N1-C2-N3	-8.20	122.50	128.40
1	A	2504	PSU	N1-C2-N3	-8.15	122.54	128.40
1	A	2604	PSU	N1-C2-N3	-8.11	122.56	128.40
1	A	955	PSU	N1-C2-N3	-8.06	122.60	128.40
1	A	2457	PSU	N1-C2-N3	-8.02	122.63	128.40
32	a	516	PSU	N1-C2-N3	-7.87	122.74	128.40
1	A	1911	PSU	N1-C2-N3	-7.83	122.76	128.40
32	a	516	PSU	C5-C4-N3	-7.57	119.22	125.43
1	A	1911	PSU	C5-C4-N3	-7.49	119.29	125.43
1	A	746	PSU	C5-C4-N3	-7.39	119.37	125.43
1	A	955	PSU	C5-C4-N3	-7.38	119.38	125.43
1	A	2604	PSU	C5-C4-N3	-7.38	119.38	125.43
58	y	54	5MU	C5-C6-N1	-7.35	114.19	122.15
1	A	2457	PSU	C5-C4-N3	-7.32	119.42	125.43
1	A	1917	PSU	C5-C4-N3	-7.27	119.47	125.43
1	A	2504	PSU	C5-C4-N3	-7.22	119.50	125.43
58	y	55	PSU	C5-C4-N3	-7.18	119.54	125.43
1	A	2605	PSU	C5-C4-N3	-7.17	119.55	125.43
52	x	55	PSU	C5-C4-N3	-7.09	119.61	125.43
1	A	1939	5MU	C5-C6-N1	-7.07	114.50	122.15
1	A	2580	PSU	C5-C4-N3	-6.97	119.71	125.43
52	x	54	5MU	C5-C6-N1	-6.86	114.72	122.15
32	a	1519	MA6	N3-C2-N1	-5.79	123.82	128.86
32	a	1518	MA6	N3-C2-N1	-5.40	124.16	128.86
1	A	2069	7MG	C5-C4-N3	-5.23	117.75	126.47
58	y	16	H2U	C4-N3-C2	-5.16	121.39	125.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	y	17	H2U	C4-N3-C2	-5.02	121.51	125.81
32	a	527	7MG	C5-C4-N3	-4.81	118.44	126.47
1	A	2449	H2U	C4-N3-C2	-4.71	121.78	125.81
52	x	20	H2U	C4-N3-C2	-4.71	121.78	125.81
58	y	20	H2U	C4-N3-C2	-4.61	121.86	125.81
58	y	46	7MG	C5-C4-N3	-4.33	119.24	126.47
1	A	1835	2MG	C6-C5-C4	-4.05	116.82	120.84
58	y	37	YG	O23-C21-O22	-4.01	119.11	124.60
32	a	966	2MG	C6-C5-C4	-3.85	117.02	120.84
1	A	745	1MG	C4-C5-N7	-3.83	105.71	109.41
1	A	1915	3TD	C5-C6-N1	-3.80	119.46	124.39
32	a	1207	2MG	C6-C5-C4	-3.74	117.13	120.84
1	A	2030	6MZ	C9-N6-C6	-3.73	119.66	122.85
1	A	2445	2MG	C6-C5-C4	-3.68	117.18	120.84
1	A	745	1MG	C6-C5-C4	-3.65	117.40	119.92
32	a	1402	4OC	CM4-N4-C4	-3.59	119.84	122.94
1	A	1835	2MG	C4-C5-N7	-3.54	105.99	109.41
32	a	1516	2MG	C6-C5-C4	-3.50	117.36	120.84
1	A	1835	2MG	CM2-N2-C2	-3.40	119.50	123.63
1	A	1618	6MZ	C9-N6-C6	-3.37	119.97	122.85
32	a	967	5MC	C5-C6-N1	-3.33	118.54	122.15
1	A	2604	PSU	C5-C6-N1	-3.31	120.09	124.39
32	a	966	2MG	C4-C5-N7	-3.29	106.24	109.41
1	A	747	5MC	C5-C6-N1	-3.27	118.61	122.15
1	A	2445	2MG	CM2-N2-C2	-3.26	119.66	123.63
1	A	1962	5MC	C5-C6-N1	-3.26	118.62	122.15
32	a	1407	5MC	C5-C6-N1	-3.25	118.64	122.15
1	A	1939	5MU	C5-C4-N3	-3.22	121.69	125.24
32	a	1207	2MG	CM2-N2-C2	-3.21	119.72	123.63
32	a	966	2MG	N3-C2-N1	-3.20	121.39	126.23
32	a	966	2MG	CM2-N2-C2	-3.20	119.73	123.63
1	A	746	PSU	C5-C6-N1	-3.20	120.24	124.39
58	y	17	H2U	O2-C2-N1	-3.15	119.17	123.12
1	A	1835	2MG	N3-C2-N1	-3.15	121.47	126.23
1	A	2457	PSU	C5-C6-N1	-3.14	120.32	124.39
1	A	2445	2MG	C4-C5-N7	-3.12	106.39	109.41
32	a	1207	2MG	N3-C2-N1	-3.11	121.53	126.23
32	a	516	PSU	C5-C6-N1	-3.10	120.37	124.39
1	A	746	PSU	C5-C1'-C2'	-3.10	110.20	115.55
1	A	2504	PSU	C5-C6-N1	-3.10	120.37	124.39
32	a	1207	2MG	C4-C5-N7	-3.08	106.43	109.41
1	A	1911	PSU	C5-C6-N1	-3.07	120.41	124.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2445	2MG	N3-C2-N1	-3.07	121.59	126.23
32	a	1516	2MG	CM2-N2-C2	-3.07	119.90	123.63
52	x	54	5MU	C5-C4-N3	-3.04	121.89	125.24
1	A	2251	OMG	C5-C6-N1	-3.04	119.16	123.48
32	a	1516	2MG	C4-C5-N7	-3.03	106.48	109.41
32	a	1516	2MG	N3-C2-N1	-3.03	121.64	126.23
32	a	1519	MA6	C4-C5-N7	-3.03	106.48	109.41
1	A	2580	PSU	C5-C6-N1	-2.98	120.52	124.39
1	A	955	PSU	C5-C6-N1	-2.98	120.53	124.39
52	x	8	4SU	C5-C4-N3	-2.97	119.98	123.73
1	A	2251	OMG	C4-C5-N7	-2.94	106.57	109.41
58	y	37	YG	C13-C12-C11	-2.92	125.58	130.66
1	A	1917	PSU	C5-C6-N1	-2.92	120.60	124.39
1	A	2251	OMG	C6-C5-C4	-2.90	117.96	120.84
58	y	54	5MU	C5-C4-N3	-2.89	122.05	125.24
1	A	2251	OMG	N3-C2-N1	-2.85	123.30	127.46
1	A	2605	PSU	C5-C6-N1	-2.77	120.79	124.39
1	A	2030	6MZ	C4-C5-N7	-2.76	106.74	109.41
32	a	1518	MA6	C4-C5-N7	-2.75	106.76	109.41
58	y	16	H2U	O2-C2-N1	-2.74	119.68	123.12
1	A	1618	6MZ	C4-C5-N7	-2.66	106.84	109.41
32	a	1402	4OC	C5-C4-N3	-2.64	118.80	123.21
52	x	55	PSU	C5-C6-N1	-2.63	120.98	124.39
58	y	55	PSU	C5-C6-N1	-2.60	121.02	124.39
1	A	2503	2MA	C4-C5-N7	-2.59	106.90	109.41
1	A	1939	5MU	C5M-C5-C6	-2.41	113.86	118.67
1	A	1915	3TD	C5-C1'-C2'	-2.39	111.42	115.55
58	y	54	5MU	C5M-C5-C6	-2.39	113.91	118.67
52	x	54	5MU	C5M-C5-C6	-2.38	113.92	118.67
58	y	37	YG	O18-C16-O17	-2.29	119.20	123.82
58	y	37	YG	C3-N3-C2	-2.26	115.09	118.31
32	a	1207	2MG	C5-C6-N1	-2.24	120.29	123.48
1	A	1835	2MG	C1'-N9-C4	-2.24	122.77	126.64
32	a	1516	2MG	C5-C6-N1	-2.24	120.30	123.48
1	A	2445	2MG	C5-C6-N1	-2.23	120.31	123.48
32	a	966	2MG	C5-C6-N1	-2.19	120.37	123.48
58	y	46	7MG	C5-C6-N1	-2.11	120.06	123.37
1	A	1835	2MG	C5-C6-N1	-2.05	120.57	123.48
52	x	20	H2U	O2-C2-N1	-2.02	120.59	123.12
1	A	2069	7MG	C5-C6-N1	-2.01	120.21	123.37
1	A	2449	H2U	O2-C2-N3	-2.01	117.69	121.50
32	a	966	2MG	N2-C2-N3	2.07	118.97	116.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a	1207	2MG	N2-C2-N3	2.13	119.02	116.95
1	A	2445	2MG	N2-C2-N3	2.18	119.07	116.95
1	A	1915	3TD	O4'-C1'-C2'	2.19	107.97	104.45
1	A	2604	PSU	O4'-C1'-C2'	2.20	107.99	104.45
32	a	1516	2MG	N2-C2-N3	2.23	119.12	116.95
32	a	967	5MC	N4-C4-N3	2.24	120.31	117.00
1	A	1962	5MC	N4-C4-N3	2.25	120.32	117.00
1	A	2580	PSU	O4'-C1'-C5	2.25	113.41	109.93
32	a	1407	5MC	N4-C4-N3	2.27	120.36	117.00
1	A	747	5MC	N4-C4-N3	2.27	120.36	117.00
32	a	1516	2MG	N2-C2-N1	2.35	119.24	116.95
58	y	55	PSU	C4-C5-C1'	2.43	125.85	121.15
1	A	2445	2MG	N2-C2-N1	2.46	119.34	116.95
1	A	2498	OMC	N4-C4-N3	2.47	120.79	116.64
58	y	20	H2U	C5-C4-N3	2.47	119.18	116.72
58	y	46	7MG	C2-N3-C4	2.50	120.98	113.95
52	x	20	H2U	C5-C4-N3	2.53	119.24	116.72
1	A	2449	H2U	C5-C4-N3	2.55	119.26	116.72
32	a	1207	2MG	N2-C2-N1	2.58	119.46	116.95
58	y	17	H2U	C5-C4-N3	2.63	119.34	116.72
32	a	1519	MA6	N1-C6-N6	2.72	119.88	117.00
32	a	527	7MG	C2-N3-C4	2.73	121.61	113.95
1	A	2069	7MG	C6-N1-C2	2.73	119.99	116.06
58	y	16	H2U	C5-C4-N3	2.76	119.47	116.72
32	a	966	2MG	N2-C2-N1	2.77	119.64	116.95
1	A	1835	2MG	N2-C2-N1	2.78	119.65	116.95
1	A	1835	2MG	C6-N1-C2	2.78	120.16	115.18
32	a	1516	2MG	C6-N1-C2	2.81	120.21	115.18
1	A	2069	7MG	C2-N3-C4	2.82	121.86	113.95
1	A	2445	2MG	C6-N1-C2	2.83	120.25	115.18
32	a	527	7MG	C6-N1-C2	2.84	120.14	116.06
32	a	966	2MG	C6-N1-C2	2.85	120.29	115.18
1	A	1911	PSU	C6-N1-C2	2.86	119.94	115.36
32	a	1207	2MG	C6-N1-C2	2.87	120.32	115.18
32	a	516	PSU	C6-N1-C2	2.88	119.97	115.36
1	A	955	PSU	C6-N1-C2	2.89	119.99	115.36
1	A	1917	PSU	C6-N1-C2	2.90	120.00	115.36
1	A	2605	PSU	C6-N1-C2	2.91	120.02	115.36
58	y	55	PSU	C6-N1-C2	2.94	120.07	115.36
1	A	2457	PSU	C6-N1-C2	2.95	120.08	115.36
52	x	55	PSU	C6-N1-C2	2.97	120.11	115.36
1	A	2504	PSU	C6-N1-C2	2.98	120.13	115.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	746	PSU	C6-N1-C2	2.99	120.15	115.36
58	y	46	7MG	C6-N1-C2	2.99	120.36	116.06
1	A	2580	PSU	C6-N1-C2	3.00	120.16	115.36
1	A	2251	OMG	C6-N1-C2	3.06	120.46	116.06
1	A	2069	7MG	C4-N9-C1'	3.06	133.97	126.58
1	A	2604	PSU	C6-N1-C2	3.07	120.27	115.36
32	a	1518	MA6	C2-N1-C6	3.08	119.38	111.82
32	a	1518	MA6	N1-C6-N6	3.12	120.31	117.00
1	A	1915	3TD	C6-N1-C2	3.16	120.41	115.36
32	a	1519	MA6	C2-N1-C6	3.19	119.64	111.82
58	y	37	YG	O18-C16-C15	3.22	120.04	111.54
58	y	37	YG	O23-C21-N20	3.61	117.73	110.82
58	y	37	YG	C24-O23-C21	3.73	120.28	115.68
52	x	8	4SU	C2-N3-C4	3.88	120.83	115.11
58	y	37	YG	C3-N3-C4	3.98	123.98	118.31
1	A	2251	OMG	C2-N3-C4	4.37	120.26	115.16
58	y	16	H2U	N3-C2-N1	4.83	121.54	116.73
58	y	20	H2U	N3-C2-N1	4.84	121.55	116.73
1	A	2449	H2U	N3-C2-N1	4.84	121.55	116.73
52	x	20	H2U	N3-C2-N1	4.88	121.58	116.73
1	A	745	1MG	C2-N3-C4	4.90	120.88	115.16
58	y	17	H2U	N3-C2-N1	5.08	121.79	116.73
58	y	46	7MG	N3-C4-N9	5.65	134.19	126.98
32	a	527	7MG	N3-C4-N9	6.26	134.97	126.98
32	a	1207	2MG	C2-N3-C4	6.36	122.37	115.11
1	A	2445	2MG	C2-N3-C4	6.39	122.41	115.11
32	a	1516	2MG	C2-N3-C4	6.40	122.41	115.11
1	A	2604	PSU	C4-N3-C2	6.42	120.78	115.16
1	A	2457	PSU	C4-N3-C2	6.46	120.81	115.16
32	a	966	2MG	C2-N3-C4	6.47	122.49	115.11
1	A	1911	PSU	C4-N3-C2	6.47	120.82	115.16
1	A	2504	PSU	C4-N3-C2	6.49	120.83	115.16
1	A	1835	2MG	C2-N3-C4	6.50	122.53	115.11
32	a	516	PSU	C4-N3-C2	6.54	120.88	115.16
1	A	746	PSU	C4-N3-C2	6.59	120.92	115.16
1	A	955	PSU	C4-N3-C2	6.59	120.93	115.16
1	A	2580	PSU	C4-N3-C2	6.68	121.00	115.16
1	A	2503	2MA	C2-N3-C4	6.72	121.22	115.41
1	A	2605	PSU	C4-N3-C2	6.75	121.07	115.16
1	A	1917	PSU	C4-N3-C2	6.81	121.11	115.16
1	A	2069	7MG	N3-C4-N9	6.89	135.78	126.98
58	y	55	PSU	C4-N3-C2	7.10	121.37	115.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	x	55	PSU	C4-N3-C2	7.15	121.41	115.16
1	A	2030	6MZ	C2-N1-C6	7.28	121.27	116.53
1	A	1618	6MZ	C2-N1-C6	7.31	121.29	116.53
1	A	1939	5MU	C5M-C5-C4	7.36	128.67	120.17
58	y	54	5MU	C5M-C5-C4	7.43	128.75	120.17
52	x	54	5MU	C5M-C5-C4	7.46	128.78	120.17
1	A	2552	OMU	C4-N3-C2	8.20	121.17	114.13
58	y	16	H2U	C5-C6-N1	8.89	119.94	110.70
58	y	17	H2U	C5-C6-N1	9.22	120.28	110.70
52	x	20	H2U	C5-C6-N1	9.41	120.48	110.70
1	A	2449	H2U	C5-C6-N1	9.45	120.52	110.70
58	y	20	H2U	C5-C6-N1	9.45	120.53	110.70

All (70) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
52	x	8	4SU	C4'
52	x	8	4SU	C2'
52	x	8	4SU	C3'
32	a	1498	UR3	C2'
32	a	1498	UR3	C3'
58	y	46	7MG	C1'
32	a	516	PSU	C4'
32	a	516	PSU	C2'
1	A	2457	PSU	C4'
1	A	2457	PSU	C2'
1	A	1835	2MG	C2'
1	A	1835	2MG	C3'
32	a	1402	4OC	C2'
32	a	1402	4OC	C1'
1	A	2449	H2U	C1'
1	A	955	PSU	C4'
1	A	955	PSU	C2'
32	a	1516	2MG	C2'
32	a	1516	2MG	C3'
58	y	16	H2U	C1'
1	A	746	PSU	C4'
1	A	746	PSU	C2'
52	x	55	PSU	C4'
52	x	55	PSU	C2'
32	a	527	7MG	C1'
32	a	1519	MA6	C2'

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Mol	Chain	Res	Type	Atom
32	a	1519	MA6	C3'
1	A	2445	2MG	C2'
1	A	2445	2MG	C3'
58	y	17	H2U	C1'
1	A	2069	7MG	C1'
1	A	1917	PSU	C4'
1	A	1917	PSU	C2'
1	A	2580	PSU	C4'
1	A	2580	PSU	C2'
1	A	2498	OMC	C4'
1	A	2498	OMC	C2'
32	a	966	2MG	C2'
32	a	966	2MG	C3'
1	A	1915	3TD	C4'
58	y	55	PSU	C4'
58	y	55	PSU	C2'
1	A	2552	OMU	C4'
52	x	20	H2U	C1'
1	A	2251	OMG	C3'
1	A	2251	OMG	C1'
1	A	2605	PSU	C4'
1	A	2605	PSU	C2'
1	A	1911	PSU	C4'
1	A	1911	PSU	C2'
52	x	54	5MU	C4'
52	x	54	5MU	C2'
52	x	54	5MU	C3'
58	y	54	5MU	C4'
58	y	54	5MU	C2'
58	y	54	5MU	C3'
32	a	1207	2MG	C2'
32	a	1207	2MG	C3'
1	A	1939	5MU	C4'
1	A	1939	5MU	C2'
1	A	1939	5MU	C3'
1	A	2503	2MA	C2'
1	A	2503	2MA	C1'
32	a	1518	MA6	C2'
32	a	1518	MA6	C3'
1	A	2604	PSU	C4'
1	A	2604	PSU	C2'
1	A	2504	PSU	C4'

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Mol	Chain	Res	Type	Atom
1	A	2504	PSU	C2'
58	y	20	H2U	C1'

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1915	3TD	3	0
1	A	1962	5MC	1	0
1	A	2030	6MZ	1	0
1	A	2069	7MG	3	0
1	A	2251	OMG	1	0
1	A	2503	2MA	2	0
1	A	2504	PSU	1	0
1	A	2552	OMU	1	0
1	A	2580	PSU	2	0
1	A	745	1MG	2	0
1	A	746	PSU	2	0
1	A	747	5MC	3	0
1	A	955	PSU	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
57	z	6

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	z	517:UNK	C	518:UNK	N	39.33
1	z	561:UNK	C	663:ALA	N	37.34
1	z	493:UNK	C	494:UNK	N	34.24
1	z	547:UNK	C	548:UNK	N	30.19
1	z	526:UNK	C	527:UNK	N	18.32
1	z	535:UNK	C	536:UNK	N	8.04