



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:53 PM GMT

PDB ID : 4W2G  
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with pactamycin (soaked), mRNA and three deacylated tRNAs in the A, P and E sites  
Authors : Polikanov, Y.S.; Osterman, I.A.; Szal, T.; Tashlitsky, V.N.; Serebryakova, M.V.; Kusochev, P.; Bulkley, D.; Malanicheva, I.A.; Efimenko, T.A.; Efremenkova, O.V.; Konevega, A.L.; Shaw, K.J.; Bogdanov, A.A.; Rodnina, M.V.; Dontsova, O.A.; Mankin, A.S.; Steitz, T.A.; Sergiev, P.V.  
Deposited on : 2014-09-12  
Resolution : 2.55 Å(reported)

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

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

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

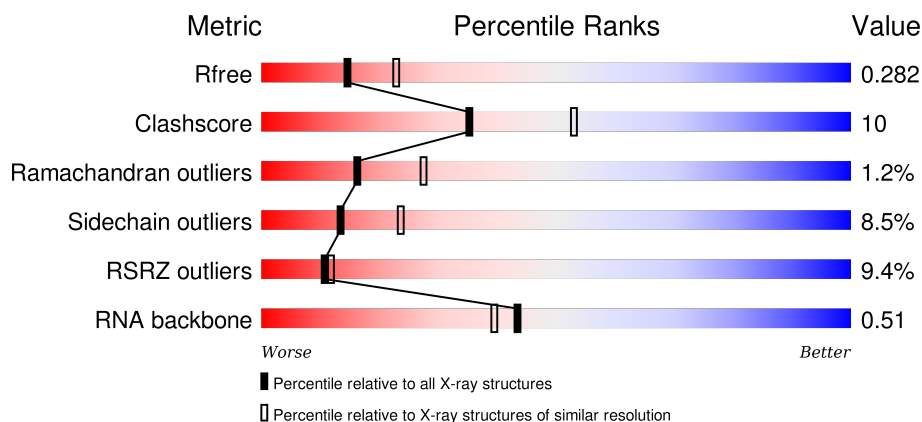
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 Å.

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



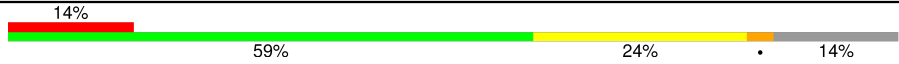

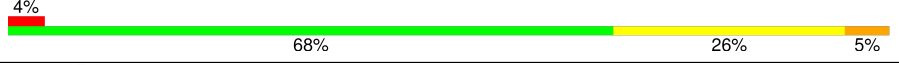

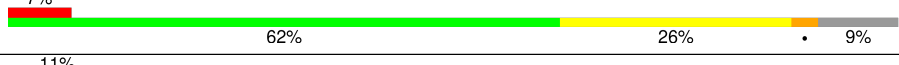
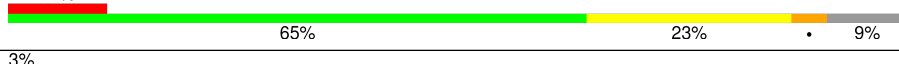
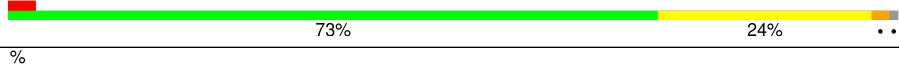

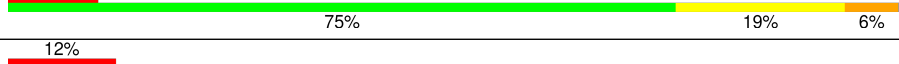


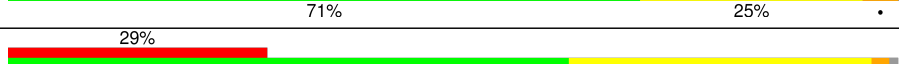

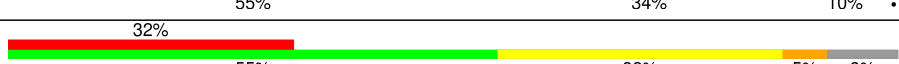

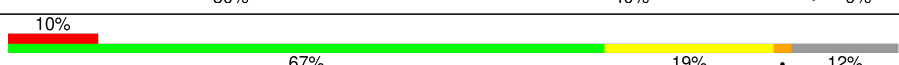
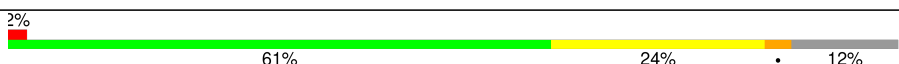
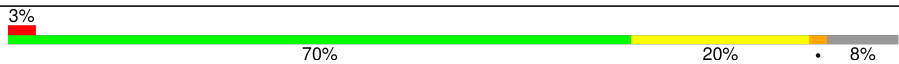
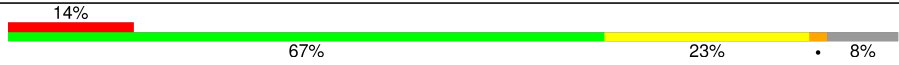


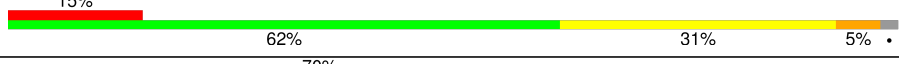
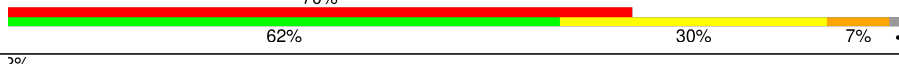


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	4549 (2.58-2.50)
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)
RSRZ outliers	91569	4561 (2.58-2.50)
RNA backbone	2183	1093 (3.00-2.08)

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

Mol	Chain	Length	Quality of chain
1	AA	1521	<div> <div>4%</div> <div>55%</div> <div>32%</div> <div>10%</div> <div>..</div> </div>
1	CA	1521	<div> <div>4%</div> <div>50%</div> <div>37%</div> <div>10%</div> <div>..</div> </div>
2	AB	256	<div> <div>19%</div> <div>48%</div> <div>36%</div> <div>5%</div> <div>10%</div> </div>
2	CB	256	<div> <div>31%</div> <div>47%</div> <div>37%</div> <div>6%</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	132	
12	CL	132	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	

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Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	24	
22	CV	24	
23	AW	76	
23	AY	76	
23	CW	76	
23	CY	76	
24	AX	77	
24	CX	77	
25	BA	2915	
25	DA	2915	
26	BB	121	
26	DB	121	

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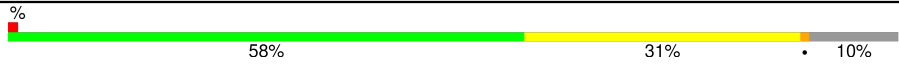








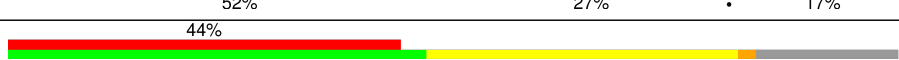





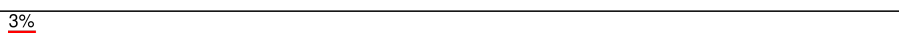
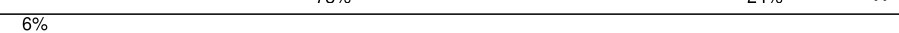










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Mol	Chain	Length	Quality of chain
27	BD	276	
27	DD	276	
28	BE	206	
28	DE	206	
29	BF	210	
29	DF	210	
30	BG	182	
30	DG	182	
31	BH	180	
31	DH	180	
32	BI	148	
32	DI	148	
33	BN	140	
33	DN	140	
34	BO	122	
34	DO	122	
35	BP	150	
35	DP	150	
36	BQ	141	
36	DQ	141	
37	BR	118	
37	DR	118	
38	BS	112	
38	DS	112	
39	BT	146	



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Mol	Chain	Length	Quality of chain
39	DT	146	
40	BU	118	
40	DU	118	
41	BV	101	
41	DV	101	
42	BW	113	
42	DW	113	
43	BX	96	
43	DX	96	
44	BY	110	
44	DY	110	
45	BZ	206	
45	DZ	206	
46	B0	85	
46	D0	85	
47	B1	98	
47	D1	98	
48	B2	72	
48	D2	72	
49	B3	60	
49	D3	60	
50	B4	71	
50	D4	71	
51	B5	60	
51	D5	60	

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Mol	Chain	Length	Quality of chain
52	B6	54	
52	D6	54	
53	B7	49	
53	D7	49	
54	B8	65	
54	D8	65	
55	B9	37	
55	D9	37	

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
56	MG	AA	3009	-	-	-	X
56	MG	AA	3012	-	-	-	X
56	MG	AA	3029	-	-	-	X
56	MG	AA	3043	-	-	-	X
56	MG	AA	3072	-	-	-	X
56	MG	AA	3073	-	-	-	X
56	MG	AA	3086	-	-	-	X
56	MG	AA	3087	-	-	-	X
56	MG	AA	3092	-	-	-	X
56	MG	AA	3104	-	-	-	X
56	MG	AA	3113	-	-	-	X
56	MG	AA	3133	-	-	-	X
56	MG	AA	3161	-	-	-	X
56	MG	AA	3162	-	-	-	X
56	MG	AA	3164	-	-	-	X
56	MG	AA	3209	-	-	-	X
56	MG	AA	3218	-	-	-	X
56	MG	AA	3219	-	-	-	X
56	MG	AA	3223	-	-	-	X
56	MG	AA	3229	-	-	-	X
56	MG	AF	3001	-	-	-	X
56	MG	AK	202	-	-	-	X
56	MG	AX	3013	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	BA	3001	-	-	-	X
56	MG	BA	3007	-	-	-	X
56	MG	BA	3008	-	-	-	X
56	MG	BA	3013	-	-	-	X
56	MG	BA	3016	-	-	-	X
56	MG	BA	3022	-	-	-	X
56	MG	BA	3024	-	-	-	X
56	MG	BA	3038	-	-	-	X
56	MG	BA	3039	-	-	-	X
56	MG	BA	3041	-	-	-	X
56	MG	BA	3043	-	-	-	X
56	MG	BA	3044	-	-	-	X
56	MG	BA	3048	-	-	-	X
56	MG	BA	3051	-	-	-	X
56	MG	BA	3053	-	-	-	X
56	MG	BA	3083	-	-	-	X
56	MG	BA	3101	-	-	-	X
56	MG	BA	3103	-	-	-	X
56	MG	BA	3105	-	-	-	X
56	MG	BA	3109	-	-	-	X
56	MG	BA	3117	-	-	-	X
56	MG	BA	3126	-	-	-	X
56	MG	BA	3133	-	-	-	X
56	MG	BA	3148	-	-	-	X
56	MG	BA	3151	-	-	-	X
56	MG	BA	3161	-	-	-	X
56	MG	BA	3181	-	-	-	X
56	MG	BA	3182	-	-	-	X
56	MG	BA	3205	-	-	-	X
56	MG	BA	3211	-	-	-	X
56	MG	BA	3227	-	-	-	X
56	MG	BA	3240	-	-	-	X
56	MG	BA	3242	-	-	-	X
56	MG	BA	3245	-	-	-	X
56	MG	BA	3247	-	-	-	X
56	MG	BA	3264	-	-	-	X
56	MG	BA	3272	-	-	-	X
56	MG	BA	3282	-	-	-	X
56	MG	BA	3294	-	-	-	X
56	MG	BA	3318	-	-	-	X
56	MG	BA	3320	-	-	-	X
56	MG	BA	3325	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	BA	3334	-	-	-	X
56	MG	BA	3347	-	-	-	X
56	MG	BA	3352	-	-	-	X
56	MG	BA	3362	-	-	-	X
56	MG	BA	3372	-	-	-	X
56	MG	BA	3384	-	-	-	X
56	MG	BA	3386	-	-	-	X
56	MG	BA	3393	-	-	-	X
56	MG	BA	3403	-	-	-	X
56	MG	BA	3412	-	-	-	X
56	MG	BA	3414	-	-	-	X
56	MG	BA	3417	-	-	-	X
56	MG	BA	3425	-	-	-	X
56	MG	BA	3428	-	-	-	X
56	MG	BA	3430	-	-	-	X
56	MG	BA	3431	-	-	-	X
56	MG	BA	3440	-	-	-	X
56	MG	BA	3441	-	-	-	X
56	MG	BA	3450	-	-	-	X
56	MG	BA	3452	-	-	-	X
56	MG	BA	3469	-	-	-	X
56	MG	BA	3484	-	-	-	X
56	MG	BA	3487	-	-	-	X
56	MG	BA	3512	-	-	-	X
56	MG	BA	3514	-	-	-	X
56	MG	BA	3533	-	-	-	X
56	MG	BA	3534	-	-	-	X
56	MG	BA	3545	-	-	-	X
56	MG	BA	3546	-	-	-	X
56	MG	BA	3552	-	-	-	X
56	MG	BA	3555	-	-	-	X
56	MG	BA	3568	-	-	-	X
56	MG	BA	3572	-	-	-	X
56	MG	BA	3584	-	-	-	X
56	MG	BA	3585	-	-	-	X
56	MG	BA	3596	-	-	-	X
56	MG	BA	3607	-	-	-	X
56	MG	BA	3609	-	-	-	X
56	MG	BA	3615	-	-	-	X
56	MG	BA	3724	-	-	-	X
56	MG	BA	3740	-	-	-	X
56	MG	BA	3762	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	BA	3763	-	-	-	X
56	MG	BA	3770	-	-	-	X
56	MG	BA	3811	-	-	-	X
56	MG	BA	3814	-	-	-	X
56	MG	BA	3829	-	-	-	X
56	MG	BA	3831	-	-	-	X
56	MG	BA	3835	-	-	-	X
56	MG	BB	3001	-	-	-	X
56	MG	BD	306	-	-	-	X
56	MG	BD	308	-	-	-	X
56	MG	BF	305	-	-	-	X
56	MG	BF	306	-	-	-	X
56	MG	BF	310	-	-	-	X
56	MG	BN	3001	-	-	-	X
56	MG	BN	3005	-	-	-	X
56	MG	BP	201	-	-	-	X
56	MG	BU	206	-	-	-	X
56	MG	BX	102	-	-	-	X
56	MG	CA	3007	-	-	-	X
56	MG	CA	3037	-	-	-	X
56	MG	CA	3039	-	-	-	X
56	MG	CA	3047	-	-	-	X
56	MG	CA	3059	-	-	-	X
56	MG	CA	3062	-	-	-	X
56	MG	CA	3098	-	-	-	X
56	MG	CA	3111	-	-	-	X
56	MG	CA	3119	-	-	-	X
56	MG	CA	3121	-	-	-	X
56	MG	CA	3142	-	-	-	X
56	MG	CA	3174	-	-	-	X
56	MG	CF	3001	-	-	-	X
56	MG	DA	3003	-	-	-	X
56	MG	DA	3015	-	-	-	X
56	MG	DA	3022	-	-	-	X
56	MG	DA	3024	-	-	-	X
56	MG	DA	3030	-	-	-	X
56	MG	DA	3033	-	-	-	X
56	MG	DA	3035	-	-	-	X
56	MG	DA	3050	-	-	-	X
56	MG	DA	3068	-	-	-	X
56	MG	DA	3070	-	-	-	X
56	MG	DA	3084	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	DA	3095	-	-	-	X
56	MG	DA	3097	-	-	-	X
56	MG	DA	3098	-	-	-	X
56	MG	DA	3100	-	-	-	X
56	MG	DA	3103	-	-	-	X
56	MG	DA	3108	-	-	-	X
56	MG	DA	3112	-	-	-	X
56	MG	DA	3115	-	-	-	X
56	MG	DA	3122	-	-	-	X
56	MG	DA	3138	-	-	-	X
56	MG	DA	3146	-	-	-	X
56	MG	DA	3148	-	-	-	X
56	MG	DA	3152	-	-	-	X
56	MG	DA	3155	-	-	-	X
56	MG	DA	3157	-	-	-	X
56	MG	DA	3158	-	-	-	X
56	MG	DA	3165	-	-	-	X
56	MG	DA	3171	-	-	-	X
56	MG	DA	3172	-	-	-	X
56	MG	DA	3182	-	-	-	X
56	MG	DA	3193	-	-	-	X
56	MG	DA	3201	-	-	-	X
56	MG	DA	3202	-	-	-	X
56	MG	DA	3209	-	-	-	X
56	MG	DA	3233	-	-	-	X
56	MG	DA	3241	-	-	-	X
56	MG	DA	3254	-	-	-	X
56	MG	DA	3257	-	-	-	X
56	MG	DA	3267	-	-	-	X
56	MG	DA	3270	-	-	-	X
56	MG	DA	3278	-	-	-	X
56	MG	DA	3299	-	-	-	X
56	MG	DA	3310	-	-	-	X
56	MG	DA	3322	-	-	-	X
56	MG	DA	3324	-	-	-	X
56	MG	DA	3332	-	-	-	X
56	MG	DA	3340	-	-	-	X
56	MG	DA	3343	-	-	-	X
56	MG	DA	3350	-	-	-	X
56	MG	DA	3354	-	-	-	X
56	MG	DA	3356	-	-	-	X
56	MG	DA	3362	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	DA	3374	-	-	-	X
56	MG	DA	3383	-	-	-	X
56	MG	DA	3400	-	-	-	X
56	MG	DA	3401	-	-	-	X
56	MG	DA	3402	-	-	-	X
56	MG	DA	3404	-	-	-	X
56	MG	DA	3415	-	-	-	X
56	MG	DA	3416	-	-	-	X
56	MG	DA	3424	-	-	-	X
56	MG	DA	3434	-	-	-	X
56	MG	DA	3446	-	-	-	X
56	MG	DA	3453	-	-	-	X
56	MG	DA	3468	-	-	-	X
56	MG	DA	3497	-	-	-	X
56	MG	DA	3522	-	-	-	X
56	MG	DA	3534	-	-	-	X
56	MG	DA	3538	-	-	-	X
56	MG	DA	3562	-	-	-	X
56	MG	DA	3593	-	-	-	X
56	MG	DA	3607	-	-	-	X
56	MG	DA	3634	-	-	-	X
56	MG	DA	3647	-	-	-	X
56	MG	DA	3663	-	-	-	X
56	MG	DA	3669	-	-	-	X
56	MG	DA	3674	-	-	-	X
56	MG	DB	3005	-	-	-	X
56	MG	DB	3006	-	-	-	X
56	MG	DD	303	-	-	-	X
56	MG	DD	304	-	-	-	X
56	MG	DD	306	-	-	-	X
56	MG	DE	301	-	-	-	X
56	MG	DE	302	-	-	-	X
56	MG	DU	3002	-	-	-	X
56	MG	DV	3001	-	-	-	X
56	MG	DV	3002	-	-	-	X
56	MG	DW	3002	-	-	-	X



## 2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 297273 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1498	Total	C	N	O	P	0	0	0
			32205	14333	5970	10404	1498			
1	CA	1503	Total	C	N	O	P	0	0	0
			32312	14381	5990	10438	1503			

- Molecule 2 is a protein called 30S Ribosomal Protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	231	Total	C	N	O	S	0	0	0
			1846	1179	331	331	5			
2	CB	231	Total	C	N	O	S	0	0	0
			1825	1167	326	327	5			

- Molecule 3 is a protein called 30S Ribosomal Protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0	0
			1552	976	302	273	1			
3	CC	206	Total	C	N	O	S	0	0	0
			1542	968	300	273	1			

- Molecule 4 is a protein called 30S Ribosomal Protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	208	Total	C	N	O	S	0	0	0
			1659	1040	326	286	7			
4	CD	208	Total	C	N	O	S	0	0	0
			1674	1050	333	284	7			

- Molecule 5 is a protein called 30S Ribosomal Protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	148	Total	C	N	O	S	0	0	0
			1129	714	213	198	4			
5	CE	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			

- Molecule 6 is a protein called 30S Ribosomal Protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	100	Total	C	N	O	S	0	0	0
			806	511	143	149	3			
6	CF	100	Total	C	N	O	S	0	0	0
			816	516	146	151	3			

- Molecule 7 is a protein called 30S Ribosomal Protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	155	Total	C	N	O	S	0	0	0
			1231	766	243	216	6			
7	CG	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			

- Molecule 8 is a protein called 30S Ribosomal Protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			
8	CH	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			

- Molecule 9 is a protein called 30S Ribosomal Protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O		0	0	0
			983	623	193	167				
9	CI	127	Total	C	N	O		0	0	0
			978	619	190	169				

- Molecule 10 is a protein called 30S Ribosomal Protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	97	Total	C	N	O		0	0	0
			709	440	138	131				

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	CJ	96	Total	C	N	O			
			714	445	138	131	0	0	0

- Molecule 11 is a protein called 30S Ribosomal Protein S11.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	AK	114	Total	C	N	O	S		
			829	516	155	155	3	0	0
11	CK	114	Total	C	N	O	S		
			833	519	156	155	3	0	0

- Molecule 12 is a protein called 30S Ribosomal Protein S12.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	AL	122	Total	C	N	O	S		
			930	585	185	159	1	0	0
12	CL	122	Total	C	N	O	S		
			930	585	185	159	1	0	0

- Molecule 13 is a protein called 30S Ribosomal Protein S13.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	AM	123	Total	C	N	O	S		
			958	592	198	166	2	0	0
13	CM	122	Total	C	N	O	S		
			950	586	197	165	2	0	0

- Molecule 14 is a protein called 30S Ribosomal Protein S14.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	AN	60	Total	C	N	O	S		
			492	312	104	72	4	0	0
14	CN	60	Total	C	N	O	S		
			492	312	104	72	4	0	0

- Molecule 15 is a protein called 30S Ribosomal Protein S15.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S		
			728	456	144	126	2	0	0
15	CO	88	Total	C	N	O	S		
			728	456	144	126	2	0	0

- Molecule 16 is a protein called 30S Ribosomal Protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	82	Total	C	N	O	S	0	0	0
			681	433	134	113	1			
16	CP	82	Total	C	N	O	S	0	0	0
			677	430	133	113	1			

- Molecule 17 is a protein called 30S Ribosomal Protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
17	CQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 18 is a protein called 30S Ribosomal Protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	68	Total	C	N	O	0	0	0
			555	355	108	92			
18	CR	68	Total	C	N	O	0	0	0
			555	355	108	92			

- Molecule 19 is a protein called 30S Ribosomal Protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	83	Total	C	N	O	S	0	0	0
			652	417	120	113	2			
19	CS	83	Total	C	N	O	S	0	0	0
			646	412	119	113	2			

- Molecule 20 is a protein called 30S Ribosomal Protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	96	Total	C	N	O	S	0	0	0
			728	446	156	124	2			
20	CT	96	Total	C	N	O	S	0	0	0
			727	446	155	124	2			

- Molecule 21 is a protein called 30S Ribosomal Protein THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	23	Total	C	N	O	0	0	0
			199	122	48	29			
21	CU	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			
22	CV	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			

- Molecule 23 is a RNA chain called A/P-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
23	AW	74	Total	C	N	O	P	S	0	0	0
			1588	713	285	515	73	2			
23	AY	74	Total	C	N	O	P	S	0	0	0
			1581	707	285	515	73	1			
23	CW	72	Total	C	N	O	P	S	0	0	0
			1541	688	278	502	72	1			
23	CY	73	Total	C	N	O	P	S	0	0	0
			1561	698	283	507	72	1			

- Molecule 24 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
24	AX	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			
24	CX	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			

- Molecule 25 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BA	2819	Total	C	N	O	P	0	0	0
			60729	27026	11370	19515	2818			
25	DA	2800	Total	C	N	O	P	0	0	0
			60311	26840	11284	19388	2799			

- Molecule 26 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			
26	DB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

- Molecule 27 is a protein called 50S Ribosomal Protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BD	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			
27	DD	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

- Molecule 28 is a protein called 50S Ribosomal Protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BE	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			
28	DE	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			

- Molecule 29 is a protein called 50S Ribosomal Protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BF	203	Total	C	N	O	S	0	0	1
			1584	1009	298	275	2			
29	DF	203	Total	C	N	O	S	0	0	1
			1580	1007	297	274	2			

- Molecule 30 is a protein called 50S Ribosomal Protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BG	181	Total	C	N	O	S	0	0	0
			1425	914	256	251	4			
30	DG	181	Total	C	N	O	S	0	0	0
			1424	911	258	251	4			

- Molecule 31 is a protein called 50S Ribosomal Protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BH	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	DH	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

- Molecule 32 is a protein called 50S Ribosomal Protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BI	146	Total	C	N	O	S	0	0	0
			1085	693	189	202	1			
32	DI	146	Total	C	N	O	S	0	0	0
			1061	680	186	194	1			

- Molecule 33 is a protein called 50S Ribosomal Protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BN	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			
33	DN	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			

- Molecule 34 is a protein called 50S Ribosomal Protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
34	DO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 35 is a protein called 50S Ribosomal Protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BP	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			
35	DP	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			

- Molecule 36 is a protein called 50S Ribosomal Protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
36	DQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 37 is a protein called 50S Ribosomal Protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
37	DR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 38 is a protein called 50S Ribosomal Protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BS	110	Total	C	N	O		0	0	0
			877	553	175	149				
38	DS	110	Total	C	N	O		0	0	0
			870	549	173	148				

- Molecule 39 is a protein called 50S Ribosomal Protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BT	131	Total	C	N	O	S	0	0	0
			1091	680	225	185	1			
39	DT	131	Total	C	N	O	S	0	0	0
			1083	675	224	183	1			

- Molecule 40 is a protein called 50S Ribosomal Protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			
40	DU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

- Molecule 41 is a protein called 50S Ribosomal Protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BV	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			
41	DV	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

- Molecule 42 is a protein called 50S Ribosomal Protein L22.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BW	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			
42	DW	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			

- Molecule 43 is a protein called 50S Ribosomal Protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BX	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
43	DX	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			

- Molecule 44 is a protein called 50S Ribosomal Protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BY	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			
44	DY	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			

- Molecule 45 is a protein called 50S Ribosomal Protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BZ	171	Total	C	N	O	S	0	0	0
			1349	862	243	242	2			
45	DZ	174	Total	C	N	O	S	0	0	0
			1360	870	243	245	2			

- Molecule 46 is a protein called 50S Ribosomal Protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	B0	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			
46	D0	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			

- Molecule 47 is a protein called 50S Ribosomal Protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	B1	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	D1	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			

- Molecule 48 is a protein called 50S Ribosomal Protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	B2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			
48	D2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

- Molecule 49 is a protein called 50S Ribosomal Protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	B3	59	Total	C	N	O	0	0	0
			469	298	90	81			
49	D3	59	Total	C	N	O	0	0	0
			464	296	90	78			

- Molecule 50 is a protein called 50S Ribosomal Protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B4	69	Total	C	N	O	S	0	0	0
			558	352	102	99	5			
50	D4	69	Total	C	N	O	S	0	0	0
			532	339	97	91	5			

- Molecule 51 is a protein called 50S Ribosomal Protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B5	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			
51	D5	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			

- Molecule 52 is a protein called 50S Ribosomal Protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
52	D6	53	Total	C	N	O	S	0	0	0
			449	279	91	75	4			

- Molecule 53 is a protein called 50S Ribosomal Protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
53	D7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 54 is a protein called 50S Ribosomal Protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B8	64	Total	C	N	O	S	0	0	0
			511	328	99	82	2			
54	D8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 55 is a protein called 50S Ribosomal Protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	B9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
55	D9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	B4	1	Total	Mg	0	0
			1	1		
56	BA	839	Total	Mg	0	0
			839	839		
56	AK	2	Total	Mg	0	0
			2	2		
56	DQ	4	Total	Mg	0	0
			4	4		
56	D3	1	Total	Mg	0	0
			1	1		
56	DF	5	Total	Mg	0	0
			5	5		
56	CV	1	Total	Mg	0	0
			1	1		
56	B8	3	Total	Mg	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	BE	8	Total 8	Mg 8	0	0
56	AW	7	Total 7	Mg 7	0	0
56	DU	2	Total 2	Mg 2	0	0
56	B1	2	Total 2	Mg 2	0	0
56	AN	1	Total 1	Mg 1	0	0
56	BP	3	Total 3	Mg 3	0	0
56	AX	12	Total 12	Mg 12	0	0
56	DN	1	Total 1	Mg 1	0	0
56	CY	1	Total 1	Mg 1	0	0
56	CA	177	Total 177	Mg 177	0	0
56	B5	4	Total 4	Mg 4	0	0
56	BB	23	Total 23	Mg 23	0	0
56	D8	1	Total 1	Mg 1	0	0
56	AE	1	Total 1	Mg 1	0	0
56	DG	1	Total 1	Mg 1	0	0
56	B9	1	Total 1	Mg 1	0	0
56	BF	12	Total 12	Mg 12	0	0
56	AV	1	Total 1	Mg 1	0	0
56	BX	2	Total 2	Mg 2	0	0
56	B2	1	Total 1	Mg 1	0	0
56	AA	230	Total 230	Mg 230	0	0

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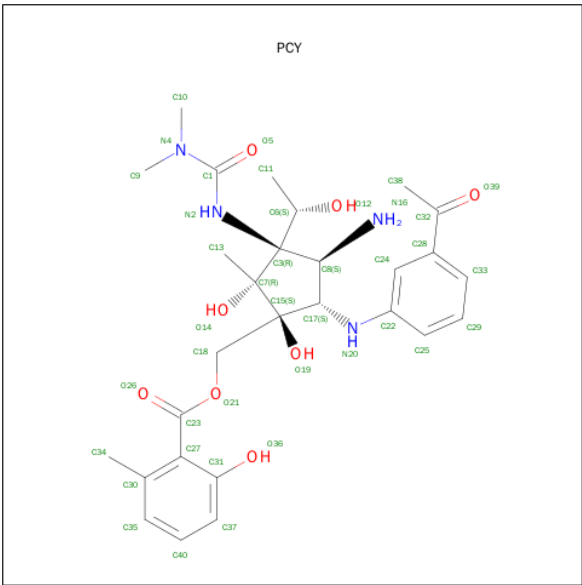
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56	CX	5	Total 5	Mg 5	0	0
56	DV	3	Total 3	Mg 3	0	0
56	B6	2	Total 2	Mg 2	0	0
56	AM	1	Total 1	Mg 1	0	0
56	BU	9	Total 9	Mg 9	0	0
56	DR	1	Total 1	Mg 1	0	0
56	AD	1	Total 1	Mg 1	0	0
56	BN	5	Total 5	Mg 5	0	0
56	CT	1	Total 1	Mg 1	0	0
56	D0	2	Total 2	Mg 2	0	0
56	BG	3	Total 3	Mg 3	0	0
56	BY	1	Total 1	Mg 1	0	0
56	DE	4	Total 4	Mg 4	0	0
56	B3	3	Total 3	Mg 3	0	0
56	CJ	1	Total 1	Mg 1	0	0
56	BR	5	Total 5	Mg 5	0	0
56	DA	675	Total 675	Mg 675	0	0
56	DW	3	Total 3	Mg 3	0	0
56	B7	2	Total 2	Mg 2	0	0

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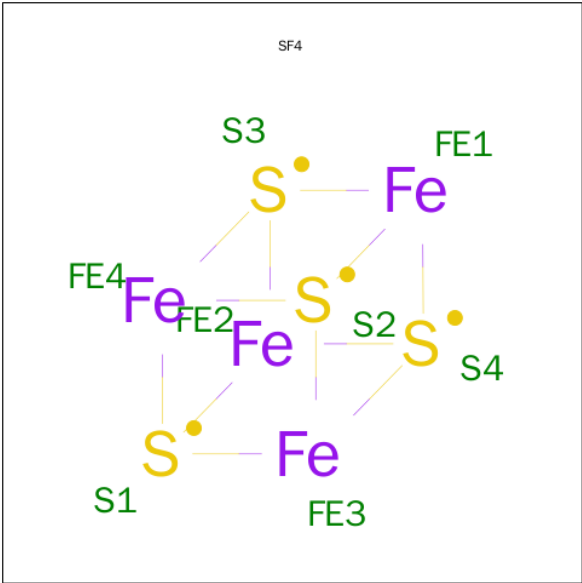
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56	BO	1	Total 1	Mg 1	0	0
56	BZ	1	Total 1	Mg 1	0	0
56	DY	1	Total 1	Mg 1	0	0
56	CW	2	Total 2	Mg 2	0	0
56	BD	11	Total 11	Mg 11	0	0
56	B0	3	Total 3	Mg 3	0	0
56	CE	2	Total 2	Mg 2	0	0
56	BW	3	Total 3	Mg 3	0	0
56	AY	3	Total 3	Mg 3	0	0
56	DD	7	Total 7	Mg 7	0	0
56	AF	1	Total 1	Mg 1	0	0
56	DB	11	Total 11	Mg 11	0	0

- Molecule 57 is Pactamycin (three-letter code: PCY) (formula:  $C_{28}H_{38}N_4O_8$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
57	AA	1	Total	C	N	O	0	0
			40	28	4	8		
57	CA	1	Total	C	N	O	0	0
			40	28	4	8		

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	AD	1	Total	Fe	S	0	0
			8	4	4		
58	CD	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	B5	1	Total 1	Zn 1	0	0
59	B4	1	Total 1	Zn 1	0	0
59	CN	1	Total 1	Zn 1	0	0
59	BY	1	Total 1	Zn 1	0	0
59	B9	1	Total 1	Zn 1	0	0
59	DY	1	Total 1	Zn 1	0	0
59	D5	1	Total 1	Zn 1	0	0
59	D4	1	Total 1	Zn 1	0	0
59	AN	1	Total 1	Zn 1	0	0
59	D6	1	Total 1	Zn 1	0	0
59	D9	1	Total 1	Zn 1	0	0
59	B6	1	Total 1	Zn 1	0	0

- Molecule 60 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AX	1	Total 1	K 1	0	0
60	CX	1	Total 1	K 1	0	0

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	AA	226	Total 226	O 226	0	0
61	AE	3	Total 3	O 3	0	0
61	AJ	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	AL	4	Total 4	O 4	0	0
61	AM	1	Total 1	O 1	0	0
61	AV	4	Total 4	O 4	0	0
61	AW	6	Total 6	O 6	0	0
61	AX	8	Total 8	O 8	0	0
61	AY	3	Total 3	O 3	0	0
61	BA	1411	Total 1411	O 1411	0	0
61	BB	36	Total 36	O 36	0	0
61	BD	16	Total 16	O 16	0	0
61	BE	13	Total 13	O 13	0	0
61	BF	7	Total 7	O 7	0	0
61	BG	3	Total 3	O 3	0	0
61	BI	1	Total 1	O 1	0	0
61	BN	2	Total 2	O 2	0	0
61	BO	3	Total 3	O 3	0	0
61	BP	17	Total 17	O 17	0	0
61	BQ	2	Total 2	O 2	0	0
61	BR	2	Total 2	O 2	0	0
61	BT	1	Total 1	O 1	0	0
61	BU	6	Total 6	O 6	0	0
61	BV	2	Total 2	O 2	0	0

*Continued on next page...*

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	BW	4	Total 4	O 4	0	0
61	BX	1	Total 1	O 1	0	0
61	B0	4	Total 4	O 4	0	0
61	B1	2	Total 2	O 2	0	0
61	B3	2	Total 2	O 2	0	0
61	B5	5	Total 5	O 5	0	0
61	B6	1	Total 1	O 1	0	0
61	B7	3	Total 3	O 3	0	0
61	B8	11	Total 11	O 11	0	0
61	CA	173	Total 173	O 173	0	0
61	CJ	2	Total 2	O 2	0	0
61	CL	1	Total 1	O 1	0	0
61	CV	2	Total 2	O 2	0	0
61	CW	1	Total 1	O 1	0	0
61	CX	4	Total 4	O 4	0	0
61	DA	1002	Total 1002	O 1002	0	0
61	DB	10	Total 10	O 10	0	0
61	DD	17	Total 17	O 17	0	0
61	DE	11	Total 11	O 11	0	0
61	DF	5	Total 5	O 5	0	0
61	DN	2	Total 2	O 2	0	0

*Continued on next page...*

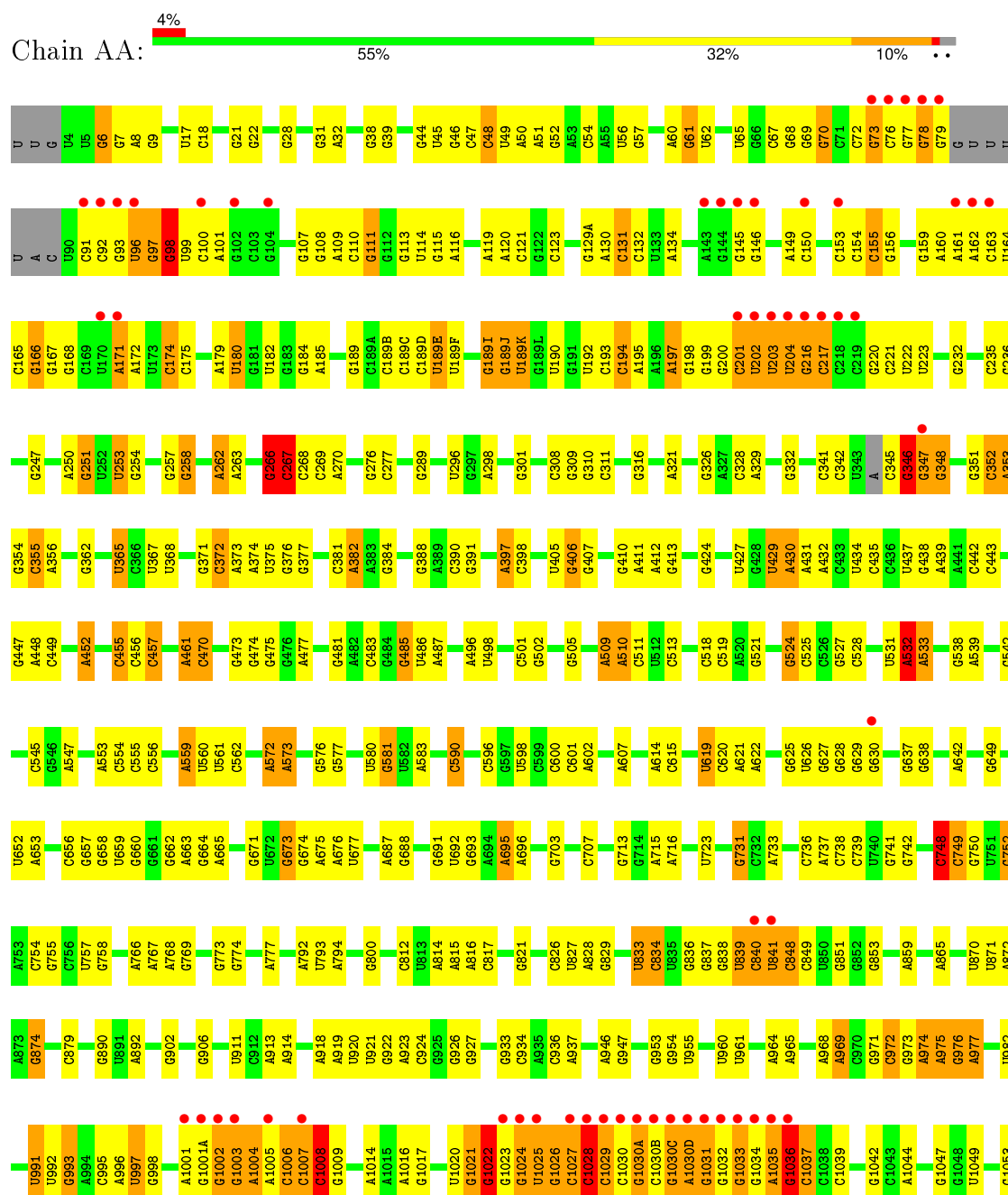
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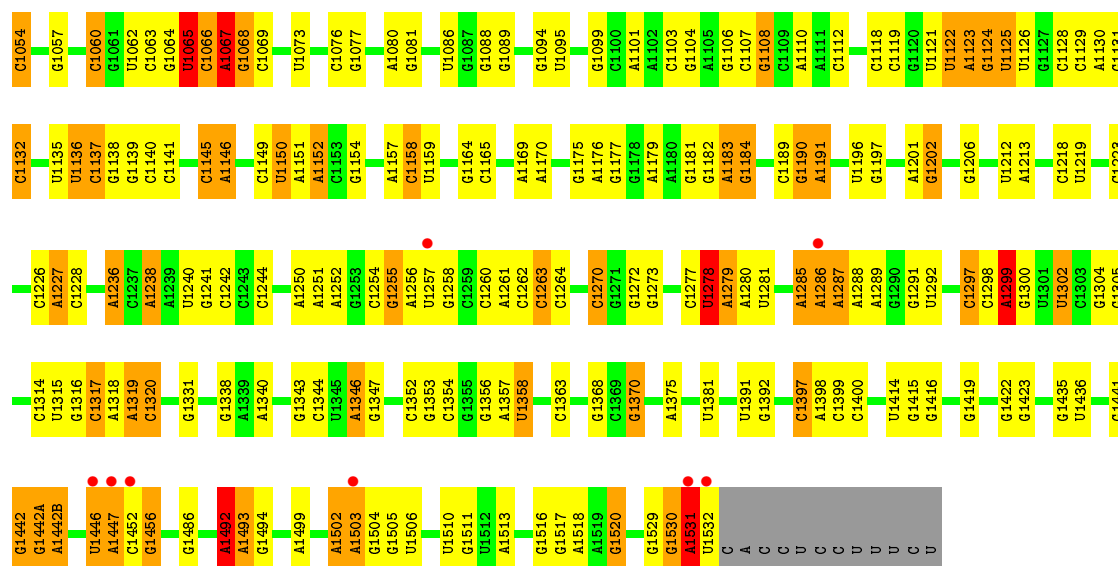
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	DO	2	Total	O	0	0
			2	2		
61	DP	8	Total	O	0	0
			8	8		
61	DQ	1	Total	O	0	0
			1	1		
61	DR	1	Total	O	0	0
			1	1		
61	DU	2	Total	O	0	0
			2	2		
61	DW	1	Total	O	0	0
			1	1		
61	DY	1	Total	O	0	0
			1	1		
61	D0	5	Total	O	0	0
			5	5		
61	D3	1	Total	O	0	0
			1	1		
61	D7	3	Total	O	0	0
			3	3		
61	D8	4	Total	O	0	0
			4	4		

### 3 Residue-property plots

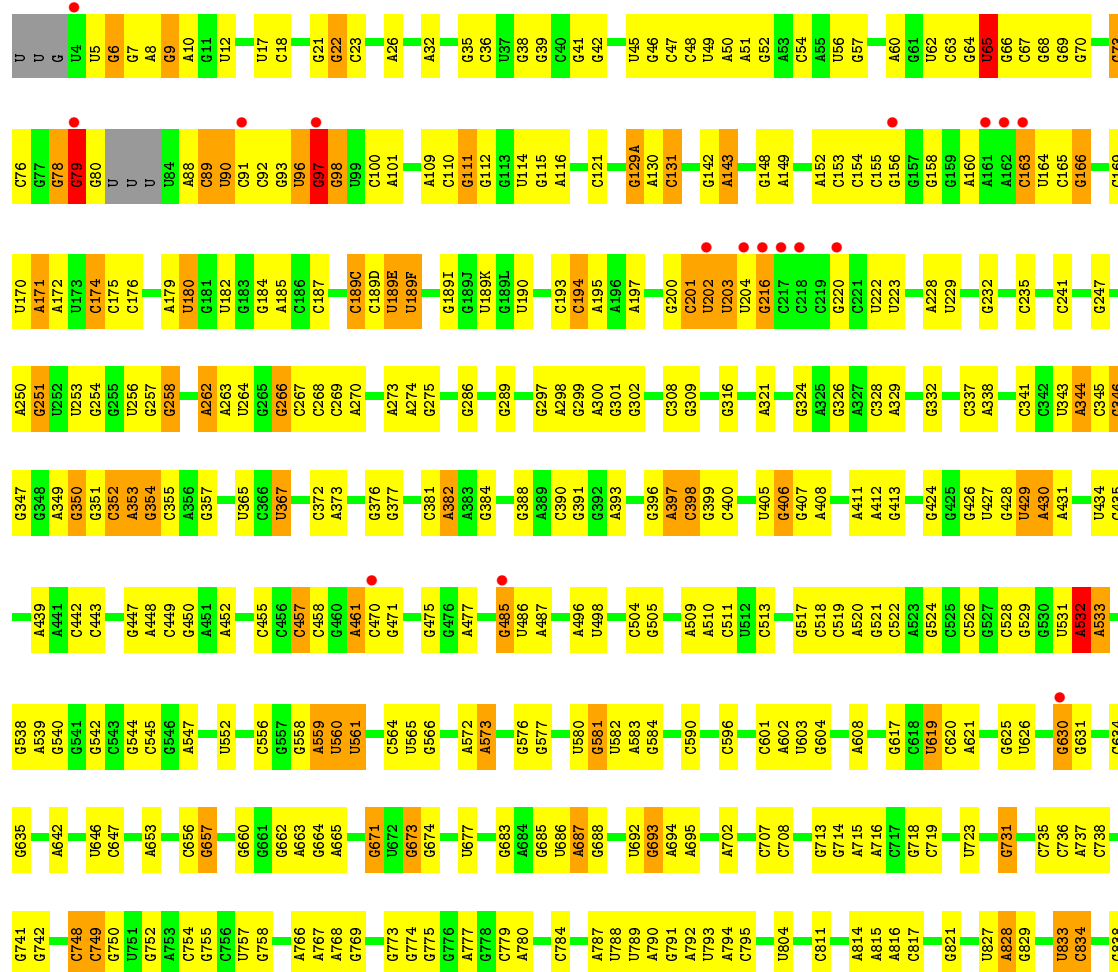
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

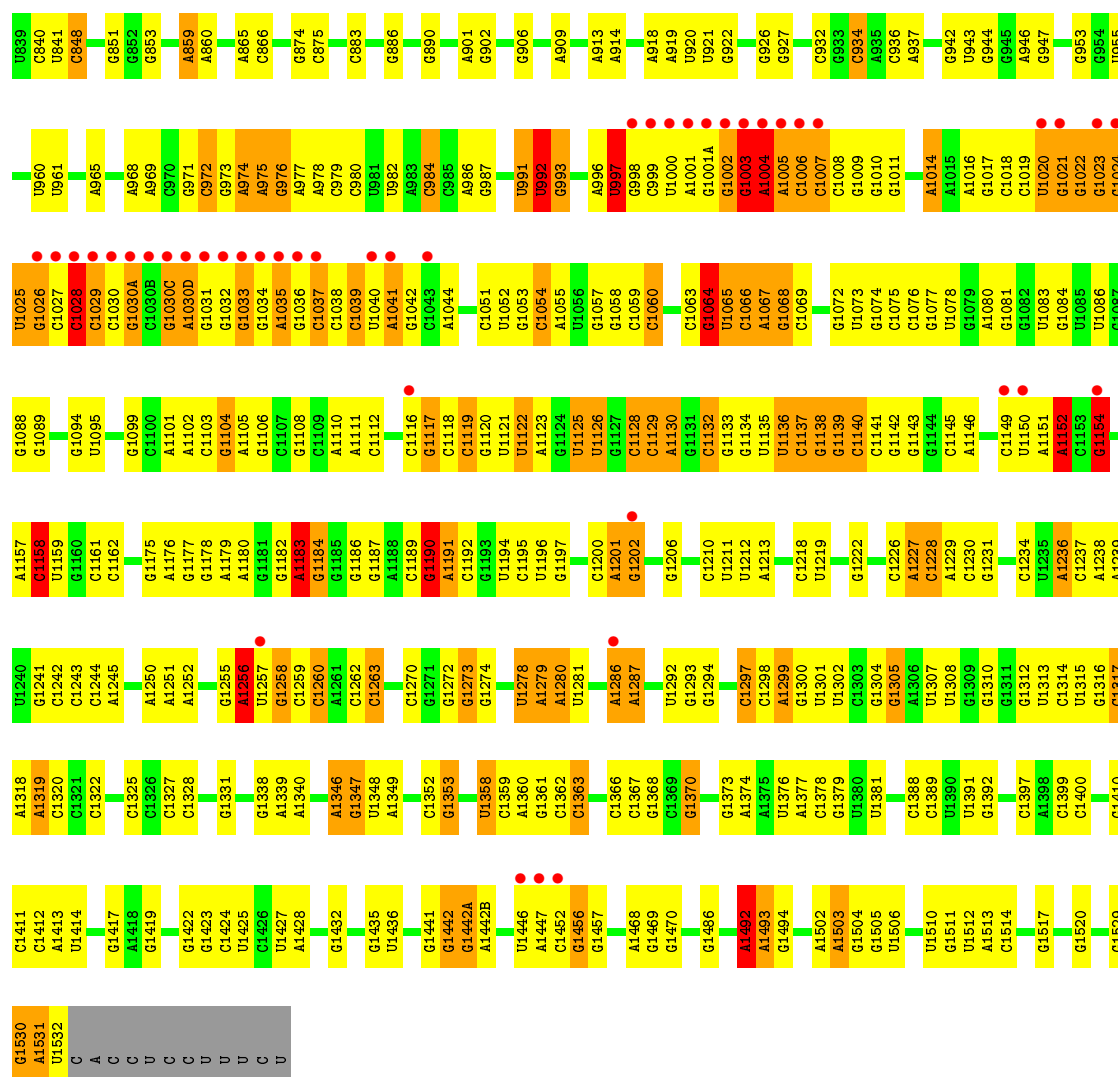
#### • Molecule 1: 16S Ribosomal RNA



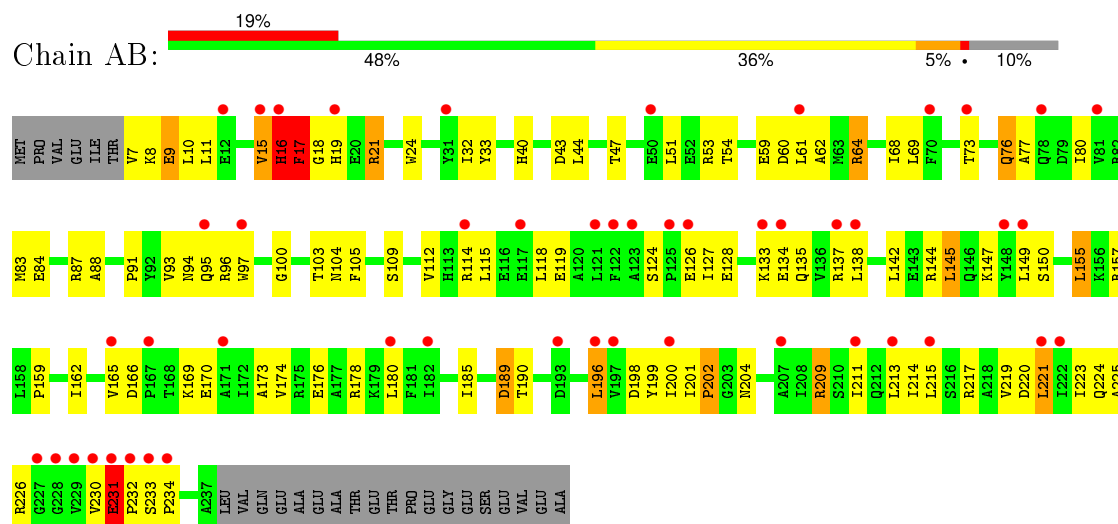


### • Molecule 1: 16S Ribosomal RNA

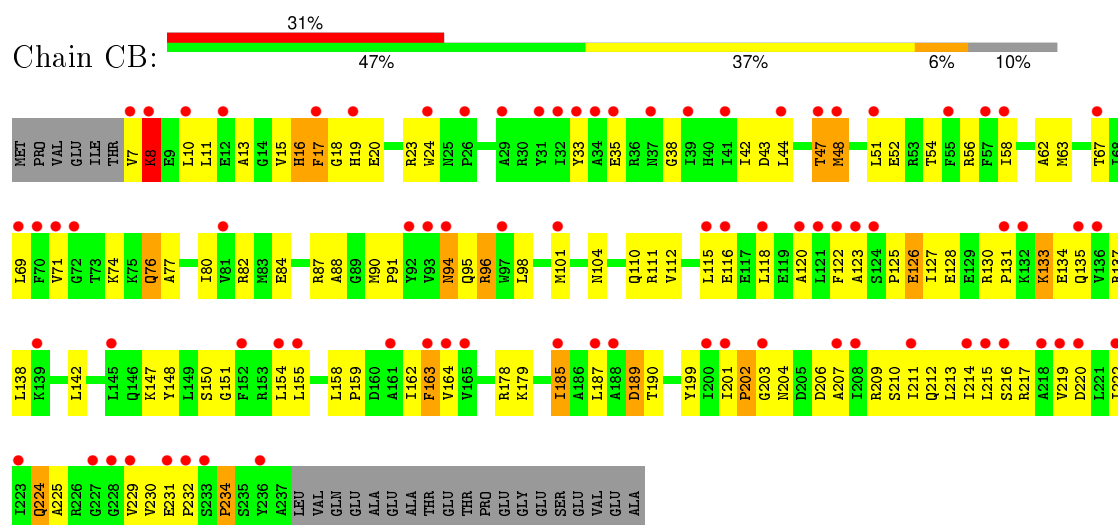




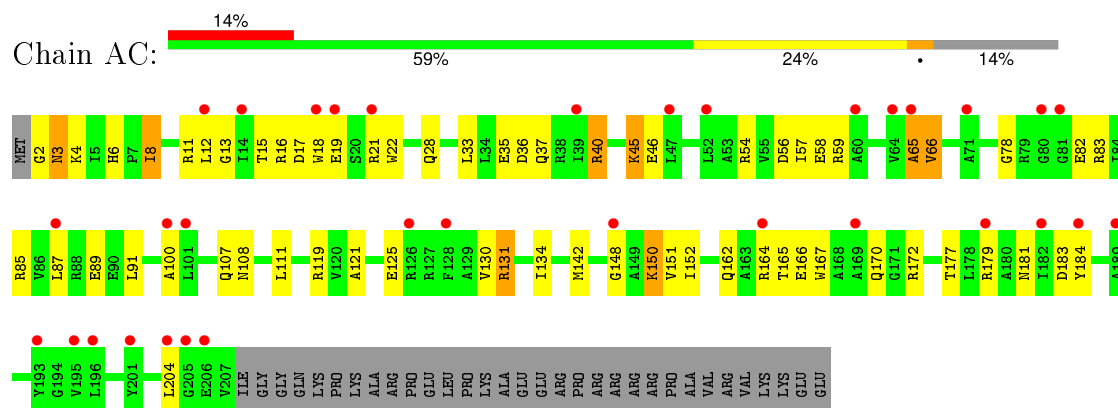
- Molecule 2: 30S Ribosomal Protein S2



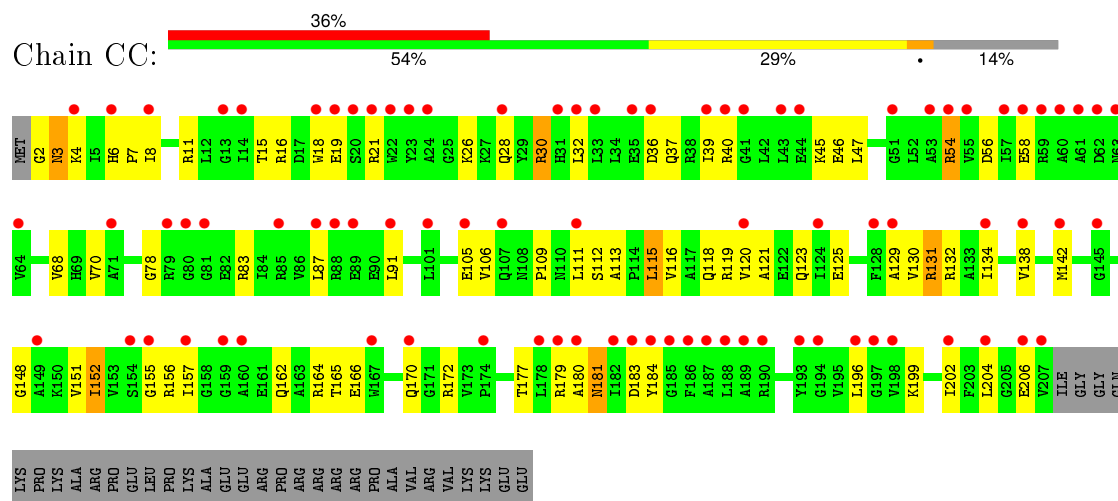
- Molecule 2: 30S Ribosomal Protein S2



- Molecule 3: 30S Ribosomal Protein S3



- Molecule 3: 30S Ribosomal Protein S3



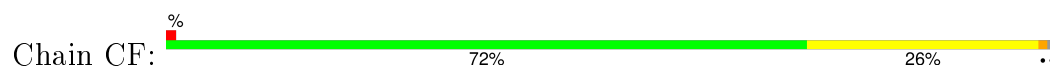
- Molecule 4: 30S Ribosomal Protein S4



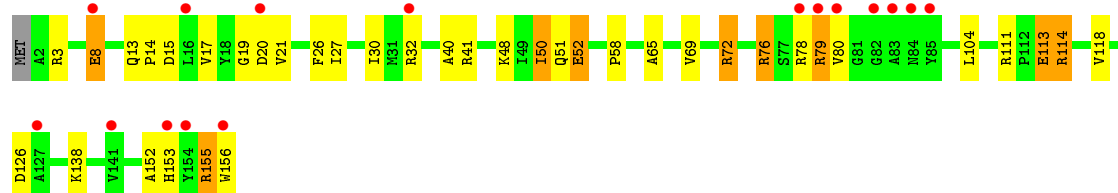
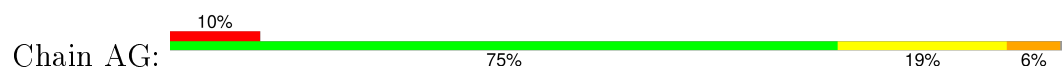




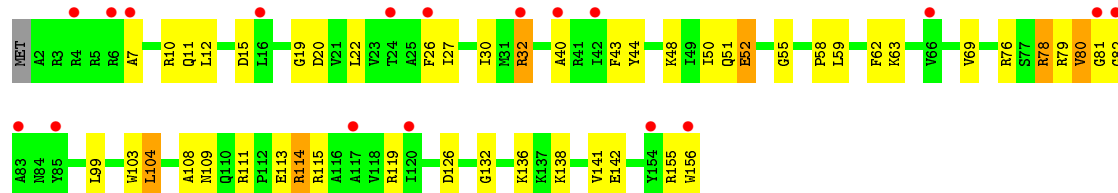
- Molecule 6: 30S Ribosomal Protein S6



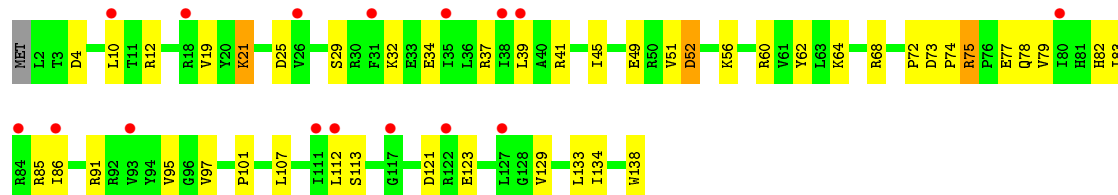
- Molecule 7: 30S Ribosomal Protein S7



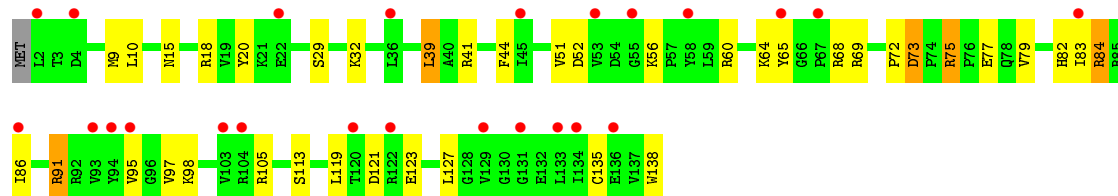
- Molecule 7: 30S Ribosomal Protein S7



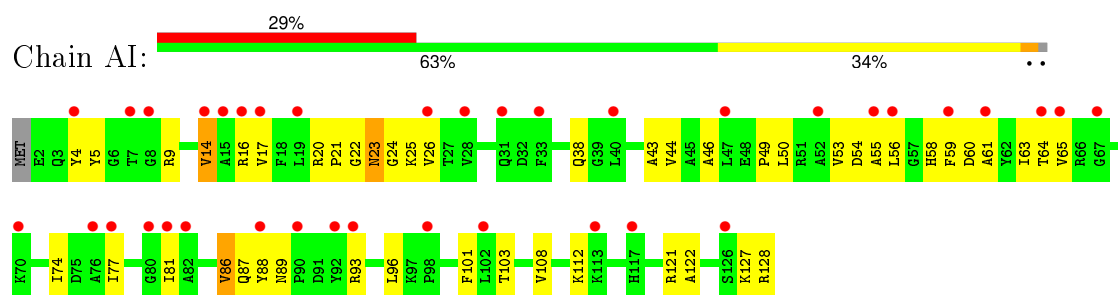
- Molecule 8: 30S Ribosomal Protein S8



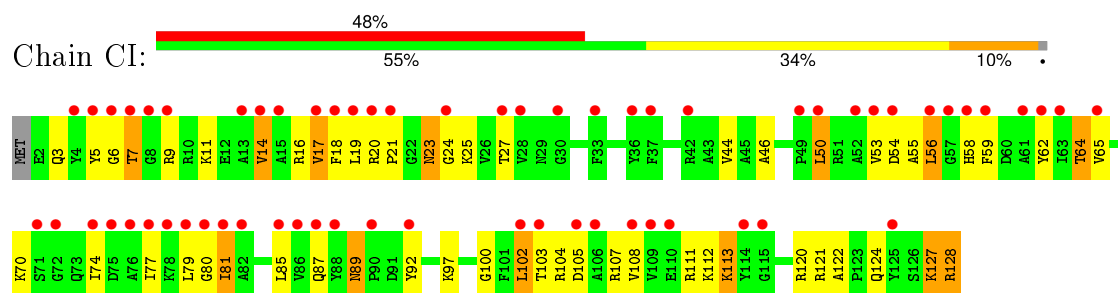
- Molecule 8: 30S Ribosomal Protein S8



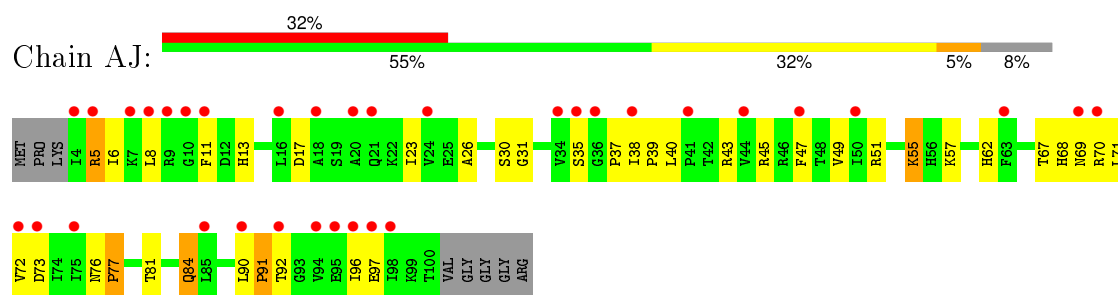
- Molecule 9: 30S Ribosomal Protein S9



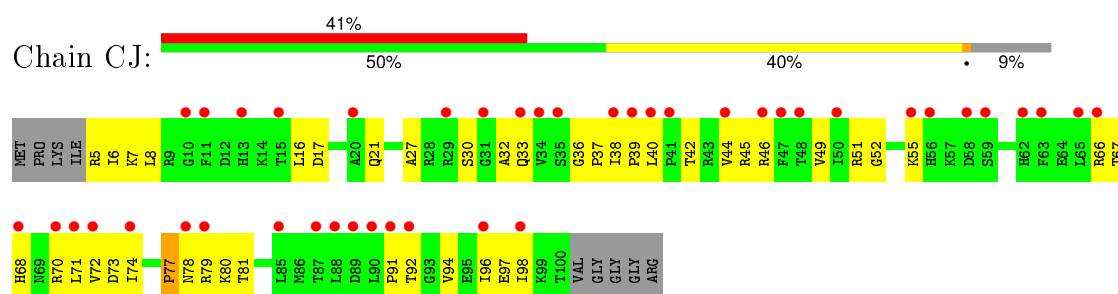
• Molecule 9: 30S Ribosomal Protein S9



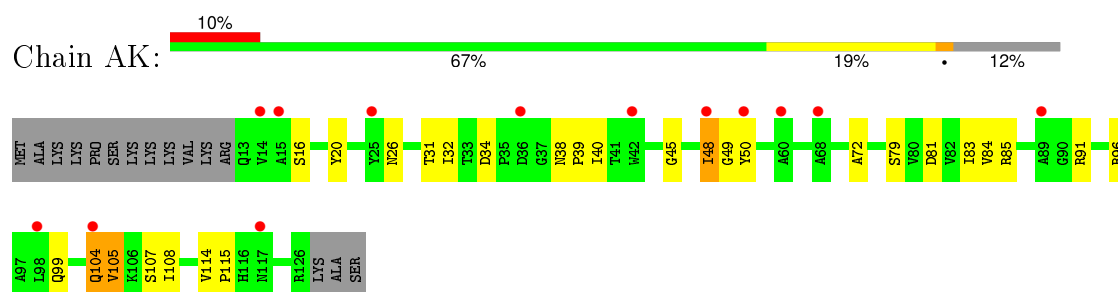
• Molecule 10: 30S Ribosomal Protein S10



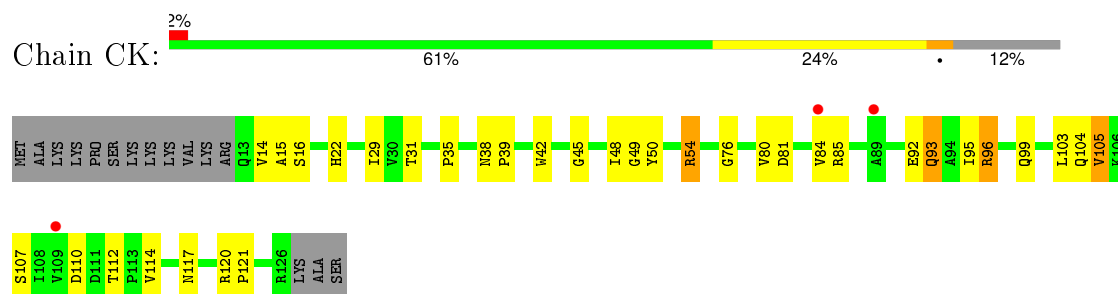
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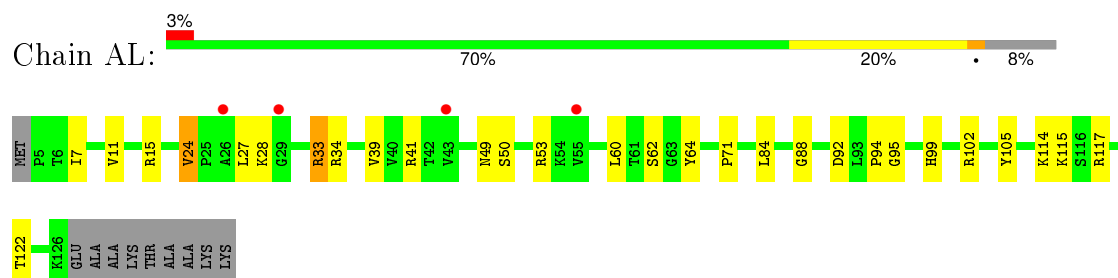
• Molecule 11: 30S Ribosomal Protein S11



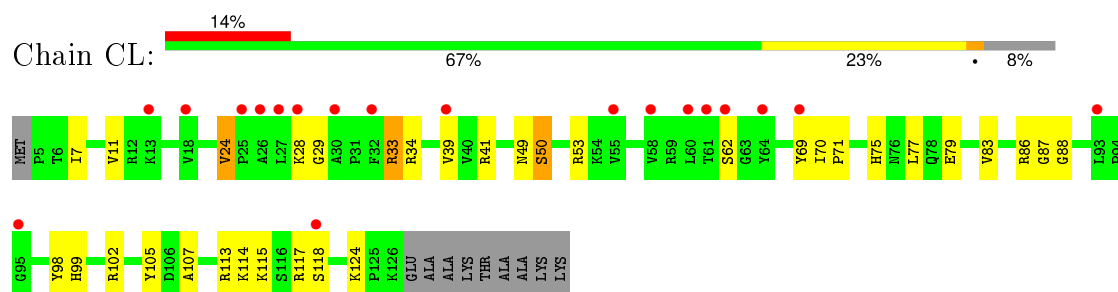
- Molecule 11: 30S Ribosomal Protein S11



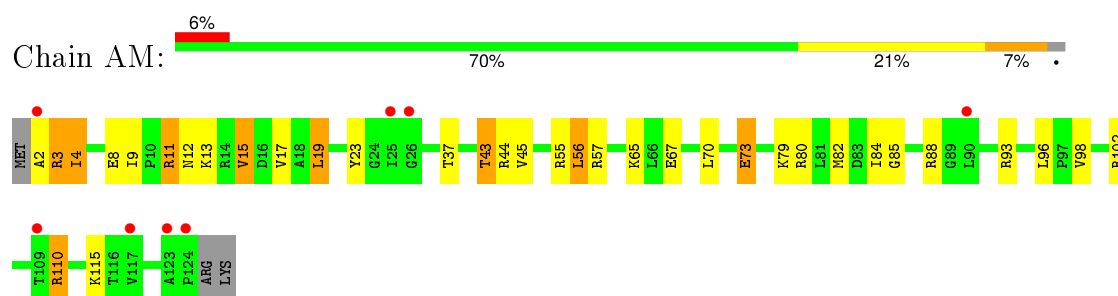
- Molecule 12: 30S Ribosomal Protein S12



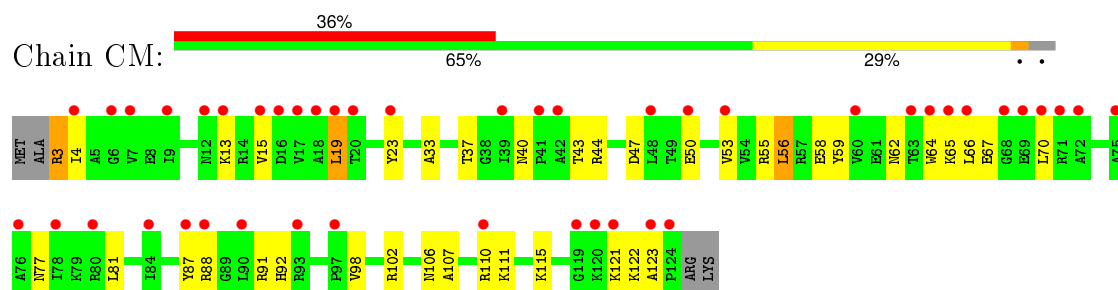
- Molecule 12: 30S Ribosomal Protein S12



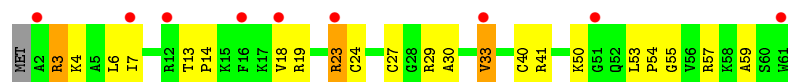
- Molecule 13: 30S Ribosomal Protein S13



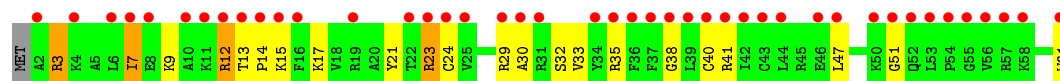
- Molecule 13: 30S Ribosomal Protein S13



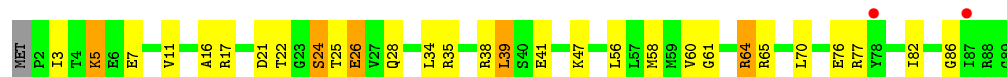
- Molecule 14: 30S Ribosomal Protein S14



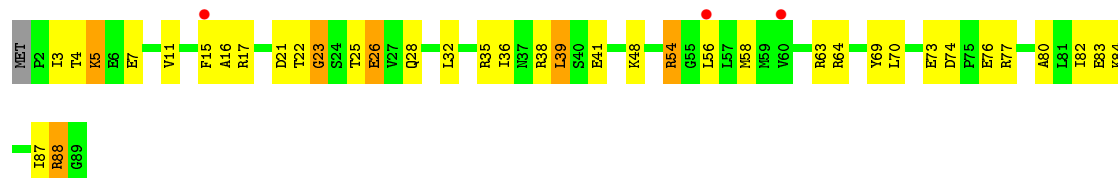
- Molecule 14: 30S Ribosomal Protein S14



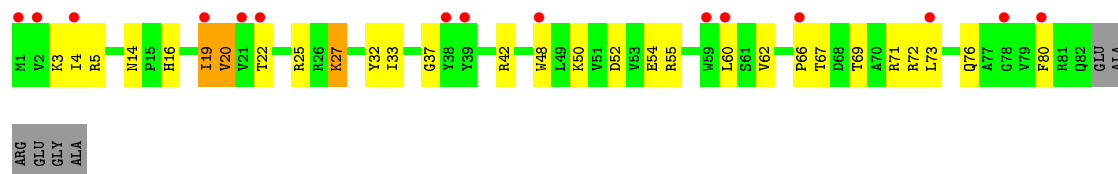
- Molecule 15: 30S Ribosomal Protein S15



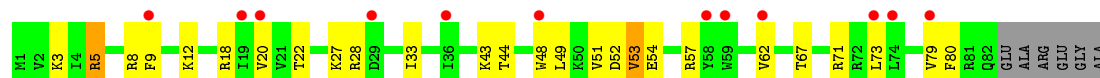
- Molecule 15: 30S Ribosomal Protein S15



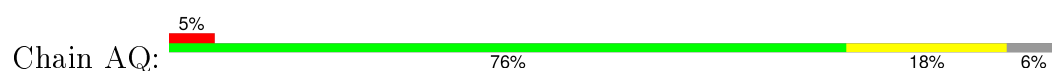
- Molecule 16: 30S Ribosomal Protein S16

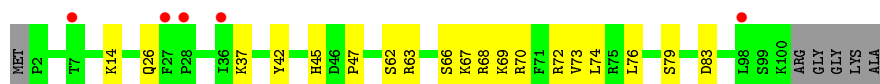


- Molecule 16: 30S Ribosomal Protein S16

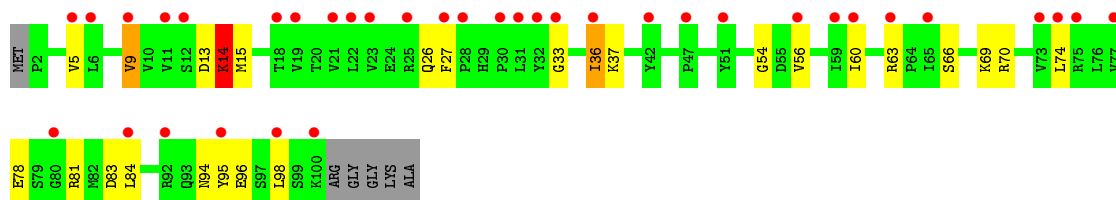


- Molecule 17: 30S Ribosomal Protein S17

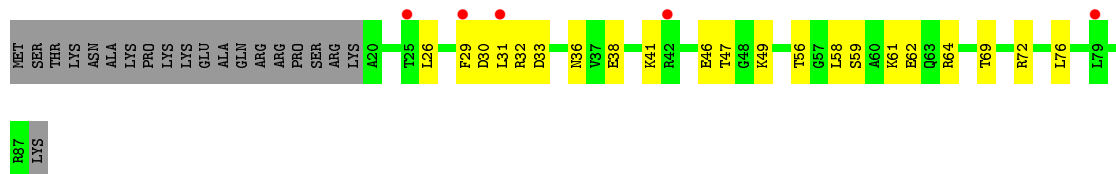




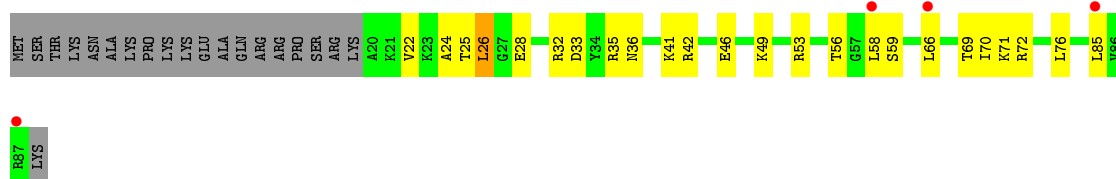
• Molecule 17: 30S Ribosomal Protein S17



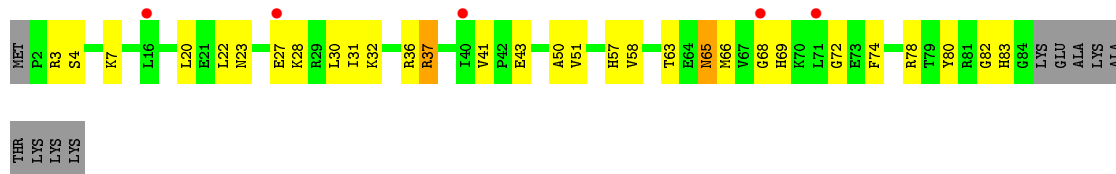
• Molecule 18: 30S Ribosomal Protein S18



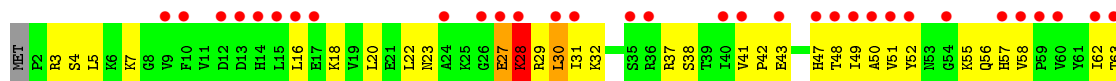
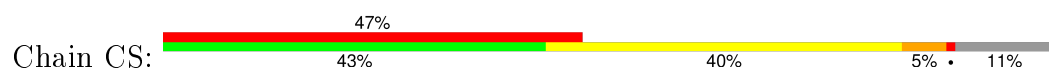
• Molecule 18: 30S Ribosomal Protein S18

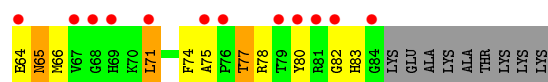


• Molecule 19: 30S Ribosomal Protein S19

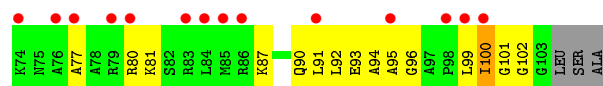
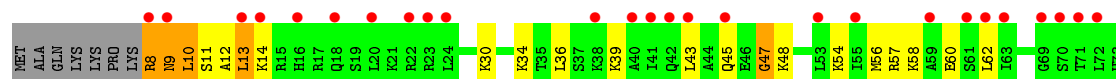
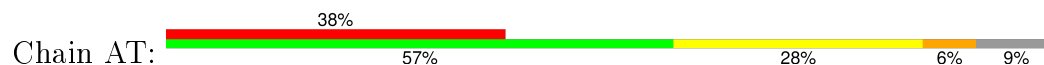


• Molecule 19: 30S Ribosomal Protein S19

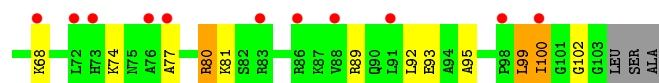
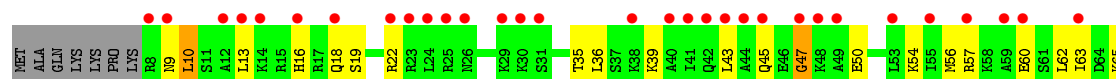




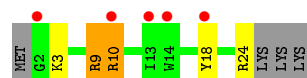
• Molecule 20: 30S Ribosomal Protein S20



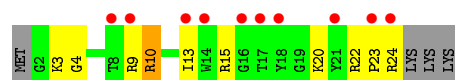
• Molecule 20: 30S Ribosomal Protein S20



• Molecule 21: 30S Ribosomal Protein THX



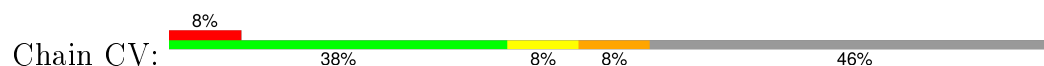
• Molecule 21: 30S Ribosomal Protein THX



• Molecule 22: mRNA

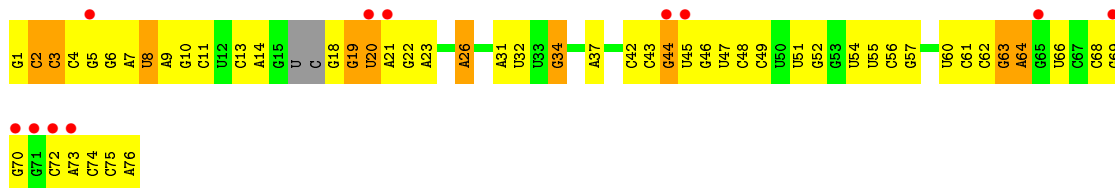


• Molecule 22: mRNA

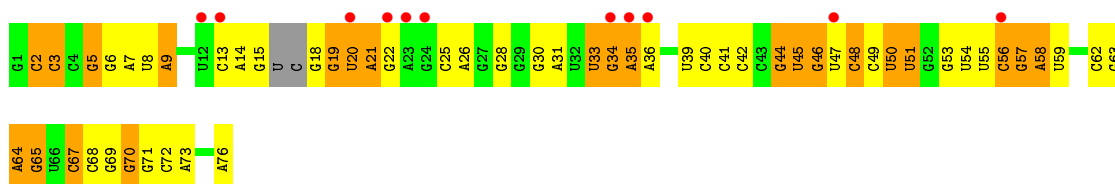




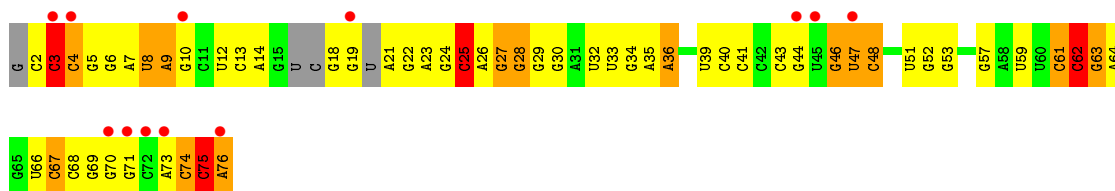
• Molecule 23: A/P-site tRNA



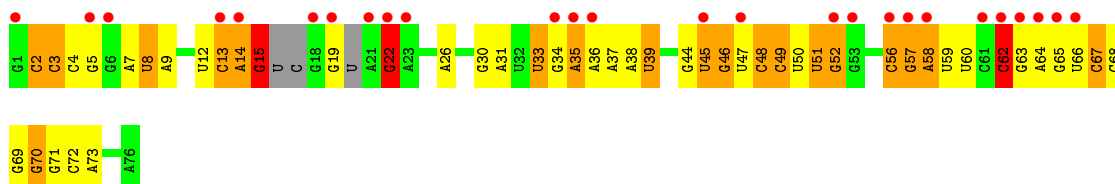
• Molecule 23: A/P-site tRNA



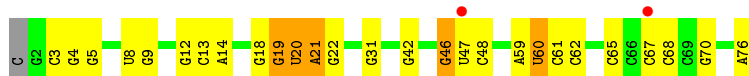
• Molecule 23: A/P-site tRNA



• Molecule 23: A/P-site tRNA



• Molecule 24: E-site tRNA



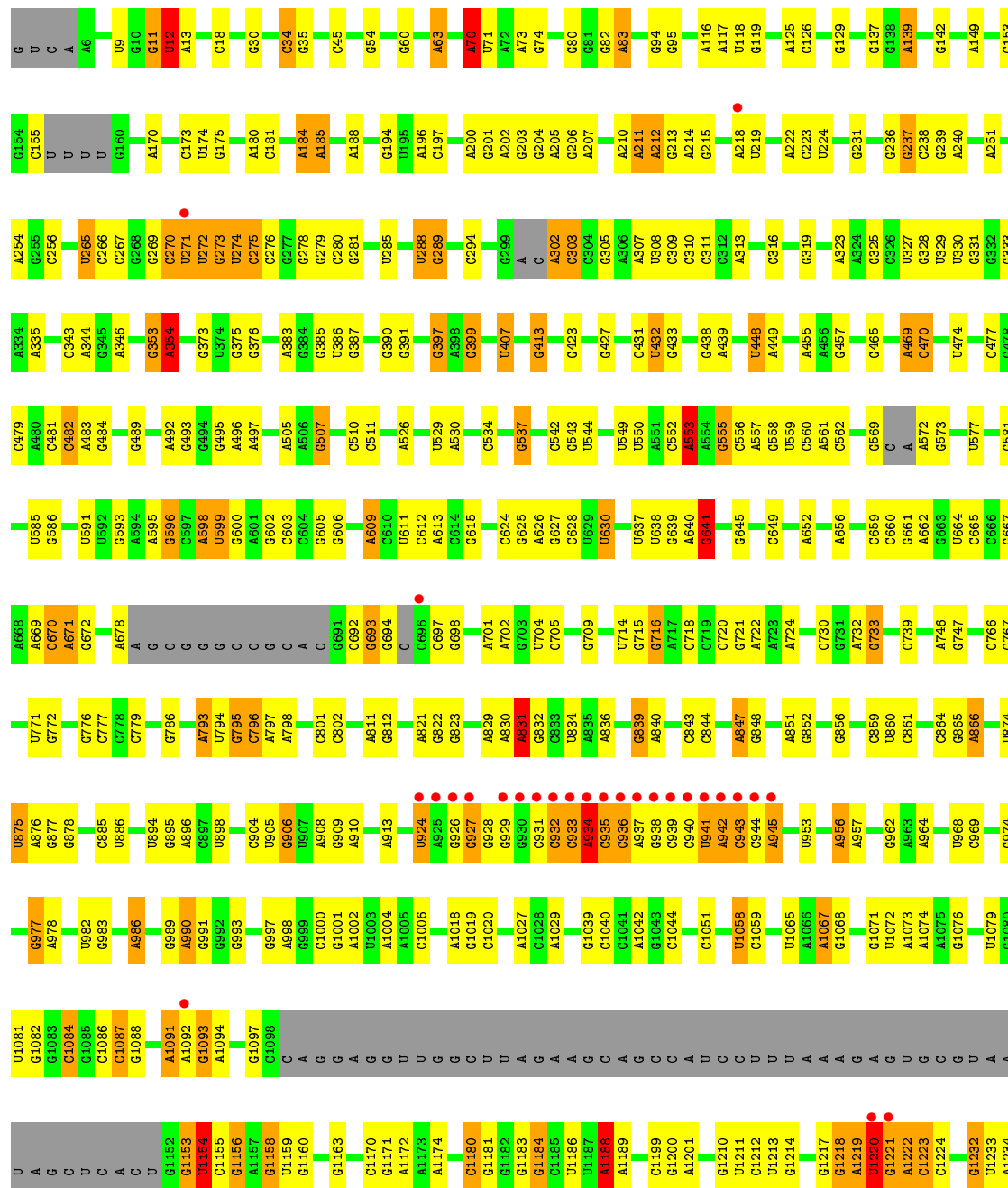
• Molecule 24: E-site tRNA

Chain CX: 

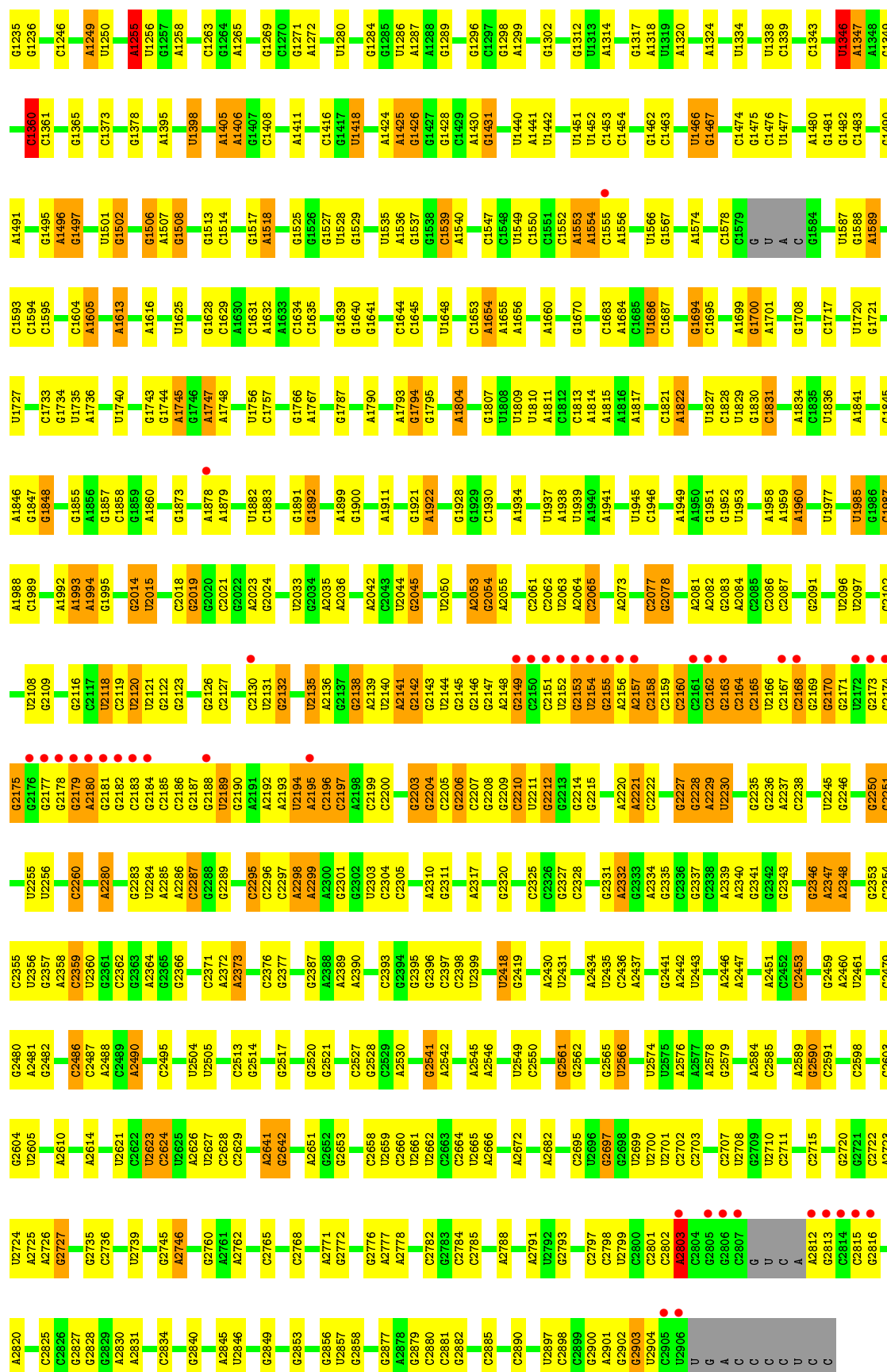


• Molecule 25: 23S Ribosomal RNA

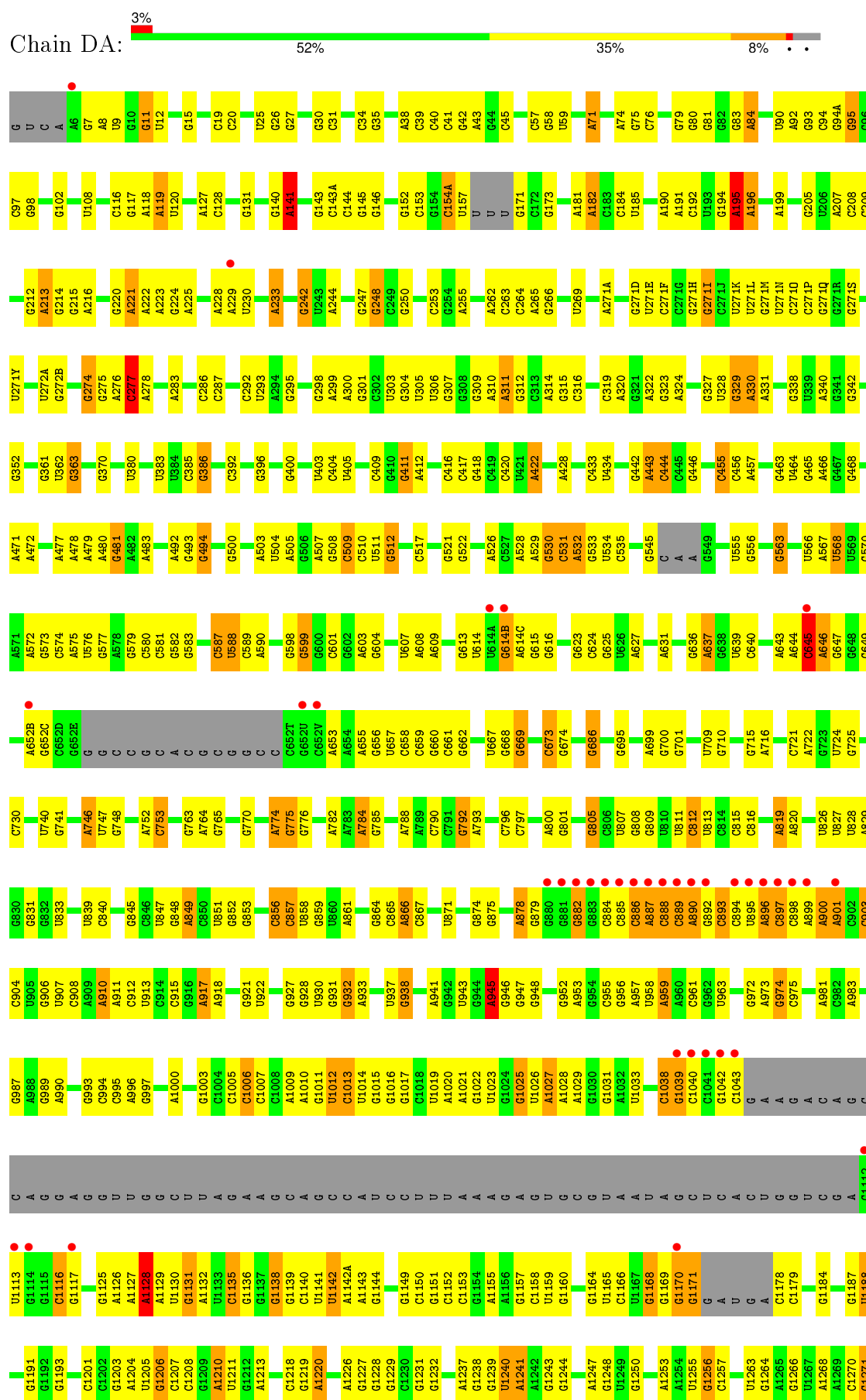
Chain BA: 



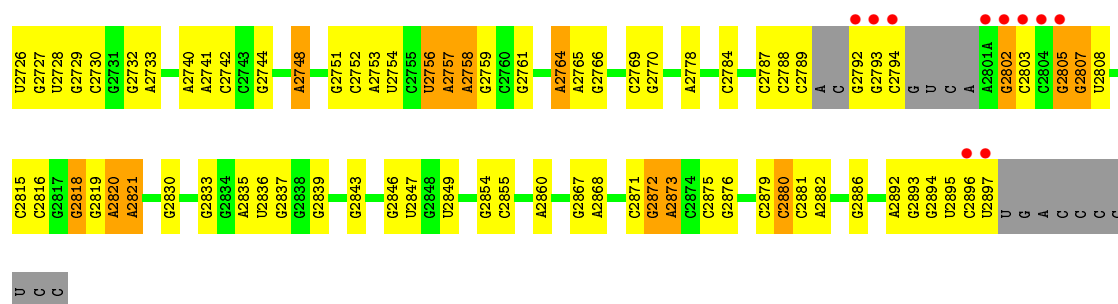




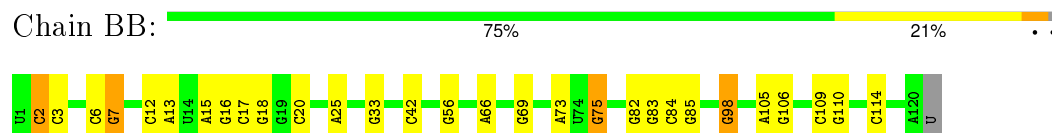
• Molecule 25: 23S Ribosomal RNA



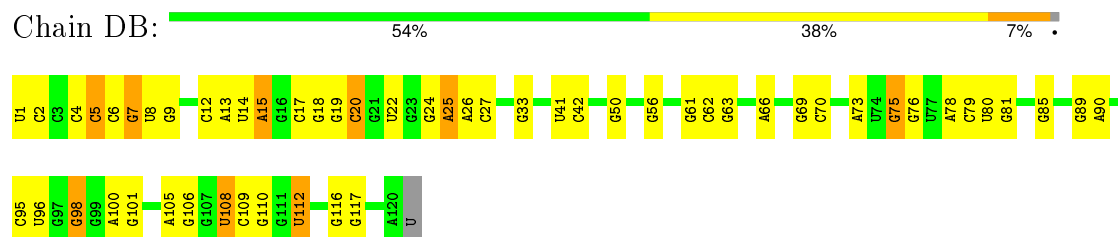
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C2643	C2540	G2447	C2355	C2285	G2168	C2108	A2005	G1896	A1785	A1670	G1559	C1451	C1363	U1273
U2649	A2541	A2448	C2356	A2286	A2170	G2110	C2006	G1899	A1786	U1671	A1566	G1459	G1364	A1274
A2650	A2542	U2449	U2357	A2287	A2171	C2111	G2012	A1900	A1789	G1674	A1569	A1461	A1365	A1278
C2651	G2543	C2449	C2358	A2288	U2172	G2112	A2013	G1899	A1790	C1685	C1577	G1465	G1368	G1283
C2652	G2544	A2450	C2359	G2289	A2173	U2113	A2014	A1903	A1791	C1686	U1578	G1466	G1369	A1284
U2653	G2550	A2453	A2360	G2290	C2174	A2114	G2018	G1903	U1794	G1687	U1579	A1467	G1370	G1285
A2654	C2551	U2457	G2364	C2292	C2175	G2115	A2019	G1906	C1795	U1688	A1579	C1467	G1371	A1286
G2655	U2552	U2457	G2365	U2296	C2176	A2116	G2020	G1906	U1796	A1689	A1580	U1372	U1372	A1287
G2659	G2553	U2457	G2366	U2297	C2177	A2117	G2021	G1906	U1797	U1692	A1583	A1471	G1373	U1288
A2660	U2554	C2461	A2369	G2299	C2178	U2118	G2022	A1912	U1798	C1685	A1584	A1472	G1374	U1292
G2661	U2555	U2462	G2300	G2300	U2180	G2120	G2023	C1914	G1799	U1693	C1586	G1473	C1375	C1293
A2662	C2556	C2465	C2301	C2302	C2183	U2122	C2026	G1922	U1794	C1694	A1587	C1474	C1375	
G2664	C2557	G2465	G2303	G2303	C2184	G2123	G2027	G1922	C1795	G1687	U1578	G1466	G1370	
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A2679	C2680		C2316	C2316	A2198	G2133	G2046	A1938	G1826	U1706	U1602	U1497	G1404	A1308
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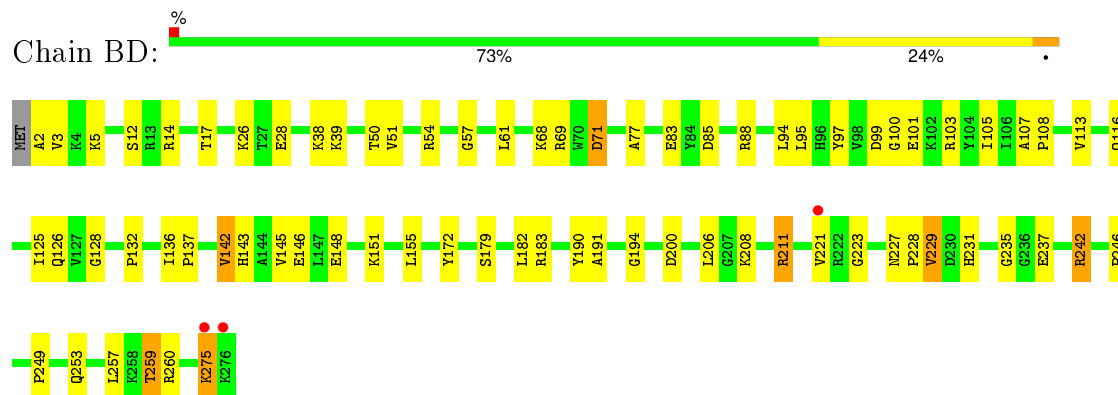
- Molecule 26: 5S Ribosomal RNA



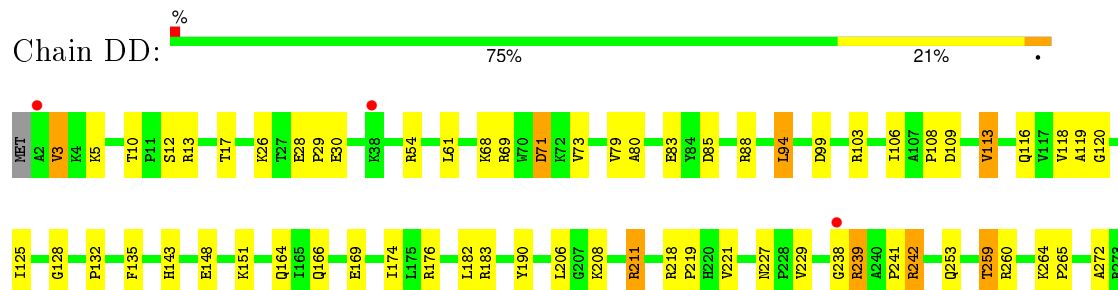
- Molecule 26: 5S Ribosomal RNA



- Molecule 27: 50S Ribosomal Protein L2



- Molecule 27: 50S Ribosomal Protein L2





• Molecule 28: 50S Ribosomal Protein L3

Chain BE: 2% 70% 24% 5%



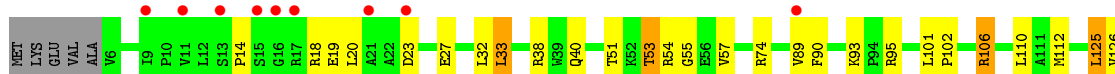
• Molecule 28: 50S Ribosomal Protein L3

Chain DE: 71% 21% 7%



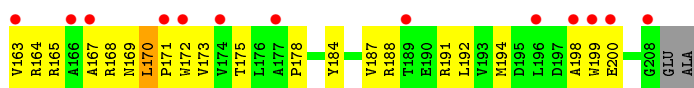
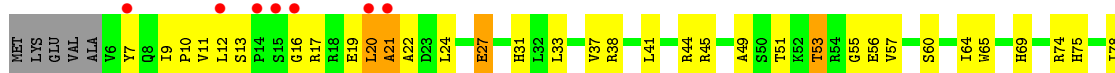
• Molecule 29: 50S Ribosomal Protein L4

Chain BF: 6% 71% 22%



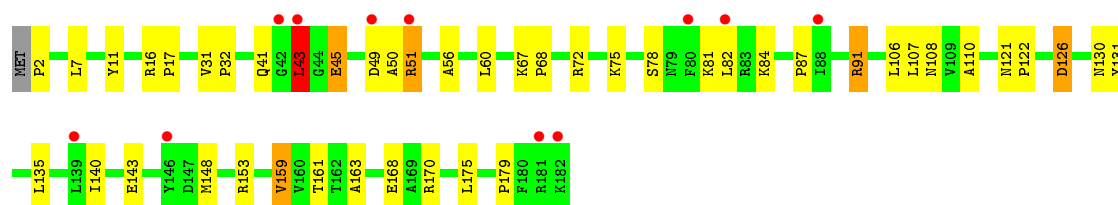
• Molecule 29: 50S Ribosomal Protein L4

Chain DF: 14% 55% 38%

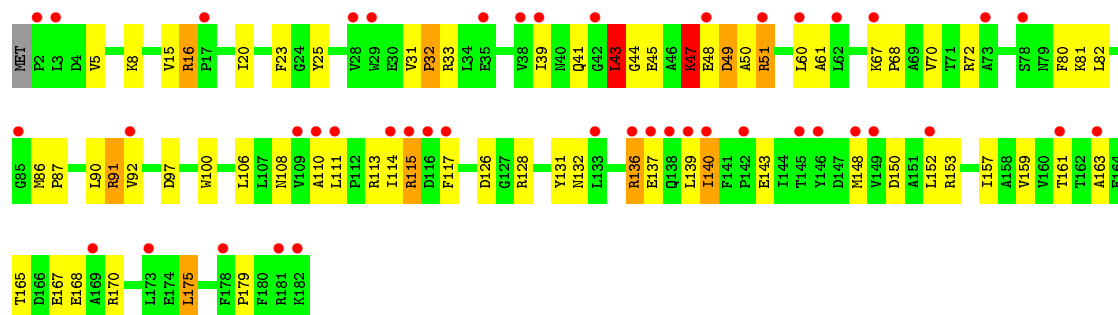


• Molecule 30: 50S Ribosomal Protein L5

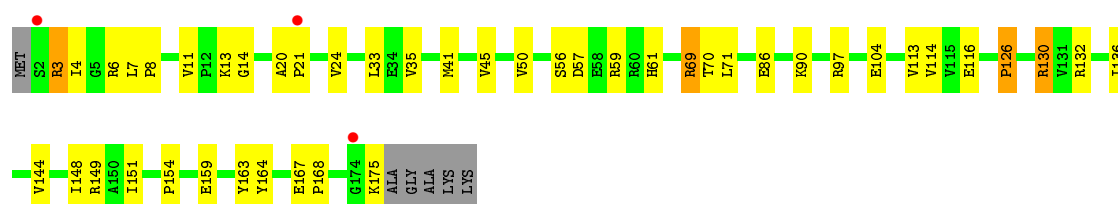
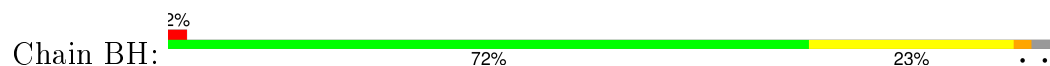
Chain BG: 6% 74% 22%



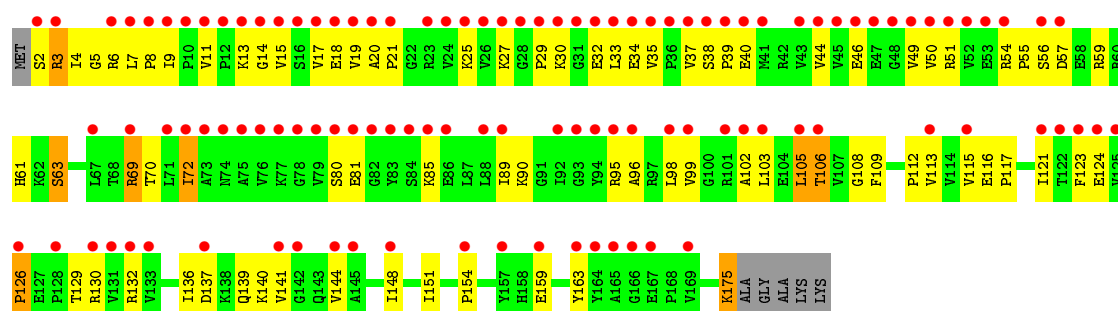
● Molecule 30: 50S Ribosomal Protein L5



● Molecule 31: 50S Ribosomal Protein L6

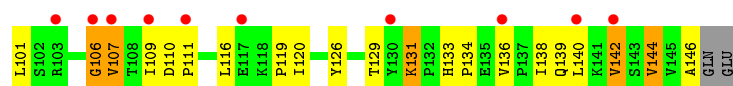


● Molecule 31: 50S Ribosomal Protein L6

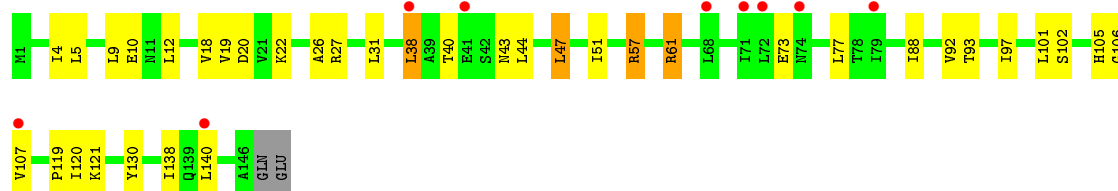
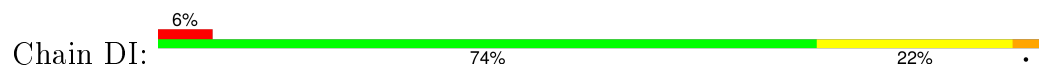


● Molecule 32: 50S Ribosomal Protein L9

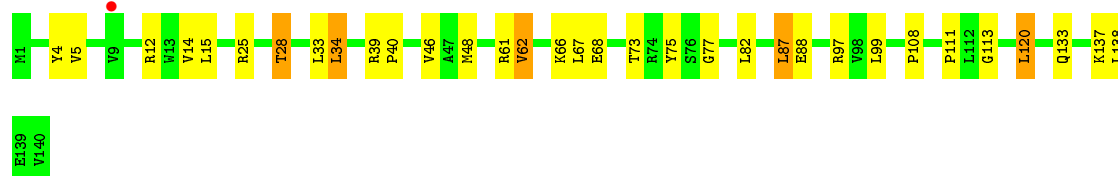
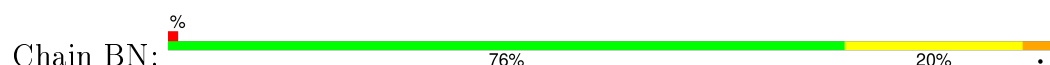




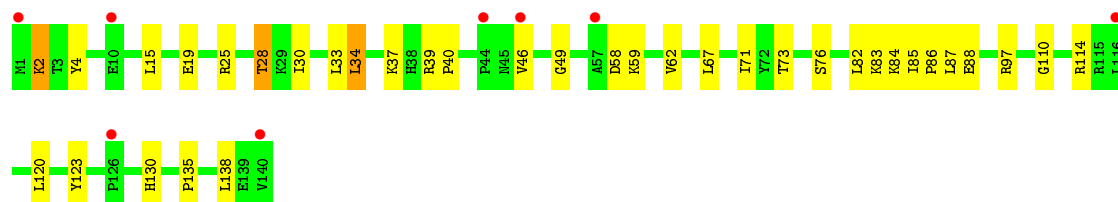
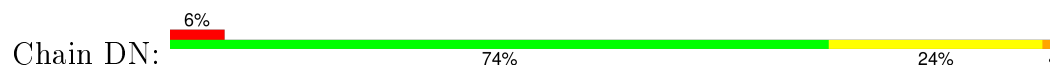
• Molecule 32: 50S Ribosomal Protein L9



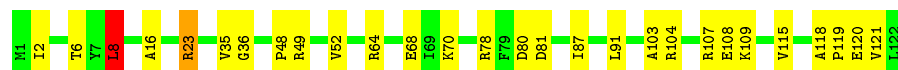
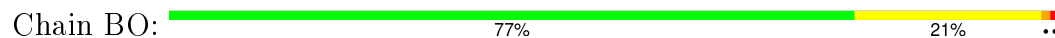
• Molecule 33: 50S Ribosomal Protein L13



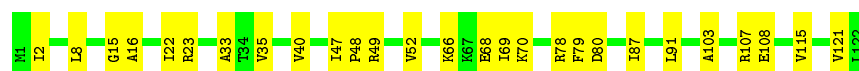
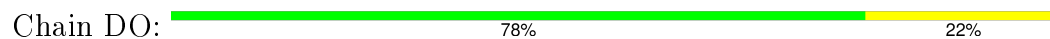
• Molecule 33: 50S Ribosomal Protein L13



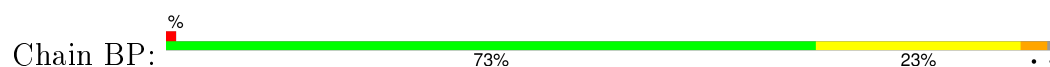
• Molecule 34: 50S Ribosomal Protein L14

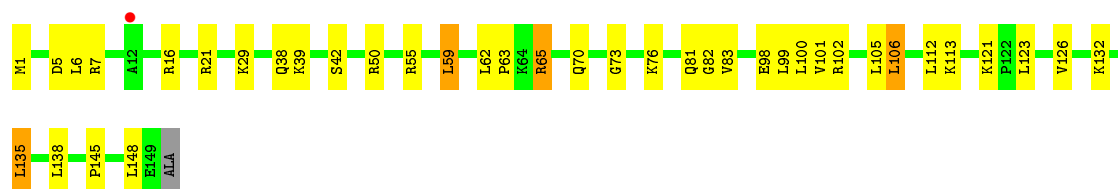


• Molecule 34: 50S Ribosomal Protein L14

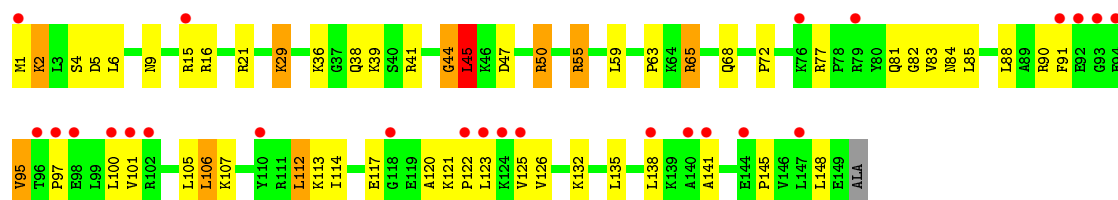


• Molecule 35: 50S Ribosomal Protein L15

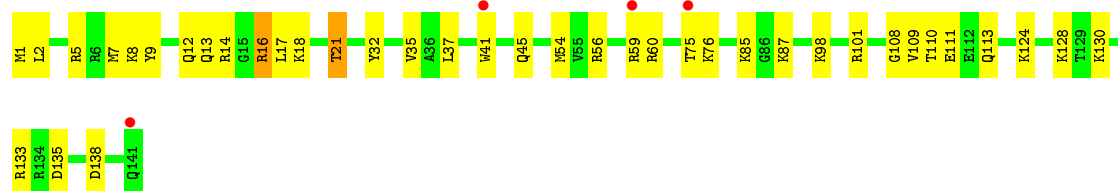
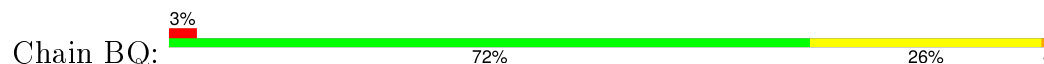




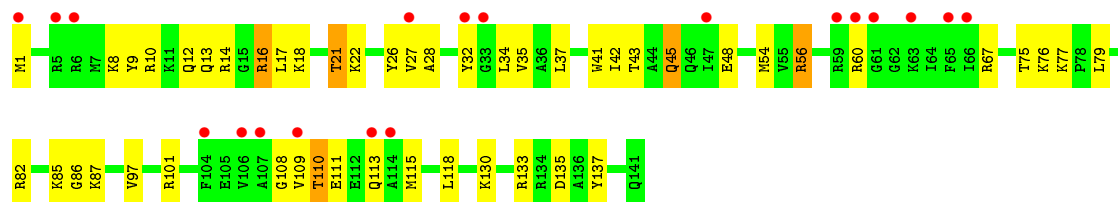
• Molecule 35: 50S Ribosomal Protein L15



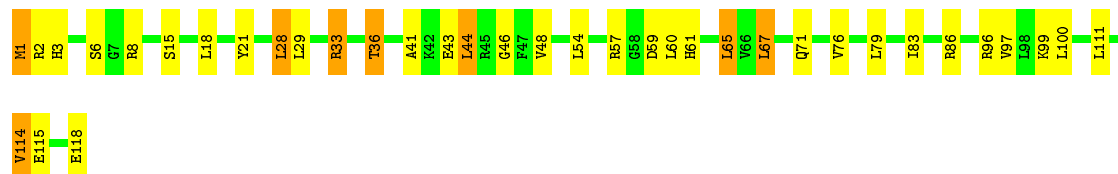
• Molecule 36: 50S Ribosomal Protein L16



• Molecule 36: 50S Ribosomal Protein L16



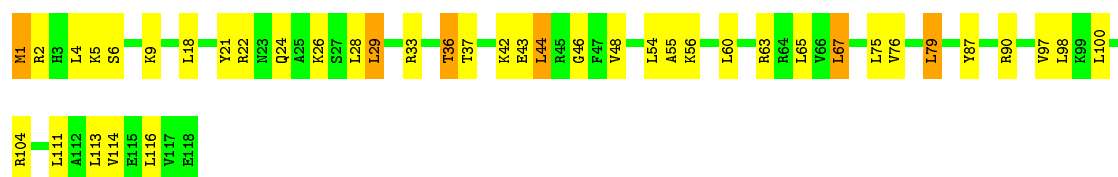
• Molecule 37: 50S Ribosomal Protein L17



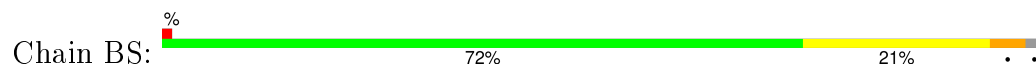
• Molecule 37: 50S Ribosomal Protein L17



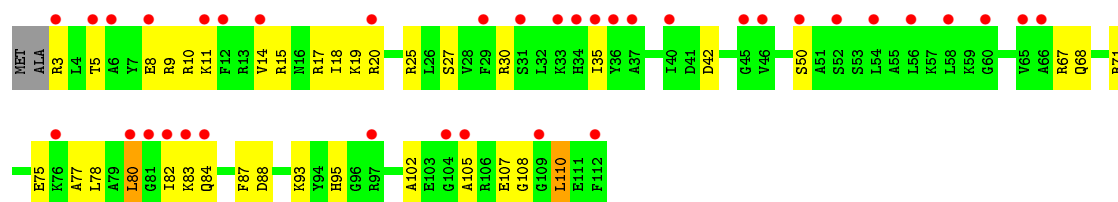




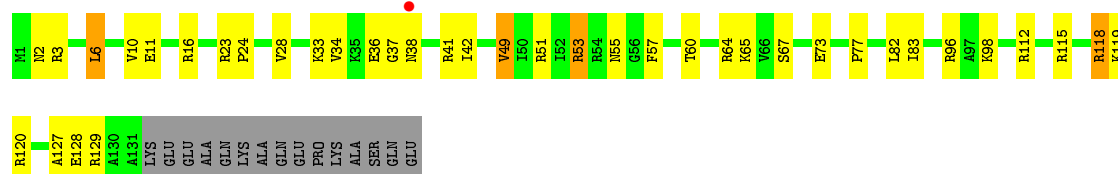
- Molecule 38: 50S Ribosomal Protein L18



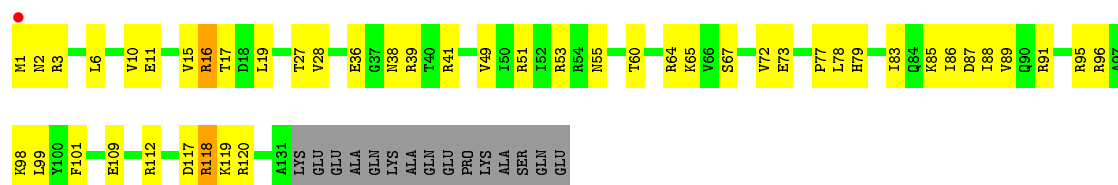
- Molecule 38: 50S Ribosomal Protein L18



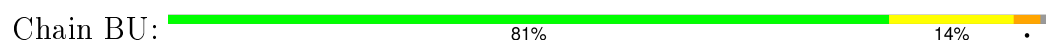
- Molecule 39: 50S Ribosomal Protein L19



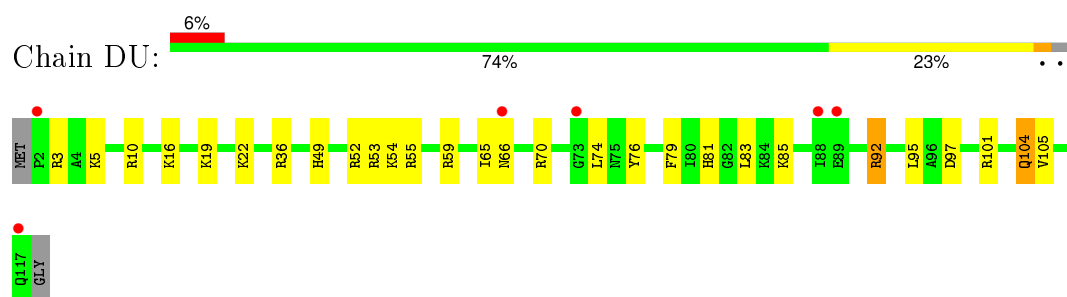
- Molecule 39: 50S Ribosomal Protein L19



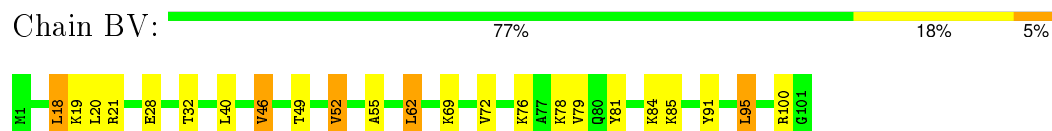
- Molecule 40: 50S Ribosomal Protein L20



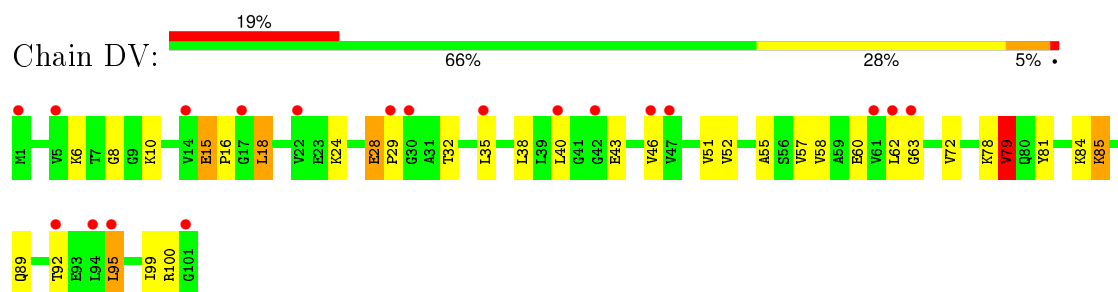
- Molecule 40: 50S Ribosomal Protein L20



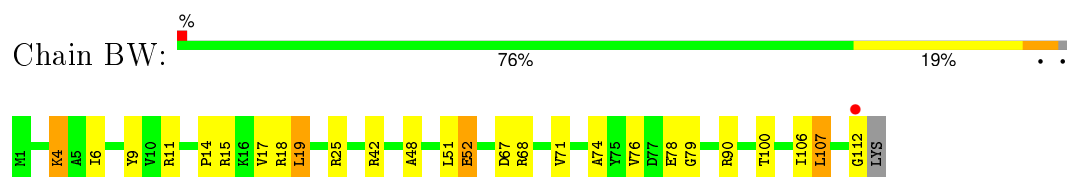
- Molecule 41: 50S Ribosomal Protein L21



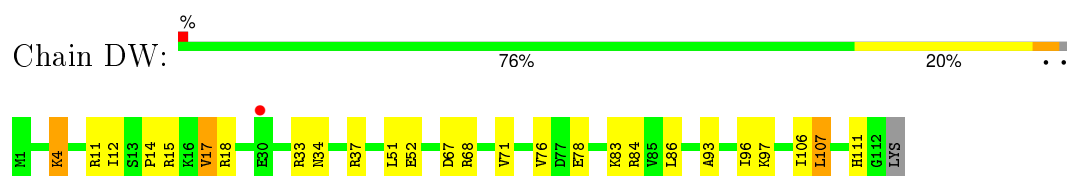
- Molecule 41: 50S Ribosomal Protein L21



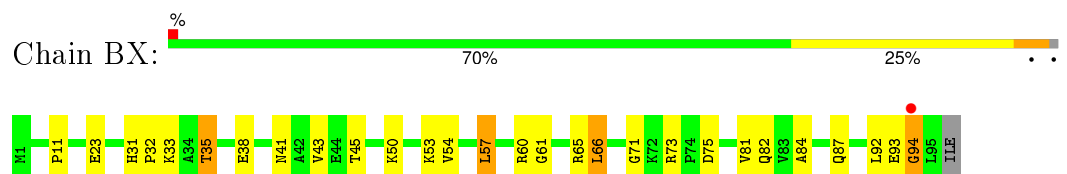
- Molecule 42: 50S Ribosomal Protein L22



- Molecule 42: 50S Ribosomal Protein L22

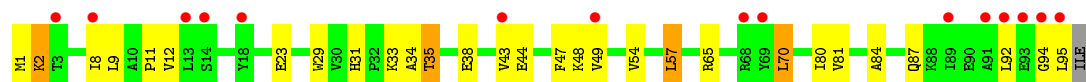


- Molecule 43: 50S Ribosomal Protein L23



- Molecule 43: 50S Ribosomal Protein L23

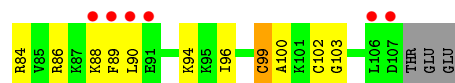
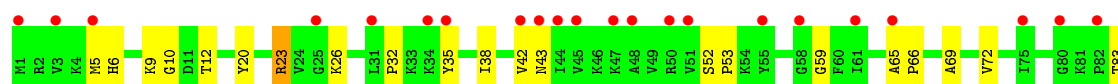




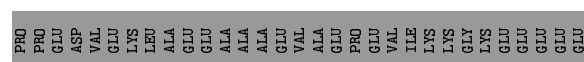
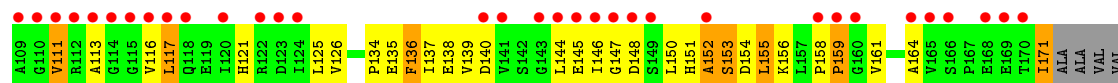
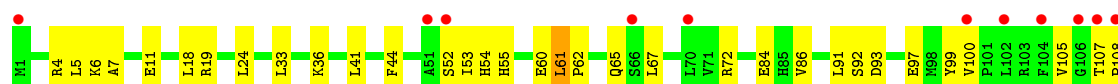
• Molecule 44: 50S Ribosomal Protein L24



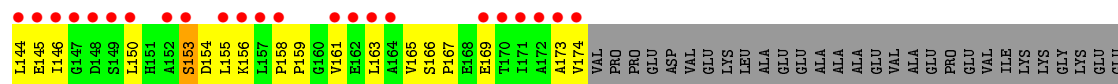
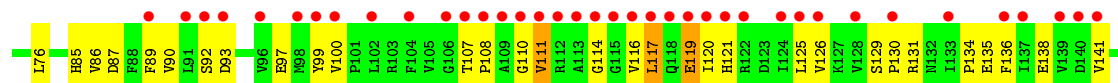
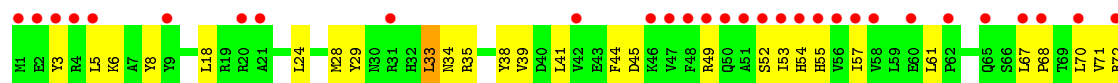
• Molecule 44: 50S Ribosomal Protein L24



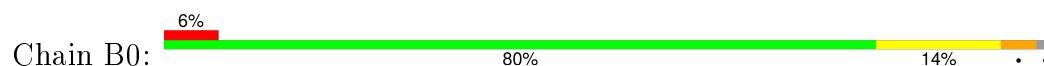
• Molecule 45: 50S Ribosomal Protein L25



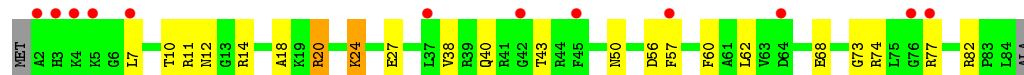
• Molecule 45: 50S Ribosomal Protein L25



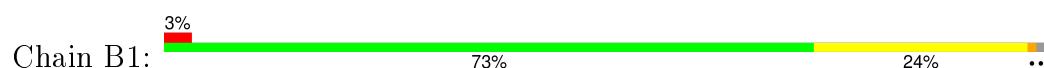
## • Molecule 46: 50S Ribosomal Protein L27



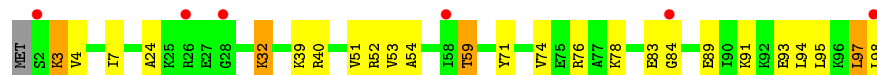
## • Molecule 46: 50S Ribosomal Protein L27



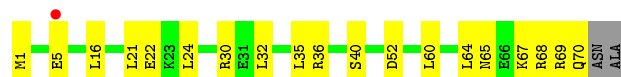
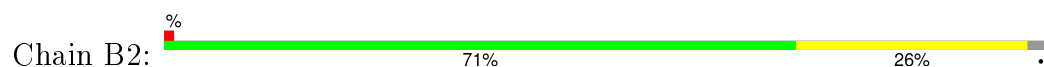
## • Molecule 47: 50S Ribosomal Protein L28



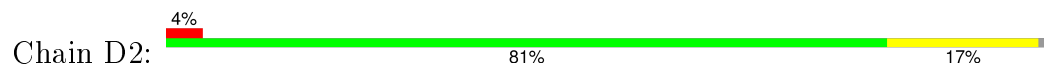
## • Molecule 47: 50S Ribosomal Protein L28



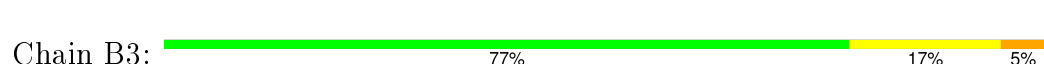
## • Molecule 48: 50S Ribosomal Protein L29



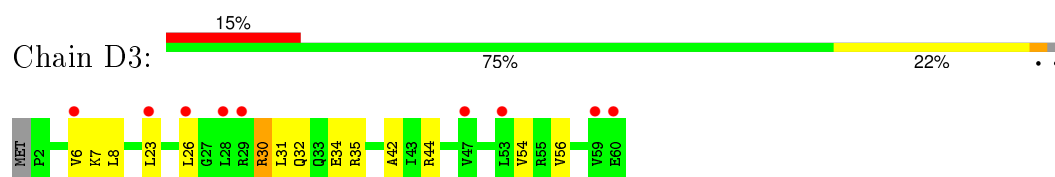
## • Molecule 48: 50S Ribosomal Protein L29



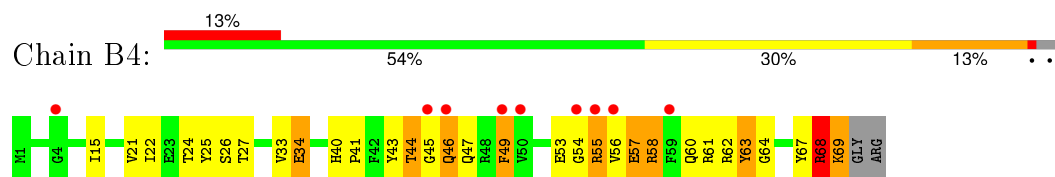
## • Molecule 49: 50S Ribosomal Protein L30



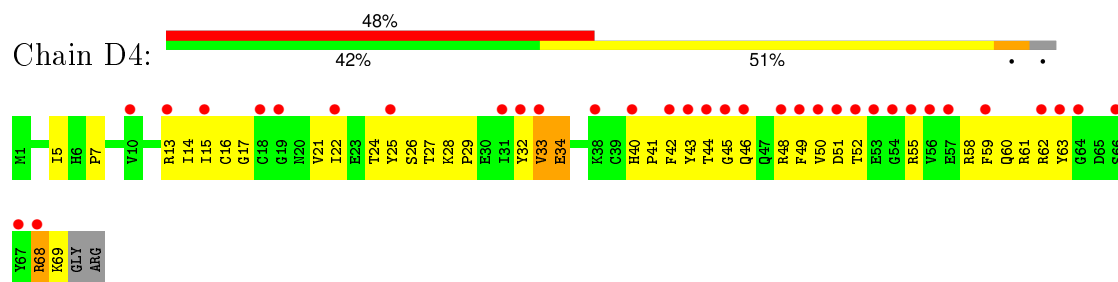
## • Molecule 49: 50S Ribosomal Protein L30



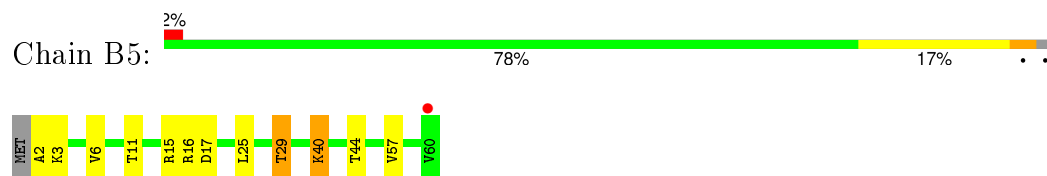
- Molecule 50: 50S Ribosomal Protein L31



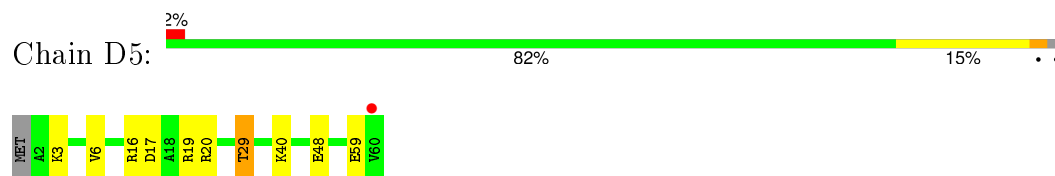
- Molecule 50: 50S Ribosomal Protein L31



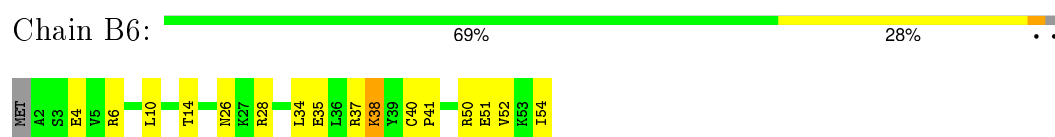
- Molecule 51: 50S Ribosomal Protein L32



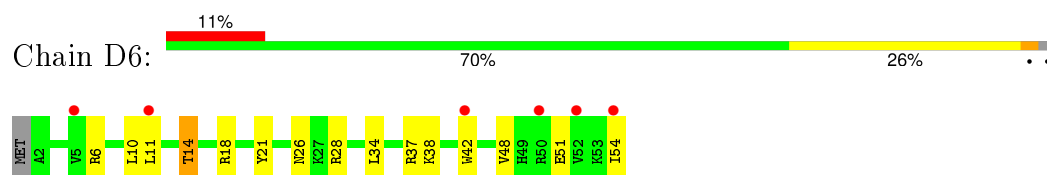
- Molecule 51: 50S Ribosomal Protein L32



- Molecule 52: 50S Ribosomal Protein L33



- Molecule 52: 50S Ribosomal Protein L33




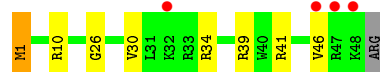
## ● Molecule 53: 50S Ribosomal Protein L34

Chain B7:  4% 67% 29% ..




## ● Molecule 53: 50S Ribosomal Protein L34

Chain D7:  8% 82% 14% ..



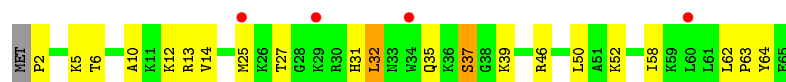
## ● Molecule 54: 50S Ribosomal Protein L35

Chain B8:  66% 32% .




## ● Molecule 54: 50S Ribosomal Protein L35

Chain D8:  6% 66% 29% ..




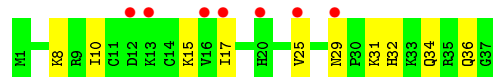
## ● Molecule 55: 50S Ribosomal Protein L36

Chain B9:  3% 86% 14%



## ● Molecule 55: 50S Ribosomal Protein L36

Chain D9:  19% 73% 27%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.35Å 449.01Å 621.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	145.52 – 2.55 145.52 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.0 (145.52-2.55) 99.0 (145.52-2.55)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.28 (at 2.55Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.225 , 0.273 0.237 , 0.282	Depositor DCC
$R_{free}$ test set	93275 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	48.2	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 58.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 1857518 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	297273	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.48% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, ZN, PCY, MIA, SF4, MG, 5MC, 4SU, 7MG, K, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	AA	0.43	0/36049	0.93	45/56261 (0.1%)
1	CA	0.42	2/36170 (0.0%)	0.95	52/56452 (0.1%)
2	AB	0.31	0/1881	0.62	1/2542 (0.0%)
2	CB	0.32	0/1860	0.59	0/2518
3	AC	0.30	0/1576	0.52	0/2130
3	CC	0.31	0/1566	0.55	0/2119
4	AD	0.32	0/1689	0.53	0/2267
4	CD	0.32	0/1704	0.55	0/2284
5	AE	0.31	0/1145	0.54	0/1543
5	CE	0.33	0/1149	0.59	0/1548
6	AF	0.32	0/819	0.53	0/1111
6	CF	0.30	0/829	0.52	0/1123
7	AG	0.30	0/1250	0.49	0/1679
7	CG	0.30	0/1254	0.50	0/1683
8	AH	0.30	0/1108	0.51	0/1494
8	CH	0.30	0/1108	0.53	0/1494
9	AI	0.32	0/1002	0.56	0/1346
9	CI	0.32	0/997	0.59	0/1343
10	AJ	0.30	0/722	0.56	0/982
10	CJ	0.31	0/727	0.60	0/988
11	AK	0.31	0/844	0.54	0/1145
11	CK	0.30	0/848	0.54	0/1149
12	AL	0.33	0/946	0.53	0/1274
12	CL	0.32	0/946	0.57	0/1274
13	AM	0.30	0/969	0.57	0/1302
13	CM	0.30	0/961	0.53	0/1291
14	AN	0.34	0/501	0.50	0/664
14	CN	0.33	0/501	0.56	0/664
15	AO	0.30	0/739	0.56	0/985
15	CO	0.31	0/739	0.54	0/985
16	AP	0.32	0/697	0.53	0/939
16	CP	0.31	0/693	0.50	0/935



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AQ	0.31	0/836	0.49	0/1117
17	CQ	0.30	0/836	0.52	0/1117
18	AR	0.32	0/560	0.55	0/746
18	CR	0.28	0/560	0.49	0/746
19	AS	0.30	0/667	0.54	0/900
19	CS	0.34	0/661	0.66	0/893
20	AT	0.29	0/730	0.57	0/965
20	CT	0.30	0/729	0.53	0/965
21	AU	0.33	0/203	0.50	0/266
21	CU	0.34	0/203	0.53	0/266
22	AV	0.48	0/310	1.00	0/480
22	CV	0.45	0/310	0.91	2/480 (0.4%)
23	AW	0.48	0/1602	1.06	0/2493
23	AY	0.52	0/1602	1.16	4/2493 (0.2%)
23	CW	0.52	0/1556	1.19	10/2418 (0.4%)
23	CY	0.54	0/1579	1.18	5/2455 (0.2%)
24	AX	0.55	2/1725 (0.1%)	1.16	12/2689 (0.4%)
24	CX	0.56	1/1725 (0.1%)	1.18	18/2689 (0.7%)
25	BA	0.60	6/68013 (0.0%)	1.02	122/106165 (0.1%)
25	DA	0.49	0/67542	0.98	62/105428 (0.1%)
26	BB	0.49	0/2878	0.91	0/4490
26	DB	0.51	0/2878	0.96	1/4490 (0.0%)
27	BD	0.41	0/2186	0.64	1/2944 (0.0%)
27	DD	0.38	0/2186	0.59	1/2944 (0.0%)
28	BE	0.42	0/1592	0.58	0/2149
28	DE	0.36	0/1592	0.58	1/2149 (0.0%)
29	BF	0.40	0/1619	0.58	0/2193
29	DF	0.36	0/1615	0.59	0/2188
30	BG	0.33	0/1450	0.56	1/1959 (0.1%)
30	DG	0.33	0/1449	0.56	0/1958
31	BH	0.34	0/1356	0.52	0/1834
31	DH	0.32	0/1356	0.53	0/1834
32	BI	0.31	0/1100	0.57	0/1501
32	DI	0.29	0/1076	0.56	0/1471
33	BN	0.39	0/1144	0.56	0/1543
33	DN	0.35	0/1144	0.56	0/1543
34	BO	0.42	0/943	0.60	1/1269 (0.1%)
34	DO	0.34	0/943	0.51	0/1269
35	BP	0.38	0/1152	0.59	0/1533
35	DP	0.35	0/1152	0.61	1/1533 (0.1%)
36	BQ	0.41	0/1143	0.55	0/1527
36	DQ	0.36	0/1143	0.55	0/1527
37	BR	0.42	0/982	0.65	0/1312

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
37	DR	0.31	0/982	0.54	0/1312
38	BS	0.34	0/887	0.59	0/1180
38	DS	0.32	0/880	0.55	0/1172
39	BT	0.39	0/1105	0.60	0/1477
39	DT	0.31	0/1097	0.52	0/1468
40	BU	0.45	0/977	0.62	1/1301 (0.1%)
40	DU	0.32	0/977	0.52	0/1301
41	BV	0.44	0/782	0.61	0/1049
41	DV	0.33	0/782	0.54	0/1049
42	BW	0.44	0/897	0.61	0/1205
42	DW	0.33	0/897	0.53	0/1205
43	BX	0.44	0/764	0.64	1/1025 (0.1%)
43	DX	0.36	0/764	0.57	1/1025 (0.1%)
44	BY	0.42	0/819	0.64	0/1095
44	DY	0.33	0/819	0.52	0/1095
45	BZ	0.35	0/1379	0.60	0/1873
45	DZ	0.33	0/1390	0.56	0/1890
46	B0	0.40	0/662	0.66	1/881 (0.1%)
46	D0	0.33	0/662	0.52	0/881
47	B1	0.40	0/762	0.57	0/1014
47	D1	0.34	0/762	0.56	0/1014
48	B2	0.37	0/590	0.65	0/781
48	D2	0.30	0/590	0.47	0/781
49	B3	0.42	0/474	0.62	0/635
49	D3	0.30	0/469	0.53	0/630
50	B4	0.39	0/571	0.66	0/768
50	D4	0.33	0/545	0.60	0/737
51	B5	0.39	0/469	0.64	0/635
51	D5	0.33	0/469	0.58	0/635
52	B6	0.42	0/460	0.58	0/613
52	D6	0.36	0/456	0.49	0/608
53	B7	0.45	0/426	0.66	0/561
53	D7	0.36	0/426	0.52	0/561
54	B8	0.41	0/519	0.62	0/684
54	D8	0.33	0/525	0.55	0/691
55	B9	0.44	0/310	0.52	0/407
55	D9	0.34	0/310	0.57	0/407
All	All	0.47	11/316672 (0.0%)	0.90	344/474091 (0.1%)

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
2	AB	0	1
7	AG	0	1
7	CG	0	1
19	CS	0	1
27	DD	0	1
38	BS	0	1
44	BY	0	1
All	All	0	7

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	354	A	N9-C4	-7.89	1.33	1.37
1	CA	1154	G	C6-N1	-7.66	1.34	1.39
25	BA	1188	A	N9-C4	-7.63	1.33	1.37
25	BA	1067	A	N9-C4	-6.49	1.33	1.37
24	AX	14	A	N7-C5	-6.24	1.35	1.39
24	AX	14	A	C8-N7	-6.01	1.27	1.31
25	BA	553	A	N9-C4	-5.68	1.34	1.37
24	CX	22	G	N7-C5	5.39	1.42	1.39
25	BA	593	G	C6-O6	-5.35	1.19	1.24
1	CA	1154	G	N1-C2	-5.31	1.33	1.37
25	BA	990	A	N9-C4	-5.25	1.34	1.37

All (344) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CA	1154	G	C5-C6-O6	17.34	139.00	128.60
1	CA	1119	C	C2-N3-C4	16.52	128.16	119.90
1	CA	1154	G	N3-C2-N2	14.11	129.78	119.90
1	CA	1119	C	N1-C2-O2	14.07	127.34	118.90
1	CA	1154	G	N1-C6-O6	-11.05	113.27	119.90
1	CA	1154	G	N1-C2-N2	-10.96	106.33	116.20
25	BA	354	A	C2-N3-C4	-10.77	105.21	110.60
1	CA	79	G	C5-C6-O6	10.57	134.94	128.60
24	AX	14	A	C4-C5-C6	10.08	122.04	117.00
1	CA	1119	C	N3-C4-C5	-10.03	117.89	121.90
1	CA	1154	G	C6-N1-C2	9.98	131.09	125.10
25	BA	848	G	O5'-P-OP2	-9.83	96.86	105.70
24	AX	46	G	C6-N1-C2	-9.82	119.21	125.10
24	CX	46	G	C6-N1-C2	-9.78	119.23	125.10
1	CA	1119	C	C5-C4-N4	9.74	127.02	120.20
1	CA	1004	A	O4'-C1'-N9	9.72	115.98	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BA	1067	A	C2-N3-C4	-9.68	105.76	110.60
24	AX	14	A	C5-N7-C8	9.60	108.70	103.90
25	DA	2585	U	C5-C4-O4	-9.26	120.35	125.90
25	DA	1776	G	O5'-P-OP2	-9.18	97.44	105.70
25	BA	2162	C	N1-C2-O2	8.97	124.28	118.90
25	BA	1686	U	O5'-P-OP2	-8.95	97.64	105.70
24	CX	14	A	C4-C5-C6	8.89	121.45	117.00
23	AY	64	A	C5-C6-N6	8.55	130.54	123.70
25	BA	593	G	C5-C6-O6	-8.55	123.47	128.60
25	BA	599	U	O5'-P-OP1	-8.44	98.10	105.70
25	BA	2697	G	N1-C6-O6	-8.39	114.86	119.90
1	CA	997	U	C5-C4-O4	8.29	130.87	125.90
25	BA	537	G	O4'-C1'-N9	8.28	114.83	108.20
25	BA	2566	U	O5'-P-OP1	-8.24	98.28	105.70
24	AX	14	A	C5-C6-N1	-8.12	113.64	117.70
25	BA	139	A	N7-C8-N9	8.08	117.84	113.80
24	CX	14	A	C5-N7-C8	8.04	107.92	103.90
25	BA	2160	C	N1-C2-O2	8.02	123.71	118.90
25	BA	2162	C	C2-N1-C1'	8.01	127.61	118.80
25	DA	1352	U	O5'-P-OP1	-7.92	98.57	105.70
23	AY	64	A	N1-C6-N6	-7.87	113.88	118.60
24	AX	22	G	C5-N7-C8	-7.87	100.37	104.30
25	BA	2014	G	P-O3'-C3'	7.82	129.08	119.70
25	BA	1067	A	N1-C2-N3	7.75	133.18	129.30
25	DA	2155	G	N3-C2-N2	7.64	125.25	119.90
1	CA	1119	C	N3-C2-O2	-7.61	116.57	121.90
1	CA	1154	G	C5-C6-N1	-7.61	107.69	111.50
25	BA	990	A	C2-N3-C4	-7.54	106.83	110.60
25	BA	354	A	N3-C4-N9	-7.54	121.37	127.40
25	BA	553	A	C2-N3-C4	-7.54	106.83	110.60
25	BA	2605	U	N3-C4-O4	-7.47	114.17	119.40
24	CX	22	G	C5-N7-C8	-7.45	100.57	104.30
25	BA	1660	A	O5'-P-OP1	-7.41	99.03	105.70
25	BA	139	A	C5-N7-C8	-7.39	100.20	103.90
24	CX	14	A	C5-C6-N1	-7.31	114.04	117.70
1	CA	1119	C	C5-C6-N1	7.31	124.65	121.00
24	CX	22	G	N1-C6-O6	-7.29	115.52	119.90
23	CY	48	C	N1-C2-O2	7.29	123.27	118.90
25	BA	354	A	N1-C2-N3	7.25	132.92	129.30
25	BA	12	U	C2-N1-C1'	7.23	126.38	117.70
25	BA	593	G	C5-C6-N1	7.18	115.09	111.50
1	AA	365	U	C5-C6-N1	-7.12	119.14	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	DA	2585	U	C2-N1-C1'	7.11	126.23	117.70
1	AA	1397	C	O4'-C1'-N1	7.10	113.88	108.20
1	AA	991	U	P-O3'-C3'	7.09	128.21	119.70
25	BA	2162	C	N3-C2-O2	-7.05	116.96	121.90
25	BA	215	G	O4'-C1'-N9	7.05	113.84	108.20
1	AA	254	G	O5'-P-OP1	-7.05	99.36	105.70
23	CW	3	C	N1-C2-O2	7.02	123.11	118.90
1	AA	1030(B)	C	C2-N1-C1'	6.98	126.47	118.80
25	BA	1807	G	O5'-P-OP2	-6.97	99.42	105.70
25	BA	2162	C	C6-N1-C2	-6.95	117.52	120.30
1	CA	1119	C	C6-N1-C2	-6.91	117.54	120.30
25	BA	354	A	N3-C4-C5	6.88	131.62	126.80
25	BA	2260	C	O5'-P-OP2	-6.88	99.50	105.70
1	CA	1004	A	N1-C6-N6	-6.88	114.47	118.60
25	BA	1346	U	P-O3'-C3'	6.87	127.94	119.70
24	AX	46	G	C5-C6-N1	6.87	114.93	111.50
25	BA	1154	U	N3-C2-O2	-6.86	117.40	122.20
27	BD	257	LEU	CA-CB-CG	6.86	131.07	115.30
1	CA	1003	G	N7-C8-N9	6.85	116.53	113.10
25	BA	1188	A	C2-N3-C4	-6.82	107.19	110.60
25	DA	2585	U	C6-N1-C1'	-6.81	111.67	121.20
25	DA	1372	U	N3-C4-O4	6.78	124.15	119.40
25	DA	1698	A	O4'-C1'-N9	6.78	113.62	108.20
1	CA	79	G	N1-C6-O6	-6.77	115.84	119.90
25	DA	2136	C	N1-C2-O2	6.73	122.94	118.90
34	BO	8	LEU	CA-CB-CG	6.73	130.77	115.30
1	CA	1183	A	P-O3'-C3'	6.72	127.76	119.70
25	DA	1372	U	C5-C4-O4	-6.71	121.87	125.90
25	DA	1639	U	O5'-P-OP2	-6.70	99.67	105.70
1	AA	98	G	N3-C4-N9	6.68	130.01	126.00
25	BA	1188	A	N3-C4-C5	6.66	131.46	126.80
1	AA	1278	U	C5-C6-N1	6.64	126.02	122.70
25	BA	139	A	C8-N9-C4	-6.64	103.15	105.80
25	BA	2160	C	N3-C2-O2	-6.63	117.26	121.90
43	BX	57	LEU	CA-CB-CG	6.63	130.56	115.30
1	CA	532	A	P-O3'-C3'	6.62	127.64	119.70
25	DA	2155	G	C6-N1-C2	6.56	129.04	125.10
1	CA	991	U	P-O3'-C3'	6.53	127.53	119.70
1	AA	1002	G	N3-C4-N9	6.53	129.92	126.00
1	AA	98	G	C6-C5-N7	-6.51	126.49	130.40
25	DA	277	C	C6-N1-C2	-6.47	117.71	120.30
1	AA	1030(B)	C	O4'-C1'-N1	6.47	113.37	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CA	79	G	C6-N1-C2	6.46	128.98	125.10
1	AA	1397	C	C2-N1-C1'	6.42	125.86	118.80
25	BA	989	G	N3-C4-N9	6.42	129.85	126.00
1	CA	754	C	C2-N1-C1'	6.42	125.86	118.80
25	BA	2298	A	N7-C8-N9	6.42	117.01	113.80
25	BA	1188	A	N3-C4-N9	-6.39	122.29	127.40
25	DA	512	G	O4'-C1'-N9	6.38	113.31	108.20
24	CX	20	U	C2-N1-C1'	6.37	125.34	117.70
24	CX	22	G	C4-C5-C6	-6.36	114.98	118.80
1	CA	754	C	N1-C2-O2	6.35	122.71	118.90
25	BA	989	G	N9-C4-C5	-6.33	102.87	105.40
25	BA	2803	A	C2-N3-C4	6.31	113.76	110.60
25	DA	2585	U	N3-C4-O4	6.31	123.82	119.40
25	DA	614	U	N3-C2-O2	-6.30	117.79	122.20
25	BA	1418	U	C5-C4-O4	-6.29	122.12	125.90
25	BA	1154	U	N1-C2-O2	6.29	127.20	122.80
25	BA	986	A	O5'-P-OP1	-6.24	100.08	105.70
25	BA	989	G	C6-C5-N7	-6.23	126.66	130.40
25	BA	2160	C	C6-N1-C2	-6.23	117.81	120.30
25	BA	399	G	O4'-C1'-N9	6.22	113.18	108.20
25	BA	990	A	C5-N7-C8	-6.21	100.79	103.90
22	CV	19	U	C5-C4-O4	6.18	129.61	125.90
1	CA	1492	A	P-O3'-C3'	6.13	127.06	119.70
25	DA	2140	C	N1-C2-O2	6.13	122.58	118.90
1	AA	98	G	N7-C8-N9	6.13	116.17	113.10
1	AA	365	U	C2-N1-C1'	-6.12	110.35	117.70
25	BA	1398	U	O5'-P-OP1	-6.11	100.20	105.70
25	BA	184	A	P-O3'-C3'	6.11	127.03	119.70
25	DA	1191	G	O5'-P-OP2	-6.11	100.20	105.70
1	CA	1003	G	C4-N9-C1'	6.10	134.43	126.50
25	BA	1232	G	N1-C6-O6	-6.09	116.24	119.90
1	CA	1003	G	C8-N9-C4	-6.09	103.96	106.40
25	BA	2050	U	N3-C4-O4	-6.07	115.15	119.40
25	DA	2207	G	C6-C5-N7	-6.04	126.78	130.40
23	CY	4	C	C5-C4-N4	6.03	124.42	120.20
25	BA	2610	A	O5'-P-OP1	-6.02	100.28	105.70
25	BA	553	A	C5-N7-C8	-6.02	100.89	103.90
1	CA	1064	G	P-O3'-C3'	6.02	126.92	119.70
25	BA	2565	G	N3-C4-N9	5.98	129.59	126.00
25	BA	793	A	O4'-C1'-N9	5.98	112.98	108.20
25	BA	1958	A	O4'-C1'-N9	5.96	112.97	108.20
1	AA	1036	G	N1-C6-O6	-5.96	116.32	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	CW	36	A	C6-N1-C2	5.96	122.17	118.60
25	BA	139	A	O4'-C1'-N9	5.96	112.96	108.20
25	DA	2685	G	N1-C6-O6	-5.95	116.33	119.90
1	CA	79	G	N3-C4-N9	-5.95	122.43	126.00
25	BA	1539	C	N1-C2-O2	5.94	122.47	118.90
25	BA	2015	U	O5'-P-OP1	-5.94	100.36	105.70
23	CW	67	C	C2-N3-C4	5.93	122.87	119.90
25	BA	637	U	N3-C2-O2	-5.93	118.05	122.20
1	AA	1002	G	N3-C4-C5	-5.92	125.64	128.60
24	CX	46	G	C5-C6-N1	5.92	114.46	111.50
1	CA	90	U	N1-C2-O2	-5.90	118.67	122.80
25	BA	254	A	O4'-C1'-N9	5.87	112.89	108.20
23	CW	25	C	O4'-C1'-N1	5.86	112.89	108.20
25	BA	2014	G	O4'-C1'-N9	-5.85	103.52	108.20
23	AY	64	A	C6-N1-C2	5.84	122.11	118.60
1	CA	1158	C	N1-C2-O2	5.84	122.41	118.90
25	DA	1300	U	P-O3'-C3'	5.84	126.71	119.70
25	BA	1067	A	C5-N7-C8	-5.83	100.98	103.90
25	DA	1128	A	C8-N9-C4	5.82	108.13	105.80
1	AA	98	G	N3-C4-C5	-5.81	125.69	128.60
24	CX	20	U	N1-C2-O2	5.81	126.86	122.80
25	BA	989	G	C8-N9-C1'	-5.80	119.46	127.00
22	CV	19	U	C2-N3-C4	5.77	130.46	127.00
25	DA	2275	C	O4'-C1'-N1	-5.77	103.59	108.20
30	BG	82	LEU	CA-CB-CG	5.76	128.55	115.30
1	AA	267	C	O5'-P-OP1	-5.74	100.54	105.70
25	DA	1368	G	O5'-P-OP2	-5.74	100.54	105.70
1	AA	98	G	C4-N9-C1'	5.73	133.95	126.50
1	AA	1502	A	N7-C8-N9	5.73	116.66	113.80
25	DA	2554	U	O5'-P-OP2	-5.71	100.56	105.70
25	BA	2697	G	C5-C6-O6	5.71	132.02	128.60
26	DB	1	U	C2-N1-C1'	5.70	124.54	117.70
1	CA	1260	C	C6-N1-C2	-5.68	118.03	120.30
25	DA	141	A	N7-C8-N9	5.68	116.64	113.80
23	AY	50	U	C2-N3-C4	5.67	130.40	127.00
25	BA	1745	A	C2-N3-C4	-5.67	107.76	110.60
24	AX	14	A	C8-N9-C1'	-5.66	117.52	127.70
43	DX	57	LEU	CA-CB-CG	5.65	128.29	115.30
25	BA	834	U	O5'-P-OP1	-5.65	100.62	105.70
1	AA	1067	A	P-O3'-C3'	5.64	126.47	119.70
25	DA	2805	G	O4'-C1'-N9	5.64	112.72	108.20
1	AA	266	G	P-O3'-C3'	5.64	126.47	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BA	137	G	C5-N7-C8	5.64	107.12	104.30
25	DA	1313	U	C2-N1-C1'	5.63	124.46	117.70
25	DA	242	G	N1-C6-O6	-5.62	116.53	119.90
25	DA	2585	U	O4'-C1'-N1	-5.62	103.70	108.20
25	BA	285	U	O4'-C1'-N1	5.62	112.69	108.20
28	DE	72	VAL	C-N-CA	5.62	135.74	121.70
23	CW	67	C	N1-C2-O2	5.60	122.26	118.90
1	AA	1007	C	C2-N3-C4	5.59	122.70	119.90
25	DA	673	C	N1-C2-O2	-5.59	115.55	118.90
25	BA	2189	U	C2-N1-C1'	5.58	124.40	117.70
25	DA	195	A	P-O3'-C3'	5.58	126.39	119.70
1	AA	346	G	C4-N9-C1'	5.57	133.74	126.50
25	BA	1686	U	OP1-P-OP2	5.57	127.95	119.60
24	CX	14	A	C4-N9-C1'	5.56	136.31	126.30
25	BA	978	A	O4'-C1'-N9	5.55	112.64	108.20
25	DA	141	A	O4'-C1'-N9	5.55	112.64	108.20
25	BA	593	G	C4-C5-N7	5.55	113.02	110.80
23	CY	15	G	N3-C2-N2	-5.55	116.01	119.90
25	DA	945	A	C5-N7-C8	-5.55	101.13	103.90
1	AA	1299	A	O5'-P-OP1	5.55	117.36	110.70
23	CW	75	C	P-O3'-C3'	5.54	126.35	119.70
1	AA	1190	G	OP2-P-O3'	5.54	117.39	105.20
23	CW	62	C	C5-C6-N1	5.52	123.76	121.00
25	DA	1992	G	P-O3'-C3'	5.52	126.32	119.70
1	AA	754	C	C2-N1-C1'	5.51	124.86	118.80
24	AX	22	G	N7-C8-N9	5.50	115.85	113.10
25	DA	1996	C	OP1-P-O3'	5.50	117.30	105.20
1	CA	992	U	P-O3'-C3'	5.49	126.29	119.70
1	CA	532	A	OP1-P-O3'	5.48	117.26	105.20
1	AA	1008	C	C2-N3-C4	5.48	122.64	119.90
1	AA	1007	C	N1-C2-O2	5.48	122.19	118.90
25	BA	2298	A	C8-N9-C4	-5.47	103.61	105.80
25	BA	1360	C	O5'-P-OP1	-5.47	100.78	105.70
25	BA	2858	G	O4'-C1'-N9	5.46	112.56	108.20
24	CX	22	G	C5-C6-N1	5.46	114.23	111.50
25	BA	1067	A	N7-C8-N9	5.45	116.52	113.80
1	AA	1022	G	N3-C2-N2	5.45	123.71	119.90
24	CX	46	G	N1-C2-N3	5.44	127.17	123.90
25	BA	1694	G	O4'-C1'-N9	-5.44	103.85	108.20
1	CA	984	C	C2-N3-C4	5.44	122.62	119.90
1	CA	1152	A	O4'-C1'-N9	5.44	112.55	108.20
25	DA	1791	A	O5'-P-OP1	-5.44	100.80	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CA	1183	A	OP1-P-O3'	5.44	117.16	105.20
25	BA	978	A	C5-N7-C8	-5.43	101.19	103.90
25	DA	753	C	O5'-P-OP1	-5.43	100.82	105.70
1	AA	1397	C	C6-N1-C1'	-5.42	114.30	120.80
25	BA	1720	U	C5-C6-N1	-5.42	119.99	122.70
25	BA	993	G	O5'-P-OP1	-5.42	100.83	105.70
23	CY	22	G	N3-C4-N9	5.41	129.25	126.00
25	BA	553	A	N3-C4-N9	-5.41	123.07	127.40
25	DA	2110	G	OP2-P-O3'	5.41	117.10	105.20
2	AB	9	GLU	N-CA-C	5.41	125.60	111.00
25	BA	2162	C	C5-C6-N1	5.41	123.70	121.00
25	DA	277	C	N1-C2-O2	5.41	122.14	118.90
1	CA	65	U	P-O3'-C3'	5.40	126.18	119.70
1	CA	1028	C	C5-C6-N1	5.40	123.70	121.00
24	AX	14	A	C4-N9-C1'	5.40	136.02	126.30
25	BA	2697	G	C6-C5-N7	5.40	133.64	130.40
25	BA	989	G	C4-N9-C1'	5.40	133.51	126.50
1	CA	1190	G	OP2-P-O3'	5.39	117.07	105.20
25	DA	614	U	C5-C4-O4	5.39	129.14	125.90
1	AA	1002	G	C4-N9-C1'	5.38	133.50	126.50
25	DA	2028	U	N3-C4-O4	-5.38	115.64	119.40
1	AA	1285	A	P-O3'-C3'	5.37	126.14	119.70
25	BA	1539	C	C2-N1-C1'	5.37	124.71	118.80
25	BA	70	A	P-O3'-C3'	5.37	126.14	119.70
25	DA	2287	A	C2-N3-C4	-5.36	107.92	110.60
1	CA	97	G	O4'-C1'-N9	5.35	112.48	108.20
25	DA	945	A	N1-C6-N6	5.35	121.81	118.60
25	BA	1539	C	N3-C2-O2	-5.35	118.16	121.90
25	BA	637	U	C5-C4-O4	5.35	129.11	125.90
25	DA	801	G	O5'-P-OP2	-5.35	100.89	105.70
25	DA	1131	G	O4'-C1'-N9	5.34	112.48	108.20
25	DA	277	C	N3-C2-O2	-5.34	118.16	121.90
24	AX	22	G	C4-C5-C6	-5.33	115.60	118.80
1	CA	1158	C	C2-N1-C1'	5.33	124.66	118.80
24	CX	22	G	N7-C8-N9	5.32	115.76	113.10
1	AA	346	G	O4'-C1'-N9	5.32	112.46	108.20
25	DA	1298	C	O5'-P-OP2	-5.32	100.91	105.70
1	AA	1036	G	C4-N9-C1'	5.32	133.42	126.50
25	DA	2155	G	C5-C6-O6	5.31	131.79	128.60
1	CA	1190	G	P-O3'-C3'	5.31	126.07	119.70
24	CX	14	A	C4-C5-N7	-5.30	108.05	110.70
25	DA	574	C	C2-N1-C1'	-5.30	112.97	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BA	1255	A	P-O3'-C3'	5.30	126.06	119.70
24	CX	14	A	C8-N9-C1'	-5.30	118.17	127.70
25	BA	1249	A	O4'-C1'-N9	5.29	112.44	108.20
1	CA	1119	C	C2-N1-C1'	5.29	124.62	118.80
25	BA	1154	U	C2-N1-C1'	5.29	124.05	117.70
25	DA	646	A	O4'-C1'-N9	5.27	112.42	108.20
1	AA	532	A	P-O3'-C3'	5.27	126.03	119.70
25	BA	1233	U	N1-C2-O2	5.27	126.49	122.80
1	CA	1026	G	C4-N9-C1'	5.27	133.35	126.50
25	BA	1235	G	C5-N7-C8	5.26	106.93	104.30
25	DA	271(Y)	U	O4'-C1'-N1	5.26	112.41	108.20
25	BA	1830	G	C4-C5-N7	-5.26	108.69	110.80
25	DA	2136	C	N3-C2-O2	-5.26	118.22	121.90
1	AA	1492	A	P-O3'-C3'	5.26	126.01	119.70
1	AA	1028	C	C6-N1-C2	-5.25	118.20	120.30
25	BA	2287	C	OP1-P-O3'	5.24	116.72	105.20
23	CW	25	C	C6-N1-C1'	5.24	127.08	120.80
27	DD	275	LYS	N-CA-C	-5.23	96.87	111.00
1	AA	98	G	C8-N9-C4	-5.22	104.31	106.40
25	BA	840	A	O5'-P-OP2	-5.22	101.00	105.70
25	BA	2050	U	N1-C2-O2	5.21	126.45	122.80
24	CX	17	C	C2-N1-C1'	5.21	124.53	118.80
25	BA	553	A	N3-C4-C5	5.21	130.44	126.80
25	BA	641	G	N1-C6-O6	-5.21	116.78	119.90
25	BA	598	A	O5'-P-OP1	-5.20	101.02	105.70
25	BA	2347	A	O4'-C1'-N9	5.20	112.36	108.20
25	DA	2447	G	N1-C6-O6	-5.19	116.79	119.90
1	CA	1158	C	C6-N1-C2	-5.18	118.23	120.30
1	AA	1042	G	O4'-C1'-N9	5.18	112.34	108.20
35	DP	44	GLY	C-N-CA	5.18	134.65	121.70
23	CY	62	C	C5-C4-N4	5.18	123.82	120.20
25	BA	1220	U	P-O3'-C3'	5.17	125.91	119.70
24	AX	46	G	C5-C6-O6	-5.17	125.50	128.60
1	AA	1531	A	O4'-C1'-N9	-5.17	104.06	108.20
25	DA	645	C	N1-C2-O2	5.17	122.00	118.90
1	CA	1256	A	O4'-C1'-N9	-5.16	104.07	108.20
25	BA	2163	G	C5-C6-O6	5.16	131.70	128.60
46	B0	12	ASN	N-CA-C	5.15	124.90	111.00
25	BA	593	G	C6-N1-C2	-5.14	122.02	125.10
23	CW	25	C	C2-N1-C1'	-5.14	113.14	118.80
25	BA	649	C	O5'-P-OP1	-5.14	101.08	105.70
1	CA	1154	G	N7-C8-N9	5.13	115.67	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	DA	746	A	O4'-C1'-N9	5.12	112.29	108.20
25	BA	2513	C	C2-N1-C1'	-5.11	113.18	118.80
25	BA	934	A	O4'-C1'-N9	5.11	112.28	108.20
24	CX	46	G	C5-C6-O6	-5.10	125.54	128.60
40	BU	74	LEU	CA-CB-CG	5.10	127.03	115.30
25	BA	1720	U	C2-N1-C1'	-5.10	111.58	117.70
25	BA	1670	G	N1-C6-O6	-5.10	116.84	119.90
25	BA	1985	U	C2-N1-C1'	5.09	123.80	117.70
1	CA	1007	C	C5-C6-N1	5.08	123.54	121.00
25	DA	1558	A	P-O3'-C3'	5.08	125.79	119.70
1	AA	1150	U	C2-N3-C4	5.07	130.04	127.00
24	AX	14	A	N1-C6-N6	5.07	121.64	118.60
1	AA	1502	A	C5-N7-C8	-5.07	101.36	103.90
25	BA	2078	G	O4'-C1'-N9	-5.07	104.15	108.20
25	BA	2298	A	C6-C5-N7	-5.07	128.75	132.30
25	DA	2206	G	C4-N9-C1'	-5.07	119.91	126.50
25	DA	1142	U	C2-N1-C1'	5.06	123.77	117.70
25	DA	748	G	C4-N9-C1'	-5.06	119.93	126.50
1	CA	997	U	N3-C4-O4	-5.05	115.86	119.40
25	BA	847	A	O5'-P-OP1	-5.05	101.16	105.70
25	BA	831	A	OP1-P-O3'	5.05	116.31	105.20
25	BA	2162	C	C6-N1-C1'	-5.05	114.74	120.80
25	DA	2572	A	C8-N9-C4	5.05	107.82	105.80
25	BA	831	A	O4'-C1'-N9	5.04	112.23	108.20
25	BA	2298	A	C5-N7-C8	-5.04	101.38	103.90
1	AA	1065	U	P-O3'-C3'	5.04	125.75	119.70
25	DA	2207	G	C4-N9-C1'	5.03	133.04	126.50
25	BA	1220	U	OP1-P-O3'	5.02	116.25	105.20
23	CW	3	C	C2-N1-C1'	5.02	124.32	118.80
1	AA	1278	U	C6-N1-C2	-5.01	117.99	121.00
25	BA	2077	C	OP1-P-O3'	5.01	116.22	105.20
1	AA	748	C	P-O3'-C3'	5.00	125.71	119.70
25	BA	875	U	C2-N1-C1'	-5.00	111.70	117.70
1	CA	687	A	P-O3'-C3'	5.00	125.70	119.70

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	231	GLU	Peptide
7	AG	78	ARG	Peptide
38	BS	58	LEU	Peptide

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Mol	Chain	Res	Type	Group
44	BY	54	LYS	Peptide
7	CG	78	ARG	Peptide
19	CS	28	LYS	Peptide
27	DD	274	ARG	Peptide

## 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	AA	32205	0	16255	434	0
1	CA	32312	0	16307	550	0
2	AB	1846	0	1867	70	0
2	CB	1825	0	1828	90	0
3	AC	1552	0	1546	45	0
3	CC	1542	0	1517	56	0
4	AD	1659	0	1676	53	0
4	CD	1674	0	1714	54	0
5	AE	1129	0	1185	33	0
5	CE	1133	0	1191	30	0
6	AF	806	0	793	18	0
6	CF	816	0	808	17	0
7	AG	1231	0	1238	22	0
7	CG	1235	0	1249	31	0
8	AH	1088	0	1126	32	0
8	CH	1088	0	1126	31	0
9	AI	983	0	986	28	0
9	CI	978	0	966	46	0
10	AJ	709	0	650	32	0
10	CJ	714	0	672	36	0
11	AK	829	0	825	15	0
11	CK	833	0	836	22	0
12	AL	930	0	980	18	0
12	CL	930	0	980	23	0
13	AM	958	0	1002	26	0
13	CM	950	0	988	24	0
14	AN	492	0	529	20	0
14	CN	492	0	529	17	0
15	AO	728	0	760	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	CO	728	0	760	31	0
16	AP	681	0	697	21	0
16	CP	677	0	686	17	0
17	AQ	823	0	891	16	0
17	CQ	823	0	891	19	0
18	AR	555	0	618	12	0
18	CR	555	0	618	13	0
19	AS	652	0	662	35	0
19	CS	646	0	644	34	0
20	AT	728	0	798	19	0
20	CT	727	0	796	20	0
21	AU	199	0	208	5	0
21	CU	199	0	208	8	0
22	AV	277	0	140	2	0
22	CV	277	0	140	2	0
23	AW	1588	0	820	30	0
23	AY	1581	0	805	57	0
23	CW	1541	0	784	50	0
23	CY	1561	0	796	46	0
24	AX	1625	0	828	11	0
24	CX	1625	0	828	28	0
25	BA	60729	0	30622	619	0
25	DA	60311	0	30414	867	0
26	BB	2573	0	1306	18	0
26	DB	2573	0	1306	38	0
27	BD	2136	0	2218	52	0
27	DD	2136	0	2218	51	0
28	BE	1559	0	1618	38	0
28	DE	1559	0	1618	41	0
29	BF	1584	0	1625	33	0
29	DF	1580	0	1619	64	0
30	BG	1425	0	1443	23	0
30	DG	1424	0	1434	47	0
31	BH	1330	0	1407	26	0
31	DH	1330	0	1407	61	0
32	BI	1085	0	1114	26	0
32	DI	1061	0	1080	19	0
33	BN	1117	0	1184	15	0
33	DN	1117	0	1184	24	0
34	BO	933	0	996	21	0
34	DO	933	0	996	18	0
35	BP	1135	0	1212	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	DP	1135	0	1212	50	0
36	BQ	1122	0	1179	23	0
36	DQ	1122	0	1179	38	0
37	BR	968	0	1033	25	0
37	DR	968	0	1033	26	0
38	BS	877	0	938	26	0
38	DS	870	0	923	23	0
39	BT	1091	0	1151	29	0
39	DT	1083	0	1136	30	0
40	BU	959	0	1019	14	0
40	DU	959	0	1019	28	0
41	BV	771	0	830	17	0
41	DV	771	0	830	21	0
42	BW	886	0	940	15	0
42	DW	886	0	940	13	0
43	BX	750	0	814	23	0
43	DX	750	0	814	22	0
44	BY	806	0	881	21	0
44	DY	806	0	881	20	0
45	BZ	1349	0	1355	41	0
45	DZ	1360	0	1363	63	0
46	B0	653	0	674	16	0
46	D0	653	0	674	24	0
47	B1	755	0	826	17	0
47	D1	755	0	826	15	0
48	B2	588	0	643	9	0
48	D2	588	0	643	8	0
49	B3	469	0	518	8	0
49	D3	464	0	514	9	0
50	B4	558	0	544	34	0
50	D4	532	0	503	25	0
51	B5	455	0	465	11	0
51	D5	455	0	465	8	0
52	B6	453	0	473	7	0
52	D6	449	0	469	8	0
53	B7	418	0	467	11	0
53	D7	418	0	467	6	0
54	B8	511	0	571	18	0
54	D8	517	0	582	21	0
55	B9	307	0	335	4	0
55	D9	307	0	335	8	0
56	AA	230	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	AD	1	0	0	0	0
56	AE	1	0	0	0	0
56	AF	1	0	0	0	0
56	AK	2	0	0	0	0
56	AM	1	0	0	0	0
56	AN	1	0	0	0	0
56	AV	1	0	0	0	0
56	AW	7	0	0	0	0
56	AX	12	0	0	0	0
56	AY	3	0	0	0	0
56	B0	3	0	0	0	0
56	B1	2	0	0	0	0
56	B2	1	0	0	0	0
56	B3	3	0	0	0	0
56	B4	1	0	0	0	0
56	B5	4	0	0	0	0
56	B6	2	0	0	0	0
56	B7	2	0	0	0	0
56	B8	3	0	0	0	0
56	B9	1	0	0	0	0
56	BA	839	0	0	0	0
56	BB	23	0	0	0	0
56	BD	11	0	0	0	0
56	BE	8	0	0	0	0
56	BF	12	0	0	0	0
56	BG	3	0	0	0	0
56	BN	5	0	0	0	0
56	BO	1	0	0	0	0
56	BP	3	0	0	0	0
56	BQ	5	0	0	0	0
56	BR	5	0	0	0	0
56	BU	9	0	0	0	0
56	BV	5	0	0	0	0
56	BW	3	0	0	0	0
56	BX	2	0	0	0	0
56	BY	1	0	0	0	0
56	BZ	1	0	0	0	0
56	CA	177	0	0	0	0
56	CE	2	0	0	0	0
56	CF	1	0	0	0	0
56	CJ	1	0	0	0	0
56	CT	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	CV	1	0	0	0	0
56	CW	2	0	0	0	0
56	CX	5	0	0	0	0
56	CY	1	0	0	0	0
56	D0	2	0	0	0	0
56	D3	1	0	0	0	0
56	D7	2	0	0	0	0
56	D8	1	0	0	0	0
56	DA	675	0	0	0	0
56	DB	11	0	0	0	0
56	DD	7	0	0	0	0
56	DE	4	0	0	0	0
56	DF	5	0	0	0	0
56	DG	1	0	0	0	0
56	DN	1	0	0	0	0
56	DO	1	0	0	0	0
56	DQ	4	0	0	0	0
56	DR	1	0	0	0	0
56	DU	2	0	0	0	0
56	DV	3	0	0	0	0
56	DW	3	0	0	0	0
56	DY	1	0	0	0	0
57	AA	40	0	37	7	0
57	CA	40	0	37	9	0
58	AD	8	0	0	0	0
58	CD	8	0	0	0	0
59	AN	1	0	0	0	0
59	B4	1	0	0	0	0
59	B5	1	0	0	0	0
59	B6	1	0	0	0	0
59	B9	1	0	0	0	0
59	BY	1	0	0	0	0
59	CN	1	0	0	0	0
59	D4	1	0	0	0	0
59	D5	1	0	0	0	0
59	D6	1	0	0	0	0
59	D9	1	0	0	0	0
59	DY	1	0	0	0	0
60	AX	1	0	0	0	0
60	CX	1	0	0	0	0
61	AA	226	0	0	17	0
61	AE	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	AJ	1	0	0	0	0
61	AL	4	0	0	1	0
61	AM	1	0	0	0	0
61	AV	4	0	0	0	0
61	AW	6	0	0	0	0
61	AX	8	0	0	0	0
61	AY	3	0	0	0	0
61	B0	4	0	0	0	0
61	B1	2	0	0	0	0
61	B3	2	0	0	0	0
61	B5	5	0	0	1	0
61	B6	1	0	0	0	0
61	B7	3	0	0	1	0
61	B8	11	0	0	1	0
61	BA	1411	0	0	69	0
61	BB	36	0	0	1	0
61	BD	16	0	0	2	0
61	BE	13	0	0	2	0
61	BF	7	0	0	0	0
61	BG	3	0	0	0	0
61	BI	1	0	0	0	0
61	BN	2	0	0	0	0
61	BO	3	0	0	0	0
61	BP	17	0	0	1	0
61	BQ	2	0	0	0	0
61	BR	2	0	0	0	0
61	BT	1	0	0	0	0
61	BU	6	0	0	0	0
61	BV	2	0	0	0	0
61	BW	4	0	0	0	0
61	BX	1	0	0	0	0
61	CA	173	0	0	15	0
61	CJ	2	0	0	2	0
61	CL	1	0	0	0	0
61	CV	2	0	0	0	0
61	CW	1	0	0	0	0
61	CX	4	0	0	2	0
61	D0	5	0	0	0	0
61	D3	1	0	0	0	0
61	D7	3	0	0	1	0
61	D8	4	0	0	0	0
61	DA	1002	0	0	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	DB	10	0	0	0	0
61	DD	17	0	0	1	0
61	DE	11	0	0	0	0
61	DF	5	0	0	0	0
61	DN	2	0	0	0	0
61	DO	2	0	0	0	0
61	DP	8	0	0	1	0
61	DQ	1	0	0	0	0
61	DR	1	0	0	0	0
61	DU	2	0	0	0	0
61	DW	1	0	0	0	0
61	DY	1	0	0	0	0
All	All	297273	0	196306	4649	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 10.

All (4649) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1256:A:H61	1:CA:1278:U:H1'	1.25	1.02
1:CA:999:C:N4	1:CA:1042:G:H1	1.59	1.00
1:AA:1025:U:O2	1:AA:1036:G:O6	1.82	0.98
23:CW:27:G:H1	23:CW:43:C:N4	1.62	0.97
1:CA:1029:C:N4	1:CA:1032:G:C6	2.33	0.97
23:CW:27:G:H1	23:CW:43:C:H42	1.01	0.97
23:CY:7:A:H61	23:CY:66:U:H3	1.12	0.97
25:BA:2158:C:H42	25:BA:2177:G:H1	0.98	0.96
25:BA:2145:G:H1	25:BA:2197:C:N4	1.63	0.96
25:DA:83:G:H1	25:DA:102:G:HO2'	1.11	0.95
23:CY:15:G:H22	23:CY:48:C:H42	1.11	0.94
23:AY:2:C:H42	23:AY:71:G:H1	1.15	0.94
23:AY:51:U:H3	23:AY:63:G:H1	0.97	0.93
23:CY:50:U:H3	23:CY:64:A:H61	1.14	0.92
25:DA:1798:U:H5'	27:DD:259:THR:HG22	1.49	0.92
25:DA:826:U:OP1	61:DA:4666:HOH:O	1.88	0.91
25:BA:1736:A:H62	25:BA:1745:A:H2	1.19	0.91
25:BA:591:U:O4	61:BA:4279:HOH:O	1.89	0.90
1:CA:1502:A:H2	1:CA:1505:G:H1	1.20	0.90
23:AY:19:G:N2	23:AY:56:C:N3	2.20	0.90
6:CF:81:ILE:HD11	27:DD:125:ILE:HB	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AY:26:A:H61	23:AY:44:G:H1	0.96	0.89
25:BA:2145:G:H1	25:BA:2197:C:H42	0.90	0.89
23:AY:26:A:N6	23:AY:44:G:H1	1.69	0.89
2:AB:16:HIS:HB2	2:AB:204:ASN:HB3	1.54	0.89
7:AG:50:ILE:HD11	7:AG:58:PRO:HA	1.55	0.89
1:AA:376:G:H5''	16:AP:5:ARG:HG2	1.54	0.88
1:CA:532:A:O2'	1:CA:533:A:OP1	1.90	0.88
1:AA:266:G:H5''	1:AA:268:C:H41	1.37	0.88
1:CA:999:C:H42	1:CA:1042:G:H1	0.88	0.88
25:BA:656:A:OP1	35:BP:65:ARG:NH1	2.07	0.88
1:AA:1502:A:H2	1:AA:1505:G:H1	1.19	0.88
53:B7:24:THR:HG22	53:B7:27:GLY:H	1.37	0.88
25:BA:786:G:OP1	61:BA:5273:HOH:O	1.92	0.87
29:DF:53:THR:HG22	29:DF:56:GLU:HG3	1.56	0.87
40:DU:76:TYR:OH	40:DU:92:ARG:NH1	2.06	0.87
25:DA:1315:C:OP2	61:DA:4468:HOH:O	1.91	0.87
39:BT:16:ARG:NH2	39:BT:83:ILE:O	2.08	0.86
46:B0:11:ARG:O	46:B0:14:ARG:NH2	2.08	0.86
25:BA:2118:U:H3	25:BA:2215:G:H1	1.24	0.86
46:B0:10:THR:HG22	46:B0:12:ASN:H	1.39	0.86
25:DA:740:U:OP2	61:DA:4516:HOH:O	1.92	0.86
25:BA:2158:C:N4	25:BA:2177:G:H1	1.72	0.86
30:BG:161:THR:HG22	30:BG:163:ALA:H	1.39	0.86
26:DB:66:A:H61	26:DB:109:C:H5'	1.39	0.86
25:BA:2299:A:H62	25:BA:2356:U:H3	1.22	0.85
1:AA:1025:U:H3	1:AA:1036:G:H1	1.24	0.85
2:CB:18:GLY:HA2	2:CB:42:ILE:HG13	1.57	0.85
1:CA:1189:C:OP1	10:CJ:51:ARG:NH2	2.10	0.85
23:CY:15:G:N2	23:CY:48:C:H42	1.75	0.85
25:BA:1829:U:H5'	27:BD:259:THR:HG22	1.59	0.84
13:CM:23:TYR:HB3	13:CM:67:GLU:HA	1.59	0.84
25:DA:1689:A:H62	25:DA:1698:A:H2	1.25	0.84
23:CY:56:C:H2'	23:CY:57:G:H8	1.42	0.84
33:DN:123:TYR:HH	33:DN:130:HIS:HE2	1.13	0.84
1:CA:1024:G:H2'	1:CA:1025:U:H5''	1.59	0.84
1:CA:1422:G:H5''	34:DO:48:PRO:HB3	1.60	0.83
25:DA:301:G:OP2	44:DY:84:ARG:NH2	2.11	0.83
19:AS:20:LEU:HD23	19:AS:23:ASN:HD22	1.43	0.83
1:CA:1029:C:N3	1:CA:1032:G:C2	2.46	0.82
1:CA:390:C:O3'	16:CP:28:ARG:NH2	2.12	0.82
25:DA:2427:C:OP1	61:DA:4666:HOH:O	1.95	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:DZ:153:SER:HB3	45:DZ:167:PRO:HB3	1.62	0.82
35:BP:126:VAL:HG12	35:BP:148:LEU:HD22	1.59	0.82
1:AA:1086:U:H3	1:AA:1099:G:H22	1.23	0.82
30:DG:161:THR:HG22	30:DG:163:ALA:H	1.45	0.82
23:CY:15:G:H22	23:CY:48:C:N4	1.78	0.81
23:AY:2:C:N4	23:AY:71:G:H1	1.78	0.81
29:DF:53:THR:HG23	29:DF:55:GLY:H	1.42	0.81
1:AA:1004:A:N7	1:AA:1036:G:N2	2.28	0.81
23:CY:50:U:H3	23:CY:64:A:N6	1.78	0.81
1:AA:1158:C:H5	1:AA:1181:G:H1	1.28	0.81
25:BA:1094:A:OP2	25:BA:1155:C:N4	2.11	0.81
25:DA:882:G:N2	25:DA:894:C:O2	2.14	0.81
1:AA:1314:C:OP2	19:AS:4:SER:OG	1.97	0.81
1:CA:1029:C:C4	1:CA:1032:G:N1	2.48	0.81
25:DA:1648:C:OP1	61:DA:4508:HOH:O	1.97	0.81
23:CW:27:G:N2	23:CW:43:C:N3	2.28	0.81
2:CB:128:GLU:HG3	2:CB:135:GLN:HE22	1.45	0.81
1:CA:972:C:OP1	61:CA:4155:HOH:O	1.97	0.81
25:BA:2443:U:OP2	61:BA:4398:HOH:O	1.98	0.81
25:DA:2126:A:N6	25:DA:2162:G:O2'	2.13	0.81
25:DA:912:C:OP1	36:DQ:8:LYS:NZ	2.14	0.80
8:AH:41:ARG:NH2	8:AH:123:GLU:OE2	2.15	0.80
3:CC:58:GLU:HB3	10:CJ:92:THR:HG21	1.61	0.80
1:CA:742:G:OP2	15:CO:35:ARG:NH2	2.14	0.80
45:DZ:72:ARG:NH2	45:DZ:97:GLU:O	2.13	0.80
36:BQ:21:THR:HG21	36:BQ:101:ARG:HD3	1.62	0.80
17:CQ:26:GLN:HG2	17:CQ:37:LYS:HG2	1.62	0.80
1:CA:1151:A:HO2'	1:CA:1152:A:H8	1.29	0.80
25:BA:2723:A:OP1	61:BA:4496:HOH:O	2.00	0.80
38:BS:25:ARG:NH1	38:BS:42:ASP:OD1	2.15	0.80
25:DA:2541:A:N7	61:DA:4301:HOH:O	2.14	0.80
1:CA:1352:C:OP1	21:CU:3:LYS:NZ	2.13	0.80
25:DA:994:C:OP1	40:DU:53:ARG:NH2	2.14	0.80
1:AA:1182:G:H4'	1:AA:1183:A:H5'	1.61	0.80
25:DA:2121:G:H1	25:DA:2177:C:H42	1.29	0.80
32:BI:92:VAL:HG13	32:BI:120:ILE:HB	1.65	0.79
47:D1:51:VAL:HG11	47:D1:74:VAL:HG21	1.64	0.79
23:AY:2:C:N3	23:AY:71:G:N2	2.30	0.79
1:CA:953:G:H5'	1:CA:965:A:H61	1.47	0.79
41:DV:40:LEU:HB2	41:DV:46:VAL:HG13	1.65	0.79
25:DA:793:A:O2'	61:DA:4544:HOH:O	1.99	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2802:C:O2	25:BA:2903:G:N1	2.14	0.79
1:AA:1008:C:N3	1:AA:1021:G:O6	2.16	0.79
27:BD:71:ASP:HB3	27:BD:103:ARG:HH22	1.48	0.79
1:CA:838:G:H1	1:CA:848:C:H42	1.30	0.79
46:D0:10:THR:HG22	46:D0:12:ASN:H	1.47	0.79
25:DA:2150:U:H2'	25:DA:2151:G:C8	2.18	0.79
1:AA:1422:G:H5''	34:BO:48:PRO:HB3	1.65	0.79
10:CJ:52:GLY:O	14:CN:41:ARG:NH2	2.16	0.79
3:CC:120:VAL:HA	3:CC:123:GLN:HE21	1.45	0.79
1:AA:1503:A:O2'	22:AV:13:A:N1	2.16	0.79
1:CA:349:A:H2'	1:CA:350:G:H5''	1.64	0.79
25:BA:615:G:O6	61:BA:5039:HOH:O	1.99	0.79
45:DZ:126:VAL:HG11	45:DZ:161:VAL:HG23	1.64	0.79
29:DF:140:LEU:HD21	29:DF:170:LEU:HD11	1.65	0.79
25:BA:237:G:OP1	61:BA:5347:HOH:O	2.00	0.78
25:BA:894:U:OP2	61:BA:4544:HOH:O	2.01	0.78
41:BV:72:VAL:HG13	41:BV:85:LYS:HB3	1.66	0.78
1:CA:38:G:H22	1:CA:397:A:H5''	1.48	0.78
25:DA:981:A:OP1	61:DA:4416:HOH:O	2.02	0.78
15:CO:87:ILE:HG22	15:CO:88:ARG:H	1.48	0.78
23:CY:7:A:N6	23:CY:66:U:H3	1.81	0.78
25:BA:1189:A:OP1	33:BN:25:ARG:NH2	2.16	0.78
1:CA:671:G:H5'	6:CF:77:ARG:HH22	1.48	0.78
32:BI:92:VAL:HG11	32:BI:144:VAL:HG11	1.66	0.78
1:AA:160:A:N6	1:AA:345:C:OP2	2.15	0.78
1:CA:504:C:OP1	61:CA:4009:HOH:O	2.02	0.78
51:D5:16:ARG:NH1	51:D5:17:ASP:OD1	2.17	0.78
1:CA:79:G:H1	1:CA:90:U:H3	1.32	0.78
25:DA:956:G:OP2	36:DQ:14:ARG:NH2	2.17	0.78
25:DA:857:C:OP2	46:D0:77:ARG:NH2	2.17	0.77
36:DQ:26:TYR:O	36:DQ:67:ARG:NH1	2.17	0.77
25:BA:1361:C:OP2	61:BA:4775:HOH:O	2.03	0.77
25:DA:2206:G:H3'	25:DA:2207:G:C8	2.20	0.77
25:DA:1031:G:H5''	55:D9:8:LYS:HE3	1.65	0.77
25:DA:1970:A:OP1	61:DA:4260:HOH:O	2.02	0.77
23:CW:18:G:O2'	23:CW:57:G:N2	2.15	0.77
2:AB:155:LEU:HD21	2:AB:159:PRO:HG3	1.65	0.77
9:AI:50:LEU:HD13	9:AI:56:LEU:HA	1.67	0.77
1:AA:1189:C:OP1	10:AJ:51:ARG:NH2	2.15	0.77
25:BA:479:C:OP1	61:BA:4437:HOH:O	2.01	0.77
23:CW:4:C:N3	23:CW:69:G:N2	2.32	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:1010:A:OP2	61:DA:4483:HOH:O	2.01	0.77
1:CA:656:C:O2'	15:CO:28:GLN:NE2	2.17	0.77
25:BA:2562:G:OP1	61:BA:5207:HOH:O	2.02	0.77
1:AA:1108:G:O6	61:AA:4156:HOH:O	2.03	0.77
45:DZ:144:LEU:HD22	45:DZ:174:VAL:HG23	1.66	0.77
25:DA:2123:G:H1	25:DA:2175:C:H42	1.32	0.77
1:CA:1083:U:OP2	61:CA:4106:HOH:O	2.02	0.77
8:AH:34:GLU:OE1	8:AH:37:ARG:NH1	2.17	0.77
1:CA:64:G:H4'	1:CA:65:U:H3'	1.67	0.77
25:DA:563:G:OP2	61:DA:4472:HOH:O	2.03	0.76
1:CA:1065:U:OP2	1:CA:1190:G:N2	2.17	0.76
1:AA:975:A:H4'	1:AA:976:G:H5''	1.66	0.76
25:DA:1171:G:H1	25:DA:1178:C:H42	1.31	0.76
25:DA:81:G:N7	61:DA:4462:HOH:O	2.18	0.76
23:AY:50:U:H3	23:AY:64:A:H2	1.31	0.76
24:CX:50:U:H3	24:CX:64:G:H1	1.34	0.76
25:DA:250:G:OP2	54:D8:13:ARG:NH2	2.19	0.76
2:CB:179:LYS:HA	8:CH:72:PRO:HG3	1.66	0.76
43:DX:35:THR:HG22	43:DX:38:GLU:H	1.51	0.76
25:BA:1296:G:OP2	35:BP:21:ARG:NH1	2.18	0.76
25:DA:2285:C:OP2	52:D6:6:ARG:NH1	2.19	0.76
25:DA:2357:U:OP1	46:D0:20:ARG:NH1	2.19	0.76
34:DO:35:VAL:HG11	34:DO:103:ALA:HB3	1.67	0.76
25:BA:1067:A:H62	25:BA:1186:U:H3	1.34	0.76
1:CA:1503:A:O2'	22:CV:13:A:N1	2.19	0.76
20:AT:10:LEU:HB3	20:AT:12:ALA:H	1.49	0.76
25:DA:2151:G:H2'	25:DA:2152:G:H8	1.51	0.75
25:BA:2459:G:OP2	61:BA:4688:HOH:O	2.03	0.75
1:CA:1029:C:C4	1:CA:1032:G:C2	2.75	0.75
25:DA:2139:C:H42	25:DA:2152:G:H1	1.32	0.75
23:CY:26:A:N1	23:CY:44:G:O6	2.20	0.75
2:AB:69:LEU:HB3	2:AB:162:ILE:HG22	1.68	0.75
27:DD:238:GLY:O	61:DD:409:HOH:O	2.03	0.75
25:DA:2171:A:N3	25:DA:2172:U:N3	2.35	0.75
25:BA:2720:G:H1'	37:BR:71:GLN:HE22	1.51	0.75
10:CJ:32:ALA:HB1	10:CJ:33:GLN:HA	1.69	0.75
1:CA:975:A:H4'	1:CA:976:G:H5''	1.69	0.75
25:DA:154(A):C:N4	25:DA:171:G:O6	2.20	0.75
25:DA:2317:C:N4	25:DA:2318:G:O6	2.20	0.75
20:CT:60:GLU:HG3	20:CT:81:LYS:HD2	1.69	0.75
45:DZ:117:LEU:HA	45:DZ:174:VAL:HA	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:33:TYR:HB2	2:AB:43:ASP:HB2	1.66	0.74
53:B7:34:ARG:NH2	61:B7:201:HOH:O	2.19	0.74
1:AA:201:C:H42	1:AA:216:G:H1	1.35	0.74
16:CP:51:VAL:HG12	16:CP:53:VAL:H	1.52	0.74
35:DP:126:VAL:HG12	35:DP:148:LEU:HD22	1.69	0.74
1:AA:406:G:H5'	4:AD:5:ILE:HD11	1.69	0.74
9:CI:97:LYS:HA	9:CI:102:LEU:HG	1.68	0.74
25:BA:878:G:O2'	35:BP:38:GLN:NE2	2.21	0.74
25:DA:847:U:OP2	61:DA:4326:HOH:O	2.04	0.74
10:CJ:8:LEU:HB2	10:CJ:70:ARG:HB2	1.67	0.74
26:DB:20:C:N4	26:DB:63:G:O6	2.20	0.74
2:AB:16:HIS:CD2	2:AB:17:PHE:H	2.05	0.74
1:CA:152:A:N6	1:CA:169:C:N3	2.35	0.74
23:CW:76:A:OP1	61:DA:4820:HOH:O	2.04	0.74
42:BW:19:LEU:HB3	51:B5:25:LEU:HD11	1.70	0.74
25:DA:1170:G:H1	25:DA:1179:C:H42	1.36	0.74
25:BA:715:G:N7	61:BA:4010:HOH:O	2.20	0.74
25:BA:2479:C:OP2	61:BA:5182:HOH:O	2.05	0.74
1:AA:1069:C:OP2	61:AA:4012:HOH:O	2.05	0.73
23:CY:51:U:O2	23:CY:63:G:N2	2.20	0.73
43:DX:11:PRO:HB3	43:DX:92:LEU:HD11	1.69	0.73
36:DQ:21:THR:HG21	36:DQ:101:ARG:HD3	1.69	0.73
23:AY:26:A:N1	23:AY:44:G:N2	2.35	0.73
43:BX:11:PRO:HB3	43:BX:92:LEU:HD11	1.68	0.73
1:CA:353:A:H8	1:CA:353:A:H5'	1.53	0.73
1:CA:693:G:N7	57:CA:3178:PCY:N16	2.37	0.73
1:CA:838:G:H1	1:CA:848:C:N4	1.87	0.73
25:BA:2849:G:H5'	37:BR:46:GLY:HA2	1.70	0.73
25:BA:1648:U:O4	61:BA:4366:HOH:O	2.05	0.73
1:AA:742:G:OP2	15:AO:35:ARG:NH2	2.22	0.73
25:DA:2287:A:H62	25:DA:2344:U:H3	1.34	0.73
11:CK:93:GLN:HA	11:CK:93:GLN:HE21	1.54	0.73
45:BZ:139:VAL:HG22	45:BZ:155:LEU:HD11	1.71	0.73
1:AA:677:U:H3	1:AA:713:G:H22	1.36	0.73
1:CA:999:C:N3	1:CA:1042:G:N2	2.34	0.73
1:CA:922:G:H4'	5:CE:20:GLN:HA	1.70	0.73
45:DZ:45:ASP:OD1	45:DZ:49:ARG:NH1	2.22	0.73
1:CA:1255:G:OP1	10:CJ:45:ARG:NH2	2.22	0.73
23:CW:4:C:N4	23:CW:69:G:N1	2.37	0.72
30:BG:108:ASN:HB3	50:B4:22:ILE:HD13	1.71	0.72
19:CS:50:ALA:HB1	19:CS:57:HIS:HB3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1000:U:H3	1:CA:1041:A:H61	1.36	0.72
25:DA:2839:G:H5'	37:DR:46:GLY:HA2	1.70	0.72
1:CA:1028:C:N3	1:CA:1033:G:C6	2.56	0.72
1:CA:539:A:OP2	12:CL:115:LYS:NZ	2.22	0.72
3:CC:109:PRO:HB3	3:CC:115:LEU:HD23	1.71	0.72
25:DA:2130:U:H4'	25:DA:2133:G:H4'	1.71	0.72
25:DA:2138:C:H42	25:DA:2153:G:H1	1.38	0.72
16:CP:52:ASP:O	16:CP:54:GLU:N	2.20	0.72
25:DA:2100:G:H1	25:DA:2189:U:H3	1.34	0.72
12:AL:71:PRO:O	12:AL:102:ARG:NH1	2.21	0.72
25:BA:1018:A:OP2	61:BA:4279:HOH:O	2.08	0.72
25:DA:1602:U:O4	61:DA:4192:HOH:O	2.07	0.72
9:CI:5:TYR:H	9:CI:87:GLN:HE22	1.38	0.72
1:AA:1183:A:O2'	1:AA:1184:G:OP1	2.08	0.72
53:B7:34:ARG:NH1	53:B7:41:ARG:O	2.23	0.72
1:AA:664:G:H22	1:AA:741:G:H1	1.38	0.72
25:BA:542:C:OP1	51:B5:16:ARG:NH2	2.23	0.72
25:DA:2880:C:O3'	37:DR:90:ARG:NH1	2.23	0.72
25:DA:1313:U:OP1	61:DA:4343:HOH:O	2.08	0.72
25:BA:839:G:O6	61:BA:4760:HOH:O	2.06	0.72
24:CX:75:C:OP1	61:CX:4003:HOH:O	2.06	0.72
54:B8:6:THR:HG22	54:B8:63:PRO:HD2	1.72	0.72
2:AB:88:ALA:HB2	2:AB:219:VAL:HG13	1.71	0.72
23:AY:8:4SU:H4'	23:AY:48:C:H4'	1.72	0.72
57:CA:3178:PCY:N2	57:CA:3178:PCY:O19	2.21	0.72
25:BA:2776:G:OP2	61:BA:4827:HOH:O	2.06	0.72
2:CB:88:ALA:HB2	2:CB:219:VAL:HG13	1.70	0.72
1:CA:1029:C:N4	1:CA:1032:G:N1	2.37	0.72
25:BA:2145:G:N2	25:BA:2197:C:N3	2.32	0.72
25:DA:1352:U:OP2	61:DA:4084:HOH:O	2.08	0.72
4:CD:25:ARG:NH1	4:CD:30:LYS:O	2.23	0.71
17:AQ:26:GLN:HG2	17:AQ:37:LYS:HG2	1.70	0.71
25:BA:1001:G:OP2	36:BQ:14:ARG:NH2	2.22	0.71
50:B4:53:GLU:C	50:B4:55:ARG:H	1.94	0.71
1:CA:78:G:H2'	1:CA:79:G:H5''	1.71	0.71
1:AA:1030(C):G:N7	1:AA:1031:G:N2	2.38	0.71
25:BA:2877:G:OP2	39:BT:119:LYS:NZ	2.23	0.71
32:BI:93:THR:HG22	32:BI:119:PRO:HB3	1.72	0.71
25:BA:2162:C:C2	25:BA:2173:G:N2	2.59	0.71
25:BA:2396:G:OP2	46:B0:55:ARG:NH1	2.21	0.71
36:BQ:14:ARG:HG2	36:BQ:41:TRP:HH2	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:CX:49:G:H1	24:CX:65:C:H42	1.35	0.71
3:AC:6:HIS:HD2	3:AC:8:ILE:H	1.36	0.71
9:CI:127:LYS:O	9:CI:128:ARG:HB3	1.91	0.71
25:DA:2110:G:O2'	25:DA:2120:G:OP2	2.08	0.71
45:DZ:144:LEU:HD21	45:DZ:173:ALA:HA	1.72	0.71
15:CO:54:ARG:NH1	15:CO:58:MET:SD	2.63	0.71
27:BD:148:GLU:HB2	27:BD:151:LYS:HD2	1.73	0.71
1:CA:427:U:OP1	4:CD:13:ARG:NH2	2.24	0.71
42:DW:33:ARG:NH2	42:DW:52:GLU:OE1	2.23	0.71
1:CA:6:G:H4'	1:CA:298:A:H4'	1.73	0.70
11:AK:79:SER:HA	11:AK:104:GLN:HB2	1.71	0.70
25:DA:320:A:OP2	29:DF:137:LYS:NZ	2.20	0.70
25:BA:1378:G:OP1	61:BA:4775:HOH:O	2.08	0.70
25:BA:465:G:N7	61:BA:4522:HOH:O	2.24	0.70
36:BQ:109:VAL:HG13	36:BQ:113:GLN:HB3	1.71	0.70
25:BA:2157:A:H61	25:BA:2178:G:H1'	1.56	0.70
25:BA:2251:G:OP2	61:BA:4470:HOH:O	2.08	0.70
57:AA:3231:PCY:O19	57:AA:3231:PCY:N2	2.24	0.70
29:BF:101:LEU:O	29:BF:106:ARG:NH1	2.25	0.70
25:BA:2146:G:H1	25:BA:2196:C:H42	1.39	0.70
3:AC:78:GLY:HA3	3:AC:83:ARG:H	1.56	0.70
1:CA:346:G:OP1	39:DT:41:ARG:NH2	2.23	0.70
1:CA:201:C:H42	1:CA:216:G:H1	1.37	0.70
25:DA:1671:U:OP2	61:DA:4069:HOH:O	2.08	0.70
50:B4:61:ARG:HG3	50:B4:62:ARG:H	1.56	0.70
27:BD:69:ARG:NH2	27:BD:128:GLY:O	2.25	0.70
25:BA:1249:A:H2	25:BA:1287:A:H62	1.39	0.70
23:CY:51:U:N3	23:CY:63:G:N1	2.39	0.70
29:DF:101:LEU:O	29:DF:106:ARG:NH1	2.25	0.70
30:DG:80:PHE:O	30:DG:82:LEU:N	2.24	0.70
25:DA:2503:A:O2'	25:DA:2505:G:OP2	2.09	0.70
1:CA:97:G:O2'	1:CA:98:G:O5'	2.09	0.70
25:BA:30:G:OP2	40:BU:5:LYS:NZ	2.23	0.70
47:D1:76:ARG:HH11	47:D1:97:LEU:HD22	1.56	0.70
1:CA:1116:C:H2'	1:CA:1117:G:H5''	1.73	0.70
25:BA:1700:G:H3'	37:BR:2:ARG:HD3	1.74	0.70
25:DA:1670:C:OP1	61:DA:4069:HOH:O	2.10	0.70
1:CA:1118:C:H2'	1:CA:1119:C:H6	1.55	0.70
5:AE:85:GLY:O	5:AE:87:SER:N	2.24	0.70
25:DA:2447:G:OP2	61:DA:4707:HOH:O	2.10	0.70
27:DD:71:ASP:HB3	27:DD:103:ARG:HH22	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:1395:A:OP1	61:BA:5097:HOH:O	2.10	0.70
35:BP:42:SER:O	61:BP:303:HOH:O	2.10	0.70
1:CA:559:A:OP1	5:CE:126:ARG:NH2	2.24	0.69
3:AC:150:LYS:HE2	3:AC:152:ILE:HD11	1.71	0.69
35:DP:36:LYS:O	61:DP:201:HOH:O	2.09	0.69
25:BA:2143:G:H1	25:BA:2199:C:H42	1.40	0.69
25:DA:2355:C:H4'	46:D0:24:LYS:HD3	1.74	0.69
44:BY:92:ASN:HB3	44:BY:94:LYS:H	1.56	0.69
9:AI:16:ARG:HB2	9:AI:64:THR:HB	1.74	0.69
25:DA:2682:U:OP2	61:DA:4147:HOH:O	2.10	0.69
25:BA:2130:C:H2'	25:BA:2131:U:H6	1.57	0.69
25:DA:601:C:O2'	29:DF:104:LYS:NZ	2.24	0.69
25:BA:1922:A:OP2	61:BA:4461:HOH:O	2.09	0.69
1:AA:538:G:H5''	12:AL:114:LYS:HB2	1.73	0.69
19:AS:63:THR:OG1	19:AS:65:ASN:ND2	2.25	0.69
1:AA:1353:G:OP1	21:AU:10:ARG:NH1	2.25	0.69
25:DA:2807:G:N2	25:DA:2893:G:O6	2.25	0.69
25:BA:1039:G:OP1	40:BU:50:ARG:NH2	2.25	0.69
1:AA:1129:C:H5''	9:AI:16:ARG:HH12	1.57	0.69
11:CK:48:ILE:O	11:CK:50:TYR:N	2.22	0.69
15:CO:22:THR:OG1	15:CO:23:GLY:N	2.21	0.69
1:AA:836:G:OP1	18:AR:61:LYS:NZ	2.23	0.69
25:BA:2081:A:OP2	61:BA:4472:HOH:O	2.11	0.69
11:CK:54:ARG:NH2	23:CY:39:PSU:O2'	2.26	0.69
1:CA:1125:U:O2'	1:CA:1126:U:H2'	1.93	0.69
25:DA:1783:A:OP1	61:DA:4516:HOH:O	2.11	0.69
25:DA:2327:A:H2'	25:DA:2328:A:C8	2.28	0.69
1:AA:812:C:N3	61:AA:4050:HOH:O	2.25	0.69
1:AA:922:G:H4'	5:AE:20:GLN:HA	1.75	0.69
23:AY:19:G:N1	23:AY:56:C:N4	2.38	0.69
25:DA:2125:G:H22	25:DA:2172:U:H5'	1.57	0.69
25:DA:2135:A:H61	25:DA:2157:G:H21	1.37	0.69
28:BE:47:VAL:HG21	28:BE:86:PRO:HD2	1.73	0.69
23:CW:2:C:N3	23:CW:71:G:O6	2.26	0.69
37:DR:67:LEU:HD13	37:DR:76:VAL:HG21	1.75	0.69
23:AY:67:C:H2'	23:AY:68:C:C6	2.28	0.69
25:DA:2162:G:H4'	25:DA:2172:U:H2'	1.75	0.69
25:DA:2122:U:O4	25:DA:2176:A:N1	2.24	0.69
25:DA:9:U:H3	25:DA:2629:A:H2	1.39	0.69
25:BA:139:A:H8	25:BA:1454:C:HO2'	1.40	0.69
1:CA:1314:C:OP2	19:CS:4:SER:OG	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AY:44:G:O2'	23:AY:45:U:OP1	2.10	0.68
1:AA:200:G:H1	1:AA:217:C:H42	1.40	0.68
1:AA:1423:G:OP1	34:BO:49:ARG:NH2	2.26	0.68
1:AA:539:A:OP2	12:AL:115:LYS:NZ	2.26	0.68
25:DA:2167:U:O2'	25:DA:2168:G:N3	2.25	0.68
25:BA:1065:U:HO2'	25:BA:1067:A:H2	1.41	0.68
25:DA:1012:U:H5	33:DN:28:THR:HG21	1.59	0.68
23:CY:13:C:N3	23:CY:22:G:O6	2.26	0.68
25:DA:601:C:OP1	29:DF:108:LYS:NZ	2.27	0.68
25:DA:1021:A:H62	25:DA:1141:U:H3	1.39	0.68
25:DA:943:U:OP2	61:DA:4576:HOH:O	2.11	0.68
1:AA:1034:G:H2'	1:AA:1035:A:C8	2.27	0.68
25:BA:1717:C:OP2	61:BA:5207:HOH:O	2.12	0.68
1:CA:1129:C:OP1	9:CI:16:ARG:NH1	2.25	0.68
1:AA:44:G:O6	61:AA:4055:HOH:O	2.09	0.68
42:BW:14:PRO:HG2	42:BW:78:GLU:HG2	1.74	0.68
25:BA:667:G:N2	25:BA:670:C:OP2	2.27	0.68
1:AA:1151:A:HO2'	1:AA:1152:A:H8	1.41	0.68
23:CW:29:G:H1	23:CW:41:C:H42	1.42	0.68
25:DA:1817:G:OP1	27:DD:88:ARG:NH2	2.26	0.68
12:AL:49:ASN:ND2	12:AL:92:ASP:OD2	2.22	0.68
10:AJ:30:SER:O	10:AJ:81:THR:OG1	2.11	0.68
23:AY:50:U:O4	23:AY:64:A:N1	2.27	0.68
26:DB:13:A:N1	26:DB:69:G:O2'	2.24	0.68
25:DA:370:G:OP2	61:DA:4103:HOH:O	2.12	0.68
25:DA:2552:U:H2'	25:DA:2554:U:OP2	1.93	0.68
1:AA:972:C:O2'	10:AJ:55:LYS:O	2.10	0.68
25:BA:1044:C:OP1	61:BA:4784:HOH:O	2.11	0.68
25:DA:1031:G:H21	55:D9:36:GLN:HE22	1.40	0.68
48:D2:22:GLU:OE2	48:D2:68:ARG:NH2	2.27	0.68
25:DA:20:C:OP1	40:DU:22:LYS:NZ	2.23	0.68
25:BA:932:C:H3'	25:BA:933:C:H5''	1.75	0.68
25:BA:2695:C:O2	34:BO:70:LYS:NZ	2.25	0.68
55:D9:25:VAL:HB	55:D9:34:GLN:HB2	1.76	0.68
25:BA:2138:G:N7	25:BA:2187:G:N2	2.42	0.68
25:BA:427:G:N7	61:BA:5099:HOH:O	2.26	0.68
9:CI:17:VAL:HG11	9:CI:81:ILE:HA	1.76	0.68
23:CY:52:G:O6	23:CY:62:C:N3	2.27	0.68
1:AA:1297:C:O2'	7:AG:114:ARG:NH2	2.27	0.68
25:DA:805:G:OP1	61:DA:4971:HOH:O	2.12	0.68
25:DA:400:G:N7	61:DA:4682:HOH:O	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:1271:G:OP2	61:DA:4508:HOH:O	2.11	0.67
25:DA:2134:A:O2'	25:DA:2159:G:N3	2.26	0.67
4:AD:173:TRP:CE3	4:AD:174:LEU:HG	2.29	0.67
39:DT:65:LYS:HE2	39:DT:67:SER:HB2	1.76	0.67
1:CA:1075:C:OP1	2:CB:179:LYS:NZ	2.26	0.67
25:BA:2122:G:H1	25:BA:2211:U:H3	1.41	0.67
10:CJ:44:VAL:HG13	10:CJ:66:ARG:HG2	1.76	0.67
32:BI:133:HIS:ND1	32:BI:134:PRO:O	2.26	0.67
8:CH:10:LEU:HD22	8:CH:83:ILE:HD11	1.76	0.67
26:DB:75:G:N2	45:DZ:87:ASP:OD1	2.25	0.67
3:CC:54:ARG:HH11	3:CC:54:ARG:HB3	1.58	0.67
25:DA:2507:C:H5''	25:DA:2573:C:N4	2.09	0.67
1:CA:766:A:OP2	61:CA:4022:HOH:O	2.11	0.67
1:CA:1301:U:O2'	1:CA:1302:U:H5'	1.94	0.67
28:DE:47:VAL:HG11	28:DE:86:PRO:HD2	1.76	0.67
1:CA:7:G:O2'	5:CE:120:THR:O	2.13	0.67
36:DQ:110:THR:HG23	36:DQ:113:GLN:HB2	1.76	0.67
10:CJ:5:ARG:N	61:CJ:5101:HOH:O	2.28	0.67
29:DF:21:ALA:HB3	29:DF:22:ALA:HA	1.76	0.67
25:BA:70:A:H3'	25:BA:70:A:OP2	1.94	0.67
1:AA:1352:C:OP1	21:AU:3:LYS:NZ	2.23	0.67
19:AS:41:VAL:HG12	19:AS:43:GLU:H	1.60	0.67
25:DA:796:C:H2'	25:DA:797:C:C6	2.30	0.67
5:CE:143:ARG:NH1	8:CH:77:GLU:OE1	2.28	0.67
3:CC:6:HIS:HD2	3:CC:8:ILE:H	1.42	0.67
25:DA:517:C:OP1	51:D5:16:ARG:NH2	2.28	0.67
1:CA:986:A:N3	19:CS:52:TYR:OH	2.25	0.67
29:DF:103:LYS:HA	29:DF:106:ARG:HG3	1.76	0.67
2:CB:69:LEU:HB3	2:CB:162:ILE:HG22	1.76	0.67
9:AI:20:ARG:O	9:AI:60:ASP:N	2.23	0.67
1:CA:1312:G:H1	1:CA:1325:C:H42	1.41	0.67
29:DF:184:TYR:CE2	29:DF:188:ARG:HD2	2.29	0.67
3:CC:129:ALA:HB3	3:CC:132:ARG:HB2	1.76	0.67
25:DA:81:G:HO2'	25:DA:295:G:HO2'	1.40	0.67
18:CR:22:VAL:HB	18:CR:56:THR:HA	1.77	0.67
27:DD:206:LEU:HD22	27:DD:211:ARG:HG2	1.76	0.67
25:BA:2788:A:N7	61:BA:4672:HOH:O	2.27	0.67
37:BR:67:LEU:HD13	37:BR:76:VAL:HG21	1.77	0.67
25:BA:2793:G:OP1	61:BA:4974:HOH:O	2.13	0.67
25:BA:2153:G:H5''	25:BA:2154:U:H3'	1.75	0.67
1:AA:1416:G:N7	61:AA:4106:HOH:O	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:2060:A:N3	61:DA:4409:HOH:O	2.28	0.67
25:BA:701:A:N7	61:BA:4847:HOH:O	2.28	0.67
25:BA:325:G:OP2	44:BY:84:ARG:NH2	2.28	0.66
32:DI:92:VAL:HG22	32:DI:120:ILE:HB	1.77	0.66
4:CD:140:VAL:HG11	4:CD:146:ILE:HD11	1.77	0.66
19:AS:68:GLY:H	50:B4:58:ARG:HH12	1.41	0.66
25:BA:2387:G:N7	61:BA:4876:HOH:O	2.29	0.66
1:AA:1392:G:N2	1:AA:1502:A:H8	1.94	0.66
1:CA:1002:G:H1	1:CA:1038:C:H42	1.43	0.66
25:DA:1218:C:H42	25:DA:1231:G:H1	1.43	0.66
27:BD:237:GLU:OE2	61:BD:412:HOH:O	2.14	0.66
1:AA:572:A:OP1	61:AA:4102:HOH:O	2.12	0.66
1:CA:1086:U:H3	1:CA:1099:G:H22	1.43	0.66
25:DA:2006:C:OP2	61:DA:4803:HOH:O	2.13	0.66
1:CA:947:G:H1	1:CA:1234:C:H42	1.41	0.66
25:DA:2046:G:H5'	51:D5:19:ARG:HA	1.76	0.66
25:DA:1188:U:H5''	41:DV:79:VAL:HG13	1.76	0.66
1:AA:1152:A:OP1	10:AJ:68:HIS:ND1	2.27	0.66
25:DA:271(I):G:N2	25:DA:271(O):C:O2	2.27	0.66
1:AA:1238:A:OP2	61:AA:4145:HOH:O	2.12	0.66
26:BB:33:G:H5'	30:BG:2:PRO:HD3	1.77	0.66
1:AA:1255:G:OP1	10:AJ:45:ARG:NH2	2.29	0.66
25:DA:1243:G:O2'	35:DP:4:SER:O	2.13	0.66
1:AA:953:G:H5'	1:AA:965:A:H61	1.60	0.66
25:DA:1658:C:OP1	61:DA:4502:HOH:O	2.12	0.66
1:CA:1360:A:OP2	14:CN:35:ARG:NH2	2.29	0.66
26:DB:12:C:H2'	46:D0:73:GLY:HA3	1.78	0.66
25:DA:1332:G:OP1	61:DA:4468:HOH:O	2.13	0.66
1:CA:972:C:O2'	10:CJ:55:LYS:O	2.14	0.66
1:CA:1029:C:N3	1:CA:1032:G:N2	2.44	0.66
1:CA:67:C:H2'	1:CA:68:G:C8	2.31	0.66
1:AA:1025:U:O2'	1:AA:1026:G:O4'	2.14	0.66
1:CA:539:A:H2'	1:CA:540:G:C8	2.31	0.66
19:AS:68:GLY:HA3	50:B4:58:ARG:HH22	1.61	0.66
9:AI:17:VAL:HG23	9:AI:63:ILE:HG12	1.78	0.66
19:CS:42:PRO:HG3	50:D4:61:ARG:HG3	1.78	0.66
43:DX:65:ARG:HG3	43:DX:70:LEU:HG	1.77	0.66
31:BH:149:ARG:NH1	31:BH:167:GLU:OE2	2.29	0.66
25:DA:304:G:O6	61:DA:4486:HOH:O	2.11	0.66
3:CC:181:ASN:HD21	3:CC:204:LEU:HD12	1.61	0.66
27:BD:206:LEU:HD22	27:BD:211:ARG:HG2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AW:51:U:H2'	23:AW:52:G:C8	2.30	0.66
25:BA:2158:C:N3	25:BA:2177:G:N2	2.43	0.66
1:AA:310:G:OP2	16:AP:27:LYS:NZ	2.27	0.66
45:BZ:72:ARG:NH2	45:BZ:97:GLU:O	2.28	0.66
28:BE:29:GLY:HA3	61:BE:406:HOH:O	1.96	0.66
25:DA:307:G:N2	25:DA:310:A:O5'	2.26	0.66
2:AB:47:THR:HA	2:AB:202:PRO:HG2	1.77	0.66
25:DA:526:A:OP1	61:DA:4488:HOH:O	2.14	0.66
25:BA:2362:C:OP2	61:BA:4189:HOH:O	2.13	0.66
23:CW:61:C:O2'	23:CW:62:C:O5'	2.09	0.66
1:AA:1392:G:H21	1:AA:1502:A:H8	1.45	0.65
45:BZ:117:LEU:HD11	45:BZ:144:LEU:HB3	1.78	0.65
25:BA:2772:G:N7	61:BA:4262:HOH:O	2.28	0.65
25:BA:2419:G:OP1	61:BA:4387:HOH:O	2.13	0.65
13:CM:40:ASN:HB3	13:CM:43:THR:HG23	1.78	0.65
4:AD:15:GLU:HG2	4:AD:63:LYS:HB3	1.78	0.65
1:CA:79:G:N2	1:CA:90:U:O2	2.27	0.65
24:CX:64:G:H4'	36:DQ:10:ARG:HH12	1.60	0.65
25:BA:2184:G:H5''	25:BA:2194:U:H2'	1.78	0.65
10:CJ:77:PRO:O	10:CJ:81:THR:OG1	2.14	0.65
39:BT:65:LYS:HE2	39:BT:67:SER:HB2	1.76	0.65
1:AA:427:U:OP1	4:AD:13:ARG:NH2	2.29	0.65
25:DA:1996:C:H4'	25:DA:1997:G:OP1	1.96	0.65
1:AA:656:C:O2'	15:AO:28:GLN:NE2	2.30	0.65
1:AA:1530:G:H2'	1:AA:1531:A:O4'	1.96	0.65
45:DZ:108:PRO:HB2	45:DZ:111:VAL:HG23	1.77	0.65
1:CA:1028:C:C4	1:CA:1033:G:O6	2.49	0.65
1:CA:1002:G:C4	1:CA:1003:G:H8	2.14	0.65
43:BX:31:HIS:HD2	43:BX:33:LYS:H	1.44	0.65
23:AW:19:G:N2	23:AW:56:C:N3	2.44	0.65
1:AA:76:C:N3	1:AA:93:G:O6	2.29	0.65
25:DA:42:G:OP2	61:DA:4954:HOH:O	2.14	0.65
36:DQ:111:GLU:OE1	36:DQ:133:ARG:NH2	2.26	0.65
25:DA:30:G:OP2	40:DU:5:LYS:NZ	2.25	0.65
1:CA:1218:C:OP2	14:CN:9:LYS:NZ	2.29	0.65
30:DG:114:ILE:HA	30:DG:140:ILE:HD11	1.79	0.65
5:AE:33:VAL:HG21	5:AE:109:ILE:HA	1.77	0.65
13:CM:37:THR:O	13:CM:55:ARG:NH1	2.29	0.65
1:AA:1002:G:H3'	1:AA:1003:G:O4'	1.97	0.65
25:DA:1019:U:H3	25:DA:1142(A):A:H62	1.45	0.65
31:DH:3:ARG:NH2	31:DH:5:GLY:H	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:D4:44:THR:O	50:D4:46:GLN:N	2.30	0.65
12:AL:24:VAL:HG11	12:AL:27:LEU:HD22	1.78	0.65
55:B9:25:VAL:HB	55:B9:34:GLN:HB2	1.78	0.65
1:AA:837:G:H1	1:AA:849:C:H42	1.45	0.65
19:CS:28:LYS:HB2	19:CS:29:ARG:HA	1.78	0.65
1:CA:1417:G:O6	61:CA:4051:HOH:O	2.12	0.65
1:CA:1245:A:H61	1:CA:1292:U:H3	1.45	0.65
23:CW:51:U:H3	23:CW:63:G:H1	1.45	0.65
34:DO:68:GLU:HB3	34:DO:78:ARG:HB2	1.79	0.65
5:CE:122:GLU:O	5:CE:126:ARG:NH1	2.30	0.64
2:CB:178:ARG:HH22	8:CH:68:ARG:HH12	1.44	0.64
2:AB:201:ILE:HG21	2:AB:214:ILE:HG21	1.80	0.64
25:DA:1204:A:H2	25:DA:1241:A:H62	1.46	0.64
25:BA:11:G:H2'	25:BA:12:U:H5''	1.79	0.64
30:DG:15:VAL:HG22	30:DG:175:LEU:HB3	1.79	0.64
33:DN:30:ILE:HG22	33:DN:34:LEU:HD22	1.78	0.64
1:AA:78:G:N2	1:AA:91:C:N3	2.46	0.64
25:DA:631:A:OP1	35:DP:65:ARG:NH1	2.30	0.64
25:BA:2340:A:H2'	25:BA:2341:G:C8	2.32	0.64
19:CS:63:THR:OG1	19:CS:65:ASN:ND2	2.30	0.64
1:CA:1149:C:O2'	1:CA:1280:A:N1	2.31	0.64
1:AA:1136:U:H5''	1:AA:1137:C:C4	2.31	0.64
1:AA:346:G:OP1	39:BT:41:ARG:NH1	2.26	0.64
9:AI:53:VAL:O	9:AI:55:ALA:N	2.31	0.64
3:AC:58:GLU:HB3	10:AJ:92:THR:HG21	1.79	0.64
1:AA:1456:G:O3'	20:AT:39:LYS:NZ	2.30	0.64
4:CD:157:LEU:O	4:CD:161:ASN:ND2	2.30	0.64
25:BA:2164:C:N3	25:BA:2171:G:O6	2.31	0.64
1:AA:1008:C:O2	1:AA:1021:G:N1	2.27	0.64
25:DA:1013:C:H2'	25:DA:1014:U:H6	1.62	0.64
7:AG:111:ARG:NH1	7:AG:113:GLU:OE2	2.27	0.64
1:AA:97:G:O2'	1:AA:98:G:O4'	2.14	0.64
33:BN:67:LEU:HB3	33:BN:88:GLU:HG3	1.79	0.64
25:BA:1451:U:H2'	25:BA:1452:U:C6	2.32	0.64
37:BR:97:VAL:HG22	37:BR:114:VAL:HG13	1.80	0.64
1:CA:1456:G:O6	20:CT:54:LYS:NZ	2.25	0.64
15:AO:25:THR:HG21	15:AO:70:LEU:HB2	1.79	0.64
25:DA:1283:G:N2	25:DA:1286:A:OP2	2.31	0.64
25:BA:1222:A:H3'	25:BA:1223:C:C6	2.32	0.64
2:CB:16:HIS:HB2	2:CB:204:ASN:HB3	1.80	0.64
9:CI:16:ARG:HB2	9:CI:64:THR:HG22	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:CY:5:G:H1	23:CY:68:C:H42	1.46	0.64
12:AL:34:ARG:NH2	61:AL:201:HOH:O	2.30	0.64
29:DF:24:LEU:HD23	29:DF:115:ALA:HA	1.79	0.64
25:DA:2431:U:OP1	61:DA:4215:HOH:O	2.15	0.64
23:CY:50:U:O2	23:CY:64:A:N1	2.31	0.64
46:D0:11:ARG:O	46:D0:14:ARG:NH2	2.31	0.64
15:CO:22:THR:HG1	15:CO:23:GLY:H	1.46	0.64
25:DA:143(A):C:O2'	43:DX:2:LYS:NZ	2.30	0.64
4:AD:177:ASP:HB3	4:AD:182:LYS:HG2	1.78	0.64
1:AA:352:C:OP2	61:AA:4109:HOH:O	2.15	0.64
25:DA:2023:G:H5'	25:DA:2617:C:H4'	1.79	0.64
1:CA:1029:C:C2	1:CA:1032:G:N2	2.66	0.64
25:DA:1958:C:OP2	61:DA:4696:HOH:O	2.15	0.64
3:CC:164:ARG:NH1	3:CC:166:GLU:OE1	2.31	0.64
1:AA:1183:A:H3'	1:AA:1184:G:H5''	1.80	0.63
45:BZ:138:GLU:H	45:BZ:156:LYS:HD3	1.62	0.63
25:DA:330:A:H2	25:DA:1210:A:HO2'	1.43	0.63
23:AW:19:G:H1	23:AW:56:C:H42	1.43	0.63
1:CA:165:C:H2'	1:CA:166:G:H8	1.62	0.63
25:DA:1266:G:O5'	42:DW:15:ARG:NH2	2.31	0.63
45:BZ:126:VAL:HG11	45:BZ:161:VAL:HG23	1.81	0.63
25:DA:2123:G:H1	25:DA:2175:C:N4	1.97	0.63
25:DA:2299:G:H2'	25:DA:2300:G:H8	1.64	0.63
1:AA:812:C:O2	61:AA:4048:HOH:O	2.14	0.63
25:DA:2360:A:OP2	61:DA:4626:HOH:O	2.15	0.63
16:AP:22:THR:HA	16:AP:33:ILE:HG13	1.80	0.63
2:CB:47:THR:HA	2:CB:202:PRO:HG2	1.79	0.63
25:BA:1219:A:H4'	25:BA:1220:U:OP1	1.97	0.63
25:BA:1431:G:O2'	25:BA:1442:U:O2	2.11	0.63
50:B4:68:ARG:HD2	50:B4:69:LYS:H	1.63	0.63
24:CX:76:A:H5'	25:DA:2585:U:H5	1.63	0.63
19:CS:27:GLU:HG2	19:CS:47:HIS:NE2	2.14	0.63
1:AA:159:G:N2	1:AA:162:A:OP2	2.32	0.63
1:AA:353:A:H5'	1:AA:353:A:H8	1.63	0.63
51:B5:40:LYS:NZ	51:B5:44:THR:O	2.22	0.63
48:D2:1:MET:N	48:D2:52:ASP:OD1	2.23	0.63
1:CA:1003:G:N2	1:CA:1025:U:O4	2.31	0.63
25:DA:307:G:N1	25:DA:310:A:OP2	2.32	0.63
28:BE:143:ASN:HD22	28:BE:147:PRO:HD3	1.64	0.63
25:DA:468:G:N7	53:D7:39:ARG:NH2	2.44	0.63
15:AO:39:LEU:HD13	15:AO:56:LEU:HB2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:545:C:OP1	4:AD:61:LYS:NZ	2.31	0.63
25:BA:1480:A:H61	25:BA:1605:A:H62	1.45	0.63
26:DB:4:C:H42	26:DB:117:G:H1	1.44	0.63
25:DA:2867:G:OP2	39:DT:119:LYS:NZ	2.32	0.63
28:DE:36:ARG:HG2	28:DE:47:VAL:HG12	1.80	0.63
2:AB:118:LEU:HB3	2:AB:142:LEU:HD12	1.79	0.63
1:CA:920:U:H2'	1:CA:921:U:C6	2.33	0.63
26:DB:22:U:H3	26:DB:61:G:H1	1.46	0.63
1:AA:78:G:N1	1:AA:91:C:N4	2.47	0.63
25:DA:900:A:H2'	25:DA:901:A:H8	1.64	0.63
25:BA:302:A:O2'	25:BA:303:C:OP1	2.17	0.63
13:CM:58:GLU:O	13:CM:62:ASN:ND2	2.27	0.63
23:AY:19:G:H3'	23:AY:20:U:H6	1.64	0.63
25:BA:2164:C:O2	25:BA:2171:G:N1	2.27	0.63
25:DA:1283:G:O2'	25:DA:1285:G:N7	2.26	0.63
37:BR:44:LEU:HD22	37:BR:48:VAL:HG23	1.81	0.63
1:AA:134:A:H61	16:AP:25:ARG:NH1	1.97	0.63
45:BZ:92:SER:OG	45:BZ:93:ASP:N	2.31	0.63
34:BO:35:VAL:HG11	34:BO:103:ALA:HB3	1.80	0.63
1:CA:1028:C:C2	1:CA:1033:G:N1	2.67	0.62
1:CA:1132:C:H42	1:CA:1142:G:H1	1.46	0.62
25:DA:2502:G:N7	61:DA:4706:HOH:O	2.31	0.62
27:DD:12:SER:HB3	27:DD:208:LYS:HB3	1.80	0.62
38:BS:59:LYS:HD2	38:BS:60:GLY:H	1.64	0.62
15:CO:5:LYS:HZ2	15:CO:5:LYS:H	1.47	0.62
25:DA:7:G:H2'	25:DA:8:A:C8	2.34	0.62
40:DU:76:TYR:HH	40:DU:92:ARG:NH1	1.96	0.62
28:DE:34:VAL:HG11	28:DE:78:LEU:HD11	1.81	0.62
23:AW:7:A:H61	23:AW:66:U:H3	1.45	0.62
25:BA:1312:G:O5'	42:BW:15:ARG:NH2	2.32	0.62
10:AJ:37:PRO:HA	10:AJ:72:VAL:HG12	1.80	0.62
25:DA:1815:A:P	27:DD:54:ARG:HH22	2.22	0.62
1:AA:1002:G:C4	1:AA:1003:G:H1'	2.34	0.62
1:CA:1120:G:C6	1:CA:1154:G:N2	2.67	0.62
1:CA:345:C:OP2	39:DT:39:ARG:NH2	2.32	0.62
29:DF:157:VAL:HB	29:DF:194:MET:HG2	1.81	0.62
1:AA:1103:C:OP1	2:AB:96:ARG:NH2	2.32	0.62
2:CB:178:ARG:NH2	8:CH:68:ARG:HH12	1.97	0.62
25:BA:265:U:H2'	25:BA:266:C:C6	2.34	0.62
26:BB:84:C:OP1	49:B3:15:TYR:OH	2.18	0.62
50:D4:24:THR:OG1	50:D4:25:TYR:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2163:G:H1	25:BA:2171:G:H22	1.46	0.62
25:DA:2141:G:O6	25:DA:2150:U:O2	2.17	0.62
3:CC:152:ILE:HG23	3:CC:199:LYS:HB2	1.82	0.62
25:DA:221:A:N1	25:DA:265:A:O2'	2.32	0.62
1:AA:316:G:OP2	1:AA:351:G:O2'	2.17	0.62
13:CM:33:ALA:HA	13:CM:59:TYR:HE2	1.64	0.62
4:CD:191:ARG:NH1	4:CD:191:ARG:O	2.32	0.62
25:BA:2164:C:H2'	25:BA:2165:C:C6	2.35	0.62
1:AA:45:U:H2'	1:AA:46:G:C8	2.35	0.62
25:DA:952:G:OP1	36:DQ:16:ARG:NH2	2.33	0.62
25:BA:278:G:OP1	47:B1:76:ARG:NH1	2.31	0.62
8:AH:10:LEU:HD22	8:AH:83:ILE:HD11	1.80	0.62
2:CB:185:ILE:HG22	2:CB:199:TYR:HB2	1.82	0.62
4:CD:15:GLU:OE2	4:CD:66:ARG:NH1	2.31	0.62
7:AG:27:ILE:HD12	7:AG:40:ALA:HA	1.82	0.62
25:DA:2591:C:OP1	27:DD:239:ARG:HD2	2.00	0.62
24:CX:21:A:H61	24:CX:46:G:H2'	1.65	0.62
1:AA:519:C:OP2	12:AL:50:SER:OG	2.17	0.62
3:CC:138:VAL:HG23	3:CC:151:VAL:HG23	1.82	0.62
2:AB:16:HIS:O	2:AB:18:GLY:N	2.32	0.62
25:BA:2163:G:C4	25:BA:2164:C:H1'	2.33	0.62
37:DR:97:VAL:HG22	37:DR:114:VAL:HG13	1.80	0.62
25:BA:1848:G:OP1	27:BD:88:ARG:NH2	2.33	0.62
20:AT:57:ARG:HH12	20:AT:100:ILE:HD12	1.64	0.62
25:DA:1842:G:O2'	27:DD:253:GLN:NE2	2.33	0.62
27:DD:182:LEU:HB2	27:DD:272:ALA:HB3	1.80	0.62
9:AI:46:ALA:HB2	9:AI:74:ILE:HG23	1.82	0.62
25:DA:2141:G:H2'	25:DA:2142:C:O4'	2.00	0.62
23:CW:74:C:N4	25:DA:2507:C:O2'	2.31	0.62
36:DQ:109:VAL:HG13	36:DQ:113:GLN:HB3	1.81	0.62
37:DR:104:ARG:HG3	37:DR:111:LEU:HD11	1.82	0.62
25:BA:2801:C:OP1	28:BE:61:ARG:NH2	2.28	0.62
1:CA:352:C:O2'	1:CA:354:G:OP1	2.14	0.62
1:CA:266:G:H5''	1:CA:268:C:H41	1.64	0.62
54:D8:6:THR:HG22	54:D8:63:PRO:HD2	1.81	0.62
18:CR:56:THR:HB	18:CR:58:LEU:HD23	1.81	0.62
7:AG:111:ARG:NH2	7:AG:126:ASP:OD2	2.32	0.62
46:B0:18:ALA:HB3	46:B0:20:ARG:HH21	1.65	0.62
25:BA:493:G:OP1	53:B7:33:ARG:NH1	2.33	0.62
3:AC:3:ASN:OD1	3:AC:3:ASN:N	2.33	0.62
45:DZ:92:SER:OG	45:DZ:93:ASP:N	2.27	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:CD:104:VAL:HG11	4:CD:146:ILE:HD13	1.82	0.62
25:BA:1223:C:H2'	25:BA:1224:C:H6	1.65	0.62
25:DA:910:A:H62	36:DQ:12:GLN:HA	1.65	0.62
38:DS:14:VAL:O	38:DS:18:ILE:HG12	2.00	0.62
1:CA:406:G:H5'	4:CD:5:ILE:HD11	1.81	0.62
25:DA:2141:G:C6	25:DA:2150:U:O2	2.52	0.61
1:CA:1129:C:H2'	1:CA:1139:G:N7	2.15	0.61
25:DA:886:C:O2'	25:DA:889:C:N4	2.32	0.61
1:CA:377:G:OP1	16:CP:3:LYS:HD2	1.99	0.61
53:D7:34:ARG:NH1	53:D7:41:ARG:O	2.32	0.61
20:CT:57:ARG:HH12	20:CT:100:ILE:HD12	1.65	0.61
3:CC:47:LEU:HD12	3:CC:68:VAL:HG11	1.81	0.61
43:BX:31:HIS:CD2	43:BX:33:LYS:H	2.18	0.61
14:AN:23:ARG:HH11	14:AN:30:ALA:HB2	1.64	0.61
27:DD:148:GLU:HB2	27:DD:151:LYS:HD2	1.82	0.61
1:AA:1435:G:H2'	1:AA:1436:U:C6	2.35	0.61
25:BA:1425:A:H4'	25:BA:1426:G:OP2	2.00	0.61
49:B3:3:ARG:NH1	49:B3:60:GLU:OE2	2.29	0.61
17:CQ:66:SER:O	17:CQ:70:ARG:NH1	2.33	0.61
8:AH:51:VAL:HG21	8:AH:60:ARG:HH11	1.65	0.61
25:DA:2121:G:H1	25:DA:2177:C:N4	1.97	0.61
1:AA:189(B):C:H42	1:AA:189(I):G:H1	1.48	0.61
4:CD:165:MET:SD	4:CD:168:ARG:NH1	2.72	0.61
23:CW:9:A:H5'	23:CW:46:7MG:HN22	1.64	0.61
1:CA:942:G:H21	9:CI:124:GLN:NE2	1.98	0.61
1:CA:148:G:H2'	1:CA:149:A:H8	1.65	0.61
25:BA:1284:G:OP2	61:BA:5106:HOH:O	2.16	0.61
1:AA:452:A:H4'	16:AP:72:ARG:NH1	2.15	0.61
1:CA:1422:G:O3'	34:DO:49:ARG:NH1	2.31	0.61
1:CA:1441:G:H5''	1:CA:1442:G:H5'	1.81	0.61
16:CP:71:ARG:HG3	16:CP:80:PHE:HE2	1.66	0.61
2:AB:53:ARG:NH2	2:AB:198:ASP:O	2.32	0.61
25:BA:288:U:O2'	25:BA:289:G:OP1	2.17	0.61
25:BA:2121:U:H3	25:BA:2212:G:H1	1.47	0.61
20:AT:60:GLU:HG3	20:AT:81:LYS:HD2	1.80	0.61
25:DA:2843:G:N7	61:DA:4550:HOH:O	2.31	0.61
25:DA:2758:A:C2	25:DA:2759:G:H1'	2.36	0.61
25:BA:1993:A:OP1	61:BA:4467:HOH:O	2.15	0.61
48:B2:65:ASN:OD1	48:B2:69:ARG:NH1	2.30	0.61
2:AB:93:VAL:HG21	2:AB:97:TRP:CD1	2.36	0.61
19:AS:32:LYS:HA	19:AS:50:ALA:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:100:C:H2'	1:AA:101:A:C8	2.36	0.61
25:DA:2611:U:C4	51:D5:3:LYS:HG2	2.35	0.61
1:AA:1305:G:N2	1:AA:1331:G:H1'	2.16	0.61
19:AS:68:GLY:H	50:B4:58:ARG:NH1	1.99	0.61
24:CX:21:A:N6	24:CX:46:G:H2'	2.16	0.61
7:CG:32:ARG:HH12	7:CG:109:ASN:HD21	1.47	0.61
25:BA:2303:U:H2'	25:BA:2304:C:C6	2.36	0.61
25:DA:831:G:O2'	35:DP:38:GLN:NE2	2.34	0.61
4:CD:72:GLU:OE1	4:CD:207:TYR:OH	2.18	0.61
1:CA:1004:A:N6	1:CA:1037:C:C2	2.69	0.61
38:BS:27:SER:HA	38:BS:88:ASP:HB3	1.82	0.61
25:DA:2110:G:H4'	25:DA:2111:C:OP2	2.00	0.61
2:AB:185:ILE:HG22	2:AB:199:TYR:HB2	1.83	0.61
25:DA:307:G:N7	61:DA:4267:HOH:O	2.31	0.61
1:CA:992:U:H3	1:CA:1044:A:H62	1.49	0.61
31:BH:3:ARG:HG2	31:BH:6:ARG:HG2	1.82	0.61
1:AA:276:G:O3'	17:AQ:68:ARG:NH1	2.33	0.61
13:CM:88:ARG:HG3	13:CM:98:VAL:HG11	1.83	0.61
36:BQ:108:GLY:HA3	45:BZ:116:VAL:HG13	1.82	0.61
1:CA:1030(A):G:H2'	1:CA:1030(C):G:OP2	2.00	0.61
23:AW:18:G:O2'	23:AW:57:G:N2	2.24	0.61
3:AC:13:GLY:HA3	14:AN:57:ARG:NH2	2.16	0.61
3:AC:8:ILE:HD13	3:AC:184:TYR:HB3	1.83	0.61
19:CS:4:SER:HB3	19:CS:7:LYS:HG3	1.82	0.61
2:AB:93:VAL:HG21	2:AB:97:TRP:HD1	1.66	0.61
17:AQ:66:SER:O	17:AQ:70:ARG:NH1	2.34	0.61
31:BH:56:SER:HB3	31:BH:61:HIS:ND1	2.16	0.61
23:CY:9:A:H5''	23:CY:46:7MG:H1'	1.81	0.61
3:AC:162:GLN:NE2	22:AV:24:A:O2'	2.33	0.61
1:CA:36:C:N4	61:CA:4168:HOH:O	2.33	0.61
25:DA:644:A:H4'	25:DA:645:C:C5	2.36	0.61
47:D1:7:ILE:HG23	47:D1:98:LEU:HD11	1.82	0.61
25:BA:1343:C:OP1	61:BA:4495:HOH:O	2.16	0.61
19:CS:32:LYS:HA	19:CS:50:ALA:HB3	1.83	0.61
43:BX:35:THR:HG22	43:BX:38:GLU:H	1.65	0.61
23:AW:1:G:O6	23:AW:72:C:N3	2.34	0.61
25:DA:1023:U:OP2	61:DA:4898:HOH:O	2.16	0.61
4:AD:128:VAL:N	4:AD:131:ARG:O	2.30	0.61
1:AA:559:A:OP1	5:AE:126:ARG:NH2	2.25	0.61
1:AA:1381:U:H1'	7:AG:79:ARG:HG3	1.83	0.61
2:CB:15:VAL:O	2:CB:17:PHE:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:DZ:145:GLU:HG3	45:DZ:146:ILE:H	1.66	0.60
1:CA:148:G:H2'	1:CA:149:A:C8	2.36	0.60
25:DA:2723:C:H5''	37:DR:1:MET:HE2	1.83	0.60
29:DF:78:ILE:HA	29:DF:83:PHE:CD1	2.36	0.60
25:BA:1211:U:H2'	25:BA:1212:C:C6	2.36	0.60
31:DH:99:VAL:N	31:DH:102:ALA:O	2.34	0.60
25:DA:2118:U:C4	25:DA:2149:G:H1'	2.37	0.60
29:DF:158:THR:O	29:DF:164:ARG:NH1	2.32	0.60
13:AM:84:ILE:HG13	13:AM:85:GLY:HA2	1.81	0.60
25:BA:1071:G:C4	25:BA:1180:C:H1'	2.36	0.60
17:AQ:76:LEU:HD21	17:AQ:79:SER:HB2	1.83	0.60
1:AA:1441:G:H5''	1:AA:1442:G:H5'	1.82	0.60
1:AA:1442:G:O2'	1:AA:1442(A):G:OP1	2.19	0.60
43:BX:60:ARG:HH22	53:B7:47:ARG:HH22	1.49	0.60
25:BA:354:A:H2	25:BA:1255:A:H2'	1.66	0.60
25:BA:956:A:H62	36:BQ:12:GLN:HA	1.66	0.60
3:CC:142:MET:HG3	3:CC:170:GLN:HB3	1.84	0.60
50:D4:50:VAL:O	50:D4:52:THR:N	2.33	0.60
25:BA:1218:G:O2'	25:BA:1219:A:O4'	2.19	0.60
25:DA:509:C:OP1	61:DA:4614:HOH:O	2.15	0.60
3:AC:12:LEU:HD23	3:AC:16:ARG:HB3	1.83	0.60
1:CA:1305:G:N2	1:CA:1331:G:H1'	2.17	0.60
32:DI:27:ARG:HD2	47:D1:71:TYR:CE1	2.37	0.60
19:CS:38:SER:HB2	19:CS:71:LEU:HD22	1.83	0.60
25:BA:1846:A:P	27:BD:54:ARG:HH22	2.23	0.60
10:AJ:26:ALA:O	10:AJ:84:GLN:NE2	2.34	0.60
25:BA:1513:G:HO2'	25:BA:1593:C:HO2'	1.46	0.60
25:DA:1220:A:OP2	40:DU:19:LYS:NZ	2.31	0.60
1:CA:1028:C:N3	1:CA:1033:G:O6	2.34	0.60
25:DA:1012:U:C5	33:DN:28:THR:HG21	2.37	0.60
31:BH:86:GLU:OE2	31:BH:132:ARG:NH2	2.34	0.60
1:CA:1007:C:N3	1:CA:1022:G:O6	2.35	0.60
1:CA:1132:C:H2'	1:CA:1133:G:H8	1.65	0.60
25:BA:1159:U:H2'	25:BA:1160:G:C8	2.36	0.60
25:DA:993:G:H21	41:DV:89:GLN:HE22	1.50	0.60
25:DA:1355:G:O6	61:DA:4421:HOH:O	2.15	0.60
1:AA:800:G:O6	61:AA:4021:HOH:O	2.12	0.60
16:CP:22:THR:HA	16:CP:33:ILE:HG13	1.82	0.60
25:BA:2173:G:H2'	25:BA:2174:G:C8	2.37	0.60
46:D0:12:ASN:HA	46:D0:14:ARG:HH21	1.66	0.60
25:DA:299:A:N1	25:DA:322:A:O2'	2.28	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:DZ:55:HIS:CE1	45:DZ:135:GLU:HG3	2.36	0.60
25:BA:2166:U:O2'	25:BA:2167:C:H2'	2.01	0.60
25:BA:1834:A:O2'	27:BD:259:THR:HG21	2.00	0.60
1:CA:657:G:H21	15:CO:22:THR:HG1	1.49	0.60
1:AA:976:G:H5'	1:AA:1358:U:O2'	2.00	0.60
27:DD:85:ASP:OD2	27:DD:88:ARG:NH1	2.34	0.60
31:DH:3:ARG:HH22	31:DH:5:GLY:H	1.49	0.60
45:DZ:163:LEU:HG	45:DZ:165:VAL:HG22	1.83	0.60
27:DD:69:ARG:NH2	27:DD:128:GLY:O	2.35	0.60
1:CA:17:U:H2'	1:CA:18:C:C6	2.37	0.60
5:AE:151:LEU:HD22	8:AH:79:VAL:HG22	1.84	0.60
47:D1:59:THR:O	47:D1:91:LYS:NZ	2.34	0.60
25:DA:1297:C:OP2	61:DA:4287:HOH:O	2.15	0.60
47:B1:7:ILE:HG23	47:B1:98:LEU:HD11	1.83	0.60
2:CB:84:GLU:HB3	2:CB:219:VAL:HG21	1.84	0.60
25:DA:322:A:OP2	29:DF:169:ASN:HB2	2.02	0.60
30:DG:150:ASP:OD2	30:DG:153:ARG:NH1	2.35	0.60
27:BD:179:SER:O	27:BD:275:LYS:HB2	2.02	0.60
25:DA:1721:G:H8	25:DA:1741:A:H62	1.48	0.60
26:BB:6:C:H2'	26:BB:7:G:H5''	1.83	0.60
1:CA:1138:G:C6	1:CA:1140:C:H1'	2.37	0.60
25:DA:392:C:OP1	61:DA:4693:HOH:O	2.16	0.60
25:DA:987:G:O2'	25:DA:1000:A:N3	2.32	0.60
20:AT:43:LEU:O	20:AT:47:GLY:N	2.35	0.60
45:BZ:4:ARG:NE	45:BZ:60:GLU:OE1	2.32	0.60
31:DH:7:LEU:HD12	31:DH:8:PRO:HD2	1.84	0.60
2:AB:84:GLU:HB3	2:AB:219:VAL:HG21	1.84	0.59
29:DF:21:ALA:CB	29:DF:22:ALA:HA	2.32	0.59
25:DA:2875:C:O2'	39:DT:2:ASN:OD1	2.19	0.59
1:CA:1376:U:H2'	1:CA:1377:A:C8	2.37	0.59
1:CA:1001:A:H2'	1:CA:1001(A):G:H8	1.66	0.59
25:DA:2495:G:H5''	36:DQ:82:ARG:HG2	1.84	0.59
6:AF:42:GLU:OE1	6:AF:59:TYR:OH	2.13	0.59
14:AN:3:ARG:HH21	14:AN:3:ARG:HB3	1.66	0.59
3:CC:30:ARG:HH21	14:CN:38:GLY:HA2	1.67	0.59
1:AA:625:G:H4'	16:AP:16:HIS:CD2	2.36	0.59
19:AS:20:LEU:HD13	50:B4:69:LYS:HE2	1.84	0.59
23:CW:29:G:H1	23:CW:41:C:N4	1.99	0.59
12:AL:88:GLY:O	12:AL:99:HIS:HD2	1.84	0.59
25:DA:1639:U:H2'	25:DA:1640:C:H5''	1.84	0.59
1:CA:811:C:N4	61:CA:4024:HOH:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:646:U:H2'	1:CA:647:C:C6	2.36	0.59
1:CA:1112:C:H1'	3:CC:179:ARG:HG2	1.83	0.59
4:AD:129:ASN:OD1	4:AD:145:GLU:N	2.33	0.59
25:BA:83:A:H5'	44:BY:8:LYS:HG2	1.83	0.59
5:AE:110:LEU:HD13	5:AE:118:ILE:HG21	1.84	0.59
9:CI:53:VAL:O	9:CI:55:ALA:N	2.35	0.59
38:DS:25:ARG:NH1	38:DS:42:ASP:OD1	2.35	0.59
35:DP:121:LYS:HB3	35:DP:123:LEU:HG	1.84	0.59
25:BA:1201:A:OP1	40:BU:55:ARG:HD3	2.02	0.59
51:B5:11:THR:HG23	51:B5:15:ARG:HB3	1.83	0.59
4:CD:98:GLU:HG2	4:CD:189:PRO:HG2	1.83	0.59
41:BV:76:LYS:HB2	41:BV:81:TYR:HB3	1.84	0.59
25:DA:2169:A:H2'	25:DA:2170:A:C8	2.37	0.59
2:CB:91:PRO:HD3	2:CB:154:LEU:HD12	1.84	0.59
25:DA:784:A:C6	27:DD:229:VAL:HG11	2.37	0.59
1:CA:934:C:OP1	61:CA:4152:HOH:O	2.17	0.59
25:BA:553:A:N1	25:BA:2064:A:H2'	2.16	0.59
23:CY:33:U:H2'	23:CY:35:A:OP2	2.01	0.59
25:DA:2139:C:N4	25:DA:2152:G:H1	2.00	0.59
25:DA:303:U:H2'	25:DA:304:G:H8	1.67	0.59
44:BY:102:CYS:SG	44:BY:103:GLY:N	2.75	0.59
54:B8:42:ARG:HD2	61:B8:207:HOH:O	2.02	0.59
1:CA:1412:C:H2'	1:CA:1413:A:C8	2.37	0.59
23:CY:62:C:H2'	23:CY:63:G:C8	2.38	0.59
45:BZ:152:ALA:HB2	45:BZ:171:ILE:HG21	1.84	0.59
25:DA:2135:A:H61	25:DA:2157:G:N2	2.00	0.59
25:DA:2137:C:H42	25:DA:2154:G:H1	1.51	0.59
25:BA:302:A:H2'	25:BA:303:C:C6	2.38	0.59
1:CA:450:G:OP1	16:CP:43:LYS:NZ	2.34	0.59
25:DA:1796:U:H2'	25:DA:1797:C:C6	2.38	0.59
1:CA:976:G:OP1	14:CN:32:SER:N	2.33	0.59
30:DG:136:ARG:HD2	30:DG:137:GLU:HG3	1.85	0.59
25:DA:613:G:O2'	25:DA:614(C):A:N1	2.30	0.59
44:DY:102:CYS:SG	44:DY:103:GLY:N	2.76	0.59
25:BA:611:U:H2'	25:BA:612:C:C6	2.37	0.59
10:CJ:7:LYS:HE3	10:CJ:71:LEU:HD13	1.84	0.59
1:AA:97:G:O2'	1:AA:98:G:H8	1.86	0.59
25:BA:2584:A:N7	28:BE:144:ARG:HD2	2.18	0.59
27:DD:132:PRO:HG2	27:DD:135:PHE:CD2	2.37	0.59
6:CF:45:LEU:HD12	6:CF:59:TYR:HD2	1.68	0.59
25:DA:2140:C:H1'	25:DA:2152:G:N2	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1128:C:O2'	1:CA:1129:C:OP1	2.17	0.59
1:CA:1218:C:H2'	1:CA:1219:U:C6	2.38	0.59
28:DE:72:VAL:HG13	28:DE:73:GLU:O	2.03	0.59
4:CD:153:ARG:HB2	4:CD:181:MET:SD	2.43	0.59
3:AC:57:ILE:HG12	3:AC:66:VAL:HG22	1.84	0.59
4:AD:155:LEU:HD13	4:AD:158:ILE:HD11	1.84	0.59
25:DA:1800:C:OP2	27:DD:183:ARG:NH2	2.35	0.59
1:CA:316:G:OP2	1:CA:351:G:O2'	2.20	0.59
30:DG:41:GLN:HE22	30:DG:153:ARG:HB3	1.66	0.59
1:CA:448:A:P	1:CA:485:G:H22	2.26	0.59
38:DS:71:ARG:NH1	38:DS:107:GLU:OE1	2.36	0.59
25:DA:2651:C:H42	25:DA:2669:G:H1	1.51	0.59
1:AA:1492:A:O2'	1:AA:1493:A:O5'	2.10	0.59
8:CH:51:VAL:HG21	8:CH:60:ARG:HB2	1.84	0.59
25:DA:957:A:H5'	36:DQ:76:LYS:HG3	1.84	0.59
45:BZ:24:LEU:HB2	45:BZ:41:LEU:HD23	1.84	0.59
1:AA:1008:C:N3	1:AA:1021:G:C6	2.71	0.58
27:BD:17:THR:O	27:BD:211:ARG:NH2	2.36	0.58
1:CA:1059:C:OP2	3:CC:199:LYS:NZ	2.33	0.58
31:BH:7:LEU:HD12	31:BH:8:PRO:HD2	1.85	0.58
1:AA:1125:U:H4'	10:AJ:5:ARG:NH2	2.18	0.58
25:BA:2045:G:H5'	25:BA:2629:C:H4'	1.84	0.58
9:CI:50:LEU:HB2	9:CI:56:LEU:HD23	1.84	0.58
25:DA:927:G:H2'	25:DA:928:G:O4'	2.02	0.58
24:CX:76:A:OP1	61:CX:4003:HOH:O	2.17	0.58
10:CJ:30:SER:O	10:CJ:81:THR:HG23	2.04	0.58
28:BE:3:GLY:HA3	28:BE:81:ILE:HD12	1.83	0.58
29:DF:116:ASP:OD1	29:DF:119:ARG:NH2	2.35	0.58
5:AE:143:ARG:NH1	8:AH:77:GLU:OE1	2.36	0.58
25:BA:1232:G:H5''	41:BV:81:TYR:CE1	2.37	0.58
25:DA:2646:C:OP2	25:DA:2732:G:O2'	2.17	0.58
24:AX:59:A:H2'	24:AX:60:U:H5'	1.83	0.58
23:CY:36:A:H2'	23:CY:37:MIA:O4'	2.03	0.58
25:DA:1803:A:O2'	27:DD:259:THR:HG21	2.03	0.58
28:BE:47:VAL:HG23	28:BE:84:PHE:O	2.03	0.58
25:BA:1452:U:H2'	25:BA:1453:C:C6	2.38	0.58
32:DI:31:LEU:HD21	32:DI:38:LEU:HG	1.84	0.58
25:DA:1359:A:H61	25:DA:1372:U:H3	1.50	0.58
1:CA:405:U:O4	4:CD:2:GLY:N	2.36	0.58
7:CG:27:ILE:HD12	7:CG:40:ALA:HA	1.85	0.58
25:BA:1218:G:O2'	25:BA:1219:A:O5'	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AH:73:ASP:OD1	8:AH:75:ARG:HD3	2.03	0.58
50:B4:61:ARG:HG3	50:B4:62:ARG:N	2.19	0.58
25:BA:2130:C:H2'	25:BA:2131:U:C6	2.37	0.58
32:BI:27:ARG:HD2	47:B1:71:TYR:CE1	2.39	0.58
17:AQ:45:HIS:CD2	17:AQ:47:PRO:HG3	2.39	0.58
25:DA:613:G:N2	25:DA:614(C):A:O2'	2.37	0.58
33:DN:15:LEU:HB2	33:DN:135:PRO:HB2	1.85	0.58
28:BE:111:ARG:HG3	28:BE:160:TYR:CD2	2.39	0.58
25:DA:871:U:O2	25:DA:906:G:N2	2.30	0.58
1:CA:545:C:OP2	4:CD:65:ARG:NH2	2.37	0.58
25:DA:1204:A:H5'	25:DA:1206:G:H1'	1.86	0.58
13:CM:33:ALA:HA	13:CM:59:TYR:CE2	2.39	0.58
25:DA:1250:G:OP2	35:DP:21:ARG:NH1	2.37	0.58
25:DA:1711:C:H2'	25:DA:1712:C:C6	2.38	0.58
1:AA:997:U:H3	1:AA:1044:A:H61	1.51	0.58
34:DO:107:ARG:CZ	39:DT:36:GLU:HG2	2.34	0.58
1:AA:200:G:H1	1:AA:217:C:N4	2.02	0.58
25:DA:972:G:OP2	25:DA:973:A:O2'	2.17	0.58
50:B4:57:GLU:HB3	50:B4:58:ARG:HG2	1.86	0.58
25:BA:1272:A:OP1	41:BV:84:LYS:HE2	2.04	0.58
25:BA:1827:U:H2'	25:BA:1828:C:C6	2.39	0.58
25:DA:900:A:H2'	25:DA:901:A:C8	2.38	0.58
25:BA:303:C:H42	25:BA:385:G:H1	1.51	0.58
52:D6:14:THR:OG1	52:D6:48:VAL:O	2.22	0.58
26:DB:81:G:H1	26:DB:96:U:H3	1.51	0.58
6:CF:9:VAL:HB	6:CF:87:ARG:HB2	1.85	0.58
12:CL:88:GLY:O	12:CL:99:HIS:HD2	1.85	0.58
25:DA:2291:U:H2'	25:DA:2292:C:C6	2.39	0.58
1:CA:517:G:N1	1:CA:533:A:OP2	2.28	0.57
25:BA:2152:U:H2'	25:BA:2153:G:N2	2.19	0.57
25:BA:83:A:H5''	44:BY:8:LYS:HE3	1.86	0.57
1:CA:775:G:N2	1:CA:804:U:O4	2.36	0.57
9:AI:9:ARG:HG2	9:AI:14:VAL:HG12	1.86	0.57
32:BI:126:TYR:HB2	32:BI:142:VAL:HG23	1.86	0.57
25:BA:2820:A:N6	25:BA:2900:G:O2'	2.36	0.57
25:DA:131:G:OP1	61:DA:4107:HOH:O	2.17	0.57
2:CB:95:GLN:HG3	2:CB:147:LYS:HD3	1.86	0.57
24:CX:49:G:H1	24:CX:65:C:N4	2.02	0.57
25:DA:324:A:N6	25:DA:338:G:O2'	2.37	0.57
25:DA:2379:G:O2'	38:DS:17:ARG:NH2	2.22	0.57
8:CH:64:LYS:HG2	8:CH:79:VAL:HG21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:CT:13:LEU:H	20:CT:13:LEU:HD12	1.68	0.57
3:CC:18:TRP:H	3:CC:18:TRP:HE3	1.52	0.57
50:B4:53:GLU:O	50:B4:55:ARG:N	2.35	0.57
11:CK:31:THR:HG23	11:CK:42:TRP:HB3	1.85	0.57
25:BA:129:G:OP1	61:BA:4198:HOH:O	2.17	0.57
20:CT:9:ASN:O	20:CT:10:LEU:HB2	2.04	0.57
1:AA:619:U:C2	4:AD:135:LEU:HD22	2.40	0.57
1:AA:1391:U:H2'	1:AA:1392:G:C8	2.40	0.57
25:BA:2299:A:N6	25:BA:2356:U:H3	1.98	0.57
25:BA:2162:C:C4	25:BA:2173:G:N1	2.71	0.57
1:CA:1001:A:H2'	1:CA:1001(A):G:C8	2.38	0.57
39:BT:24:PRO:HA	39:BT:49:VAL:HG22	1.86	0.57
25:DA:833:U:O2	35:DP:55:ARG:NH2	2.36	0.57
25:DA:570:G:H2'	25:DA:2030:A:C5	2.39	0.57
14:AN:27:CYS:SG	14:AN:29:ARG:HB2	2.44	0.57
1:CA:1029:C:N4	1:CA:1032:G:C5	2.72	0.57
1:CA:1348:U:H2'	1:CA:1349:A:H8	1.70	0.57
27:DD:26:LYS:NZ	27:DD:30:GLU:OE1	2.31	0.57
25:BA:2227:G:H5'	25:BA:2228:G:N7	2.19	0.57
38:DS:27:SER:HA	38:DS:88:ASP:HB3	1.87	0.57
24:AX:21:A:N6	24:AX:46:G:H2'	2.19	0.57
23:AY:63:G:H2'	23:AY:64:A:O4'	2.05	0.57
1:AA:1183:A:HO2'	1:AA:1184:G:P	2.27	0.57
35:DP:97:PRO:HD3	35:DP:126:VAL:O	2.04	0.57
35:BP:63:PRO:HG2	54:B8:25:MET:HB2	1.85	0.57
25:DA:1539:G:H2'	25:DA:1540:U:O4'	2.04	0.57
25:DA:1400:G:H2'	25:DA:1401:G:C8	2.38	0.57
1:CA:1151:A:O4'	10:CJ:39:PRO:HB2	2.03	0.57
25:DA:2142:C:H2'	25:DA:2143:C:C6	2.40	0.57
25:BA:667:G:H21	25:BA:671:A:H2	1.52	0.57
50:D4:61:ARG:O	50:D4:63:TYR:N	2.38	0.57
25:DA:1400:G:H2'	25:DA:1401:G:H8	1.70	0.57
1:AA:1191:A:H5''	3:AC:4:LYS:NZ	2.20	0.57
25:BA:2126:G:H2'	25:BA:2127:C:C6	2.40	0.57
13:CM:13:LYS:HA	13:CM:44:ARG:HH11	1.70	0.57
15:AO:11:VAL:HG21	15:AO:34:LEU:HD22	1.86	0.57
11:CK:110:ASP:HB3	18:CR:85:LEU:HB3	1.86	0.57
30:DG:39:ILE:HG12	30:DG:157:ILE:HG12	1.87	0.57
23:AY:20:U:H4'	23:AY:21:A:OP1	2.04	0.57
9:CI:128:ARG:NH2	24:CX:33:U:OP2	2.38	0.57
37:BR:28:LEU:HD12	37:BR:48:VAL:HG21	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:784:A:C5	27:DD:229:VAL:HG11	2.40	0.57
38:BS:20:ARG:NH2	46:B0:48:GLY:O	2.37	0.57
7:CG:15:ASP:OD2	7:CG:44:TYR:OH	2.18	0.57
2:AB:178:ARG:HG2	8:AH:72:PRO:HA	1.85	0.57
7:CG:69:VAL:HG21	7:CG:104:LEU:HD11	1.87	0.57
10:AJ:38:ILE:HD11	10:AJ:71:LEU:HD23	1.87	0.57
1:AA:222:U:H2'	1:AA:223:U:C6	2.39	0.57
38:DS:87:PHE:CE1	38:DS:102:ALA:HB2	2.40	0.57
48:D2:35:LEU:HD12	48:D2:53:LEU:HD12	1.87	0.57
25:DA:250:G:P	54:D8:13:ARG:HH22	2.28	0.57
1:AA:78:G:C6	1:AA:91:C:N4	2.73	0.57
13:CM:81:LEU:HD13	13:CM:88:ARG:HG2	1.87	0.57
1:CA:1030(A):G:N2	1:CA:1030(D):A:OP2	2.37	0.57
25:DA:1359:A:N6	25:DA:1372:U:H3	2.03	0.57
25:DA:1530:C:N4	25:DA:1539:G:H1	2.03	0.57
1:AA:1510:U:H2'	1:AA:1511:G:C8	2.40	0.57
6:AF:97:PHE:N	18:AR:30:ASP:OD1	2.37	0.57
1:AA:7:G:O2'	5:AE:120:THR:O	2.23	0.57
25:BA:572:A:H61	41:BV:19:LYS:H	1.53	0.57
25:DA:639:U:H2'	25:DA:640:C:C6	2.40	0.57
29:DF:11:VAL:HG22	29:DF:125:LEU:HB2	1.86	0.57
1:CA:673:G:H2'	1:CA:674:G:C8	2.40	0.57
1:CA:1317:C:OP1	14:CN:17:LYS:HG2	2.05	0.57
34:DO:2:ILE:HB	34:DO:33:ALA:HB3	1.87	0.57
1:CA:1392:G:H21	1:CA:1502:A:H8	1.50	0.57
26:DB:15:A:OP2	26:DB:69:G:N2	2.37	0.57
1:AA:972:C:OP1	61:AA:4158:HOH:O	2.18	0.57
10:CJ:78:ASN:O	10:CJ:80:LYS:N	2.38	0.57
27:BD:108:PRO:HB3	27:BD:143:HIS:CE1	2.40	0.57
35:BP:81:GLN:NE2	35:BP:105:LEU:O	2.36	0.57
7:CG:78:ARG:NH1	7:CG:79:ARG:HH12	2.03	0.57
25:BA:1027:A:OP1	61:BA:4709:HOH:O	2.18	0.57
2:CB:74:LYS:HG3	2:CB:77:ALA:HB3	1.86	0.57
29:BF:53:THR:HG22	29:BF:55:GLY:H	1.70	0.57
25:BA:2736:C:OP1	37:BR:3:HIS:ND1	2.22	0.57
25:BA:613:A:OP1	29:BF:95:ARG:NH1	2.38	0.57
45:DZ:110:GLY:O	45:DZ:146:ILE:HG13	2.04	0.56
25:DA:528:A:C2	25:DA:2042:A:H2'	2.40	0.56
36:DQ:32:TYR:OH	36:DQ:111:GLU:OE1	2.13	0.56
25:BA:1475:G:H2'	25:BA:1476:C:C6	2.39	0.56
34:DO:87:ILE:HD12	34:DO:91:LEU:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:1346:U:H4'	25:BA:1347:A:C5'	2.35	0.56
25:BA:1065:U:O2'	25:BA:1067:A:H2	1.88	0.56
25:DA:2138:C:N4	25:DA:2153:G:H1	2.03	0.56
24:CX:76:A:H5'	25:DA:2585:U:C5	2.41	0.56
25:DA:1204:A:N6	25:DA:1240:U:H2'	2.20	0.56
25:BA:2840:G:OP1	28:BE:76:ARG:NH2	2.38	0.56
1:AA:838:G:H2'	1:AA:839:U:H2'	1.86	0.56
25:DA:1430:C:H2'	25:DA:1431:U:C6	2.39	0.56
31:BH:113:VAL:HG11	31:BH:151:ILE:HD13	1.87	0.56
34:DO:115:VAL:HG13	34:DO:121:VAL:HG21	1.87	0.56
1:AA:405:U:OP2	4:AD:3:ARG:NH2	2.38	0.56
25:BA:346:A:OP1	29:BF:168:ARG:HD2	2.05	0.56
25:BA:2331:G:H22	38:BS:3:ARG:NE	2.03	0.56
1:AA:977:A:H1'	1:AA:982:U:O4	2.06	0.56
1:AA:1064:G:H4'	1:AA:1065:U:OP1	2.06	0.56
2:CB:118:LEU:HB3	2:CB:142:LEU:HD12	1.87	0.56
50:B4:33:VAL:HG12	50:B4:34:GLU:H	1.71	0.56
1:CA:1151:A:O2'	1:CA:1152:A:H8	1.88	0.56
25:DA:994:C:OP2	40:DU:54:LYS:NZ	2.33	0.56
52:D6:6:ARG:NH1	52:D6:26:ASN:HB2	2.20	0.56
25:DA:2506:U:OP1	28:DE:144:ARG:NH2	2.38	0.56
23:CY:62:C:H2'	23:CY:63:G:H8	1.69	0.56
23:AY:33:U:H2'	23:AY:35:A:OP2	2.04	0.56
3:CC:15:THR:HG21	3:CC:181:ASN:HA	1.87	0.56
25:BA:1613:A:OP1	27:BD:211:ARG:NH1	2.39	0.56
25:BA:1513:G:H2'	25:BA:1594:C:N4	2.20	0.56
8:CH:51:VAL:HG11	8:CH:60:ARG:NH1	2.20	0.56
38:DS:68:GLN:HE21	38:DS:71:ARG:HD3	1.69	0.56
31:DH:96:ALA:HB1	31:DH:103:LEU:HD11	1.87	0.56
25:DA:1300:U:H4'	25:DA:1301:A:H5'	1.88	0.56
20:CT:92:LEU:HA	20:CT:95:ALA:HB3	1.87	0.56
25:BA:2310:A:H2'	25:BA:2311:G:O4'	2.05	0.56
19:CS:30:LEU:HA	19:CS:48:THR:O	2.06	0.56
8:CH:41:ARG:NH2	8:CH:123:GLU:OE2	2.38	0.56
3:AC:33:LEU:HD21	14:AN:53:LEU:HD22	1.85	0.56
25:BA:1817:A:H1'	25:BA:1960:A:N6	2.20	0.56
5:AE:79:GLU:HG3	5:AE:93:PRO:HD2	1.87	0.56
25:BA:273:G:H4'	25:BA:274:U:OP1	2.04	0.56
15:CO:25:THR:HG21	15:CO:70:LEU:HB2	1.86	0.56
25:DA:2193:G:H2'	25:DA:2194:G:H8	1.71	0.56
1:CA:1492:A:O2'	1:CA:1493:A:O5'	2.16	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:BF:140:LEU:HD21	29:BF:170:LEU:HD11	1.86	0.56
25:DA:1434:A:H61	25:DA:1558:A:H62	1.53	0.56
25:DA:1594:G:H2'	25:DA:1595:G:O4'	2.05	0.56
2:AB:100:GLY:N	2:AB:176:GLU:OE2	2.27	0.56
2:AB:15:VAL:HG21	2:AB:209:ARG:HG2	1.87	0.56
1:AA:1007:C:N3	1:AA:1022:G:O6	2.37	0.56
25:DA:1231:G:H2'	25:DA:1232:G:C8	2.41	0.56
25:DA:1518:U:H2'	25:DA:1519:G:O4'	2.05	0.56
41:DV:43:GLU:OE2	41:DV:43:GLU:N	2.37	0.56
3:AC:54:ARG:NH1	3:AC:56:ASP:OD2	2.38	0.56
25:BA:173:C:H2'	25:BA:174:U:C6	2.40	0.56
57:AA:3231:PCY:O26	57:AA:3231:PCY:O36	2.22	0.56
1:CA:201:C:N4	1:CA:216:G:H1	2.04	0.56
4:AD:108:LEU:HD22	4:AD:174:LEU:HD13	1.88	0.56
25:DA:2611:U:H5'	25:DA:2611:U:H6	1.71	0.56
30:DG:43:LEU:HD11	30:DG:153:ARG:HG2	1.86	0.56
1:CA:685:G:N1	1:CA:686:U:O4	2.39	0.56
18:AR:56:THR:HB	18:AR:58:LEU:HD23	1.87	0.56
36:BQ:111:GLU:OE1	36:BQ:133:ARG:NH2	2.38	0.56
9:CI:18:PHE:HD2	9:CI:62:TYR:HD2	1.52	0.56
14:CN:12:ARG:HE	14:CN:14:PRO:HB3	1.71	0.56
15:AO:64:ARG:HH11	15:AO:64:ARG:HB3	1.70	0.56
29:BF:157:VAL:HB	29:BF:194:MET:HG2	1.88	0.56
1:AA:17:U:H2'	1:AA:18:C:C6	2.40	0.56
25:BA:1428:G:N7	61:BA:5233:HOH:O	2.33	0.56
25:BA:2825:C:H5'	51:B5:29:THR:HG21	1.87	0.56
23:CW:23:A:H2'	23:CW:24:G:C8	2.40	0.56
36:DQ:111:GLU:O	36:DQ:115:MET:HG2	2.05	0.56
1:CA:1014:A:OP1	19:CS:18:LYS:NZ	2.30	0.56
18:CR:32:ARG:HA	18:CR:69:THR:HG21	1.86	0.56
23:AW:4:C:H2'	23:AW:5:G:H8	1.71	0.56
23:AY:19:G:H3'	23:AY:20:U:C6	2.39	0.56
1:AA:924:C:O2'	1:AA:1502:A:N6	2.37	0.56
25:DA:1203:G:OP2	25:DA:1204:A:O2'	2.20	0.56
25:DA:131:G:OP1	61:DA:4106:HOH:O	2.18	0.56
19:CS:22:LEU:HD22	19:CS:31:ILE:HD11	1.86	0.56
29:DF:167:ALA:HB1	29:DF:173:VAL:HG11	1.87	0.56
25:DA:1226:A:OP1	41:DV:84:LYS:HE2	2.05	0.56
25:BA:1084:C:H42	25:BA:1163:G:H1	1.54	0.56
25:BA:2289:G:OP2	46:B0:10:THR:HG21	2.05	0.56
37:DR:56:LYS:NZ	37:DR:90:ARG:O	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:DE:72:VAL:HA	28:DE:73:GLU:HB3	1.88	0.56
25:DA:1414:G:N2	25:DA:1588:C:O2	2.37	0.56
28:BE:24:THR:HG22	28:BE:186:GLY:O	2.06	0.56
25:DA:649:G:H4'	54:D8:46:ARG:HH22	1.70	0.56
23:CW:39:PSU:H2'	23:CW:40:C:H6	1.71	0.56
11:CK:81:ASP:OD1	11:CK:107:SER:OG	2.21	0.56
52:B6:35:GLU:OE2	52:B6:50:ARG:NH1	2.39	0.56
2:CB:87:ARG:HH12	2:CB:230:VAL:HG11	1.70	0.56
1:CA:1029:C:C4	1:CA:1033:G:C6	2.94	0.56
25:DA:1798:U:OP2	27:DD:274:ARG:NH2	2.39	0.56
45:DZ:120:ILE:HG13	45:DZ:173:ALA:HB3	1.88	0.56
25:BA:2157:A:N1	25:BA:2178:G:O2'	2.32	0.56
9:CI:9:ARG:HG2	9:CI:14:VAL:HG12	1.88	0.56
13:CM:92:HIS:CE1	13:CM:98:VAL:HG21	2.41	0.56
25:DA:1721:G:N1	25:DA:1739:U:OP2	2.39	0.56
29:BF:125:LEU:HD12	29:BF:194:MET:HB2	1.88	0.56
25:DA:2303:G:O2'	30:DG:132:ASN:HB2	2.06	0.56
13:AM:3:ARG:HD2	13:AM:9:ILE:HG12	1.88	0.56
1:CA:1513:A:H2'	1:CA:1514:C:C6	2.41	0.56
23:AW:8:4SU:H6	23:AW:8:4SU:O5'	2.06	0.56
25:BA:796:C:OP2	61:BA:5333:HOH:O	2.18	0.56
38:BS:14:VAL:O	38:BS:18:ILE:HG12	2.06	0.56
2:AB:16:HIS:CG	2:AB:17:PHE:N	2.74	0.55
1:CA:1442(A):G:C8	39:DT:118:ARG:HG2	2.41	0.55
19:AS:50:ALA:HB1	19:AS:57:HIS:HB3	1.87	0.55
3:AC:17:ASP:O	3:AC:54:ARG:NH2	2.40	0.55
1:CA:1073:U:O2	2:CB:104:ASN:ND2	2.38	0.55
45:DZ:33:LEU:HD11	45:DZ:90:VAL:HG21	1.87	0.55
1:CA:45:U:H2'	1:CA:46:G:C8	2.42	0.55
2:CB:189:ASP:N	2:CB:189:ASP:OD1	2.34	0.55
25:BA:795:G:H2'	25:BA:797:A:OP2	2.06	0.55
1:CA:1051:C:H2'	1:CA:1052:U:C6	2.41	0.55
1:CA:1122:U:N3	1:CA:1123:A:N7	2.55	0.55
27:DD:242:ARG:N	27:DD:242:ARG:HD3	2.20	0.55
25:DA:1300:U:H4'	25:DA:1301:A:C5'	2.37	0.55
1:AA:60:A:H4'	1:AA:61:G:H5'	1.88	0.55
25:DA:27:G:N2	25:DA:512:G:H1'	2.20	0.55
32:BI:72:LEU:O	32:BI:74:ASN:N	2.39	0.55
11:CK:92:GLU:HB3	11:CK:96:ARG:HH21	1.72	0.55
25:DA:2177:C:H2'	25:DA:2178:C:O4'	2.06	0.55
1:CA:838:G:N2	1:CA:848:C:N3	2.52	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:CJ:8:LEU:HB3	10:CJ:16:LEU:HD22	1.88	0.55
25:DA:330:A:HO2'	25:DA:331:A:H8	1.53	0.55
1:CA:352:C:OP2	61:CA:4054:HOH:O	2.17	0.55
27:DD:218:ARG:HB3	27:DD:219:PRO:HD2	1.88	0.55
25:BA:559:U:H2'	25:BA:560:C:C6	2.42	0.55
37:BR:96:ARG:NH1	37:BR:118:GLU:OE2	2.37	0.55
19:CS:41:VAL:HG12	19:CS:43:GLU:H	1.71	0.55
20:CT:43:LEU:O	20:CT:47:GLY:N	2.39	0.55
36:DQ:37:LEU:HD21	36:DQ:130:LYS:HE2	1.89	0.55
25:DA:1406:U:H2'	25:DA:1407:C:C6	2.41	0.55
25:DA:878:A:N6	25:DA:899:A:O2'	2.39	0.55
1:AA:1392:G:N2	1:AA:1502:A:C8	2.74	0.55
25:DA:2273:A:H2'	25:DA:2274:A:C8	2.41	0.55
25:BA:641:G:OP1	29:BF:40:GLN:HG2	2.07	0.55
1:CA:1469:G:H2'	1:CA:1470:G:C8	2.42	0.55
8:CH:69:ARG:NH2	8:CH:75:ARG:O	2.39	0.55
2:CB:98:LEU:H	2:CB:98:LEU:HD22	1.71	0.55
25:BA:431:C:H4'	25:BA:432:U:H5'	1.87	0.55
1:AA:975:A:H5'	1:AA:975:A:H8	1.70	0.55
25:DA:2296:U:OP2	38:DS:9:ARG:NH2	2.39	0.55
25:DA:1266:G:O2'	25:DA:2012:G:O6	2.20	0.55
35:DP:38:GLN:O	35:DP:39:LYS:HB3	2.05	0.55
9:AI:22:GLY:N	9:AI:58:HIS:O	2.31	0.55
25:BA:1735:U:O2	25:BA:1747:A:H5'	2.06	0.55
25:BA:661:G:OP1	35:BP:132:LYS:HE2	2.07	0.55
1:AA:715:A:H2'	1:AA:716:A:C8	2.41	0.55
1:AA:356:A:N3	1:AA:368:U:O2'	2.33	0.55
1:CA:1006:C:H2'	1:CA:1007:C:C6	2.41	0.55
25:DA:143:G:H4'	43:DX:35:THR:HG21	1.87	0.55
32:BI:93:THR:OG1	32:BI:96:ASP:OD1	2.16	0.55
6:AF:91:VAL:HG11	18:AR:72:ARG:NH1	2.20	0.55
1:CA:677:U:H3	1:CA:713:G:H22	1.53	0.55
31:DH:30:LYS:HG3	31:DH:80:SER:O	2.06	0.55
1:AA:509:A:O2'	1:AA:510:A:OP1	2.18	0.55
1:AA:165:C:H2'	1:AA:166:G:C8	2.42	0.55
61:BA:5082:HOH:O	35:BP:39:LYS:HE3	2.06	0.55
47:B1:89:GLU:O	47:B1:93:GLU:HG2	2.07	0.55
25:BA:333:G:N3	25:BA:353:G:O2'	2.36	0.55
23:CW:29:G:H2'	23:CW:30:G:H8	1.72	0.55
25:BA:1222:A:H2'	25:BA:1222:A:N3	2.21	0.55
1:CA:1469:G:H2'	1:CA:1470:G:H8	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:814:A:H2'	1:CA:816:A:H5''	1.87	0.55
25:BA:906:G:O2'	25:BA:962:G:O6	2.21	0.55
1:AA:1025:U:C2	1:AA:1036:G:O6	2.59	0.55
4:AD:190:ASP:HB2	4:AD:193:ASP:OD2	2.07	0.55
25:DA:2683:C:P	39:DT:53:ARG:HH22	2.30	0.55
25:DA:2022:U:O2'	25:DA:2617:C:H5'	2.07	0.55
25:DA:1579:A:H2'	25:DA:1580:A:C8	2.42	0.55
25:BA:206:G:OP2	61:BA:5143:HOH:O	2.18	0.55
1:AA:407:G:OP1	4:AD:115:ARG:NH2	2.39	0.55
1:CA:1010:G:H2'	1:CA:1011:G:H8	1.71	0.55
26:BB:66:A:H61	26:BB:109:C:H5'	1.71	0.55
3:CC:37:GLN:HE22	3:CC:40:ARG:HD2	1.72	0.55
14:CN:23:ARG:NH1	14:CN:30:ALA:HB2	2.21	0.55
24:CX:19:G:H4'	24:CX:20:U:OP2	2.07	0.55
1:CA:1370:G:O6	61:CA:4006:HOH:O	2.16	0.55
25:BA:479:C:O2	25:BA:483:A:O2'	2.23	0.55
25:BA:139:A:H8	25:BA:1454:C:O2'	1.90	0.55
3:CC:7:PRO:O	3:CC:11:ARG:NH1	2.38	0.55
42:DW:4:LYS:HB2	42:DW:106:ILE:HG12	1.89	0.55
25:BA:272:U:OP1	32:BI:50:ARG:NH1	2.40	0.55
1:AA:1414:U:H3	1:AA:1486:G:H1	1.54	0.55
25:DA:674:G:H1'	29:DF:74:ARG:HD3	1.89	0.55
25:DA:191:A:H2'	25:DA:192:C:C6	2.41	0.55
25:BA:704:U:H2'	25:BA:705:C:C6	2.42	0.55
50:B4:63:TYR:N	50:B4:64:GLY:HA2	2.20	0.55
43:DX:31:HIS:CD2	43:DX:33:LYS:H	2.24	0.55
1:CA:1121:U:C4	1:CA:1122:U:C4	2.96	0.55
40:DU:49:HIS:HA	40:DU:52:ARG:HB3	1.88	0.55
10:CJ:38:ILE:HD11	10:CJ:71:LEU:HB3	1.89	0.55
3:CC:134:ILE:HG23	3:CC:151:VAL:HB	1.88	0.55
5:AE:151:LEU:HD11	8:AH:77:GLU:HG2	1.88	0.55
5:AE:91:LEU:HG	5:AE:118:ILE:HD11	1.89	0.55
9:CI:23:ASN:HD22	9:CI:25:LYS:HG2	1.72	0.55
43:DX:8:ILE:O	48:D2:36:ARG:NH2	2.40	0.55
20:AT:36:LEU:HD13	20:AT:58:LYS:HG3	1.88	0.55
25:DA:2641:G:H5''	33:DN:76:SER:HB3	1.88	0.55
33:BN:15:LEU:HD12	33:BN:137:LYS:HG3	1.89	0.55
50:D4:59:PHE:HA	50:D4:60:GLN:C	2.27	0.55
25:BA:1873:G:O2'	27:BD:253:GLN:NE2	2.39	0.55
10:AJ:17:ASP:OD1	10:AJ:70:ARG:NH1	2.39	0.55
25:DA:829:A:N7	25:DA:2247:A:O2'	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:189:ASP:OD1	2:AB:189:ASP:N	2.30	0.55
1:AA:1007:C:H2'	1:AA:1008:C:H5''	1.88	0.54
1:CA:76:C:H42	1:CA:93:G:H1	1.55	0.54
31:DH:80:SER:OG	31:DH:81:GLU:N	2.40	0.54
25:DA:2666:C:N4	31:DH:108:GLY:O	2.39	0.54
9:AI:21:PRO:HA	9:AI:59:PHE:HA	1.90	0.54
25:DA:896:A:H62	45:DZ:146:ILE:HD13	1.72	0.54
26:DB:19:G:H2'	26:DB:20:C:O4'	2.06	0.54
23:CW:51:U:H2'	23:CW:52:G:H8	1.72	0.54
23:CY:67:C:H2'	23:CY:68:C:C6	2.42	0.54
23:CY:9:A:O3'	23:CY:45:U:O2'	2.25	0.54
24:AX:19:G:H4'	24:AX:20:U:OP2	2.07	0.54
25:DA:829:A:N7	25:DA:2248:C:H5'	2.22	0.54
34:BO:64:ARG:NH1	34:BO:81:ASP:OD1	2.40	0.54
34:BO:104:ARG:CZ	39:BT:34:VAL:HG21	2.37	0.54
3:AC:134:ILE:HG23	3:AC:151:VAL:HB	1.89	0.54
1:AA:69:G:H2'	1:AA:70:G:C8	2.42	0.54
29:BF:14:PRO:HD2	29:BF:127:GLU:OE2	2.07	0.54
23:AY:40:C:H2'	23:AY:41:C:H6	1.72	0.54
3:AC:164:ARG:NH1	3:AC:166:GLU:OE1	2.40	0.54
35:BP:1:MET:HE3	35:BP:5:ASP:HB3	1.89	0.54
26:DB:66:A:N6	26:DB:109:C:H5'	2.14	0.54
1:CA:664:G:H22	1:CA:741:G:H1	1.53	0.54
25:DA:807:U:O2'	25:DA:2060:A:N1	2.40	0.54
1:AA:165:C:H2'	1:AA:166:G:H8	1.72	0.54
25:BA:714:U:O2	54:B8:2:PRO:HD2	2.06	0.54
39:BT:112:ARG:HG3	39:BT:115:ARG:NH2	2.23	0.54
3:AC:11:ARG:NH2	3:AC:177:THR:O	2.41	0.54
1:AA:153:C:H2'	1:AA:154:C:C6	2.42	0.54
25:DA:2167:U:H2'	25:DA:2168:G:H21	1.73	0.54
1:CA:1063:C:OP2	1:CA:1064:G:O2'	2.23	0.54
1:CA:976:G:H5'	1:CA:1358:U:O2'	2.07	0.54
25:BA:2146:G:H1	25:BA:2196:C:N4	2.05	0.54
23:CW:51:U:H2'	23:CW:52:G:C8	2.42	0.54
25:DA:2183:C:H2'	25:DA:2184:G:H8	1.72	0.54
25:DA:1889:A:H2'	25:DA:1890:A:C8	2.43	0.54
34:BO:80:ASP:OD1	39:BT:64:ARG:NH2	2.40	0.54
1:AA:749:C:H2'	1:AA:750:G:H8	1.72	0.54
1:CA:1183:A:O2'	1:CA:1184:G:OP1	2.22	0.54
1:AA:1112:C:H1'	3:AC:179:ARG:HG2	1.88	0.54
4:AD:98:GLU:HG2	4:AD:189:PRO:HG2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:731:G:H5'	1:AA:766:A:H4'	1.89	0.54
25:DA:2430:A:H2'	25:DA:2430:A:N3	2.22	0.54
25:DA:864:G:H21	25:DA:866:A:H61	1.54	0.54
1:AA:637:G:H2'	1:AA:638:G:H8	1.71	0.54
25:BA:2298:A:H4'	25:BA:2299:A:O4'	2.07	0.54
50:B4:53:GLU:HG3	50:B4:55:ARG:H	1.72	0.54
25:DA:2721:A:OP1	61:DA:4147:HOH:O	2.18	0.54
1:CA:1456:G:O3'	20:CT:39:LYS:NZ	2.40	0.54
15:CO:5:LYS:NZ	15:CO:5:LYS:H	2.06	0.54
7:CG:32:ARG:HH12	7:CG:109:ASN:ND2	2.05	0.54
1:CA:448:A:O5'	1:CA:485:G:N2	2.40	0.54
32:BI:72:LEU:C	32:BI:74:ASN:H	2.08	0.54
40:BU:108:GLU:O	40:BU:112:ARG:HG2	2.07	0.54
28:DE:116:VAL:HG13	28:DE:122:PHE:HB2	1.90	0.54
2:AB:83:MET:HB3	2:AB:234:PRO:HG2	1.88	0.54
45:DZ:70:LEU:O	45:DZ:89:PHE:N	2.38	0.54
25:BA:602:G:H2'	25:BA:603:C:C6	2.43	0.54
45:DZ:117:LEU:HD12	45:DZ:174:VAL:HG22	1.89	0.54
25:DA:2447:G:N2	25:DA:2450:A:OP2	2.40	0.54
28:DE:73:GLU:HG3	28:DE:73:GLU:O	2.06	0.54
4:CD:162:LEU:HD13	4:CD:181:MET:HG2	1.90	0.54
25:BA:552:C:H5	61:BA:4972:HOH:O	1.90	0.54
23:AY:76:A:N6	25:BA:2434:A:O4'	2.40	0.54
33:BN:4:TYR:CD2	40:BU:100:VAL:HG11	2.42	0.54
1:AA:376:G:O3'	16:AP:5:ARG:HD2	2.07	0.54
19:CS:52:TYR:HB2	19:CS:57:HIS:CE1	2.42	0.54
25:DA:303:U:H2'	25:DA:304:G:C8	2.42	0.54
25:BA:2227:G:O2'	25:BA:2228:G:OP1	2.24	0.54
2:CB:201:ILE:HG21	2:CB:214:ILE:HG21	1.89	0.54
6:AF:8:ILE:HD11	6:AF:79:LEU:HD13	1.89	0.54
25:BA:2373:A:OP1	54:B8:27:THR:OG1	2.18	0.54
23:CW:27:G:H2'	23:CW:28:G:C8	2.43	0.54
23:AY:55:PSU:C2	23:AY:57:G:H5'	2.43	0.54
2:AB:162:ILE:O	2:AB:185:ILE:HG12	2.07	0.54
1:CA:1118:C:H1'	1:CA:1179:A:C5	2.43	0.54
3:AC:181:ASN:HD21	3:AC:204:LEU:HD12	1.73	0.54
25:DA:323:G:HO2'	25:DA:1205:U:H3	0.67	0.54
29:BF:184:TYR:CE2	29:BF:188:ARG:HD2	2.43	0.54
10:AJ:49:VAL:HG23	14:AN:41:ARG:HB2	1.89	0.54
4:AD:168:ARG:H	4:AD:168:ARG:CD	2.21	0.54
25:DA:2659:G:H4'	31:DH:175:LYS:HD3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:CK:22:HIS:HB3	11:CK:29:ILE:HB	1.90	0.54
44:BY:20:TYR:CE1	44:BY:43:ASN:HA	2.41	0.54
25:BA:2255:U:H2'	25:BA:2256:U:C6	2.43	0.54
25:BA:310:C:H2'	25:BA:311:C:H6	1.72	0.54
1:AA:532:A:O2'	1:AA:533:A:OP1	2.22	0.54
28:DE:38:THR:HG23	28:DE:41:LYS:HB3	1.90	0.54
1:CA:1003:G:H1	1:CA:1035:A:N6	2.06	0.54
23:CW:21:A:N6	23:CW:46:7MG:N3	2.56	0.54
39:DT:64:ARG:HB2	39:DT:73:GLU:HG2	1.89	0.54
1:CA:1028:C:O2	1:CA:1033:G:N1	2.41	0.54
25:DA:319:C:H2'	25:DA:320:A:O4'	2.08	0.54
25:BA:2178:G:H2'	25:BA:2179:G:C4	2.42	0.54
1:CA:160:A:H1'	1:CA:344:A:N7	2.23	0.54
36:DQ:16:ARG:HG2	36:DQ:18:LYS:HE2	1.89	0.54
31:BH:56:SER:OG	31:BH:57:ASP:N	2.41	0.54
25:BA:2227:G:H3'	25:BA:2228:G:C8	2.42	0.54
15:CO:70:LEU:HD11	15:CO:77:ARG:HB2	1.89	0.54
47:B1:85:LEU:HD22	47:B1:89:GLU:HG3	1.90	0.54
37:DR:21:TYR:CZ	37:DR:43:GLU:HG2	2.43	0.54
30:BG:72:ARG:NH1	30:BG:87:PRO:HG3	2.23	0.54
1:AA:1218:C:H2'	1:AA:1219:U:C6	2.43	0.54
1:CA:41:G:H2'	1:CA:42:G:H8	1.73	0.54
1:CA:41:G:H2'	1:CA:42:G:C8	2.43	0.54
1:AA:676:A:H1'	11:AK:115:PRO:HB3	1.88	0.54
32:DI:57:ARG:HA	32:DI:61:ARG:HH21	1.72	0.54
1:CA:35:G:O2'	12:CL:118:SER:O	2.19	0.54
25:DA:2141:G:O4'	25:DA:2151:G:N2	2.41	0.53
1:AA:134:A:H61	16:AP:25:ARG:HH12	1.56	0.53
27:DD:132:PRO:HD3	27:DD:190:TYR:CZ	2.42	0.53
1:CA:158:G:N2	1:CA:163:C:O2	2.41	0.53
25:BA:1653:C:H4'	25:BA:1654:A:O5'	2.07	0.53
13:AM:93:ARG:HD2	25:BA:935:C:OP1	2.08	0.53
34:BO:16:ALA:HB2	34:BO:52:VAL:HG21	1.89	0.53
25:BA:2549:U:H2'	25:BA:2550:C:C6	2.43	0.53
25:DA:770:G:OP2	61:DA:4559:HOH:O	2.19	0.53
11:AK:99:GLN:HG2	11:AK:105:VAL:HG21	1.90	0.53
30:DG:113:ARG:NH1	30:DG:139:LEU:O	2.37	0.53
25:BA:354:A:H2	25:BA:1255:A:C2'	2.21	0.53
31:DH:9:ILE:HG12	31:DH:69:ARG:HD2	1.90	0.53
1:AA:1494:G:O2'	25:BA:1934:A:O2'	2.27	0.53
2:AB:178:ARG:HH21	8:AH:74:PRO:HB3	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BD:145:VAL:HG12	27:BD:146:GLU:O	2.07	0.53
1:CA:21:G:H2'	1:CA:22:G:C8	2.43	0.53
25:BA:1740:U:O2'	27:BD:14:ARG:NH2	2.41	0.53
48:B2:24:LEU:HD23	48:B2:60:LEU:HD21	1.89	0.53
25:BA:718:C:N4	61:BA:5006:HOH:O	2.40	0.53
1:CA:788:U:O2'	57:CA:3178:PCY:O14	2.20	0.53
1:CA:692:U:O2'	1:CA:694:A:N7	2.30	0.53
23:CW:52:G:H2'	23:CW:53:G:O4'	2.08	0.53
45:BZ:117:LEU:HD21	45:BZ:144:LEU:HD13	1.89	0.53
19:CS:27:GLU:HG2	19:CS:47:HIS:CE1	2.43	0.53
15:CO:26:GLU:OE2	15:CO:77:ARG:NH2	2.35	0.53
7:CG:111:ARG:NH1	7:CG:113:GLU:OE2	2.40	0.53
1:AA:110:C:H2'	1:AA:111:G:O4'	2.07	0.53
25:DA:709:U:H2'	25:DA:710:G:C8	2.44	0.53
13:AM:37:THR:O	13:AM:55:ARG:NH1	2.42	0.53
35:DP:84:ASN:OD1	35:DP:117:GLU:HB2	2.08	0.53
25:BA:236:G:H4'	25:BA:413:G:C5	2.42	0.53
25:BA:794:U:O2	25:BA:2036:A:H1'	2.07	0.53
23:CY:8:4SU:H6	23:CY:8:4SU:H5''	1.91	0.53
25:BA:968:U:H2'	25:BA:969:C:C6	2.44	0.53
31:DH:90:LYS:HD3	31:DH:159:GLU:HG2	1.91	0.53
41:DV:6:LYS:HB2	41:DV:38:LEU:HD21	1.90	0.53
1:AA:933:G:O6	7:AG:3:ARG:NH2	2.39	0.53
1:CA:187:C:O2'	20:CT:89:ARG:NH2	2.39	0.53
1:AA:1001:A:H2'	1:AA:1001(A):G:C8	2.43	0.53
25:DA:2206:G:H3'	25:DA:2207:G:N7	2.22	0.53
25:BA:1067:A:H3'	25:BA:1067:A:C8	2.43	0.53
1:AA:1305:G:H22	1:AA:1331:G:H1'	1.72	0.53
1:AA:1494:G:HO2'	25:BA:1934:A:HO2'	1.56	0.53
31:DH:103:LEU:HB3	31:DH:115:VAL:HB	1.89	0.53
39:BT:23:ARG:HG3	39:BT:120:ARG:NH1	2.23	0.53
25:DA:660:G:H5'	29:DF:99:TYR:CE2	2.43	0.53
25:BA:927:G:H2'	25:BA:928:G:H8	1.74	0.53
25:BA:1000:C:OP1	36:BQ:87:LYS:HE3	2.08	0.53
25:DA:811:U:OP2	35:DP:29:LYS:N	2.35	0.53
4:AD:101:LEU:HB2	4:AD:138:TYR:HB3	1.90	0.53
31:DH:113:VAL:HG11	31:DH:151:ILE:HD13	1.89	0.53
1:AA:1027:C:N4	1:AA:1033:G:O6	2.42	0.53
40:DU:76:TYR:HH	40:DU:92:ARG:HH11	1.56	0.53
26:DB:17:C:H2'	26:DB:18:G:O4'	2.09	0.53
36:DQ:14:ARG:HG2	36:DQ:41:TRP:HH2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:254:G:OP1	17:CQ:66:SER:OG	2.21	0.53
1:AA:1124:G:N7	1:AA:1145:C:O2'	2.40	0.53
10:AJ:5:ARG:NH2	10:AJ:73:ASP:OD2	2.32	0.53
23:AW:4:C:N3	23:AW:69:G:O6	2.42	0.53
25:DA:2483:C:H2'	25:DA:2484:G:O4'	2.07	0.53
29:DF:129:PHE:CD2	29:DF:163:VAL:HG21	2.44	0.53
25:BA:1058:U:C5	33:BN:28:THR:HG21	2.44	0.53
25:DA:1292:U:H2'	25:DA:1293:C:C6	2.44	0.53
25:DA:247:G:H4'	25:DA:386:G:C5	2.44	0.53
15:CO:16:ALA:HB1	15:CO:21:ASP:HB3	1.89	0.53
26:DB:6:C:H2'	26:DB:7:G:H5''	1.89	0.53
1:CA:142:G:H2'	1:CA:143:A:C8	2.44	0.53
1:AA:1004:A:H5''	1:AA:1025:U:C5	2.43	0.53
10:CJ:17:ASP:OD1	10:CJ:70:ARG:NH1	2.42	0.53
51:B5:16:ARG:NH1	51:B5:17:ASP:OD1	2.41	0.53
23:AY:67:C:H2'	23:AY:68:C:H6	1.71	0.53
27:DD:26:LYS:HE2	27:DD:28:GLU:O	2.08	0.53
27:BD:77:ALA:HB2	27:BD:97:TYR:CD2	2.44	0.53
28:BE:28:ALA:HB3	28:BE:93:VAL:HG12	1.91	0.53
23:AW:26:A:H61	23:AW:44:G:H1	1.55	0.53
9:AI:86:VAL:HG13	9:AI:96:LEU:HD12	1.91	0.53
1:AA:954:G:H21	1:AA:1227:A:H62	1.56	0.53
25:BA:2798:C:OP1	28:BE:41:LYS:NZ	2.39	0.53
36:DQ:85:LYS:HG2	46:D0:7:LEU:HB3	1.90	0.53
24:CX:8:4SU:O5'	24:CX:8:4SU:H6	2.08	0.53
25:BA:238:C:O2	54:B8:12:LYS:NZ	2.33	0.53
1:CA:91:C:H2'	1:CA:92:C:C6	2.43	0.53
3:CC:37:GLN:NE2	3:CC:40:ARG:HD2	2.23	0.53
40:DU:79:PHE:CZ	40:DU:83:LEU:HD21	2.43	0.53
1:CA:1077:G:N2	1:CA:1080:A:OP2	2.42	0.53
1:CA:49:U:O4	1:CA:365:U:H5	1.89	0.53
45:BZ:11:GLU:O	45:BZ:36:LYS:NZ	2.31	0.53
25:DA:774:A:N3	25:DA:774:A:H2'	2.24	0.53
25:BA:239:G:OP2	54:B8:13:ARG:NH2	2.42	0.53
1:AA:1176:A:H2'	1:AA:1177:G:C8	2.43	0.53
25:BA:2589:A:H5''	25:BA:2590:G:H5'	1.90	0.53
25:DA:1247:A:OP1	29:DF:95:ARG:NH2	2.40	0.53
25:DA:403:U:H4'	25:DA:404:C:H5'	1.89	0.53
44:BY:54:LYS:H	44:BY:56:PRO:HD3	1.73	0.53
15:AO:82:ILE:O	15:AO:86:GLY:N	2.41	0.53
25:DA:956:G:N2	25:DA:959:A:H3'	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:993:G:H21	41:DV:89:GLN:NE2	2.06	0.53
16:CP:9:PHE:CE1	16:CP:18:ARG:HD2	2.44	0.53
25:DA:2567:G:H2'	25:DA:2568:C:C6	2.43	0.53
42:DW:86:LEU:HD22	42:DW:96:ILE:HD11	1.91	0.53
1:CA:396:G:O2'	1:CA:398:C:OP1	2.09	0.53
9:AI:23:ASN:ND2	9:AI:25:LYS:HG2	2.24	0.53
25:DA:1496:A:N3	25:DA:1577:C:O2'	2.40	0.53
8:AH:4:ASP:OD2	8:AH:85:ARG:NH1	2.41	0.53
40:DU:92:ARG:HA	40:DU:95:LEU:HB2	1.90	0.53
25:BA:1154:U:O2'	25:BA:1155:C:O4'	2.27	0.53
26:DB:105:A:OP1	45:DZ:72:ARG:NH1	2.42	0.53
30:DG:115:ARG:HD2	30:DG:136:ARG:HH21	1.73	0.53
23:AY:40:C:H2'	23:AY:41:C:C6	2.44	0.53
25:DA:323:G:C8	29:DF:171:PRO:HG3	2.44	0.53
1:CA:1435:G:H2'	1:CA:1436:U:C6	2.44	0.53
38:BS:34:HIS:O	38:BS:97:ARG:NH2	2.41	0.53
25:DA:455:C:N3	25:DA:472:A:H2'	2.24	0.53
1:CA:428:G:OP2	4:CD:10:ARG:NH1	2.42	0.53
25:DA:39:C:H2'	25:DA:40:C:C6	2.44	0.53
6:AF:68:PRO:HB2	6:AF:71:ARG:HG3	1.90	0.53
25:BA:1338:U:H2'	25:BA:1339:C:C6	2.44	0.53
44:BY:6:HIS:CD2	44:BY:6:HIS:H	2.26	0.53
30:DG:16:ARG:O	30:DG:20:ILE:HG13	2.07	0.53
1:AA:78:G:C2	1:AA:91:C:N3	2.77	0.53
29:DF:117:ARG:HH12	35:DP:1:MET:H2	1.55	0.53
1:AA:1149:C:P	9:AI:9:ARG:HH21	2.32	0.53
25:DA:1405:U:H2'	25:DA:1406:U:C6	2.43	0.53
39:BT:64:ARG:HB2	39:BT:73:GLU:HG2	1.90	0.53
25:BA:1634:C:H2'	25:BA:1635:C:H6	1.74	0.53
1:AA:562:C:H1'	12:AL:15:ARG:HB3	1.91	0.53
8:AH:112:LEU:HA	8:AH:134:ILE:HG12	1.91	0.53
25:BA:2346:G:H5'	38:BS:9:ARG:HG2	1.90	0.53
25:BA:2604:G:OP1	61:BA:4863:HOH:O	2.18	0.53
25:DA:2881:C:H2'	25:DA:2882:A:O4'	2.09	0.53
5:CE:60:TYR:OH	5:CE:64:ARG:NH2	2.41	0.53
1:AA:253:U:OP1	17:AQ:67:LYS:NZ	2.42	0.52
25:BA:1159:U:H2'	25:BA:1160:G:H8	1.74	0.52
50:B4:15:ILE:O	50:B4:33:VAL:N	2.40	0.52
25:BA:1634:C:H2'	25:BA:1635:C:C6	2.44	0.52
25:BA:2490:A:H5'	55:B9:31:LYS:HE2	1.92	0.52
1:AA:67:C:H2'	1:AA:68:G:C8	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:179:A:H2'	1:CA:180:U:C6	2.44	0.52
25:DA:1278:A:OP1	37:DR:36:THR:HG23	2.08	0.52
39:BT:51:ARG:HG3	39:BT:98:LYS:HD2	1.91	0.52
49:B3:8:LEU:HD13	49:B3:31:LEU:HD23	1.91	0.52
23:AW:20:U:H4'	23:AW:20:U:OP1	2.07	0.52
25:BA:2364:A:N6	25:BA:2377:G:O2'	2.42	0.52
25:DA:918:A:H5''	26:DB:98:G:O2'	2.09	0.52
1:CA:1256:A:N6	1:CA:1278:U:H1'	2.09	0.52
4:AD:173:TRP:HE1	4:AD:193:ASP:HB3	1.74	0.52
3:CC:54:ARG:NH1	3:CC:56:ASP:OD1	2.42	0.52
1:CA:165:C:H2'	1:CA:166:G:C8	2.44	0.52
17:CQ:66:SER:OG	17:CQ:69:LYS:HB2	2.08	0.52
25:BA:1346:U:H4'	25:BA:1347:A:H5'	1.91	0.52
8:CH:73:ASP:OD1	8:CH:75:ARG:HD3	2.10	0.52
36:DQ:85:LYS:HD3	46:D0:7:LEU:HG	1.92	0.52
35:BP:82:GLY:HA2	35:BP:113:LYS:O	2.09	0.52
43:BX:53:LYS:HB3	43:BX:82:GLN:HB3	1.90	0.52
25:DA:937:U:H2'	25:DA:938:G:O4'	2.08	0.52
25:BA:2169:G:H2'	25:BA:2170:G:O4'	2.09	0.52
25:DA:2836:U:H2'	25:DA:2837:G:C8	2.44	0.52
32:BI:65:ALA:HB1	32:BI:136:VAL:HG11	1.91	0.52
26:BB:83:G:OP1	49:B3:19:GLN:NE2	2.41	0.52
6:CF:91:VAL:HG11	18:CR:72:ARG:NH1	2.24	0.52
31:DH:89:ILE:O	31:DH:129:THR:HG23	2.09	0.52
25:BA:599:U:H2'	25:BA:600:G:C8	2.44	0.52
20:AT:90:GLN:O	20:AT:93:GLU:HB3	2.09	0.52
28:DE:170:LEU:HB3	28:DE:184:VAL:HG22	1.91	0.52
40:DU:104:GLN:OE1	40:DU:105:VAL:N	2.39	0.52
1:AA:741:G:H2'	1:AA:742:G:O4'	2.09	0.52
1:CA:1325:C:OP1	21:CU:15:ARG:NE	2.40	0.52
2:AB:54:THR:HG21	2:AB:201:ILE:HD11	1.89	0.52
6:AF:45:LEU:HD12	6:AF:59:TYR:HD2	1.74	0.52
25:BA:2228:G:O2'	25:BA:2229:A:OP1	2.25	0.52
25:BA:934:A:H2	25:BA:936:C:H2'	1.74	0.52
25:BA:2603:C:H2'	25:BA:2604:G:C8	2.44	0.52
25:DA:220:G:O2'	25:DA:233:A:N3	2.39	0.52
25:DA:1149:G:H2'	25:DA:1150:C:C6	2.45	0.52
11:AK:32:ILE:HG13	11:AK:72:ALA:HB2	1.91	0.52
43:BX:43:VAL:HG21	43:BX:81:VAL:HG11	1.91	0.52
1:AA:1179:A:H4'	9:AI:103:THR:HA	1.90	0.52
29:BF:143:ALA:HB1	29:BF:148:LEU:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:833:U:H2'	1:CA:834:C:H6	1.73	0.52
43:DX:84:ALA:HB3	43:DX:87:GLN:NE2	2.24	0.52
42:DW:14:PRO:HG2	42:DW:78:GLU:HG2	1.92	0.52
23:AY:18:G:H1	23:AY:55:PSU:H1'	1.74	0.52
1:CA:185:A:N3	20:CT:81:LYS:NZ	2.58	0.52
25:DA:2136:C:O2'	25:DA:2137:C:O5'	2.23	0.52
51:B5:16:ARG:HG2	51:B5:16:ARG:HH11	1.74	0.52
2:CB:163:PHE:HA	2:CB:185:ILE:HG12	1.92	0.52
1:CA:1111:A:N1	3:CC:177:THR:OG1	2.33	0.52
10:AJ:35:SER:HB3	10:AJ:73:ASP:HB2	1.91	0.52
36:BQ:32:TYR:OH	36:BQ:111:GLU:OE1	2.22	0.52
25:BA:1405:A:H2'	25:BA:1406:A:H5'	1.90	0.52
25:BA:957:A:H2'	36:BQ:9:TYR:OH	2.10	0.52
1:CA:642:A:N3	8:CH:113:SER:OG	2.43	0.52
1:CA:735:C:H2'	1:CA:736:C:H6	1.73	0.52
25:DA:1913:A:H4'	25:DA:1914:C:O5'	2.09	0.52
1:AA:410:G:OP1	4:AD:30:LYS:NZ	2.29	0.52
41:DV:35:LEU:HB2	41:DV:57:VAL:HG22	1.91	0.52
25:BA:469:A:H1'	25:BA:1246:C:O4'	2.08	0.52
1:AA:1442(B):A:N3	39:BT:118:ARG:NH2	2.57	0.52
52:B6:34:LEU:HB2	52:B6:51:GLU:HB2	1.91	0.52
25:DA:2712:U:H2'	25:DA:2714:G:H5''	1.91	0.52
25:BA:1094:A:N1	25:BA:1158:G:O2'	2.36	0.52
25:DA:1971:A:OP2	27:DD:242:ARG:NH2	2.42	0.52
57:CA:3178:PCY:H381	7:CG:82:GLY:O	2.10	0.52
10:CJ:30:SER:HB2	10:CJ:80:LYS:CB	2.39	0.52
33:DN:34:LEU:O	33:DN:49:GLY:HA3	2.09	0.52
1:CA:992:U:OP1	1:CA:992:U:H3'	2.08	0.52
3:AC:16:ARG:NH2	3:AC:183:ASP:OD1	2.36	0.52
25:DA:590:A:OP1	29:DF:95:ARG:NH1	2.43	0.52
6:CF:76:ALA:O	6:CF:80:ARG:HG3	2.09	0.52
36:DQ:34:LEU:HB2	36:DQ:118:LEU:HD22	1.91	0.52
1:CA:1192:C:OP2	3:CC:4:LYS:NZ	2.36	0.52
33:BN:14:VAL:HG11	33:BN:138:LEU:HD12	1.91	0.52
25:DA:361:G:O2'	25:DA:362:U:H5'	2.09	0.52
37:DR:44:LEU:HD22	37:DR:48:VAL:HG23	1.91	0.52
25:BA:924:U:H3	25:BA:945:A:H2	1.56	0.52
1:AA:438:G:H4'	4:AD:123:HIS:ND1	2.24	0.52
5:CE:31:LEU:HD22	5:CE:43:LEU:HD11	1.90	0.52
25:BA:847:A:OP1	25:BA:847:A:H8	1.92	0.52
5:AE:74:GLY:HA3	5:AE:116:THR:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:153:C:OP2	47:B1:92:LYS:NZ	2.43	0.52
1:CA:1002:G:H1	1:CA:1038:C:N4	2.07	0.52
1:AA:346:G:C2	1:AA:347:G:H1'	2.44	0.52
1:AA:347:G:H2'	1:AA:348:G:C8	2.44	0.52
1:CA:97:G:O2'	1:CA:98:G:H8	1.93	0.52
1:AA:76:C:H2'	1:AA:77:G:C8	2.44	0.52
25:DA:1324:G:C2	25:DA:1331:A:C2	2.97	0.52
25:DA:1607:C:H4'	25:DA:1608:A:O5'	2.10	0.52
1:AA:1320:C:O2	19:AS:36:ARG:NH2	2.38	0.52
45:DZ:100:VAL:HG21	45:DZ:134:PRO:HG2	1.91	0.52
28:DE:7:VAL:HG12	28:DE:27:LEU:HB3	1.90	0.52
38:DS:77:ALA:HB1	38:DS:82:ILE:HB	1.91	0.52
1:AA:1158:C:H5	1:AA:1181:G:N1	2.02	0.52
1:CA:1117:G:N2	1:CA:1180:A:O2'	2.42	0.52
25:BA:2331:G:H22	38:BS:3:ARG:CZ	2.23	0.52
13:AM:3:ARG:HG3	13:AM:8:GLU:HA	1.92	0.52
5:CE:12:LEU:HB3	5:CE:31:LEU:HB2	1.91	0.52
33:BN:73:THR:HG23	33:BN:82:LEU:HD11	1.91	0.52
8:CH:39:LEU:HD12	8:CH:44:PHE:HB2	1.91	0.52
47:D1:89:GLU:O	47:D1:93:GLU:HG2	2.10	0.52
1:AA:946:A:H2'	1:AA:947:G:C8	2.44	0.52
47:B1:3:LYS:HB2	47:B1:61:ARG:HH12	1.75	0.52
18:AR:26:LEU:HD23	18:AR:29:PHE:CE2	2.45	0.52
25:BA:1699:A:OP1	37:BR:8:ARG:NH1	2.36	0.52
25:DA:2143:C:H2'	25:DA:2144:U:O4'	2.10	0.52
23:CY:52:G:N1	23:CY:62:C:O2	2.33	0.52
1:CA:353:A:C8	1:CA:353:A:H5'	2.40	0.52
25:BA:2148:A:N6	25:BA:2184:G:O2'	2.43	0.52
38:BS:10:ARG:O	38:BS:14:VAL:HG13	2.09	0.52
31:DH:90:LYS:HD2	31:DH:163:TYR:CE1	2.45	0.52
1:CA:1222:G:OP1	19:CS:77:THR:HG21	2.10	0.52
6:CF:8:ILE:HD11	6:CF:79:LEU:HD13	1.91	0.52
25:BA:482:C:H4'	61:BA:4038:HOH:O	2.09	0.52
25:BA:2797:C:H1'	28:BE:37:ARG:NH1	2.25	0.52
1:AA:1499:A:H1'	1:AA:1520:G:H5'	1.90	0.52
1:AA:1251:A:H2'	1:AA:1252:A:C8	2.45	0.52
25:DA:492:A:H2'	25:DA:493:G:O4'	2.09	0.52
25:DA:1786:A:H1'	25:DA:1938:A:N6	2.24	0.52
25:DA:190:A:OP2	47:D1:39:LYS:HE3	2.09	0.52
23:CY:13:C:O2	23:CY:22:G:N1	2.33	0.52
26:BB:105:A:OP1	45:BZ:72:ARG:NH1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AH:51:VAL:HG12	8:AH:52:ASP:H	1.75	0.52
2:CB:87:ARG:NH2	2:CB:220:ASP:OD1	2.43	0.52
43:BX:54:VAL:HG22	43:BX:81:VAL:HG12	1.92	0.52
2:CB:122:PHE:HD1	2:CB:123:ALA:H	1.56	0.52
34:BO:2:ILE:HD12	34:BO:6:THR:HG21	1.92	0.52
45:DZ:117:LEU:HD23	45:DZ:119:GLU:HG2	1.92	0.52
1:AA:189(I):G:H2'	1:AA:189(J):G:H5''	1.92	0.52
25:BA:427:G:O6	61:BA:5098:HOH:O	2.16	0.52
4:CD:173:TRP:CD1	4:CD:189:PRO:HG3	2.45	0.52
25:BA:310:C:H2'	25:BA:311:C:C6	2.45	0.52
44:DY:23:ARG:HG2	44:DY:42:VAL:HG22	1.91	0.52
25:DA:1859:A:N6	25:DA:1883:G:O2'	2.42	0.52
25:DA:1939:U:OP1	25:DA:2604:U:O2'	2.27	0.52
25:DA:242:G:C8	54:D8:5:LYS:HG2	2.45	0.52
15:AO:26:GLU:OE2	15:AO:77:ARG:NE	2.31	0.52
45:BZ:55:HIS:CE1	45:BZ:135:GLU:HG3	2.45	0.52
25:DA:2820:A:O2'	25:DA:2821:A:OP1	2.27	0.52
1:CA:110:C:H2'	1:CA:111:G:O4'	2.10	0.52
25:BA:1804:A:OP2	61:BA:4855:HOH:O	2.19	0.52
1:CA:1120:G:C6	1:CA:1121:U:C4	2.98	0.51
43:BX:31:HIS:CD2	43:BX:33:LYS:HB2	2.45	0.51
25:BA:2339:A:H2'	25:BA:2340:A:C8	2.45	0.51
25:DA:812:C:H2'	25:DA:813:U:H6	1.74	0.51
29:DF:20:LEU:HD12	29:DF:125:LEU:HD13	1.92	0.51
1:CA:1512:U:H2'	1:CA:1513:A:C8	2.46	0.51
34:DO:80:ASP:OD1	39:DT:64:ARG:NH2	2.43	0.51
37:DR:36:THR:HG22	37:DR:37:THR:H	1.75	0.51
2:CB:71:VAL:HB	2:CB:164:VAL:HA	1.91	0.51
17:CQ:78:GLU:OE2	17:CQ:81:ARG:NH1	2.41	0.51
1:AA:309:G:O2'	1:AA:607:A:N1	2.42	0.51
25:DA:911:A:H2'	36:DQ:9:TYR:OH	2.10	0.51
25:DA:1386:C:H2'	25:DA:1387:C:C6	2.45	0.51
13:CM:3:ARG:N	50:D4:34:GLU:OE1	2.43	0.51
25:DA:1028:A:N6	25:DA:1125:G:H2'	2.24	0.51
51:D5:16:ARG:HG2	51:D5:16:ARG:HH11	1.74	0.51
1:CA:1312:G:H1	1:CA:1325:C:N4	2.07	0.51
25:DA:2683:C:O2	34:DO:70:LYS:NZ	2.39	0.51
2:CB:185:ILE:HG22	2:CB:199:TYR:CD2	2.45	0.51
27:BD:242:ARG:HD3	27:BD:242:ARG:N	2.25	0.51
16:CP:43:LYS:HA	16:CP:48:TRP:HB3	1.91	0.51
24:AX:59:A:C2'	24:AX:60:U:H5'	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:572:A:N6	41:BV:19:LYS:H	2.07	0.51
25:DA:1429:G:H2'	25:DA:1430:C:C6	2.45	0.51
25:DA:938:G:OP1	54:D8:52:LYS:HD2	2.10	0.51
13:AM:19:LEU:HD21	13:AM:56:LEU:HD11	1.91	0.51
25:DA:668:G:H5'	25:DA:669:G:OP2	2.11	0.51
1:AA:583:A:OP2	61:AA:4025:HOH:O	2.19	0.51
25:BA:595:A:OP2	41:BV:78:LYS:NZ	2.43	0.51
1:AA:250:A:H4'	1:AA:251:G:O5'	2.10	0.51
23:CW:4:C:N4	23:CW:69:G:C6	2.77	0.51
25:DA:330:A:H2	25:DA:1210:A:O2'	1.93	0.51
25:BA:1604:C:OP2	25:BA:1605:A:O2'	2.22	0.51
20:AT:54:LYS:HB2	20:AT:100:ILE:HD11	1.93	0.51
1:AA:28:G:O2'	1:AA:296:U:OP1	2.26	0.51
7:CG:50:ILE:HD11	7:CG:58:PRO:HA	1.93	0.51
25:BA:2623:U:C4	51:B5:3:LYS:HG2	2.44	0.51
2:AB:77:ALA:HB2	2:AB:165:VAL:HG11	1.92	0.51
7:CG:138:LYS:NZ	7:CG:142:GLU:OE1	2.42	0.51
7:AG:48:LYS:O	7:AG:52:GLU:HG2	2.11	0.51
6:CF:41:GLU:OE1	18:CR:35:ARG:NH2	2.42	0.51
28:BE:105:THR:OG1	28:BE:199:ARG:NH2	2.43	0.51
1:AA:1036:G:H3'	1:AA:1037:C:C6	2.45	0.51
45:DZ:97:GLU:HB2	45:DZ:125:LEU:HD11	1.92	0.51
9:AI:77:ILE:O	9:AI:81:ILE:HG22	2.10	0.51
23:AY:34:G:H2'	23:AY:35:A:C8	2.45	0.51
25:DA:1005:C:H2'	25:DA:1006:C:C6	2.44	0.51
1:CA:1014:A:C2	1:CA:1219:U:H1'	2.45	0.51
54:D8:63:PRO:HG2	54:D8:64:TYR:CD2	2.44	0.51
25:BA:1212:C:O2'	61:BA:4755:HOH:O	2.19	0.51
37:BR:21:TYR:OH	37:BR:43:GLU:HG2	2.10	0.51
25:BA:489:G:O6	61:BA:4635:HOH:O	2.18	0.51
42:DW:12:ILE:HD13	42:DW:17:VAL:HG13	1.93	0.51
1:CA:1053:G:N7	1:CA:1200:C:H5''	2.26	0.51
26:DB:14:U:OP2	26:DB:70:C:O2'	2.25	0.51
25:BA:1091:A:OP1	25:BA:1091:A:H4'	2.10	0.51
38:BS:15:ARG:O	38:BS:19:LYS:HG2	2.09	0.51
25:BA:2143:G:H1	25:BA:2199:C:N4	2.08	0.51
25:DA:2727:G:O2'	34:DO:70:LYS:NZ	2.42	0.51
1:CA:920:U:H2'	1:CA:921:U:H6	1.72	0.51
28:DE:72:VAL:HA	28:DE:73:GLU:CB	2.41	0.51
25:DA:637:A:H5''	35:DP:117:GLU:HG2	1.92	0.51
1:CA:142:G:H2'	1:CA:143:A:H8	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2797:C:H1'	28:BE:37:ARG:HH12	1.74	0.51
18:CR:24:ALA:O	18:CR:26:LEU:N	2.39	0.51
26:BB:2:C:H2'	26:BB:3:C:C6	2.45	0.51
9:AI:93:ARG:HB2	9:AI:93:ARG:HH11	1.75	0.51
8:CH:121:ASP:OD1	8:CH:121:ASP:N	2.41	0.51
25:DA:580:C:H2'	25:DA:581:C:H6	1.74	0.51
25:DA:1771:C:OP1	61:DA:4530:HOH:O	2.19	0.51
3:CC:121:ALA:O	3:CC:125:GLU:HG3	2.11	0.51
1:AA:49:U:O4	1:AA:365:U:H5	1.94	0.51
38:BS:15:ARG:NE	38:BS:88:ASP:OD2	2.37	0.51
1:CA:1132:C:H2'	1:CA:1133:G:C8	2.45	0.51
44:BY:92:ASN:N	44:BY:93:GLY:HA2	2.26	0.51
29:DF:24:LEU:HD21	29:DF:114:VAL:HG12	1.92	0.51
1:CA:1512:U:H2'	1:CA:1513:A:H8	1.76	0.51
31:DH:80:SER:OG	31:DH:81:GLU:OE1	2.26	0.51
29:DF:156:LEU:HD21	29:DF:163:VAL:HG12	1.92	0.51
25:DA:2640:G:N7	61:DA:4154:HOH:O	2.34	0.51
1:CA:56:U:H2'	1:CA:57:G:C8	2.45	0.51
25:DA:852:G:H2'	25:DA:853:G:C8	2.45	0.51
40:DU:66:ASN:O	40:DU:70:ARG:HG3	2.10	0.51
25:DA:2299:G:N1	25:DA:2318:G:N7	2.59	0.51
25:BA:1223:C:H2'	25:BA:1224:C:C6	2.45	0.51
14:AN:23:ARG:NH1	14:AN:30:ALA:HB2	2.25	0.51
9:CI:3:GLN:OE1	9:CI:20:ARG:NH2	2.43	0.51
35:DP:44:GLY:CA	35:DP:45:LEU:HB2	2.40	0.51
25:DA:625:G:O6	35:DP:107:LYS:NZ	2.35	0.51
15:AO:21:ASP:OD2	15:AO:24:SER:HB3	2.10	0.51
1:AA:757:U:H2'	1:AA:758:G:O4'	2.11	0.51
33:DN:19:GLU:HA	33:DN:59:LYS:HB2	1.93	0.51
3:CC:3:ASN:N	3:CC:3:ASN:OD1	2.41	0.51
6:AF:70:ASP:OD1	6:AF:70:ASP:N	2.36	0.51
28:BE:9:VAL:HB	39:BT:3:ARG:HG2	1.93	0.51
1:AA:581:G:OP1	15:AO:65:ARG:NH2	2.43	0.51
16:AP:71:ARG:HG3	16:AP:80:PHE:HE2	1.75	0.51
23:AW:18:G:N2	23:AW:57:G:H2'	2.25	0.51
23:AW:18:G:H4'	23:AW:60:U:C5	2.46	0.51
1:AA:1202:G:O4'	14:AN:29:ARG:NH1	2.43	0.51
25:DA:1530:C:H42	25:DA:1539:G:H1	1.58	0.51
1:CA:833:U:H2'	1:CA:834:C:C6	2.46	0.51
25:DA:362:U:O2'	25:DA:363:G:H5''	2.11	0.51
25:DA:1507:A:O2'	25:DA:1508:A:O5'	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:720:C:OP1	29:BF:54:ARG:NH1	2.42	0.51
25:DA:2630:G:H2'	25:DA:2631:G:C8	2.45	0.51
1:AA:381:C:H2'	1:AA:382:A:O4'	2.10	0.51
2:AB:21:ARG:HH21	2:AB:21:ARG:H	1.59	0.51
1:CA:426:G:OP1	4:CD:38:TYR:OH	2.21	0.51
54:B8:23:VAL:HG11	54:B8:47:LYS:HD3	1.93	0.51
19:AS:65:ASN:HD22	19:AS:65:ASN:N	2.07	0.51
1:AA:437:U:H5'	4:AD:155:LEU:HD21	1.93	0.51
2:CB:95:GLN:HB2	2:CB:148:TYR:HD1	1.76	0.51
25:DA:2193:G:H2'	25:DA:2194:G:C8	2.46	0.51
28:BE:11:MET:HG2	28:BE:24:THR:HB	1.93	0.51
47:B1:85:LEU:HB3	47:B1:89:GLU:HG3	1.93	0.51
25:BA:704:U:H2'	25:BA:705:C:H6	1.76	0.51
25:DA:608:A:H2'	25:DA:609:A:C8	2.45	0.51
1:AA:1318:A:H5''	19:AS:3:ARG:NH1	2.26	0.51
37:BR:57:ARG:NE	37:BR:59:ASP:OD1	2.44	0.51
28:BE:12:THR:HG22	28:BE:13:ARG:H	1.76	0.51
39:DT:16:ARG:NH2	39:DT:83:ILE:O	2.43	0.51
12:CL:28:LYS:N	12:CL:29:GLY:HA2	2.26	0.51
1:AA:1277:C:O2'	1:AA:1279:A:H1'	2.10	0.51
25:BA:2044:U:O2'	25:BA:2629:C:H5'	2.11	0.51
1:CA:1010:G:N2	1:CA:1020:U:H1'	2.25	0.51
32:BI:81:VAL:O	32:BI:146:ALA:HA	2.10	0.51
31:DH:20:ALA:HB1	31:DH:21:PRO:HD2	1.92	0.51
30:DG:5:VAL:HG22	30:DG:8:LYS:H	1.76	0.51
45:DZ:52:SER:OG	45:DZ:53:ILE:N	2.43	0.51
1:CA:748:C:H4'	1:CA:749:C:O5'	2.11	0.51
6:AF:37:VAL:HA	6:AF:65:VAL:HG12	1.92	0.51
25:BA:865:G:O6	61:BA:4412:HOH:O	2.19	0.51
25:BA:771:U:H2'	25:BA:772:G:O4'	2.11	0.51
2:CB:134:GLU:O	2:CB:138:LEU:HG	2.10	0.51
1:AA:1001:A:H2'	1:AA:1001(A):G:H8	1.76	0.50
2:CB:15:VAL:HG13	2:CB:209:ARG:HB3	1.93	0.50
1:CA:953:G:H5'	1:CA:965:A:N6	2.23	0.50
1:CA:986:A:H2'	1:CA:987:G:C8	2.47	0.50
27:DD:17:THR:O	27:DD:211:ARG:NH2	2.41	0.50
1:AA:92:C:H2'	1:AA:93:G:C8	2.46	0.50
27:BD:85:ASP:OD2	27:BD:88:ARG:NH1	2.39	0.50
25:DA:2183:C:H2'	25:DA:2184:G:C8	2.46	0.50
6:AF:33:TYR:CD2	6:AF:75:LEU:HD23	2.46	0.50
25:DA:2819:G:N7	61:DA:4376:HOH:O	2.34	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AM:11:ARG:HA	13:AM:45:VAL:HB	1.92	0.50
12:AL:117:ARG:HB3	12:AL:122:THR:HB	1.93	0.50
25:BA:407:U:OP1	61:BA:4339:HOH:O	2.19	0.50
11:AK:84:VAL:HG11	11:AK:91:ARG:HD2	1.93	0.50
1:AA:174:C:H2'	1:AA:175:C:H6	1.77	0.50
25:DA:1025:G:C4	25:DA:1135:C:H1'	2.46	0.50
2:CB:47:THR:O	2:CB:51:LEU:N	2.44	0.50
15:CO:87:ILE:HG22	15:CO:88:ARG:N	2.23	0.50
23:CW:4:C:N4	23:CW:69:G:H1	2.10	0.50
57:AA:3231:PCY:H40	23:AY:35:A:C2	2.45	0.50
17:AQ:67:LYS:HA	17:AQ:70:ARG:HH12	1.76	0.50
3:AC:164:ARG:HG2	3:AC:165:THR:H	1.76	0.50
25:DA:2846:G:H2'	25:DA:2847:U:O4'	2.11	0.50
30:BG:75:LYS:HA	30:BG:84:LYS:HE2	1.92	0.50
26:BB:82:G:N7	61:BB:3110:HOH:O	2.34	0.50
31:DH:56:SER:OG	31:DH:57:ASP:N	2.43	0.50
25:BA:1040:C:OP1	40:BU:53:ARG:NH2	2.44	0.50
30:BG:16:ARG:HH21	30:BG:31:VAL:HG11	1.75	0.50
37:DR:29:LEU:HB3	37:DR:75:LEU:HD11	1.93	0.50
40:BU:76:TYR:CZ	40:BU:80:ILE:HG13	2.46	0.50
25:BA:801:C:H2'	25:BA:802:C:C6	2.46	0.50
1:CA:1035:A:H2'	1:CA:1036:G:H8	1.77	0.50
1:CA:78:G:C2'	1:CA:79:G:H5"	2.37	0.50
3:CC:54:ARG:HH12	3:CC:56:ASP:CG	2.14	0.50
23:CW:8:4SU:O2'	23:CW:21:A:N6	2.41	0.50
25:BA:1269:G:N2	25:BA:1272:A:OP2	2.36	0.50
2:AB:231:GLU:HB3	2:AB:232:PRO:HD3	1.93	0.50
45:BZ:52:SER:OG	45:BZ:53:ILE:N	2.45	0.50
52:D6:34:LEU:HB2	52:D6:51:GLU:HB2	1.92	0.50
25:BA:1002:A:H5'	36:BQ:76:LYS:HG3	1.92	0.50
25:DA:531:C:H4'	25:DA:532:A:H5"	1.94	0.50
25:DA:1448:G:H4'	25:DA:1542:A:OP1	2.10	0.50
25:BA:510:C:H2'	25:BA:511:C:C6	2.47	0.50
23:AY:6:G:O6	23:AY:7:A:N6	2.45	0.50
9:AI:50:LEU:HD23	9:AI:81:ILE:HD11	1.94	0.50
2:CB:80:ILE:HD11	2:CB:212:GLN:HA	1.93	0.50
23:CY:2:C:H2'	23:CY:3:C:C6	2.46	0.50
25:DA:443:A:H1'	25:DA:1201:C:O4'	2.10	0.50
25:DA:76:C:O3'	48:D2:59:ARG:HG3	2.11	0.50
1:CA:1179:A:H4'	9:CI:103:THR:HA	1.93	0.50
9:CI:9:ARG:O	9:CI:104:ARG:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:CI:9:ARG:H	9:CI:79:LEU:HD23	1.77	0.50
25:BA:2148:A:N6	25:BA:2184:G:HO2'	2.09	0.50
25:DA:2334:G:H5'	38:DS:9:ARG:HG2	1.93	0.50
25:BA:385:G:N1	25:BA:386:U:O4	2.44	0.50
30:DG:23:PHE:HB2	30:DG:25:TYR:CZ	2.47	0.50
1:AA:1254:C:H41	10:AJ:43:ARG:HH12	1.58	0.50
25:BA:721:G:O2'	29:BF:74:ARG:HD3	2.10	0.50
25:DA:2830:G:OP1	28:DE:76:ARG:NH2	2.45	0.50
8:AH:121:ASP:OD2	8:AH:121:ASP:N	2.43	0.50
6:CF:70:ASP:OD1	6:CF:70:ASP:N	2.27	0.50
25:DA:1946:U:H2'	25:DA:1947:C:C6	2.45	0.50
13:AM:88:ARG:HG3	13:AM:98:VAL:CG1	2.42	0.50
4:AD:127:THR:HA	4:AD:132:ARG:HA	1.93	0.50
31:DH:144:VAL:O	31:DH:148:ILE:HG12	2.12	0.50
17:CQ:95:TYR:HA	17:CQ:98:LEU:HD22	1.94	0.50
25:BA:1744:G:OP2	25:BA:1745:A:O2'	2.13	0.50
1:AA:93:G:H2'	1:AA:96:U:O4'	2.12	0.50
20:AT:34:LYS:HZ2	20:AT:80:ARG:HH12	1.59	0.50
1:CA:9:G:H2'	1:CA:10:A:H8	1.77	0.50
2:CB:224:GLN:HG2	2:CB:225:ALA:N	2.27	0.50
28:DE:111:ARG:HG3	28:DE:160:TYR:CD2	2.46	0.50
30:DG:48:GLU:O	30:DG:51:ARG:HG3	2.12	0.50
25:BA:470:C:H5''	61:BA:4091:HOH:O	2.10	0.50
25:BA:2132:G:C2	25:BA:2142:G:H1'	2.47	0.50
25:DA:2655:G:O2'	25:DA:2664:G:O6	2.28	0.50
1:CA:297:G:N2	1:CA:300:A:OP2	2.45	0.50
8:CH:82:HIS:N	8:CH:138:TRP:O	2.42	0.50
41:BV:40:LEU:HB2	41:BV:46:VAL:HG13	1.93	0.50
5:AE:50:GLU:HB2	5:AE:53:LEU:HD13	1.94	0.50
35:DP:81:GLN:NE2	35:DP:105:LEU:O	2.44	0.50
23:AY:5:G:H1'	23:AY:69:G:N2	2.25	0.50
1:AA:1027:C:N3	1:AA:1034:G:C6	2.80	0.50
1:AA:1027:C:O2	1:AA:1034:G:C2	2.65	0.50
1:CA:1399:C:H4'	1:CA:1400:C:O5'	2.12	0.50
23:CY:26:A:N1	23:CY:44:G:C6	2.79	0.50
23:AW:56:C:P	25:BA:943:C:H5'	2.52	0.50
1:AA:96:U:O2'	1:AA:97:G:H5'	2.11	0.50
1:CA:909:A:N3	1:CA:1413:A:O2'	2.32	0.50
1:AA:69:G:H2'	1:AA:70:G:H8	1.76	0.50
1:AA:1318:A:H5''	19:AS:3:ARG:HH12	1.77	0.50
39:DT:85:LYS:NZ	39:DT:87:ASP:OD2	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2389:A:H2'	25:BA:2390:A:C8	2.47	0.50
1:AA:833:U:H2'	1:AA:834:C:C6	2.47	0.50
1:AA:8:A:H5'	5:AE:101:ILE:HG22	1.93	0.50
11:AK:45:GLY:O	11:AK:50:TYR:HB2	2.11	0.50
25:BA:2235:G:OP1	27:BD:172:TYR:OH	2.24	0.50
25:BA:2885:C:O2'	39:BT:2:ASN:OD1	2.26	0.50
26:DB:9:G:H1	26:DB:112:U:H3	1.58	0.50
1:CA:1310:G:H5'	13:CM:77:ASN:ND2	2.26	0.50
25:BA:555:G:O4'	25:BA:555:G:N3	2.43	0.50
1:CA:1346:A:N1	1:CA:1374:A:H5''	2.27	0.50
25:BA:1298:G:OP1	40:BU:36:ARG:NH2	2.45	0.50
2:AB:109:SER:HA	2:AB:112:VAL:HG13	1.94	0.50
44:BY:55:TYR:CD2	44:BY:55:TYR:N	2.80	0.50
1:CA:222:U:H2'	1:CA:223:U:C6	2.46	0.50
25:BA:2155:G:H21	25:BA:2180:A:H62	1.58	0.50
33:BN:62:VAL:HG22	33:BN:66:LYS:HD2	1.92	0.50
1:AA:21:G:OP1	61:AA:4120:HOH:O	2.19	0.50
25:DA:1009:A:H5'	40:DU:59:ARG:HG2	1.92	0.50
1:CA:1004:A:H5''	1:CA:1025:U:C5	2.47	0.50
1:CA:349:A:C2'	1:CA:350:G:H5''	2.38	0.50
45:DZ:111:VAL:HG13	45:DZ:117:LEU:H	1.77	0.50
5:CE:140:ARG:O	5:CE:143:ARG:NH2	2.45	0.50
1:AA:97:G:HO2'	1:AA:98:G:H8	1.60	0.50
6:CF:45:LEU:HD12	6:CF:59:TYR:CD2	2.46	0.50
23:CY:8:4SU:S4	23:CY:14:A:N7	2.85	0.50
35:BP:59:LEU:HD22	54:B8:13:ARG:HD2	1.94	0.50
25:BA:489:G:OP2	61:BA:5265:HOH:O	2.20	0.50
1:CA:1347:G:N2	1:CA:1373:G:H2'	2.27	0.50
4:CD:149:ALA:HB3	4:CD:152:SER:HB2	1.94	0.50
10:AJ:11:PHE:HE1	10:AJ:67:THR:HG22	1.76	0.50
25:DA:274:G:H2'	25:DA:275:G:C8	2.46	0.50
40:BU:86:ALA:O	41:BV:49:THR:HG23	2.12	0.50
9:CI:121:ARG:NH1	9:CI:122:ALA:O	2.44	0.50
25:BA:2116:G:P	32:BI:22:LYS:HD2	2.52	0.50
3:CC:78:GLY:HA3	3:CC:83:ARG:H	1.77	0.50
1:CA:1123:A:O3'	10:CJ:36:GLY:HA3	2.12	0.49
20:CT:77:ALA:O	20:CT:81:LYS:HG3	2.11	0.49
25:DA:2502:G:H5''	25:DA:2503:A:H5''	1.94	0.49
1:CA:947:G:H1	1:CA:1234:C:N4	2.09	0.49
25:DA:1155:A:H3'	61:DA:4617:HOH:O	2.11	0.49
1:CA:811:C:O2'	1:CA:901:A:N1	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:587:C:OP2	35:DP:21:ARG:NH2	2.45	0.49
1:AA:1068:G:OP2	1:AA:1068:G:H8	1.95	0.49
38:BS:34:HIS:ND1	38:BS:53:SER:OG	2.35	0.49
25:DA:2313:C:H4'	30:DG:91:ARG:HG3	1.94	0.49
42:DW:71:VAL:HA	42:DW:107:LEU:HD12	1.94	0.49
32:BI:66:GLU:HA	32:BI:69:LYS:HB3	1.94	0.49
25:BA:2495:C:N3	36:BQ:124:LYS:NZ	2.58	0.49
1:AA:1122:U:H2'	1:AA:1123:A:O4'	2.12	0.49
25:DA:2124:G:N2	25:DA:2174:C:N3	2.58	0.49
28:DE:174:ASP:OD1	28:DE:175:VAL:N	2.45	0.49
25:DA:2741:A:H2'	25:DA:2742:C:O4'	2.12	0.49
50:B4:56:VAL:O	50:B4:60:GLN:HG3	2.12	0.49
15:CO:15:PHE:CE2	15:CO:84:LYS:HD3	2.47	0.49
1:CA:1035:A:H2'	1:CA:1036:G:C8	2.47	0.49
25:DA:2148:G:H2'	25:DA:2149:G:C8	2.47	0.49
24:CX:76:A:H3'	25:DA:2585:U:C5	2.47	0.49
1:AA:922:G:C6	1:AA:923:A:C6	3.00	0.49
25:DA:1639:U:H4'	25:DA:2699:C:H4'	1.93	0.49
7:CG:111:ARG:NH2	7:CG:126:ASP:OD2	2.45	0.49
1:AA:174:C:H2'	1:AA:175:C:C6	2.47	0.49
2:AB:231:GLU:HB3	2:AB:232:PRO:CD	2.42	0.49
38:DS:93:LYS:CD	38:DS:95:HIS:HB2	2.42	0.49
31:BH:154:PRO:HB3	31:BH:163:TYR:CZ	2.47	0.49
1:AA:590:C:O2	1:AA:649:G:N2	2.30	0.49
36:DQ:108:GLY:HA3	45:DZ:116:VAL:HG13	1.93	0.49
30:BG:131:TYR:HB3	30:BG:159:VAL:HG13	1.93	0.49
1:AA:524:G:H2'	1:AA:525:C:C6	2.47	0.49
25:BA:1517:G:H5''	25:BA:1518:A:OP1	2.12	0.49
1:CA:973:G:H3'	1:CA:974:A:H5''	1.94	0.49
25:BA:484:G:O2'	25:BA:495:G:O6	2.29	0.49
1:CA:532:A:H2	1:CA:1206:G:H21	1.60	0.49
25:BA:1155:C:H5'	25:BA:1156:G:OP2	2.11	0.49
23:CW:25:C:H2'	23:CW:26:A:H8	1.76	0.49
25:DA:921:G:H4'	25:DA:2269:A:C5	2.47	0.49
32:BI:106:GLY:HA2	32:BI:107:VAL:O	2.12	0.49
1:AA:1060:C:C5	3:AC:2:GLY:HA3	2.48	0.49
1:CA:1104:G:H4'	2:CB:111:ARG:NH1	2.26	0.49
30:DG:108:ASN:HB3	50:D4:22:ILE:HD13	1.95	0.49
38:DS:78:LEU:HD11	38:DS:108:GLY:O	2.12	0.49
3:AC:87:LEU:O	3:AC:91:LEU:N	2.36	0.49
25:BA:1067:A:H3'	25:BA:1067:A:H8	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:185:A:H5'	20:CT:74:LYS:HE2	1.94	0.49
1:CA:1178:G:N2	1:CA:1180:A:H3'	2.28	0.49
31:BH:164:TYR:N	31:BH:167:GLU:OE1	2.42	0.49
2:CB:185:ILE:HG22	2:CB:199:TYR:HD2	1.77	0.49
31:DH:4:ILE:HG22	31:DH:69:ARG:HG2	1.94	0.49
32:BI:77:LEU:HB3	32:BI:142:VAL:HG12	1.94	0.49
23:AW:4:C:H2'	23:AW:5:G:C8	2.46	0.49
25:DA:2537:U:H2'	25:DA:2538:C:C6	2.47	0.49
25:BA:2357:G:H4'	25:BA:2358:A:H5''	1.94	0.49
25:BA:2710:U:H2'	25:BA:2711:C:C6	2.47	0.49
25:DA:276:A:H5''	25:DA:277:C:H5'	1.94	0.49
28:BE:170:LEU:HB3	28:BE:184:VAL:HG22	1.93	0.49
25:DA:657:U:H2'	25:DA:658:C:C6	2.46	0.49
5:CE:38:GLN:HE21	5:CE:38:GLN:N	2.10	0.49
32:DI:130:TYR:HD2	32:DI:138:ILE:HD12	1.78	0.49
25:DA:1589:C:H2'	25:DA:1590:U:H6	1.77	0.49
25:DA:2529:G:H5''	25:DA:2530:A:H5''	1.94	0.49
2:AB:17:PHE:HB2	2:AB:44:LEU:HD21	1.94	0.49
1:AA:1399:C:C2	1:AA:1502:A:N6	2.81	0.49
25:DA:2125:G:H1	25:DA:2172:U:P	2.35	0.49
1:CA:184:G:H2'	1:CA:185:A:H8	1.77	0.49
1:CA:787:A:C2	57:CA:3178:PCY:H111	2.48	0.49
29:DF:165:ARG:HG2	29:DF:168:ARG:NH2	2.28	0.49
19:AS:3:ARG:HE	19:AS:7:LYS:HB2	1.78	0.49
25:DA:839:U:H2'	25:DA:840:C:C6	2.46	0.49
53:B7:12:ARG:NH2	53:B7:44:PRO:HB3	2.27	0.49
25:BA:739:C:O2'	27:BD:38:LYS:NZ	2.46	0.49
25:BA:2626:A:OP1	61:BA:4516:HOH:O	2.19	0.49
1:CA:193:C:H2'	1:CA:194:C:C6	2.47	0.49
18:CR:53:ARG:HH21	18:CR:59:SER:HA	1.77	0.49
39:DT:19:LEU:HD22	39:DT:86:ILE:HG13	1.93	0.49
32:BI:129:THR:HG22	32:BI:139:GLN:HE22	1.76	0.49
25:BA:125:A:H5''	25:BA:126:C:C6	2.48	0.49
2:AB:59:GLU:HB2	2:AB:221:LEU:HG	1.94	0.49
48:B2:16:LEU:O	48:B2:67:LYS:NZ	2.46	0.49
47:D1:24:ALA:HA	47:D1:32:LYS:HD2	1.95	0.49
12:CL:70:ILE:HD13	12:CL:77:LEU:HD12	1.94	0.49
1:AA:1025:U:O2	1:AA:1036:G:C6	2.62	0.49
1:AA:1034:G:H2'	1:AA:1035:A:H8	1.72	0.49
1:CA:1030:C:N4	1:CA:1032:G:O6	2.45	0.49
24:CX:47:U:N3	24:CX:50:U:OP1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:CA:3178:PCY:O36	57:CA:3178:PCY:O21	2.29	0.49
5:AE:85:GLY:C	5:AE:87:SER:H	2.13	0.49
25:DA:1006:C:C2	25:DA:1138:G:N2	2.81	0.49
25:DA:271(O):C:H2'	25:DA:271(P):C:C6	2.48	0.49
4:CD:111:ALA:HB1	4:CD:116:GLN:HB3	1.94	0.49
1:CA:1305:G:H5'	21:CU:4:GLY:HA3	1.94	0.49
8:CH:64:LYS:HD2	8:CH:79:VAL:HG11	1.94	0.49
45:DZ:52:SER:OG	45:DZ:54:HIS:ND1	2.42	0.49
45:DZ:53:ILE:HD13	45:DZ:99:TYR:HB2	1.94	0.49
25:BA:801:C:H2'	25:BA:802:C:H6	1.78	0.49
44:BY:35:TYR:CE2	44:BY:69:ALA:HB3	2.47	0.49
29:BF:89:VAL:HG12	29:BF:90:PHE:CD2	2.48	0.49
25:BA:1553:A:O2'	25:BA:1554:A:O4'	2.30	0.49
27:BD:107:ALA:O	61:BD:416:HOH:O	2.20	0.49
4:AD:175:SER:HB3	4:AD:186:LEU:HD11	1.93	0.49
25:BA:1589:A:O2'	61:BA:5331:HOH:O	2.20	0.49
21:CU:13:ILE:HG12	21:CU:22:ARG:NH2	2.28	0.49
25:DA:184:C:H2'	25:DA:185:U:C6	2.47	0.49
1:CA:1016:A:H2'	1:CA:1017:G:O4'	2.12	0.49
25:BA:779:C:OP1	61:BA:4829:HOH:O	2.19	0.49
25:BA:630:U:OP1	29:BF:102:PRO:HA	2.12	0.49
1:CA:153:C:H2'	1:CA:154:C:C6	2.47	0.49
1:CA:1149:C:H2'	1:CA:1150:U:C6	2.48	0.49
25:DA:298:G:H5''	25:DA:299:A:OP1	2.13	0.49
31:DH:3:ARG:HD3	31:DH:54:ARG:HH12	1.76	0.49
1:CA:1305:G:O2'	1:CA:1331:G:N2	2.45	0.49
1:AA:1066:C:O2'	1:AA:1067:A:H5'	2.13	0.49
39:BT:11:GLU:OE1	39:BT:57:PHE:HB3	2.13	0.49
25:DA:576:U:OP1	61:DA:4464:HOH:O	2.19	0.49
1:AA:131:C:H2'	1:AA:132:C:C6	2.48	0.49
27:BD:12:SER:HB3	27:BD:208:LYS:HB3	1.94	0.49
25:BA:2348:A:H61	46:B0:43:THR:HG22	1.78	0.49
52:B6:6:ARG:NH1	52:B6:26:ASN:HB2	2.27	0.49
27:BD:2:ALA:HA	27:BD:200:ASP:OD2	2.12	0.49
1:CA:519:C:OP2	12:CL:50:SER:OG	2.31	0.49
1:CA:1028:C:C2	1:CA:1033:G:C6	3.00	0.49
2:CB:48:MET:HA	2:CB:51:LEU:HB2	1.95	0.49
25:DA:2137:C:H2'	25:DA:2138:C:C6	2.47	0.49
26:DB:75:G:HO2'	45:DZ:85:HIS:CE1	2.27	0.49
25:DA:2650:U:H2'	25:DA:2651:C:C6	2.47	0.49
24:AX:8:4SU:H6	24:AX:8:4SU:O5'	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:BF:53:THR:CG2	29:BF:55:GLY:H	2.25	0.49
36:DQ:37:LEU:HD11	36:DQ:130:LYS:HB2	1.94	0.49
3:AC:11:ARG:HB3	3:AC:15:THR:HB	1.94	0.49
37:DR:2:ARG:NH1	37:DR:5:LYS:O	2.46	0.49
17:AQ:62:SER:HB3	17:AQ:72:ARG:HD2	1.94	0.49
25:BA:2856:G:H2'	25:BA:2857:U:O4'	2.13	0.49
35:DP:95:VAL:HG13	35:DP:125:VAL:HG12	1.94	0.49
25:BA:860:U:H2'	25:BA:861:C:C6	2.48	0.49
25:BA:709:G:H5''	35:BP:16:ARG:HG2	1.93	0.49
28:BE:59:VAL:HG21	28:BE:74:PRO:HB3	1.93	0.49
25:BA:1424:A:OP1	53:B7:10:ARG:NH2	2.46	0.49
25:DA:2784:C:H1'	28:DE:37:ARG:HH12	1.77	0.49
26:DB:13:A:O2'	26:DB:14:U:H3'	2.12	0.49
2:CB:17:PHE:HB2	2:CB:44:LEU:HD11	1.95	0.49
1:CA:946:A:H2'	1:CA:947:G:C8	2.48	0.49
50:B4:63:TYR:CD1	50:B4:63:TYR:N	2.78	0.49
25:DA:71:A:N7	43:DX:31:HIS:HE1	2.11	0.49
25:DA:146:G:O6	61:DA:4857:HOH:O	2.17	0.49
25:DA:2647:U:H2'	25:DA:2648:C:C6	2.48	0.49
38:DS:15:ARG:O	38:DS:19:LYS:HG2	2.12	0.49
25:BA:2784:C:H2'	25:BA:2785:C:C6	2.48	0.49
10:CJ:42:THR:HG23	10:CJ:68:HIS:HA	1.94	0.49
1:CA:1106:G:H5''	3:CC:172:ARG:HG2	1.94	0.49
19:CS:49:ILE:HD13	19:CS:62:ILE:HD13	1.95	0.49
1:CA:1009:G:H22	1:CA:1021:G:H1'	1.75	0.49
25:BA:2880:C:H2'	25:BA:2881:C:O4'	2.13	0.49
25:BA:2245:U:H2'	25:BA:2246:G:C8	2.47	0.49
25:DA:2078:C:C4	25:DA:2079:U:C4	3.01	0.49
25:BA:956:A:N1	25:BA:2289:G:H1'	2.28	0.49
2:CB:52:GLU:HG2	2:CB:56:ARG:HH22	1.78	0.49
45:DZ:126:VAL:CG1	45:DZ:161:VAL:HG23	2.40	0.49
1:CA:1000:U:H3	1:CA:1041:A:N6	2.05	0.49
25:DA:2156:G:H2'	25:DA:2157:G:C2	2.48	0.49
11:CK:45:GLY:O	11:CK:50:TYR:HB2	2.12	0.49
25:BA:354:A:H2	25:BA:1255:A:HO2'	1.61	0.49
5:AE:140:ARG:O	5:AE:143:ARG:NH2	2.46	0.49
17:AQ:45:HIS:NE2	17:AQ:47:PRO:HG3	2.28	0.49
25:DA:861:A:N3	26:DB:79:C:O2'	2.41	0.49
25:DA:2116:G:H5'	25:DA:2117:A:OP2	2.13	0.49
44:BY:86:ARG:HH11	44:BY:100:ALA:HB1	1.78	0.49
44:DY:5:MET:HE1	44:DY:32:PRO:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:DG:68:PRO:HB3	30:DG:92:VAL:HB	1.95	0.49
25:DA:1168:G:H2'	25:DA:1169:G:C8	2.48	0.49
29:BF:51:THR:O	29:BF:93:LYS:HE2	2.13	0.49
1:AA:1244:C:OP1	21:AU:9:ARG:HB2	2.13	0.49
26:DB:24:G:H4'	26:DB:25:A:C8	2.47	0.49
2:AB:128:GLU:HB2	2:AB:135:GLN:NE2	2.28	0.49
1:CA:662:G:H2'	1:CA:663:A:C8	2.48	0.49
1:CA:202:U:O2'	1:CA:203:U:O5'	2.26	0.49
23:AY:48:C:C2	23:AY:59:U:H1'	2.48	0.48
1:AA:972:C:OP2	10:AJ:57:LYS:NZ	2.42	0.48
25:DA:1430:C:H2'	25:DA:1431:U:H6	1.76	0.48
29:BF:185:ASP:HA	29:BF:188:ARG:HD3	1.95	0.48
25:DA:2820:A:O5'	37:DR:4:LEU:HD23	2.13	0.48
25:DA:1507:A:O2'	25:DA:1508:A:O4'	2.31	0.48
28:BE:31:CYS:HB3	28:BE:49:LEU:HG	1.95	0.48
1:CA:434:U:H2'	1:CA:435:C:C6	2.47	0.48
25:BA:1815:A:OP2	61:BA:4831:HOH:O	2.20	0.48
2:AB:32:ILE:HD13	2:AB:40:HIS:CD2	2.48	0.48
25:DA:897:C:H3'	25:DA:898:C:C6	2.46	0.48
34:BO:87:ILE:HD12	34:BO:91:LEU:HA	1.94	0.48
1:CA:189(F):U:O2	17:CQ:63:ARG:NH2	2.46	0.48
25:DA:2756:U:H1'	25:DA:2757:A:H5''	1.95	0.48
30:DG:72:ARG:NH1	30:DG:87:PRO:HG3	2.28	0.48
25:DA:947:G:H2'	25:DA:948:G:C8	2.48	0.48
25:BA:625:G:O2'	25:BA:702:A:N6	2.46	0.48
1:AA:346:G:H3'	1:AA:347:G:H4'	1.94	0.48
45:DZ:110:GLY:O	45:DZ:174:VAL:HG11	2.13	0.48
9:CI:77:ILE:O	9:CI:81:ILE:HG22	2.13	0.48
25:DA:1231:G:H2'	25:DA:1232:G:H8	1.78	0.48
1:CA:1316:G:N1	1:CA:1319:A:OP2	2.46	0.48
25:DA:1335:U:OP1	43:DX:65:ARG:NH2	2.46	0.48
25:DA:307:G:H21	25:DA:330:A:H62	1.61	0.48
25:BA:2073:A:H5'	25:BA:2590:G:O4'	2.13	0.48
1:CA:194:C:O3'	20:CT:68:LYS:HD2	2.13	0.48
25:DA:2365:G:O6	54:D8:39:LYS:HE3	2.12	0.48
25:BA:2203:G:O2'	25:BA:2204:G:OP1	2.26	0.48
25:DA:819:A:OP2	25:DA:1187:G:N2	2.31	0.48
25:BA:1733:C:H2'	25:BA:1734:G:O4'	2.13	0.48
19:CS:20:LEU:HD23	19:CS:23:ASN:HD22	1.77	0.48
5:CE:78:HIS:HA	8:CH:105:ARG:HG3	1.96	0.48
1:CA:26:A:N6	1:CA:558:G:O2'	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:D8:31:HIS:ND1	54:D8:32:LEU:HD13	2.28	0.48
25:DA:1641:A:H2'	25:DA:1642:G:O4'	2.13	0.48
1:AA:1236:A:H4'	1:AA:1304:G:H4'	1.94	0.48
23:CW:34:G:H2'	23:CW:35:A:C8	2.47	0.48
1:CA:1004:A:H2'	1:CA:1038:C:H1'	1.95	0.48
1:AA:347:G:H3'	1:AA:348:G:H5''	1.96	0.48
23:CW:76:A:H4'	25:DA:2506:U:O2'	2.12	0.48
25:BA:933:C:H4'	25:BA:933:C:OP1	2.13	0.48
14:AN:6:LEU:HB3	14:AN:23:ARG:NH2	2.28	0.48
28:DE:11:MET:HG2	28:DE:24:THR:HB	1.96	0.48
25:DA:443:A:N7	29:DF:45:ARG:HG2	2.28	0.48
10:AJ:11:PHE:HB3	14:AN:55:GLY:HA3	1.95	0.48
28:DE:9:VAL:HG22	28:DE:25:VAL:HB	1.95	0.48
1:AA:473:G:H2'	1:AA:474:G:H8	1.78	0.48
1:AA:1298:C:H4'	1:AA:1299:A:O4'	2.13	0.48
35:BP:121:LYS:HB3	35:BP:123:LEU:HG	1.95	0.48
28:DE:119:ARG:HB3	28:DE:120:TRP:CD1	2.48	0.48
1:CA:1457:G:H5''	20:CT:35:THR:HG21	1.95	0.48
25:DA:2128:C:H1'	25:DA:2173:A:O2'	2.12	0.48
1:CA:1228:C:H2'	1:CA:1229:A:H8	1.78	0.48
42:BW:79:GLY:HA3	42:BW:100:THR:HG22	1.94	0.48
27:BD:39:LYS:NZ	27:BD:57:GLY:O	2.44	0.48
42:BW:71:VAL:HA	42:BW:107:LEU:HD12	1.96	0.48
25:DA:1778:U:H2'	25:DA:1784:A:N6	2.27	0.48
1:CA:337:C:H2'	1:CA:338:A:C8	2.48	0.48
1:CA:1002:G:C5	1:CA:1003:G:C8	3.02	0.48
32:BI:116:LEU:HD21	32:BI:119:PRO:HA	1.96	0.48
1:CA:1126:U:H3	10:CJ:40:LEU:HD11	1.78	0.48
19:CS:28:LYS:HB2	19:CS:29:ARG:CA	2.42	0.48
1:CA:1317:C:OP2	14:CN:17:LYS:HE3	2.13	0.48
25:DA:323:G:O2'	25:DA:1205:U:N3	2.23	0.48
30:BG:7:LEU:HD11	30:BG:107:LEU:HD12	1.96	0.48
6:CF:2:ARG:NE	6:CF:69:GLU:HG2	2.28	0.48
25:BA:63:A:H1'	43:BX:66:LEU:HB2	1.94	0.48
25:BA:2486:C:H5''	25:BA:2487:C:OP2	2.13	0.48
1:AA:447:G:H2'	1:AA:485:G:N2	2.28	0.48
25:BA:2033:U:OP1	42:BW:42:ARG:NH1	2.43	0.48
8:AH:82:HIS:N	8:AH:138:TRP:O	2.47	0.48
23:AW:62:C:H2'	23:AW:63:G:H8	1.79	0.48
5:CE:24:ARG:NH1	22:CV:24:A:OP2	2.46	0.48
1:AA:620:C:H2'	1:AA:621:A:O4'	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1002:G:C4	1:CA:1003:G:C8	2.99	0.48
25:DA:143:G:C2	25:DA:143(A):C:C2	3.02	0.48
1:CA:986:A:H1'	19:CS:55:LYS:HA	1.95	0.48
23:AY:33:U:H3'	23:AY:34:G:H5''	1.95	0.48
1:CA:1316:G:H22	1:CA:1319:A:H5''	1.79	0.48
1:CA:601:C:H2'	1:CA:602:A:C8	2.49	0.48
9:CI:23:ASN:HB2	9:CI:25:LYS:HE3	1.94	0.48
25:BA:2482:G:OP1	36:BQ:56:ARG:NH2	2.47	0.48
30:DG:179:PRO:HB2	50:D4:42:PHE:HE1	1.78	0.48
25:BA:390:G:H2'	25:BA:391:G:C8	2.49	0.48
15:AO:5:LYS:HD2	15:AO:5:LYS:H	1.78	0.48
42:BW:25:ARG:NH2	42:BW:74:ALA:O	2.28	0.48
1:AA:1029:C:N3	1:AA:1032:G:O6	2.46	0.48
25:BA:1093:G:H2'	25:BA:1156:G:H22	1.77	0.48
1:CA:73:G:C6	1:CA:97:G:C6	3.02	0.48
25:DA:2042:A:OP1	61:DA:4181:HOH:O	2.20	0.48
25:DA:1354:A:H2'	25:DA:1355:G:O4'	2.13	0.48
25:DA:1358:G:O2'	25:DA:1359:A:H5''	2.14	0.48
7:CG:113:GLU:CG	7:CG:119:ARG:HG2	2.44	0.48
1:CA:1008:C:H2'	1:CA:1009:G:O4'	2.13	0.48
1:CA:522:C:OP2	12:CL:69:TYR:OH	2.25	0.48
42:BW:48:ALA:O	42:BW:52:GLU:HB2	2.13	0.48
1:CA:174:C:H2'	1:CA:175:C:H6	1.79	0.48
1:AA:486:U:H2'	1:AA:487:A:H8	1.77	0.48
13:AM:79:LYS:HA	13:AM:82:MET:HE2	1.95	0.48
25:DA:1991:U:H2'	25:DA:1992:G:H5''	1.95	0.48
11:CK:15:ALA:HA	11:CK:76:GLY:O	2.13	0.48
1:AA:628:G:H2'	1:AA:629:G:C8	2.49	0.48
1:CA:1103:C:OP1	2:CB:96:ARG:NH2	2.47	0.48
25:DA:997:G:OP1	40:DU:92:ARG:HG2	2.12	0.48
25:BA:2802:C:O2'	25:BA:2803:A:H4'	2.14	0.48
1:CA:1064:G:O6	1:CA:1191:A:N6	2.46	0.48
25:BA:185:A:H2'	25:BA:185:A:N3	2.29	0.48
1:CA:1129:C:H1'	1:CA:1130:A:N7	2.28	0.48
25:DA:322:A:H5'	25:DA:340:A:H1'	1.95	0.48
25:BA:671:A:H2'	25:BA:672:G:O4'	2.13	0.48
25:DA:1204:A:H61	25:DA:1240:U:H2'	1.79	0.48
1:CA:171:A:H2'	1:CA:172:A:C8	2.49	0.48
43:BX:60:ARG:HA	43:BX:75:ASP:OD2	2.14	0.48
26:BB:7:G:H5''	26:BB:7:G:H8	1.78	0.48
1:CA:1051:C:H2'	1:CA:1052:U:H6	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:CX:59:A:H2'	24:CX:60:U:H5'	1.95	0.48
25:BA:2760:G:O6	25:BA:2768:C:H5''	2.13	0.48
7:AG:153:HIS:HA	7:AG:155:ARG:NH2	2.29	0.48
25:BA:1845:G:H4'	27:BD:51:VAL:HG21	1.96	0.48
33:DN:82:LEU:HD23	33:DN:84:LYS:HE2	1.96	0.48
39:DT:11:GLU:O	39:DT:15:VAL:HG23	2.14	0.48
3:AC:18:TRP:HE3	3:AC:18:TRP:H	1.60	0.48
25:BA:821:A:H2'	25:BA:821:A:N3	2.29	0.48
25:DA:2059:A:O2'	29:DF:69:HIS:HD2	1.97	0.48
1:AA:1292:U:OP2	7:AG:41:ARG:NH2	2.47	0.48
1:AA:738:C:H2'	1:AA:739:C:H6	1.78	0.48
50:B4:53:GLU:HG3	50:B4:55:ARG:N	2.29	0.48
4:CD:150:GLU:HA	4:CD:153:ARG:HE	1.79	0.48
29:BF:164:ARG:O	29:BF:168:ARG:HB2	2.14	0.48
3:AC:181:ASN:HD22	3:AC:204:LEU:HB2	1.77	0.48
35:BP:59:LEU:HD21	54:B8:10:ALA:HA	1.95	0.48
9:CI:24:GLY:HA2	9:CI:59:PHE:O	2.14	0.48
45:BZ:65:GLN:HB3	45:BZ:67:LEU:HD21	1.95	0.48
25:BA:2627:U:H2'	25:BA:2628:C:H6	1.79	0.48
36:BQ:135:ASP:N	36:BQ:138:ASP:OD2	2.34	0.48
7:CG:132:GLY:O	7:CG:136:LYS:HG2	2.14	0.48
1:AA:1062:U:H2'	1:AA:1063:C:C6	2.49	0.48
2:CB:16:HIS:HB2	2:CB:204:ASN:CB	2.43	0.48
1:CA:1060:C:H5'	10:CJ:51:ARG:HB3	1.96	0.48
1:CA:976:G:C8	1:CA:1358:U:C2	3.02	0.48
29:DF:164:ARG:O	29:DF:168:ARG:HB2	2.14	0.48
25:DA:322:A:OP1	29:DF:168:ARG:HD2	2.13	0.48
23:CY:38:A:H2'	23:CY:39:PSU:O4'	2.13	0.48
42:BW:14:PRO:HG2	42:BW:78:GLU:CG	2.43	0.48
25:DA:2334:G:O6	46:D0:74:ARG:NH2	2.46	0.48
45:BZ:111:VAL:C	45:BZ:113:ALA:H	2.17	0.48
7:AG:111:ARG:HB3	7:AG:113:GLU:OE2	2.14	0.48
31:DH:90:LYS:HD2	31:DH:163:TYR:CD1	2.49	0.48
28:DE:24:THR:HG23	28:DE:184:VAL:HG12	1.96	0.48
1:AA:486:U:H2'	1:AA:487:A:C8	2.49	0.48
44:BY:99:CYS:HB2	44:BY:106:LEU:HD21	1.95	0.48
19:AS:51:VAL:O	19:AS:58:VAL:N	2.43	0.48
18:CR:33:ASP:OD2	18:CR:36:ASN:HB2	2.14	0.48
1:AA:1053:G:H4'	1:AA:1054:C:H5'	1.94	0.48
25:BA:2327:G:H2'	25:BA:2328:C:C6	2.49	0.48
1:CA:757:U:H2'	1:CA:758:G:O4'	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AJ:6:ILE:HA	10:AJ:97:GLU:O	2.14	0.48
25:DA:2029:G:H2'	25:DA:2031:A:OP1	2.14	0.48
50:B4:24:THR:OG1	50:B4:25:TYR:N	2.45	0.48
3:CC:164:ARG:HG2	3:CC:165:THR:H	1.79	0.48
25:DA:910:A:C5	36:DQ:13:GLN:HG3	2.48	0.48
4:CD:173:TRP:CZ3	4:CD:193:ASP:HB3	2.49	0.48
32:DI:57:ARG:HA	32:DI:61:ARG:NH2	2.28	0.48
1:CA:299:G:H2'	1:CA:300:A:C8	2.49	0.48
41:DV:29:PRO:HG3	41:DV:63:GLY:HA2	1.95	0.48
1:CA:12:U:H4'	1:CA:526:C:O2'	2.13	0.48
31:BH:4:ILE:O	31:BH:69:ARG:HG2	2.14	0.48
29:BF:33:LEU:HD22	29:BF:112:MET:HE3	1.96	0.48
13:AM:23:TYR:HB3	13:AM:67:GLU:HA	1.95	0.48
1:CA:275:G:H5'	17:CQ:14:LYS:HB3	1.96	0.48
25:DA:534:U:H2'	25:DA:535:C:C6	2.49	0.48
2:AB:60:ASP:O	2:AB:64:ARG:HB2	2.14	0.48
1:CA:1388:C:H2'	1:CA:1389:C:C6	2.49	0.48
3:CC:39:ILE:HG23	3:CC:91:LEU:HD11	1.96	0.48
7:AG:72:ARG:HG2	7:AG:72:ARG:H	1.42	0.48
2:AB:95:GLN:HG3	2:AB:147:LYS:HD3	1.96	0.48
1:CA:779:C:H2'	1:CA:780:A:O4'	2.13	0.48
1:AA:1399:C:H4'	1:AA:1400:C:O5'	2.14	0.47
1:CA:96:U:O2'	1:CA:97:G:H5'	2.14	0.47
1:CA:921:U:O2	5:CE:19:MET:HB2	2.13	0.47
31:BH:3:ARG:CG	31:BH:6:ARG:HG2	2.44	0.47
25:DA:1257:C:H4'	29:DF:83:PHE:CD2	2.49	0.47
1:AA:1118:C:H1'	1:AA:1179:A:C4	2.49	0.47
1:AA:56:U:H2'	1:AA:57:G:C8	2.49	0.47
10:AJ:8:LEU:HD22	10:AJ:96:ILE:HG12	1.95	0.47
1:CA:1176:A:H2'	1:CA:1177:G:O4'	2.14	0.47
3:AC:36:ASP:O	3:AC:40:ARG:HG3	2.14	0.47
25:DA:623:G:H2'	25:DA:624:C:C6	2.49	0.47
25:BA:1938:A:H2'	25:BA:1939:U:O4'	2.13	0.47
1:CA:376:G:H4'	16:CP:5:ARG:HD3	1.96	0.47
1:CA:1286:A:C8	1:CA:1287:A:H4'	2.49	0.47
2:AB:115:LEU:O	2:AB:119:GLU:HG2	2.14	0.47
5:AE:38:GLN:HB2	5:AE:38:GLN:HE21	1.55	0.47
26:DB:41:U:H5	30:DG:70:VAL:H	1.60	0.47
38:DS:105:ALA:O	38:DS:110:LEU:HB2	2.14	0.47
19:CS:80:TYR:CZ	19:CS:82:GLY:HA2	2.49	0.47
23:CW:9:A:O2'	23:CW:10:G:N7	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:646:U:H2'	1:CA:647:C:H6	1.78	0.47
25:DA:2331:G:O2'	46:D0:43:THR:HG22	2.14	0.47
31:BH:90:LYS:HD3	31:BH:159:GLU:HG2	1.96	0.47
1:CA:865:A:H5'	1:CA:1078:U:C5	2.49	0.47
25:BA:659:C:H2'	25:BA:660:C:C6	2.48	0.47
25:DA:1263:U:C4	25:DA:1264:G:C6	3.02	0.47
1:CA:1239:A:H62	1:CA:1299:A:H62	1.62	0.47
1:AA:1057:G:OP2	61:AA:4034:HOH:O	2.20	0.47
25:DA:851:U:O2'	49:D3:42:ALA:O	2.32	0.47
13:CM:50:GLU:HA	13:CM:53:VAL:HB	1.96	0.47
25:DA:315:G:H2'	25:DA:316:C:C6	2.49	0.47
25:DA:2127:G:N2	25:DA:2161:C:N3	2.63	0.47
25:BA:185:A:H62	35:BP:38:GLN:HE22	1.62	0.47
23:CW:46:7MG:O2'	23:CW:47:U:O5'	2.29	0.47
25:BA:1513:G:H2'	25:BA:1594:C:H41	1.80	0.47
25:DA:2651:C:C2'	25:DA:2652:C:H5'	2.45	0.47
25:DA:2651:C:H2'	25:DA:2652:C:H5'	1.97	0.47
25:BA:346:A:OP2	29:BF:169:ASN:HB2	2.14	0.47
29:BF:18:ARG:NH2	29:BF:127:GLU:OE1	2.46	0.47
45:DZ:53:ILE:HG22	45:DZ:71:VAL:O	2.14	0.47
13:AM:11:ARG:C	13:AM:13:LYS:H	2.17	0.47
1:CA:9:G:H2'	1:CA:10:A:C8	2.49	0.47
28:BE:101:ARG:CZ	28:BE:171:GLU:HB2	2.44	0.47
13:CM:122:LYS:CD	13:CM:123:ALA:H	2.27	0.47
30:BG:126:ASP:OD2	30:BG:130:ASN:ND2	2.38	0.47
3:CC:32:LEU:H	3:CC:32:LEU:HD22	1.79	0.47
12:CL:33:ARG:HD3	12:CL:62:SER:HB3	1.96	0.47
25:BA:1882:U:H2'	25:BA:1883:C:O4'	2.14	0.47
25:DA:1685:C:H2'	25:DA:1686:C:C6	2.49	0.47
45:DZ:156:LYS:HG2	45:DZ:158:PRO:HD3	1.97	0.47
33:DN:123:TYR:HH	33:DN:130:HIS:CD2	2.28	0.47
25:BA:2163:G:H1	25:BA:2171:G:N2	2.12	0.47
1:AA:342:C:C2	1:AA:348:G:N2	2.82	0.47
25:BA:2138:G:N1	25:BA:2184:G:OP1	2.31	0.47
25:DA:2684:U:O2'	34:DO:68:GLU:OE1	2.32	0.47
9:CI:85:LEU:HB3	9:CI:92:TYR:HD2	1.78	0.47
23:CW:23:A:H2'	23:CW:24:G:H8	1.80	0.47
4:AD:166:LYS:HB2	4:AD:168:ARG:NH2	2.30	0.47
25:DA:852:G:H2'	25:DA:853:G:H8	1.77	0.47
25:DA:1011:G:OP2	40:DU:70:ARG:NH2	2.48	0.47
15:AO:16:ALA:HB1	15:AO:21:ASP:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2139:A:O2'	25:BA:2140:U:H5''	2.14	0.47
1:AA:833:U:H2'	1:AA:834:C:H6	1.79	0.47
44:BY:86:ARG:NH1	44:BY:100:ALA:HB1	2.29	0.47
25:DA:1503:U:H2'	25:DA:1504:C:C6	2.50	0.47
1:AA:642:A:N3	8:AH:113:SER:OG	2.46	0.47
31:DH:18:GLU:HG2	31:DH:19:VAL:N	2.29	0.47
1:CA:1084:G:H5'	1:CA:1102:A:OP2	2.13	0.47
25:DA:2849:U:H4'	25:DA:2868:A:C2	2.49	0.47
25:DA:2532:G:H1'	25:DA:2663:G:N2	2.29	0.47
32:DI:40:THR:O	32:DI:44:LEU:HB2	2.14	0.47
49:B3:23:LEU:HD13	49:B3:50:VAL:HG11	1.96	0.47
13:AM:96:LEU:O	13:AM:110:ARG:NH1	2.32	0.47
31:DH:126:PRO:HG2	31:DH:130:ARG:HD2	1.96	0.47
25:DA:2886:G:N7	61:DA:4437:HOH:O	2.35	0.47
6:AF:69:GLU:O	6:AF:72:VAL:HG12	2.14	0.47
25:BA:2658:C:H2'	25:BA:2659:U:O4'	2.14	0.47
25:BA:211:A:H3'	25:BA:448:U:H5'	1.96	0.47
1:CA:1399:C:C2	1:CA:1502:A:N6	2.83	0.47
38:BS:11:LYS:O	38:BS:15:ARG:HG3	2.14	0.47
1:AA:625:G:H2'	1:AA:626:U:C6	2.50	0.47
9:CI:23:ASN:ND2	9:CI:23:ASN:H	2.12	0.47
25:DA:2336:A:H61	46:D0:43:THR:HG22	1.79	0.47
31:BH:90:LYS:HD2	31:BH:163:TYR:CD1	2.49	0.47
25:BA:211:A:H5''	25:BA:448:U:OP1	2.14	0.47
1:AA:1370:G:O6	61:AA:4100:HOH:O	2.20	0.47
1:CA:250:A:H4'	1:CA:251:G:O5'	2.13	0.47
1:CA:232:G:H1'	1:CA:262:A:N1	2.29	0.47
5:CE:84:PHE:N	5:CE:87:SER:O	2.48	0.47
25:DA:2461:C:H2'	25:DA:2462:U:C6	2.50	0.47
19:CS:51:VAL:O	19:CS:58:VAL:N	2.40	0.47
30:BG:43:LEU:HD11	30:BG:153:ARG:HG2	1.95	0.47
25:DA:194:G:H2'	25:DA:195:A:O4'	2.14	0.47
25:BA:1153:G:H2'	25:BA:1153:G:N3	2.29	0.47
25:DA:2320:A:N3	25:DA:2320:A:H2'	2.28	0.47
25:DA:2704:C:H2'	25:DA:2705:A:O4'	2.15	0.47
1:AA:184:G:H2'	1:AA:185:A:C8	2.50	0.47
12:AL:7:ILE:O	12:AL:11:VAL:HG23	2.14	0.47
1:AA:1004:A:H5''	1:AA:1025:U:H5	1.79	0.47
1:AA:1029:C:N4	1:AA:1030:C:H41	2.13	0.47
1:CA:1391:U:H2'	1:CA:1392:G:C8	2.50	0.47
1:CA:1392:G:N2	1:CA:1502:A:H8	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:2299:G:H2'	25:DA:2300:G:C8	2.47	0.47
19:CS:27:GLU:HB2	19:CS:28:LYS:NZ	2.28	0.47
45:BZ:126:VAL:CG1	45:BZ:161:VAL:HG23	2.43	0.47
25:DA:2748:A:H5'	31:DH:4:ILE:HD12	1.96	0.47
1:AA:6:G:H4'	1:AA:298:A:H4'	1.97	0.47
25:BA:274:U:H3'	25:BA:275:C:C5'	2.44	0.47
39:BT:112:ARG:HG3	39:BT:115:ARG:HH21	1.78	0.47
1:AA:438:G:H4'	4:AD:123:HIS:HD1	1.79	0.47
1:CA:109:A:C6	1:CA:326:G:C6	3.03	0.47
25:DA:1386:C:H2'	25:DA:1387:C:H6	1.79	0.47
25:DA:1667:G:O2'	25:DA:1991:U:O4	2.26	0.47
4:AD:162:LEU:CD1	4:AD:181:MET:HG2	2.45	0.47
47:D1:54:ALA:HB1	47:D1:83:GLU:HG3	1.96	0.47
33:DN:67:LEU:HB3	33:DN:88:GLU:HG3	1.97	0.47
1:CA:1378:C:H5	1:CA:1379:G:H1'	1.79	0.47
27:BD:26:LYS:HE2	27:BD:28:GLU:O	2.14	0.47
43:DX:54:VAL:HG22	43:DX:81:VAL:HG12	1.95	0.47
1:AA:695:A:H2'	1:AA:696:A:C8	2.49	0.47
45:BZ:105:VAL:O	45:BZ:140:ASP:HA	2.14	0.47
1:AA:501:C:H2'	1:AA:502:G:C8	2.50	0.47
4:AD:79:PHE:HE1	4:AD:204:ILE:HD13	1.80	0.47
25:BA:2175:G:H2'	25:BA:2175:G:N3	2.29	0.47
50:B4:44:THR:O	50:B4:46:GLN:N	2.47	0.47
29:DF:12:LEU:HB2	29:DF:124:LEU:HD11	1.96	0.47
25:BA:2096:U:H2'	25:BA:2097:U:C6	2.49	0.47
25:BA:898:U:O2'	49:B3:42:ALA:O	2.30	0.47
40:BU:66:ASN:O	40:BU:70:ARG:HG3	2.15	0.47
2:CB:17:PHE:HB2	2:CB:44:LEU:HD21	1.96	0.47
2:CB:207:ALA:HB3	2:CB:210:SER:HB3	1.95	0.47
2:CB:48:MET:O	2:CB:52:GLU:N	2.48	0.47
24:CX:47:U:H5'	24:CX:48:C:H5'	1.97	0.47
1:CA:1132:C:N4	1:CA:1142:G:H1	2.12	0.47
25:BA:670:C:H5'	25:BA:671:A:OP2	2.15	0.47
1:CA:408:A:H4'	4:CD:112:VAL:HG21	1.97	0.47
25:DA:2635:C:H5''	28:DE:78:LEU:O	2.15	0.47
23:AW:7:A:N6	23:AW:66:U:H3	2.10	0.47
1:CA:235:C:H5'	17:CQ:70:ARG:HG2	1.95	0.47
25:BA:1993:A:OP2	27:BD:242:ARG:NH2	2.48	0.47
25:DA:1297:C:OP1	25:DA:2710:C:H4'	2.14	0.47
25:BA:2021:C:H5''	25:BA:2736:C:O2'	2.15	0.47
2:CB:87:ARG:HD3	2:CB:234:PRO:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:BR:118:GLU:H	37:BR:118:GLU:CD	2.18	0.47
1:AA:164:U:H2'	1:AA:165:C:C6	2.50	0.47
3:CC:19:GLU:HB3	3:CC:40:ARG:NH2	2.29	0.47
1:AA:193:C:H2'	1:AA:194:C:C6	2.49	0.47
25:BA:1814:A:N7	61:BA:5150:HOH:O	2.35	0.47
9:AI:26:VAL:HG13	9:AI:61:ALA:HB3	1.96	0.47
39:DT:117:ASP:OD2	39:DT:120:ARG:NE	2.39	0.47
31:DH:46:GLU:HB2	31:DH:49:VAL:HG13	1.97	0.47
10:AJ:76:ASN:HA	10:AJ:77:PRO:HD2	1.68	0.47
25:BA:1756:U:H2'	25:BA:1757:C:C6	2.50	0.47
38:DS:80:LEU:HA	38:DS:80:LEU:HD12	1.76	0.47
12:CL:34:ARG:HG3	12:CL:105:TYR:CE2	2.50	0.47
25:DA:116:C:H2'	25:DA:117:G:O4'	2.15	0.47
1:CA:886:G:O6	61:CA:4005:HOH:O	2.18	0.47
31:DH:11:VAL:HG13	31:DH:15:VAL:HG13	1.96	0.47
41:DV:60:GLU:HB3	41:DV:95:LEU:HB3	1.97	0.47
52:B6:10:LEU:HG	52:B6:54:ILE:HG13	1.97	0.47
1:CA:538:G:H5''	12:CL:114:LYS:HB2	1.96	0.47
25:BA:1640:G:H2'	25:BA:1641:G:O4'	2.14	0.47
1:AA:841:U:C5	1:AA:848:C:H1'	2.49	0.47
39:BT:33:LYS:O	39:BT:82:LEU:HD23	2.15	0.47
28:DE:5:LEU:HD11	28:DE:79:ARG:HB2	1.96	0.47
41:DV:16:PRO:HD3	41:DV:99:ILE:HD11	1.95	0.47
36:DQ:77:LYS:NZ	36:DQ:86:GLY:O	2.46	0.47
1:CA:1187:G:P	9:CI:113:LYS:HZ1	2.38	0.47
45:BZ:145:GLU:H	45:BZ:148:ASP:HB2	1.79	0.47
2:CB:19:HIS:ND1	2:CB:20:GLU:HG2	2.29	0.47
7:CG:103:TRP:CH2	7:CG:141:VAL:HG21	2.50	0.47
25:DA:1926:U:O2'	25:DA:1928:A:N7	2.37	0.47
31:BH:20:ALA:HB1	31:BH:21:PRO:HD2	1.96	0.47
25:BA:2641:A:H1'	25:BA:2642:G:H5''	1.95	0.47
25:DA:2316:C:H1'	30:DG:128:ARG:HH21	1.79	0.47
25:BA:2745:G:OP1	28:BE:203:LYS:NZ	2.43	0.47
23:AY:54:5MU:O2	23:AY:58:A:N7	2.48	0.47
25:DA:2114:A:H8	25:DA:2168:G:HO2'	1.63	0.47
1:CA:741:G:H2'	1:CA:742:G:O4'	2.15	0.47
45:DZ:45:ASP:OD2	45:DZ:49:ARG:HD2	2.15	0.47
25:DA:1019:U:H2'	25:DA:1020:A:H8	1.79	0.47
1:CA:1245:A:N6	1:CA:1292:U:H3	2.13	0.47
25:DA:889:C:O2'	25:DA:890:A:O5'	2.29	0.47
20:AT:77:ALA:O	20:AT:81:LYS:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:997:U:H3	1:CA:1044:A:H61	1.62	0.47
8:CH:51:VAL:HG12	8:CH:52:ASP:H	1.80	0.47
8:CH:51:VAL:HG11	8:CH:60:ARG:HH12	1.79	0.47
1:CA:1054:C:C5	23:CW:34:G:H1'	2.49	0.47
7:AG:152:ALA:O	7:AG:155:ARG:HB3	2.15	0.47
25:DA:2080:G:H2'	25:DA:2081:C:C6	2.49	0.47
1:AA:920:U:H2'	1:AA:921:U:C6	2.49	0.47
32:DI:4:ILE:HG12	32:DI:18:VAL:HG22	1.97	0.47
1:CA:955:U:O2'	19:CS:83:HIS:HD2	1.98	0.47
25:DA:271(D):G:H2'	25:DA:271(E):U:C6	2.50	0.47
26:BB:75:G:H5''	26:BB:75:G:H8	1.79	0.47
19:AS:27:GLU:CD	19:AS:27:GLU:H	2.18	0.47
25:BA:2141:A:C2	25:BA:2192:A:H2'	2.50	0.47
23:AY:2:C:N4	23:AY:71:G:N1	2.39	0.47
23:AW:51:U:H2'	23:AW:52:G:H8	1.75	0.47
1:CA:685:G:C2	1:CA:686:U:C4	3.03	0.47
23:CW:39:PSU:H2'	23:CW:40:C:C6	2.50	0.47
39:BT:118:ARG:HD2	39:BT:118:ARG:HA	1.66	0.47
25:DA:493:G:H2'	25:DA:494:G:O4'	2.14	0.47
25:DA:1786:A:OP1	25:DA:1980:G:N2	2.39	0.47
25:DA:2124:G:H1	25:DA:2174:C:H42	1.59	0.47
25:DA:271(E):U:H2'	25:DA:271(F):C:C6	2.50	0.47
25:BA:2398:C:O2'	61:BA:5405:HOH:O	2.20	0.47
25:BA:1537:G:O2'	27:BD:101:GLU:HB2	2.15	0.47
1:CA:1262:C:H2'	1:CA:1263:C:C6	2.49	0.47
34:BO:107:ARG:CZ	39:BT:36:GLU:HG2	2.45	0.47
7:CG:114:ARG:HB2	7:CG:115:ARG:HH21	1.80	0.47
2:AB:61:LEU:HD23	2:AB:68:ILE:HD11	1.97	0.47
25:DA:2390:U:OP2	54:D8:35:GLN:NE2	2.32	0.47
25:BA:2230:U:O2	47:B1:52:ARG:NH2	2.48	0.47
25:DA:1471:A:H3'	25:DA:1472:A:H8	1.79	0.47
15:CO:48:LYS:HD3	15:CO:48:LYS:HA	1.69	0.47
25:BA:1694:G:OP1	61:BA:5334:HOH:O	2.20	0.47
18:AR:38:GLU:HA	18:AR:41:LYS:HD2	1.97	0.47
34:BO:68:GLU:HB3	34:BO:78:ARG:HB2	1.96	0.47
1:AA:1028:C:H2'	1:AA:1029:C:H4'	1.97	0.47
1:CA:750:G:H1'	15:CO:22:THR:OG1	2.15	0.47
25:DA:2572:A:C8	28:DE:144:ARG:HD2	2.50	0.47
25:DA:2584:U:H2'	25:DA:2585:U:H2'	1.97	0.47
13:CM:65:LYS:HA	50:D4:50:VAL:HG11	1.97	0.47
1:AA:748:C:H4'	1:AA:749:C:O5'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CB:187:LEU:HA	2:CB:201:ILE:HB	1.97	0.47
6:AF:75:LEU:O	6:AF:79:LEU:HG	2.15	0.47
25:DA:2631:G:N2	25:DA:2787:C:O2	2.38	0.47
13:AM:11:ARG:O	13:AM:13:LYS:N	2.46	0.47
1:CA:1226:C:O2'	13:CM:111:LYS:NZ	2.49	0.47
25:BA:905:U:O2	25:BA:2280:A:H2'	2.15	0.47
39:BT:127:ALA:O	39:BT:128:GLU:HB2	2.15	0.47
2:AB:145:LEU:O	2:AB:149:LEU:HB2	2.14	0.47
25:DA:286:C:H2'	25:DA:287:C:C6	2.50	0.47
25:BA:2527:C:O2'	25:BA:2528:G:H5'	2.15	0.47
26:DB:78:A:C2	26:DB:100:A:C4	3.03	0.47
1:CA:784:C:H4'	25:DA:1837:C:OP1	2.15	0.47
3:CC:70:VAL:O	3:CC:106:VAL:N	2.48	0.47
7:CG:26:PHE:CE1	7:CG:30:ILE:HD11	2.50	0.47
25:DA:2271:G:C5	25:DA:2272:U:C5	3.03	0.46
25:DA:221:A:C8	25:DA:266:G:C6	3.03	0.46
26:DB:80:U:H2'	26:DB:81:G:C8	2.49	0.46
1:AA:473:G:H2'	1:AA:474:G:C8	2.50	0.46
1:CA:1227:A:P	13:CM:111:LYS:HZ1	2.38	0.46
29:BF:129:PHE:CD2	29:BF:163:VAL:HG21	2.50	0.46
32:BI:60:GLU:HG3	32:BI:61:ARG:HD2	1.97	0.46
35:DP:68:GLN:HG3	54:D8:12:LYS:HG2	1.97	0.46
31:BH:33:LEU:HD21	31:BH:136:ILE:HG13	1.97	0.46
24:AX:13:C:O2'	25:BA:1946:C:H4'	2.15	0.46
25:DA:478:A:N1	25:DA:500:G:H4'	2.30	0.46
11:CK:99:GLN:HG2	11:CK:105:VAL:HG21	1.96	0.46
14:CN:47:LEU:O	14:CN:51:GLY:N	2.48	0.46
25:DA:963:U:OP1	61:DA:4058:HOH:O	2.21	0.46
25:BA:2720:G:H1'	37:BR:71:GLN:NE2	2.26	0.46
1:CA:1039:C:C4	1:CA:1040:U:C4	3.03	0.46
1:CA:1133:G:C4	1:CA:1134:G:C8	3.04	0.46
1:CA:1118:C:H2'	1:CA:1119:C:C6	2.42	0.46
25:DA:900:A:O2'	25:DA:901:A:OP1	2.33	0.46
25:DA:392:C:H5''	25:DA:409:C:H5''	1.97	0.46
4:AD:133:VAL:HG12	4:AD:135:LEU:H	1.79	0.46
25:BA:1475:G:H2'	25:BA:1476:C:H6	1.79	0.46
9:CI:23:ASN:ND2	9:CI:25:LYS:HG2	2.30	0.46
43:DX:9:LEU:HA	48:D2:36:ARG:HH21	1.80	0.46
2:AB:32:ILE:HG21	2:AB:40:HIS:HD2	1.79	0.46
25:DA:223:A:O2'	25:DA:420:C:O2	2.29	0.46
25:DA:1015:G:H2'	25:DA:1016:G:H8	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:662:G:H2'	1:AA:663:A:C8	2.49	0.46
16:AP:19:ILE:HG22	16:AP:37:GLY:C	2.36	0.46
3:CC:113:ALA:HB2	3:CC:202:ILE:HG13	1.97	0.46
25:DA:300:A:P	44:DY:86:ARG:HH22	2.38	0.46
25:BA:1891:G:H2'	25:BA:1892:G:O4'	2.15	0.46
1:AA:1356:G:H2'	1:AA:1357:A:C8	2.49	0.46
25:DA:955:C:OP1	36:DQ:87:LYS:HE3	2.16	0.46
25:BA:2834:C:H5	61:BA:4097:HOH:O	1.98	0.46
25:BA:2561:G:O6	61:BA:4141:HOH:O	2.20	0.46
23:AY:19:G:H1	23:AY:56:C:N4	2.09	0.46
1:AA:376:G:P	16:AP:67:THR:HG21	2.56	0.46
25:DA:1151:G:H4'	40:DU:81:HIS:CG	2.51	0.46
53:B7:30:VAL:O	53:B7:34:ARG:HG3	2.15	0.46
32:BI:96:ASP:OD1	32:BI:96:ASP:N	2.47	0.46
26:DB:12:C:O2'	46:D0:74:ARG:HG2	2.15	0.46
1:AA:76:C:O2	1:AA:93:G:N1	2.32	0.46
24:AX:8:4SU:O2	24:AX:21:A:H2	1.98	0.46
7:CG:79:ARG:HB3	7:CG:79:ARG:CZ	2.45	0.46
13:AM:57:ARG:CZ	50:B4:34:GLU:HB3	2.45	0.46
47:B1:86:SER:OG	47:B1:89:GLU:OE1	2.24	0.46
1:CA:735:C:H2'	1:CA:736:C:C6	2.50	0.46
25:DA:144:C:H2'	25:DA:145:G:H8	1.80	0.46
7:CG:48:LYS:O	7:CG:52:GLU:HG2	2.16	0.46
44:DY:20:TYR:CE1	44:DY:43:ASN:HA	2.50	0.46
2:AB:62:ALA:HB3	2:AB:225:ALA:HB3	1.97	0.46
45:DZ:3:TYR:O	45:DZ:57:ILE:HA	2.16	0.46
1:AA:236:G:H5''	17:AQ:42:TYR:OH	2.15	0.46
40:BU:104:GLN:H	40:BU:104:GLN:CD	2.18	0.46
25:DA:1857:G:C6	25:DA:1858:G:C6	3.03	0.46
25:BA:733:G:C4	53:B7:11:LYS:HG2	2.50	0.46
8:AH:39:LEU:HB3	8:AH:45:ILE:HG12	1.96	0.46
1:CA:1057:G:H2'	1:CA:1058:G:O4'	2.16	0.46
25:DA:1803:A:H4'	27:DD:259:THR:HG23	1.98	0.46
23:CW:75:C:H2'	23:CW:76:A:C4	2.50	0.46
25:BA:2331:G:N2	38:BS:3:ARG:HA	2.31	0.46
2:CB:54:THR:HG21	2:CB:201:ILE:HD11	1.97	0.46
19:AS:3:ARG:HH21	19:AS:7:LYS:HB3	1.79	0.46
23:AY:3:C:H42	23:AY:70:G:H1	1.64	0.46
1:CA:1226:C:H4'	19:CS:80:TYR:OH	2.14	0.46
1:CA:918:A:H2'	1:CA:919:A:O4'	2.16	0.46
19:CS:51:VAL:HB	19:CS:75:ALA:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:477:A:H2'	25:DA:478:A:C8	2.51	0.46
8:CH:91:ARG:NH1	17:CQ:33:GLY:HA3	2.30	0.46
9:CI:46:ALA:HB2	9:CI:74:ILE:HG23	1.97	0.46
25:BA:305:G:O2'	25:BA:383:A:N6	2.45	0.46
48:D2:16:LEU:O	48:D2:67:LYS:NZ	2.49	0.46
25:BA:2541:G:H5''	25:BA:2542:A:H5''	1.98	0.46
25:BA:876:A:N7	25:BA:2260:C:H5'	2.31	0.46
41:BV:52:VAL:HG22	41:BV:55:ALA:HB3	1.98	0.46
23:CW:29:G:H2'	23:CW:30:G:C8	2.51	0.46
25:BA:1221:G:H21	25:BA:1222:A:H4'	1.80	0.46
25:DA:1434:A:H61	25:DA:1558:A:N6	2.14	0.46
2:CB:201:ILE:O	2:CB:203:GLY:N	2.48	0.46
47:D1:83:GLU:HA	47:D1:84:GLY:HA2	1.64	0.46
1:CA:1187:G:OP1	9:CI:113:LYS:NZ	2.49	0.46
25:BA:2660:C:H2'	25:BA:2661:U:C6	2.50	0.46
25:DA:521:G:H2'	25:DA:522:G:H8	1.80	0.46
35:DP:47:ASP:OD2	35:DP:50:ARG:HD3	2.16	0.46
17:CQ:9:VAL:HG13	17:CQ:56:VAL:HG22	1.97	0.46
23:CY:71:G:H4'	25:DA:1851:U:H4'	1.97	0.46
2:CB:35:GLU:OE2	2:CB:38:GLY:HA2	2.16	0.46
25:BA:2504:U:H2'	25:BA:2505:U:C6	2.51	0.46
1:AA:870:U:H4'	1:AA:871:U:H5''	1.97	0.46
25:BA:1496:A:H5'	25:BA:1497:G:OP2	2.15	0.46
25:BA:864:C:H4'	25:BA:977:G:C5	2.51	0.46
1:CA:1202:G:O4'	14:CN:29:ARG:NH1	2.49	0.46
26:DB:33:G:C2	26:DB:50:G:C2	3.04	0.46
5:AE:121:LYS:HG3	5:AE:123:LEU:HG	1.98	0.46
25:BA:2285:A:H2'	25:BA:2286:A:C8	2.49	0.46
1:CA:407:G:OP1	4:CD:115:ARG:HD2	2.16	0.46
1:CA:1243:C:H42	1:CA:1294:G:H1	1.63	0.46
12:AL:84:LEU:HB2	12:AL:105:TYR:CE2	2.50	0.46
29:DF:187:VAL:HG11	35:DP:6:LEU:HD11	1.97	0.46
27:DD:108:PRO:HB3	27:DD:143:HIS:CE1	2.50	0.46
2:AB:16:HIS:CG	2:AB:17:PHE:H	2.30	0.46
25:DA:740:U:H2'	25:DA:741:G:C8	2.51	0.46
1:CA:1006:C:OP1	1:CA:1037:C:O2'	2.33	0.46
25:BA:1093:G:HO2'	25:BA:1094:A:H8	1.64	0.46
24:CX:64:G:H4'	36:DQ:10:ARG:NH1	2.27	0.46
23:CY:51:U:O4	23:CY:63:G:O6	2.33	0.46
25:BA:2209:G:H2'	25:BA:2210:C:O4'	2.15	0.46
3:CC:11:ARG:HB3	3:CC:15:THR:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:CC:8:ILE:HD13	3:CC:184:TYR:HB3	1.98	0.46
1:AA:1278:U:H6	1:AA:1278:U:H3'	1.81	0.46
25:DA:989:G:H4'	25:DA:990:A:OP1	2.15	0.46
24:CX:59:A:C2'	24:CX:60:U:H5'	2.46	0.46
23:CY:71:G:H2'	23:CY:72:C:C6	2.51	0.46
49:D3:6:VAL:HG13	49:D3:56:VAL:HG22	1.97	0.46
34:DO:15:GLY:O	34:DO:47:ILE:HG12	2.14	0.46
25:DA:1378:A:OP1	53:D7:10:ARG:NH2	2.49	0.46
1:AA:202:U:O2'	1:AA:203:U:O5'	2.29	0.46
9:AI:4:TYR:CE1	9:AI:88:TYR:HD1	2.34	0.46
42:BW:18:ARG:NH1	42:BW:76:VAL:O	2.49	0.46
4:AD:53:ASP:O	4:AD:57:ARG:HG3	2.16	0.46
1:CA:573:A:N3	1:CA:883:C:O2'	2.45	0.46
25:BA:2160:C:H2'	25:BA:2160:C:O2	2.15	0.46
1:AA:614:A:H2'	1:AA:615:C:O4'	2.15	0.46
24:CX:23:C:H2'	24:CX:24:U:C6	2.50	0.46
50:D4:26:SER:OG	50:D4:27:THR:N	2.49	0.46
25:BA:1289:G:O2'	35:BP:7:ARG:NH2	2.49	0.46
2:AB:17:PHE:CB	2:AB:44:LEU:HD21	2.46	0.46
25:DA:2112:G:H2'	25:DA:2113:U:O4'	2.15	0.46
1:AA:345:C:O5'	1:AA:345:C:H6	1.98	0.46
57:CA:3178:PCY:N16	57:CA:3178:PCY:O5	2.45	0.46
1:CA:1128:C:C2'	1:CA:1129:C:H5''	2.46	0.46
25:BA:139:A:C8	25:BA:1454:C:O2'	2.67	0.46
25:BA:932:C:H3'	25:BA:933:C:C5'	2.44	0.46
30:DG:114:ILE:HG23	30:DG:136:ARG:NH2	2.30	0.46
25:BA:1258:A:N3	25:BA:1284:G:O2'	2.41	0.46
1:CA:1442:G:HO2'	1:CA:1442(A):G:P	2.37	0.46
1:AA:600:C:H5'	8:AH:129:VAL:HA	1.98	0.46
25:DA:1292:U:H2'	25:DA:1293:C:H6	1.79	0.46
45:DZ:52:SER:HG	45:DZ:54:HIS:HD1	1.58	0.46
25:BA:2297:C:OP2	52:B6:6:ARG:NH1	2.49	0.46
12:CL:34:ARG:HB3	12:CL:34:ARG:HE	1.44	0.46
29:BF:126:VAL:HG21	29:BF:129:PHE:CZ	2.50	0.46
9:AI:5:TYR:O	9:AI:87:GLN:NE2	2.49	0.46
27:BD:142:VAL:HG13	27:BD:191:ALA:HB1	1.98	0.46
1:CA:1161:C:H2'	1:CA:1162:C:C6	2.51	0.46
25:DA:1336:A:H2'	25:DA:1337:G:C8	2.51	0.46
35:DP:101:VAL:HA	35:DP:106:LEU:O	2.16	0.46
25:BA:2325:C:H4'	30:BG:91:ARG:HG3	1.96	0.46
29:DF:120:GLU:HB2	29:DF:122:LYS:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:AS:80:TYR:CZ	19:AS:82:GLY:HA2	2.51	0.46
13:AM:65:LYS:NZ	13:AM:73:GLU:HG3	2.31	0.46
15:CO:17:ARG:HG3	15:CO:17:ARG:HH11	1.81	0.46
30:DG:49:ASP:N	30:DG:49:ASP:OD1	2.45	0.46
31:DH:124:GLU:OE1	31:DH:132:ARG:HD2	2.15	0.46
29:BF:195:ASP:HB3	29:BF:198:ALA:H	1.81	0.46
42:BW:4:LYS:HB2	42:BW:106:ILE:HG12	1.96	0.46
1:CA:1327:C:H2'	1:CA:1328:C:C6	2.51	0.46
1:AA:189(D):C:H2'	1:AA:189(E):U:O4'	2.16	0.46
23:AY:26:A:N6	23:AY:44:G:N1	2.42	0.46
25:DA:2170:A:H2'	25:DA:2171:A:H5'	1.98	0.46
45:DZ:97:GLU:HA	45:DZ:126:VAL:O	2.16	0.46
25:DA:981:A:N1	25:DA:2027:G:O2'	2.39	0.46
25:DA:2203:U:H4'	27:DD:151:LYS:HG2	1.96	0.46
1:CA:447:G:O6	1:CA:485:G:O2'	2.29	0.46
50:B4:15:ILE:HD12	50:B4:21:VAL:HG22	1.98	0.46
6:CF:69:GLU:O	6:CF:72:VAL:HG12	2.16	0.46
25:BA:2486:C:OP2	25:BA:2487:C:N4	2.41	0.46
1:CA:1410:G:H2'	1:CA:1411:C:C6	2.51	0.46
1:AA:184:G:H2'	1:AA:185:A:H8	1.81	0.46
45:BZ:145:GLU:O	45:BZ:147:GLY:HA2	2.16	0.46
25:DA:1325:G:OP1	25:DA:1647:G:O2'	2.21	0.46
25:BA:2018:C:H4'	25:BA:2019:G:OP1	2.15	0.46
38:BS:39:ILE:HB	38:BS:49:VAL:HG13	1.98	0.46
1:CA:1307:U:H2'	1:CA:1308:U:C6	2.51	0.46
25:BA:231:G:C8	54:B8:5:LYS:HG2	2.50	0.46
1:CA:23:C:H5	1:CA:561:U:O4	1.98	0.46
39:DT:27:THR:HB	39:DT:89:VAL:HG22	1.97	0.46
32:DI:101:LEU:HD12	32:DI:105:HIS:HD2	1.81	0.46
23:AW:2:C:H2'	23:AW:3:C:C6	2.51	0.46
23:CW:33:U:N3	23:CW:36:A:OP2	2.46	0.46
25:DA:1029:A:N1	25:DA:2465:C:O2'	2.36	0.46
2:CB:125:PRO:O	2:CB:127:ILE:N	2.49	0.46
31:DH:117:PRO:HG3	31:DH:123:PHE:CD2	2.51	0.46
5:CE:57:LYS:HG2	5:CE:61:TYR:CE2	2.51	0.46
12:AL:33:ARG:HH11	12:AL:62:SER:HB3	1.81	0.46
1:CA:1004:A:H8	1:CA:1005:A:H4'	1.79	0.46
1:AA:1030(D):A:H2'	1:AA:1031:G:O4'	2.16	0.46
1:CA:1118:C:OP1	9:CI:9:ARG:HD2	2.16	0.46
47:B1:72:GLU:O	47:B1:76:ARG:HG3	2.16	0.46
25:DA:1449:A:H8	25:DA:1449:A:OP2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:AO:7:GLU:O	15:AO:11:VAL:HG23	2.16	0.46
25:DA:639:U:H2'	25:DA:640:C:H6	1.80	0.46
25:BA:2021:C:H4'	25:BA:2736:C:O2	2.15	0.46
4:AD:98:GLU:O	4:AD:103:ASN:ND2	2.48	0.46
1:CA:1069:C:O2'	1:CA:1192:C:H1'	2.16	0.46
3:CC:83:ARG:O	3:CC:87:LEU:HG	2.16	0.46
30:DG:70:VAL:HA	30:DG:90:LEU:HD23	1.97	0.46
25:DA:747:U:O2	25:DA:2014:A:H1'	2.14	0.46
50:B4:46:GLN:HB3	50:B4:46:GLN:HE21	1.60	0.46
25:BA:2697:G:H5'	34:BO:68:GLU:OE1	2.16	0.46
1:CA:1251:A:H2'	1:CA:1252:A:C8	2.50	0.46
25:DA:2815:C:H5'	51:D5:29:THR:HG21	1.98	0.46
25:DA:2179:C:C2'	25:DA:2180:U:H5'	2.46	0.46
1:AA:573:A:OP2	61:AA:4006:HOH:O	2.20	0.46
23:AW:9:A:O2'	23:AW:10:G:N7	2.49	0.46
17:CQ:5:VAL:HG22	17:CQ:60:ILE:HG13	1.97	0.46
35:BP:138:LEU:HD23	35:BP:145:PRO:HG3	1.98	0.46
31:BH:126:PRO:HB2	31:BH:130:ARG:HH21	1.81	0.46
25:DA:479:A:H4'	25:DA:480:A:OP1	2.15	0.46
25:BA:2135:U:O4	25:BA:2136:A:N6	2.46	0.46
1:CA:1194:U:H2'	1:CA:1195:C:C6	2.51	0.46
55:D9:10:ILE:HD12	55:D9:32:HIS:HA	1.97	0.46
20:AT:87:LYS:O	20:AT:91:LEU:HG	2.16	0.46
1:CA:943:U:H2'	1:CA:944:G:H5'	1.97	0.46
25:BA:397:G:OP2	25:BA:397:G:H8	1.99	0.46
40:DU:16:LYS:HB3	40:DU:16:LYS:HE2	1.69	0.46
8:AH:101:PRO:HG3	8:AH:133:LEU:HD11	1.98	0.46
12:CL:83:VAL:HG23	12:CL:107:ALA:HB2	1.98	0.46
25:BA:1535:U:HO2'	25:BA:1536:A:H8	1.63	0.46
1:CA:1004:A:C2	1:CA:1038:C:C4	3.04	0.46
25:DA:896:A:H61	45:DZ:114:GLY:HA3	1.81	0.46
20:AT:10:LEU:HD13	20:AT:12:ALA:HB2	1.98	0.46
1:AA:922:G:H2'	1:AA:923:A:C8	2.51	0.46
25:DA:2552:U:C2	25:DA:2554:U:H5''	2.51	0.46
10:CJ:27:ALA:HA	10:CJ:81:THR:HG22	1.97	0.46
31:DH:2:SER:O	31:DH:3:ARG:HG2	2.15	0.46
7:AG:113:GLU:HG3	7:AG:118:VAL:HG12	1.98	0.46
35:BP:62:LEU:O	54:B8:13:ARG:HD3	2.15	0.46
25:DA:2336:A:H61	46:D0:43:THR:CG2	2.29	0.46
25:BA:63:A:O3'	43:BX:71:GLY:HA3	2.16	0.46
41:DV:62:LEU:HD21	41:DV:95:LEU:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BD:95:LEU:HD11	27:BD:105:ILE:HD13	1.97	0.46
1:AA:197:A:C6	1:AA:221:C:H4'	2.51	0.46
25:DA:887:A:H5'	25:DA:888:C:OP1	2.16	0.46
36:BQ:85:LYS:HG2	46:B0:7:LEU:HB3	1.98	0.46
7:AG:15:ASP:OD1	7:AG:20:ASP:N	2.40	0.46
4:CD:22:LYS:HB2	4:CD:26:CYS:SG	2.56	0.46
1:CA:1318:A:OP1	19:CS:3:ARG:NH2	2.43	0.46
50:D4:16:CYS:SG	50:D4:17:GLY:N	2.89	0.46
1:CA:544:G:P	4:CD:62:GLN:HE21	2.37	0.46
2:AB:166:ASP:OD2	2:AB:169:LYS:HB2	2.16	0.46
1:AA:38:G:H22	1:AA:397:A:H5''	1.81	0.46
12:CL:7:ILE:O	12:CL:11:VAL:HG23	2.16	0.46
57:AA:3231:PCY:O21	57:AA:3231:PCY:N20	2.49	0.45
4:CD:112:VAL:HG13	4:CD:161:ASN:OD1	2.15	0.45
25:BA:265:U:H2'	25:BA:266:C:H6	1.80	0.45
25:DA:265:A:H1'	25:DA:266:G:O4'	2.16	0.45
1:CA:713:G:H2'	1:CA:714:G:C8	2.51	0.45
25:DA:2666:C:N4	31:DH:109:PHE:HA	2.31	0.45
25:DA:2712:U:OP1	25:DA:2714:G:H4'	2.17	0.45
1:CA:583:A:H2'	1:CA:584:G:O4'	2.16	0.45
1:CA:865:A:H2	1:CA:918:A:H4'	1.81	0.45
7:AG:15:ASP:O	7:AG:19:GLY:HA2	2.16	0.45
9:AI:49:PRO:HG3	9:AI:101:PHE:CD2	2.51	0.45
25:BA:505:A:N3	25:BA:507:G:H5''	2.31	0.45
31:BH:13:LYS:HA	31:BH:14:GLY:HA2	1.54	0.45
28:DE:112:GLY:O	28:DE:159:HIS:HA	2.16	0.45
41:DV:15:GLU:O	41:DV:18:LEU:HB2	2.16	0.45
1:AA:707:C:OP1	11:AK:85:ARG:NH1	2.48	0.45
25:BA:439:A:H8	25:BA:439:A:O5'	1.99	0.45
25:DA:1669:A:H5''	25:DA:2550:G:OP1	2.16	0.45
25:DA:588:U:H2'	25:DA:589:C:C6	2.51	0.45
50:D4:15:ILE:HG23	50:D4:21:VAL:HG22	1.96	0.45
25:BA:1987:C:OP1	25:BA:1988:A:O2'	2.30	0.45
25:DA:305:U:H2'	25:DA:306:U:C6	2.51	0.45
5:CE:100:VAL:O	5:CE:107:ARG:NH2	2.28	0.45
25:DA:695:G:OP1	25:DA:1380:G:O2'	2.32	0.45
46:B0:10:THR:HG22	46:B0:12:ASN:N	2.20	0.45
10:CJ:32:ALA:CB	10:CJ:33:GLN:HA	2.43	0.45
1:AA:204:U:H4'	1:AA:216:G:O5'	2.15	0.45
23:CW:2:C:H2'	23:CW:3:C:H6	1.81	0.45
50:D4:49:PHE:HB3	50:D4:50:VAL:H	1.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:DH:4:ILE:O	31:DH:69:ARG:HG2	2.17	0.45
2:CB:230:VAL:HG22	2:CB:231:GLU:H	1.80	0.45
47:B1:3:LYS:HB3	47:B1:4:VAL:H	1.41	0.45
19:AS:3:ARG:NH2	19:AS:7:LYS:HE2	2.31	0.45
25:BA:549:U:H2'	25:BA:550:U:C6	2.51	0.45
25:DA:2191:G:H2'	25:DA:2192:G:O4'	2.16	0.45
44:DY:9:LYS:HA	44:DY:10:GLY:HA2	1.57	0.45
1:CA:62:U:H2'	1:CA:63:C:C6	2.51	0.45
36:BQ:18:LYS:O	36:BQ:98:LYS:NZ	2.31	0.45
25:BA:2430:A:H2'	25:BA:2431:U:C6	2.51	0.45
28:BE:73:GLU:HG3	28:BE:73:GLU:H	1.55	0.45
23:AY:28:G:H1	23:AY:42:C:H42	1.64	0.45
25:DA:1782:C:H1'	25:DA:2609:U:H5''	1.98	0.45
33:BN:75:TYR:CE2	33:BN:77:GLY:HA2	2.51	0.45
1:CA:1066:C:O2'	1:CA:1067:A:H5'	2.15	0.45
1:CA:1186:G:H21	14:CN:61:TRP:C	2.20	0.45
1:CA:1022:G:H4'	1:CA:1022:G:OP1	2.16	0.45
25:DA:2127:G:N1	25:DA:2161:C:N4	2.64	0.45
47:D1:53:VAL:HG22	47:D1:74:VAL:HG13	1.97	0.45
2:AB:80:ILE:HD13	2:AB:211:ILE:HG22	1.98	0.45
23:AY:48:C:OP1	23:AY:48:C:H2'	2.17	0.45
25:BA:555:G:C5	25:BA:2044:U:H5''	2.51	0.45
3:AC:15:THR:HG21	3:AC:181:ASN:HA	1.99	0.45
25:BA:2168:C:H4'	25:BA:2169:G:N3	2.31	0.45
25:BA:2357:G:N3	25:BA:2393:C:H2'	2.31	0.45
25:DA:1187:G:H5'	41:DV:81:TYR:CE1	2.51	0.45
1:AA:738:C:H2'	1:AA:739:C:C6	2.50	0.45
1:CA:1388:C:H2'	1:CA:1389:C:H6	1.81	0.45
25:BA:942:A:N7	45:BZ:146:ILE:HD12	2.31	0.45
25:DA:2080:G:H2'	25:DA:2081:C:H6	1.81	0.45
5:CE:57:LYS:HG2	5:CE:61:TYR:HE2	1.82	0.45
25:DA:2519:U:C6	25:DA:2542:A:N6	2.84	0.45
43:DX:44:GLU:O	43:DX:48:LYS:N	2.49	0.45
25:DA:892:G:H2'	25:DA:893:C:C4'	2.46	0.45
1:CA:630:G:O2'	1:CA:631:G:H5'	2.16	0.45
1:CA:1273:G:H3'	1:CA:1274:G:H8	1.81	0.45
7:AG:76:ARG:HB3	7:AG:156:TRP:HH2	1.82	0.45
25:BA:581:G:OP1	33:BN:111:PRO:HD2	2.17	0.45
1:CA:50:A:H1'	1:CA:52:G:C8	2.52	0.45
25:DA:2728:U:H2'	25:DA:2729:G:C8	2.51	0.45
50:B4:26:SER:OG	50:B4:27:THR:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:529:G:O6	12:CL:49:ASN:HA	2.16	0.45
1:AA:455:C:H6	1:AA:455:C:O5'	2.00	0.45
1:AA:434:U:H2'	1:AA:435:C:C6	2.51	0.45
49:B3:5:LYS:HE3	49:B3:55:ARG:HH12	1.82	0.45
34:DO:16:ALA:HB2	34:DO:52:VAL:HG21	1.98	0.45
29:DF:37:VAL:O	29:DF:41:LEU:HG	2.17	0.45
25:BA:1834:A:H4'	27:BD:259:THR:HG23	1.97	0.45
45:BZ:138:GLU:N	45:BZ:156:LYS:HD3	2.30	0.45
1:CA:1128:C:H2'	1:CA:1129:C:H5''	1.99	0.45
1:CA:200:G:H2'	1:CA:201:C:O4'	2.15	0.45
23:AW:19:G:H1	23:AW:56:C:N4	2.10	0.45
31:DH:6:ARG:HH22	31:DH:54:ARG:NH2	2.14	0.45
25:BA:266:C:H2'	25:BA:267:C:O4'	2.16	0.45
25:DA:196:A:H62	35:DP:38:GLN:HE22	1.63	0.45
4:AD:164:ALA:O	4:AD:168:ARG:HD3	2.16	0.45
29:DF:126:VAL:HG21	29:DF:129:PHE:CZ	2.52	0.45
28:DE:24:THR:HG22	28:DE:186:GLY:O	2.16	0.45
37:DR:44:LEU:HD23	37:DR:44:LEU:HA	1.74	0.45
3:CC:148:GLY:HA3	3:CC:172:ARG:O	2.16	0.45
25:BA:2745:G:H3'	25:BA:2746:A:O4'	2.16	0.45
5:CE:68:GLU:OE1	5:CE:70:PRO:HG3	2.16	0.45
33:DN:73:THR:HA	33:DN:83:LYS:O	2.16	0.45
1:AA:872:A:C8	1:AA:874:G:C8	3.05	0.45
26:BB:12:C:H2'	46:B0:73:GLY:HA3	1.97	0.45
35:BP:50:ARG:HD3	54:B8:7:HIS:CD2	2.51	0.45
25:BA:1170:C:H1'	55:B9:36:GLN:NE2	2.31	0.45
23:CY:57:G:H2'	23:CY:57:G:N3	2.32	0.45
25:BA:2162:C:O2'	25:BA:2174:G:N2	2.49	0.45
1:CA:1122:U:C4	1:CA:1123:A:N7	2.84	0.45
51:B5:17:ASP:OD2	61:B5:205:HOH:O	2.21	0.45
1:CA:67:C:H2'	1:CA:68:G:H8	1.81	0.45
30:DG:137:GLU:HG2	30:DG:152:LEU:HD23	1.99	0.45
50:D4:46:GLN:C	50:D4:48:ARG:H	2.20	0.45
27:DD:182:LEU:HA	27:DD:182:LEU:HD23	1.81	0.45
23:CW:47:U:O2'	23:CW:48:C:OP1	2.33	0.45
17:AQ:67:LYS:O	17:AQ:68:ARG:HB3	2.16	0.45
1:CA:1073:U:H2'	1:CA:1074:G:H8	1.82	0.45
25:DA:38:A:H2'	25:DA:39:C:C6	2.51	0.45
25:BA:904:C:N4	25:BA:905:U:O4	2.49	0.45
25:DA:500:G:N1	25:DA:503:A:OP2	2.50	0.45
25:DA:1857:G:C6	25:DA:1858:G:N1	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:BQ:16:ARG:HG3	36:BQ:17:LEU:H	1.81	0.45
25:DA:1703:G:H2'	25:DA:1704:G:C8	2.51	0.45
1:AA:390:C:H2'	1:AA:391:G:C8	2.51	0.45
31:DH:35:VAL:O	31:DH:37:VAL:HG23	2.17	0.45
25:BA:2119:C:H2'	25:BA:2120:U:O4'	2.16	0.45
9:AI:121:ARG:NH1	9:AI:122:ALA:O	2.50	0.45
23:CY:69:G:H2'	23:CY:70:G:O4'	2.17	0.45
25:BA:843:C:H2'	25:BA:844:C:C6	2.50	0.45
1:AA:1131:G:C2'	1:AA:1132:C:H5'	2.47	0.45
44:DY:88:LYS:NZ	44:DY:89:PHE:O	2.38	0.45
4:AD:23:GLY:HA3	4:AD:112:VAL:CG1	2.46	0.45
25:DA:2792:G:N3	25:DA:2792:G:H2'	2.32	0.45
12:CL:75:HIS:HA	12:CL:102:ARG:HH22	1.80	0.45
25:BA:1199:C:H2'	25:BA:1200:G:O4'	2.16	0.45
12:CL:117:ARG:NH2	12:CL:124:LYS:HB2	2.31	0.45
2:CB:16:HIS:CD2	2:CB:204:ASN:HB3	2.51	0.45
27:DD:71:ASP:CB	27:DD:103:ARG:HH22	2.28	0.45
44:BY:92:ASN:OD1	44:BY:94:LYS:HG3	2.16	0.45
23:CW:21:A:N6	23:CW:46:7MG:C4	2.85	0.45
30:DG:41:GLN:NE2	30:DG:153:ARG:HB3	2.32	0.45
1:AA:626:U:C2	1:AA:627:G:C8	3.04	0.45
29:BF:170:LEU:HG	29:BF:172:TRP:NE1	2.32	0.45
4:AD:164:ALA:C	4:AD:168:ARG:HH11	2.19	0.45
54:B8:23:VAL:CG1	54:B8:47:LYS:HD3	2.46	0.45
2:CB:63:MET:CG	2:CB:225:ALA:HB1	2.47	0.45
25:DA:656:G:H2'	25:DA:657:U:O4'	2.17	0.45
1:AA:130:A:O2'	1:AA:131:C:O5'	2.30	0.45
1:CA:264:U:H4'	17:CQ:63:ARG:HD2	1.99	0.45
25:DA:117:G:C6	25:DA:119:A:C6	3.05	0.45
35:BP:101:VAL:HA	35:BP:106:LEU:O	2.16	0.45
25:DA:2724:C:OP1	28:DE:118:LYS:NZ	2.44	0.45
25:DA:433:C:H2'	25:DA:434:U:C6	2.51	0.45
25:BA:2699:U:OP2	61:BA:4975:HOH:O	2.21	0.45
25:BA:940:C:H2'	25:BA:941:U:O4'	2.16	0.45
25:DA:1709:U:H1'	25:DA:2860:A:N3	2.32	0.45
3:AC:121:ALA:O	3:AC:125:GLU:HG3	2.17	0.45
25:DA:2514:U:H2'	25:DA:2515:C:C6	2.52	0.45
3:AC:82:GLU:HG2	3:AC:85:ARG:NH2	2.32	0.45
33:DN:39:ARG:HA	33:DN:40:PRO:HD3	1.78	0.45
2:CB:13:ALA:C	2:CB:15:VAL:H	2.20	0.45
2:CB:219:VAL:HA	2:CB:222:ILE:CG1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:171:A:H2'	1:AA:172:A:C8	2.52	0.45
25:DA:1218:C:N4	25:DA:1231:G:H1	2.13	0.45
23:CW:61:C:O2'	23:CW:62:C:H6	1.99	0.45
34:BO:120:GLU:OE1	39:BT:67:SER:OG	2.19	0.45
14:AN:6:LEU:HD12	14:AN:6:LEU:HA	1.88	0.45
1:AA:277:C:H5''	17:AQ:68:ARG:NH2	2.31	0.45
38:BS:3:ARG:HA	38:BS:3:ARG:HE	1.82	0.45
25:DA:1417:C:H2'	25:DA:1418:G:O4'	2.16	0.45
36:DQ:35:VAL:HG12	36:DQ:130:LYS:O	2.16	0.45
25:BA:939:C:H2'	25:BA:940:C:C6	2.51	0.45
49:D3:7:LYS:HB2	49:D3:34:GLU:HG2	1.98	0.45
1:CA:256:U:H2'	1:CA:257:G:C8	2.51	0.45
11:AK:34:ASP:HB3	11:AK:40:ILE:HD11	1.99	0.45
24:CX:72:A:H2'	24:CX:73:A:C8	2.52	0.45
42:DW:83:LYS:HE2	42:DW:97:LYS:HD3	1.99	0.45
25:DA:724:U:H2'	25:DA:725:G:O4'	2.17	0.45
1:AA:691:G:H2'	1:AA:692:U:C6	2.51	0.45
25:BA:1213:U:H2'	25:BA:1214:G:C8	2.52	0.45
11:AK:20:TYR:CZ	11:AK:83:ILE:HD12	2.52	0.45
23:CY:59:U:O5'	23:CY:59:U:H6	1.99	0.45
35:DP:59:LEU:HD23	54:D8:58:ILE:HD13	1.98	0.45
1:CA:130:A:O2'	1:CA:131:C:O5'	2.35	0.45
1:CA:1230:C:H2'	1:CA:1231:G:H8	1.82	0.45
36:BQ:37:LEU:HD21	36:BQ:130:LYS:HE2	1.98	0.45
25:DA:1227:G:N2	25:DA:1228:G:H1'	2.32	0.45
4:AD:157:LEU:HD22	4:AD:161:ASN:HD21	1.81	0.45
1:CA:1154:G:H8	1:CA:1154:G:H3'	1.81	0.45
25:DA:2120:G:H2'	25:DA:2121:G:H8	1.82	0.45
1:CA:1359:C:H1'	1:CA:1362:C:H41	1.82	0.45
35:DP:100:LEU:HD12	35:DP:112:LEU:HD11	1.97	0.45
45:BZ:152:ALA:HA	45:BZ:155:LEU:HD22	1.98	0.45
2:AB:215:LEU:O	2:AB:219:VAL:HG23	2.17	0.45
25:DA:30:G:H2'	25:DA:31:C:C6	2.52	0.45
19:CS:27:GLU:HG2	19:CS:47:HIS:HE2	1.81	0.45
14:CN:21:TYR:HE2	14:CN:23:ARG:NE	2.15	0.45
2:CB:63:MET:HG3	2:CB:225:ALA:HB1	1.99	0.45
43:BX:66:LEU:HD23	43:BX:66:LEU:HA	1.68	0.45
2:AB:103:THR:HA	2:AB:180:LEU:HD11	1.99	0.45
1:CA:258:G:O6	61:CA:4159:HOH:O	2.21	0.45
25:DA:1341:U:O2	43:DX:80:ILE:HD12	2.16	0.45
25:DA:572:A:OP2	41:DV:78:LYS:NZ	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:119:A:H4'	1:AA:120:A:C8	2.52	0.45
45:DZ:6:LYS:HD2	45:DZ:8:TYR:OH	2.16	0.45
4:CD:166:LYS:HD3	4:CD:178:VAL:HG11	1.99	0.45
27:DD:10:THR:OG1	27:DD:13:ARG:HG2	2.17	0.45
25:DA:2275:C:H5'	25:DA:2275:C:H6	1.82	0.45
25:DA:2518:A:OP2	61:DA:4302:HOH:O	2.21	0.45
1:AA:1002:G:O6	1:AA:1003:G:N2	2.50	0.45
25:DA:83:G:N1	25:DA:102:G:O2'	2.31	0.45
23:AY:50:U:N3	23:AY:64:A:C2	2.77	0.45
25:DA:2149:G:H3'	25:DA:2150:U:H6	1.82	0.45
25:DA:1826:G:H4'	27:DD:242:ARG:CZ	2.47	0.45
25:DA:1152:C:H2'	25:DA:1153:C:C6	2.51	0.45
25:DA:2317:C:N3	25:DA:2318:G:N7	2.65	0.45
23:CY:51:U:H2'	23:CY:52:G:O4'	2.17	0.45
1:AA:1128:C:H2'	1:AA:1129:C:H5'	1.98	0.45
25:BA:2149:G:H1	25:BA:2183:C:N4	2.15	0.45
1:AA:149:A:H2'	1:AA:150:C:C6	2.52	0.45
37:BR:41:ALA:HB1	37:BR:114:VAL:HG22	1.99	0.45
3:CC:131:ARG:HH21	3:CC:166:GLU:HB3	1.82	0.45
3:CC:179:ARG:NH1	3:CC:206:GLU:OE1	2.50	0.45
1:AA:1145:C:H4'	1:AA:1146:A:H5''	1.98	0.45
25:DA:1529:G:C6	25:DA:1530:C:N4	2.85	0.45
38:BS:3:ARG:CA	38:BS:3:ARG:HE	2.30	0.45
25:BA:274:U:H3'	25:BA:275:C:H5'	1.99	0.45
1:CA:1072:G:H2'	1:CA:1073:U:C6	2.52	0.45
1:CA:715:A:H2'	1:CA:716:A:C8	2.52	0.45
1:CA:542:G:OP1	4:CD:10:ARG:NH2	2.43	0.45
15:CO:4:THR:OG1	15:CO:7:GLU:OE1	2.20	0.45
25:BA:909:G:H2'	25:BA:910:A:O4'	2.17	0.45
25:DA:2693:A:H2'	25:DA:2694:G:H8	1.81	0.45
46:D0:38:VAL:HG12	46:D0:40:GLN:HG2	1.99	0.45
25:DA:463:G:N2	25:DA:466:A:OP2	2.46	0.45
8:CH:86:ILE:HG12	8:CH:135:CYS:HA	1.99	0.45
25:BA:327:U:H2'	25:BA:328:G:H8	1.81	0.45
25:DA:2399:G:H2'	25:DA:2400:G:O4'	2.16	0.45
25:BA:2545:A:H2'	25:BA:2546:A:O4'	2.16	0.45
1:AA:345:C:H4'	1:AA:346:G:N3	2.31	0.45
23:CW:4:C:N3	23:CW:69:G:C2	2.84	0.45
1:AA:1151:A:O4'	10:AJ:39:PRO:HB2	2.17	0.45
35:DP:63:PRO:HD3	54:D8:27:THR:HG22	1.97	0.45
25:BA:553:A:H3'	25:BA:553:A:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:DF:125:LEU:HD22	29:DF:199:TRP:HB2	1.99	0.45
25:DA:2526:G:H5'	25:DA:2742:C:O2'	2.17	0.45
13:CM:122:LYS:HD3	13:CM:123:ALA:H	1.82	0.45
30:BG:41:GLN:HE22	30:BG:153:ARG:HB3	1.82	0.45
31:DH:44:VAL:O	31:DH:50:VAL:HA	2.16	0.45
31:DH:13:LYS:HA	31:DH:14:GLY:HA2	1.61	0.45
25:BA:2054:G:O2'	28:BE:145:LYS:HE3	2.17	0.45
47:B1:2:SER:HB3	47:B1:46:LEU:HD12	1.99	0.45
27:DD:166:GLN:HB2	27:DD:174:ILE:HG22	1.99	0.45
29:BF:197:ASP:OD1	29:BF:197:ASP:N	2.49	0.45
23:AW:37:MIA:H162	23:AW:37:MIA:H122	1.87	0.45
10:CJ:6:ILE:HG12	10:CJ:98:ILE:HG13	1.99	0.45
25:DA:1007:C:P	33:DN:37:LYS:HZ1	2.40	0.45
25:DA:224:G:H2'	25:DA:225:A:O4'	2.17	0.45
44:BY:1:MET:HB2	44:BY:2:ARG:H	1.65	0.45
1:AA:1286:A:H2	21:AU:18:TYR:OH	2.00	0.45
1:AA:1036:G:H5''	1:AA:1037:C:C5	2.52	0.44
1:CA:532:A:H2	1:CA:1206:G:N2	2.14	0.44
40:DU:65:ILE:HD11	40:DU:95:LEU:HB3	1.99	0.44
25:DA:2168:G:H2'	25:DA:2169:A:C8	2.52	0.44
1:AA:1182:G:C4'	1:AA:1183:A:H5'	2.39	0.44
29:DF:7:TYR:O	29:DF:22:ALA:N	2.50	0.44
54:D8:63:PRO:HG2	54:D8:64:TYR:CE2	2.53	0.44
2:CB:95:GLN:HB2	2:CB:148:TYR:CD1	2.52	0.44
1:CA:1010:G:H2'	1:CA:1011:G:C8	2.50	0.44
25:DA:864:G:H2'	25:DA:865:C:C6	2.53	0.44
1:AA:1118:C:H2'	1:AA:1119:C:H6	1.82	0.44
25:DA:646:A:H2'	25:DA:647:G:O4'	2.17	0.44
25:BA:1639:G:H2'	25:BA:1640:G:C8	2.53	0.44
25:BA:997:G:OP1	36:BQ:16:ARG:NH2	2.48	0.44
1:AA:198:G:H2'	1:AA:199:G:H8	1.83	0.44
43:DX:47:PHE:O	43:DX:49:VAL:HG13	2.18	0.44
25:BA:2023:A:H2'	25:BA:2024:G:C8	2.51	0.44
41:DV:72:VAL:CG1	41:DV:85:LYS:HD2	2.47	0.44
45:BZ:7:ALA:HB3	45:BZ:61:LEU:HD12	1.99	0.44
1:CA:357:G:OP1	1:CA:367:U:H5''	2.17	0.44
37:BR:83:ILE:O	37:BR:86:ARG:HG2	2.17	0.44
25:DA:383:U:H2'	25:DA:385:C:H5	1.81	0.44
35:DP:122:PRO:HB3	35:DP:141:ALA:O	2.17	0.44
27:DD:169:GLU:HG3	27:DD:169:GLU:O	2.17	0.44
46:D0:68:GLU:OE1	46:D0:82:ARG:HD2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2799:U:O2'	28:BE:62:PRO:O	2.29	0.44
25:DA:93:G:H2'	25:DA:94:C:C6	2.52	0.44
1:CA:664:G:N2	1:CA:741:G:H1	2.14	0.44
25:DA:2268:A:OP1	61:DA:4433:HOH:O	2.21	0.44
25:DA:848:G:N9	25:DA:933:A:H8	2.15	0.44
44:BY:92:ASN:HB3	44:BY:94:LYS:N	2.30	0.44
25:DA:1019:U:H2'	25:DA:1020:A:C8	2.51	0.44
33:BN:67:LEU:HD13	33:BN:87:LEU:HD13	1.98	0.44
25:BA:1320:A:N3	25:BA:1343:C:H1'	2.32	0.44
2:AB:178:ARG:HH22	8:AH:68:ARG:HH22	1.66	0.44
25:BA:2735:G:H2'	25:BA:2736:C:C6	2.52	0.44
1:CA:1468:A:H2'	1:CA:1469:G:O4'	2.18	0.44
1:AA:1302:U:OP1	13:AM:13:LYS:HE3	2.17	0.44
26:DB:24:G:N3	26:DB:26:A:N6	2.65	0.44
1:AA:1054:C:C4	23:AW:34:G:H1'	2.52	0.44
33:DN:67:LEU:O	33:DN:88:GLU:HG3	2.17	0.44
25:DA:479:A:HO2'	25:DA:481:G:H8	1.64	0.44
1:CA:944:G:O2'	1:CA:1339:A:N6	2.49	0.44
1:AA:371:G:H2'	1:AA:372:C:O4'	2.17	0.44
39:BT:6:LEU:O	39:BT:10:VAL:HG23	2.18	0.44
27:BD:223:GLY:HA3	27:BD:231:HIS:CE1	2.52	0.44
1:CA:1530:G:H2'	1:CA:1531:A:O4'	2.18	0.44
25:DA:1165:U:H2'	25:DA:1166:C:C6	2.52	0.44
1:AA:673:G:H2'	1:AA:674:G:C8	2.52	0.44
28:BE:174:ASP:OD1	28:BE:175:VAL:N	2.50	0.44
7:AG:26:PHE:CE2	7:AG:30:ILE:HD11	2.53	0.44
1:AA:262:A:H2'	1:AA:263:A:C8	2.52	0.44
1:CA:1136:U:H5''	1:CA:1137:C:C5	2.52	0.44
1:AA:1262:C:H2'	1:AA:1263:C:C6	2.53	0.44
1:AA:1241:G:H2'	1:AA:1242:C:C6	2.52	0.44
25:DA:212:G:H5'	25:DA:213:A:OP2	2.17	0.44
25:DA:1127:A:C2'	25:DA:1128:A:H5''	2.48	0.44
42:DW:34:ASN:OD1	42:DW:37:ARG:NH1	2.40	0.44
23:AY:19:G:H4'	23:AY:57:G:H22	1.82	0.44
25:DA:2141:G:O6	25:DA:2150:U:C2	2.70	0.44
51:D5:16:ARG:HD2	51:D5:20:ARG:NH1	2.33	0.44
25:DA:1900:A:N1	25:DA:1970:A:C6	2.85	0.44
45:BZ:155:LEU:HD12	45:BZ:156:LYS:H	1.82	0.44
25:BA:831:A:C8	25:BA:839:G:C5	3.05	0.44
25:DA:422:A:OP2	61:DA:4103:HOH:O	2.21	0.44
25:BA:2123:G:H1	25:BA:2210:C:H42	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1315:U:H2'	1:CA:1316:G:O4'	2.17	0.44
1:AA:98:G:H5'	1:AA:99:U:OP2	2.17	0.44
1:AA:161:A:H2'	1:AA:162:A:C8	2.52	0.44
25:DA:910:A:N1	25:DA:2277:G:H1'	2.33	0.44
9:CI:55:ALA:HA	9:CI:58:HIS:CD2	2.52	0.44
32:DI:38:LEU:HD12	32:DI:38:LEU:H	1.82	0.44
1:AA:973:G:H3'	1:AA:974:A:H5''	1.99	0.44
2:CB:77:ALA:HA	2:CB:80:ILE:HG22	1.98	0.44
25:BA:174:U:H2'	25:BA:175:G:C8	2.52	0.44
43:DX:31:HIS:HD2	43:DX:33:LYS:H	1.65	0.44
4:AD:163:GLU:C	4:AD:165:MET:H	2.21	0.44
4:AD:168:ARG:H	4:AD:168:ARG:NE	2.15	0.44
23:AY:69:G:H2'	23:AY:70:G:O4'	2.17	0.44
25:DA:2648:C:H2'	25:DA:2649:U:C6	2.52	0.44
1:CA:203:U:OP2	1:CA:203:U:H2'	2.17	0.44
9:CI:21:PRO:HA	9:CI:59:PHE:HA	1.99	0.44
45:DZ:138:GLU:H	45:DZ:156:LYS:HD3	1.82	0.44
1:AA:192:U:H2'	1:AA:193:C:C6	2.52	0.44
25:DA:286:C:H2'	25:DA:287:C:H6	1.83	0.44
48:B2:1:MET:HG2	48:B2:5:GLU:OE1	2.17	0.44
1:AA:1016:A:H2'	1:AA:1017:G:O4'	2.18	0.44
34:BO:36:GLY:HA3	34:BO:109:LYS:HD2	1.99	0.44
39:BT:37:GLY:HA2	39:BT:38:ASN:HA	1.67	0.44
1:AA:767:A:H2'	1:AA:768:A:O4'	2.17	0.44
52:D6:18:ARG:HD2	52:D6:42:TRP:CE2	2.52	0.44
28:DE:101:ARG:NH1	28:DE:169:ASN:O	2.43	0.44
25:DA:2108:C:H2'	25:DA:2109:U:H6	1.82	0.44
25:BA:1324:A:OP1	37:BR:36:THR:HG23	2.17	0.44
2:CB:7:VAL:HB	2:CB:8:LYS:H	1.55	0.44
39:DT:99:LEU:HD22	39:DT:101:PHE:HE1	1.81	0.44
25:DA:1184:G:OP1	49:D3:30:ARG:HD2	2.17	0.44
29:DF:150:GLY:HA2	29:DF:172:TRP:CD2	2.52	0.44
25:BA:1360:C:OP1	61:BA:4775:HOH:O	2.21	0.44
1:AA:664:G:OP1	18:AR:64:ARG:NE	2.46	0.44
43:BX:31:HIS:HD2	43:BX:33:LYS:HB2	1.83	0.44
50:B4:57:GLU:HA	50:B4:58:ARG:HA	1.61	0.44
25:DA:307:G:H22	25:DA:310:A:P	2.39	0.44
19:CS:28:LYS:HB3	19:CS:28:LYS:HZ3	1.83	0.44
25:DA:2871:C:N4	61:DA:4551:HOH:O	2.51	0.44
25:DA:2331:G:O2'	25:DA:2336:A:N1	2.37	0.44
1:CA:779:C:O2'	11:CK:120:ARG:HD3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:DH:25:LYS:HE2	31:DH:34:GLU:OE2	2.17	0.44
25:DA:2532:G:H1'	25:DA:2663:G:H22	1.83	0.44
2:CB:19:HIS:NE2	2:CB:206:ASP:HB2	2.32	0.44
25:DA:1015:G:H2'	25:DA:1016:G:C8	2.53	0.44
25:BA:2661:U:H2'	25:BA:2662:U:C6	2.52	0.44
4:CD:58:LEU:HD22	4:CD:62:GLN:HG2	1.98	0.44
52:D6:11:LEU:HB2	52:D6:21:TYR:HB2	1.99	0.44
15:CO:39:LEU:HD13	15:CO:56:LEU:HB2	1.99	0.44
25:BA:2574:U:H1'	34:BO:23:ARG:HD3	2.00	0.44
25:BA:2221:A:OP2	25:BA:2222:C:H5	2.00	0.44
48:B2:21:LEU:HB2	48:B2:64:LEU:HD23	2.00	0.44
25:DA:908:C:OP1	36:DQ:22:LYS:HB3	2.18	0.44
25:BA:2453:C:OP2	25:BA:2598:C:O2'	2.34	0.44
1:AA:1270:C:OP2	21:AU:24:ARG:NH2	2.51	0.44
2:AB:170:GLU:O	2:AB:174:VAL:HG23	2.18	0.44
37:BR:33:ARG:NH2	51:B5:57:VAL:O	2.46	0.44
23:AY:19:G:C2	23:AY:56:C:N3	2.86	0.44
23:AY:25:C:H2'	23:AY:26:A:H8	1.82	0.44
54:B8:6:THR:HG23	54:B8:64:TYR:HD2	1.83	0.44
13:AM:84:ILE:HD12	19:AS:74:PHE:CE2	2.53	0.44
35:DP:63:PRO:HG2	54:D8:25:MET:HB2	2.00	0.44
36:DQ:18:LYS:HE3	36:DQ:18:LYS:HB2	1.74	0.44
4:AD:155:LEU:HB3	4:AD:158:ILE:HD11	1.99	0.44
7:CG:79:ARG:NE	7:CG:80:VAL:H	2.16	0.44
23:CW:24:G:C2'	23:CW:25:C:H5'	2.46	0.44
25:DA:510:C:H2'	25:DA:511:U:O4'	2.18	0.44
1:AA:154:C:C2'	1:AA:155:C:H5'	2.48	0.44
1:CA:564:C:C4	1:CA:565:U:C4	3.06	0.44
25:BA:1552:C:O2'	25:BA:1553:A:H5'	2.17	0.44
55:D9:29:ASN:HD22	55:D9:32:HIS:CE1	2.35	0.44
25:DA:887:A:H4'	25:DA:888:C:C5	2.51	0.44
1:AA:1131:G:O2'	1:AA:1132:C:H5'	2.18	0.44
38:BS:26:LEU:HB2	38:BS:85:VAL:HG21	1.99	0.44
25:BA:270:C:H4'	25:BA:271:U:OP1	2.18	0.44
28:DE:163:GLU:HG2	28:DE:164:ARG:N	2.33	0.44
1:AA:1073:U:O2'	2:AB:104:ASN:OD1	2.28	0.44
23:AW:31:A:H2'	23:AW:32:PSU:O4'	2.17	0.44
2:CB:112:VAL:O	2:CB:116:GLU:HB2	2.18	0.44
25:BA:2707:C:H2'	25:BA:2708:U:C6	2.52	0.44
25:BA:2707:C:H2'	25:BA:2708:U:H6	1.82	0.44
16:AP:14:ASN:OD1	16:AP:42:ARG:NH2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:BP:135:LEU:HD23	35:BP:135:LEU:HA	1.70	0.44
25:BA:1727:U:O2'	25:BA:1794:G:N7	2.40	0.44
1:AA:257:G:C6	1:AA:258:G:C5	3.05	0.44
25:DA:57:C:H2'	25:DA:58:G:O4'	2.18	0.44
1:AA:1169:A:C6	1:AA:1170:A:C6	3.06	0.44
18:AR:33:ASP:OD2	18:AR:36:ASN:HB2	2.17	0.44
1:CA:1244:C:H42	1:CA:1293:G:H1	1.65	0.44
25:DA:2872:G:O2'	25:DA:2873:A:H5'	2.18	0.44
1:AA:376:G:OP2	16:AP:67:THR:HG21	2.17	0.44
1:CA:532:A:O2'	1:CA:533:A:P	2.75	0.44
25:DA:973:A:H5'	25:DA:1188:U:H1'	1.99	0.44
19:AS:68:GLY:N	50:B4:58:ARG:HH12	2.13	0.44
25:DA:528:A:N1	25:DA:2042:A:H2'	2.33	0.44
2:AB:51:LEU:HD23	2:AB:201:ILE:HD12	1.99	0.44
25:BA:2062:C:H2'	25:BA:2063:U:O4'	2.18	0.44
20:AT:100:ILE:HB	20:AT:101:GLY:H	1.63	0.44
9:CI:53:VAL:HG21	9:CI:92:TYR:CE1	2.53	0.44
23:CY:33:U:OP2	23:CY:33:U:H6	2.00	0.44
1:AA:1124:G:O2'	1:AA:1145:C:C4	2.71	0.44
25:DA:1557:C:H5''	25:DA:1558:A:OP2	2.17	0.44
25:BA:934:A:O2'	25:BA:935:C:OP2	2.31	0.44
25:BA:2376:C:H2'	25:BA:2377:G:O4'	2.18	0.44
2:CB:62:ALA:HB1	2:CB:225:ALA:HB3	2.00	0.44
25:BA:1809:U:H2'	25:BA:1815:A:N6	2.33	0.44
3:CC:32:LEU:O	3:CC:36:ASP:HB2	2.17	0.44
3:CC:113:ALA:N	3:CC:183:ASP:OD2	2.45	0.44
1:AA:1226:C:H4'	19:AS:80:TYR:OH	2.17	0.44
25:DA:416:C:H2'	25:DA:417:C:O4'	2.17	0.44
1:AA:652:U:O4	1:AA:752:G:O2'	2.24	0.44
42:DW:68:ARG:HH11	42:DW:111:HIS:HA	1.81	0.44
25:DA:2557:G:H2'	25:DA:2558:C:C6	2.52	0.44
25:DA:2094:G:OP1	32:DI:22:LYS:HD2	2.18	0.44
1:AA:964:A:N3	1:AA:969:A:O2'	2.40	0.44
5:AE:8:GLU:OE2	5:AE:63:ARG:NH2	2.49	0.44
35:BP:76:LYS:HE3	35:BP:76:LYS:HB3	1.78	0.44
25:DA:583:G:OP2	40:DU:10:ARG:HD2	2.17	0.44
49:D3:26:LEU:O	49:D3:35:ARG:HD3	2.18	0.44
20:AT:92:LEU:O	20:AT:96:GLY:HA2	2.18	0.44
1:AA:1004:A:H5'	1:AA:1024:G:O6	2.17	0.44
23:AY:9:A:O3'	23:AY:45:U:O2'	2.26	0.44
1:CA:390:C:H2'	1:CA:391:G:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1006:C:H2'	1:AA:1007:C:C6	2.53	0.44
25:DA:2207:G:H3'	25:DA:2208:A:H5''	1.99	0.44
45:DZ:110:GLY:HA3	45:DZ:144:LEU:O	2.18	0.44
19:AS:66:MET:HB2	19:AS:74:PHE:CZ	2.53	0.44
31:BH:167:GLU:HA	31:BH:168:PRO:HD3	1.83	0.44
25:DA:1239:G:H2'	25:DA:1240:U:O4'	2.18	0.44
25:BA:1343:C:OP1	25:BA:2722:C:H4'	2.18	0.44
6:AF:19:LEU:HD21	6:AF:59:TYR:CE1	2.53	0.44
24:AX:20:U:H5''	24:AX:21:A:OP2	2.18	0.44
1:CA:91:C:H2'	1:CA:92:C:H6	1.83	0.44
30:DG:86:MET:HA	30:DG:87:PRO:HD3	1.89	0.44
25:DA:2849:U:OP2	39:DT:95:ARG:NH1	2.51	0.44
25:DA:903:C:H2'	25:DA:904:C:C6	2.52	0.44
1:AA:555:C:H2'	1:AA:556:C:C6	2.53	0.44
25:DA:2818:G:OP2	37:DR:42:LYS:NZ	2.46	0.44
29:DF:51:THR:HG23	29:DF:92:PRO:HG2	1.99	0.44
32:BI:110:ASP:HA	32:BI:111:PRO:HD2	1.67	0.44
1:AA:1047:G:H5''	14:AN:4:LYS:HD2	2.00	0.44
47:D1:94:LEU:HD23	47:D1:94:LEU:HA	1.76	0.44
25:DA:1632:A:H8	25:DA:1632:A:O5'	1.99	0.44
25:BA:895:G:H2'	25:BA:896:A:C8	2.53	0.44
25:DA:309:G:N3	25:DA:329:G:O2'	2.47	0.44
25:DA:2340:G:H2'	25:DA:2341:G:H8	1.82	0.44
25:BA:2295:C:H2'	25:BA:2296:C:O4'	2.17	0.44
1:AA:376:G:H5''	16:AP:5:ARG:CG	2.38	0.44
57:AA:3231:PCY:H37	23:AY:34:G:O6	2.17	0.44
37:DR:63:ARG:O	37:DR:67:LEU:HB2	2.18	0.44
25:DA:2023:G:H4'	25:DA:2617:C:O3'	2.18	0.44
1:CA:160:A:H1'	1:CA:344:A:C8	2.53	0.44
25:DA:2591:C:H2'	25:DA:2592:G:C8	2.53	0.44
25:DA:885:C:H2'	25:DA:886:C:H4'	1.98	0.44
25:BA:1210:G:H2'	25:BA:1211:U:C6	2.53	0.44
25:DA:1449:A:O2'	25:DA:1529:G:N2	2.23	0.44
25:BA:2343:G:O2'	46:B0:43:THR:HG22	2.18	0.44
1:CA:1105:A:H2'	1:CA:1106:G:H8	1.83	0.44
26:DB:24:G:N2	26:DB:27:C:N3	2.47	0.44
29:BF:33:LEU:HB3	35:BP:6:LEU:HD21	2.00	0.44
1:CA:1327:C:H2'	1:CA:1328:C:H6	1.83	0.44
8:AH:86:ILE:HG13	8:AH:133:LEU:HD22	2.00	0.44
49:D3:7:LYS:NZ	49:D3:32:GLN:O	2.50	0.44
1:AA:1286:A:C8	1:AA:1287:A:H4'	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:BH:11:VAL:HG21	31:BH:50:VAL:HG23	1.99	0.44
25:DA:1450(A):C:N4	25:DA:1451:C:H41	2.15	0.44
1:CA:936:C:H2'	1:CA:937:A:O4'	2.18	0.44
4:CD:184:LYS:HE3	4:CD:186:LEU:HD23	2.00	0.44
13:AM:115:LYS:HB2	13:AM:115:LYS:HE2	1.84	0.44
1:CA:1068:G:H8	1:CA:1068:G:OP2	2.01	0.44
1:CA:603:U:H2'	1:CA:604:G:H8	1.83	0.44
1:CA:1256:A:OP2	3:CC:26:LYS:NZ	2.51	0.44
1:AA:1003:G:C2	1:AA:1004:A:N3	2.86	0.44
1:AA:1032:G:H2'	1:AA:1033:G:C8	2.53	0.44
1:CA:1005:A:H3'	1:CA:1006:C:O4'	2.17	0.44
1:AA:1353:G:H2'	1:AA:1354:C:H6	1.83	0.44
25:BA:2695:C:OP1	39:BT:53:ARG:NH2	2.51	0.44
25:BA:2148:A:H4'	25:BA:2149:G:H5'	2.00	0.44
35:DP:2:LYS:HG2	35:DP:5:ASP:CG	2.38	0.44
25:DA:528:A:C2'	25:DA:529:A:H5''	2.48	0.44
25:BA:2762:A:P	31:BH:3:ARG:HH21	2.39	0.44
7:CG:27:ILE:HD11	7:CG:43:PHE:HB3	2.00	0.44
23:CY:8:4SU:H5'	23:CY:49:C:H5''	2.00	0.44
1:AA:840:C:H4'	1:AA:841:U:OP1	2.18	0.44
2:CB:19:HIS:HD1	2:CB:20:GLU:HG2	1.83	0.44
12:CL:71:PRO:O	12:CL:102:ARG:HD2	2.18	0.44
6:CF:3:ARG:HD3	6:CF:64:GLN:NE2	2.32	0.44
25:BA:1822:A:H8	25:BA:1822:A:OP2	2.00	0.44
43:BX:50:LYS:N	43:BX:87:GLN:OE1	2.47	0.44
25:BA:280:C:H2'	25:BA:281:G:H8	1.83	0.44
45:DZ:29:TYR:HB3	45:DZ:34:ASN:HD22	1.83	0.44
25:BA:664:U:H2'	25:BA:665:C:C6	2.53	0.44
25:DA:721:C:H2'	25:DA:722:A:C8	2.53	0.44
38:BS:110:LEU:HD12	38:BS:110:LEU:HA	1.73	0.44
25:BA:2371:C:H2'	25:BA:2372:A:O4'	2.18	0.44
5:AE:92:LYS:HB3	5:AE:119:LEU:HB2	1.99	0.44
25:BA:537:G:OP1	25:BA:1280:U:O2'	2.23	0.44
1:AA:1008:C:H2'	1:AA:1009:G:O4'	2.17	0.43
25:DA:2572:A:N7	28:DE:145:LYS:HB2	2.33	0.43
45:BZ:152:ALA:O	45:BZ:155:LEU:HB2	2.18	0.43
25:BA:831:A:C6	27:BD:229:VAL:HG11	2.52	0.43
23:AY:34:G:C6	23:AY:35:A:C6	3.06	0.43
4:AD:170:VAL:CG1	4:AD:174:LEU:HB2	2.48	0.43
4:AD:174:LEU:HD23	4:AD:185:PHE:HA	2.00	0.43
25:DA:1013:C:O2'	25:DA:1014:U:H5'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:DD:68:LYS:O	27:DD:69:ARG:HB2	2.18	0.43
30:DG:43:LEU:HD12	30:DG:43:LEU:HA	1.85	0.43
1:AA:167:G:H2'	1:AA:168:G:H8	1.82	0.43
42:DW:84:ARG:O	42:DW:96:ILE:N	2.50	0.43
3:AC:82:GLU:HA	3:AC:85:ARG:CZ	2.48	0.43
6:CF:35:ALA:HA	6:CF:67:MET:HB3	2.00	0.43
4:CD:64:LEU:HD22	4:CD:198:VAL:HG11	1.99	0.43
23:AY:46:7MG:H2'	23:AY:46:7MG:H81	1.75	0.43
45:DZ:150:LEU:HD12	45:DZ:150:LEU:HA	1.80	0.43
36:DQ:56:ARG:O	36:DQ:56:ARG:HD3	2.18	0.43
25:BA:1836:U:O2	27:BD:50:THR:HB	2.17	0.43
1:AA:736:C:H2'	1:AA:737:A:C8	2.53	0.43
25:BA:2173:G:C2	25:BA:2174:G:C6	3.06	0.43
1:CA:1121:U:H2'	1:CA:1122:U:O4'	2.18	0.43
1:CA:1123:A:H4'	10:CJ:37:PRO:HD2	2.00	0.43
1:CA:1353:G:OP1	21:CU:10:ARG:NH1	2.51	0.43
45:DZ:146:ILE:H	45:DZ:146:ILE:HD12	1.83	0.43
1:CA:184:G:H2'	1:CA:185:A:C8	2.53	0.43
25:DA:848:G:C4	25:DA:933:A:H8	2.36	0.43
1:AA:1129:C:H5''	9:AI:16:ARG:NH1	2.29	0.43
25:DA:528:A:H2'	25:DA:529:A:H5''	1.99	0.43
25:BA:1218:G:H2'	25:BA:1218:G:OP2	2.18	0.43
25:BA:1086:C:H2'	25:BA:1087:C:O4'	2.17	0.43
38:DS:25:ARG:HD3	38:DS:42:ASP:OD2	2.17	0.43
8:CH:82:HIS:CE1	8:CH:84:ARG:HG2	2.53	0.43
10:AJ:11:PHE:CE1	10:AJ:67:THR:HG22	2.53	0.43
41:BV:49:THR:HG22	41:BV:49:THR:O	2.19	0.43
45:DZ:158:PRO:HA	45:DZ:159:PRO:HD3	1.90	0.43
7:CG:99:LEU:HD22	7:CG:103:TRP:CZ2	2.54	0.43
17:CQ:27:PHE:CE2	17:CQ:36:ILE:HD11	2.52	0.43
45:DZ:166:SER:O	45:DZ:169:GLU:HB2	2.18	0.43
6:CF:100:ASN:HB2	18:CR:28:GLU:HA	2.00	0.43
4:CD:81:GLU:O	4:CD:85:LYS:HB2	2.18	0.43
45:BZ:100:VAL:HG21	45:BZ:134:PRO:HG2	2.00	0.43
1:CA:1210:C:H2'	1:CA:1211:U:H5''	1.99	0.43
3:CC:155:GLY:O	3:CC:157:ILE:N	2.48	0.43
46:B0:38:VAL:HG12	46:B0:40:GLN:HG2	1.99	0.43
25:DA:2474:C:H5''	25:DA:2475:C:OP2	2.17	0.43
1:AA:72:C:H2'	1:AA:73:G:O4'	2.17	0.43
45:BZ:125:LEU:HG	45:BZ:164:ALA:HB3	2.00	0.43
16:CP:49:LEU:HD22	16:CP:73:LEU:HD22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:DY:83:THR:HG21	44:DY:99:CYS:HB2	2.01	0.43
38:DS:30:ARG:HG3	38:DS:35:ILE:HD12	2.00	0.43
1:AA:109:A:H2'	1:AA:326:G:N2	2.33	0.43
1:AA:429:U:H4'	1:AA:430:A:O5'	2.18	0.43
30:BG:179:PRO:HG3	50:B4:43:TYR:OH	2.18	0.43
7:AG:65:ALA:O	7:AG:69:VAL:HG23	2.17	0.43
14:CN:3:ARG:O	14:CN:7:ILE:HG23	2.17	0.43
39:DT:78:LEU:HD12	39:DT:79:HIS:NE2	2.33	0.43
25:BA:956:A:C5	36:BQ:13:GLN:HG3	2.53	0.43
16:CP:8:ARG:HB3	16:CP:28:ARG:NH1	2.32	0.43
1:CA:1352:C:H2'	1:CA:1353:G:C8	2.52	0.43
2:AB:155:LEU:HD11	2:AB:159:PRO:HD3	2.00	0.43
25:DA:2590:A:OP2	27:DD:238:GLY:HA2	2.18	0.43
1:CA:1040:U:H2'	1:CA:1041:A:H5''	2.00	0.43
25:DA:2133:G:HO2'	25:DA:2134:A:P	2.42	0.43
25:DA:2135:A:C6	25:DA:2136:C:N4	2.86	0.43
10:AJ:13:HIS:HB3	10:AJ:68:HIS:CE1	2.54	0.43
23:CY:5:G:H1	23:CY:68:C:N4	2.12	0.43
25:DA:468:G:H5''	29:DF:60:SER:HB2	2.00	0.43
3:CC:130:VAL:O	3:CC:134:ILE:HG12	2.18	0.43
29:DF:116:ASP:OD2	35:DP:1:MET:N	2.40	0.43
25:BA:1476:C:H2'	25:BA:1477:U:C6	2.52	0.43
1:AA:532:A:N6	1:AA:1206:G:O2'	2.52	0.43
25:BA:692:C:H2'	25:BA:693:G:O4'	2.18	0.43
25:DA:1038:C:C4	25:DA:1039:G:N7	2.86	0.43
30:BG:16:ARG:HB2	30:BG:17:PRO:HD3	1.99	0.43
25:DA:2538:C:H2'	25:DA:2539:C:H6	1.83	0.43
25:DA:182:A:N3	25:DA:433:C:O2'	2.45	0.43
41:DV:55:ALA:HA	41:DV:100:ARG:O	2.18	0.43
25:BA:1547:C:O4'	27:BD:100:GLY:HA2	2.17	0.43
25:DA:1157:G:C2	25:DA:1158:C:C2	3.06	0.43
7:CG:22:LEU:HG	7:CG:62:PHE:CE2	2.54	0.43
25:DA:11:G:N7	61:DA:4572:HOH:O	2.36	0.43
1:CA:393:A:OP2	16:CP:12:LYS:HD2	2.17	0.43
45:BZ:19:ARG:NH1	45:BZ:84:GLU:O	2.51	0.43
1:CA:875:C:H1'	8:CH:15:ASN:HD21	1.82	0.43
25:DA:662:G:H5''	35:DP:16:ARG:HG2	2.00	0.43
25:DA:141:A:C8	25:DA:1408:C:O2'	2.70	0.43
25:BA:2651:A:OP2	61:BA:4267:HOH:O	2.21	0.43
15:CO:82:ILE:HB	15:CO:87:ILE:HB	2.00	0.43
1:AA:44:G:C2	1:AA:45:U:H1'	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:159:G:N2	1:AA:161:A:H3'	2.33	0.43
36:DQ:16:ARG:HG3	36:DQ:17:LEU:H	1.82	0.43
25:DA:196:A:H2'	25:DA:196:A:N3	2.33	0.43
8:AH:72:PRO:O	8:AH:74:PRO:HD3	2.19	0.43
1:AA:7:G:H5'	1:AA:298:A:O4'	2.18	0.43
19:CS:64:GLU:HB2	50:D4:59:PHE:CE1	2.53	0.43
49:B3:19:GLN:OE1	49:B3:52:HIS:NE2	2.48	0.43
1:CA:60:A:N6	1:CA:110:C:N3	2.64	0.43
17:CQ:81:ARG:NH2	17:CQ:84:LEU:HD21	2.32	0.43
25:BA:2879:G:H2'	25:BA:2880:C:O4'	2.19	0.43
12:CL:11:VAL:HG11	17:CQ:36:ILE:HG21	2.00	0.43
50:B4:40:HIS:HA	50:B4:41:PRO:HD2	1.70	0.43
16:AP:48:TRP:HH2	16:AP:76:GLN:HE22	1.65	0.43
4:CD:88:VAL:HA	5:CE:97:GLY:HA3	1.99	0.43
12:AL:39:VAL:HG11	12:AL:41:ARG:NH1	2.33	0.43
25:DA:614(B):G:H2'	29:DF:44:ARG:HH11	1.82	0.43
20:CT:63:ILE:HD13	20:CT:80:ARG:HB3	1.99	0.43
25:BA:1501:U:O2'	25:BA:1502:G:N7	2.51	0.43
25:DA:2753:A:N3	55:D9:15:LYS:NZ	2.64	0.43
25:DA:2018:G:H2'	25:DA:2019:A:O4'	2.18	0.43
54:B8:62:LEU:HB3	54:B8:65:GLU:HG2	2.00	0.43
44:DY:35:TYR:CE2	44:DY:69:ALA:HB3	2.54	0.43
25:BA:201:G:H2'	25:BA:202:A:O4'	2.19	0.43
1:AA:1317:C:N3	19:AS:37:ARG:NH2	2.65	0.43
14:AN:24:CYS:HB2	14:AN:40:CYS:HB3	1.99	0.43
1:CA:719:C:N4	18:CR:71:LYS:HE2	2.33	0.43
23:CW:32:PSU:H2'	23:CW:32:PSU:O4	2.18	0.43
25:BA:645:G:N3	25:BA:645:G:H5'	2.33	0.43
25:DA:207:A:H2'	25:DA:208:C:O4'	2.18	0.43
38:DS:5:THR:OG1	38:DS:8:GLU:OE2	2.23	0.43
25:DA:94(A):G:C6	25:DA:95:G:C5	3.06	0.43
1:CA:1134:G:N3	1:CA:1134:G:H2'	2.33	0.43
25:DA:616:G:OP2	29:DF:106:ARG:NE	2.40	0.43
25:DA:2507:C:H2'	25:DA:2508:G:O4'	2.18	0.43
1:AA:1493:A:H5''	1:AA:1494:G:OP2	2.19	0.43
25:DA:1359:A:N1	25:DA:1372:U:O4	2.52	0.43
25:DA:140:G:N2	25:DA:1596:A:H4'	2.34	0.43
25:DA:866:A:C2	25:DA:867:C:C5	3.06	0.43
11:AK:48:ILE:O	11:AK:50:TYR:N	2.46	0.43
25:DA:974:G:N2	25:DA:989:G:H1'	2.34	0.43
6:AF:2:ARG:NE	6:AF:69:GLU:HG2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AK:34:ASP:OD2	11:AK:38:ASN:HB2	2.18	0.43
1:AA:1346:A:N6	1:AA:1375:A:OP2	2.51	0.43
26:BB:13:A:N1	26:BB:69:G:O2'	2.40	0.43
25:DA:1886:C:H2'	25:DA:1887:C:H6	1.84	0.43
29:DF:178:PRO:HB3	29:DF:198:ALA:HA	2.00	0.43
25:DA:2096:U:H2'	25:DA:2097:C:C6	2.54	0.43
1:AA:481:G:O2'	1:AA:483:C:N4	2.48	0.43
10:AJ:40:LEU:HB2	10:AJ:69:ASN:HB2	2.00	0.43
25:DA:2391:G:O6	25:DA:2425:A:H8	2.02	0.43
25:DA:2854:G:H2'	25:DA:2855:C:C6	2.53	0.43
26:BB:114:C:H4'	38:BS:46:VAL:HG22	2.00	0.43
25:BA:1490:G:N2	25:BA:1595:C:C2	2.87	0.43
25:BA:1921:G:H2'	25:BA:1921:G:N3	2.33	0.43
25:DA:2243:U:H2'	25:DA:2244:U:C6	2.54	0.43
1:AA:814:A:H2'	1:AA:816:A:H5''	2.00	0.43
19:AS:30:LEU:HG	19:AS:31:ILE:N	2.33	0.43
1:CA:552:U:O3'	12:CL:87:GLY:HA3	2.19	0.43
51:D5:16:ARG:HG2	51:D5:16:ARG:NH1	2.34	0.43
10:CJ:16:LEU:HD23	10:CJ:16:LEU:HA	1.85	0.43
25:DA:2572:A:N7	28:DE:144:ARG:HD2	2.33	0.43
43:BX:92:LEU:HA	43:BX:92:LEU:HD12	1.79	0.43
1:CA:694:A:N1	1:CA:787:A:O2'	2.52	0.43
3:CC:109:PRO:C	3:CC:111:LEU:H	2.22	0.43
25:DA:820:A:N3	25:DA:943:U:H4'	2.33	0.43
8:AH:25:ASP:OD1	8:AH:60:ARG:HG3	2.18	0.43
26:BB:7:G:C5'	26:BB:7:G:H8	2.32	0.43
25:DA:1155:A:H5''	40:DU:55:ARG:HD3	2.00	0.43
7:CG:15:ASP:O	7:CG:19:GLY:HA2	2.18	0.43
7:CG:15:ASP:OD1	7:CG:20:ASP:N	2.43	0.43
25:DA:637:A:H8	35:DP:117:GLU:HG3	1.84	0.43
25:BA:2346:G:H4'	25:BA:2347:A:OP2	2.19	0.43
25:DA:253:C:OP2	54:D8:5:LYS:NZ	2.38	0.43
17:CQ:54:GLY:O	17:CQ:81:ARG:N	2.46	0.43
30:BG:11:TYR:CZ	30:BG:16:ARG:HD3	2.54	0.43
25:DA:658:C:H2'	25:DA:659:C:C6	2.53	0.43
2:CB:76:GLN:HG3	2:CB:206:ASP:O	2.18	0.43
4:CD:166:LYS:HD3	4:CD:166:LYS:HA	1.73	0.43
25:DA:2693:A:H2'	25:DA:2694:G:C8	2.54	0.43
2:AB:170:GLU:HB3	2:AB:173:ALA:HB3	2.01	0.43
2:AB:87:ARG:NE	2:AB:233:SER:HB3	2.33	0.43
25:BA:180:A:H2'	25:BA:181:C:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:699:A:H2'	25:DA:700:G:O4'	2.17	0.43
25:DA:567:A:H4'	25:DA:808:G:OP1	2.19	0.43
41:BV:21:ARG:HG2	41:BV:91:TYR:CD1	2.54	0.43
25:DA:456:C:H4'	61:DA:4011:HOH:O	2.18	0.43
1:CA:189(D):C:H2'	1:CA:189(E):U:O4'	2.19	0.43
25:BA:2334:A:H2'	25:BA:2335:G:O4'	2.19	0.43
13:CM:115:LYS:HB2	13:CM:115:LYS:HE2	1.72	0.43
5:AE:31:LEU:HD23	5:AE:31:LEU:HA	1.91	0.43
4:AD:107:ARG:HD2	4:AD:107:ARG:HA	1.88	0.43
25:DA:2685:G:P	39:DT:51:ARG:HH12	2.42	0.43
25:DA:763:G:H1'	25:DA:765:G:O4'	2.18	0.43
13:CM:19:LEU:HD21	13:CM:56:LEU:HD11	2.00	0.43
32:DI:88:ILE:O	32:DI:121:LYS:NZ	2.34	0.43
1:AA:269:C:H2'	1:AA:270:A:C8	2.54	0.43
17:CQ:13:ASP:C	17:CQ:15:MET:H	2.20	0.43
1:CA:979:C:H2'	1:CA:980:C:H5'	2.01	0.43
28:BE:51:PHE:O	28:BE:77:ILE:HD12	2.18	0.43
25:DA:1833:U:O2'	25:DA:1969:A:N1	2.45	0.43
25:DA:1693:U:O2'	25:DA:1695:G:O6	2.32	0.43
23:CY:56:C:H2'	23:CY:57:G:C8	2.35	0.43
1:CA:1004:A:N6	1:CA:1037:C:N3	2.66	0.43
1:CA:1150:U:C2'	1:CA:1151:A:H5'	2.48	0.43
45:DZ:111:VAL:CG2	45:DZ:117:LEU:HB2	2.49	0.43
1:AA:664:G:N2	1:AA:741:G:H1	2.11	0.43
2:CB:219:VAL:HA	2:CB:222:ILE:HG12	2.01	0.43
1:CA:580:U:H5''	15:CO:58:MET:HG2	2.01	0.43
4:AD:173:TRP:CZ3	4:AD:174:LEU:HG	2.53	0.43
29:DF:64:ILE:HG21	29:DF:78:ILE:HG23	1.99	0.43
8:AH:64:LYS:HG2	8:AH:79:VAL:HG21	1.99	0.43
29:DF:117:ARG:HH12	35:DP:1:MET:N	2.16	0.43
25:DA:1371:G:H2'	25:DA:1372:U:H5	1.83	0.43
25:DA:812:C:H1'	25:DA:1250:G:C2	2.53	0.43
29:BF:164:ARG:HD2	29:BF:175:THR:HG23	2.00	0.43
25:BA:2168:C:H4'	25:BA:2169:G:C4	2.54	0.43
25:DA:1608:A:H1'	25:DA:1610:A:OP2	2.19	0.43
25:BA:2627:U:H2'	25:BA:2628:C:C6	2.54	0.43
1:CA:1410:G:H2'	1:CA:1411:C:H6	1.83	0.43
25:BA:1810:U:H2'	61:BA:5150:HOH:O	2.17	0.43
25:BA:9:U:O4	25:BA:2641:A:H2	2.02	0.43
1:AA:232:G:H1'	1:AA:262:A:N1	2.33	0.43
1:CA:603:U:H2'	1:CA:604:G:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:D4:40:HIS:HA	50:D4:41:PRO:HD2	1.79	0.43
13:AM:15:VAL:HG22	13:AM:43:THR:O	2.18	0.43
1:AA:936:C:H2'	1:AA:937:A:O4'	2.18	0.43
25:BA:313:A:N6	25:BA:375:G:O2'	2.52	0.43
30:BG:121:ASN:HA	30:BG:122:PRO:HD3	1.90	0.43
25:DA:244:A:C2	25:DA:255:A:C4	3.07	0.43
1:CA:308:C:H2'	1:CA:309:G:C8	2.54	0.43
20:CT:18:GLN:O	20:CT:22:ARG:HG3	2.19	0.43
1:CA:1297:C:H1'	1:CA:1298:C:H5	1.83	0.43
53:D7:1:MET:HB2	53:D7:1:MET:HE2	1.88	0.43
25:BA:609:A:N1	25:BA:856:G:O2'	2.44	0.43
39:DT:60:THR:HG22	39:DT:77:PRO:HA	2.00	0.43
25:DA:1688:U:O2	25:DA:1700:A:H5'	2.19	0.43
1:AA:890:G:O2'	1:AA:906:G:O6	2.18	0.43
25:BA:1994:A:H2'	25:BA:1995:G:H8	1.83	0.43
25:DA:2802:G:H2'	25:DA:2803:C:O4'	2.19	0.43
52:D6:10:LEU:HG	52:D6:54:ILE:HG13	2.00	0.43
23:AY:71:G:H2'	23:AY:72:C:C6	2.54	0.43
23:AY:25:C:H2'	23:AY:26:A:C8	2.54	0.43
2:CB:42:ILE:HG21	2:CB:202:PRO:O	2.19	0.43
38:BS:15:ARG:HE	38:BS:88:ASP:CG	2.19	0.43
45:DZ:108:PRO:HG3	45:DZ:141:VAL:HB	2.00	0.43
1:CA:788:U:O3'	57:CA:3178:PCY:H25	2.18	0.43
32:BI:93:THR:O	32:BI:97:ILE:HG13	2.19	0.43
37:DR:97:VAL:CG2	37:DR:114:VAL:HG13	2.49	0.43
25:DA:2722:G:H2'	25:DA:2723:C:C6	2.53	0.43
31:DH:8:PRO:HA	31:DH:51:ARG:HG2	2.00	0.43
1:AA:1149:C:H2'	1:AA:1150:U:C6	2.53	0.43
1:AA:974:A:OP1	1:AA:974:A:H8	2.01	0.43
25:DA:1528(A):A:H2'	25:DA:1529:G:O4'	2.19	0.43
29:BF:150:GLY:HA2	29:BF:172:TRP:CE3	2.53	0.43
25:DA:1418:G:OP1	25:DA:1588:C:H4'	2.19	0.43
27:BD:145:VAL:HB	27:BD:155:LEU:HB2	2.00	0.43
4:AD:99:SER:O	4:AD:140:VAL:HG23	2.19	0.43
1:AA:1302:U:C5	13:AM:17:VAL:HG21	2.53	0.43
38:DS:93:LYS:HD3	38:DS:95:HIS:HB2	1.99	0.43
3:AC:19:GLU:HB3	3:AC:40:ARG:NH2	2.34	0.43
25:BA:2284:U:H5''	25:BA:2285:A:OP1	2.18	0.43
36:BQ:16:ARG:HG2	36:BQ:18:LYS:HE2	2.00	0.43
25:DA:892:G:H2'	25:DA:893:C:O4'	2.19	0.43
25:DA:2729:G:C6	25:DA:2730:C:C4	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:130:A:H1'	1:CA:263:A:O2'	2.18	0.43
4:AD:157:LEU:HD22	4:AD:161:ASN:ND2	2.34	0.43
41:BV:62:LEU:HD21	41:BV:95:LEU:HB2	2.01	0.43
25:BA:2102:G:OP1	47:B1:35:THR:HG21	2.18	0.43
1:CA:707:C:H2'	1:CA:708:C:C6	2.53	0.43
34:BO:115:VAL:HG13	34:BO:121:VAL:HG21	2.01	0.43
19:CS:66:MET:HB2	19:CS:74:PHE:CZ	2.54	0.43
27:DD:80:ALA:HB3	27:DD:94:LEU:HB3	2.01	0.43
25:BA:561:A:H2'	25:BA:562:C:C6	2.54	0.43
11:CK:80:VAL:HG13	11:CK:103:LEU:HD12	1.99	0.43
39:BT:60:THR:HG22	39:BT:77:PRO:HA	1.99	0.43
25:BA:1587:U:H2'	25:BA:1588:G:O4'	2.18	0.43
33:BN:34:LEU:HD21	33:BN:120:LEU:HB2	2.01	0.43
44:BY:14:LEU:HB2	44:BY:75:ILE:HD11	2.01	0.43
45:BZ:151:HIS:O	45:BZ:153:SER:N	2.49	0.43
25:DA:2238:G:H2'	25:DA:2238:G:N3	2.33	0.43
35:DP:138:LEU:HD23	35:DP:145:PRO:HG3	2.01	0.43
1:AA:1164:G:H2'	1:AA:1165:C:C6	2.53	0.43
25:DA:2487:G:H2'	25:DA:2488:A:C8	2.53	0.43
25:BA:964:A:H5''	26:BB:98:G:O2'	2.19	0.43
25:DA:686:G:N2	25:DA:788:A:H61	2.17	0.43
25:DA:2432:A:C6	25:DA:2433:A:C6	3.07	0.43
1:AA:456:C:H2'	1:AA:457:C:C6	2.53	0.43
30:BG:49:ASP:O	30:BG:51:ARG:N	2.51	0.43
52:B6:40:CYS:HA	52:B6:41:PRO:HD3	1.84	0.43
1:AA:1316:G:H22	1:AA:1319:A:H5''	1.84	0.43
25:DA:2026:C:H2'	25:DA:2027:G:O4'	2.19	0.43
36:DQ:135:ASP:OD2	45:DZ:49:ARG:NH2	2.51	0.43
12:CL:113:ARG:NE	12:CL:115:LYS:O	2.43	0.43
9:CI:5:TYR:OH	9:CI:16:ARG:HG2	2.19	0.43
3:CC:180:ALA:O	3:CC:181:ASN:C	2.56	0.43
25:DA:2683:C:H4'	28:DE:13:ARG:CZ	2.49	0.43
20:CT:50:GLU:O	20:CT:100:ILE:HD11	2.18	0.43
25:DA:1741:A:H2'	25:DA:1742:G:O4'	2.18	0.43
25:DA:2875:C:OP1	39:DT:3:ARG:NH2	2.51	0.43
13:AM:2:ALA:N	13:AM:8:GLU:OE1	2.52	0.43
37:DR:2:ARG:HG2	37:DR:5:LYS:HB2	2.01	0.43
25:DA:2787:C:H1'	28:DE:62:PRO:HG3	2.01	0.43
25:DA:576:U:H2'	25:DA:577:G:C8	2.54	0.43
1:CA:1054:C:C4	23:CW:34:G:H1'	2.54	0.43
28:DE:9:VAL:HG13	28:DE:25:VAL:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AW:62:C:H2'	23:AW:63:G:C8	2.54	0.43
25:BA:2398:C:H2'	25:BA:2399:U:C6	2.54	0.43
44:DY:43:ASN:OD1	44:DY:65:ALA:HB3	2.19	0.43
42:BW:4:LYS:HE2	42:BW:6:ILE:HD11	2.00	0.43
25:DA:1164:G:H2'	25:DA:1165:U:C6	2.54	0.43
25:BA:200:A:H2'	25:BA:201:G:O4'	2.18	0.43
25:DA:2443:C:H2'	25:DA:2444:G:H8	1.84	0.43
28:DE:1:MET:HE1	28:DE:199:ARG:HD2	2.00	0.43
3:AC:45:LYS:HG3	3:AC:46:GLU:N	2.34	0.43
25:DA:1533:G:H22	25:DA:1536:C:H1'	1.82	0.43
11:CK:38:ASN:HA	11:CK:39:PRO:HD3	1.77	0.43
25:DA:1363:C:H2'	25:DA:1364:G:H8	1.82	0.43
25:BA:212:A:O4'	25:BA:449:A:H5'	2.19	0.43
25:BA:2897:U:H2'	25:BA:2898:C:C6	2.54	0.43
28:BE:40:GLU:CD	28:BE:40:GLU:H	2.22	0.43
2:AB:196:LEU:HA	2:AB:196:LEU:HD12	1.80	0.43
29:DF:93:LYS:HD3	29:DF:93:LYS:HA	1.79	0.43
25:BA:2250:G:H2'	25:BA:2250:G:N3	2.34	0.43
1:CA:228:A:H2'	1:CA:229:U:O4'	2.19	0.43
1:AA:1240:U:O2'	7:AG:32:ARG:NH2	2.51	0.43
18:AR:32:ARG:HA	18:AR:69:THR:HG21	2.01	0.43
1:CA:789:U:H2'	1:CA:791:G:OP2	2.19	0.43
25:BA:1440:U:H2'	25:BA:1441:A:O4'	2.19	0.43
5:AE:145:LYS:O	5:AE:149:GLU:HG2	2.19	0.43
23:AY:54:5MU:C4	23:AY:55:PSU:C2	3.07	0.43
1:AA:1315:U:H2'	1:AA:1316:G:O4'	2.19	0.43
25:DA:2141:G:C8	25:DA:2151:G:N2	2.86	0.43
25:BA:323:A:N1	25:BA:346:A:O2'	2.43	0.43
8:CH:119:LEU:HB3	8:CH:123:GLU:HB3	2.01	0.43
2:CB:98:LEU:HB2	2:CB:101:MET:HG3	2.01	0.43
11:AK:99:GLN:HE21	11:AK:108:ILE:HD11	1.83	0.43
44:BY:6:HIS:HE1	44:BY:72:VAL:O	2.02	0.43
1:AA:1118:C:H2'	1:AA:1119:C:C6	2.53	0.43
1:AA:411:A:OP2	4:AD:30:LYS:HD2	2.19	0.43
15:AO:61:GLY:O	15:AO:65:ARG:HG3	2.19	0.43
7:CG:26:PHE:O	7:CG:30:ILE:HG13	2.18	0.43
44:DY:86:ARG:NH1	44:DY:100:ALA:HB1	2.34	0.43
31:DH:116:GLU:HA	31:DH:117:PRO:HD3	1.79	0.43
49:D3:7:LYS:HE3	49:D3:32:GLN:NE2	2.34	0.43
25:DA:2086:U:H2'	25:DA:2087:G:C8	2.54	0.43
1:CA:1258:G:O2'	1:CA:1259:C:H5'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:1566:U:H2'	25:BA:1567:G:O4'	2.19	0.43
1:AA:955:U:O2'	19:AS:83:HIS:HD2	2.01	0.43
25:BA:596:G:N1	25:BA:2053:A:OP2	2.38	0.43
12:CL:39:VAL:HG11	12:CL:41:ARG:NH1	2.34	0.43
27:BD:5:LYS:HE3	27:BD:5:LYS:HB3	1.80	0.43
25:DA:845:G:N2	25:DA:845:G:OP2	2.41	0.43
27:DD:5:LYS:HE3	27:DD:5:LYS:HB3	1.81	0.43
1:CA:347:G:H8	1:CA:347:G:OP2	2.01	0.43
6:AF:81:ILE:HD11	27:BD:125:ILE:HB	2.00	0.43
1:CA:1236:A:H2'	1:CA:1237:C:C6	2.54	0.43
28:BE:119:ARG:HD2	28:BE:120:TRP:CE2	2.54	0.43
25:BA:343:C:H2'	25:BA:344:A:O4'	2.19	0.43
1:CA:1005:A:H5''	1:CA:1006:C:C5	2.54	0.42
25:DA:2161:C:H2'	25:DA:2162:G:C8	2.54	0.42
25:DA:959:A:N3	25:DA:2457:U:O2'	2.43	0.42
10:CJ:8:LEU:CD2	10:CJ:96:ILE:HG12	2.49	0.42
13:AM:84:ILE:HD12	19:AS:74:PHE:CZ	2.54	0.42
25:DA:271(H):G:O6	25:DA:271(Q):G:C6	2.72	0.42
4:CD:112:VAL:HG22	4:CD:116:GLN:OE1	2.18	0.42
25:DA:265:A:C8	25:DA:266:G:HI1'	2.54	0.42
25:BA:1831:C:OP2	27:BD:183:ARG:NH2	2.51	0.42
1:CA:170:U:O2'	1:CA:171:A:H5'	2.19	0.42
25:BA:1087:C:H42	25:BA:1160:G:H1	1.67	0.42
26:DB:80:U:H2'	26:DB:81:G:N7	2.34	0.42
2:AB:178:ARG:HH22	8:AH:68:ARG:HH12	1.66	0.42
25:DA:511:U:O4	25:DA:512:G:N1	2.51	0.42
1:AA:154:C:N3	1:AA:168:G:C2	2.87	0.42
31:DH:56:SER:HB3	31:DH:61:HIS:ND1	2.33	0.42
21:CU:9:ARG:O	21:CU:13:ILE:HG13	2.18	0.42
1:AA:448:A:O5'	1:AA:485:G:N2	2.45	0.42
1:CA:376:G:H5''	16:CP:5:ARG:HB2	2.00	0.42
1:CA:1226:C:H4'	19:CS:80:TYR:CZ	2.53	0.42
2:AB:73:THR:OG1	2:AB:170:GLU:OE1	2.31	0.42
1:CA:1236:A:O2'	1:CA:1304:G:H4'	2.19	0.42
1:AA:553:A:H2'	1:AA:554:C:C6	2.54	0.42
25:DA:2350:C:H2'	25:DA:2351:G:O4'	2.19	0.42
44:BY:98:VAL:HG12	44:BY:105:ALA:HA	2.00	0.42
1:CA:1432:G:O6	61:CA:4070:HOH:O	2.21	0.42
5:AE:152:ARG:NH2	8:AH:107:LEU:O	2.52	0.42
25:DA:2543:G:H2'	25:DA:2544:G:C8	2.54	0.42
31:BH:97:ARG:NE	31:BH:104:GLU:OE1	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:DI:12:LEU:HD22	32:DI:19:VAL:HG21	2.01	0.42
25:DA:152:G:H2'	25:DA:153:C:C6	2.54	0.42
1:AA:113:G:H2'	1:AA:114:U:C6	2.54	0.42
25:DA:446:G:OP1	40:DU:3:ARG:NH1	2.52	0.42
24:AX:12:G:H4'	25:BA:1930:C:O2	2.19	0.42
35:DP:82:GLY:HA2	35:DP:113:LYS:O	2.19	0.42
41:DV:28:GLU:HG2	41:DV:28:GLU:H	1.58	0.42
44:BY:19:LYS:HB3	44:BY:19:LYS:HE2	1.90	0.42
25:BA:2724:U:OP1	25:BA:2727:G:H4'	2.19	0.42
25:DA:775:G:N3	61:DA:4545:HOH:O	2.37	0.42
52:B6:37:ARG:O	52:B6:38:LYS:HD2	2.19	0.42
2:CB:67:THR:HG22	2:CB:90:MET:HE2	2.01	0.42
2:CB:16:HIS:CG	2:CB:17:PHE:N	2.87	0.42
30:DG:33:ARG:O	30:DG:161:THR:HG23	2.19	0.42
25:DA:1010:A:N3	25:DA:1153:C:H1'	2.35	0.42
3:AC:6:HIS:CD2	3:AC:8:ILE:HB	2.54	0.42
25:DA:1012:U:O2	33:DN:25:ARG:NH2	2.50	0.42
1:AA:149:A:H2'	1:AA:150:C:H6	1.84	0.42
38:BS:59:LYS:CD	38:BS:60:GLY:H	2.30	0.42
38:DS:10:ARG:O	38:DS:14:VAL:HG13	2.19	0.42
1:AA:993:G:H2'	1:AA:995:C:H41	1.84	0.42
25:DA:2203:U:O4'	27:DD:151:LYS:HE2	2.19	0.42
25:BA:1846:A:OP1	25:BA:1846:A:H8	2.02	0.42
27:DD:132:PRO:HG2	27:DD:135:PHE:HD2	1.80	0.42
25:DA:2184:G:H2'	25:DA:2185:C:C6	2.54	0.42
25:BA:239:G:C6	25:BA:240:A:C6	3.08	0.42
25:DA:2820:A:OP1	37:DR:2:ARG:NH2	2.51	0.42
1:CA:581:G:O2'	1:CA:582:U:H5'	2.19	0.42
25:DA:2648:C:H2'	25:DA:2649:U:H6	1.83	0.42
13:AM:96:LEU:C	13:AM:110:ARG:HG2	2.39	0.42
25:DA:117:G:C6	25:DA:119:A:N6	2.87	0.42
25:DA:1027:A:C2	25:DA:2488:A:H5'	2.54	0.42
25:BA:2724:U:H2'	25:BA:2727:G:H5''	2.00	0.42
3:AC:22:TRP:CZ2	14:AN:54:PRO:HG3	2.55	0.42
1:CA:619:U:N3	4:CD:134:ASP:OD1	2.45	0.42
3:AC:35:GLU:CD	3:AC:59:ARG:HH22	2.22	0.42
25:DA:1255:U:O5'	25:DA:1256:G:H5''	2.20	0.42
44:DY:52:SER:HB2	44:DY:53:PRO:HD2	2.02	0.42
1:CA:859:A:H2'	1:CA:860:A:O4'	2.19	0.42
25:DA:1268:A:C2	25:DA:2013:A:C4	3.06	0.42
25:DA:1903:G:OP1	27:DD:241:PRO:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1446:U:O2'	1:AA:1447:A:O5'	2.37	0.42
29:DF:31:HIS:HB2	35:DP:9:ASN:OD1	2.20	0.42
23:AY:51:U:O2	23:AY:63:G:N2	2.47	0.42
1:CA:1005:A:H5''	1:CA:1006:C:C6	2.53	0.42
25:BA:1093:G:H2'	25:BA:1156:G:N2	2.34	0.42
1:CA:1142:G:H2'	1:CA:1143:G:O4'	2.18	0.42
2:AB:88:ALA:O	2:AB:226:ARG:NH1	2.52	0.42
1:CA:93:G:O2'	1:CA:96:U:H5'	2.19	0.42
1:CA:97:G:HO2'	1:CA:98:G:P	2.42	0.42
25:DA:529:A:H62	25:DA:2041:U:H3	1.67	0.42
36:DQ:111:GLU:CD	36:DQ:133:ARG:HH21	2.18	0.42
31:DH:3:ARG:CZ	31:DH:5:GLY:H	2.32	0.42
15:AO:56:LEU:O	15:AO:60:VAL:HG23	2.19	0.42
25:BA:302:A:HO2'	25:BA:303:C:P	2.40	0.42
25:BA:1857:G:H2'	25:BA:1858:C:O4'	2.18	0.42
9:CI:89:ASN:O	9:CI:92:TYR:HB2	2.19	0.42
25:DA:784:A:C8	25:DA:792:G:C5	3.07	0.42
25:DA:566:U:H5''	35:DP:29:LYS:HE3	2.01	0.42
25:DA:39:C:H2'	25:DA:40:C:H6	1.82	0.42
25:DA:580:C:H2'	25:DA:581:C:C6	2.53	0.42
35:DP:45:LEU:HD22	35:DP:45:LEU:HA	1.61	0.42
1:CA:300:A:H1'	1:CA:565:U:O2	2.19	0.42
31:DH:44:VAL:HG12	31:DH:46:GLU:HG2	2.00	0.42
25:DA:1668:A:O2'	25:DA:1674:G:N7	2.43	0.42
25:DA:208:C:H2'	25:DA:209:C:C6	2.54	0.42
1:CA:828:A:H5''	1:CA:859:A:C2	2.54	0.42
35:BP:98:GLU:OE1	35:BP:102:ARG:NH1	2.53	0.42
25:DA:411:G:C5	35:DP:72:PRO:HB3	2.54	0.42
5:CE:91:LEU:HG	5:CE:118:ILE:HD11	2.02	0.42
27:BD:228:PRO:HD3	27:BD:235:GLY:CA	2.49	0.42
30:BG:67:LYS:HE3	30:BG:68:PRO:O	2.19	0.42
6:AF:6:VAL:HG13	6:AF:90:VAL:HG22	2.01	0.42
7:CG:59:LEU:HD11	7:CG:63:LYS:HE2	2.00	0.42
31:DH:38:SER:HA	31:DH:39:PRO:HD3	1.83	0.42
8:CH:20:TYR:HA	8:CH:65:TYR:CZ	2.54	0.42
44:DY:38:ILE:HD11	44:DY:66:PRO:HG3	2.00	0.42
35:DP:88:LEU:HD11	35:DP:114:ILE:HD12	2.01	0.42
1:CA:1494:G:HO2'	25:DA:1912:A:HO2'	1.66	0.42
2:AB:76:GLN:H	2:AB:76:GLN:CD	2.21	0.42
45:BZ:150:LEU:HA	45:BZ:150:LEU:HD12	1.86	0.42
1:AA:1343:G:H2'	1:AA:1344:C:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AM:80:ARG:HH21	19:AS:69:HIS:HE1	1.66	0.42
29:DF:13:SER:OG	29:DF:16:GLY:O	2.23	0.42
25:DA:1308:A:H2'	25:DA:1309:G:O4'	2.19	0.42
1:CA:978:A:O2'	1:CA:1322:C:N3	2.40	0.42
33:BN:108:PRO:O	33:BN:113:GLY:HA3	2.18	0.42
1:CA:1510:U:H2'	1:CA:1511:G:C8	2.54	0.42
1:CA:1241:G:H2'	1:CA:1242:C:C6	2.54	0.42
25:BA:1081:U:H2'	25:BA:1082:G:C8	2.53	0.42
1:CA:1022:G:C6	1:CA:1023:G:C6	3.07	0.42
1:CA:1353:G:C2	1:CA:1370:G:C2	3.07	0.42
23:CW:68:C:H2'	23:CW:69:G:H8	1.85	0.42
1:AA:975:A:C8	1:AA:975:A:H5'	2.53	0.42
25:BA:1700:G:O3'	37:BR:2:ARG:HB2	2.18	0.42
19:AS:63:THR:O	19:AS:66:MET:HG2	2.18	0.42
25:DA:2328:A:H2'	25:DA:2329:G:C8	2.55	0.42
23:CY:12:U:C2	23:CY:13:C:H1'	2.53	0.42
4:AD:170:VAL:HG12	4:AD:174:LEU:HB2	2.01	0.42
27:BD:242:ARG:HG2	27:BD:246:PRO:HG3	2.01	0.42
15:AO:26:GLU:HG2	15:AO:26:GLU:H	1.38	0.42
25:DA:2847:U:OP1	39:DT:98:LYS:HE3	2.19	0.42
5:AE:36:ASP:OD2	5:AE:40:ARG:HB2	2.19	0.42
1:CA:1227:A:OP2	13:CM:111:LYS:HE3	2.19	0.42
1:CA:1262:C:H2'	1:CA:1263:C:H6	1.83	0.42
53:B7:11:LYS:HE3	53:B7:15:THR:OG1	2.18	0.42
25:BA:1199:C:OP1	40:BU:92:ARG:NH1	2.52	0.42
5:AE:148:VAL:HG21	8:AH:107:LEU:HB3	2.00	0.42
1:AA:377:G:OP1	16:AP:3:LYS:HD2	2.19	0.42
26:DB:89:G:C6	26:DB:90:A:C6	3.07	0.42
3:AC:142:MET:HG3	3:AC:170:GLN:HB3	2.00	0.42
25:DA:1618:A:H5'	61:DA:4351:HOH:O	2.19	0.42
25:DA:995:C:N3	33:DN:2:LYS:HA	2.34	0.42
1:CA:1366:C:H2'	1:CA:1367:C:C6	2.54	0.42
48:B2:32:LEU:HD13	48:B2:36:ARG:HH11	1.84	0.42
31:DH:106:THR:HG23	31:DH:112:PRO:HB3	2.01	0.42
25:DA:2740:A:C6	25:DA:2764:A:C8	3.07	0.42
25:DA:1473:G:C6	25:DA:1474:C:C4	3.07	0.42
25:BA:605:G:H2'	25:BA:606:G:C8	2.54	0.42
2:CB:82:ARG:HB3	2:CB:94:ASN:OD1	2.20	0.42
25:DA:598:G:C6	25:DA:599:G:C5	3.07	0.42
1:CA:532:A:HO2'	1:CA:533:A:P	2.37	0.42
33:DN:123:TYR:OH	33:DN:130:HIS:NE2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1003:G:H2'	1:CA:1004:A:H1'	2.01	0.42
25:DA:1171:G:H1	25:DA:1178:C:N4	2.06	0.42
25:DA:2271:G:OP1	46:D0:18:ALA:HB1	2.20	0.42
11:CK:93:GLN:CA	11:CK:93:GLN:HE21	2.28	0.42
25:DA:2134:A:O2'	25:DA:2135:A:OP1	2.37	0.42
25:DA:2136:C:O2'	25:DA:2137:C:H6	2.02	0.42
10:CJ:7:LYS:HB2	10:CJ:97:GLU:HB2	2.01	0.42
1:AA:922:G:N3	1:AA:1398:A:H2	2.18	0.42
1:CA:1319:A:H61	1:CA:1361:G:H21	1.67	0.42
45:BZ:111:VAL:HG13	45:BZ:117:LEU:H	1.84	0.42
28:BE:143:ASN:HD22	28:BE:147:PRO:CD	2.31	0.42
25:DA:2723:C:OP2	28:DE:109:LYS:NZ	2.52	0.42
35:DP:21:ARG:HA	35:DP:21:ARG:HD3	1.68	0.42
25:DA:570:G:H2'	25:DA:2030:A:N7	2.35	0.42
10:AJ:70:ARG:HA	10:AJ:70:ARG:HD3	1.71	0.42
25:DA:2659:G:H2'	25:DA:2661:G:OP2	2.19	0.42
1:AA:1219:U:OP1	14:AN:19:ARG:NH2	2.47	0.42
4:AD:138:TYR:HE1	4:AD:140:VAL:HA	1.83	0.42
37:DR:29:LEU:HA	37:DR:29:LEU:HD12	1.81	0.42
1:CA:519:C:H2'	1:CA:520:A:O4'	2.19	0.42
25:DA:1264:G:H2'	25:DA:2014:A:N6	2.33	0.42
31:DH:11:VAL:HG21	31:DH:50:VAL:HG23	2.02	0.42
25:DA:444:C:H4'	29:DF:49:ALA:HB2	2.01	0.42
4:CD:58:LEU:O	4:CD:62:GLN:HG2	2.19	0.42
25:BA:2699:U:H2'	25:BA:2700:U:O4'	2.20	0.42
1:CA:719:C:O2'	18:CR:49:LYS:HB3	2.20	0.42
1:CA:189(C):C:H2'	1:CA:189(D):C:O4'	2.20	0.42
12:AL:28:LYS:HE2	12:AL:64:TYR:CE1	2.54	0.42
25:BA:1549:U:H2'	25:BA:1550:C:C6	2.54	0.42
25:BA:1644:C:H2'	25:BA:1645:C:H6	1.85	0.42
25:BA:746:A:H2'	25:BA:747:G:O4'	2.20	0.42
31:DH:40:GLU:O	31:DH:55:PRO:HG3	2.20	0.42
1:CA:381:C:H2'	1:CA:382:A:O4'	2.19	0.42
1:CA:8:A:H5'	5:CE:101:ILE:HG22	2.01	0.42
25:BA:1683:C:H2'	25:BA:1684:A:C8	2.54	0.42
48:B2:22:GLU:OE2	48:B2:68:ARG:NH2	2.53	0.42
25:DA:856:C:O4'	46:D0:27:GLU:HB3	2.19	0.42
28:BE:116:VAL:HG13	28:BE:122:PHE:HB2	2.00	0.42
2:CB:130:ARG:HA	2:CB:131:PRO:HD3	1.92	0.42
24:CX:10:G:C2	24:CX:26:G:H1'	2.54	0.42
1:CA:429:U:H4'	1:CA:430:A:O5'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:241:C:C2	1:CA:286:G:C2	3.08	0.42
41:DV:8:GLY:O	41:DV:10:LYS:NZ	2.50	0.42
2:CB:210:SER:OG	2:CB:211:ILE:N	2.52	0.42
2:CB:211:ILE:O	2:CB:215:LEU:HB2	2.20	0.42
1:AA:1314:C:H2'	1:AA:1315:U:C6	2.54	0.42
1:CA:1064:G:H4'	1:CA:1065:U:O5'	2.20	0.42
1:CA:114:U:H1'	1:CA:353:A:H1'	2.02	0.42
2:AB:211:ILE:HG22	2:AB:215:LEU:HD12	2.00	0.42
1:AA:1030(A):G:O2'	1:AA:1030(C):G:N7	2.53	0.42
10:AJ:45:ARG:HG2	10:AJ:47:PHE:CZ	2.55	0.42
23:CW:61:C:OP2	23:CW:61:C:H2'	2.20	0.42
29:DF:64:ILE:HG13	29:DF:65:TRP:N	2.34	0.42
31:DH:69:ARG:HG3	31:DH:70:THR:N	2.33	0.42
2:CB:91:PRO:HA	2:CB:151:GLY:O	2.19	0.42
4:CD:158:ILE:HG22	4:CD:162:LEU:HD12	2.02	0.42
50:D4:33:VAL:HG12	50:D4:34:GLU:H	1.85	0.42
25:DA:1992:G:O5'	25:DA:1992:G:C8	2.73	0.42
25:BA:2576:A:C2	25:BA:2659:U:H4'	2.54	0.42
39:BT:33:LYS:HA	39:BT:42:ILE:HD13	2.00	0.42
9:CI:111:ARG:O	9:CI:113:LYS:HD2	2.19	0.42
29:DF:150:GLY:HA2	29:DF:172:TRP:CE3	2.54	0.42
25:DA:141:A:H8	25:DA:1408:C:O2'	2.01	0.42
25:DA:1027:A:N6	25:DA:1126:A:C4	2.87	0.42
8:CH:9:MET:SD	8:CH:32:LYS:HD3	2.59	0.42
25:BA:2418:U:H6	25:BA:2418:U:H2'	1.70	0.42
29:BF:132:VAL:HA	29:BF:138:GLU:HB3	2.01	0.42
1:CA:273:A:N6	1:CA:274:A:C6	2.87	0.42
1:AA:123:C:OP1	1:AA:311:C:O2'	2.32	0.42
1:AA:598:U:O4	61:AA:4079:HOH:O	2.21	0.42
25:DA:2393:A:H2'	25:DA:2394:C:O4'	2.19	0.42
47:B1:50:ARG:HG2	47:B1:59:THR:HB	2.02	0.42
16:AP:20:VAL:HG21	16:AP:32:TYR:CD2	2.55	0.42
1:CA:767:A:H2'	1:CA:768:A:O4'	2.20	0.42
25:DA:800:A:OP1	25:DA:800:A:H8	2.03	0.42
14:CN:24:CYS:HB2	14:CN:40:CYS:HB3	2.01	0.42
31:DH:121:ILE:HD11	31:DH:140:LYS:HG2	1.99	0.42
1:CA:1423:G:P	34:DO:49:ARG:HH12	2.42	0.42
1:AA:1316:G:N1	1:AA:1319:A:OP2	2.49	0.42
2:AB:69:LEU:HD12	2:AB:91:PRO:O	2.19	0.42
57:CA:3178:PCY:H24	57:CA:3178:PCY:H17	1.67	0.42
9:CI:16:ARG:HD3	9:CI:64:THR:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:2805:G:H2'	25:DA:2807:G:C8	2.54	0.42
25:DA:807:U:OP2	35:DP:41:ARG:NH2	2.52	0.42
35:DP:2:LYS:HG2	35:DP:5:ASP:OD2	2.20	0.42
45:BZ:111:VAL:O	45:BZ:113:ALA:N	2.49	0.42
31:DH:3:ARG:HB3	31:DH:6:ARG:HG2	2.01	0.42
31:DH:8:PRO:O	31:DH:69:ARG:NH1	2.53	0.42
4:CD:150:GLU:CD	4:CD:151:LYS:H	2.22	0.42
1:CA:1348:U:H4'	9:CI:120:ARG:HD2	2.02	0.42
37:BR:96:ARG:HD2	37:BR:115:GLU:OE1	2.20	0.42
25:BA:1405:A:C2	25:BA:1418:U:O4	2.72	0.42
4:AD:188:LEU:HA	4:AD:189:PRO:HD3	1.85	0.42
19:AS:36:ARG:HB3	19:AS:72:GLY:HA3	2.02	0.42
1:AA:757:U:O2'	1:AA:879:C:O2	2.34	0.42
20:CT:65:LYS:HA	20:CT:68:LYS:HD3	2.00	0.42
25:BA:1495:G:H1'	25:BA:1574:A:N1	2.34	0.42
29:BF:93:LYS:HD3	29:BF:93:LYS:HA	1.79	0.42
42:BW:9:TYR:HA	42:BW:100:THR:HG23	2.01	0.42
32:BI:57:ARG:O	32:BI:61:ARG:HD3	2.20	0.42
49:D3:7:LYS:HZ3	49:D3:34:GLU:HG3	1.84	0.42
1:AA:262:A:C6	1:AA:263:A:C6	3.08	0.42
1:AA:1169:A:H2'	1:AA:1170:A:C8	2.54	0.42
1:CA:189(D):C:H6	1:CA:189(D):C:O5'	2.03	0.42
25:DA:1794:U:H2'	25:DA:1795:C:C6	2.55	0.42
32:DI:93:THR:HG22	32:DI:119:PRO:HB3	2.01	0.42
1:CA:890:G:O2'	1:CA:906:G:O6	2.27	0.42
45:DZ:24:LEU:N	45:DZ:39:VAL:O	2.50	0.42
40:DU:97:ASP:OD1	40:DU:101:ARG:HD2	2.20	0.42
25:DA:2004:G:H2'	25:DA:2005:A:O4'	2.20	0.42
25:DA:1356:G:OP1	61:DA:4817:HOH:O	2.21	0.42
47:D1:78:LYS:HE3	47:D1:78:LYS:HB2	1.86	0.42
15:AO:17:ARG:HH11	15:AO:17:ARG:HG3	1.84	0.42
3:CC:112:SER:O	3:CC:116:VAL:HG23	2.20	0.42
25:BA:1527:G:C6	25:BA:1528:U:C4	3.08	0.42
1:CA:1278:U:H5'	1:CA:1279:A:C5'	2.50	0.42
45:DZ:111:VAL:HG22	45:DZ:174:VAL:HG22	2.02	0.42
25:DA:2061:G:H5''	25:DA:2503:A:C2	2.54	0.42
25:DA:796:C:H2'	25:DA:797:C:H6	1.80	0.42
53:D7:34:ARG:NH2	61:D7:203:HOH:O	2.53	0.42
13:CM:65:LYS:N	50:D4:50:VAL:HG21	2.35	0.42
25:DA:471:A:H2'	25:DA:472:A:O4'	2.20	0.42
1:AA:1118:C:H1'	1:AA:1179:A:C5	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:736:C:H2'	1:CA:737:A:C8	2.55	0.42
34:BO:6:THR:HG22	34:BO:8:LEU:HD22	2.01	0.42
25:BA:495:G:O6	53:B7:37:LYS:HE2	2.20	0.42
25:DA:921:G:H2'	25:DA:922:U:H6	1.85	0.42
25:BA:1553:A:O2'	25:BA:1554:A:O5'	2.25	0.42
5:CE:93:PRO:HG2	8:CH:105:ARG:HE	1.85	0.42
25:BA:1821:C:H5''	25:BA:1822:A:OP1	2.20	0.42
25:DA:141:A:H8	25:DA:1408:C:HO2'	1.57	0.42
47:D1:3:LYS:HB3	47:D1:4:VAL:H	1.58	0.42
25:DA:1364:G:C5	47:D1:3:LYS:HE2	2.55	0.42
5:AE:145:LYS:HB3	5:AE:145:LYS:HE2	1.82	0.42
25:BA:2108:U:H2'	25:BA:2109:G:C8	2.55	0.42
1:CA:431:A:OP2	61:CA:4140:HOH:O	2.21	0.42
37:DR:98:LEU:HB2	37:DR:113:LEU:HD11	2.02	0.42
25:DA:1983:C:H4'	25:DA:2606:C:H4'	2.00	0.42
45:DZ:28:MET:HE3	45:DZ:35:ARG:HB2	2.02	0.42
1:CA:457:C:H2'	1:CA:458:C:C6	2.54	0.42
25:DA:262:A:H2'	25:DA:263:C:O4'	2.20	0.42
30:DG:106:LEU:HA	30:DG:110:ALA:HB3	2.01	0.42
9:CI:105:ASP:HB2	9:CI:107:ARG:HG3	2.02	0.42
1:CA:1018:C:H2'	1:CA:1019:C:O4'	2.20	0.42
35:DP:85:LEU:HD13	35:DP:120:ALA:HB2	2.02	0.42
2:CB:58:ILE:HD13	2:CB:58:ILE:HA	1.83	0.42
25:BA:886:U:H1'	25:BA:1236:G:H1'	2.02	0.42
25:DA:568:U:H5'	25:DA:945:A:N1	2.34	0.42
29:DF:9:ILE:HA	29:DF:10:PRO:HD3	1.79	0.42
20:AT:13:LEU:HD12	20:AT:14:LYS:N	2.35	0.42
18:AR:47:THR:HG23	18:AR:49:LYS:HG3	2.02	0.42
1:AA:918:A:H2'	1:AA:919:A:O4'	2.19	0.42
1:AA:1002:G:C5	1:AA:1003:G:H1'	2.54	0.42
2:CB:52:GLU:HG2	2:CB:56:ARG:NH2	2.34	0.42
41:BV:72:VAL:HG11	41:BV:85:LYS:HD2	2.01	0.42
11:CK:93:GLN:NE2	11:CK:93:GLN:HA	2.29	0.42
50:B4:53:GLU:HG2	50:B4:55:ARG:HD2	2.02	0.42
50:B4:55:ARG:HA	50:B4:55:ARG:HD2	1.83	0.42
25:BA:669:A:H4'	25:BA:670:C:H5	1.85	0.42
23:CW:29:G:N2	23:CW:41:C:N3	2.67	0.42
3:CC:181:ASN:ND2	3:CC:204:LEU:HD12	2.30	0.42
1:AA:1530:G:H4'	1:AA:1530:G:OP1	2.19	0.42
25:DA:1796:U:H2'	25:DA:1797:C:H6	1.84	0.42
25:DA:2652:C:O2	25:DA:2668:G:N2	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:2646:C:O5'	25:DA:2646:C:H6	2.03	0.42
27:BD:143:HIS:ND1	27:BD:194:GLY:O	2.43	0.42
23:CW:25:C:H2'	23:CW:26:A:C8	2.54	0.42
1:CA:769:G:H4'	1:CA:1513:A:H4'	2.02	0.42
1:CA:324:G:N2	1:CA:326:G:H3'	2.35	0.42
26:BB:2:C:H2'	26:BB:3:C:H6	1.85	0.42
25:DA:1187:G:OP2	25:DA:1187:G:H8	2.02	0.42
1:AA:1291:G:O2'	9:AI:38:GLN:OE1	2.30	0.42
1:AA:501:C:H2'	1:AA:502:G:H8	1.84	0.42
1:CA:1273:G:H3'	1:CA:1274:G:C8	2.54	0.42
45:BZ:7:ALA:O	45:BZ:62:PRO:HD3	2.20	0.42
25:BA:895:G:O6	25:BA:974:G:H2'	2.20	0.42
4:AD:22:LYS:HB2	4:AD:26:CYS:SG	2.60	0.42
52:D6:37:ARG:O	52:D6:38:LYS:HD2	2.20	0.42
30:DG:111:LEU:HB3	30:DG:117:PHE:CE2	2.55	0.42
32:BI:131:LYS:H	32:BI:138:ILE:H	1.67	0.42
25:BA:2086:C:H2'	25:BA:2087:C:C6	2.55	0.42
48:B2:35:LEU:HA	48:B2:35:LEU:HD23	1.84	0.42
36:DQ:79:LEU:HA	36:DQ:79:LEU:HD23	1.94	0.42
25:DA:2419:U:H2'	25:DA:2420:C:C6	2.55	0.42
6:CF:22:GLU:O	6:CF:26:ILE:HG13	2.20	0.42
25:DA:2335:A:C8	25:DA:2337:G:C5	3.08	0.42
25:DA:667:U:O2	54:D8:2:PRO:HD2	2.20	0.42
30:BG:163:ALA:HB1	30:BG:168:GLU:HB2	2.01	0.42
26:DB:14:U:H1'	26:DB:108:U:O2'	2.20	0.42
25:BA:1091:A:O2'	25:BA:1093:G:C4	2.66	0.42
1:CA:1120:G:O6	1:CA:1154:G:N2	2.53	0.42
10:CJ:37:PRO:HA	10:CJ:72:VAL:HG12	2.02	0.42
25:DA:2149:G:H3'	25:DA:2150:U:C6	2.55	0.42
1:CA:397:A:H3'	1:CA:397:A:N3	2.34	0.42
25:DA:1171:G:H8	25:DA:1171:G:OP2	2.03	0.42
25:DA:848:G:H2'	25:DA:849:A:C8	2.54	0.42
43:DX:92:LEU:C	43:DX:94:GLY:H	2.23	0.42
43:BX:92:LEU:O	43:BX:94:GLY:N	2.44	0.42
25:DA:2135:A:N6	25:DA:2157:G:H21	2.12	0.42
3:AC:6:HIS:CD2	3:AC:8:ILE:H	2.27	0.42
1:CA:1111:A:H2'	1:CA:1112:C:C6	2.54	0.42
8:CH:73:ASP:OD2	8:CH:75:ARG:NH1	2.53	0.42
1:CA:714:G:H2'	1:CA:715:A:C8	2.55	0.42
25:BA:1405:A:H61	25:BA:1418:U:H3	1.68	0.42
1:CA:737:A:H2'	1:CA:738:C:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:1913:A:H4'	25:DA:1914:C:C5'	2.50	0.42
25:DA:2787:C:H2'	25:DA:2788:C:C6	2.55	0.42
2:AB:230:VAL:HG22	2:AB:231:GLU:H	1.84	0.42
1:AA:130:A:H5'	17:AQ:63:ARG:NE	2.35	0.42
29:BF:32:LEU:HB3	29:BF:112:MET:HE1	2.02	0.42
25:BA:1945:U:H2'	25:BA:1946:C:C6	2.54	0.42
25:DA:2514:U:H2'	25:DA:2515:C:H6	1.84	0.42
25:DA:1027:A:C6	25:DA:1126:A:C4	3.07	0.42
35:BP:99:LEU:HD22	35:BP:102:ARG:NH2	2.35	0.42
32:BI:40:THR:O	32:BI:44:LEU:HB2	2.19	0.42
27:DD:118:VAL:HG22	27:DD:119:ALA:H	1.85	0.42
1:CA:625:G:H2'	1:CA:626:U:C6	2.55	0.42
1:AA:107:G:H2'	1:AA:108:G:O4'	2.20	0.42
25:BA:196:A:H2'	25:BA:197:C:O4'	2.18	0.42
41:BV:18:LEU:HD13	41:BV:20:LEU:HB2	2.02	0.42
25:BA:213:G:H2'	25:BA:214:A:O4'	2.19	0.42
2:AB:220:ASP:O	2:AB:224:GLN:HG3	2.20	0.42
35:BP:100:LEU:HA	35:BP:100:LEU:HD23	1.85	0.42
6:CF:82:ARG:HA	6:CF:82:ARG:HD2	1.90	0.42
37:DR:55:ALA:HB2	37:DR:79:LEU:HD13	2.02	0.42
1:AA:431:A:H2'	1:AA:432:A:O4'	2.20	0.42
25:BA:329:U:H2'	25:BA:330:U:C6	2.55	0.42
28:DE:31:CYS:HA	28:DE:32:PRO:HD2	1.86	0.42
8:AH:29:SER:HB3	8:AH:32:LYS:HG3	2.02	0.42
25:BA:316:C:C2	25:BA:373:G:C2	3.08	0.42
30:DG:165:THR:OG1	30:DG:168:GLU:HG3	2.20	0.42
43:DX:12:VAL:HG22	43:DX:29:TRP:CE2	2.55	0.42
25:DA:2114:A:H2'	25:DA:2114:A:N3	2.35	0.41
12:AL:92:ASP:O	12:AL:94:PRO:HD3	2.19	0.41
5:AE:41:VAL:HG11	5:AE:109:ILE:O	2.20	0.41
25:BA:354:A:H2	25:BA:1255:A:O2'	2.03	0.41
25:BA:553:A:C2	25:BA:2065:C:H4'	2.55	0.41
16:CP:43:LYS:HB3	16:CP:48:TRP:CD1	2.55	0.41
2:CB:229:VAL:HG12	2:CB:230:VAL:N	2.35	0.41
7:CG:113:GLU:HG2	7:CG:119:ARG:HG2	2.01	0.41
23:AW:26:A:N6	23:AW:44:G:H1	2.18	0.41
39:BT:118:ARG:HH11	39:BT:118:ARG:HG3	1.85	0.41
8:CH:39:LEU:HA	8:CH:39:LEU:HD13	1.85	0.41
17:CQ:94:ASN:O	17:CQ:98:LEU:HD13	2.20	0.41
25:BA:2348:A:H61	46:B0:43:THR:CG2	2.33	0.41
5:AE:36:ASP:OD1	5:AE:38:GLN:N	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:BZ:146:ILE:HA	45:BZ:147:GLY:HA2	1.77	0.41
33:DN:4:TYR:HB2	40:DU:101:ARG:NH1	2.35	0.41
25:DA:1213:A:H1'	25:DA:1238:G:N3	2.35	0.41
1:AA:50:A:H1'	1:AA:52:G:C8	2.55	0.41
1:CA:620:C:H2'	1:CA:621:A:O4'	2.20	0.41
1:AA:1368:G:OP2	9:AI:112:LYS:HG3	2.19	0.41
1:AA:1106:G:C6	1:AA:1107:C:C4	3.08	0.41
25:DA:25:U:H2'	25:DA:26:G:O4'	2.20	0.41
25:BA:1855:G:O3'	27:BD:249:PRO:HD3	2.20	0.41
25:BA:766:C:H2'	25:BA:767:C:C6	2.54	0.41
31:BH:144:VAL:O	31:BH:148:ILE:HG13	2.20	0.41
10:AJ:90:LEU:HA	10:AJ:91:PRO:HD3	1.95	0.41
11:AK:81:ASP:OD1	11:AK:107:SER:OG	2.25	0.41
8:AH:19:VAL:HG23	8:AH:21:LYS:HD3	2.02	0.41
2:AB:133:LYS:O	2:AB:137:ARG:HG3	2.19	0.41
8:AH:56:LYS:HD3	8:AH:56:LYS:HA	1.87	0.41
20:AT:48:LYS:HD3	20:AT:48:LYS:HA	1.85	0.41
1:CA:718:G:H5'	11:CK:117:ASN:ND2	2.35	0.41
25:BA:2815:C:H2'	25:BA:2816:G:C8	2.55	0.41
5:CE:13:ILE:HA	5:CE:29:GLY:O	2.19	0.41
30:DG:131:TYR:HB3	30:DG:159:VAL:CG2	2.50	0.41
9:CI:6:GLY:HA3	9:CI:80:GLY:O	2.19	0.41
13:CM:64:TRP:HB2	13:CM:66:LEU:HD21	2.00	0.41
1:AA:31:G:O2'	1:AA:48:C:N4	2.53	0.41
25:DA:2144:U:O2	25:DA:2148:G:N1	2.54	0.41
10:CJ:49:VAL:HG23	14:CN:41:ARG:HB2	2.01	0.41
35:DP:97:PRO:HG3	35:DP:112:LEU:HD12	2.02	0.41
1:CA:7:G:H5'	1:CA:298:A:O4'	2.20	0.41
26:DB:4:C:N4	26:DB:117:G:H1	2.15	0.41
26:DB:61:G:C6	26:DB:62:C:C4	3.08	0.41
1:CA:344:A:H4'	1:CA:345:C:OP2	2.21	0.41
25:DA:1274:A:N3	25:DA:1297:C:H1'	2.35	0.41
4:CD:98:GLU:OE1	4:CD:103:ASN:ND2	2.37	0.41
4:CD:65:ARG:HD3	4:CD:70:ILE:O	2.20	0.41
25:BA:2126:G:H2'	25:BA:2127:C:H6	1.82	0.41
25:DA:1404:C:O2'	25:DA:1405:U:H5'	2.20	0.41
25:BA:239:G:P	54:B8:13:ARG:HH22	2.43	0.41
37:BR:21:TYR:CZ	37:BR:43:GLU:HG2	2.55	0.41
9:AI:93:ARG:HB2	9:AI:93:ARG:NH1	2.35	0.41
23:CY:2:C:H2'	23:CY:3:C:H6	1.85	0.41
30:DG:47:LYS:HB3	30:DG:48:GLU:H	1.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:2526:G:H2'	25:DA:2527:C:H6	1.85	0.41
25:DA:2769:C:H2'	25:DA:2770:G:O4'	2.20	0.41
1:AA:1292:U:H5'	9:AI:38:GLN:OE1	2.19	0.41
1:CA:407:G:H5''	4:CD:115:ARG:HB3	2.02	0.41
25:DA:1336:A:H2'	25:DA:1337:G:H8	1.84	0.41
25:BA:327:U:H2'	25:BA:328:G:C8	2.54	0.41
15:CO:36:ILE:HG23	15:CO:56:LEU:HD11	2.02	0.41
28:DE:51:PHE:O	28:DE:77:ILE:HD12	2.20	0.41
27:DD:79:VAL:O	27:DD:113:VAL:HG23	2.19	0.41
15:CO:32:LEU:HD13	15:CO:63:ARG:HB2	2.02	0.41
27:DD:164:GLN:NE2	27:DD:176:ARG:HH22	2.17	0.41
25:DA:1848:A:C4	25:DA:1849:G:C8	3.09	0.41
31:DH:27:LYS:NZ	31:DH:32:GLU:OE2	2.45	0.41
34:DO:66:LYS:HA	34:DO:79:PHE:O	2.21	0.41
25:BA:1506:G:H5''	25:BA:1507:A:OP2	2.20	0.41
25:BA:1506:G:C6	25:BA:1508:G:C5	3.08	0.41
28:BE:7:VAL:HG12	28:BE:27:LEU:HB3	2.02	0.41
45:BZ:54:HIS:HD2	45:BZ:99:TYR:O	2.03	0.41
2:AB:134:GLU:O	2:AB:138:LEU:HG	2.20	0.41
9:CI:19:LEU:HD23	9:CI:19:LEU:HA	1.89	0.41
50:B4:47:GLN:HG2	50:B4:49:PHE:H	1.85	0.41
1:CA:399:G:H2'	1:CA:400:C:C6	2.54	0.41
16:AP:52:ASP:HB3	16:AP:55:ARG:HB2	2.02	0.41
5:CE:51:VAL:HG23	5:CE:52:PRO:HD3	2.01	0.41
1:AA:266:G:O2'	1:AA:267:C:OP2	2.33	0.41
38:BS:19:LYS:HE3	38:BS:42:ASP:OD1	2.20	0.41
1:AA:1022:G:H4'	1:AA:1022:G:OP1	2.21	0.41
25:DA:2135:A:H2'	25:DA:2136:C:C6	2.55	0.41
25:DA:2156:G:H2'	25:DA:2157:G:N3	2.35	0.41
9:CI:5:TYR:CE2	9:CI:7:THR:HG23	2.55	0.41
25:BA:1249:A:N6	25:BA:1286:U:H2'	2.36	0.41
9:CI:100:GLY:O	9:CI:103:THR:HG22	2.20	0.41
25:BA:2122:G:H2'	25:BA:2123:G:C8	2.56	0.41
1:AA:92:C:H2'	1:AA:93:G:H8	1.84	0.41
30:DG:115:ARG:HH11	30:DG:115:ARG:H	1.68	0.41
25:BA:2584:A:C8	28:BE:144:ARG:HD2	2.55	0.41
24:AX:21:A:H61	24:AX:46:G:H2'	1.84	0.41
3:AC:130:VAL:O	3:AC:134:ILE:HG13	2.20	0.41
4:AD:166:LYS:HB2	4:AD:168:ARG:CZ	2.50	0.41
7:CG:108:ALA:HA	7:CG:111:ARG:HD2	2.02	0.41
1:AA:1278:U:H5'	1:AA:1279:A:C5'	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AY:69:G:C2	23:AY:70:G:H1'	2.55	0.41
30:DG:179:PRO:HG3	50:D4:43:TYR:OH	2.20	0.41
39:DT:88:ILE:HG13	39:DT:91:ARG:NH2	2.35	0.41
43:BX:84:ALA:HB3	43:BX:87:GLN:NE2	2.35	0.41
25:DA:2097:C:H2'	25:DA:2098:U:O4'	2.20	0.41
1:CA:552:U:H4'	12:CL:86:ARG:HD2	2.02	0.41
31:BH:104:GLU:HG3	31:BH:114:VAL:HG22	2.03	0.41
2:CB:158:LEU:HA	2:CB:159:PRO:HD3	1.88	0.41
15:CO:69:TYR:O	15:CO:73:GLU:HG2	2.21	0.41
25:DA:1614:A:C2	42:DW:93:ALA:HB2	2.54	0.41
15:CO:74:ASP:OD1	15:CO:76:GLU:HB2	2.20	0.41
44:DY:90:LEU:HD11	44:DY:96:ILE:HG23	2.02	0.41
25:BA:18:C:O2'	25:BA:577:U:OP1	2.33	0.41
12:CL:24:VAL:HG12	12:CL:98:TYR:CE1	2.56	0.41
4:CD:45:GLN:HB2	4:CD:46:LYS:H	1.73	0.41
25:BA:1686:U:O2'	25:BA:1687:C:H5'	2.20	0.41
1:CA:984:C:O5'	1:CA:984:C:H6	2.03	0.41
5:CE:33:VAL:HA	5:CE:42:GLY:O	2.20	0.41
1:AA:1028:C:N3	1:AA:1029:C:H1'	2.35	0.41
26:DB:66:A:N6	26:DB:108:U:H3'	2.34	0.41
2:CB:16:HIS:HB3	2:CB:210:SER:HB3	2.03	0.41
25:BA:1091:A:C8	25:BA:1093:G:N2	2.88	0.41
45:DZ:97:GLU:HG2	45:DZ:97:GLU:H	1.61	0.41
25:BA:2849:G:C5'	37:BR:46:GLY:HA2	2.46	0.41
57:AA:3231:PCY:H40	23:AY:35:A:N1	2.36	0.41
25:BA:2186:C:H5	25:BA:2187:G:C4	2.37	0.41
10:CJ:5:ARG:HA	10:CJ:73:ASP:OD1	2.19	0.41
27:DD:3:VAL:HG13	27:DD:17:THR:HB	2.02	0.41
25:DA:271(H):G:N3	25:DA:271(I):G:C8	2.88	0.41
25:BA:1221:G:H1'	25:BA:1222:A:O5'	2.21	0.41
4:CD:15:GLU:OE1	4:CD:63:LYS:HG3	2.21	0.41
1:CA:1441:G:O5'	1:CA:1441:G:H8	2.04	0.41
25:BA:288:U:O2'	25:BA:289:G:P	2.79	0.41
23:AW:1:G:H2'	23:AW:1:G:N3	2.34	0.41
33:DN:15:LEU:HB2	33:DN:135:PRO:CB	2.49	0.41
1:AA:601:C:H2'	1:AA:602:A:H8	1.84	0.41
28:DE:27:LEU:HD22	39:DT:1:MET:HE1	2.02	0.41
23:CY:3:C:O5'	23:CY:3:C:H6	2.04	0.41
30:BG:56:ALA:HA	30:BG:153:ARG:HH21	1.85	0.41
33:DN:67:LEU:C	33:DN:88:GLU:HG3	2.41	0.41
39:DT:91:ARG:HD2	39:DT:120:ARG:NH1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:362:G:O3'	12:AL:33:ARG:NH2	2.53	0.41
25:DA:2815:C:H2'	25:DA:2816:C:H6	1.85	0.41
25:BA:2574:U:H1'	34:BO:23:ARG:HH11	1.86	0.41
1:CA:129(A):G:C6	1:CA:189(E):U:H4'	2.55	0.41
32:DI:93:THR:O	32:DI:97:ILE:HG13	2.20	0.41
1:AA:865:A:H2	1:AA:918:A:H4'	1.85	0.41
34:BO:118:ALA:HA	34:BO:119:PRO:HD2	1.80	0.41
18:AR:59:SER:OG	18:AR:62:GLU:HG2	2.20	0.41
25:BA:543:G:H2'	25:BA:544:U:C6	2.55	0.41
1:AA:658:G:H2'	1:AA:659:U:C6	2.55	0.41
33:DN:110:GLY:O	33:DN:114:ARG:HG3	2.20	0.41
14:AN:13:THR:HA	14:AN:14:PRO:HD3	1.95	0.41
25:DA:2001:A:H2'	25:DA:2002:G:C8	2.55	0.41
30:DG:61:ALA:O	50:D4:7:PRO:HG2	2.21	0.41
7:AG:14:PRO:HG3	7:AG:21:VAL:HG13	2.02	0.41
11:CK:85:ARG:HG2	11:CK:112:THR:HA	2.02	0.41
1:CA:1313:U:P	19:CS:5:LEU:HG	2.60	0.41
28:DE:28:ALA:HB3	28:DE:93:VAL:HG12	2.02	0.41
37:DR:87:TYR:OH	37:DR:116:LEU:HB3	2.20	0.41
40:BU:83:LEU:HD13	40:BU:113:ALA:HB2	2.01	0.41
5:AE:83:GLU:HG2	5:AE:88:LYS:HB2	2.02	0.41
27:BD:132:PRO:HG3	27:BD:190:TYR:CE1	2.55	0.41
1:AA:911:U:OP1	12:AL:95:GLY:HA2	2.20	0.41
25:BA:1074:A:N6	25:BA:1171:G:H2'	2.36	0.41
1:AA:1001(A):G:C6	1:AA:1002:G:N7	2.89	0.41
1:CA:1023:G:C5	1:CA:1024:G:C8	3.08	0.41
25:DA:1270:C:H5''	25:DA:1271:G:O5'	2.20	0.41
1:CA:89:C:H2'	1:CA:90:U:O4'	2.21	0.41
25:DA:2356:C:O3'	46:D0:20:ARG:HD3	2.21	0.41
3:AC:152:ILE:HG23	3:AC:167:TRP:HB3	2.02	0.41
25:DA:1005:C:H4'	25:DA:1012:U:C6	2.55	0.41
25:DA:1817:G:H2'	25:DA:1818:U:H5'	2.03	0.41
50:B4:58:ARG:HB3	50:B4:58:ARG:CZ	2.49	0.41
1:CA:1360:A:H2'	1:CA:1361:G:O4'	2.21	0.41
25:BA:2195:A:H2'	25:BA:2195:A:N3	2.35	0.41
25:DA:248:G:C2	25:DA:2431:U:H4'	2.55	0.41
25:DA:2758:A:H2'	25:DA:2759:G:O4'	2.21	0.41
31:DH:9:ILE:HD13	31:DH:72:ILE:HG21	2.03	0.41
1:AA:1049:U:OP1	14:AN:3:ARG:HB2	2.20	0.41
1:AA:1125:U:H4'	10:AJ:5:ARG:HH22	1.83	0.41
3:AC:131:ARG:NE	3:AC:166:GLU:OE2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:DU:79:PHE:CE2	40:DU:83:LEU:HD21	2.55	0.41
1:CA:982:U:O2	1:CA:1222:G:N1	2.39	0.41
25:DA:579:G:H2'	25:DA:580:C:C6	2.56	0.41
38:DS:11:LYS:O	38:DS:15:ARG:HG3	2.20	0.41
24:CX:15:G:H2'	24:CX:59:A:N1	2.35	0.41
11:CK:120:ARG:HA	11:CK:121:PRO:HD3	1.95	0.41
25:DA:1707:G:C5	25:DA:1756:G:C6	3.08	0.41
43:DX:43:VAL:HG21	43:DX:81:VAL:HG11	2.03	0.41
1:AA:691:G:OP2	11:AK:26:ASN:ND2	2.43	0.41
45:DZ:8:TYR:HB2	45:DZ:38:TYR:CE2	2.55	0.41
25:DA:1127:A:H2'	25:DA:1128:A:H5''	2.02	0.41
25:DA:930:U:O4'	25:DA:931:G:C2	2.74	0.41
25:BA:1183:G:H2'	25:BA:1184:G:O4'	2.20	0.41
25:DA:1159:U:O2'	25:DA:1160:G:H5'	2.20	0.41
25:DA:1706:U:O2	25:DA:1757:U:H5'	2.20	0.41
50:D4:68:ARG:O	50:D4:69:LYS:HB3	2.20	0.41
1:AA:892:A:O2'	1:AA:1415:G:H4'	2.20	0.41
45:DZ:44:PHE:CZ	45:DZ:86:VAL:HG11	2.56	0.41
1:AA:1516:G:H2'	1:AA:1518:A:OP2	2.21	0.41
25:BA:2827:G:OP1	37:BR:99:LYS:HE2	2.21	0.41
1:CA:1414:U:H3	1:CA:1486:G:H1	1.68	0.41
42:BW:68:ARG:NH1	42:BW:112:GLY:H	2.19	0.41
2:CB:133:LYS:O	2:CB:137:ARG:HG3	2.20	0.41
25:DA:2319:G:N2	38:DS:3:ARG:HA	2.35	0.41
25:DA:1131:G:N2	25:DA:1132:A:N3	2.68	0.41
25:BA:2162:C:H1'	25:BA:2174:G:H22	1.85	0.41
39:BT:53:ARG:NH1	39:BT:53:ARG:HB3	2.35	0.41
25:DA:271(H):G:O2'	25:DA:271(I):G:C8	2.69	0.41
16:AP:27:LYS:HE3	16:AP:27:LYS:HB2	1.72	0.41
25:DA:42:G:H2'	25:DA:43:A:O4'	2.19	0.41
1:CA:164:U:H2'	1:CA:165:C:C6	2.56	0.41
1:AA:1145:C:H4'	1:AA:1146:A:C5'	2.51	0.41
25:DA:1593:G:H2'	25:DA:1594:G:C8	2.55	0.41
9:CI:18:PHE:CD2	9:CI:62:TYR:HD2	2.36	0.41
9:AI:24:GLY:HA2	9:AI:59:PHE:O	2.20	0.41
4:AD:163:GLU:O	4:AD:166:LYS:HG2	2.20	0.41
1:CA:542:G:P	4:CD:10:ARG:HH22	2.43	0.41
50:D4:14:ILE:HB	50:D4:22:ILE:HB	2.03	0.41
45:DZ:156:LYS:HE2	45:DZ:158:PRO:HB3	2.02	0.41
5:CE:84:PHE:CE2	5:CE:133:TYR:HD2	2.39	0.41
25:DA:263:C:H2'	25:DA:264:C:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:BZ:107:THR:HA	45:BZ:108:PRO:HD3	1.63	0.41
20:CT:16:HIS:O	20:CT:19:SER:OG	2.27	0.41
53:D7:26:GLY:O	53:D7:30:VAL:HG23	2.21	0.41
36:DQ:42:ILE:HD13	36:DQ:97:VAL:HB	2.02	0.41
41:DV:24:LYS:HA	41:DV:92:THR:OG1	2.21	0.41
25:DA:1810:A:H2'	25:DA:1811:G:O4'	2.20	0.41
45:BZ:136:PHE:O	45:BZ:137:ILE:HG13	2.20	0.41
25:BA:308:U:H2'	25:BA:309:C:C6	2.55	0.41
25:BA:80:G:HO2'	25:BA:319:G:HO2'	1.66	0.41
44:DY:94:LYS:HA	44:DY:94:LYS:HD2	1.84	0.41
25:BA:2591:C:H6	25:BA:2591:C:O5'	2.04	0.41
55:D9:17:ILE:HD12	55:D9:17:ILE:HA	1.82	0.41
46:D0:56:ASP:O	46:D0:57:PHE:HB2	2.20	0.41
25:BA:982:U:H2'	25:BA:983:G:O4'	2.21	0.41
46:D0:50:ASN:HA	46:D0:62:LEU:HD12	2.03	0.41
50:D4:28:LYS:HA	50:D4:29:PRO:HD3	1.93	0.41
28:DE:48:GLN:HA	28:DE:80:GLU:HA	2.03	0.41
1:CA:1028:C:O2	1:CA:1034:G:H1'	2.20	0.41
1:CA:1055:A:C5	1:CA:1206:G:C2	3.09	0.41
2:CB:16:HIS:CB	2:CB:204:ASN:HB3	2.50	0.41
25:BA:1065:U:H3	25:BA:1188:A:H62	1.66	0.41
25:BA:715:G:H5'	25:BA:716:G:OP2	2.20	0.41
1:CA:411:A:OP2	4:CD:25:ARG:NH2	2.54	0.41
37:BR:1:MET:HB2	37:BR:2:ARG:H	1.74	0.41
5:AE:122:GLU:O	5:AE:126:ARG:NH1	2.53	0.41
29:DF:64:ILE:HD11	29:DF:75:HIS:HB2	2.02	0.41
2:CB:80:ILE:HD11	2:CB:212:GLN:CA	2.51	0.41
14:CN:13:THR:HA	14:CN:14:PRO:HD3	1.88	0.41
26:BB:17:C:H2'	26:BB:18:G:O4'	2.21	0.41
20:CT:89:ARG:O	20:CT:93:GLU:HB2	2.20	0.41
25:DA:1494:A:C6	25:DA:1495:A:C6	3.09	0.41
1:CA:583:A:N6	1:CA:758:G:O2'	2.54	0.41
44:DY:86:ARG:HH11	44:DY:100:ALA:HB1	1.85	0.41
25:DA:1379:A:H4'	25:DA:1380:G:OP2	2.21	0.41
14:AN:33:VAL:HA	14:AN:40:CYS:HA	2.03	0.41
24:CX:67:C:H2'	24:CX:68:C:H5'	2.03	0.41
13:CM:87:TYR:O	13:CM:91:ARG:HG2	2.21	0.41
4:CD:92:VAL:O	4:CD:96:LEU:HD22	2.21	0.41
25:DA:2643:G:H2'	25:DA:2644:G:O4'	2.21	0.41
1:CA:302:G:N3	1:CA:556:C:H4'	2.35	0.41
25:DA:2489:G:C2'	25:DA:2490:G:H5'	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:DZ:129:SER:HA	45:DZ:130:PRO:HD3	1.92	0.41
25:DA:673:C:H5''	29:DF:81:PRO:HD2	2.02	0.41
3:AC:148:GLY:HA3	3:AC:172:ARG:O	2.20	0.41
25:DA:2516:G:C6	25:DA:2517:C:C4	3.08	0.41
25:DA:1316:U:H2'	25:DA:1317:A:C8	2.55	0.41
1:CA:1029:C:N4	1:CA:1032:G:C2	2.87	0.41
23:AY:64:A:H2'	23:AY:65:G:C8	2.56	0.41
40:DU:49:HIS:O	40:DU:53:ARG:N	2.54	0.41
25:DA:2120:G:H2'	25:DA:2121:G:C8	2.56	0.41
3:CC:120:VAL:HA	3:CC:123:GLN:NE2	2.25	0.41
1:CA:657:G:H4'	15:CO:28:GLN:HG2	2.02	0.41
45:DZ:107:THR:HA	45:DZ:108:PRO:HD3	1.81	0.41
1:CA:788:U:O2	1:CA:795:C:N4	2.53	0.41
25:DA:2153:G:H2'	25:DA:2154:G:C8	2.55	0.41
1:CA:1116:C:C2'	1:CA:1117:G:H5''	2.46	0.41
6:AF:44:GLY:HA2	6:AF:59:TYR:CE2	2.56	0.41
9:CI:55:ALA:HA	9:CI:58:HIS:HD2	1.86	0.41
25:DA:784:A:O4'	27:DD:227:ASN:ND2	2.53	0.41
17:AQ:45:HIS:O	17:AQ:73:VAL:HG23	2.21	0.41
6:AF:91:VAL:HG11	18:AR:72:ARG:HH12	1.86	0.41
31:DH:154:PRO:HB3	31:DH:163:TYR:CZ	2.54	0.41
25:DA:247:G:H4'	25:DA:386:G:C6	2.55	0.41
25:DA:861:A:C2	25:DA:917:A:C4	3.09	0.41
1:CA:109:A:H5'	1:CA:110:C:C5	2.56	0.41
25:BA:2141:A:N1	25:BA:2192:A:H2'	2.36	0.41
39:BT:127:ALA:C	39:BT:129:ARG:H	2.24	0.41
9:CI:70:LYS:O	9:CI:74:ILE:HG13	2.21	0.41
25:BA:2159:C:H2'	25:BA:2160:C:C6	2.56	0.41
1:AA:674:G:H2'	1:AA:675:A:C8	2.56	0.41
1:AA:1261:A:H3'	1:AA:1262:C:C6	2.56	0.41
50:B4:40:HIS:HB3	50:B4:43:TYR:CD2	2.55	0.41
2:CB:94:ASN:HD22	2:CB:94:ASN:HA	1.54	0.41
25:DA:1794:U:H2'	25:DA:1795:C:H6	1.86	0.41
25:BA:2853:G:N7	61:BA:4892:HOH:O	2.37	0.41
25:BA:1334:U:C4	25:BA:1373:C:H1'	2.56	0.41
20:AT:8:ARG:O	20:AT:9:ASN:HB2	2.21	0.41
37:BR:61:HIS:O	37:BR:65:LEU:HD22	2.21	0.41
15:CO:80:ALA:O	15:CO:83:GLU:HB3	2.21	0.41
31:DH:59:ARG:O	31:DH:63:SER:OG	2.29	0.41
25:BA:492:A:N3	25:BA:730:C:H1'	2.35	0.41
54:D8:10:ALA:HB3	54:D8:62:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:746:A:H2'	25:DA:2612:C:H5''	2.03	0.41
31:DH:98:LEU:HA	31:DH:98:LEU:HD12	1.85	0.41
49:D3:31:LEU:HA	49:D3:31:LEU:HD23	1.92	0.41
25:DA:636:G:OP1	35:DP:132:LYS:HE2	2.21	0.41
25:BA:1076:G:OP2	36:BQ:128:LYS:NZ	2.49	0.41
16:AP:69:THR:O	16:AP:73:LEU:HG	2.21	0.41
1:CA:1424:C:H2'	1:CA:1425:U:O4'	2.21	0.41
23:AY:44:G:H3'	23:AY:45:U:C6	2.56	0.41
29:DF:53:THR:HG23	29:DF:55:GLY:N	2.23	0.41
40:DU:92:ARG:H	40:DU:92:ARG:HG2	1.56	0.41
2:AB:105:PHE:CZ	2:AB:155:LEU:HD12	2.56	0.41
25:DA:1151:G:C6	25:DA:1152:C:N3	2.89	0.41
25:DA:2356:C:P	46:D0:24:LYS:HZ1	2.44	0.41
1:CA:976:G:H22	1:CA:1363:C:H5''	1.86	0.41
1:AA:216:G:C2	1:AA:217:C:C4	3.08	0.41
10:CJ:16:LEU:HD23	10:CJ:94:VAL:HG13	2.03	0.41
25:DA:299:A:N3	25:DA:319:C:O2'	2.51	0.41
57:AA:3231:PCY:H17	57:AA:3231:PCY:H24	1.77	0.41
25:BA:70:A:N7	43:BX:31:HIS:HE1	2.18	0.41
43:BX:31:HIS:HA	43:BX:32:PRO:HD3	1.93	0.41
35:DP:2:LYS:HG3	35:DP:4:SER:OG	2.21	0.41
25:BA:2283:G:OP1	46:B0:18:ALA:HB1	2.21	0.41
25:BA:142:G:H4'	43:BX:35:THR:HG21	2.01	0.41
30:DG:43:LEU:HB3	30:DG:44:GLY:H	1.53	0.41
9:CI:85:LEU:HB3	9:CI:92:TYR:CD2	2.56	0.41
5:AE:110:LEU:HD13	5:AE:118:ILE:HD13	2.02	0.41
10:AJ:35:SER:N	10:AJ:73:ASP:O	2.38	0.41
26:DB:95:C:H2'	26:DB:96:U:C6	2.56	0.41
1:AA:974:A:OP2	14:AN:29:ARG:NH2	2.53	0.41
1:AA:1191:A:OP1	3:AC:4:LYS:NZ	2.45	0.41
2:CB:118:LEU:HD13	2:CB:142:LEU:HB2	2.03	0.41
13:AM:3:ARG:HD3	13:AM:4:ILE:HG22	2.02	0.41
25:DA:1149:G:H2'	25:DA:1150:C:H6	1.85	0.41
28:DE:27:LEU:HD22	39:DT:1:MET:CE	2.51	0.41
1:AA:308:C:H2'	1:AA:309:G:C8	2.56	0.41
25:DA:2323:G:C6	25:DA:2324:C:C4	3.09	0.41
2:AB:223:ILE:HD12	2:AB:230:VAL:HG12	2.03	0.41
25:BA:2132:G:OP1	25:BA:2140:U:N3	2.51	0.41
30:DG:91:ARG:HB3	30:DG:91:ARG:HE	1.60	0.41
1:AA:1121:U:H2'	1:AA:1122:U:O4'	2.21	0.41
28:BE:101:ARG:HA	28:BE:170:LEU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:776:G:C6	27:BD:208:LYS:HB2	2.56	0.41
25:DA:2365:G:H4'	46:D0:60:PHE:CZ	2.56	0.41
54:D8:37:SER:OG	54:D8:39:LYS:HB3	2.21	0.41
25:DA:2364:C:H2'	25:DA:2365:G:O4'	2.21	0.41
1:AA:621:A:H2'	1:AA:622:A:C8	2.56	0.41
1:CA:175:C:H2'	1:CA:176:C:C6	2.56	0.41
1:CA:866:C:O2'	1:CA:919:A:OP1	2.26	0.41
31:DH:18:GLU:OE2	31:DH:25:LYS:HD3	2.21	0.41
6:AF:2:ARG:HG3	6:AF:69:GLU:HG3	2.03	0.41
27:BD:26:LYS:HB3	27:BD:83:GLU:HG2	2.02	0.41
31:DH:17:VAL:HG11	31:DH:50:VAL:HG21	2.03	0.41
25:BA:904:C:H1'	46:B0:26:TYR:CE2	2.56	0.41
7:CG:52:GLU:H	7:CG:52:GLU:HG2	1.47	0.41
25:DA:1379:A:O5'	25:DA:1379:A:H8	2.04	0.41
45:DZ:8:TYR:HB2	45:DZ:38:TYR:CZ	2.56	0.41
1:AA:1261:A:H5''	1:AA:1262:C:OP2	2.21	0.41
4:CD:196:LEU:O	4:CD:198:VAL:N	2.48	0.41
1:CA:309:G:H1'	1:CA:608:A:C2	2.56	0.41
1:CA:429:U:H3'	4:CD:9:CYS:SG	2.60	0.41
25:BA:2418:U:N3	35:BP:73:GLY:O	2.37	0.41
25:DA:2418:A:C2	25:DA:2419:U:C2	3.09	0.41
1:CA:718:G:H5'	11:CK:117:ASN:CG	2.41	0.41
25:DA:97:C:O3'	48:D2:2:LYS:HA	2.20	0.41
28:BE:36:ARG:NH2	28:BE:88:GLY:O	2.54	0.41
25:DA:816:C:O2'	25:DA:932:G:O6	2.31	0.41
25:BA:798:A:H5'	42:BW:90:ARG:HA	2.03	0.41
1:CA:269:C:H2'	1:CA:270:A:C8	2.56	0.41
25:BA:1466:U:O2'	25:BA:1467:G:OP1	2.33	0.41
25:DA:715:G:H2'	25:DA:716:A:O4'	2.21	0.41
1:AA:1223:C:P	19:AS:78:ARG:HH21	2.43	0.41
25:DA:483:A:O2'	44:DY:59:GLY:N	2.53	0.41
25:BA:1481:G:H2'	25:BA:1482:G:O4'	2.20	0.41
25:BA:119:G:H4'	25:BA:149:A:H5'	2.03	0.41
32:DI:102:SER:O	32:DI:106:GLY:N	2.54	0.41
1:CA:993:G:H2'	1:CA:993:G:N3	2.36	0.41
25:DA:1899:G:N3	25:DA:1899:G:H2'	2.36	0.41
25:DA:1207:C:H2'	25:DA:1208:C:C6	2.56	0.41
26:DB:5:C:H42	26:DB:116:G:H1	1.69	0.41
25:DA:311:A:C6	25:DA:328:U:C4	3.09	0.41
25:DA:2070:G:H2'	25:DA:2071:A:O4'	2.21	0.41
1:AA:189:G:H1	1:AA:189(K):U:H3	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2664:C:H2'	25:BA:2665:U:O4'	2.21	0.41
25:BA:2205:C:C2	25:BA:2206:G:C8	3.09	0.41
35:DP:90:ARG:HG2	35:DP:91:PHE:CD1	2.55	0.41
42:DW:18:ARG:NH1	42:DW:76:VAL:O	2.54	0.41
39:DT:6:LEU:O	39:DT:10:VAL:HG23	2.21	0.41
11:CK:16:SER:O	11:CK:35:PRO:HD3	2.21	0.41
25:BA:722:A:C8	25:BA:851:A:C6	3.09	0.41
25:DA:2671:A:H2'	25:DA:2672:G:O4'	2.21	0.41
1:CA:100:C:H2'	1:CA:101:A:O4'	2.20	0.41
25:DA:464:U:H2'	25:DA:465:G:O4'	2.21	0.41
1:AA:826:C:H4'	8:AH:12:ARG:HG2	2.02	0.41
3:CC:45:LYS:HG3	3:CC:46:GLU:N	2.36	0.41
44:DY:6:HIS:CD2	44:DY:6:HIS:H	2.39	0.41
27:BD:182:LEU:HA	27:BD:182:LEU:HD23	1.77	0.41
8:AH:49:GLU:HG2	8:AH:62:TYR:HE1	1.86	0.41
1:AA:1077:G:N2	1:AA:1080:A:OP2	2.45	0.41
1:CA:1002:G:C5	1:CA:1003:G:H8	2.39	0.41
19:AS:20:LEU:HD23	19:AS:23:ASN:ND2	2.23	0.41
40:BU:50:ARG:HH12	41:BV:72:VAL:HA	1.85	0.41
45:DZ:145:GLU:HG3	45:DZ:146:ILE:N	2.36	0.41
43:DX:94:GLY:N	43:DX:95:LEU:HA	2.36	0.41
1:CA:1129:C:O2'	1:CA:1139:G:O6	2.31	0.41
25:BA:2148:A:N6	25:BA:2185:C:O4'	2.54	0.41
3:CC:54:ARG:NH1	3:CC:54:ARG:HB3	2.29	0.41
20:AT:99:LEU:HA	20:AT:100:ILE:O	2.21	0.41
25:BA:2304:C:H2'	25:BA:2305:C:C6	2.56	0.41
25:BA:331:G:H21	25:BA:354:A:H62	1.69	0.41
1:CA:461:A:O2'	1:CA:471:G:N7	2.42	0.41
4:CD:173:TRP:CD1	4:CD:174:LEU:HG	2.56	0.41
25:DA:79:G:C6	25:DA:80:G:C5	3.09	0.41
10:AJ:35:SER:CB	10:AJ:73:ASP:HB2	2.49	0.41
1:AA:61:G:H2'	1:AA:62:U:O4'	2.21	0.41
2:AB:189:ASP:HB2	2:AB:190:THR:H	1.73	0.41
1:AA:601:C:H2'	1:AA:602:A:C8	2.56	0.41
5:CE:31:LEU:HA	5:CE:31:LEU:HD23	1.93	0.41
34:BO:2:ILE:HG23	34:BO:6:THR:HG21	2.02	0.41
25:BA:865:G:H4'	25:BA:885:C:O3'	2.21	0.41
25:DA:974:G:OP1	25:DA:1187:G:O2'	2.21	0.41
1:AA:193:C:H2'	1:AA:194:C:H6	1.85	0.41
25:DA:582:G:H2'	25:DA:583:G:C8	2.56	0.41
1:CA:790:A:C6	1:CA:791:G:C6	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:108:U:OP1	25:DA:293:U:O2'	2.36	0.41
27:DD:73:VAL:HG13	27:DD:120:GLY:HA3	2.03	0.41
25:BA:223:C:H2'	25:BA:224:U:H6	1.85	0.41
27:DD:29:PRO:HA	27:DD:83:GLU:OE1	2.20	0.41
1:AA:542:G:H5'	4:AD:41:GLY:HA3	2.03	0.41
45:BZ:44:PHE:CZ	45:BZ:86:VAL:HG11	2.56	0.41
3:AC:108:ASN:HB3	3:AC:111:LEU:HD12	2.03	0.41
3:AC:65:ALA:HA	3:AC:100:ALA:HB3	2.03	0.41
25:DA:1374:G:H2'	25:DA:1375:C:C6	2.56	0.41
25:DA:530:G:N3	25:DA:530:G:O4'	2.53	0.41
26:DB:76:G:N2	26:DB:101:G:O6	2.42	0.41
4:AD:134:ASP:O	4:AD:136:PRO:HD3	2.21	0.41
25:DA:127:A:H5''	25:DA:128:C:C6	2.55	0.41
11:CK:84:VAL:HG21	11:CK:95:ILE:HD11	2.03	0.41
25:BA:251:A:N3	25:BA:457:G:O2'	2.48	0.41
25:BA:1073:A:C6	25:BA:1172:A:C4	3.09	0.41
1:AA:1003:G:O3'	1:AA:1004:A:H4'	2.22	0.40
1:CA:1005:A:N6	1:CA:1024:G:O2'	2.54	0.40
50:B4:69:LYS:HE3	50:B4:69:LYS:HB3	1.83	0.40
25:BA:2163:G:N1	25:BA:2164:C:O2	2.55	0.40
25:DA:912:C:N4	25:DA:913:U:O4	2.54	0.40
25:DA:1171:G:N2	25:DA:1178:C:N3	2.50	0.40
1:CA:1358:U:H2'	1:CA:1359:C:O4'	2.21	0.40
43:DX:92:LEU:HA	43:DX:92:LEU:HD12	1.91	0.40
23:AY:35:A:H2'	23:AY:36:A:C8	2.57	0.40
27:BD:68:LYS:O	27:BD:69:ARG:HB2	2.21	0.40
25:DA:1140:C:O3'	33:DN:25:ARG:NH1	2.53	0.40
25:DA:19:C:H2'	25:DA:20:C:C6	2.55	0.40
23:CW:9:A:H5'	23:CW:46:7MG:N2	2.34	0.40
4:CD:174:LEU:HD23	4:CD:185:PHE:HA	2.03	0.40
47:B1:86:SER:O	47:B1:89:GLU:HG2	2.20	0.40
2:AB:19:HIS:HE1	2:AB:189:ASP:HB3	1.86	0.40
23:CY:8:4SU:S4	23:CY:14:A:C8	3.14	0.40
25:DA:566:U:O2'	25:DA:809:G:OP2	2.27	0.40
25:DA:1495:A:H2'	25:DA:1496:A:C8	2.56	0.40
1:CA:865:A:C2	1:CA:918:A:H4'	2.56	0.40
25:DA:314:A:H2'	25:DA:315:G:C8	2.57	0.40
25:DA:2320:A:H1'	25:DA:2321:G:C2	2.56	0.40
19:AS:22:LEU:C	19:AS:27:GLU:HG3	2.41	0.40
25:DA:144:C:H2'	25:DA:145:G:C8	2.56	0.40
1:CA:1201:A:H4'	1:CA:1202:G:O5'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:CE:53:LEU:O	5:CE:57:LYS:HB2	2.21	0.40
1:AA:1263:C:H5''	1:AA:1264:C:OP2	2.21	0.40
25:DA:2108:C:H2'	25:DA:2109:U:C6	2.55	0.40
24:CX:9:G:H21	24:CX:45:G:H3'	1.86	0.40
25:DA:1790:C:H5''	25:DA:1791:A:OP1	2.20	0.40
45:BZ:158:PRO:HA	45:BZ:159:PRO:HD3	1.85	0.40
33:DN:71:ILE:HA	33:DN:86:PRO:HA	2.02	0.40
25:BA:2353:G:H2'	25:BA:2354:C:C6	2.57	0.40
25:DA:643:A:N1	25:DA:2369:A:O2'	2.43	0.40
23:AW:54:5MU:H73	23:AW:55:PSU:O2	2.22	0.40
25:BA:1314:A:C2	25:BA:2035:A:C4	3.09	0.40
25:DA:1877:A:OP2	25:DA:1877:A:H8	2.04	0.40
47:B1:80:LEU:HD22	47:B1:97:LEU:HD11	2.03	0.40
31:BH:24:VAL:HG22	31:BH:35:VAL:HB	2.03	0.40
25:DA:84:A:N1	25:DA:98:G:O2'	2.46	0.40
33:BN:39:ARG:HA	33:BN:40:PRO:HD3	1.91	0.40
24:CX:13:C:O2'	25:DA:1924:C:H4'	2.21	0.40
1:CA:1060:C:N4	3:CC:2:GLY:HA2	2.36	0.40
1:AA:1007:C:N3	1:AA:1022:G:C6	2.89	0.40
15:CO:87:ILE:CG2	15:CO:88:ARG:H	2.26	0.40
25:DA:1971:A:OP1	61:DA:4260:HOH:O	2.21	0.40
1:AA:1128:C:C2'	1:AA:1129:C:H5'	2.51	0.40
19:AS:65:ASN:ND2	19:AS:65:ASN:N	2.68	0.40
10:CJ:40:LEU:HD23	10:CJ:40:LEU:HA	1.93	0.40
39:DT:65:LYS:O	39:DT:72:VAL:N	2.47	0.40
25:DA:2684:U:H1'	34:DO:70:LYS:HD2	2.03	0.40
25:BA:12:U:O2	25:BA:12:U:H2'	2.21	0.40
38:BS:59:LYS:HG3	38:BS:59:LYS:H	1.77	0.40
48:B2:65:ASN:OD1	48:B2:69:ARG:HD3	2.22	0.40
29:DF:78:ILE:HA	29:DF:83:PHE:CE1	2.56	0.40
25:DA:1711:C:H2'	25:DA:1712:C:H6	1.85	0.40
25:BA:2331:G:C2	38:BS:3:ARG:HA	2.56	0.40
43:DX:31:HIS:HB3	43:DX:34:ALA:HB2	2.03	0.40
25:DA:660:G:C6	25:DA:661:C:C4	3.10	0.40
23:AW:43:C:H2'	23:AW:44:G:C8	2.56	0.40
25:DA:2529:G:O6	55:D9:31:LYS:NZ	2.54	0.40
25:DA:1777:U:O2'	25:DA:1778:U:H5'	2.21	0.40
1:CA:174:C:H2'	1:CA:175:C:C6	2.56	0.40
38:DS:105:ALA:HB1	38:DS:110:LEU:HD23	2.02	0.40
31:DH:85:LYS:O	31:DH:132:ARG:HA	2.21	0.40
36:BQ:85:LYS:HD3	46:B0:7:LEU:HG	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:1668:A:H4'	25:DA:1669:A:O5'	2.21	0.40
25:DA:1782:C:O2	25:DA:2608:G:O2'	2.31	0.40
25:DA:2679:A:C2	25:DA:2729:G:C2	3.09	0.40
27:DD:264:LYS:HA	27:DD:265:PRO:HD3	1.95	0.40
29:DF:154:VAL:HG22	29:DF:191:ARG:HB2	2.03	0.40
25:BA:2672:A:N7	31:BH:175:LYS:NZ	2.68	0.40
10:AJ:62:HIS:HB3	14:AN:59:ALA:HB3	2.03	0.40
25:BA:1408:C:O2'	25:BA:1841:A:O2'	2.35	0.40
1:CA:560:U:H5'	1:CA:566:G:N2	2.36	0.40
32:DI:47:LEU:O	32:DI:51:ILE:HG13	2.21	0.40
2:CB:33:TYR:HB2	2:CB:43:ASP:HB2	2.02	0.40
25:DA:815:C:N3	25:DA:1193:G:C2	2.89	0.40
25:DA:1288:U:C2	25:DA:1327:C:O2	2.74	0.40
45:DZ:67:LEU:HA	45:DZ:68:PRO:HD3	1.77	0.40
1:CA:683:G:O6	61:CA:4133:HOH:O	2.21	0.40
55:B9:17:ILE:HD12	55:B9:17:ILE:HA	1.90	0.40
3:CC:16:ARG:HA	3:CC:16:ARG:HD2	1.96	0.40
25:BA:2332:A:H2'	25:BA:2332:A:N3	2.37	0.40
5:AE:105:VAL:HB	5:AE:106:PRO:HD3	2.03	0.40
25:BA:2812:A:N3	25:BA:2904:U:H1'	2.37	0.40
31:DH:137:ASP:O	31:DH:141:VAL:HG23	2.21	0.40
5:AE:82:VAL:HG21	5:AE:138:ALA:HA	2.03	0.40
1:CA:69:G:H2'	1:CA:70:G:C8	2.56	0.40
1:AA:179:A:C5	1:AA:180:U:C4	3.09	0.40
25:BA:2624:C:OP2	51:B5:2:ALA:N	2.54	0.40
25:BA:624:C:O2'	25:BA:628:C:H5''	2.21	0.40
25:DA:2140:C:H2'	25:DA:2140:C:O2	2.22	0.40
25:DA:857:C:H2'	25:DA:858:U:C6	2.56	0.40
20:AT:10:LEU:HD22	20:AT:11:SER:H	1.86	0.40
1:CA:1125:U:C2	10:CJ:38:ILE:HD13	2.56	0.40
1:CA:731:G:OP1	1:CA:766:A:H1'	2.22	0.40
3:CC:6:HIS:HA	3:CC:7:PRO:HD3	1.84	0.40
4:AD:63:LYS:HG3	4:AD:64:LEU:H	1.87	0.40
25:DA:41:C:H2'	25:DA:42:G:H8	1.86	0.40
15:CO:5:LYS:N	15:CO:5:LYS:HD3	2.36	0.40
17:AQ:66:SER:OG	17:AQ:69:LYS:HB2	2.22	0.40
8:CH:51:VAL:CG2	8:CH:60:ARG:HB2	2.51	0.40
1:AA:1068:G:N2	1:AA:1191:A:N3	2.60	0.40
1:CA:1381:U:H1'	7:CG:79:ARG:HD3	2.03	0.40
25:DA:1434:A:H2'	25:DA:1435:G:C8	2.56	0.40
25:DA:2666:C:H42	31:DH:109:PHE:HA	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:DH:105:LEU:N	31:DH:113:VAL:O	2.45	0.40
30:DG:67:LYS:HG2	30:DG:68:PRO:HD2	2.04	0.40
32:DI:101:LEU:HG	32:DI:107:VAL:HB	2.03	0.40
26:BB:16:G:C6	26:BB:69:G:C2	3.09	0.40
25:DA:1692:U:O2'	25:DA:1693:U:H2'	2.21	0.40
1:CA:1158:C:O3'	2:CB:133:LYS:NZ	2.54	0.40
25:DA:1789:A:H2'	25:DA:1790:C:O4'	2.21	0.40
1:AA:374:A:C6	1:AA:375:U:C4	3.09	0.40
5:CE:106:PRO:O	5:CE:110:LEU:HG	2.21	0.40
30:BG:106:LEU:HA	30:BG:110:ALA:HB3	2.01	0.40
1:AA:461:A:O2'	1:AA:470:C:H5'	2.22	0.40
25:BA:34:C:H5''	25:BA:35:G:OP2	2.22	0.40
16:CP:57:ARG:HH21	16:CP:79:VAL:HA	1.85	0.40
25:DA:1344:G:C2	25:DA:1385:G:C8	3.09	0.40
37:DR:22:ARG:O	37:DR:26:LYS:HG3	2.21	0.40
36:DQ:43:THR:OG1	36:DQ:45:GLN:HG2	2.22	0.40
28:BE:162:ALA:HB3	61:BE:409:HOH:O	2.21	0.40
25:BA:2236:G:H4'	25:BA:2238:C:C2	2.56	0.40
25:BA:2359:C:H2'	25:BA:2360:U:C6	2.56	0.40
25:DA:1446:C:H42	25:DA:1465:G:H1	1.69	0.40
1:CA:486:U:H2'	1:CA:487:A:C8	2.57	0.40
25:BA:866:A:C4	25:BA:1234:A:C2	3.09	0.40
18:CR:66:LEU:O	18:CR:70:ILE:HG13	2.21	0.40
1:AA:769:G:H4'	1:AA:1513:A:H4'	2.04	0.40
7:AG:8:GLU:HG3	7:AG:8:GLU:H	1.63	0.40
25:DA:1866:C:H6	25:DA:1866:C:O5'	2.05	0.40
29:DF:27:GLU:HA	29:DF:27:GLU:OE2	2.20	0.40
54:D8:50:LEU:HD23	54:D8:50:LEU:HA	1.86	0.40
43:BX:41:ASN:O	43:BX:45:THR:HG23	2.21	0.40
32:BI:10:GLU:O	32:BI:12:LEU:N	2.54	0.40
16:AP:4:ILE:HB	16:AP:66:PRO:HA	2.03	0.40
39:DT:109:GLU:HG2	39:DT:112:ARG:NH2	2.36	0.40
27:BD:136:ILE:HA	27:BD:137:PRO:HD3	1.88	0.40
1:AA:1035:A:H2	1:AA:1036:G:C5	2.39	0.40
2:AB:15:VAL:O	2:AB:16:HIS:HB3	2.22	0.40
2:CB:16:HIS:O	2:CB:18:GLY:N	2.55	0.40
25:BA:2162:C:O2	25:BA:2162:C:H2'	2.21	0.40
25:DA:2176:A:H2'	25:DA:2177:C:C5	2.56	0.40
46:D0:18:ALA:HB3	46:D0:20:ARG:HH21	1.87	0.40
2:CB:84:GLU:OE1	2:CB:216:SER:HA	2.21	0.40
10:CJ:74:ILE:HG22	61:CJ:5101:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:DP:65:ARG:HG3	54:D8:25:MET:CG	2.52	0.40
25:BA:1857:G:H4'	27:BD:242:ARG:CZ	2.51	0.40
1:AA:235:C:H5'	17:AQ:70:ARG:HG2	2.03	0.40
25:DA:1000:A:C6	25:DA:1155:A:C8	3.09	0.40
25:DA:2699:C:H2'	25:DA:2700:C:O4'	2.21	0.40
4:CD:162:LEU:HA	4:CD:162:LEU:HD23	1.89	0.40
25:BA:174:U:H2'	25:BA:175:G:H8	1.85	0.40
25:DA:1116:C:H2'	25:DA:1117:G:C8	2.57	0.40
25:DA:1786:A:C4	25:DA:1938:A:C6	3.09	0.40
13:AM:13:LYS:O	13:AM:44:ARG:HA	2.22	0.40
25:BA:2155:G:H21	25:BA:2180:A:N6	2.19	0.40
25:DA:921:G:H2'	25:DA:922:U:C6	2.57	0.40
23:AW:63:G:H2'	23:AW:64:A:O4'	2.21	0.40
31:BH:69:ARG:HG3	31:BH:70:THR:N	2.35	0.40
25:DA:2461:C:H2'	25:DA:2462:U:H6	1.85	0.40
25:DA:90:U:H1'	25:DA:92:A:C8	2.56	0.40
25:DA:2550:G:C6	25:DA:2551:C:C4	3.09	0.40
11:AK:38:ASN:HA	11:AK:39:PRO:HD3	1.79	0.40
25:DA:875:G:N2	25:DA:903:C:C2	2.89	0.40
30:BG:67:LYS:HG2	30:BG:68:PRO:HD2	2.03	0.40
30:DG:106:LEU:O	30:DG:110:ALA:HB3	2.21	0.40
25:BA:207:A:C2	25:BA:224:U:H4'	2.57	0.40
1:CA:617:G:H4'	16:CP:44:THR:O	2.22	0.40
25:BA:1271:G:OP1	41:BV:69:LYS:NZ	2.45	0.40
34:DO:22:ILE:HD11	34:DO:40:VAL:HG12	2.03	0.40
30:DG:97:ASP:HA	30:DG:100:TRP:HD1	1.86	0.40
7:CG:76:ARG:HG2	7:CG:156:TRP:CH2	2.55	0.40
25:DA:1922:G:H2'	25:DA:1923:U:O4'	2.21	0.40
25:DA:1653:G:C4	37:DR:9:LYS:HD2	2.56	0.40
25:BA:2520:G:H2'	25:BA:2521:G:O4'	2.22	0.40
25:BA:155:C:O5'	25:BA:155:C:H6	2.03	0.40
30:BG:45:GLU:HG2	30:BG:45:GLU:H	1.53	0.40
25:BA:2765:C:O5'	25:BA:2765:C:H6	2.05	0.40
36:DQ:137:TYR:HB3	45:DZ:76:LEU:HD21	2.04	0.40
24:CX:43:A:H2'	24:CX:44:A:C8	2.56	0.40
23:AY:57:G:N3	23:AY:57:G:H2'	2.35	0.40
1:CA:1004:A:H5''	1:CA:1024:G:H22	1.87	0.40
25:DA:2126:A:H4'	25:DA:2127:G:OP1	2.20	0.40
25:BA:1790:A:H1'	25:BA:2723:A:C2	2.57	0.40
25:DA:858:U:O2	25:DA:2268:A:H2'	2.21	0.40
25:DA:2133:G:O2'	25:DA:2134:A:P	2.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1133:G:H2'	1:CA:1134:G:O4'	2.22	0.40
25:BA:831:A:O4'	27:BD:227:ASN:ND2	2.54	0.40
26:DB:75:G:H21	45:DZ:85:HIS:HD1	1.68	0.40
23:CW:53:G:H1	23:CW:61:C:H42	1.69	0.40
30:DG:113:ARG:HD2	30:DG:140:ILE:O	2.21	0.40
25:DA:2359:C:H2'	25:DA:2360:A:O4'	2.21	0.40
32:DI:26:ALA:O	32:DI:31:LEU:HB2	2.22	0.40
1:AA:355:C:C4	1:AA:356:A:N7	2.89	0.40
61:BA:4080:HOH:O	33:BN:28:THR:HG23	2.21	0.40
15:CO:11:VAL:O	15:CO:15:PHE:HD1	2.04	0.40
21:CU:13:ILE:HG12	21:CU:22:ARG:CZ	2.51	0.40
28:BE:56:PRO:HG3	28:BE:74:PRO:HG2	2.04	0.40
25:DA:947:G:H2'	25:DA:948:G:H8	1.87	0.40
2:CB:20:GLU:HB2	2:CB:190:THR:OG1	2.22	0.40
1:CA:1327:C:OP1	21:CU:20:LYS:N	2.55	0.40
50:D4:15:ILE:HB	50:D4:32:TYR:CD1	2.56	0.40
41:DV:58:VAL:HG21	41:DV:100:ARG:HH11	1.87	0.40
5:CE:33:VAL:HG21	5:CE:109:ILE:HA	2.02	0.40
1:AA:1288:A:H2'	1:AA:1289:A:C8	2.57	0.40
43:BX:61:GLY:HA3	43:BX:73:ARG:O	2.22	0.40
30:DG:31:VAL:HA	30:DG:32:PRO:HD2	1.78	0.40
4:CD:128:VAL:N	4:CD:131:ARG:O	2.51	0.40
23:CY:58:A:H1'	23:CY:60:U:O2	2.22	0.40
1:CA:634:C:H2'	1:CA:635:G:H8	1.86	0.40
1:CA:1368:G:OP2	9:CI:112:LYS:NZ	2.50	0.40
54:B8:54:GLU:O	54:B8:58:ILE:HG13	2.22	0.40
1:AA:580:U:H5''	15:AO:58:MET:HG2	2.03	0.40
24:AX:4:G:H2'	24:AX:5:G:C8	2.55	0.40
2:CB:110:GLN:O	2:CB:110:GLN:HG2	2.21	0.40
24:CX:38:A:O5'	24:CX:38:A:H8	2.04	0.40
30:DG:167:GLU:H	30:DG:167:GLU:CD	2.25	0.40
40:DU:85:LYS:HE2	40:DU:85:LYS:HB3	1.82	0.40
8:CH:56:LYS:HD3	8:CH:56:LYS:HA	1.82	0.40
25:DA:2055:C:H5'	25:DA:2056:G:O5'	2.22	0.40
44:DY:12:THR:OG1	44:DY:26:LYS:HE2	2.22	0.40
1:CA:1427:U:H2'	1:CA:1428:A:C8	2.56	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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	229/256 (90%)	200 (87%)	19 (8%)	10 (4%)	3	3
2	CB	229/256 (90%)	195 (85%)	24 (10%)	10 (4%)	3	3
3	AC	204/239 (85%)	184 (90%)	17 (8%)	3 (2%)	13	22
3	CC	204/239 (85%)	180 (88%)	22 (11%)	2 (1%)	19	33
4	AD	206/209 (99%)	192 (93%)	12 (6%)	2 (1%)	19	33
4	CD	206/209 (99%)	189 (92%)	16 (8%)	1 (0%)	34	54
5	AE	146/162 (90%)	134 (92%)	9 (6%)	3 (2%)	9	13
5	CE	146/162 (90%)	138 (94%)	7 (5%)	1 (1%)	26	44
6	AF	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
6	CF	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
7	AG	153/156 (98%)	143 (94%)	8 (5%)	2 (1%)	15	25
7	CG	153/156 (98%)	140 (92%)	9 (6%)	4 (3%)	7	9
8	AH	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
8	CH	135/138 (98%)	129 (96%)	5 (4%)	1 (1%)	26	44
9	AI	125/128 (98%)	111 (89%)	11 (9%)	3 (2%)	7	11
9	CI	125/128 (98%)	114 (91%)	8 (6%)	3 (2%)	7	11
10	AJ	95/105 (90%)	83 (87%)	9 (10%)	3 (3%)	5	6
10	CJ	94/105 (90%)	81 (86%)	10 (11%)	3 (3%)	5	6
11	AK	112/129 (87%)	106 (95%)	4 (4%)	2 (2%)	11	17
11	CK	112/129 (87%)	107 (96%)	3 (3%)	2 (2%)	11	17
12	AL	120/132 (91%)	115 (96%)	5 (4%)	0	100	100
12	CL	120/132 (91%)	116 (97%)	4 (3%)	0	100	100
13	AM	121/126 (96%)	110 (91%)	9 (7%)	2 (2%)	11	18
13	CM	120/126 (95%)	108 (90%)	9 (8%)	3 (2%)	7	10
14	AN	58/61 (95%)	54 (93%)	4 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	CN	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
15	AO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
15	CO	86/89 (97%)	80 (93%)	4 (5%)	2 (2%)	8	11
16	AP	80/88 (91%)	78 (98%)	2 (2%)	0	100	100
16	CP	80/88 (91%)	77 (96%)	2 (2%)	1 (1%)	15	25
17	AQ	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
17	CQ	97/105 (92%)	91 (94%)	5 (5%)	1 (1%)	19	33
18	AR	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
18	CR	66/88 (75%)	65 (98%)	0	1 (2%)	13	22
19	AS	81/93 (87%)	72 (89%)	9 (11%)	0	100	100
19	CS	81/93 (87%)	71 (88%)	10 (12%)	0	100	100
20	AT	94/106 (89%)	84 (89%)	3 (3%)	7 (7%)	1	1
20	CT	94/106 (89%)	84 (89%)	5 (5%)	5 (5%)	2	2
21	AU	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
21	CU	21/27 (78%)	18 (86%)	2 (10%)	1 (5%)	3	3
27	BD	273/276 (99%)	257 (94%)	15 (6%)	1 (0%)	39	60
27	DD	273/276 (99%)	258 (94%)	13 (5%)	2 (1%)	26	44
28	BE	202/206 (98%)	193 (96%)	8 (4%)	1 (0%)	34	54
28	DE	202/206 (98%)	191 (95%)	9 (4%)	2 (1%)	19	33
29	BF	201/210 (96%)	197 (98%)	3 (2%)	1 (0%)	34	54
29	DF	201/210 (96%)	195 (97%)	4 (2%)	2 (1%)	19	33
30	BG	179/182 (98%)	167 (93%)	7 (4%)	5 (3%)	6	8
30	DG	179/182 (98%)	165 (92%)	7 (4%)	7 (4%)	4	4
31	BH	172/180 (96%)	159 (92%)	12 (7%)	1 (1%)	30	48
31	DH	172/180 (96%)	157 (91%)	13 (8%)	2 (1%)	16	27
32	BI	144/148 (97%)	123 (85%)	16 (11%)	5 (4%)	4	5
32	DI	144/148 (97%)	126 (88%)	17 (12%)	1 (1%)	26	44
33	BN	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
33	DN	138/140 (99%)	133 (96%)	4 (3%)	1 (1%)	26	44
34	BO	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
34	DO	120/122 (98%)	115 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	BP	147/150 (98%)	138 (94%)	8 (5%)	1 (1%)	26	44
35	DP	147/150 (98%)	135 (92%)	10 (7%)	2 (1%)	14	23
36	BQ	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
36	DQ	139/141 (99%)	129 (93%)	8 (6%)	2 (1%)	14	23
37	BR	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
37	DR	116/118 (98%)	107 (92%)	9 (8%)	0	100	100
38	BS	108/112 (96%)	102 (94%)	6 (6%)	0	100	100
38	DS	108/112 (96%)	104 (96%)	3 (3%)	1 (1%)	21	36
39	BT	129/146 (88%)	121 (94%)	7 (5%)	1 (1%)	24	40
39	DT	129/146 (88%)	123 (95%)	5 (4%)	1 (1%)	24	40
40	BU	114/118 (97%)	114 (100%)	0	0	100	100
40	DU	114/118 (97%)	114 (100%)	0	0	100	100
41	BV	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	19	33
41	DV	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	19	33
42	BW	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
42	DW	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
43	BX	93/96 (97%)	90 (97%)	1 (1%)	2 (2%)	8	12
43	DX	93/96 (97%)	90 (97%)	2 (2%)	1 (1%)	17	30
44	BY	105/110 (96%)	96 (91%)	9 (9%)	0	100	100
44	DY	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
45	BZ	169/206 (82%)	143 (85%)	24 (14%)	2 (1%)	16	27
45	DZ	172/206 (84%)	149 (87%)	22 (13%)	1 (1%)	30	48
46	B0	81/85 (95%)	77 (95%)	3 (4%)	1 (1%)	16	27
46	D0	81/85 (95%)	75 (93%)	6 (7%)	0	100	100
47	B1	95/98 (97%)	91 (96%)	4 (4%)	0	100	100
47	D1	95/98 (97%)	91 (96%)	4 (4%)	0	100	100
48	B2	68/72 (94%)	68 (100%)	0	0	100	100
48	D2	68/72 (94%)	68 (100%)	0	0	100	100
49	B3	57/60 (95%)	57 (100%)	0	0	100	100
49	D3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
50	B4	67/71 (94%)	50 (75%)	11 (16%)	6 (9%)	1	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	D4	67/71 (94%)	51 (76%)	12 (18%)	4 (6%)	2	1
51	B5	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
51	D5	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
52	B6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
52	D6	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
53	B7	46/49 (94%)	46 (100%)	0	0	100	100
53	D7	46/49 (94%)	45 (98%)	0	1 (2%)	8	12
54	B8	62/65 (95%)	62 (100%)	0	0	100	100
54	D8	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
55	B9	35/37 (95%)	35 (100%)	0	0	100	100
55	D9	35/37 (95%)	35 (100%)	0	0	100	100
All	All	11409/12128 (94%)	10643 (93%)	629 (6%)	137 (1%)	16	27

All (137) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	9	GLU
2	AB	15	VAL
2	AB	16	HIS
2	AB	17	PHE
2	AB	126	GLU
2	AB	231	GLU
3	AC	65	ALA
9	AI	44	VAL
9	AI	54	ASP
10	AJ	77	PRO
20	AT	47	GLY
27	BD	275	LYS
29	BF	130	ALA
30	BG	50	ALA
50	B4	55	ARG
50	B4	57	GLU
2	CB	16	HIS
2	CB	17	PHE
2	CB	126	GLU
7	CG	7	ALA
9	CI	44	VAL
9	CI	54	ASP

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Mol	Chain	Res	Type
10	CJ	79	ARG
13	CM	107	ALA
20	CT	10	LEU
29	DF	21	ALA
29	DF	130	ALA
30	DG	47	LYS
30	DG	81	LYS
31	DH	29	PRO
31	DH	126	PRO
32	DI	10	GLU
35	DP	45	LEU
50	D4	45	GLY
50	D4	51	ASP
50	D4	62	ARG
53	D7	46	VAL
3	AC	66	VAL
5	AE	85	GLY
5	AE	86	ALA
9	AI	43	ALA
10	AJ	31	GLY
10	AJ	91	PRO
11	AK	49	GLY
30	BG	43	LEU
30	BG	126	ASP
31	BH	126	PRO
32	BI	11	ASN
32	BI	106	GLY
41	BV	79	VAL
45	BZ	152	ALA
45	BZ	159	PRO
50	B4	45	GLY
50	B4	54	GLY
50	B4	68	ARG
2	CB	10	LEU
3	CC	181	ASN
7	CG	81	GLY
10	CJ	77	PRO
11	CK	49	GLY
13	CM	106	ASN
15	CO	23	GLY
16	CP	53	VAL
20	CT	47	GLY

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Mol	Chain	Res	Type
28	DE	73	GLU
30	DG	43	LEU
30	DG	51	ARG
30	DG	126	ASP
41	DV	79	VAL
45	DZ	117	LEU
2	AB	150	SER
4	AD	166	LYS
4	AD	173	TRP
13	AM	12	ASN
20	AT	9	ASN
20	AT	10	LEU
20	AT	94	ALA
20	AT	100	ILE
20	AT	102	GLY
28	BE	52	LEU
46	B0	13	GLY
2	CB	8	LYS
2	CB	150	SER
4	CD	45	GLN
5	CE	69	VAL
8	CH	73	ASP
9	CI	11	LYS
20	CT	99	LEU
27	DD	3	VAL
28	DE	52	LEU
33	DN	2	LYS
36	DQ	28	ALA
38	DS	84	GLN
2	AB	10	LEU
3	AC	107	GLN
5	AE	69	VAL
7	AG	80	VAL
13	AM	11	ARG
30	BG	32	PRO
30	BG	51	ARG
32	BI	73	GLU
39	BT	55	ASN
43	BX	93	GLU
15	CO	88	ARG
17	CQ	14	LYS
27	DD	239	ARG

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Mol	Chain	Res	Type
30	DG	32	PRO
39	DT	55	ASN
43	DX	2	LYS
50	D4	55	ARG
2	AB	124	SER
11	AK	105	VAL
20	AT	95	ALA
32	BI	107	VAL
35	BP	29	LYS
50	B4	44	THR
2	CB	120	ALA
2	CB	234	PRO
3	CC	156	ARG
7	CG	55	GLY
18	CR	25	THR
20	CT	102	GLY
30	DG	50	ALA
2	AB	202	PRO
2	CB	202	PRO
2	CB	232	PRO
20	CT	100	ILE
35	DP	29	LYS
43	BX	94	GLY
11	CK	105	VAL
7	AG	17	VAL
10	CJ	91	PRO
21	CU	23	PRO
7	CG	80	VAL
13	CM	4	ILE
36	DQ	27	VAL
32	BI	131	LYS

### 5.3.2 Protein sidechains ⓘ

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	192/220 (87%)	169 (88%)	23 (12%)	6	11
2	CB	187/220 (85%)	168 (90%)	19 (10%)	9	16
3	AC	143/188 (76%)	132 (92%)	11 (8%)	16	28
3	CC	140/188 (74%)	127 (91%)	13 (9%)	11	19
4	AD	170/181 (94%)	155 (91%)	15 (9%)	12	22
4	CD	173/181 (96%)	160 (92%)	13 (8%)	17	30
5	AE	113/123 (92%)	106 (94%)	7 (6%)	23	39
5	CE	114/123 (93%)	105 (92%)	9 (8%)	15	27
6	AF	83/90 (92%)	77 (93%)	6 (7%)	18	31
6	CF	85/90 (94%)	81 (95%)	4 (5%)	32	54
7	AG	119/127 (94%)	106 (89%)	13 (11%)	8	13
7	CG	120/127 (94%)	111 (92%)	9 (8%)	17	30
8	AH	114/119 (96%)	107 (94%)	7 (6%)	23	40
8	CH	114/119 (96%)	104 (91%)	10 (9%)	12	22
9	AI	90/99 (91%)	82 (91%)	8 (9%)	12	22
9	CI	89/99 (90%)	73 (82%)	16 (18%)	2	3
10	AJ	66/92 (72%)	62 (94%)	4 (6%)	23	40
10	CJ	69/92 (75%)	66 (96%)	3 (4%)	35	59
11	AK	82/99 (83%)	76 (93%)	6 (7%)	17	31
11	CK	83/99 (84%)	77 (93%)	6 (7%)	18	31
12	AL	97/109 (89%)	93 (96%)	4 (4%)	37	61
12	CL	97/109 (89%)	92 (95%)	5 (5%)	29	49
13	AM	93/101 (92%)	83 (89%)	10 (11%)	8	14
13	CM	92/101 (91%)	83 (90%)	9 (10%)	10	17
14	AN	49/50 (98%)	43 (88%)	6 (12%)	6	10
14	CN	49/50 (98%)	43 (88%)	6 (12%)	6	10
15	AO	78/80 (98%)	67 (86%)	11 (14%)	4	7
15	CO	78/80 (98%)	70 (90%)	8 (10%)	9	15
16	AP	69/74 (93%)	62 (90%)	7 (10%)	9	16
16	CP	68/74 (92%)	63 (93%)	5 (7%)	17	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	AQ	94/97 (97%)	91 (97%)	3 (3%)	46	72
17	CQ	94/97 (97%)	88 (94%)	6 (6%)	22	38
18	AR	59/77 (77%)	56 (95%)	3 (5%)	29	50
18	CR	59/77 (77%)	54 (92%)	5 (8%)	13	23
19	AS	69/80 (86%)	66 (96%)	3 (4%)	35	59
19	CS	67/80 (84%)	57 (85%)	10 (15%)	4	6
20	AT	70/82 (85%)	64 (91%)	6 (9%)	13	23
20	CT	70/82 (85%)	64 (91%)	6 (9%)	13	23
21	AU	18/22 (82%)	16 (89%)	2 (11%)	8	13
21	CU	18/22 (82%)	16 (89%)	2 (11%)	8	13
27	BD	215/218 (99%)	200 (93%)	15 (7%)	19	33
27	DD	215/218 (99%)	202 (94%)	13 (6%)	24	41
28	BE	164/166 (99%)	147 (90%)	17 (10%)	9	15
28	DE	164/166 (99%)	145 (88%)	19 (12%)	7	12
29	BF	160/166 (96%)	142 (89%)	18 (11%)	7	12
29	DF	159/166 (96%)	142 (89%)	17 (11%)	8	14
30	BG	143/156 (92%)	130 (91%)	13 (9%)	12	20
30	DG	142/156 (91%)	128 (90%)	14 (10%)	10	17
31	BH	144/148 (97%)	136 (94%)	8 (6%)	26	45
31	DH	144/148 (97%)	133 (92%)	11 (8%)	16	29
32	BI	110/124 (89%)	92 (84%)	18 (16%)	3	4
32	DI	104/124 (84%)	93 (89%)	11 (11%)	8	15
33	BN	118/119 (99%)	103 (87%)	15 (13%)	5	9
33	DN	118/119 (99%)	107 (91%)	11 (9%)	11	19
34	BO	100/100 (100%)	97 (97%)	3 (3%)	48	74
34	DO	100/100 (100%)	96 (96%)	4 (4%)	38	62
35	BP	115/116 (99%)	107 (93%)	8 (7%)	19	33
35	DP	115/116 (99%)	103 (90%)	12 (10%)	9	15
36	BQ	111/111 (100%)	97 (87%)	14 (13%)	5	9
36	DQ	111/111 (100%)	101 (91%)	10 (9%)	12	21
37	BR	101/101 (100%)	84 (83%)	17 (17%)	2	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	DR	101/101 (100%)	86 (85%)	15 (15%)	4	6
38	BS	87/88 (99%)	78 (90%)	9 (10%)	9	15
38	DS	85/88 (97%)	78 (92%)	7 (8%)	14	25
39	BT	115/127 (91%)	109 (95%)	6 (5%)	29	49
39	DT	113/127 (89%)	106 (94%)	7 (6%)	23	39
40	BU	93/94 (99%)	86 (92%)	7 (8%)	17	30
40	DU	93/94 (99%)	88 (95%)	5 (5%)	27	47
41	BV	80/82 (98%)	72 (90%)	8 (10%)	9	17
41	DV	80/82 (98%)	71 (89%)	9 (11%)	7	12
42	BW	90/92 (98%)	82 (91%)	8 (9%)	12	22
42	DW	90/92 (98%)	84 (93%)	6 (7%)	20	35
43	BX	77/78 (99%)	72 (94%)	5 (6%)	21	37
43	DX	77/78 (99%)	72 (94%)	5 (6%)	21	37
44	BY	85/91 (93%)	80 (94%)	5 (6%)	24	42
44	DY	85/91 (93%)	82 (96%)	3 (4%)	43	68
45	BZ	145/179 (81%)	131 (90%)	14 (10%)	10	18
45	DZ	145/179 (81%)	132 (91%)	13 (9%)	12	21
46	B0	65/67 (97%)	63 (97%)	2 (3%)	47	73
46	D0	65/67 (97%)	63 (97%)	2 (3%)	47	73
47	B1	80/83 (96%)	75 (94%)	5 (6%)	22	38
47	D1	80/83 (96%)	73 (91%)	7 (9%)	12	22
48	B2	65/67 (97%)	61 (94%)	4 (6%)	23	39
48	D2	65/67 (97%)	64 (98%)	1 (2%)	72	90
49	B3	51/52 (98%)	47 (92%)	4 (8%)	16	28
49	D3	50/52 (96%)	45 (90%)	5 (10%)	9	17
50	B4	60/63 (95%)	52 (87%)	8 (13%)	5	8
50	D4	53/63 (84%)	47 (89%)	6 (11%)	7	12
51	B5	50/52 (96%)	47 (94%)	3 (6%)	24	41
51	D5	50/52 (96%)	45 (90%)	5 (10%)	9	17
52	B6	51/52 (98%)	46 (90%)	5 (10%)	10	17
52	D6	50/52 (96%)	48 (96%)	2 (4%)	38	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	B7	41/42 (98%)	38 (93%)	3 (7%)	17	31
53	D7	41/42 (98%)	40 (98%)	1 (2%)	57	81
54	B8	53/55 (96%)	50 (94%)	3 (6%)	25	44
54	D8	54/55 (98%)	51 (94%)	3 (6%)	26	45
55	B9	34/34 (100%)	34 (100%)	0	100	100
55	D9	34/34 (100%)	34 (100%)	0	100	100
All	All	9320/10066 (93%)	8532 (92%)	788 (8%)	13	23

All (788) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AB	7	VAL
2	AB	8	LYS
2	AB	11	LEU
2	AB	16	HIS
2	AB	17	PHE
2	AB	21	ARG
2	AB	24	TRP
2	AB	64	ARG
2	AB	76	GLN
2	AB	94	ASN
2	AB	114	ARG
2	AB	127	ILE
2	AB	144	ARG
2	AB	145	LEU
2	AB	155	LEU
2	AB	157	ARG
2	AB	189	ASP
2	AB	196	LEU
2	AB	200	ILE
2	AB	209	ARG
2	AB	213	LEU
2	AB	217	ARG
2	AB	221	LEU
3	AC	3	ASN
3	AC	8	ILE
3	AC	21	ARG
3	AC	28	GLN
3	AC	37	GLN
3	AC	40	ARG

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Mol	Chain	Res	Type
3	AC	45	LYS
3	AC	89	GLU
3	AC	119	ARG
3	AC	131	ARG
3	AC	150	LYS
4	AD	5	ILE
4	AD	15	GLU
4	AD	19	LEU
4	AD	31	CYS
4	AD	49	ARG
4	AD	58	LEU
4	AD	115	ARG
4	AD	127	THR
4	AD	135	LEU
4	AD	140	VAL
4	AD	141	ARG
4	AD	150	GLU
4	AD	157	LEU
4	AD	158	ILE
4	AD	168	ARG
5	AE	31	LEU
5	AE	38	GLN
5	AE	41	VAL
5	AE	47	LYS
5	AE	51	VAL
5	AE	73	ASN
5	AE	151	LEU
6	AF	36	ARG
6	AF	55	ASP
6	AF	70	ASP
6	AF	74	ASP
6	AF	75	LEU
6	AF	82	ARG
7	AG	8	GLU
7	AG	13	GLN
7	AG	50	ILE
7	AG	51	GLN
7	AG	52	GLU
7	AG	72	ARG
7	AG	76	ARG
7	AG	79	ARG
7	AG	104	LEU

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Mol	Chain	Res	Type
7	AG	113	GLU
7	AG	114	ARG
7	AG	138	LYS
7	AG	155	ARG
8	AH	21	LYS
8	AH	52	ASP
8	AH	75	ARG
8	AH	78	GLN
8	AH	91	ARG
8	AH	95	VAL
8	AH	97	VAL
9	AI	14	VAL
9	AI	23	ASN
9	AI	65	VAL
9	AI	86	VAL
9	AI	89	ASN
9	AI	108	VAL
9	AI	127	LYS
9	AI	128	ARG
10	AJ	5	ARG
10	AJ	23	ILE
10	AJ	55	LYS
10	AJ	84	GLN
11	AK	16	SER
11	AK	31	THR
11	AK	48	ILE
11	AK	96	ARG
11	AK	104	GLN
11	AK	114	VAL
12	AL	24	VAL
12	AL	33	ARG
12	AL	53	ARG
12	AL	60	LEU
13	AM	3	ARG
13	AM	4	ILE
13	AM	15	VAL
13	AM	19	LEU
13	AM	43	THR
13	AM	56	LEU
13	AM	70	LEU
13	AM	73	GLU
13	AM	102	ARG

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Mol	Chain	Res	Type
13	AM	110	ARG
14	AN	3	ARG
14	AN	7	ILE
14	AN	18	VAL
14	AN	23	ARG
14	AN	33	VAL
14	AN	50	LYS
15	AO	3	ILE
15	AO	5	LYS
15	AO	22	THR
15	AO	24	SER
15	AO	26	GLU
15	AO	38	ARG
15	AO	39	LEU
15	AO	41	GLU
15	AO	47	LYS
15	AO	64	ARG
15	AO	76	GLU
16	AP	19	ILE
16	AP	20	VAL
16	AP	27	LYS
16	AP	50	LYS
16	AP	54	GLU
16	AP	60	LEU
16	AP	62	VAL
17	AQ	14	LYS
17	AQ	74	LEU
17	AQ	83	ASP
18	AR	31	LEU
18	AR	46	GLU
18	AR	76	LEU
19	AS	28	LYS
19	AS	37	ARG
19	AS	65	ASN
20	AT	8	ARG
20	AT	13	LEU
20	AT	30	LYS
20	AT	45	GLN
20	AT	56	MET
20	AT	62	LEU
21	AU	9	ARG
21	AU	10	ARG

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Mol	Chain	Res	Type
27	BD	3	VAL
27	BD	61	LEU
27	BD	71	ASP
27	BD	94	LEU
27	BD	99	ASP
27	BD	113	VAL
27	BD	116	GLN
27	BD	126	GLN
27	BD	142	VAL
27	BD	211	ARG
27	BD	221	VAL
27	BD	229	VAL
27	BD	242	ARG
27	BD	259	THR
27	BD	260	ARG
28	BE	12	THR
28	BE	21	VAL
28	BE	24	THR
28	BE	40	GLU
28	BE	73	GLU
28	BE	77	ILE
28	BE	78	LEU
28	BE	82	ARG
28	BE	89	ASP
28	BE	97	LYS
28	BE	111	ARG
28	BE	116	VAL
28	BE	119	ARG
28	BE	144	ARG
28	BE	154	LYS
28	BE	163	GLU
28	BE	175	VAL
29	BF	19	GLU
29	BF	20	LEU
29	BF	23	ASP
29	BF	27	GLU
29	BF	33	LEU
29	BF	38	ARG
29	BF	53	THR
29	BF	57	VAL
29	BF	106	ARG
29	BF	110	LEU

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Mol	Chain	Res	Type
29	BF	125	LEU
29	BF	158	THR
29	BF	170	LEU
29	BF	175	THR
29	BF	192	LEU
29	BF	195	ASP
29	BF	197	ASP
29	BF	200	GLU
30	BG	43	LEU
30	BG	45	GLU
30	BG	60	LEU
30	BG	78	SER
30	BG	81	LYS
30	BG	91	ARG
30	BG	135	LEU
30	BG	140	ILE
30	BG	143	GLU
30	BG	148	MET
30	BG	159	VAL
30	BG	170	ARG
30	BG	175	LEU
31	BH	3	ARG
31	BH	41	MET
31	BH	45	VAL
31	BH	59	ARG
31	BH	69	ARG
31	BH	71	LEU
31	BH	116	GLU
31	BH	130	ARG
32	BI	5	LEU
32	BI	10	GLU
32	BI	20	ASP
32	BI	38	LEU
32	BI	43	ASN
32	BI	47	LEU
32	BI	50	ARG
32	BI	57	ARG
32	BI	60	GLU
32	BI	66	GLU
32	BI	77	LEU
32	BI	92	VAL
32	BI	96	ASP

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Mol	Chain	Res	Type
32	BI	101	LEU
32	BI	109	ILE
32	BI	140	LEU
32	BI	142	VAL
32	BI	144	VAL
33	BN	5	VAL
33	BN	12	ARG
33	BN	28	THR
33	BN	33	LEU
33	BN	34	LEU
33	BN	46	VAL
33	BN	48	MET
33	BN	61	ARG
33	BN	62	VAL
33	BN	68	GLU
33	BN	87	LEU
33	BN	97	ARG
33	BN	99	LEU
33	BN	120	LEU
33	BN	133	GLN
34	BO	8	LEU
34	BO	23	ARG
34	BO	108	GLU
35	BP	55	ARG
35	BP	59	LEU
35	BP	65	ARG
35	BP	70	GLN
35	BP	83	VAL
35	BP	106	LEU
35	BP	112	LEU
35	BP	135	LEU
36	BQ	1	MET
36	BQ	2	LEU
36	BQ	5	ARG
36	BQ	7	MET
36	BQ	8	LYS
36	BQ	16	ARG
36	BQ	21	THR
36	BQ	35	VAL
36	BQ	45	GLN
36	BQ	54	MET
36	BQ	59	ARG

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Mol	Chain	Res	Type
36	BQ	60	ARG
36	BQ	75	THR
36	BQ	110	THR
37	BR	1	MET
37	BR	6	SER
37	BR	15	SER
37	BR	18	LEU
37	BR	28	LEU
37	BR	29	LEU
37	BR	33	ARG
37	BR	36	THR
37	BR	44	LEU
37	BR	54	LEU
37	BR	60	LEU
37	BR	65	LEU
37	BR	67	LEU
37	BR	79	LEU
37	BR	100	LEU
37	BR	111	LEU
37	BR	114	VAL
38	BS	14	VAL
38	BS	20	ARG
38	BS	49	VAL
38	BS	50	SER
38	BS	57	LYS
38	BS	59	LYS
38	BS	69	VAL
38	BS	78	LEU
38	BS	110	LEU
39	BT	6	LEU
39	BT	28	VAL
39	BT	49	VAL
39	BT	53	ARG
39	BT	96	ARG
39	BT	118	ARG
40	BU	8	VAL
40	BU	36	ARG
40	BU	59	ARG
40	BU	74	LEU
40	BU	83	LEU
40	BU	95	LEU
40	BU	104	GLN

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Mol	Chain	Res	Type
41	BV	18	LEU
41	BV	28	GLU
41	BV	32	THR
41	BV	46	VAL
41	BV	52	VAL
41	BV	62	LEU
41	BV	95	LEU
41	BV	100	ARG
42	BW	4	LYS
42	BW	11	ARG
42	BW	17	VAL
42	BW	19	LEU
42	BW	51	LEU
42	BW	52	GLU
42	BW	67	ASP
42	BW	107	LEU
43	BX	23	GLU
43	BX	35	THR
43	BX	57	LEU
43	BX	65	ARG
43	BX	66	LEU
44	BY	23	ARG
44	BY	55	TYR
44	BY	73	ARG
44	BY	90	LEU
44	BY	99	CYS
45	BZ	5	LEU
45	BZ	6	LYS
45	BZ	18	LEU
45	BZ	33	LEU
45	BZ	61	LEU
45	BZ	91	LEU
45	BZ	111	VAL
45	BZ	117	LEU
45	BZ	121	HIS
45	BZ	136	PHE
45	BZ	153	SER
45	BZ	154	ASP
45	BZ	155	LEU
45	BZ	171	ILE
46	B0	14	ARG
46	B0	20	ARG

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Mol	Chain	Res	Type
47	B1	40	ARG
47	B1	59	THR
47	B1	75	GLU
47	B1	78	LYS
47	B1	95	LEU
48	B2	30	ARG
48	B2	40	SER
48	B2	52	ASP
48	B2	70	GLN
49	B3	8	LEU
49	B3	23	LEU
49	B3	54	VAL
49	B3	60	GLU
50	B4	34	GLU
50	B4	46	GLN
50	B4	49	PHE
50	B4	58	ARG
50	B4	63	TYR
50	B4	67	TYR
50	B4	68	ARG
50	B4	69	LYS
51	B5	6	VAL
51	B5	29	THR
51	B5	40	LYS
52	B6	4	GLU
52	B6	14	THR
52	B6	28	ARG
52	B6	38	LYS
52	B6	52	VAL
53	B7	1	MET
53	B7	24	THR
53	B7	43	THR
54	B8	14	VAL
54	B8	31	HIS
54	B8	32	LEU
2	CB	8	LYS
2	CB	11	LEU
2	CB	23	ARG
2	CB	24	TRP
2	CB	47	THR
2	CB	48	MET
2	CB	76	GLN

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Mol	Chain	Res	Type
2	CB	94	ASN
2	CB	96	ARG
2	CB	115	LEU
2	CB	126	GLU
2	CB	133	LYS
2	CB	155	LEU
2	CB	163	PHE
2	CB	185	ILE
2	CB	189	ASP
2	CB	213	LEU
2	CB	217	ARG
2	CB	224	GLN
3	CC	3	ASN
3	CC	21	ARG
3	CC	28	GLN
3	CC	30	ARG
3	CC	54	ARG
3	CC	105	GLU
3	CC	115	LEU
3	CC	118	GLN
3	CC	119	ARG
3	CC	131	ARG
3	CC	152	ILE
3	CC	162	GLN
3	CC	196	LEU
4	CD	31	CYS
4	CD	34	GLU
4	CD	47	ARG
4	CD	58	LEU
4	CD	61	LYS
4	CD	96	LEU
4	CD	108	LEU
4	CD	135	LEU
4	CD	141	ARG
4	CD	150	GLU
4	CD	155	LEU
4	CD	157	LEU
4	CD	194	LEU
5	CE	24	ARG
5	CE	31	LEU
5	CE	38	GLN
5	CE	41	VAL

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Mol	Chain	Res	Type
5	CE	47	LYS
5	CE	51	VAL
5	CE	64	ARG
5	CE	78	HIS
5	CE	79	GLU
6	CF	10	LEU
6	CF	28	ARG
6	CF	70	ASP
6	CF	75	LEU
7	CG	10	ARG
7	CG	11	GLN
7	CG	12	LEU
7	CG	32	ARG
7	CG	51	GLN
7	CG	52	GLU
7	CG	104	LEU
7	CG	114	ARG
7	CG	155	ARG
8	CH	18	ARG
8	CH	29	SER
8	CH	39	LEU
8	CH	75	ARG
8	CH	84	ARG
8	CH	91	ARG
8	CH	95	VAL
8	CH	97	VAL
8	CH	98	LYS
8	CH	127	LEU
9	CI	7	THR
9	CI	14	VAL
9	CI	17	VAL
9	CI	23	ASN
9	CI	27	THR
9	CI	50	LEU
9	CI	56	LEU
9	CI	64	THR
9	CI	65	VAL
9	CI	81	ILE
9	CI	89	ASN
9	CI	102	LEU
9	CI	108	VAL
9	CI	113	LYS

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Mol	Chain	Res	Type
9	CI	127	LYS
9	CI	128	ARG
10	CJ	21	GLN
10	CJ	46	ARG
10	CJ	67	THR
11	CK	14	VAL
11	CK	54	ARG
11	CK	93	GLN
11	CK	96	ARG
11	CK	104	GLN
11	CK	114	VAL
12	CL	24	VAL
12	CL	33	ARG
12	CL	50	SER
12	CL	53	ARG
12	CL	79	GLU
13	CM	3	ARG
13	CM	15	VAL
13	CM	19	LEU
13	CM	47	ASP
13	CM	56	LEU
13	CM	70	LEU
13	CM	102	ARG
13	CM	110	ARG
13	CM	121	LYS
14	CN	3	ARG
14	CN	7	ILE
14	CN	12	ARG
14	CN	15	LYS
14	CN	23	ARG
14	CN	33	VAL
15	CO	3	ILE
15	CO	5	LYS
15	CO	26	GLU
15	CO	38	ARG
15	CO	39	LEU
15	CO	41	GLU
15	CO	54	ARG
15	CO	64	ARG
16	CP	5	ARG
16	CP	20	VAL
16	CP	27	LYS

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Mol	Chain	Res	Type
16	CP	62	VAL
16	CP	67	THR
17	CQ	9	VAL
17	CQ	14	LYS
17	CQ	36	ILE
17	CQ	74	LEU
17	CQ	83	ASP
17	CQ	96	GLU
18	CR	26	LEU
18	CR	41	LYS
18	CR	42	ARG
18	CR	46	GLU
18	CR	76	LEU
19	CS	16	LEU
19	CS	27	GLU
19	CS	28	LYS
19	CS	30	LEU
19	CS	37	ARG
19	CS	56	GLN
19	CS	65	ASN
19	CS	71	LEU
19	CS	77	THR
19	CS	78	ARG
20	CT	36	LEU
20	CT	45	GLN
20	CT	56	MET
20	CT	62	LEU
20	CT	80	ARG
20	CT	99	LEU
21	CU	10	ARG
21	CU	24	ARG
27	DD	61	LEU
27	DD	71	ASP
27	DD	94	LEU
27	DD	99	ASP
27	DD	106	ILE
27	DD	109	ASP
27	DD	113	VAL
27	DD	116	GLN
27	DD	211	ARG
27	DD	221	VAL
27	DD	242	ARG

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Mol	Chain	Res	Type
27	DD	259	THR
27	DD	260	ARG
28	DE	9	VAL
28	DE	12	THR
28	DE	21	VAL
28	DE	24	THR
28	DE	34	VAL
28	DE	38	THR
28	DE	52	LEU
28	DE	73	GLU
28	DE	75	VAL
28	DE	77	ILE
28	DE	78	LEU
28	DE	82	ARG
28	DE	111	ARG
28	DE	116	VAL
28	DE	119	ARG
28	DE	144	ARG
28	DE	154	LYS
28	DE	163	GLU
28	DE	175	VAL
29	DF	17	ARG
29	DF	19	GLU
29	DF	20	LEU
29	DF	27	GLU
29	DF	33	LEU
29	DF	38	ARG
29	DF	53	THR
29	DF	57	VAL
29	DF	106	ARG
29	DF	107	LYS
29	DF	108	LYS
29	DF	110	LEU
29	DF	158	THR
29	DF	170	LEU
29	DF	175	THR
29	DF	192	LEU
29	DF	200	GLU
30	DG	16	ARG
30	DG	43	LEU
30	DG	45	GLU
30	DG	47	LYS

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Mol	Chain	Res	Type
30	DG	49	ASP
30	DG	60	LEU
30	DG	91	ARG
30	DG	115	ARG
30	DG	136	ARG
30	DG	140	ILE
30	DG	143	GLU
30	DG	148	MET
30	DG	170	ARG
30	DG	175	LEU
31	DH	3	ARG
31	DH	33	LEU
31	DH	63	SER
31	DH	69	ARG
31	DH	72	ILE
31	DH	95	ARG
31	DH	105	LEU
31	DH	106	THR
31	DH	136	ILE
31	DH	139	GLN
31	DH	175	LYS
32	DI	5	LEU
32	DI	9	LEU
32	DI	20	ASP
32	DI	38	LEU
32	DI	43	ASN
32	DI	47	LEU
32	DI	57	ARG
32	DI	61	ARG
32	DI	73	GLU
32	DI	77	LEU
32	DI	140	LEU
33	DN	28	THR
33	DN	33	LEU
33	DN	34	LEU
33	DN	46	VAL
33	DN	58	ASP
33	DN	62	VAL
33	DN	85	ILE
33	DN	87	LEU
33	DN	97	ARG
33	DN	120	LEU

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Mol	Chain	Res	Type
33	DN	138	LEU
34	DO	8	LEU
34	DO	23	ARG
34	DO	69	ILE
34	DO	108	GLU
35	DP	2	LYS
35	DP	15	ARG
35	DP	45	LEU
35	DP	50	ARG
35	DP	55	ARG
35	DP	65	ARG
35	DP	77	ARG
35	DP	83	VAL
35	DP	95	VAL
35	DP	106	LEU
35	DP	112	LEU
35	DP	135	LEU
36	DQ	1	MET
36	DQ	16	ARG
36	DQ	21	THR
36	DQ	45	GLN
36	DQ	48	GLU
36	DQ	54	MET
36	DQ	56	ARG
36	DQ	60	ARG
36	DQ	75	THR
36	DQ	110	THR
37	DR	1	MET
37	DR	6	SER
37	DR	18	LEU
37	DR	24	GLN
37	DR	28	LEU
37	DR	29	LEU
37	DR	33	ARG
37	DR	36	THR
37	DR	44	LEU
37	DR	54	LEU
37	DR	60	LEU
37	DR	65	LEU
37	DR	67	LEU
37	DR	79	LEU
37	DR	100	LEU

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Mol	Chain	Res	Type
38	DS	20	ARG
38	DS	50	SER
38	DS	67	ARG
38	DS	75	GLU
38	DS	80	LEU
38	DS	83	LYS
38	DS	110	LEU
39	DT	16	ARG
39	DT	17	THR
39	DT	28	VAL
39	DT	38	ASN
39	DT	49	VAL
39	DT	96	ARG
39	DT	118	ARG
40	DU	36	ARG
40	DU	74	LEU
40	DU	92	ARG
40	DU	104	GLN
40	DU	108	GLU
41	DV	15	GLU
41	DV	18	LEU
41	DV	28	GLU
41	DV	32	THR
41	DV	51	VAL
41	DV	52	VAL
41	DV	79	VAL
41	DV	85	LYS
41	DV	95	LEU
42	DW	4	LYS
42	DW	11	ARG
42	DW	17	VAL
42	DW	51	LEU
42	DW	67	ASP
42	DW	107	LEU
43	DX	1	MET
43	DX	23	GLU
43	DX	35	THR
43	DX	57	LEU
43	DX	70	LEU
44	DY	23	ARG
44	DY	72	VAL
44	DY	99	CYS

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Mol	Chain	Res	Type
45	DZ	5	LEU
45	DZ	18	LEU
45	DZ	33	LEU
45	DZ	41	LEU
45	DZ	61	LEU
45	DZ	111	VAL
45	DZ	119	GLU
45	DZ	121	HIS
45	DZ	131	ARG
45	DZ	136	PHE
45	DZ	153	SER
45	DZ	154	ASP
45	DZ	155	LEU
46	D0	20	ARG
46	D0	24	LYS
47	D1	3	LYS
47	D1	32	LYS
47	D1	40	ARG
47	D1	52	ARG
47	D1	59	THR
47	D1	95	LEU
47	D1	97	LEU
48	D2	70	GLN
49	D3	8	LEU
49	D3	23	LEU
49	D3	30	ARG
49	D3	44	ARG
49	D3	54	VAL
50	D4	5	ILE
50	D4	13	ARG
50	D4	33	VAL
50	D4	34	GLU
50	D4	58	ARG
50	D4	68	ARG
51	D5	6	VAL
51	D5	29	THR
51	D5	40	LYS
51	D5	48	GLU
51	D5	59	GLU
52	D6	14	THR
52	D6	28	ARG
53	D7	1	MET

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Mol	Chain	Res	Type
54	D8	14	VAL
54	D8	32	LEU
54	D8	37	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (122) such sidechains are listed below:

Mol	Chain	Res	Type
2	AB	16	HIS
2	AB	19	HIS
2	AB	40	HIS
2	AB	94	ASN
3	AC	6	HIS
3	AC	28	GLN
3	AC	37	GLN
3	AC	98	ASN
3	AC	102	ASN
3	AC	104	GLN
3	AC	123	GLN
3	AC	136	GLN
3	AC	162	GLN
3	AC	181	ASN
4	AD	45	GLN
4	AD	77	ASN
4	AD	125	HIS
5	AE	38	GLN
5	AE	141	GLN
6	AF	100	ASN
7	AG	28	ASN
7	AG	97	GLN
9	AI	23	ASN
9	AI	58	HIS
10	AJ	56	HIS
11	AK	99	GLN
11	AK	104	GLN
12	AL	78	GLN
12	AL	99	HIS
15	AO	28	GLN
17	AQ	16	GLN
19	AS	23	ASN
19	AS	65	ASN
19	AS	69	HIS
19	AS	83	HIS

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Mol	Chain	Res	Type
20	AT	42	GLN
20	AT	45	GLN
27	BD	87	ASN
27	BD	253	GLN
28	BE	85	ASN
28	BE	143	ASN
29	BF	69	HIS
29	BF	169	ASN
29	BF	203	GLN
30	BG	26	GLN
32	BI	43	ASN
32	BI	74	ASN
35	BP	38	GLN
36	BQ	12	GLN
36	BQ	57	HIS
37	BR	71	GLN
39	BT	43	GLN
39	BT	123	GLN
40	BU	94	ASN
43	BX	31	HIS
43	BX	82	GLN
44	BY	6	HIS
45	BZ	34	ASN
45	BZ	55	HIS
45	BZ	118	GLN
48	B2	70	GLN
49	B3	32	GLN
50	B4	46	GLN
55	B9	36	GLN
2	CB	135	GLN
2	CB	224	GLN
3	CC	6	HIS
3	CC	28	GLN
3	CC	37	GLN
3	CC	104	GLN
3	CC	123	GLN
3	CC	136	GLN
4	CD	77	ASN
4	CD	125	HIS
5	CE	38	GLN
5	CE	73	ASN
5	CE	141	GLN

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Mol	Chain	Res	Type
6	CF	73	ASN
6	CF	100	ASN
7	CG	51	GLN
7	CG	97	GLN
8	CH	15	ASN
9	CI	23	ASN
9	CI	31	GLN
9	CI	58	HIS
9	CI	87	GLN
9	CI	89	ASN
9	CI	124	GLN
10	CJ	13	HIS
10	CJ	21	GLN
11	CK	93	GLN
12	CL	78	GLN
12	CL	99	HIS
13	CM	77	ASN
15	CO	28	GLN
19	CS	23	ASN
19	CS	65	ASN
19	CS	69	HIS
19	CS	83	HIS
20	CT	90	GLN
27	DD	164	GLN
27	DD	253	GLN
29	DF	69	HIS
29	DF	169	ASN
29	DF	203	GLN
30	DG	26	GLN
30	DG	40	ASN
32	DI	105	HIS
34	DO	89	ASN
35	DP	38	GLN
36	DQ	45	GLN
36	DQ	57	HIS
37	DR	13	HIS
38	DS	68	GLN
39	DT	123	GLN
41	DV	64	HIS
41	DV	89	GLN
42	DW	60	ASN
43	DX	31	HIS

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Mol	Chain	Res	Type
43	DX	82	GLN
45	DZ	55	HIS
55	D9	36	GLN

### 5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1495/1521 (98%)	306 (20%)	21 (1%)
1	CA	1501/1521 (98%)	310 (20%)	23 (1%)
22	AV	12/24 (50%)	3 (25%)	0
22	CV	12/24 (50%)	3 (25%)	0
23	AW	71/76 (93%)	30 (42%)	2 (2%)
23	AY	71/76 (93%)	33 (46%)	1 (1%)
23	CW	68/76 (89%)	30 (44%)	3 (4%)
23	CY	69/76 (90%)	28 (40%)	0
24	AX	75/77 (97%)	18 (24%)	1 (1%)
24	CX	75/77 (97%)	19 (25%)	0
25	BA	2811/2915 (96%)	433 (15%)	27 (0%)
25	DA	2791/2915 (95%)	499 (17%)	33 (1%)
26	BB	119/121 (98%)	13 (10%)	0
26	DB	119/121 (98%)	17 (14%)	0
All	All	9289/9620 (96%)	1742 (18%)	111 (1%)

All (1742) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	9	G
1	AA	22	G
1	AA	32	A
1	AA	39	G
1	AA	47	C
1	AA	48	C
1	AA	51	A
1	AA	54	C
1	AA	61	G
1	AA	65	U
1	AA	70	G
1	AA	73	G
1	AA	78	G
1	AA	79	G

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Mol	Chain	Res	Type
1	AA	96	U
1	AA	97	G
1	AA	98	G
1	AA	111	G
1	AA	116	A
1	AA	121	C
1	AA	129(A)	G
1	AA	131	C
1	AA	145	G
1	AA	146	G
1	AA	155	C
1	AA	156	G
1	AA	163	C
1	AA	166	G
1	AA	171	A
1	AA	174	C
1	AA	180	U
1	AA	182	U
1	AA	189(C)	C
1	AA	189(E)	U
1	AA	189(F)	U
1	AA	189(I)	G
1	AA	189(J)	G
1	AA	189(K)	U
1	AA	190	U
1	AA	194	C
1	AA	195	A
1	AA	197	A
1	AA	201	C
1	AA	202	U
1	AA	203	U
1	AA	204	U
1	AA	216	G
1	AA	217	C
1	AA	220	G
1	AA	247	G
1	AA	251	G
1	AA	253	U
1	AA	258	G
1	AA	262	A
1	AA	266	G
1	AA	267	C

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Mol	Chain	Res	Type
1	AA	289	G
1	AA	301	G
1	AA	321	A
1	AA	328	C
1	AA	329	A
1	AA	332	G
1	AA	341	C
1	AA	346	G
1	AA	347	G
1	AA	348	G
1	AA	352	C
1	AA	353	A
1	AA	354	G
1	AA	355	C
1	AA	367	U
1	AA	372	C
1	AA	373	A
1	AA	382	A
1	AA	384	G
1	AA	388	G
1	AA	397	A
1	AA	398	C
1	AA	406	G
1	AA	412	A
1	AA	413	G
1	AA	424	G
1	AA	429	U
1	AA	430	A
1	AA	439	A
1	AA	442	C
1	AA	443	C
1	AA	449	C
1	AA	452	A
1	AA	455	C
1	AA	457	C
1	AA	461	A
1	AA	470	C
1	AA	475	G
1	AA	477	A
1	AA	485	G
1	AA	496	A
1	AA	498	U

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Mol	Chain	Res	Type
1	AA	505	G
1	AA	509	A
1	AA	510	A
1	AA	511	C
1	AA	513	C
1	AA	518	C
1	AA	521	G
1	AA	524	G
1	AA	527	G
1	AA	528	C
1	AA	531	U
1	AA	532	A
1	AA	533	A
1	AA	547	A
1	AA	559	A
1	AA	561	U
1	AA	572	A
1	AA	573	A
1	AA	576	G
1	AA	577	G
1	AA	581	G
1	AA	590	C
1	AA	596	C
1	AA	619	U
1	AA	630	G
1	AA	653	A
1	AA	657	G
1	AA	660	G
1	AA	665	A
1	AA	671	G
1	AA	673	G
1	AA	687	A
1	AA	688	G
1	AA	693	G
1	AA	695	A
1	AA	703	G
1	AA	723	U
1	AA	731	G
1	AA	733	A
1	AA	749	C
1	AA	752	G
1	AA	755	G

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Mol	Chain	Res	Type
1	AA	773	G
1	AA	774	G
1	AA	777	A
1	AA	792	A
1	AA	793	U
1	AA	794	A
1	AA	815	A
1	AA	817	C
1	AA	821	G
1	AA	827	U
1	AA	828	A
1	AA	829	G
1	AA	833	U
1	AA	834	C
1	AA	840	C
1	AA	841	U
1	AA	848	C
1	AA	851	G
1	AA	853	G
1	AA	859	A
1	AA	874	G
1	AA	902	G
1	AA	914	A
1	AA	926	G
1	AA	927	G
1	AA	934	C
1	AA	960	U
1	AA	961	U
1	AA	968	A
1	AA	969	A
1	AA	971	G
1	AA	972	C
1	AA	974	A
1	AA	975	A
1	AA	976	G
1	AA	977	A
1	AA	991	U
1	AA	992	U
1	AA	993	G
1	AA	996	A
1	AA	997	U
1	AA	998	G

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Mol	Chain	Res	Type
1	AA	1003	G
1	AA	1004	A
1	AA	1005	A
1	AA	1006	C
1	AA	1008	C
1	AA	1014	A
1	AA	1020	U
1	AA	1021	G
1	AA	1022	G
1	AA	1023	G
1	AA	1024	G
1	AA	1025	U
1	AA	1026	G
1	AA	1027	C
1	AA	1028	C
1	AA	1029	C
1	AA	1030(A)	G
1	AA	1030(C)	G
1	AA	1030(D)	A
1	AA	1031	G
1	AA	1033	G
1	AA	1035	A
1	AA	1037	C
1	AA	1039	C
1	AA	1054	C
1	AA	1060	C
1	AA	1065	U
1	AA	1066	C
1	AA	1068	G
1	AA	1076	C
1	AA	1081	G
1	AA	1088	G
1	AA	1089	G
1	AA	1094	G
1	AA	1095	U
1	AA	1101	A
1	AA	1104	G
1	AA	1108	G
1	AA	1110	A
1	AA	1122	U
1	AA	1123	A
1	AA	1124	G

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Mol	Chain	Res	Type
1	AA	1125	U
1	AA	1126	U
1	AA	1130	A
1	AA	1132	C
1	AA	1135	U
1	AA	1136	U
1	AA	1137	C
1	AA	1138	G
1	AA	1139	G
1	AA	1140	C
1	AA	1141	C
1	AA	1145	C
1	AA	1146	A
1	AA	1152	A
1	AA	1154	G
1	AA	1157	A
1	AA	1158	C
1	AA	1159	U
1	AA	1175	G
1	AA	1183	A
1	AA	1184	G
1	AA	1191	A
1	AA	1196	U
1	AA	1197	G
1	AA	1202	G
1	AA	1212	U
1	AA	1213	A
1	AA	1227	A
1	AA	1228	C
1	AA	1236	A
1	AA	1238	A
1	AA	1250	A
1	AA	1255	G
1	AA	1256	A
1	AA	1257	U
1	AA	1258	G
1	AA	1260	C
1	AA	1263	C
1	AA	1270	C
1	AA	1272	G
1	AA	1273	G
1	AA	1278	U

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Mol	Chain	Res	Type
1	AA	1279	A
1	AA	1280	A
1	AA	1281	U
1	AA	1286	A
1	AA	1287	A
1	AA	1297	C
1	AA	1299	A
1	AA	1300	G
1	AA	1302	U
1	AA	1317	C
1	AA	1319	A
1	AA	1320	C
1	AA	1338	G
1	AA	1340	A
1	AA	1346	A
1	AA	1347	G
1	AA	1358	U
1	AA	1363	C
1	AA	1370	G
1	AA	1397	C
1	AA	1419	G
1	AA	1442	G
1	AA	1442(A)	G
1	AA	1442(B)	A
1	AA	1446	U
1	AA	1447	A
1	AA	1452	C
1	AA	1456	G
1	AA	1492	A
1	AA	1493	A
1	AA	1503	A
1	AA	1504	G
1	AA	1506	U
1	AA	1517	G
1	AA	1520	G
1	AA	1529	G
1	AA	1530	G
1	AA	1531	A
1	AA	1532	U
22	AV	13	A
22	AV	14	A
22	AV	24	A

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Mol	Chain	Res	Type
23	AW	2	C
23	AW	3	C
23	AW	6	G
23	AW	8	4SU
23	AW	11	C
23	AW	13	C
23	AW	14	A
23	AW	19	G
23	AW	20	U
23	AW	21	A
23	AW	22	G
23	AW	23	A
23	AW	26	A
23	AW	34	G
23	AW	42	C
23	AW	44	G
23	AW	45	U
23	AW	46	7MG
23	AW	47	U
23	AW	48	C
23	AW	49	C
23	AW	61	C
23	AW	63	G
23	AW	64	A
23	AW	68	C
23	AW	70	G
23	AW	73	A
23	AW	74	C
23	AW	75	C
23	AW	76	A
24	AX	3	C
24	AX	9	G
24	AX	18	G
24	AX	19	G
24	AX	20	U
24	AX	21	A
24	AX	31	G
24	AX	42	G
24	AX	47	U
24	AX	48	C
24	AX	60	U
24	AX	61	C

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Mol	Chain	Res	Type
24	AX	62	C
24	AX	65	C
24	AX	67	C
24	AX	68	C
24	AX	70	G
24	AX	76	A
23	AY	2	C
23	AY	3	C
23	AY	5	G
23	AY	9	A
23	AY	13	C
23	AY	14	A
23	AY	15	G
23	AY	19	G
23	AY	20	U
23	AY	21	A
23	AY	22	G
23	AY	30	G
23	AY	31	A
23	AY	33	U
23	AY	34	G
23	AY	35	A
23	AY	39	PSU
23	AY	44	G
23	AY	45	U
23	AY	46	7MG
23	AY	47	U
23	AY	48	C
23	AY	49	C
23	AY	51	U
23	AY	53	G
23	AY	56	C
23	AY	57	G
23	AY	58	A
23	AY	62	C
23	AY	65	G
23	AY	67	C
23	AY	70	G
23	AY	73	A
25	BA	11	G
25	BA	12	U
25	BA	13	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
25	BA	34	C
25	BA	45	C
25	BA	54	G
25	BA	60	G
25	BA	63	A
25	BA	70	A
25	BA	71	U
25	BA	73	A
25	BA	74	G
25	BA	82	G
25	BA	83	A
25	BA	94	G
25	BA	95	G
25	BA	116	A
25	BA	117	A
25	BA	118	U
25	BA	170	A
25	BA	185	A
25	BA	188	A
25	BA	194	G
25	BA	203	G
25	BA	204	G
25	BA	205	A
25	BA	210	A
25	BA	211	A
25	BA	212	A
25	BA	218	A
25	BA	219	U
25	BA	222	A
25	BA	237	G
25	BA	256	C
25	BA	265	U
25	BA	269	G
25	BA	271	U
25	BA	272	U
25	BA	273	G
25	BA	274	U
25	BA	275	C
25	BA	276	C
25	BA	279	G
25	BA	289	G
25	BA	294	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
25	BA	303	C
25	BA	307	A
25	BA	335	A
25	BA	353	G
25	BA	354	A
25	BA	376	G
25	BA	387	G
25	BA	397	G
25	BA	399	G
25	BA	407	U
25	BA	413	G
25	BA	423	G
25	BA	432	U
25	BA	433	G
25	BA	438	G
25	BA	448	U
25	BA	455	A
25	BA	469	A
25	BA	470	C
25	BA	474	U
25	BA	477	C
25	BA	481	C
25	BA	482	C
25	BA	496	A
25	BA	497	A
25	BA	507	G
25	BA	526	A
25	BA	529	U
25	BA	530	A
25	BA	534	C
25	BA	553	A
25	BA	555	G
25	BA	556	C
25	BA	557	A
25	BA	558	G
25	BA	569	G
25	BA	573	G
25	BA	585	U
25	BA	586	G
25	BA	596	G
25	BA	598	A
25	BA	609	A

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Mol	Chain	Res	Type
25	BA	626	A
25	BA	627	G
25	BA	630	U
25	BA	638	U
25	BA	639	G
25	BA	640	A
25	BA	641	G
25	BA	652	A
25	BA	662	A
25	BA	670	C
25	BA	671	A
25	BA	678	A
25	BA	693	G
25	BA	694	G
25	BA	697	C
25	BA	698	G
25	BA	716	G
25	BA	724	A
25	BA	733	G
25	BA	777	C
25	BA	795	G
25	BA	796	C
25	BA	811	A
25	BA	812	G
25	BA	822	G
25	BA	823	G
25	BA	829	A
25	BA	830	A
25	BA	831	A
25	BA	832	G
25	BA	836	A
25	BA	839	G
25	BA	852	G
25	BA	859	C
25	BA	866	A
25	BA	874	U
25	BA	875	U
25	BA	877	G
25	BA	906	G
25	BA	908	A
25	BA	913	A
25	BA	924	U

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Mol	Chain	Res	Type
25	BA	926	G
25	BA	927	G
25	BA	929	G
25	BA	931	C
25	BA	932	C
25	BA	933	C
25	BA	934	A
25	BA	935	C
25	BA	936	C
25	BA	937	A
25	BA	938	G
25	BA	941	U
25	BA	942	A
25	BA	943	C
25	BA	944	C
25	BA	945	A
25	BA	953	U
25	BA	956	A
25	BA	977	G
25	BA	986	A
25	BA	990	A
25	BA	991	G
25	BA	998	A
25	BA	1004	A
25	BA	1006	C
25	BA	1019	G
25	BA	1020	C
25	BA	1029	A
25	BA	1042	A
25	BA	1051	C
25	BA	1058	U
25	BA	1059	C
25	BA	1068	G
25	BA	1072	U
25	BA	1079	U
25	BA	1084	C
25	BA	1087	C
25	BA	1088	G
25	BA	1091	A
25	BA	1092	A
25	BA	1093	G
25	BA	1097	G

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Mol	Chain	Res	Type
25	BA	1153	G
25	BA	1154	U
25	BA	1156	G
25	BA	1158	G
25	BA	1174	A
25	BA	1180	C
25	BA	1181	G
25	BA	1184	G
25	BA	1217	G
25	BA	1218	G
25	BA	1219	A
25	BA	1220	U
25	BA	1221	G
25	BA	1222	A
25	BA	1223	C
25	BA	1250	U
25	BA	1255	A
25	BA	1256	U
25	BA	1263	C
25	BA	1265	A
25	BA	1299	A
25	BA	1302	G
25	BA	1317	G
25	BA	1318	A
25	BA	1346	U
25	BA	1347	A
25	BA	1349	G
25	BA	1360	C
25	BA	1365	G
25	BA	1398	U
25	BA	1405	A
25	BA	1406	A
25	BA	1411	A
25	BA	1416	C
25	BA	1426	G
25	BA	1430	A
25	BA	1431	G
25	BA	1462	G
25	BA	1463	C
25	BA	1466	U
25	BA	1467	G
25	BA	1474	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
25	BA	1483	C
25	BA	1491	A
25	BA	1496	A
25	BA	1497	G
25	BA	1502	G
25	BA	1506	G
25	BA	1508	G
25	BA	1514	C
25	BA	1518	A
25	BA	1525	G
25	BA	1529	G
25	BA	1539	C
25	BA	1540	A
25	BA	1553	A
25	BA	1554	A
25	BA	1555	C
25	BA	1556	A
25	BA	1578	C
25	BA	1589	A
25	BA	1605	A
25	BA	1613	A
25	BA	1616	A
25	BA	1625	U
25	BA	1628	G
25	BA	1629	C
25	BA	1631	C
25	BA	1632	A
25	BA	1654	A
25	BA	1655	A
25	BA	1656	A
25	BA	1695	C
25	BA	1701	A
25	BA	1708	G
25	BA	1721	G
25	BA	1743	G
25	BA	1747	A
25	BA	1748	A
25	BA	1766	G
25	BA	1767	A
25	BA	1787	G
25	BA	1794	G
25	BA	1795	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
25	BA	1804	A
25	BA	1811	A
25	BA	1813	C
25	BA	1822	A
25	BA	1831	C
25	BA	1847	G
25	BA	1848	G
25	BA	1860	A
25	BA	1878	A
25	BA	1879	A
25	BA	1892	G
25	BA	1899	A
25	BA	1900	G
25	BA	1911	A
25	BA	1922	A
25	BA	1928	G
25	BA	1937	U
25	BA	1941	A
25	BA	1949	A
25	BA	1951	G
25	BA	1952	G
25	BA	1953	U
25	BA	1959	A
25	BA	1960	A
25	BA	1977	U
25	BA	1985	U
25	BA	1987	C
25	BA	1989	C
25	BA	1992	A
25	BA	1993	A
25	BA	1994	A
25	BA	2014	G
25	BA	2015	U
25	BA	2019	G
25	BA	2042	A
25	BA	2045	G
25	BA	2053	A
25	BA	2054	G
25	BA	2055	A
25	BA	2061	C
25	BA	2065	C
25	BA	2077	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
25	BA	2078	G
25	BA	2082	A
25	BA	2083	G
25	BA	2084	A
25	BA	2091	G
25	BA	2118	U
25	BA	2120	U
25	BA	2132	G
25	BA	2135	U
25	BA	2138	G
25	BA	2141	A
25	BA	2142	G
25	BA	2144	U
25	BA	2147	G
25	BA	2149	G
25	BA	2151	C
25	BA	2153	G
25	BA	2154	U
25	BA	2155	G
25	BA	2156	A
25	BA	2157	A
25	BA	2158	C
25	BA	2164	C
25	BA	2165	C
25	BA	2168	C
25	BA	2170	G
25	BA	2175	G
25	BA	2179	G
25	BA	2180	A
25	BA	2181	G
25	BA	2182	G
25	BA	2188	G
25	BA	2189	U
25	BA	2190	G
25	BA	2193	A
25	BA	2194	U
25	BA	2195	A
25	BA	2196	C
25	BA	2197	C
25	BA	2200	C
25	BA	2203	G
25	BA	2204	G

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Mol	Chain	Res	Type
25	BA	2206	G
25	BA	2207	C
25	BA	2208	G
25	BA	2210	C
25	BA	2212	G
25	BA	2214	G
25	BA	2220	A
25	BA	2221	A
25	BA	2227	G
25	BA	2228	G
25	BA	2229	A
25	BA	2230	U
25	BA	2237	A
25	BA	2250	G
25	BA	2251	G
25	BA	2280	A
25	BA	2287	C
25	BA	2295	C
25	BA	2299	A
25	BA	2301	G
25	BA	2317	A
25	BA	2320	G
25	BA	2332	A
25	BA	2337	G
25	BA	2346	G
25	BA	2348	A
25	BA	2355	C
25	BA	2359	C
25	BA	2366	G
25	BA	2373	A
25	BA	2395	G
25	BA	2397	C
25	BA	2418	U
25	BA	2435	U
25	BA	2436	C
25	BA	2437	A
25	BA	2441	G
25	BA	2442	A
25	BA	2446	A
25	BA	2447	A
25	BA	2451	A
25	BA	2453	C

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Mol	Chain	Res	Type
25	BA	2460	A
25	BA	2461	U
25	BA	2480	G
25	BA	2481	A
25	BA	2486	C
25	BA	2488	A
25	BA	2490	A
25	BA	2514	G
25	BA	2517	G
25	BA	2530	A
25	BA	2541	G
25	BA	2561	G
25	BA	2566	U
25	BA	2578	A
25	BA	2579	G
25	BA	2585	C
25	BA	2590	G
25	BA	2614	A
25	BA	2621	U
25	BA	2623	U
25	BA	2624	C
25	BA	2641	A
25	BA	2642	G
25	BA	2653	G
25	BA	2666	A
25	BA	2682	A
25	BA	2701	U
25	BA	2702	C
25	BA	2703	C
25	BA	2715	C
25	BA	2725	A
25	BA	2726	A
25	BA	2727	G
25	BA	2739	U
25	BA	2746	A
25	BA	2771	A
25	BA	2777	A
25	BA	2778	A
25	BA	2782	C
25	BA	2791	A
25	BA	2803	A
25	BA	2813	G

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Mol	Chain	Res	Type
25	BA	2828	G
25	BA	2830	A
25	BA	2831	A
25	BA	2845	A
25	BA	2846	U
25	BA	2882	G
25	BA	2890	C
25	BA	2901	A
25	BA	2902	G
25	BA	2903	G
26	BB	2	C
26	BB	7	G
26	BB	15	A
26	BB	20	C
26	BB	25	A
26	BB	42	C
26	BB	56	G
26	BB	73	A
26	BB	75	G
26	BB	85	G
26	BB	98	G
26	BB	106	G
26	BB	110	G
1	CA	5	U
1	CA	6	G
1	CA	9	G
1	CA	22	G
1	CA	32	A
1	CA	39	G
1	CA	47	C
1	CA	48	C
1	CA	51	A
1	CA	54	C
1	CA	65	U
1	CA	66	G
1	CA	73	G
1	CA	78	G
1	CA	79	G
1	CA	80	G
1	CA	88	A
1	CA	89	C
1	CA	96	U

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Mol	Chain	Res	Type
1	CA	97	G
1	CA	98	G
1	CA	111	G
1	CA	112	G
1	CA	116	A
1	CA	121	C
1	CA	129(A)	G
1	CA	131	C
1	CA	143	A
1	CA	155	C
1	CA	156	G
1	CA	163	C
1	CA	166	G
1	CA	171	A
1	CA	174	C
1	CA	180	U
1	CA	182	U
1	CA	189(C)	C
1	CA	189(E)	U
1	CA	189(F)	U
1	CA	189(I)	G
1	CA	189(K)	U
1	CA	190	U
1	CA	194	C
1	CA	195	A
1	CA	197	A
1	CA	201	C
1	CA	202	U
1	CA	203	U
1	CA	204	U
1	CA	216	G
1	CA	220	G
1	CA	247	G
1	CA	251	G
1	CA	253	U
1	CA	258	G
1	CA	262	A
1	CA	266	G
1	CA	267	C
1	CA	289	G
1	CA	301	G
1	CA	321	A

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Mol	Chain	Res	Type
1	CA	328	C
1	CA	329	A
1	CA	332	G
1	CA	341	C
1	CA	343	U
1	CA	344	A
1	CA	346	G
1	CA	350	G
1	CA	352	C
1	CA	353	A
1	CA	354	G
1	CA	355	C
1	CA	367	U
1	CA	372	C
1	CA	373	A
1	CA	382	A
1	CA	384	G
1	CA	388	G
1	CA	397	A
1	CA	398	C
1	CA	406	G
1	CA	412	A
1	CA	413	G
1	CA	424	G
1	CA	429	U
1	CA	430	A
1	CA	439	A
1	CA	442	C
1	CA	443	C
1	CA	449	C
1	CA	452	A
1	CA	455	C
1	CA	457	C
1	CA	461	A
1	CA	470	C
1	CA	475	G
1	CA	477	A
1	CA	485	G
1	CA	496	A
1	CA	498	U
1	CA	505	G
1	CA	509	A

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Mol	Chain	Res	Type
1	CA	510	A
1	CA	511	C
1	CA	513	C
1	CA	518	C
1	CA	521	G
1	CA	524	G
1	CA	528	C
1	CA	531	U
1	CA	532	A
1	CA	533	A
1	CA	547	A
1	CA	559	A
1	CA	561	U
1	CA	572	A
1	CA	573	A
1	CA	576	G
1	CA	577	G
1	CA	581	G
1	CA	590	C
1	CA	596	C
1	CA	619	U
1	CA	630	G
1	CA	653	A
1	CA	657	G
1	CA	660	G
1	CA	665	A
1	CA	671	G
1	CA	673	G
1	CA	687	A
1	CA	688	G
1	CA	693	G
1	CA	695	A
1	CA	702	A
1	CA	723	U
1	CA	731	G
1	CA	749	C
1	CA	752	G
1	CA	755	G
1	CA	773	G
1	CA	774	G
1	CA	777	A
1	CA	792	A

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Mol	Chain	Res	Type
1	CA	793	U
1	CA	794	A
1	CA	815	A
1	CA	817	C
1	CA	821	G
1	CA	827	U
1	CA	828	A
1	CA	829	G
1	CA	833	U
1	CA	834	C
1	CA	840	C
1	CA	841	U
1	CA	848	C
1	CA	851	G
1	CA	853	G
1	CA	859	A
1	CA	874	G
1	CA	902	G
1	CA	914	A
1	CA	926	G
1	CA	927	G
1	CA	932	C
1	CA	934	C
1	CA	960	U
1	CA	961	U
1	CA	968	A
1	CA	969	A
1	CA	971	G
1	CA	972	C
1	CA	974	A
1	CA	975	A
1	CA	976	G
1	CA	977	A
1	CA	991	U
1	CA	992	U
1	CA	993	G
1	CA	996	A
1	CA	997	U
1	CA	998	G
1	CA	1002	G
1	CA	1003	G
1	CA	1004	A

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Mol	Chain	Res	Type
1	CA	1005	A
1	CA	1006	C
1	CA	1014	A
1	CA	1020	U
1	CA	1021	G
1	CA	1022	G
1	CA	1023	G
1	CA	1024	G
1	CA	1025	U
1	CA	1026	G
1	CA	1027	C
1	CA	1028	C
1	CA	1029	C
1	CA	1030(A)	G
1	CA	1030(C)	G
1	CA	1030(D)	A
1	CA	1031	G
1	CA	1033	G
1	CA	1035	A
1	CA	1037	C
1	CA	1039	C
1	CA	1041	A
1	CA	1054	C
1	CA	1060	C
1	CA	1065	U
1	CA	1066	C
1	CA	1068	G
1	CA	1076	C
1	CA	1081	G
1	CA	1088	G
1	CA	1089	G
1	CA	1094	G
1	CA	1095	U
1	CA	1101	A
1	CA	1104	G
1	CA	1108	G
1	CA	1110	A
1	CA	1117	G
1	CA	1122	U
1	CA	1125	U
1	CA	1126	U
1	CA	1129	C

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Mol	Chain	Res	Type
1	CA	1130	A
1	CA	1132	C
1	CA	1135	U
1	CA	1136	U
1	CA	1137	C
1	CA	1138	G
1	CA	1139	G
1	CA	1140	C
1	CA	1141	C
1	CA	1145	C
1	CA	1146	A
1	CA	1152	A
1	CA	1154	G
1	CA	1157	A
1	CA	1158	C
1	CA	1159	U
1	CA	1175	G
1	CA	1182	G
1	CA	1183	A
1	CA	1184	G
1	CA	1191	A
1	CA	1196	U
1	CA	1197	G
1	CA	1201	A
1	CA	1202	G
1	CA	1212	U
1	CA	1213	A
1	CA	1227	A
1	CA	1228	C
1	CA	1236	A
1	CA	1238	A
1	CA	1250	A
1	CA	1256	A
1	CA	1257	U
1	CA	1258	G
1	CA	1260	C
1	CA	1263	C
1	CA	1270	C
1	CA	1272	G
1	CA	1273	G
1	CA	1278	U
1	CA	1279	A

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Mol	Chain	Res	Type
1	CA	1280	A
1	CA	1281	U
1	CA	1286	A
1	CA	1287	A
1	CA	1297	C
1	CA	1299	A
1	CA	1300	G
1	CA	1305	G
1	CA	1317	C
1	CA	1319	A
1	CA	1320	C
1	CA	1338	G
1	CA	1340	A
1	CA	1346	A
1	CA	1347	G
1	CA	1353	G
1	CA	1358	U
1	CA	1363	C
1	CA	1370	G
1	CA	1397	C
1	CA	1419	G
1	CA	1442	G
1	CA	1442(A)	G
1	CA	1442(B)	A
1	CA	1446	U
1	CA	1447	A
1	CA	1452	C
1	CA	1456	G
1	CA	1492	A
1	CA	1493	A
1	CA	1503	A
1	CA	1504	G
1	CA	1506	U
1	CA	1517	G
1	CA	1520	G
1	CA	1529	G
1	CA	1530	G
1	CA	1531	A
1	CA	1532	U
22	CV	13	A
22	CV	14	A
22	CV	24	A

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Mol	Chain	Res	Type
23	CW	3	C
23	CW	5	G
23	CW	6	G
23	CW	7	A
23	CW	8	4SU
23	CW	9	A
23	CW	12	U
23	CW	13	C
23	CW	14	A
23	CW	19	G
23	CW	22	G
23	CW	25	C
23	CW	27	G
23	CW	28	G
23	CW	44	G
23	CW	46	7MG
23	CW	47	U
23	CW	48	C
23	CW	59	U
23	CW	61	C
23	CW	62	C
23	CW	63	G
23	CW	64	A
23	CW	66	U
23	CW	67	C
23	CW	70	G
23	CW	73	A
23	CW	74	C
23	CW	75	C
23	CW	76	A
24	CX	3	C
24	CX	9	G
24	CX	13	C
24	CX	18	G
24	CX	19	G
24	CX	20	U
24	CX	21	A
24	CX	31	G
24	CX	42	G
24	CX	47	U
24	CX	48	C
24	CX	60	U

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Mol	Chain	Res	Type
24	CX	61	C
24	CX	62	C
24	CX	65	C
24	CX	67	C
24	CX	68	C
24	CX	70	G
24	CX	76	A
23	CY	2	C
23	CY	3	C
23	CY	8	4SU
23	CY	13	C
23	CY	14	A
23	CY	15	G
23	CY	19	G
23	CY	22	G
23	CY	30	G
23	CY	31	A
23	CY	33	U
23	CY	34	G
23	CY	35	A
23	CY	39	PSU
23	CY	45	U
23	CY	46	7MG
23	CY	47	U
23	CY	49	C
23	CY	51	U
23	CY	52	G
23	CY	56	C
23	CY	57	G
23	CY	58	A
23	CY	62	C
23	CY	65	G
23	CY	67	C
23	CY	70	G
23	CY	73	A
25	DA	11	G
25	DA	12	U
25	DA	15	G
25	DA	34	C
25	DA	35	G
25	DA	45	C
25	DA	59	U

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Mol	Chain	Res	Type
25	DA	71	A
25	DA	74	A
25	DA	75	G
25	DA	84	A
25	DA	95	G
25	DA	118	A
25	DA	119	A
25	DA	120	U
25	DA	141	A
25	DA	154(A)	C
25	DA	157	U
25	DA	173	G
25	DA	181	A
25	DA	182	A
25	DA	196	A
25	DA	199	A
25	DA	205	G
25	DA	213	A
25	DA	214	G
25	DA	215	G
25	DA	216	A
25	DA	221	A
25	DA	222	A
25	DA	229	A
25	DA	230	U
25	DA	233	A
25	DA	248	G
25	DA	269	U
25	DA	271(A)	A
25	DA	271(I)	G
25	DA	271(K)	U
25	DA	271(L)	U
25	DA	271(M)	G
25	DA	271(N)	U
25	DA	271(S)	G
25	DA	272(A)	U
25	DA	272(B)	G
25	DA	274	G
25	DA	277	C
25	DA	278	A
25	DA	283	A
25	DA	292	C

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Mol	Chain	Res	Type
25	DA	311	A
25	DA	312	G
25	DA	327	G
25	DA	329	G
25	DA	330	A
25	DA	342	G
25	DA	352	G
25	DA	363	G
25	DA	380	U
25	DA	386	G
25	DA	396	G
25	DA	405	U
25	DA	411	G
25	DA	412	A
25	DA	418	G
25	DA	422	A
25	DA	428	A
25	DA	442	G
25	DA	443	A
25	DA	444	C
25	DA	455	C
25	DA	457	A
25	DA	481	G
25	DA	494	G
25	DA	504	U
25	DA	505	A
25	DA	507	A
25	DA	508	G
25	DA	509	C
25	DA	530	G
25	DA	531	C
25	DA	532	A
25	DA	533	G
25	DA	545	G
25	DA	555	U
25	DA	556	G
25	DA	563	G
25	DA	568	U
25	DA	573	G
25	DA	575	A
25	DA	588	U
25	DA	599	G

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Mol	Chain	Res	Type
25	DA	603	A
25	DA	604	G
25	DA	607	U
25	DA	614(B)	G
25	DA	615	G
25	DA	627	A
25	DA	637	A
25	DA	645	C
25	DA	652(B)	A
25	DA	652(C)	G
25	DA	653	A
25	DA	655	A
25	DA	669	G
25	DA	686	G
25	DA	701	G
25	DA	730	C
25	DA	753	C
25	DA	775	G
25	DA	776	G
25	DA	782	A
25	DA	784	A
25	DA	785	G
25	DA	790	C
25	DA	792	G
25	DA	805	G
25	DA	812	C
25	DA	819	A
25	DA	827	U
25	DA	828	U
25	DA	849	A
25	DA	857	C
25	DA	859	G
25	DA	866	A
25	DA	874	G
25	DA	878	A
25	DA	879	G
25	DA	882	G
25	DA	884	C
25	DA	886	C
25	DA	887	A
25	DA	888	C
25	DA	889	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
25	DA	890	A
25	DA	893	C
25	DA	895	U
25	DA	896	A
25	DA	897	C
25	DA	900	A
25	DA	901	A
25	DA	903	C
25	DA	907	U
25	DA	910	A
25	DA	915	C
25	DA	917	A
25	DA	932	G
25	DA	938	G
25	DA	941	A
25	DA	945	A
25	DA	946	G
25	DA	953	A
25	DA	958	U
25	DA	959	A
25	DA	961	C
25	DA	974	G
25	DA	975	C
25	DA	983	A
25	DA	996	A
25	DA	1003	G
25	DA	1006	C
25	DA	1012	U
25	DA	1013	C
25	DA	1017	G
25	DA	1022	G
25	DA	1025	G
25	DA	1026	U
25	DA	1027	A
25	DA	1033	U
25	DA	1038	C
25	DA	1039	G
25	DA	1040	C
25	DA	1042	G
25	DA	1043	C
25	DA	1113	U
25	DA	1116	C

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Mol	Chain	Res	Type
25	DA	1128	A
25	DA	1129	A
25	DA	1130	U
25	DA	1135	C
25	DA	1136	G
25	DA	1138	G
25	DA	1139	G
25	DA	1142	U
25	DA	1143	A
25	DA	1144	G
25	DA	1168	G
25	DA	1170	G
25	DA	1171	G
25	DA	1188	U
25	DA	1206	G
25	DA	1211	U
25	DA	1219	G
25	DA	1220	A
25	DA	1229	G
25	DA	1237	A
25	DA	1241	A
25	DA	1244	G
25	DA	1248	G
25	DA	1253	A
25	DA	1256	G
25	DA	1271	G
25	DA	1272	A
25	DA	1284	A
25	DA	1286	A
25	DA	1287	A
25	DA	1300	U
25	DA	1301	A
25	DA	1303	G
25	DA	1305	C
25	DA	1314	C
25	DA	1345	C
25	DA	1352	U
25	DA	1359	A
25	DA	1360	A
25	DA	1365	A
25	DA	1370	C
25	DA	1384	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
25	DA	1385	G
25	DA	1408	C
25	DA	1416	G
25	DA	1417	C
25	DA	1419	A
25	DA	1420	U
25	DA	1421	G
25	DA	1428	C
25	DA	1435	G
25	DA	1437	C
25	DA	1445	A
25	DA	1449	A
25	DA	1450	G
25	DA	1459	G
25	DA	1461	G
25	DA	1467	C
25	DA	1471	A
25	DA	1482	G
25	DA	1487	G
25	DA	1490	A
25	DA	1493	C
25	DA	1494	A
25	DA	1496	A
25	DA	1497	U
25	DA	1505	C
25	DA	1508	A
25	DA	1509	C
25	DA	1509(A)	A
25	DA	1531	C
25	DA	1533	G
25	DA	1541	G
25	DA	1542	A
25	DA	1545	A
25	DA	1547	C
25	DA	1558	A
25	DA	1559	G
25	DA	1566	A
25	DA	1569	A
25	DA	1578	U
25	DA	1580	A
25	DA	1583	A
25	DA	1584	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
25	DA	1586	A
25	DA	1598	C
25	DA	1608	A
25	DA	1610	A
25	DA	1616	A
25	DA	1639	U
25	DA	1640	C
25	DA	1648	C
25	DA	1654	A
25	DA	1664	A
25	DA	1674	G
25	DA	1696	G
25	DA	1700	A
25	DA	1701	A
25	DA	1721	G
25	DA	1722	A
25	DA	1740	G
25	DA	1756	G
25	DA	1762	A
25	DA	1763	G
25	DA	1764	G
25	DA	1773	A
25	DA	1780	A
25	DA	1782	C
25	DA	1791	A
25	DA	1797	C
25	DA	1800	C
25	DA	1801	G
25	DA	1816	G
25	DA	1829	A
25	DA	1835	G
25	DA	1847	A
25	DA	1848	A
25	DA	1877	A
25	DA	1878	G
25	DA	1896	G
25	DA	1900	A
25	DA	1906	G
25	DA	1913	A
25	DA	1914	C
25	DA	1929	G
25	DA	1930	G

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Mol	Chain	Res	Type
25	DA	1937	A
25	DA	1938	A
25	DA	1955	U
25	DA	1963	U
25	DA	1967	C
25	DA	1970	A
25	DA	1971	A
25	DA	1972	A
25	DA	1993	U
25	DA	1995	U
25	DA	1996	C
25	DA	1997	G
25	DA	2005	A
25	DA	2023	G
25	DA	2031	A
25	DA	2032	G
25	DA	2033	A
25	DA	2043	C
25	DA	2046	G
25	DA	2055	C
25	DA	2056	G
25	DA	2060	A
25	DA	2061	G
25	DA	2062	A
25	DA	2069	G
25	DA	2070	G
25	DA	2082	A
25	DA	2099	U
25	DA	2103	C
25	DA	2107	C
25	DA	2110	G
25	DA	2111	C
25	DA	2113	U
25	DA	2115	G
25	DA	2116	G
25	DA	2117	A
25	DA	2119	A
25	DA	2122	U
25	DA	2124	G
25	DA	2126	A
25	DA	2127	G
25	DA	2129	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
25	DA	2132	U
25	DA	2133	G
25	DA	2134	A
25	DA	2135	A
25	DA	2136	C
25	DA	2137	C
25	DA	2141	G
25	DA	2142	C
25	DA	2145	C
25	DA	2146	C
25	DA	2148	G
25	DA	2153	G
25	DA	2154	G
25	DA	2156	G
25	DA	2157	G
25	DA	2158	A
25	DA	2159	G
25	DA	2163	C
25	DA	2164	C
25	DA	2165	G
25	DA	2166	G
25	DA	2167	U
25	DA	2168	G
25	DA	2169	A
25	DA	2172	U
25	DA	2173	A
25	DA	2175	C
25	DA	2176	A
25	DA	2177	C
25	DA	2178	C
25	DA	2180	U
25	DA	2188	C
25	DA	2189	U
25	DA	2192	G
25	DA	2198	A
25	DA	2206	G
25	DA	2207	G
25	DA	2208	A
25	DA	2218	U
25	DA	2225	A
25	DA	2238	G
25	DA	2268	A

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Mol	Chain	Res	Type
25	DA	2272	U
25	DA	2275	C
25	DA	2279	G
25	DA	2283	C
25	DA	2287	A
25	DA	2289	G
25	DA	2302	G
25	DA	2303	G
25	DA	2305	A
25	DA	2308	G
25	DA	2312	U
25	DA	2318	G
25	DA	2319	G
25	DA	2320	A
25	DA	2325	G
25	DA	2327	A
25	DA	2334	G
25	DA	2336	A
25	DA	2343	C
25	DA	2347	C
25	DA	2350	C
25	DA	2354	G
25	DA	2355	C
25	DA	2376	A
25	DA	2383	G
25	DA	2385	C
25	DA	2393	A
25	DA	2406	U
25	DA	2410	G
25	DA	2414	G
25	DA	2422	A
25	DA	2423	U
25	DA	2425	A
25	DA	2428	G
25	DA	2429	G
25	DA	2430	A
25	DA	2431	U
25	DA	2434	A
25	DA	2435	A
25	DA	2439	A
25	DA	2441	C
25	DA	2448	A

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Mol	Chain	Res	Type
25	DA	2453	A
25	DA	2469	A
25	DA	2474	C
25	DA	2476	A
25	DA	2478	A
25	DA	2487	G
25	DA	2490	G
25	DA	2494	G
25	DA	2502	G
25	DA	2505	G
25	DA	2506	U
25	DA	2507	C
25	DA	2518	A
25	DA	2529	G
25	DA	2554	U
25	DA	2556	C
25	DA	2566	A
25	DA	2567	G
25	DA	2573	C
25	DA	2602	A
25	DA	2611	U
25	DA	2612	C
25	DA	2615	U
25	DA	2629	A
25	DA	2630	G
25	DA	2647	U
25	DA	2652	C
25	DA	2654	A
25	DA	2663	G
25	DA	2681	C
25	DA	2689	U
25	DA	2690	C
25	DA	2691	C
25	DA	2702	U
25	DA	2703	C
25	DA	2712(A)	A
25	DA	2713	A
25	DA	2726	U
25	DA	2733	A
25	DA	2744	G
25	DA	2748	A
25	DA	2751	G

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Mol	Chain	Res	Type
25	DA	2752	C
25	DA	2754	U
25	DA	2757	A
25	DA	2758	A
25	DA	2761	G
25	DA	2764	A
25	DA	2765	A
25	DA	2766	G
25	DA	2778	A
25	DA	2789	C
25	DA	2793	G
25	DA	2794	C
25	DA	2802	G
25	DA	2807	G
25	DA	2808	U
25	DA	2818	G
25	DA	2820	A
25	DA	2821	A
25	DA	2833	G
25	DA	2835	A
25	DA	2872	G
25	DA	2873	A
25	DA	2876	G
25	DA	2879	C
25	DA	2880	C
25	DA	2892	A
25	DA	2894	G
25	DA	2895	U
25	DA	2896	C
25	DA	2897	U
26	DB	2	C
26	DB	5	C
26	DB	7	G
26	DB	8	U
26	DB	15	A
26	DB	20	C
26	DB	25	A
26	DB	42	C
26	DB	56	G
26	DB	73	A
26	DB	75	G
26	DB	85	G

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Mol	Chain	Res	Type
26	DB	98	G
26	DB	106	G
26	DB	108	U
26	DB	110	G
26	DB	112	U

All (111) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	97	G
1	AA	115	G
1	AA	266	G
1	AA	429	U
1	AA	509	A
1	AA	532	A
1	AA	560	U
1	AA	687	A
1	AA	748	C
1	AA	839	U
1	AA	913	A
1	AA	991	U
1	AA	1036	G
1	AA	1065	U
1	AA	1067	A
1	AA	1190	G
1	AA	1201	A
1	AA	1285	A
1	AA	1299	A
1	AA	1442	G
1	AA	1492	A
23	AW	13	C
23	AW	22	G
24	AX	47	U
23	AY	44	G
25	BA	70	A
25	BA	184	A
25	BA	185	A
25	BA	270	C
25	BA	271	U
25	BA	273	G
25	BA	288	U
25	BA	302	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
25	BA	732	A
25	BA	793	A
25	BA	795	G
25	BA	811	A
25	BA	1019	G
25	BA	1188	A
25	BA	1219	A
25	BA	1220	U
25	BA	1221	G
25	BA	1255	A
25	BA	1346	U
25	BA	1425	A
25	BA	1466	U
25	BA	1700	G
25	BA	1793	A
25	BA	2014	G
25	BA	2203	G
25	BA	2418	U
25	BA	2701	U
1	CA	65	U
1	CA	115	G
1	CA	266	G
1	CA	429	U
1	CA	509	A
1	CA	532	A
1	CA	560	U
1	CA	687	A
1	CA	748	C
1	CA	913	A
1	CA	991	U
1	CA	992	U
1	CA	1064	G
1	CA	1065	U
1	CA	1067	A
1	CA	1128	C
1	CA	1183	A
1	CA	1190	G
1	CA	1201	A
1	CA	1212	U
1	CA	1256	A
1	CA	1442	G
1	CA	1492	A

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Mol	Chain	Res	Type
23	CW	4	C
23	CW	13	C
23	CW	75	C
25	DA	195	A
25	DA	196	A
25	DA	228	A
25	DA	271(K)	U
25	DA	271(M)	G
25	DA	277	C
25	DA	587	C
25	DA	752	A
25	DA	764	A
25	DA	774	A
25	DA	827	U
25	DA	856	C
25	DA	900	A
25	DA	1026	U
25	DA	1210	A
25	DA	1240	U
25	DA	1300	U
25	DA	1420	U
25	DA	1427	A
25	DA	1493	C
25	DA	1530	C
25	DA	1558	A
25	DA	1653	G
25	DA	1663	C
25	DA	1913	A
25	DA	1992	G
25	DA	2110	G
25	DA	2116	G
25	DA	2335	A
25	DA	2406	U
25	DA	2430	A
25	DA	2689	U
25	DA	2756	U

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

36 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
23	PSU	AW	32	56,23	13,21,22	1.15	1 (7%)	18,30,33	3.58	6 (33%)
23	MIA	AW	37	23	21,31,32	1.85	2 (9%)	26,44,47	1.34	5 (19%)
23	PSU	AW	39	23	13,21,22	1.21	1 (7%)	18,30,33	3.31	6 (33%)
23	7MG	AW	46	23	19,26,27	1.06	1 (5%)	24,39,42	3.10	7 (29%)
23	5MU	AW	54	23	12,22,23	0.25	0	14,32,35	2.77	2 (14%)
23	PSU	AW	55	23	13,21,22	1.19	1 (7%)	18,30,33	3.55	6 (33%)
23	4SU	AW	8	23	11,21,22	1.14	1 (9%)	13,30,33	1.25	1 (7%)
24	5MC	AX	32	24	13,22,23	1.38	1 (7%)	15,32,35	1.06	1 (6%)
24	5MU	AX	54	24,56	12,22,23	0.38	0	14,32,35	2.28	2 (14%)
24	PSU	AX	55	24	13,21,22	1.49	1 (7%)	18,30,33	3.38	6 (33%)
24	4SU	AX	8	24	11,21,22	1.10	1 (9%)	13,30,33	1.88	1 (7%)
23	PSU	AY	32	23	13,21,22	1.29	1 (7%)	18,30,33	3.35	6 (33%)
23	MIA	AY	37	23	15,24,32	1.24	2 (13%)	16,35,47	2.08	2 (12%)
23	PSU	AY	39	23	13,21,22	1.25	2 (15%)	18,30,33	3.76	5 (27%)
23	7MG	AY	46	23	19,26,27	1.17	2 (10%)	24,39,42	3.23	7 (29%)
23	5MU	AY	54	23	12,22,23	0.27	0	14,32,35	2.92	2 (14%)
23	PSU	AY	55	23	13,21,22	1.26	1 (7%)	18,30,33	3.36	5 (27%)
23	4SU	AY	8	23	11,21,22	1.10	1 (9%)	13,30,33	1.52	1 (7%)
23	PSU	CW	32	23	13,21,22	0.80	1 (7%)	18,30,33	3.50	6 (33%)
23	MIA	CW	37	23	15,24,32	1.15	2 (13%)	16,35,47	2.35	2 (12%)
23	PSU	CW	39	23	13,21,22	1.12	1 (7%)	18,30,33	3.83	6 (33%)
23	7MG	CW	46	23	19,26,27	1.03	1 (5%)	24,39,42	3.07	7 (29%)
23	5MU	CW	54	23	12,22,23	0.40	0	14,32,35	2.49	2 (14%)
23	PSU	CW	55	23	13,21,22	1.07	1 (7%)	18,30,33	3.39	6 (33%)
23	4SU	CW	8	56,23	11,21,22	1.19	1 (9%)	13,30,33	1.37	1 (7%)
24	5MC	CX	32	24	13,22,23	1.33	1 (7%)	15,32,35	1.11	1 (6%)
24	5MU	CX	54	24	12,22,23	0.36	0	14,32,35	2.31	2 (14%)
24	PSU	CX	55	24	13,21,22	0.90	1 (7%)	18,30,33	3.41	5 (27%)
24	4SU	CX	8	24	11,21,22	1.04	1 (9%)	13,30,33	1.96	1 (7%)
23	PSU	CY	32	23	13,21,22	1.03	1 (7%)	18,30,33	3.41	6 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	MIA	CY	37	23	15,24,32	1.25	2 (13%)	16,35,47	2.07	2 (12%)
23	PSU	CY	39	23	13,21,22	1.42	2 (15%)	18,30,33	3.36	6 (33%)
23	7MG	CY	46	23	19,26,27	1.07	1 (5%)	24,39,42	3.10	7 (29%)
23	5MU	CY	54	23	12,22,23	0.34	0	14,32,35	2.56	2 (14%)
23	PSU	CY	55	23	13,21,22	1.18	1 (7%)	18,30,33	3.20	6 (33%)
23	4SU	CY	8	23	11,21,22	1.23	1 (9%)	13,30,33	1.19	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PSU	AW	32	56,23	-	0/7/25/26	0/2/2/2
23	MIA	AW	37	23	-	0/11/33/34	0/3/3/3
23	PSU	AW	39	23	-	0/7/25/26	0/2/2/2
23	7MG	AW	46	23	-	0/7/37/38	0/3/3/3
23	5MU	AW	54	23	-	0/3/25/26	0/2/2/2
23	PSU	AW	55	23	-	0/7/25/26	0/2/2/2
23	4SU	AW	8	23	-	0/3/25/26	0/2/2/2
24	5MC	AX	32	24	-	0/3/25/26	0/2/2/2
24	5MU	AX	54	24,56	-	0/3/25/26	0/2/2/2
24	PSU	AX	55	24	-	0/7/25/26	0/2/2/2
24	4SU	AX	8	24	-	0/3/25/26	0/2/2/2
23	PSU	AY	32	23	-	0/7/25/26	0/2/2/2
23	MIA	AY	37	23	-	0/3/25/34	0/3/3/3
23	PSU	AY	39	23	-	0/7/25/26	0/2/2/2
23	7MG	AY	46	23	-	0/7/37/38	0/3/3/3
23	5MU	AY	54	23	-	0/3/25/26	0/2/2/2
23	PSU	AY	55	23	-	0/7/25/26	0/2/2/2
23	4SU	AY	8	23	-	0/3/25/26	0/2/2/2
23	PSU	CW	32	23	-	0/7/25/26	0/2/2/2
23	MIA	CW	37	23	-	0/3/25/34	0/3/3/3
23	PSU	CW	39	23	-	0/7/25/26	0/2/2/2
23	7MG	CW	46	23	-	0/7/37/38	0/3/3/3
23	5MU	CW	54	23	-	0/3/25/26	0/2/2/2
23	PSU	CW	55	23	-	0/7/25/26	0/2/2/2
23	4SU	CW	8	56,23	-	0/3/25/26	0/2/2/2
24	5MC	CX	32	24	-	0/3/25/26	0/2/2/2
24	5MU	CX	54	24	-	0/3/25/26	0/2/2/2
24	PSU	CX	55	24	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	4SU	CX	8	24	-	0/3/25/26	0/2/2/2
23	PSU	CY	32	23	-	0/7/25/26	0/2/2/2
23	MIA	CY	37	23	-	0/3/25/34	0/3/3/3
23	PSU	CY	39	23	-	0/7/25/26	0/2/2/2
23	7MG	CY	46	23	-	0/7/37/38	0/3/3/3
23	5MU	CY	54	23	-	0/3/25/26	0/2/2/2
23	PSU	CY	55	23	-	0/7/25/26	0/2/2/2
23	4SU	CY	8	23	-	0/3/25/26	0/2/2/2

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AW	37	MIA	C2-S10	-7.32	1.69	1.75
24	AX	55	PSU	C5-C1'	-4.89	1.48	1.52
23	CY	39	PSU	C5-C1'	-4.20	1.48	1.52
23	AY	32	PSU	C5-C1'	-4.11	1.48	1.52
23	AY	55	PSU	C5-C1'	-4.05	1.48	1.52
23	CY	8	4SU	C4-S4	-3.87	1.60	1.67
23	AW	39	PSU	C5-C1'	-3.84	1.48	1.52
23	AW	32	PSU	C5-C1'	-3.77	1.49	1.52
23	AW	55	PSU	C5-C1'	-3.75	1.49	1.52
23	CY	55	PSU	C5-C1'	-3.68	1.49	1.52
23	AW	8	4SU	C4-S4	-3.63	1.60	1.67
23	AY	39	PSU	C5-C1'	-3.46	1.49	1.52
24	AX	8	4SU	C4-S4	-3.45	1.60	1.67
23	CW	8	4SU	C4-S4	-3.45	1.60	1.67
23	CW	39	PSU	C5-C1'	-3.43	1.49	1.52
23	AY	8	4SU	C4-S4	-3.37	1.60	1.67
23	CW	55	PSU	C5-C1'	-3.33	1.49	1.52
24	CX	8	4SU	C4-S4	-3.29	1.61	1.67
23	CY	32	PSU	C5-C1'	-3.09	1.49	1.52
24	CX	55	PSU	C5-C1'	-2.63	1.49	1.52
23	AY	39	PSU	O4'-C1'	-2.40	1.40	1.44
23	CW	32	PSU	C5-C1'	-2.33	1.50	1.52
23	CY	39	PSU	O4'-C1'	-2.22	1.40	1.44
23	AY	46	7MG	CM7-N7	2.01	1.49	1.46
23	CW	37	MIA	C2-N3	2.31	1.36	1.32
23	AY	37	MIA	C2-N3	2.37	1.36	1.32
23	CY	37	MIA	C2-N3	2.38	1.36	1.32
23	AW	37	MIA	C5-C4	3.02	1.47	1.40
23	CW	46	7MG	C5-C4	3.10	1.47	1.39
23	CW	37	MIA	C5-C4	3.13	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AW	46	7MG	C5-C4	3.16	1.48	1.39
23	CY	46	7MG	C5-C4	3.21	1.48	1.39
23	AY	46	7MG	C5-C4	3.49	1.49	1.39
23	AY	37	MIA	C5-C4	3.51	1.48	1.40
23	CY	37	MIA	C5-C4	3.53	1.48	1.40
24	CX	32	5MC	C5-C4	4.58	1.48	1.41
24	AX	32	5MC	C5-C4	4.74	1.48	1.41

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	CW	39	PSU	N1-C2-N3	-12.28	120.50	128.33
23	AY	39	PSU	N1-C2-N3	-12.10	120.61	128.33
23	CW	32	PSU	N1-C2-N3	-11.17	121.21	128.33
24	CX	55	PSU	N1-C2-N3	-11.11	121.24	128.33
23	AW	32	PSU	N1-C2-N3	-11.00	121.31	128.33
23	CY	32	PSU	N1-C2-N3	-10.83	121.42	128.33
23	AY	55	PSU	N1-C2-N3	-10.64	121.55	128.33
23	AW	39	PSU	N1-C2-N3	-10.49	121.64	128.33
24	AX	55	PSU	N1-C2-N3	-10.48	121.65	128.33
23	CY	39	PSU	N1-C2-N3	-10.43	121.68	128.33
23	AW	55	PSU	N1-C2-N3	-10.32	121.75	128.33
23	CY	55	PSU	N1-C2-N3	-9.99	121.96	128.33
23	AY	32	PSU	N1-C2-N3	-9.99	121.96	128.33
23	CW	46	7MG	C5-C4-N3	-9.88	117.19	126.82
23	CW	55	PSU	N1-C2-N3	-9.69	122.15	128.33
23	AW	46	7MG	C5-C4-N3	-9.03	118.01	126.82
23	AY	46	7MG	C5-C4-N3	-9.01	118.04	126.82
23	CY	46	7MG	C5-C4-N3	-8.51	118.53	126.82
23	CW	37	MIA	N3-C2-N1	-8.28	122.55	128.89
23	AY	37	MIA	N3-C2-N1	-7.31	123.30	128.89
23	CY	37	MIA	N3-C2-N1	-7.29	123.32	128.89
24	CX	8	4SU	C5-C4-N3	-6.60	117.16	123.63
24	AX	8	4SU	C5-C4-N3	-6.41	117.35	123.63
23	AY	54	5MU	C5-C4-N3	-6.03	118.42	125.14
23	AW	55	PSU	C5-C1'-C2'	-6.00	104.87	115.52
23	AW	54	5MU	C5-C4-N3	-5.91	118.55	125.14
23	AY	46	7MG	C5-C6-N1	-5.69	114.72	123.46
23	CY	46	7MG	C5-C6-N1	-5.55	114.93	123.46
23	CW	54	5MU	C5-C4-N3	-5.51	119.00	125.14
23	CY	54	5MU	C5-C4-N3	-5.46	119.06	125.14
23	CW	55	PSU	C5-C1'-C2'	-5.44	105.86	115.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	CX	54	5MU	C5-C4-N3	-5.43	119.09	125.14
23	AW	46	7MG	C5-C6-N1	-5.27	115.35	123.46
23	AY	8	4SU	C5-C4-N3	-5.14	118.60	123.63
24	AX	54	5MU	C5-C4-N3	-5.10	119.46	125.14
23	AY	32	PSU	C5-C1'-C2'	-4.75	107.09	115.52
23	CW	46	7MG	C5-C6-N1	-4.74	116.17	123.46
23	CW	8	4SU	C5-C4-N3	-4.41	119.31	123.63
23	AW	32	PSU	C5-C1'-C2'	-4.35	107.79	115.52
23	AW	8	4SU	C5-C4-N3	-4.06	119.65	123.63
23	AY	55	PSU	C5-C6-N1	-3.87	118.94	124.39
24	CX	55	PSU	C5-C6-N1	-3.85	118.96	124.39
23	AY	32	PSU	C5-C6-N1	-3.66	119.22	124.39
24	AX	55	PSU	C5-C6-N1	-3.63	119.26	124.39
23	AW	39	PSU	C5-C6-N1	-3.57	119.36	124.39
23	CW	55	PSU	C5-C6-N1	-3.52	119.42	124.39
23	AW	55	PSU	C5-C6-N1	-3.41	119.58	124.39
23	CY	8	4SU	C5-C4-N3	-3.40	120.30	123.63
23	CW	37	MIA	C4-C5-N7	-3.29	106.45	109.48
23	CY	32	PSU	C5-C6-N1	-3.23	119.83	124.39
23	AW	32	PSU	C5-C6-N1	-3.23	119.84	124.39
23	CW	39	PSU	C5-C6-N1	-3.17	119.91	124.39
23	CY	55	PSU	C5-C6-N1	-3.11	120.00	124.39
24	AX	55	PSU	C5-C1'-C2'	-3.07	110.08	115.52
23	CY	39	PSU	C5-C1'-C2'	-3.03	110.15	115.52
23	AW	37	MIA	C5-C6-N1	-2.99	117.40	120.48
23	CY	39	PSU	C5-C6-N1	-2.85	120.37	124.39
23	AY	37	MIA	C4-C5-N7	-2.81	106.89	109.48
23	CW	32	PSU	C5-C6-N1	-2.75	120.51	124.39
23	AY	46	7MG	CM7-N7-C8	-2.70	112.86	120.52
23	AW	46	7MG	CM7-N7-C8	-2.69	112.89	120.52
23	CY	37	MIA	C4-C5-N7	-2.69	107.00	109.48
23	CY	46	7MG	CM7-N7-C8	-2.68	112.91	120.52
23	CW	46	7MG	CM7-N7-C8	-2.67	112.95	120.52
23	CW	39	PSU	C5-C1'-C2'	-2.63	110.86	115.52
23	AW	37	MIA	C4-C5-N7	-2.51	107.17	109.48
23	CY	55	PSU	C5-C1'-C2'	-2.41	111.24	115.52
23	CY	32	PSU	C5-C1'-C2'	-2.39	111.28	115.52
23	AW	39	PSU	C5-C1'-C2'	-2.33	111.37	115.52
23	AY	39	PSU	C5-C6-N1	-2.29	121.15	124.39
23	AY	46	7MG	C5-C4-N9	-2.25	102.86	106.18
23	AW	46	7MG	C5-C4-N9	-2.14	103.03	106.18
23	CY	46	7MG	C5-C4-N9	-2.12	103.06	106.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	AW	37	MIA	N3-C2-N1	-2.05	122.87	126.79
23	CW	46	7MG	C2-N3-C4	2.05	120.50	114.53
23	CW	46	7MG	CM7-N7-C5	2.11	131.16	124.09
23	CY	39	PSU	O4'-C1'-C2'	2.13	106.90	104.73
23	AW	46	7MG	CM7-N7-C5	2.15	131.30	124.09
23	CY	46	7MG	CM7-N7-C5	2.22	131.51	124.09
23	CW	32	PSU	O4'-C1'-C2'	2.27	107.04	104.73
23	AY	46	7MG	CM7-N7-C5	2.31	131.81	124.09
23	AW	32	PSU	O4'-C1'-C2'	2.33	107.10	104.73
23	AW	55	PSU	O4'-C1'-C2'	2.38	107.16	104.73
23	AY	39	PSU	O4'-C1'-C2'	2.59	107.37	104.73
23	AW	39	PSU	O4'-C1'-C2'	2.60	107.38	104.73
24	CX	32	5MC	N4-C4-N3	2.65	120.79	116.95
24	CX	55	PSU	O4'-C1'-C2'	2.77	107.55	104.73
23	AY	32	PSU	O4'-C1'-C2'	2.77	107.55	104.73
24	AX	55	PSU	O4'-C1'-C2'	2.77	107.55	104.73
23	CW	55	PSU	O4'-C1'-C2'	2.77	107.56	104.73
23	CY	32	PSU	O4'-C1'-C2'	2.84	107.62	104.73
24	AX	32	5MC	N4-C4-N3	2.86	121.09	116.95
23	CW	32	PSU	C4-C5-C1'	2.98	126.67	121.23
23	CW	39	PSU	O4'-C1'-C2'	3.03	107.82	104.73
23	CY	55	PSU	O4'-C1'-C2'	3.05	107.84	104.73
23	AW	37	MIA	C2-N1-C6	3.06	122.32	113.35
23	AY	55	PSU	O4'-C1'-C2'	3.24	108.03	104.73
23	AW	37	MIA	N6-C6-N1	3.28	122.75	118.52
23	AY	39	PSU	C6-N1-C2	3.59	121.24	115.47
23	CY	39	PSU	C6-N1-C2	3.62	121.30	115.47
23	CY	55	PSU	C6-N1-C2	3.87	121.69	115.47
23	CW	55	PSU	C6-N1-C2	3.89	121.72	115.47
23	CY	32	PSU	C6-N1-C2	4.02	121.93	115.47
23	AW	55	PSU	C6-N1-C2	4.04	121.97	115.47
23	AW	32	PSU	C6-N1-C2	4.07	122.02	115.47
23	AY	32	PSU	C6-N1-C2	4.09	122.04	115.47
24	AX	55	PSU	C6-N1-C2	4.13	122.12	115.47
23	AY	55	PSU	C6-N1-C2	4.14	122.13	115.47
23	CW	39	PSU	C6-N1-C2	4.20	122.22	115.47
23	AW	39	PSU	C6-N1-C2	4.23	122.27	115.47
23	CW	32	PSU	C6-N1-C2	4.23	122.28	115.47
23	CW	46	7MG	C6-N1-C2	4.38	122.02	115.94
24	CX	55	PSU	C6-N1-C2	4.63	122.92	115.47
23	AW	46	7MG	C6-N1-C2	5.38	123.41	115.94
24	CX	55	PSU	C4-N3-C2	5.90	120.35	115.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	CY	46	7MG	C6-N1-C2	6.02	124.29	115.94
23	AY	32	PSU	C4-N3-C2	6.11	120.53	115.25
23	AY	55	PSU	C4-N3-C2	6.15	120.56	115.25
23	AY	46	7MG	C6-N1-C2	6.17	124.50	115.94
23	AW	39	PSU	C4-N3-C2	6.29	120.68	115.25
24	CX	54	5MU	C4-N3-C2	6.38	120.76	115.25
23	CY	55	PSU	C4-N3-C2	6.40	120.78	115.25
23	CW	55	PSU	C4-N3-C2	6.43	120.81	115.25
23	AW	55	PSU	C4-N3-C2	6.45	120.82	115.25
24	AX	54	5MU	C4-N3-C2	6.53	120.89	115.25
24	AX	55	PSU	C4-N3-C2	6.58	120.93	115.25
23	CW	32	PSU	C4-N3-C2	6.86	121.17	115.25
23	CY	32	PSU	C4-N3-C2	6.92	121.22	115.25
23	AW	32	PSU	C4-N3-C2	7.18	121.46	115.25
23	CW	54	5MU	C4-N3-C2	7.19	121.46	115.25
23	CY	39	PSU	C4-N3-C2	7.35	121.60	115.25
23	CY	54	5MU	C4-N3-C2	7.57	121.79	115.25
23	CY	46	7MG	N3-C4-N9	7.75	138.38	126.75
23	CW	46	7MG	N3-C4-N9	7.94	138.66	126.75
23	AW	46	7MG	N3-C4-N9	8.13	138.96	126.75
23	CW	39	PSU	C4-N3-C2	8.14	122.28	115.25
23	AY	46	7MG	N3-C4-N9	8.22	139.09	126.75
23	AW	54	5MU	C4-N3-C2	8.23	122.36	115.25
23	AY	39	PSU	C4-N3-C2	8.69	122.76	115.25
23	AY	54	5MU	C4-N3-C2	8.90	122.94	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

19 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	AW	32	PSU	1	0
23	AW	37	MIA	1	0
23	AW	54	5MU	1	0
23	AW	55	PSU	1	0
23	AW	8	4SU	1	0
24	AX	8	4SU	2	0
23	AY	46	7MG	1	0
23	AY	54	5MU	2	0
23	AY	55	PSU	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	AY	8	4SU	1	0
23	CW	32	PSU	1	0
23	CW	39	PSU	2	0
23	CW	46	7MG	5	0
23	CW	8	4SU	1	0
24	CX	8	4SU	1	0
23	CY	37	MIA	1	0
23	CY	39	PSU	2	0
23	CY	46	7MG	1	0
23	CY	8	4SU	4	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2152 ligands modelled in this entry, 2148 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
57	PCY	AA	3231	-	36,42,42	1.61	5 (13%)	41,65,65	1.47	9 (21%)
58	SF4	AD	501	4	0,12,12	0.00	-	0,24,24	0.00	-
57	PCY	CA	3178	-	36,42,42	1.58	4 (11%)	41,65,65	1.33	3 (7%)
58	SF4	CD	501	4	0,12,12	0.00	-	0,24,24	0.00	-

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
57	PCY	AA	3231	-	-	0/33/67/67	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	SF4	AD	501	4	-	0/0/48/48	0/6/5/5
57	PCY	CA	3178	-	-	0/33/67/67	0/3/3/3
58	SF4	CD	501	4	-	0/0/48/48	0/6/5/5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	CA	3178	PCY	C28-C32	-5.52	1.39	1.49
57	AA	3231	PCY	C28-C32	-5.37	1.39	1.49
57	AA	3231	PCY	C34-C30	-5.18	1.40	1.51
57	CA	3178	PCY	C34-C30	-5.15	1.40	1.51
57	AA	3231	PCY	C27-C23	-3.73	1.40	1.50
57	CA	3178	PCY	C27-C23	-3.34	1.41	1.50
57	CA	3178	PCY	C22-N20	-3.08	1.33	1.39
57	AA	3231	PCY	C22-N20	-2.80	1.34	1.39
57	AA	3231	PCY	C17-N20	2.20	1.48	1.45

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	CA	3178	PCY	C8-C17-N20	-4.69	106.12	113.17
57	AA	3231	PCY	C18-O21-C23	-4.45	107.00	116.64
57	AA	3231	PCY	C8-C17-N20	-3.78	107.50	113.17
57	CA	3178	PCY	C18-O21-C23	-3.40	109.27	116.64
57	AA	3231	PCY	O36-C31-C27	-2.16	116.91	121.10
57	AA	3231	PCY	C34-C30-C35	-2.08	116.08	120.33
57	AA	3231	PCY	C30-C27-C23	2.09	126.64	120.42
57	AA	3231	PCY	C10-N4-C9	2.12	122.22	115.74
57	CA	3178	PCY	C10-N4-C9	2.17	122.35	115.74
57	AA	3231	PCY	C34-C30-C27	2.19	124.53	121.77
57	AA	3231	PCY	O21-C18-C15	2.54	112.92	108.23
57	AA	3231	PCY	O21-C23-C27	2.85	119.12	112.45

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	AA	3231	PCY	7	0
57	CA	3178	PCY	9	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AA	1498/1521 (98%)	0.40	66 (4%) 38 44	40, 67, 92, 106	0
1	CA	1503/1521 (98%)	0.29	61 (4%) 41 47	43, 69, 92, 106	0
2	AB	231/256 (90%)	1.29	49 (21%) 1 1	63, 80, 90, 94	0
2	CB	231/256 (90%)	1.57	80 (34%) 0 0	64, 82, 89, 96	0
3	AC	206/239 (86%)	1.18	33 (16%) 3 2	61, 74, 84, 92	0
3	CC	206/239 (86%)	1.87	86 (41%) 0 0	64, 76, 86, 92	0
4	AD	208/209 (99%)	0.54	9 (4%) 39 45	56, 68, 79, 87	0
4	CD	208/209 (99%)	1.15	36 (17%) 2 2	57, 68, 78, 87	0
5	AE	148/162 (91%)	0.86	12 (8%) 15 16	56, 67, 77, 91	0
5	CE	148/162 (91%)	0.97	18 (12%) 5 6	57, 69, 79, 92	0
6	AF	100/101 (99%)	0.46	3 (3%) 54 60	53, 66, 76, 82	0
6	CF	100/101 (99%)	0.36	1 (1%) 84 87	54, 66, 76, 82	0
7	AG	155/156 (99%)	0.95	16 (10%) 9 9	61, 71, 83, 93	0
7	CG	155/156 (99%)	1.02	18 (11%) 6 7	62, 73, 84, 96	0
8	AH	137/138 (99%)	0.89	16 (11%) 6 6	57, 69, 75, 83	0
8	CH	137/138 (99%)	1.13	24 (17%) 2 2	59, 71, 77, 84	0
9	AI	127/128 (99%)	1.60	37 (29%) 1 0	56, 78, 85, 90	0
9	CI	127/128 (99%)	2.16	62 (48%) 0 0	62, 79, 86, 89	0
10	AJ	97/105 (92%)	1.56	34 (35%) 0 0	57, 78, 90, 91	0
10	CJ	96/105 (91%)	1.96	43 (44%) 0 0	60, 80, 91, 93	0
11	AK	114/129 (88%)	0.96	13 (11%) 7 7	47, 67, 80, 83	0
11	CK	114/129 (88%)	0.45	3 (2%) 59 64	47, 67, 79, 83	0
12	AL	122/132 (92%)	0.59	4 (3%) 50 56	42, 56, 69, 75	0
12	CL	122/132 (92%)	1.02	19 (15%) 3 3	45, 58, 71, 75	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AM	123/126 (97%)	0.65	8 (6%) 22 25	42, 63, 75, 80	0
13	CM	122/126 (96%)	1.69	45 (36%) 0 0	66, 79, 86, 90	0
14	AN	60/61 (98%)	1.22	9 (15%) 3 3	60, 70, 77, 81	0
14	CN	60/61 (98%)	2.91	43 (71%) 0 0	64, 73, 80, 83	0
15	AO	88/89 (98%)	0.40	2 (2%) 64 69	50, 66, 76, 82	0
15	CO	88/89 (98%)	0.63	3 (3%) 49 55	53, 68, 77, 82	0
16	AP	82/88 (93%)	1.12	15 (18%) 2 2	52, 68, 76, 80	0
16	CP	82/88 (93%)	1.17	12 (14%) 3 3	51, 68, 76, 79	0
17	AQ	99/105 (94%)	0.73	5 (5%) 32 37	55, 68, 77, 79	0
17	CQ	99/105 (94%)	1.63	36 (36%) 0 0	57, 69, 77, 80	0
18	AR	68/88 (77%)	0.88	5 (7%) 17 20	58, 66, 76, 80	0
18	CR	68/88 (77%)	0.60	4 (5%) 26 30	59, 68, 77, 80	0
19	AS	83/93 (89%)	0.89	5 (6%) 25 29	63, 73, 81, 91	0
19	CS	83/93 (89%)	2.11	44 (53%) 0 0	66, 76, 84, 92	0
20	AT	96/106 (90%)	1.82	40 (41%) 0 0	57, 68, 80, 86	0
20	CT	96/106 (90%)	1.79	42 (43%) 0 0	58, 68, 82, 87	0
21	AU	23/27 (85%)	1.38	5 (21%) 1 1	63, 66, 72, 75	0
21	CU	23/27 (85%)	1.69	10 (43%) 0 0	65, 68, 74, 77	0
22	AV	13/24 (54%)	1.15	1 (7%) 16 18	52, 64, 82, 98	0
22	CV	13/24 (54%)	0.66	2 (15%) 3 3	56, 67, 85, 99	0
23	AW	67/76 (88%)	1.16	11 (16%) 2 2	47, 84, 97, 104	0
23	AY	67/76 (88%)	1.20	11 (16%) 2 2	38, 97, 101, 104	0
23	CW	65/76 (85%)	1.13	12 (18%) 2 2	68, 91, 102, 104	0
23	CY	66/76 (86%)	1.70	26 (39%) 0 0	43, 97, 101, 104	0
24	AX	72/77 (93%)	0.74	2 (2%) 56 62	39, 68, 85, 93	0
24	CX	72/77 (93%)	0.14	0 100 100	43, 71, 86, 94	0
25	BA	2819/2915 (96%)	0.61	69 (2%) 62 67	23, 42, 88, 104	0
25	DA	2800/2915 (96%)	0.09	94 (3%) 49 55	27, 47, 89, 108	0
26	BB	120/121 (99%)	0.14	0 100 100	35, 56, 70, 86	0
26	DB	120/121 (99%)	0.15	0 100 100	42, 62, 73, 87	0
27	BD	275/276 (99%)	0.79	3 (1%) 82 85	23, 40, 55, 79	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
27	DD	275/276 (99%)	0.47	3 (1%) 82 85	26, 42, 56, 77	0
28	BE	204/206 (99%)	0.75	4 (1%) 68 73	22, 47, 66, 76	0
28	DE	204/206 (99%)	0.27	3 (1%) 76 80	28, 50, 67, 77	0
29	BF	203/210 (96%)	0.79	12 (5%) 26 30	23, 49, 73, 88	0
29	DF	203/210 (96%)	0.89	29 (14%) 4 4	27, 55, 75, 88	0
30	BG	181/182 (99%)	0.57	11 (6%) 25 28	44, 64, 78, 90	0
30	DG	181/182 (99%)	1.36	44 (24%) 1 1	50, 67, 80, 90	0
31	BH	174/180 (96%)	0.49	3 (1%) 73 77	51, 65, 76, 85	0
31	DH	174/180 (96%)	2.77	111 (63%) 0 0	57, 70, 80, 86	0
32	BI	146/148 (98%)	0.99	22 (15%) 3 3	50, 71, 82, 86	0
32	DI	146/148 (98%)	0.54	9 (6%) 24 27	53, 71, 82, 85	0
33	BN	140/140 (100%)	0.60	1 (0%) 89 91	32, 47, 68, 75	0
33	DN	140/140 (100%)	0.73	8 (5%) 27 32	36, 52, 70, 77	0
34	BO	122/122 (100%)	0.41	0 100 100	25, 38, 59, 65	0
34	DO	122/122 (100%)	0.57	0 100 100	47, 59, 74, 79	0
35	BP	149/150 (99%)	0.52	1 (0%) 89 91	24, 55, 74, 81	0
35	DP	149/150 (99%)	0.95	25 (16%) 2 2	29, 59, 76, 82	0
36	BQ	141/141 (100%)	0.84	4 (2%) 56 62	31, 50, 66, 77	0
36	DQ	141/141 (100%)	0.93	19 (13%) 4 4	38, 54, 69, 80	0
37	BR	118/118 (100%)	0.34	0 100 100	21, 32, 50, 58	0
37	DR	118/118 (100%)	0.30	0 100 100	38, 53, 64, 74	0
38	BS	110/112 (98%)	0.51	1 (0%) 85 88	32, 48, 64, 67	0
38	DS	110/112 (98%)	1.57	37 (33%) 0 0	58, 69, 80, 85	0
39	BT	131/146 (89%)	0.26	1 (0%) 87 89	31, 42, 68, 89	0
39	DT	131/146 (89%)	0.35	1 (0%) 87 89	51, 64, 78, 84	0
40	BU	116/118 (98%)	0.31	0 100 100	17, 28, 47, 65	0
40	DU	116/118 (98%)	0.62	7 (6%) 25 29	40, 62, 76, 82	0
41	BV	101/101 (100%)	0.21	0 100 100	15, 35, 54, 67	0
41	DV	101/101 (100%)	1.11	19 (18%) 2 2	39, 74, 81, 88	0
42	BW	112/113 (99%)	0.39	1 (0%) 85 88	17, 28, 53, 79	0
42	DW	112/113 (99%)	0.62	1 (0%) 85 88	38, 51, 68, 86	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
43	BX	95/96 (98%)	0.38	1 (1%) 82 85	21, 35, 60, 75	0
43	DX	95/96 (98%)	1.08	15 (15%) 3 3	38, 56, 76, 85	0
44	BY	107/110 (97%)	0.26	2 (1%) 70 74	30, 46, 65, 83	0
44	DY	107/110 (97%)	1.44	28 (26%) 1 1	57, 71, 83, 86	0
45	BZ	171/206 (83%)	1.77	44 (25%) 1 1	35, 67, 94, 105	0
45	DZ	174/206 (84%)	2.93	91 (52%) 0 0	65, 83, 97, 103	0
46	B0	83/85 (97%)	0.49	5 (6%) 25 29	20, 36, 57, 76	0
46	D0	83/85 (97%)	1.18	12 (14%) 3 3	44, 64, 74, 79	0
47	B1	97/98 (98%)	0.56	3 (3%) 52 58	24, 45, 70, 73	0
47	D1	97/98 (98%)	0.75	6 (6%) 24 27	37, 56, 75, 86	0
48	B2	70/72 (97%)	0.53	1 (1%) 78 81	30, 45, 58, 78	0
48	D2	70/72 (97%)	0.65	3 (4%) 39 45	53, 66, 78, 82	0
49	B3	59/60 (98%)	0.24	0 100 100	19, 31, 58, 75	0
49	D3	59/60 (98%)	0.93	9 (15%) 3 3	54, 66, 78, 88	0
50	B4	69/71 (97%)	0.67	9 (13%) 5 5	51, 70, 89, 99	0
50	D4	69/71 (97%)	2.13	34 (49%) 0 0	72, 82, 92, 93	0
51	B5	59/60 (98%)	0.43	1 (1%) 73 77	17, 27, 43, 54	0
51	D5	59/60 (98%)	0.44	1 (1%) 73 77	35, 50, 66, 74	0
52	B6	53/54 (98%)	0.24	0 100 100	28, 39, 56, 67	0
52	D6	53/54 (98%)	0.77	6 (11%) 7 7	48, 59, 71, 76	0
53	B7	48/49 (97%)	0.69	2 (4%) 40 46	18, 26, 62, 72	0
53	D7	48/49 (97%)	0.98	4 (8%) 14 15	30, 41, 61, 78	0
54	B8	64/65 (98%)	0.24	0 100 100	19, 31, 40, 63	0
54	D8	64/65 (98%)	0.84	4 (6%) 23 27	44, 54, 65, 71	0
55	B9	37/37 (100%)	0.69	1 (2%) 58 63	26, 47, 63, 70	0
55	D9	37/37 (100%)	1.39	7 (18%) 2 2	45, 57, 68, 75	0
All	All	20900/21748 (96%)	0.70	1973 (9%) 11 12	15, 61, 87, 108	0

All (1973) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
45	BZ	108	PRO	16.3
45	DZ	116	VAL	13.7

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Mol	Chain	Res	Type	RSRZ
45	DZ	115	GLY	12.9
45	DZ	114	GLY	11.5
45	BZ	111	VAL	11.4
45	DZ	107	THR	11.4
7	CG	82	GLY	11.2
45	DZ	144	LEU	11.2
45	DZ	108	PRO	10.8
45	BZ	115	GLY	10.2
45	DZ	113	ALA	10.0
45	DZ	171	ILE	9.4
45	BZ	114	GLY	9.4
45	BZ	113	ALA	9.3
45	BZ	116	VAL	8.9
45	DZ	112	ARG	8.9
25	DA	888	C	8.7
45	DZ	155	LEU	8.6
25	BA	942	A	8.6
25	DA	883	G	8.3
45	DZ	147	GLY	8.3
45	DZ	149	SER	8.2
25	DA	896	A	8.1
23	AW	71	G	8.1
45	DZ	141	VAL	7.9
25	DA	229	A	7.9
45	DZ	170	THR	7.8
25	BA	931	C	7.7
1	CA	1030(B)	C	7.7
13	AM	124	PRO	7.7
50	D4	49	PHE	7.6
43	DX	92	LEU	7.6
31	DH	48	GLY	7.6
3	CC	198	VAL	7.6
25	DA	2802	G	7.5
45	BZ	106	GLY	7.5
14	CN	39	LEU	7.5
1	AA	1030(B)	C	7.4
7	AG	79	ARG	7.4
45	BZ	141	VAL	7.3
25	DA	884	C	7.3
13	CM	124	PRO	7.3
13	CM	123	ALA	7.3
44	DY	1	MET	7.1

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Mol	Chain	Res	Type	RSRZ
36	DQ	109	VAL	7.0
10	CJ	10	GLY	7.0
14	CN	37	PHE	6.8
25	BA	932	C	6.8
45	DZ	111	VAL	6.8
23	CY	36	A	6.7
45	BZ	143	GLY	6.7
10	CJ	47	PHE	6.7
10	CJ	85	LEU	6.7
45	BZ	112	ARG	6.6
31	DH	76	VAL	6.6
31	DH	82	GLY	6.5
45	DZ	139	VAL	6.5
9	CI	8	GLY	6.5
23	AY	36	A	6.5
45	DZ	156	LYS	6.5
2	CB	165	VAL	6.5
25	BA	934	A	6.5
23	AW	20	U	6.4
45	BZ	144	LEU	6.4
31	DH	44	VAL	6.3
23	CW	71	G	6.3
2	AB	232	PRO	6.3
23	AW	44	G	6.3
1	AA	1532	U	6.2
45	DZ	173	ALA	6.2
25	BA	2153	G	6.2
44	DY	65	ALA	6.2
14	CN	34	TYR	6.2
25	BA	943	C	6.2
25	DA	885	C	6.2
31	DH	25	LYS	6.2
25	BA	930	G	6.2
2	CB	207	ALA	6.1
31	DH	45	VAL	6.1
50	D4	59	PHE	6.1
14	CN	38	GLY	6.1
14	CN	25	VAL	6.0
45	DZ	172	ALA	6.0
9	CI	4	TYR	6.0
23	AY	34	G	6.0
31	DH	24	VAL	6.0

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Mol	Chain	Res	Type	RSRZ
31	DH	49	VAL	5.9
7	CG	16	LEU	5.9
1	CA	1030(A)	G	5.9
7	AG	84	ASN	5.9
3	CC	182	ILE	5.7
1	AA	1030(C)	G	5.7
1	CA	1001(A)	G	5.7
47	B1	2	SER	5.7
45	DZ	174	VAL	5.6
25	DA	2160	G	5.6
19	CS	80	TYR	5.6
10	CJ	63	PHE	5.6
25	DA	2145	C	5.6
31	DH	32	GLU	5.6
3	CC	145	GLY	5.6
31	DH	51	ARG	5.6
45	BZ	110	GLY	5.6
31	DH	47	GLU	5.6
14	CN	51	GLY	5.6
50	D4	50	VAL	5.6
45	BZ	146	ILE	5.5
45	DZ	146	ILE	5.5
45	DZ	4	ARG	5.5
2	CB	34	ALA	5.5
45	BZ	107	THR	5.5
13	AM	123	ALA	5.5
30	BG	146	TYR	5.5
45	DZ	145	GLU	5.4
29	DF	208	GLY	5.4
9	AI	15	ALA	5.4
7	CG	156	TRP	5.4
31	DH	43	VAL	5.4
25	DA	887	A	5.4
25	DA	2125	G	5.4
45	DZ	96	VAL	5.4
3	AC	80	GLY	5.4
31	DH	105	LEU	5.3
25	DA	2146	C	5.3
45	DZ	9	TYR	5.3
31	DH	20	ALA	5.3
45	BZ	104	PHE	5.3
23	AY	13	C	5.2

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Mol	Chain	Res	Type	RSRZ
25	BA	936	C	5.2
13	CM	68	GLY	5.2
7	CG	83	ALA	5.2
1	AA	1257	U	5.2
30	DG	115	ARG	5.2
23	CY	34	G	5.2
45	BZ	120	ILE	5.2
44	DY	45	VAL	5.2
1	CA	1257	U	5.2
1	CA	1034	G	5.2
2	CB	51	LEU	5.2
3	AC	65	ALA	5.2
45	DZ	51	ALA	5.2
45	DZ	47	VAL	5.2
19	CS	16	LEU	5.1
25	BA	2806	G	5.1
12	CL	39	VAL	5.1
31	DH	52	VAL	5.1
1	AA	163	C	5.1
7	AG	82	GLY	5.1
20	CT	9	ASN	5.1
3	CC	39	ILE	5.1
31	DH	79	VAL	5.1
31	DH	7	LEU	5.1
20	AT	55	ILE	5.1
1	CA	1030(C)	G	5.0
45	DZ	57	ILE	5.0
25	BA	929	G	5.0
31	DH	18	GLU	5.0
9	CI	19	LEU	5.0
2	AB	227	GLY	5.0
1	AA	1031	G	5.0
25	BA	938	G	5.0
14	CN	35	ARG	5.0
45	DZ	118	GLN	5.0
45	DZ	120	ILE	5.0
31	DH	8	PRO	5.0
2	CB	92	TYR	4.9
9	CI	106	ALA	4.9
9	CI	90	PRO	4.9
1	AA	204	U	4.9
30	DG	139	LEU	4.9

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Mol	Chain	Res	Type	RSRZ
3	CC	60	ALA	4.9
1	AA	1446	U	4.9
1	CA	1036	G	4.9
25	DA	2133	G	4.9
2	CB	32	ILE	4.9
3	CC	157	ILE	4.9
25	BA	2180	A	4.8
46	D0	42	GLY	4.8
25	DA	2159	G	4.8
9	CI	56	LEU	4.8
31	DH	35	VAL	4.8
46	D0	2	ALA	4.8
25	BA	1221	G	4.8
13	CM	87	TYR	4.8
25	BA	935	C	4.8
38	DS	58	LEU	4.8
2	CB	123	ALA	4.8
9	CI	15	ALA	4.8
25	DA	2794	C	4.8
45	DZ	50	GLN	4.8
9	CI	80	GLY	4.7
45	BZ	147	GLY	4.7
45	DZ	148	ASP	4.7
45	BZ	149	SER	4.7
3	CC	186	PHE	4.7
25	BA	2154	U	4.7
1	AA	1030(D)	A	4.7
25	BA	1555	C	4.7
14	CN	61	TRP	4.7
25	BA	2162	C	4.7
31	DH	128	PRO	4.7
3	CC	64	VAL	4.7
19	CS	63	THR	4.7
31	DH	106	THR	4.7
9	AI	19	LEU	4.7
25	DA	2128	C	4.7
31	DH	123	PHE	4.7
25	DA	2793	G	4.7
25	BA	2168	C	4.7
33	DN	140	VAL	4.7
50	D4	18	CYS	4.6
44	DY	5	MET	4.6

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Mol	Chain	Res	Type	RSRZ
25	DA	882	G	4.6
30	DG	182	LYS	4.6
25	DA	886	C	4.6
3	CC	91	LEU	4.6
9	CI	9	ARG	4.6
3	AC	87	LEU	4.6
23	CW	44	G	4.6
23	CY	52	G	4.6
7	AG	156	TRP	4.6
19	CS	71	LEU	4.6
7	AG	83	ALA	4.6
50	B4	59	PHE	4.6
10	CJ	74	ILE	4.6
45	DZ	42	VAL	4.5
25	DA	652(B)	A	4.5
3	CC	101	LEU	4.5
31	DH	71	LEU	4.5
13	CM	4	ILE	4.5
12	CL	55	VAL	4.5
1	AA	1036	G	4.5
30	DG	136	ARG	4.5
31	DH	31	GLY	4.5
9	AI	90	PRO	4.5
51	D5	60	VAL	4.5
25	DA	2154	G	4.5
31	DH	13	LYS	4.5
31	DH	17	VAL	4.5
25	BA	941	U	4.5
2	AB	228	GLY	4.5
9	CI	76	ALA	4.5
9	CI	27	THR	4.5
13	CM	90	LEU	4.5
1	AA	1447	A	4.5
21	CU	16	GLY	4.4
19	CS	13	ASP	4.4
9	AI	65	VAL	4.4
10	AJ	90	LEU	4.4
20	CT	26	ASN	4.4
1	AA	841	U	4.4
41	DV	30	GLY	4.4
45	BZ	164	ALA	4.4
8	CH	133	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
20	AT	43	LEU	4.4
44	DY	61	ILE	4.4
45	BZ	109	ALA	4.4
2	CB	232	PRO	4.4
25	DA	2155	G	4.4
31	DH	36	PRO	4.4
14	CN	36	PHE	4.4
25	BA	933	C	4.4
29	DF	196	LEU	4.4
31	DH	141	VAL	4.4
23	AY	35	A	4.4
9	CI	103	THR	4.4
15	CO	60	VAL	4.3
44	DY	75	ILE	4.3
25	DA	2161	C	4.3
1	CA	1002	G	4.3
17	CQ	23	VAL	4.3
31	DH	73	ALA	4.3
50	D4	52	THR	4.3
2	AB	222	ILE	4.3
9	CI	36	TYR	4.3
31	DH	11	VAL	4.3
12	CL	95	GLY	4.3
20	CT	47	GLY	4.3
23	CY	47	U	4.3
3	CC	87	LEU	4.3
12	CL	18	VAL	4.3
50	D4	43	TYR	4.3
9	CI	52	ALA	4.3
19	CS	40	ILE	4.3
45	DZ	89	PHE	4.3
13	CM	7	VAL	4.3
31	DH	75	ALA	4.3
23	CW	70	G	4.3
1	AA	1027	C	4.3
25	DA	897	C	4.3
25	DA	2896	C	4.3
45	DZ	58	VAL	4.2
9	CI	62	TYR	4.2
45	DZ	3	TYR	4.2
7	CG	7	ALA	4.2
9	AI	26	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
9	AI	82	ALA	4.2
3	CC	57	ILE	4.2
14	CN	55	GLY	4.2
1	CA	1021	G	4.2
45	DZ	109	ALA	4.2
9	AI	80	GLY	4.2
9	AI	81	ILE	4.2
8	CH	2	LEU	4.2
45	BZ	118	GLN	4.2
1	CA	1030(D)	A	4.2
9	AI	14	VAL	4.2
20	CT	59	ALA	4.2
14	CN	53	LEU	4.2
44	DY	43	ASN	4.2
3	AC	81	GLY	4.2
9	CI	28	VAL	4.2
17	AQ	27	PHE	4.2
31	DH	16	SER	4.2
31	DH	14	GLY	4.2
13	CM	15	VAL	4.1
1	CA	1001	A	4.1
31	DH	159	GLU	4.1
45	DZ	163	LEU	4.1
9	AI	76	ALA	4.1
50	D4	44	THR	4.1
12	CL	64	TYR	4.1
31	DH	10	PRO	4.1
3	CC	134	ILE	4.1
25	BA	2181	G	4.1
14	AN	2	ALA	4.1
31	DH	46	GLU	4.1
14	CN	42	ILE	4.1
1	AA	1024	G	4.1
23	CY	53	G	4.1
9	CI	109	VAL	4.1
29	DF	15	SER	4.1
1	CA	1035	A	4.1
29	DF	12	LEU	4.1
45	DZ	117	LEU	4.1
11	AK	14	VAL	4.1
9	CI	81	ILE	4.1
31	DH	72	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
23	CW	45	U	4.1
4	CD	188	LEU	4.1
9	AI	47	LEU	4.1
23	CY	1	G	4.0
25	DA	2127	G	4.0
20	CT	63	ILE	4.0
2	CB	187	LEU	4.0
31	DH	98	LEU	4.0
36	DQ	114	ALA	4.0
45	DZ	152	ALA	4.0
2	CB	211	ILE	4.0
10	CJ	90	LEU	4.0
53	B7	48	LYS	4.0
31	DH	6	ARG	4.0
9	CI	17	VAL	4.0
23	AY	47	U	4.0
45	DZ	93	ASP	4.0
19	AS	71	LEU	4.0
45	BZ	170	THR	4.0
1	CA	1030	C	4.0
29	BF	16	GLY	4.0
3	CC	202	ILE	4.0
17	AQ	36	ILE	4.0
3	AC	52	LEU	4.0
3	CC	197	GLY	4.0
1	AA	1003	G	4.0
25	DA	2138	C	4.0
39	BT	38	ASN	4.0
4	CD	135	LEU	4.0
45	BZ	1	MET	4.0
47	D1	2	SER	4.0
1	AA	202	U	4.0
45	BZ	169	GLU	4.0
13	AM	90	LEU	4.0
40	DU	88	ILE	4.0
25	BA	926	G	3.9
14	CN	7	ILE	3.9
25	DA	2167	U	3.9
7	AG	80	VAL	3.9
13	CM	88	ARG	3.9
5	CE	12	LEU	3.9
35	DP	91	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
31	DH	145	ALA	3.9
25	BA	2167	C	3.9
31	DH	142	GLY	3.9
16	CP	59	TRP	3.9
31	DH	29	PRO	3.9
2	CB	228	GLY	3.9
31	DH	2	SER	3.9
31	DH	34	GLU	3.9
38	DS	20	ARG	3.9
25	BA	271	U	3.9
45	DZ	99	TYR	3.9
1	AA	162	A	3.9
1	CA	485	G	3.9
7	CG	4	ARG	3.9
44	DY	55	TYR	3.9
3	AC	101	LEU	3.9
36	DQ	106	VAL	3.9
25	BA	2183	C	3.9
19	CS	14	HIS	3.8
2	AB	61	LEU	3.8
10	CJ	71	LEU	3.8
45	DZ	157	LEU	3.8
20	AT	100	ILE	3.8
45	DZ	121	HIS	3.8
30	DG	42	GLY	3.8
3	CC	28	GLN	3.8
17	AQ	98	LEU	3.8
53	D7	46	VAL	3.8
5	CE	11	ILE	3.8
30	DG	39	ILE	3.8
45	DZ	133	ILE	3.8
35	DP	1	MET	3.8
9	CI	61	ALA	3.8
23	CW	72	C	3.8
41	DV	17	GLY	3.8
10	CJ	91	PRO	3.8
27	BD	276	LYS	3.8
3	CC	184	TYR	3.8
4	CD	87	GLY	3.8
1	AA	1030(A)	G	3.8
46	D0	3	HIS	3.8
20	AT	74	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
45	DZ	128	VAL	3.8
10	AJ	4	ILE	3.8
4	CD	152	SER	3.8
5	CE	99	GLY	3.8
36	DQ	33	GLY	3.8
2	CB	17	PHE	3.8
7	CG	154	TYR	3.7
21	AU	14	TRP	3.7
25	DA	2153	G	3.7
32	BI	72	LEU	3.7
31	DH	95	ARG	3.7
2	CB	208	ILE	3.7
41	DV	92	THR	3.7
3	CC	18	TRP	3.7
32	DI	74	ASN	3.7
18	AR	31	LEU	3.7
25	BA	2155	G	3.7
53	D7	48	LYS	3.7
45	DZ	140	ASP	3.7
29	BF	21	ALA	3.7
19	CS	52	TYR	3.7
20	CT	83	ARG	3.7
23	CY	62	C	3.7
25	BA	2814	C	3.7
25	DA	2792	G	3.7
17	CQ	80	GLY	3.7
43	DX	94	GLY	3.7
2	CB	37	ASN	3.7
25	DA	2144	U	3.7
2	AB	123	ALA	3.7
3	AC	179	ARG	3.7
5	AE	10	MET	3.7
8	CH	134	ILE	3.7
10	AJ	72	VAL	3.7
31	DH	15	VAL	3.7
31	DH	92	ILE	3.7
3	CC	188	LEU	3.7
23	AY	12	U	3.7
25	BA	2151	C	3.7
12	CL	30	ALA	3.7
14	CN	2	ALA	3.7
45	DZ	106	GLY	3.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	AA	216	G	3.7
46	D0	37	LEU	3.7
49	D3	29	ARG	3.7
13	CM	119	GLY	3.6
19	CS	68	GLY	3.6
40	DU	73	GLY	3.6
3	AC	184	TYR	3.6
35	DP	92	GLU	3.6
23	CY	63	G	3.6
20	AT	72	LEU	3.6
25	BA	944	C	3.6
31	DH	102	ALA	3.6
30	DG	116	ASP	3.6
3	CC	193	TYR	3.6
8	CH	65	TYR	3.6
4	CD	196	LEU	3.6
44	DY	106	LEU	3.6
50	D4	54	GLY	3.6
3	CC	187	ALA	3.6
10	CJ	72	VAL	3.6
32	BI	136	VAL	3.6
35	DP	102	ARG	3.6
2	AB	196	LEU	3.6
31	DH	103	LEU	3.6
21	CU	17	THR	3.6
23	AY	24	G	3.6
19	CS	41	VAL	3.6
19	CS	51	VAL	3.6
30	DG	140	ILE	3.6
16	CP	48	TRP	3.6
31	DH	30	LYS	3.6
25	DA	2173	A	3.6
31	DH	41	MET	3.6
44	DY	91	GLU	3.6
1	AA	1001(A)	G	3.6
10	AJ	96	ILE	3.6
2	AB	125	PRO	3.6
10	CJ	15	THR	3.6
3	CC	129	ALA	3.6
4	AD	110	PHE	3.6
4	CD	157	LEU	3.6
14	CN	4	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
18	CR	66	LEU	3.6
18	AR	25	THR	3.5
13	CM	76	ALA	3.5
43	DX	91	ALA	3.5
31	DH	50	VAL	3.5
1	CA	202	U	3.5
25	DA	2139	C	3.5
25	DA	2140	C	3.5
13	CM	64	TRP	3.5
8	CH	94	TYR	3.5
9	CI	114	TYR	3.5
2	AB	70	PHE	3.5
45	DZ	1	MET	3.5
45	DZ	169	GLU	3.5
5	CE	114	GLY	3.5
8	CH	93	VAL	3.5
19	CS	69	HIS	3.5
20	AT	41	ILE	3.5
24	AX	47	U	3.5
31	DH	26	VAL	3.5
2	AB	215	LEU	3.5
2	CB	69	LEU	3.5
10	CJ	88	LEU	3.5
18	CR	85	LEU	3.5
38	DS	56	LEU	3.5
45	DZ	125	LEU	3.5
25	BA	2163	G	3.5
25	BA	2176	G	3.5
35	DP	79	ARG	3.5
36	DQ	63	LYS	3.5
3	CC	204	LEU	3.5
19	CS	30	LEU	3.5
20	AT	84	LEU	3.5
24	AX	67	C	3.5
30	DG	3	LEU	3.5
31	DH	27	LYS	3.5
28	DE	71	GLY	3.5
23	CW	47	U	3.5
3	CC	179	ARG	3.5
53	D7	47	ARG	3.5
29	BF	15	SER	3.5
50	B4	54	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
20	AT	22	ARG	3.5
25	DA	2156	G	3.5
29	BF	17	ARG	3.5
35	DP	94	GLU	3.5
2	CB	201	ILE	3.5
19	AS	40	ILE	3.5
31	DH	37	VAL	3.5
45	DZ	5	LEU	3.5
43	DX	18	TYR	3.5
16	CP	19	ILE	3.5
31	DH	12	PRO	3.5
12	CL	28	LYS	3.5
45	BZ	102	LEU	3.5
20	CT	86	ARG	3.4
31	DH	69	ARG	3.4
50	D4	48	ARG	3.4
19	CS	79	THR	3.4
4	CD	158	ILE	3.4
10	CJ	59	SER	3.4
31	DH	89	ILE	3.4
45	DZ	153	SER	3.4
9	CI	86	VAL	3.4
41	DV	14	VAL	3.4
3	CC	170	GLN	3.4
25	DA	1039	G	3.4
9	CI	30	GLY	3.4
45	DZ	110	GLY	3.4
23	CW	4	C	3.4
25	BA	925	A	3.4
25	BA	939	C	3.4
1	CA	1446	U	3.4
2	CB	33	TYR	3.4
17	CQ	36	ILE	3.4
10	CJ	44	VAL	3.4
3	AC	196	LEU	3.4
3	CC	6	HIS	3.4
1	CA	1033	G	3.4
23	AW	70	G	3.4
25	DA	2123	G	3.4
14	CN	10	ALA	3.4
20	CT	44	ALA	3.4
25	DA	2164	C	3.4

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Mol	Chain	Res	Type	RSRZ
25	DA	2803	C	3.4
32	BI	65	ALA	3.4
33	DN	57	ALA	3.4
9	CI	18	PHE	3.4
31	DH	94	TYR	3.4
3	AC	39	ILE	3.4
45	BZ	100	VAL	3.4
43	DX	68	ARG	3.4
1	AA	1028	C	3.4
25	BA	2157	A	3.4
46	D0	4	LYS	3.4
2	CB	229	VAL	3.4
9	CI	14	VAL	3.4
16	AP	2	VAL	3.4
31	DH	19	VAL	3.4
13	CM	70	LEU	3.4
1	AA	93	G	3.4
25	DA	892	G	3.4
3	CC	41	GLY	3.4
14	AN	51	GLY	3.4
3	AC	201	TYR	3.4
2	CB	81	VAL	3.4
32	BI	103	ARG	3.4
45	BZ	165	VAL	3.4
3	CC	13	GLY	3.4
7	CG	81	GLY	3.4
9	CI	33	PHE	3.4
50	D4	42	PHE	3.4
1	AA	1030	C	3.4
38	DS	36	TYR	3.4
52	D6	50	ARG	3.4
4	CD	134	ASP	3.4
9	AI	17	VAL	3.3
13	CM	60	VAL	3.3
30	DG	145	THR	3.3
3	CC	189	ALA	3.3
9	CI	49	PRO	3.3
29	DF	131	GLY	3.3
2	CB	122	PHE	3.3
10	CJ	66	ARG	3.3
36	DQ	65	PHE	3.3
10	AJ	97	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
10	CJ	98	ILE	3.3
17	CQ	42	TYR	3.3
20	AT	63	ILE	3.3
1	CA	161	A	3.3
9	CI	79	LEU	3.3
17	CQ	74	LEU	3.3
45	DZ	161	VAL	3.3
4	CD	23	GLY	3.3
31	DH	93	GLY	3.3
36	DQ	59	ARG	3.3
45	DZ	130	PRO	3.3
3	CC	22	TRP	3.3
14	CN	58	LYS	3.3
19	CS	49	ILE	3.3
14	CN	44	LEU	3.3
30	DG	146	TYR	3.3
31	DH	33	LEU	3.3
9	AI	28	VAL	3.3
19	CS	67	VAL	3.3
44	DY	51	VAL	3.3
30	DG	2	PRO	3.3
31	DH	53	GLU	3.3
50	D4	51	ASP	3.3
20	CT	55	ILE	3.3
25	BA	2905	C	3.3
2	AB	73	THR	3.3
9	CI	57	GLY	3.3
10	CJ	87	THR	3.3
23	CY	64	A	3.3
10	CJ	39	PRO	3.3
10	AJ	47	PHE	3.3
13	CM	65	LYS	3.3
14	CN	31	ARG	3.3
30	DG	29	TRP	3.3
17	CQ	59	ILE	3.3
32	BI	68	LEU	3.3
7	AG	85	TYR	3.3
25	BA	2807	C	3.3
25	DA	894	C	3.3
50	B4	45	GLY	3.3
25	BA	2803	A	3.3
25	DA	2158	A	3.3

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Mol	Chain	Res	Type	RSRZ
25	DA	2801(A)	A	3.3
38	DS	83	LYS	3.3
1	CA	1024	G	3.3
25	DA	2115	G	3.3
25	DA	2157	G	3.3
2	AB	12	GLU	3.3
36	BQ	59	ARG	3.3
45	DZ	104	PHE	3.3
18	AR	79	LEU	3.3
20	CT	41	ILE	3.3
1	CA	1028	C	3.3
1	CA	1149	C	3.3
9	CI	75	ASP	3.3
16	AP	21	VAL	3.3
10	CJ	56	HIS	3.3
14	CN	14	PRO	3.3
45	DZ	62	PRO	3.3
7	CG	117	ALA	3.3
3	CC	44	GLU	3.3
6	AF	46	ARG	3.3
17	CQ	27	PHE	3.3
1	AA	78	G	3.3
23	CY	19	G	3.3
25	BA	927	G	3.3
3	CC	111	LEU	3.2
20	CT	53	LEU	3.2
50	D4	45	GLY	3.2
55	D9	12	ASP	3.2
45	BZ	166	SER	3.2
23	CY	61	C	3.2
30	DG	35	GLU	3.2
23	AY	23	A	3.2
8	CH	55	GLY	3.2
16	AP	78	GLY	3.2
1	CA	204	U	3.2
1	CA	998	G	3.2
45	DZ	124	ILE	3.2
9	CI	92	TYR	3.2
11	AK	42	TRP	3.2
19	CS	58	VAL	3.2
25	DA	1509	C	3.2
45	DZ	46	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
10	CJ	89	ASP	3.2
25	DA	2897	U	3.2
16	CP	79	VAL	3.2
29	DF	21	ALA	3.2
45	BZ	152	ALA	3.2
3	CC	159	GLY	3.2
1	CA	1447	A	3.2
25	DA	2126	A	3.2
2	AB	213	LEU	3.2
9	CI	71	SER	3.2
16	CP	74	LEU	3.2
3	CC	19	GLU	3.2
29	DF	127	GLU	3.2
2	AB	165	VAL	3.2
2	AB	229	VAL	3.2
13	CM	17	VAL	3.2
25	BA	2173	G	3.2
29	BF	23	ASP	3.2
50	D4	62	ARG	3.2
9	AI	113	LYS	3.2
20	AT	62	LEU	3.2
9	CI	108	VAL	3.2
20	AT	40	ALA	3.2
2	CB	31	TYR	3.2
35	DP	110	TYR	3.2
25	BA	2816	G	3.2
2	CB	48	MET	3.2
17	CQ	22	LEU	3.2
35	DP	147	LEU	3.2
8	AH	35	ILE	3.2
20	AT	23	ARG	3.2
4	CD	198	VAL	3.2
20	CT	49	ALA	3.2
27	DD	2	ALA	3.2
35	DP	101	VAL	3.2
38	DS	45	GLY	3.2
50	D4	53	GLU	3.2
10	CJ	13	HIS	3.2
23	AW	72	C	3.2
25	DA	2129	C	3.2
18	AR	29	PHE	3.2
14	CN	13	THR	3.1

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Mol	Chain	Res	Type	RSRZ
29	DF	115	ALA	3.1
31	DH	131	VAL	3.1
50	B4	50	VAL	3.1
2	AB	95	GLN	3.1
20	AT	45	GLN	3.1
36	DQ	113	GLN	3.1
8	CH	122	ARG	3.1
25	DA	889	C	3.1
25	DA	1043	C	3.1
25	DA	1042	G	3.1
2	AB	200	ILE	3.1
4	CD	5	ILE	3.1
2	AB	78	GLN	3.1
25	BA	937	A	3.1
29	DF	167	ALA	3.1
35	DP	140	ALA	3.1
17	CQ	5	VAL	3.1
3	CC	23	TYR	3.1
1	CA	1027	C	3.1
9	CI	50	LEU	3.1
10	AJ	8	LEU	3.1
3	AC	18	TRP	3.1
46	D0	76	GLY	3.1
1	AA	1002	G	3.1
13	AM	25	ILE	3.1
31	DH	9	ILE	3.1
3	CC	61	ALA	3.1
13	CM	120	LYS	3.1
14	CN	30	ALA	3.1
20	AT	95	ALA	3.1
20	CT	16	HIS	3.1
10	AJ	85	LEU	3.1
25	BA	940	C	3.1
13	CM	6	GLY	3.1
8	CH	95	VAL	3.1
10	AJ	24	VAL	3.1
25	BA	2805	G	3.1
38	DS	14	VAL	3.1
1	CA	1286	A	3.1
30	BG	80	PHE	3.1
19	CS	81	ARG	3.1
12	CL	61	THR	3.1

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Mol	Chain	Res	Type	RSRZ
3	CC	160	ALA	3.1
29	DF	113	ALA	3.1
32	DI	41	GLU	3.1
2	CB	152	PHE	3.1
9	AI	59	PHE	3.1
19	CS	59	PRO	3.1
20	AT	13	LEU	3.1
2	CB	47	THR	3.1
30	DG	161	THR	3.1
3	CC	8	ILE	3.1
3	CC	124	ILE	3.1
43	DX	89	ILE	3.1
2	CB	120	ALA	3.1
2	CB	216	SER	3.1
17	CQ	19	VAL	3.1
52	D6	52	VAL	3.1
3	CC	80	GLY	3.1
21	AU	2	GLY	3.1
44	DY	58	GLY	3.1
7	CG	85	TYR	3.0
38	DS	80	LEU	3.0
10	CJ	55	LYS	3.0
2	AB	117	GLU	3.0
10	AJ	20	ALA	3.0
13	CM	42	ALA	3.0
31	DH	23	ARG	3.0
17	CQ	21	VAL	3.0
4	CD	19	LEU	3.0
23	CY	21	A	3.0
23	CY	35	A	3.0
43	DX	69	TYR	3.0
10	AJ	50	ILE	3.0
19	CS	31	ILE	3.0
31	DH	80	SER	3.0
2	AB	50	GLU	3.0
23	CY	22	G	3.0
3	CC	53	ALA	3.0
11	AK	60	ALA	3.0
10	AJ	73	ASP	3.0
14	CN	52	GLN	3.0
10	CJ	68	HIS	3.0
45	DZ	98	MET	3.0

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Mol	Chain	Res	Type	RSRZ
9	CI	37	PHE	3.0
12	CL	60	LEU	3.0
43	DX	95	LEU	3.0
13	CM	23	TYR	3.0
23	CW	73	A	3.0
50	D4	32	TYR	3.0
2	CB	218	ALA	3.0
2	CB	222	ILE	3.0
3	CC	71	ALA	3.0
3	CC	194	GLY	3.0
13	CM	78	ILE	3.0
17	CQ	65	ILE	3.0
1	AA	91	C	3.0
1	AA	1033	G	3.0
1	CA	1031	G	3.0
25	BA	696	C	3.0
9	CI	54	ASP	3.0
5	AE	51	VAL	3.0
14	CN	23	ARG	3.0
31	DH	113	VAL	3.0
44	DY	3	VAL	3.0
52	D6	5	VAL	3.0
2	CB	8	LYS	3.0
3	CC	142	MET	3.0
46	D0	45	PHE	3.0
38	DS	60	GLY	3.0
50	D4	63	TYR	3.0
1	CA	1004	A	3.0
2	AB	207	ALA	3.0
11	AK	89	ALA	3.0
23	CW	76	A	3.0
2	AB	15	VAL	3.0
3	CC	63	ASN	3.0
20	AT	9	ASN	3.0
50	B4	56	VAL	3.0
55	D9	16	VAL	3.0
2	CB	215	LEU	3.0
48	D2	44	LEU	3.0
7	CG	32	ARG	3.0
2	AB	182	ILE	3.0
45	BZ	159	PRO	3.0
23	CY	65	G	2.9

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Mol	Chain	Res	Type	RSRZ
25	BA	2178	G	2.9
25	DA	614(B)	G	2.9
17	CQ	6	LEU	2.9
20	AT	80	ARG	2.9
50	B4	49	PHE	2.9
31	DH	57	ASP	2.9
12	CL	69	TYR	2.9
41	DV	29	PRO	2.9
14	CN	29	ARG	2.9
20	AT	42	GLN	2.9
27	BD	275	LYS	2.9
36	DQ	6	ARG	2.9
50	B4	55	ARG	2.9
2	CB	115	LEU	2.9
2	CB	55	PHE	2.9
16	CP	9	PHE	2.9
20	AT	69	GLY	2.9
31	DH	166	GLY	2.9
44	DY	25	GLY	2.9
2	CB	220	ASP	2.9
2	CB	94	ASN	2.9
9	CI	5	TYR	2.9
50	D4	67	TYR	2.9
55	D9	17	ILE	2.9
9	CI	42	ARG	2.9
5	AE	69	VAL	2.9
8	AH	39	LEU	2.9
20	AT	91	LEU	2.9
41	DV	62	LEU	2.9
48	D2	1	MET	2.9
49	D3	23	LEU	2.9
10	CJ	48	THR	2.9
25	DA	2132	U	2.9
1	AA	79	G	2.9
10	CJ	20	ALA	2.9
13	CM	12	ASN	2.9
29	DF	198	ALA	2.9
30	DG	163	ALA	2.9
45	DZ	21	ALA	2.9
31	DH	164	TYR	2.9
32	BI	111	PRO	2.9
31	DH	86	GLU	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	CC	36	ASP	2.9
10	AJ	10	GLY	2.9
29	DF	174	VAL	2.9
31	DH	115	VAL	2.9
32	BI	75	LEU	2.9
45	DZ	91	LEU	2.9
9	CI	13	ALA	2.9
1	AA	144	G	2.9
2	CB	214	ILE	2.9
10	AJ	98	ILE	2.9
30	BG	139	LEU	2.9
32	BI	117	GLU	2.9
35	DP	96	THR	2.9
13	CM	18	ALA	2.9
44	DY	44	ILE	2.9
11	AK	25	TYR	2.9
30	DG	152	LEU	2.9
41	DV	5	VAL	2.9
25	BA	2906	U	2.9
38	DS	84	GLN	2.9
19	CS	50	ALA	2.9
3	AC	148	GLY	2.9
9	AI	8	GLY	2.9
10	AJ	36	GLY	2.9
50	D4	19	GLY	2.9
3	AC	206	GLU	2.8
3	CC	190	ARG	2.8
1	CA	1003	G	2.8
20	AT	24	LEU	2.8
23	CY	18	G	2.8
55	D9	25	VAL	2.8
19	CS	47	HIS	2.8
23	CY	23	A	2.8
45	DZ	164	ALA	2.8
9	CI	110	GLU	2.8
20	CT	98	PRO	2.8
29	DF	14	PRO	2.8
50	D4	57	GLU	2.8
36	DQ	5	ARG	2.8
12	CL	62	SER	2.8
31	DH	38	SER	2.8
30	DG	60	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
3	CC	183	ASP	2.8
5	CE	6	PHE	2.8
45	BZ	148	ASP	2.8
2	AB	231	GLU	2.8
5	CE	8	GLU	2.8
10	AJ	9	ARG	2.8
13	AM	26	GLY	2.8
23	CW	3	C	2.8
25	BA	945	A	2.8
25	DA	6	A	2.8
5	CE	13	ILE	2.8
10	CJ	78	ASN	2.8
19	CS	35	SER	2.8
31	BH	2	SER	2.8
9	AI	117	HIS	2.8
20	AT	20	LEU	2.8
20	CT	24	LEU	2.8
31	DH	99	VAL	2.8
36	DQ	27	VAL	2.8
36	DQ	104	PHE	2.8
4	AD	16	GLY	2.8
3	AC	60	ALA	2.8
22	CV	24	A	2.8
25	DA	898	C	2.8
2	CB	223	ILE	2.8
3	CC	35	GLU	2.8
31	DH	81	GLU	2.8
3	AC	12	LEU	2.8
16	CP	73	LEU	2.8
36	DQ	32	TYR	2.8
46	D0	7	LEU	2.8
31	DH	144	VAL	2.8
44	BY	1	MET	2.8
14	CN	54	PRO	2.8
20	AT	59	ALA	2.8
20	AT	76	ALA	2.8
3	CC	20	SER	2.8
20	AT	61	SER	2.8
25	BA	218	A	2.8
17	CQ	60	ILE	2.8
45	BZ	123	ASP	2.8
13	CM	13	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
28	BE	195	LEU	2.8
44	DY	47	LYS	2.8
52	D6	11	LEU	2.8
2	CB	164	VAL	2.8
17	CQ	77	VAL	2.8
19	CS	9	VAL	2.8
9	AI	93	ARG	2.8
1	AA	146	G	2.8
25	DA	881	G	2.8
25	DA	895	U	2.8
20	CT	43	LEU	2.8
9	CI	6	GLY	2.8
31	DH	157	TYR	2.8
45	BZ	160	GLY	2.8
2	CB	136	VAL	2.8
4	CD	161	ASN	2.8
16	AP	66	PRO	2.8
17	CQ	30	PRO	2.8
31	DH	21	PRO	2.8
2	CB	161	ALA	2.8
1	CA	91	C	2.7
5	CE	109	ILE	2.7
10	AJ	75	ILE	2.7
1	AA	1035	A	2.7
2	CB	121	LEU	2.7
3	CC	51	GLY	2.7
12	CL	93	LEU	2.7
41	DV	101	GLY	2.7
47	B1	98	LEU	2.7
50	B4	4	GLY	2.7
4	CD	168	ARG	2.7
14	CN	12	ARG	2.7
14	CN	56	VAL	2.7
44	DY	42	VAL	2.7
54	D8	29	LYS	2.7
3	AC	100	ALA	2.7
3	CC	154	SER	2.7
11	AK	68	ALA	2.7
14	CN	40	CYS	2.7
45	DZ	137	ILE	2.7
3	AC	205	GLY	2.7
5	CE	59	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
23	CY	56	C	2.7
25	DA	1041	C	2.7
30	BG	51	ARG	2.7
50	D4	68	ARG	2.7
25	DA	2162	G	2.7
32	BI	86	THR	2.7
9	CI	105	ASP	2.7
9	AI	55	ALA	2.7
9	CI	82	ALA	2.7
20	CT	40	ALA	2.7
19	CS	28	LYS	2.7
3	CC	88	ARG	2.7
10	CJ	29	ARG	2.7
1	AA	150	C	2.7
10	CJ	65	LEU	2.7
14	CN	6	LEU	2.7
1	AA	161	A	2.7
1	AA	1503	A	2.7
19	CS	48	THR	2.7
25	BA	1878	A	2.7
2	AB	19	HIS	2.7
2	AB	230	VAL	2.7
17	CQ	28	PRO	2.7
1	AA	1023	G	2.7
9	CI	63	ILE	2.7
29	BF	9	ILE	2.7
19	CS	15	LEU	2.7
1	AA	76	C	2.7
20	CT	45	GLN	2.7
25	DA	2137	C	2.7
29	DF	171	PRO	2.7
3	CC	138	VAL	2.7
10	AJ	35	SER	2.7
20	AT	70	SER	2.7
55	D9	20	HIS	2.7
33	DN	46	VAL	2.7
16	CP	58	TYR	2.7
20	AT	79	ARG	2.7
1	AA	1032	G	2.7
3	CC	81	GLY	2.7
25	BA	2152	U	2.7
25	DA	2147	G	2.7

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Mol	Chain	Res	Type	RSRZ
29	DF	145	GLU	2.7
44	DY	80	GLY	2.7
13	CM	39	ILE	2.7
41	DV	94	LEU	2.7
46	B0	7	LEU	2.7
21	CU	24	ARG	2.7
29	DF	172	TRP	2.7
50	D4	66	SER	2.7
8	CH	129	VAL	2.7
14	AN	16	PHE	2.7
53	B7	46	VAL	2.7
4	AD	138	TYR	2.7
1	AA	203	U	2.7
1	CA	1150	U	2.7
25	BA	1220	U	2.7
25	DA	1113	U	2.7
20	CT	30	LYS	2.7
23	AY	22	G	2.7
9	CI	77	ILE	2.7
13	CM	84	ILE	2.7
32	BI	109	ILE	2.7
2	AB	138	LEU	2.7
45	DZ	150	LEU	2.7
9	CI	21	PRO	2.7
12	CL	25	PRO	2.7
4	AD	88	VAL	2.7
10	AJ	63	PHE	2.7
14	AN	33	VAL	2.7
30	DG	169	ALA	2.7
30	DG	178	PHE	2.7
31	DH	96	ALA	2.7
45	DZ	126	VAL	2.7
1	AA	1034	G	2.6
2	AB	221	LEU	2.6
9	AI	56	LEU	2.6
10	CJ	40	LEU	2.6
50	D4	40	HIS	2.6
13	CM	53	VAL	2.6
14	CN	16	PHE	2.6
41	DV	42	GLY	2.6
41	DV	63	GLY	2.6
20	AT	18	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
31	DH	133	VAL	2.6
49	D3	47	VAL	2.6
23	AW	45	U	2.6
9	CI	125	TYR	2.6
31	DH	40	GLU	2.6
38	DS	3	ARG	2.6
45	DZ	60	GLU	2.6
2	CB	39	ILE	2.6
31	DH	148	ILE	2.6
55	B9	26	ILE	2.6
2	AB	233	SER	2.6
2	AB	234	PRO	2.6
13	CM	121	LYS	2.6
29	BF	13	SER	2.6
10	CJ	92	THR	2.6
23	CY	5	G	2.6
36	DQ	1	MET	2.6
3	AC	71	ALA	2.6
3	CC	149	ALA	2.6
7	CG	40	ALA	2.6
8	AH	93	VAL	2.6
17	CQ	73	VAL	2.6
20	CT	77	ALA	2.6
31	DH	169	VAL	2.6
35	DP	141	ALA	2.6
38	DS	66	ALA	2.6
41	DV	47	VAL	2.6
47	B1	93	GLU	2.6
20	CT	8	ARG	2.6
9	AI	4	TYR	2.6
2	CB	139	LYS	2.6
2	AB	211	ILE	2.6
2	CB	185	ILE	2.6
4	CD	94	LEU	2.6
43	BX	94	GLY	2.6
18	AR	42	ARG	2.6
31	DH	101	ARG	2.6
25	DA	1114	G	2.6
32	BI	98	ALA	2.6
38	DS	12	PHE	2.6
4	CD	140	VAL	2.6
2	AB	16	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
25	DA	2135	A	2.6
13	CM	9	ILE	2.6
31	DH	56	SER	2.6
41	DV	95	LEU	2.6
19	AS	68	GLY	2.6
13	CM	71	ARG	2.6
36	DQ	60	ARG	2.6
39	DT	1	MET	2.6
1	CA	1452	C	2.6
25	BA	2815	C	2.6
45	DZ	65	GLN	2.6
17	CQ	12	SER	2.6
2	CB	145	LEU	2.6
3	CC	178	LEU	2.6
13	CM	66	LEU	2.6
16	AP	59	TRP	2.6
20	CT	91	LEU	2.6
31	DH	54	ARG	2.6
35	DP	97	PRO	2.6
35	DP	76	LYS	2.6
38	DS	33	LYS	2.6
38	DS	35	ILE	2.6
47	D1	98	LEU	2.6
50	D4	22	ILE	2.6
50	D4	64	GLY	2.6
2	CB	70	PHE	2.6
5	CE	17	ALA	2.6
15	CO	15	PHE	2.6
29	DF	118	ALA	2.6
29	DF	161	GLU	2.6
3	CC	207	VAL	2.6
17	CQ	9	VAL	2.6
38	DS	34	HIS	2.6
1	CA	1116	C	2.6
8	AH	122	ARG	2.6
45	DZ	49	ARG	2.6
1	AA	73	G	2.6
17	CQ	33	GLY	2.6
25	DA	2166	G	2.6
17	CQ	47	PRO	2.6
41	DV	35	LEU	2.6
2	CB	200	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	CA	1005	A	2.6
9	CI	7	THR	2.6
45	DZ	119	GLU	2.6
1	AA	1025	U	2.6
3	AC	169	ALA	2.6
13	AM	2	ALA	2.6
20	CT	42	GLN	2.6
46	D0	57	PHE	2.6
31	DH	85	LYS	2.5
44	DY	34	LYS	2.5
1	AA	217	C	2.5
1	AA	840	C	2.5
3	CC	155	GLY	2.5
31	DH	28	GLY	2.5
35	DP	93	GLY	2.5
45	DZ	92	SER	2.5
35	DP	122	PRO	2.5
3	AC	204	LEU	2.5
36	BQ	41	TRP	2.5
14	CN	57	ARG	2.5
30	DG	110	ALA	2.5
50	D4	13	ARG	2.5
2	AB	122	PHE	2.5
10	CJ	11	PHE	2.5
30	DG	109	VAL	2.5
38	DS	46	VAL	2.5
2	CB	124	SER	2.5
10	CJ	31	GLY	2.5
19	CS	84	GLY	2.5
31	DH	78	GLY	2.5
42	BW	112	GLY	2.5
31	DH	126	PRO	2.5
2	AB	149	LEU	2.5
3	CC	196	LEU	2.5
17	CQ	84	LEU	2.5
32	DI	68	LEU	2.5
35	DP	100	LEU	2.5
44	DY	90	LEU	2.5
49	D3	26	LEU	2.5
2	AB	133	LYS	2.5
3	CC	40	ARG	2.5
1	CA	220	G	2.5

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Mol	Chain	Res	Type	RSRZ
25	BA	2179	G	2.5
2	CB	97	TRP	2.5
14	AN	61	TRP	2.5
3	CC	128	PHE	2.5
4	CD	34	GLU	2.5
35	DP	144	GLU	2.5
5	CE	90	VAL	2.5
29	BF	11	VAL	2.5
30	DG	38	VAL	2.5
46	B0	6	GLY	2.5
10	CJ	41	PRO	2.5
33	DN	44	PRO	2.5
30	BG	43	LEU	2.5
30	DG	133	LEU	2.5
13	CM	69	GLU	2.5
45	DZ	54	HIS	2.5
1	CA	79	G	2.5
25	DA	2165	G	2.5
9	AI	33	PHE	2.5
16	AP	80	PHE	2.5
25	DA	2169	A	2.5
9	CI	78	LYS	2.5
14	CN	11	LYS	2.5
40	DU	66	ASN	2.5
3	CC	21	ARG	2.5
9	AI	98	PRO	2.5
14	AN	12	ARG	2.5
17	CQ	75	ARG	2.5
20	CT	23	ARG	2.5
30	DG	142	PRO	2.5
44	DY	50	ARG	2.5
2	CB	44	LEU	2.5
10	AJ	16	LEU	2.5
3	AC	193	TYR	2.5
7	AG	20	ASP	2.5
16	AP	22	THR	2.5
30	DG	114	ILE	2.5
44	DY	35	TYR	2.5
50	D4	15	ILE	2.5
5	AE	132	ALA	2.5
5	CE	146	ALA	2.5
7	AG	127	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
19	CS	24	ALA	2.5
4	CD	47	ARG	2.5
14	CN	19	ARG	2.5
17	CQ	11	VAL	2.5
2	CB	231	GLU	2.5
40	DU	89	GLU	2.5
45	DZ	68	PRO	2.5
8	AH	112	LEU	2.5
45	BZ	70	LEU	2.5
5	CE	131	ILE	2.5
20	AT	71	THR	2.5
20	AT	77	ALA	2.5
31	DH	124	GLU	2.5
1	AA	1286	A	2.5
45	BZ	140	ASP	2.5
28	DE	52	LEU	2.5
31	DH	88	LEU	2.5
45	DZ	70	LEU	2.5
49	D3	53	LEU	2.5
14	CN	22	THR	2.5
4	AD	70	ILE	2.5
4	CD	146	ILE	2.5
10	AJ	5	ARG	2.5
21	AU	13	ILE	2.5
47	D1	58	ILE	2.5
35	DP	118	GLY	2.5
31	DH	165	ALA	2.5
44	DY	48	ALA	2.5
38	DS	76	LYS	2.4
2	AB	197	VAL	2.4
3	CC	120	VAL	2.4
30	DG	149	VAL	2.4
23	CY	14	A	2.4
17	CQ	98	LEU	2.4
14	CN	46	GLU	2.4
20	AT	86	ARG	2.4
25	DA	652(U)	G	2.4
30	DG	137	GLU	2.4
15	AO	87	ILE	2.4
55	D9	29	ASN	2.4
16	AP	1	MET	2.4
43	DX	14	SER	2.4

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Mol	Chain	Res	Type	RSRZ
55	D9	13	LYS	2.4
9	CI	53	VAL	2.4
40	DU	117	GLN	2.4
45	DZ	122	ARG	2.4
46	D0	77	ARG	2.4
3	AC	47	LEU	2.4
13	CM	19	LEU	2.4
20	CT	13	LEU	2.4
29	DF	20	LEU	2.4
3	CC	185	GLY	2.4
8	CH	131	GLY	2.4
29	DF	199	TRP	2.4
1	CA	1026	G	2.4
20	CT	100	ILE	2.4
2	CB	101	MET	2.4
25	BA	2813	G	2.4
1	AA	92	C	2.4
1	AA	219	C	2.4
2	CB	188	ALA	2.4
12	CL	26	ALA	2.4
16	CP	29	ASP	2.4
2	AB	114	ARG	2.4
19	CS	10	PHE	2.4
33	DN	126	PRO	2.4
45	BZ	158	PRO	2.4
2	CB	71	VAL	2.4
38	DS	11	LYS	2.4
46	D0	5	LYS	2.4
4	CD	69	GLY	2.4
4	CD	78	LEU	2.4
12	AL	29	GLY	2.4
14	CN	24	CYS	2.4
20	CT	72	LEU	2.4
32	BI	106	GLY	2.4
35	DP	123	LEU	2.4
1	AA	171	A	2.4
13	CM	63	THR	2.4
2	CB	35	GLU	2.4
11	AK	36	ASP	2.4
9	AI	88	TYR	2.4
25	BA	2177	G	2.4
25	DA	645	C	2.4

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Mol	Chain	Res	Type	RSRZ
3	CC	174	PRO	2.4
14	CN	50	LYS	2.4
9	CI	24	GLY	2.4
10	AJ	34	VAL	2.4
32	BI	74	ASN	2.4
38	DS	109	GLY	2.4
2	CB	24	TRP	2.4
10	AJ	21	GLN	2.4
36	BQ	141	GLN	2.4
38	BS	77	ALA	2.4
46	B0	5	LYS	2.4
20	AT	16	HIS	2.4
45	DZ	158	PRO	2.4
1	AA	104	G	2.4
1	CA	97	G	2.4
29	DF	160	ASN	2.4
31	BH	174	GLY	2.4
31	DH	74	ASN	2.4
3	CC	32	LEU	2.4
11	CK	109	VAL	2.4
23	CY	66	U	2.4
20	AT	53	LEU	2.4
30	DG	92	VAL	2.4
32	BI	140	LEU	2.4
41	DV	22	VAL	2.4
13	CM	110	ARG	2.4
30	DG	51	ARG	2.4
30	DG	181	ARG	2.4
45	DZ	72	ARG	2.4
21	CU	14	TRP	2.4
9	AI	92	TYR	2.4
9	CI	88	TYR	2.4
19	CS	43	GLU	2.4
31	BH	21	PRO	2.4
25	DA	2804	C	2.4
8	AH	84	ARG	2.4
8	AH	127	LEU	2.4
9	CI	65	VAL	2.4
17	CQ	25	ARG	2.4
25	BA	2182	G	2.4
31	DH	132	ARG	2.4
14	CN	47	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
30	DG	173	LEU	2.4
32	DI	38	LEU	2.4
13	CM	20	THR	2.4
38	DS	52	SER	2.4
19	CS	27	GLU	2.4
43	DX	93	GLU	2.4
9	AI	52	ALA	2.4
13	CM	41	PRO	2.3
30	DG	17	PRO	2.3
2	CB	132	LYS	2.3
4	CD	20	TYR	2.3
7	CG	26	PHE	2.3
10	AJ	11	PHE	2.3
17	CQ	100	LYS	2.3
20	CT	25	ARG	2.3
1	AA	201	C	2.3
1	CA	1020	U	2.3
25	DA	2174	C	2.3
7	AG	141	VAL	2.3
9	AI	40	LEU	2.3
9	CI	85	LEU	2.3
38	DS	54	LEU	2.3
45	DZ	56	VAL	2.3
25	BA	2184	G	2.3
25	DA	2116	G	2.3
4	CD	33	MET	2.3
20	CT	12	ALA	2.3
7	CG	6	ARG	2.3
45	DZ	162	GLU	2.3
9	CI	102	LEU	2.3
18	CR	58	LEU	2.3
21	CU	8	THR	2.3
1	CA	1023	G	2.3
7	AG	32	ARG	2.3
23	AW	69	G	2.3
23	CY	57	G	2.3
19	CS	26	GLY	2.3
50	D4	31	ILE	2.3
10	CJ	33	GLN	2.3
3	CC	89	GLU	2.3
13	CM	16	ASP	2.3
30	DG	48	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
23	AY	20	U	2.3
15	AO	78	TYR	2.3
16	AP	48	TRP	2.3
25	BA	2195	A	2.3
20	AT	38	LYS	2.3
33	DN	116	LEU	2.3
45	BZ	52	SER	2.3
17	CQ	56	VAL	2.3
3	CC	59	ARG	2.3
7	AG	153	HIS	2.3
13	CM	93	ARG	2.3
31	DH	122	THR	2.3
3	CC	107	GLN	2.3
27	DD	238	GLY	2.3
29	BF	131	GLY	2.3
2	CB	29	ALA	2.3
5	CE	81	GLU	2.3
8	CH	136	GLU	2.3
13	CM	72	ALA	2.3
29	DF	177	ALA	2.3
1	CA	4	U	2.3
31	DH	77	LYS	2.3
2	CB	155	LEU	2.3
3	AC	21	ARG	2.3
3	CC	43	LEU	2.3
4	CD	115	ARG	2.3
7	AG	16	LEU	2.3
8	AH	10	LEU	2.3
20	CT	22	ARG	2.3
22	CV	12	A	2.3
25	DA	890	A	2.3
29	DF	7	TYR	2.3
30	BG	181	ARG	2.3
4	CD	56	VAL	2.3
23	CY	13	C	2.3
29	BF	89	VAL	2.3
32	DI	107	VAL	2.3
45	DZ	55	HIS	2.3
50	D4	10	VAL	2.3
2	AB	134	GLU	2.3
3	CC	105	GLU	2.3
8	AH	117	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
3	AC	189	ALA	2.3
8	CH	86	ILE	2.3
10	CJ	38	ILE	2.3
14	CN	15	LYS	2.3
1	AA	170	U	2.3
1	CA	1202	G	2.3
7	AG	78	ARG	2.3
20	AT	8	ARG	2.3
23	CY	6	G	2.3
25	DA	880	G	2.3
45	BZ	122	ARG	2.3
2	AB	121	LEU	2.3
32	DI	72	LEU	2.3
45	DZ	2	GLU	2.3
48	B2	5	GLU	2.3
2	CB	19	HIS	2.3
20	CT	18	GLN	2.3
2	CB	219	VAL	2.3
12	AL	55	VAL	2.3
14	AN	18	VAL	2.3
29	DF	189	THR	2.3
49	D3	59	VAL	2.3
1	AA	100	C	2.3
44	DY	82	PRO	2.3
2	CB	41	ILE	2.3
3	CC	14	ILE	2.3
19	CS	75	ALA	2.3
29	BF	206	ILE	2.3
20	CT	57	ARG	2.3
38	DS	97	ARG	2.3
9	AI	126	SER	2.3
20	CT	31	SER	2.3
38	DS	31	SER	2.3
2	AB	180	LEU	2.3
9	AI	70	LYS	2.3
23	CW	19	G	2.3
25	DA	2805	G	2.3
45	DZ	102	LEU	2.3
8	CH	120	THR	2.3
30	DG	85	GLY	2.3
10	AJ	44	VAL	2.3
19	CS	60	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
23	CY	58	A	2.3
25	BA	1092	A	2.3
31	DH	125	VAL	2.3
32	BI	19	VAL	2.3
1	CA	218	C	2.3
2	CB	131	PRO	2.3
20	AT	83	ARG	2.3
35	DP	15	ARG	2.3
5	AE	95	ALA	2.2
11	AK	48	ILE	2.2
16	CP	36	ILE	2.2
38	DS	37	ALA	2.2
41	DV	1	MET	2.2
49	D3	60	GLU	2.2
9	AI	31	GLN	2.2
20	CT	38	LYS	2.2
2	CB	227	GLY	2.2
4	AD	21	LEU	2.2
16	AP	73	LEU	2.2
36	DQ	61	GLY	2.2
2	CB	67	THR	2.2
11	CK	84	VAL	2.2
21	AU	18	TYR	2.2
21	CU	21	TYR	2.2
28	BE	175	VAL	2.2
38	DS	65	VAL	2.2
42	DW	30	GLU	2.2
45	DZ	20	ARG	2.2
50	D4	55	ARG	2.2
5	AE	96	PRO	2.2
21	CU	23	PRO	2.2
1	CA	217	C	2.2
1	CA	1037	C	2.2
20	CT	76	ALA	2.2
40	DU	116	ALA	2.2
9	CI	74	ILE	2.2
2	AB	193	ASP	2.2
46	B0	3	HIS	2.2
2	CB	72	GLY	2.2
5	CE	22	GLY	2.2
3	CC	33	LEU	2.2
12	CL	27	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
14	CN	8	GLU	2.2
30	DG	111	LEU	2.2
45	BZ	117	LEU	2.2
3	CC	55	VAL	2.2
17	CQ	51	TYR	2.2
27	BD	221	VAL	2.2
50	D4	56	VAL	2.2
51	B5	60	VAL	2.2
1	CA	630	G	2.2
25	DA	1170	G	2.2
22	AV	15	A	2.2
25	BA	2812	A	2.2
25	DA	899	A	2.2
50	D4	46	GLN	2.2
1	AA	1452	C	2.2
3	CC	180	ALA	2.2
11	AK	15	ALA	2.2
19	CS	62	ILE	2.2
21	CU	13	ILE	2.2
45	BZ	168	GLU	2.2
4	CD	110	PHE	2.2
19	CS	82	GLY	2.2
31	DH	3	ARG	2.2
30	DG	67	LYS	2.2
35	DP	124	LYS	2.2
10	CJ	34	VAL	2.2
10	AJ	18	ALA	2.2
1	AA	77	G	2.2
1	AA	143	A	2.2
1	CA	156	G	2.2
1	CA	162	A	2.2
1	CA	999	C	2.2
1	CA	1006	C	2.2
5	AE	136	MET	2.2
6	CF	100	ASN	2.2
25	BA	2150	C	2.2
25	BA	2161	C	2.2
25	DA	652(V)	C	2.2
25	DA	1112	G	2.2
25	DA	2131	G	2.2
30	DG	148	MET	2.2
44	BY	91	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
3	AC	126	ARG	2.2
8	AH	111	ILE	2.2
30	BG	88	ILE	2.2
45	DZ	52	SER	2.2
4	CD	167	GLY	2.2
9	AI	67	GLY	2.2
30	BG	42	GLY	2.2
3	AC	128	PHE	2.2
12	CL	32	PHE	2.2
5	CE	110	LEU	2.2
17	CQ	31	LEU	2.2
30	BG	82	LEU	2.2
32	DI	140	LEU	2.2
3	AC	19	GLU	2.2
13	CM	97	PRO	2.2
16	CP	20	VAL	2.2
16	CP	62	VAL	2.2
29	DF	200	GLU	2.2
23	CY	45	U	2.2
25	BA	924	U	2.2
25	DA	2113	U	2.2
31	DH	83	TYR	2.2
33	BN	9	VAL	2.2
41	DV	46	VAL	2.2
3	CC	62	ASP	2.2
50	D4	25	TYR	2.2
3	CC	4	LYS	2.2
8	AH	18	ARG	2.2
9	CI	20	ARG	2.2
10	CJ	79	ARG	2.2
13	CM	80	ARG	2.2
14	CN	43	CYS	2.2
27	DD	38	LYS	2.2
32	BI	57	ARG	2.2
8	CH	83	ILE	2.2
1	CA	1041	A	2.2
25	DA	2176	A	2.2
47	D1	28	GLY	2.2
45	DZ	136	PHE	2.2
10	AJ	95	GLU	2.2
44	DY	31	LEU	2.2
4	CD	122	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
19	CS	36	ARG	2.2
3	AC	64	VAL	2.2
28	DE	104	VAL	2.2
30	BG	49	ASP	2.2
3	CC	24	ALA	2.2
3	AC	14	ILE	2.2
8	AH	38	ILE	2.2
8	CH	45	ILE	2.2
10	AJ	38	ILE	2.2
36	DQ	66	ILE	2.2
2	CB	12	GLU	2.2
3	CC	206	GLU	2.2
25	BA	2130	C	2.2
31	DH	167	GLU	2.2
44	DY	89	PHE	2.2
1	AA	145	G	2.2
1	CA	1154	G	2.2
4	CD	86	LYS	2.2
25	DA	2148	G	2.2
44	DY	88	LYS	2.2
45	DZ	67	LEU	2.2
47	D1	26	ARG	2.2
10	AJ	41	PRO	2.2
17	AQ	28	PRO	2.2
44	DY	107	ASP	2.2
46	D0	64	ASP	2.2
10	CJ	62	HIS	2.1
49	D3	6	VAL	2.1
2	AB	31	TYR	2.1
2	CB	203	GLY	2.1
29	BF	166	ALA	2.1
30	DG	73	ALA	2.1
35	BP	12	ALA	2.1
38	DS	104	GLY	2.1
45	BZ	51	ALA	2.1
2	AB	126	GLU	2.1
5	CE	10	MET	2.1
20	AT	85	MET	2.1
5	AE	89	ILE	2.1
10	CJ	96	ILE	2.1
16	AP	19	ILE	2.1
45	BZ	124	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
20	CT	29	LYS	2.1
50	D4	38	LYS	2.1
1	AA	1029	C	2.1
1	CA	470	C	2.1
1	CA	1007	C	2.1
1	CA	1029	C	2.1
10	CJ	46	ARG	2.1
14	CN	41	ARG	2.1
5	AE	53	LEU	2.1
8	CH	36	LEU	2.1
31	DH	137	ASP	2.1
35	DP	138	LEU	2.1
1	AA	347	G	2.1
2	AB	167	PRO	2.1
3	CC	167	TRP	2.1
8	CH	67	PRO	2.1
9	AI	64	THR	2.1
40	DU	2	PRO	2.1
43	DX	3	THR	2.1
54	D8	34	TRP	2.1
25	BA	2149	G	2.1
3	CC	58	GLU	2.1
4	CD	121	VAL	2.1
4	CD	148	VAL	2.1
7	CG	66	VAL	2.1
12	AL	43	VAL	2.1
30	DG	138	GLN	2.1
36	DQ	107	ALA	2.1
38	DS	50	SER	2.1
45	BZ	66	SER	2.1
2	CB	236	TYR	2.1
21	CU	18	TYR	2.1
54	D8	25	MET	2.1
3	CC	79	ARG	2.1
8	AH	80	ILE	2.1
8	CH	104	ARG	2.1
9	AI	16	ARG	2.1
14	AN	7	ILE	2.1
28	BE	77	ILE	2.1
31	DH	121	ILE	2.1
32	DI	71	ILE	2.1
5	AE	119	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
17	CQ	18	THR	2.1
19	AS	27	GLU	2.1
20	AT	98	PRO	2.1
20	CT	60	GLU	2.1
23	AW	21	A	2.1
23	AW	73	A	2.1
19	CS	54	GLY	2.1
20	CT	14	LYS	2.1
30	DG	78	SER	2.1
2	AB	81	VAL	2.1
13	AM	117	VAL	2.1
13	CM	75	ALA	2.1
29	DF	163	VAL	2.1
32	BI	142	VAL	2.1
7	AG	154	TYR	2.1
3	AC	182	ILE	2.1
7	AG	8	GLU	2.1
19	CS	12	ASP	2.1
36	DQ	47	ILE	2.1
38	DS	8	GLU	2.1
1	AA	218	C	2.1
1	CA	1043	C	2.1
20	AT	14	LYS	2.1
29	DF	140	LEU	2.1
41	DV	40	LEU	2.1
43	DX	13	LEU	2.1
45	DZ	48	PHE	2.1
25	DA	1040	C	2.1
25	DA	2143	C	2.1
38	DS	5	THR	2.1
1	AA	1005	A	2.1
9	CI	72	GLY	2.1
46	B0	8	GLY	2.1
10	CJ	35	SER	2.1
10	CJ	70	ARG	2.1
4	AD	198	VAL	2.1
4	CD	147	ALA	2.1
8	CH	53	VAL	2.1
29	DF	166	ALA	2.1
32	BI	53	ALA	2.1
41	DV	61	VAL	2.1
43	DX	49	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
25	BA	2174	G	2.1
35	DP	98	GLU	2.1
2	CB	58	ILE	2.1
8	AH	86	ILE	2.1
17	CQ	32	TYR	2.1
20	CT	48	LYS	2.1
31	DH	163	TYR	2.1
38	DS	82	ILE	2.1
52	D6	54	ILE	2.1
5	AE	151	LEU	2.1
9	AI	102	LEU	2.1
30	DG	117	PHE	2.1
31	DH	67	LEU	2.1
1	AA	153	C	2.1
7	CG	24	THR	2.1
10	AJ	70	ARG	2.1
10	AJ	92	THR	2.1
36	BQ	75	THR	2.1
47	D1	84	GLY	2.1
1	AA	1001	A	2.1
25	BA	2156	A	2.1
2	AB	97	TRP	2.1
4	AD	170	VAL	2.1
38	DS	105	ALA	2.1
33	DN	1	MET	2.1
1	AA	630	G	2.1
9	AI	77	ILE	2.1
16	AP	39	TYR	2.1
23	AW	5	G	2.1
25	DA	2168	G	2.1
32	BI	130	TYR	2.1
32	DI	79	ILE	2.1
17	CQ	63	ARG	2.1
19	CS	76	PRO	2.1
48	D2	32	LEU	2.1
2	CB	116	GLU	2.1
19	CS	64	GLU	2.1
1	CA	163	C	2.1
2	CB	233	SER	2.1
10	CJ	58	ASP	2.1
5	AE	48	ALA	2.1
11	CK	89	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
12	AL	26	ALA	2.1
25	DA	2134	A	2.1
2	CB	135	GLN	2.1
35	DP	125	VAL	2.1
45	DZ	100	VAL	2.1
50	B4	46	GLN	2.1
10	AJ	69	ASN	2.1
3	CC	85	ARG	2.1
14	AN	23	ARG	2.1
21	AU	10	ARG	2.1
3	CC	31	HIS	2.1
11	AK	50	TYR	2.1
20	CT	73	HIS	2.1
32	BI	41	GLU	2.1
1	AA	102	G	2.1
2	CB	26	PRO	2.1
4	CD	64	LEU	2.1
6	AF	60	PHE	2.1
13	CM	48	LEU	2.1
23	CW	10	G	2.1
30	BG	182	LYS	2.1
31	DH	39	PRO	2.1
32	BI	35	LEU	2.1
38	DS	29	PHE	2.1
9	AI	7	THR	2.1
9	CI	87	GLN	2.0
23	AY	56	C	2.0
3	AC	195	VAL	2.0
5	CE	105	VAL	2.0
50	D4	33	VAL	2.0
4	AD	85	LYS	2.0
7	CG	42	ILE	2.0
19	CS	57	HIS	2.0
28	BE	14	ILE	2.0
29	DF	16	GLY	2.0
38	DS	81	GLY	2.0
2	AB	148	TYR	2.0
1	AA	96	U	2.0
2	CB	57	PHE	2.0
2	CB	118	LEU	2.0
2	CB	154	LEU	2.0
4	CD	142	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
2	CB	163	PHE	2.0
16	AP	60	LEU	2.0
19	AS	16	LEU	2.0
20	AT	99	LEU	2.0
30	DG	62	LEU	2.0
12	CL	118	SER	2.0
1	CA	1032	G	2.0
23	AW	65	G	2.0
2	AB	137	ARG	2.0
3	AC	164	ARG	2.0
3	CC	54	ARG	2.0
8	CH	22	GLU	2.0
21	CU	9	ARG	2.0
33	DN	10	GLU	2.0
2	AB	171	ALA	2.0
53	D7	32	LYS	2.0
8	AH	26	VAL	2.0
10	AJ	94	VAL	2.0
12	CL	58	VAL	2.0
20	CT	88	VAL	2.0
30	DG	28	VAL	2.0
32	BI	107	VAL	2.0
43	DX	43	VAL	2.0
1	AA	1531	A	2.0
9	CI	115	GLY	2.0
25	DA	901	A	2.0
16	AP	4	ILE	2.0
43	DX	8	ILE	2.0
45	DZ	53	ILE	2.0
31	DH	154	PRO	2.0
52	D6	42	TRP	2.0
1	CA	1040	U	2.0
6	AF	61	LEU	2.0
8	CH	58	TYR	2.0
13	AM	109	THR	2.0
17	AQ	7	THR	2.0
25	DA	614(A)	U	2.0
31	DH	84	SER	2.0
4	CD	153	ARG	2.0
18	CR	87	ARG	2.0
19	CS	17	GLU	2.0
45	BZ	145	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
45	DZ	31	ARG	2.0
11	AK	117	ASN	2.0
12	CL	13	LYS	2.0
1	CA	216	G	2.0
1	AA	1007	C	2.0
9	AI	61	ALA	2.0
25	BA	2188	G	2.0
25	DA	1117	G	2.0
25	DA	2319	G	2.0
38	DS	6	ALA	2.0
2	CB	7	VAL	2.0
2	CB	93	VAL	2.0
8	CH	103	VAL	2.0
9	CI	58	HIS	2.0
7	CG	120	ILE	2.0
8	CH	4	ASP	2.0
10	CJ	50	ILE	2.0
11	AK	104	GLN	2.0
25	DA	2170	A	2.0
25	DA	2310	A	2.0
13	CM	50	GLU	2.0
38	DS	40	ILE	2.0
1	CA	1000	U	2.0
2	CB	10	LEU	2.0
11	AK	98	LEU	2.0
15	CO	56	LEU	2.0
17	CQ	92	ARG	2.0
25	BA	2172	U	2.0
31	DH	130	ARG	2.0
49	D3	28	LEU	2.0
54	D8	60	LEU	2.0
4	CD	207	TYR	2.0
8	AH	31	PHE	2.0
9	CI	59	PHE	2.0
10	AJ	7	LYS	2.0
16	AP	38	TYR	2.0
17	CQ	95	TYR	2.0
20	CT	68	LYS	2.0
38	DS	112	PHE	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
23	PSU	CY	55	20/21	0.83	0.29	-	92,98,105,119	0
23	MIA	AY	37	22/30	0.82	0.25	-	72,87,104,128	0
23	7MG	AW	46	24/25	0.83	0.22	-	70,83,111,120	0
24	5MC	AX	32	21/22	0.97	0.19	-	48,54,58,72	0
24	4SU	AX	8	20/21	0.96	0.18	-	51,64,80,88	0
23	5MU	CY	54	21/22	0.69	0.40	-	78,92,113,136	0
23	MIA	AW	37	29/30	0.96	0.21	-	40,49,63,75	0
24	PSU	AX	55	20/21	0.94	0.18	-	60,67,93,94	0
23	PSU	CY	32	20/21	0.79	0.20	-	83,92,99,105	0
23	7MG	CW	46	24/25	0.80	0.30	-	85,98,110,126	0
23	4SU	AY	8	20/21	0.82	0.20	-	92,98,108,126	0
23	PSU	AW	55	20/21	0.93	0.20	-	50,70,80,81	0
23	5MU	CW	54	21/22	0.90	0.17	-	60,72,84,86	0
23	4SU	CY	8	20/21	0.70	0.19	-	83,99,114,124	0
23	PSU	CY	39	20/21	0.87	0.19	-	80,88,99,111	0
24	5MC	CX	32	21/22	0.95	0.16	-	66,71,81,83	0
24	5MU	AX	54	21/22	0.94	0.18	-	58,65,74,81	0
23	PSU	CW	39	20/21	0.96	0.17	-	63,72,81,82	0
23	MIA	CW	37	22/30	0.91	0.16	-	55,66,75,81	0
23	7MG	AY	46	24/25	0.72	0.24	-	80,94,107,121	0
24	PSU	CX	55	20/21	0.90	0.16	-	63,69,89,97	0
23	PSU	AW	39	20/21	0.96	0.20	-	49,59,65,65	0
24	5MU	CX	54	21/22	0.92	0.23	-	71,80,88,94	0
23	4SU	AW	8	20/21	0.91	0.17	-	73,85,96,105	0
23	PSU	CW	32	20/21	0.90	0.19	-	70,85,92,95	0
23	PSU	AY	32	20/21	0.85	0.24	-	83,91,98,100	0
23	PSU	AY	39	20/21	0.90	0.21	-	77,86,97,100	0
23	PSU	CW	55	20/21	0.83	0.20	-	61,83,94,94	0
24	4SU	CX	8	20/21	0.93	0.17	-	54,78,85,86	0
23	5MU	AW	54	21/22	0.95	0.16	-	42,58,69,76	0
23	5MU	AY	54	21/22	0.81	0.23	-	81,91,102,125	0
23	4SU	CW	8	20/21	0.75	0.24	-	88,94,105,122	0
23	7MG	CY	46	24/25	0.77	0.18	-	86,95,102,125	0
23	PSU	AW	32	20/21	0.95	0.16	-	50,60,69,69	0
23	PSU	AY	55	20/21	0.69	0.28	-	93,99,105,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MIA	CY	37	22/30	0.68	0.33	-	82,93,117,140	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3831	1/1	0.81	0.95	41.81	52,52,52,52	0
56	MG	DA	3434	1/1	0.88	0.46	35.58	51,51,51,51	0
56	MG	DA	3182	1/1	0.63	0.30	28.23	64,64,64,64	0
56	MG	DA	3155	1/1	0.83	0.29	23.05	40,40,40,40	0
56	MG	BA	3105	1/1	0.94	0.45	22.30	69,69,69,69	0
56	MG	DA	3497	1/1	0.91	0.32	20.90	51,51,51,51	0
56	MG	BA	3829	1/1	0.94	0.33	20.63	45,45,45,45	0
56	MG	BA	3320	1/1	0.88	0.30	20.62	60,60,60,60	0
56	MG	DA	3095	1/1	0.93	0.27	18.91	47,47,47,47	0
56	MG	DA	3663	1/1	0.92	0.25	18.89	60,60,60,60	0
56	MG	BA	3469	1/1	0.94	0.31	18.10	37,37,37,37	0
56	MG	DA	3562	1/1	0.93	0.34	17.61	58,58,58,58	0
56	MG	BA	3585	1/1	0.80	0.39	16.80	55,55,55,55	0
56	MG	DA	3193	1/1	0.96	0.33	16.77	40,40,40,40	0
56	MG	DA	3138	1/1	0.92	0.41	15.62	59,59,59,59	0
56	MG	DA	3202	1/1	0.95	0.33	15.24	50,50,50,50	0
56	MG	DA	3446	1/1	0.97	0.32	15.23	47,47,47,47	0
56	MG	BP	201	1/1	0.96	0.39	15.03	41,41,41,41	0
56	MG	BA	3038	1/1	0.96	0.31	14.68	47,47,47,47	0
56	MG	BA	3393	1/1	0.83	0.26	14.65	54,54,54,54	0
56	MG	BA	3428	1/1	0.92	0.30	14.40	38,38,38,38	0
56	MG	BA	3762	1/1	0.91	0.38	14.33	40,40,40,40	0
56	MG	DA	3024	1/1	0.97	0.44	13.94	40,40,40,40	0
56	MG	BA	3103	1/1	0.96	0.33	13.85	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3415	1/1	0.91	0.24	13.70	50,50,50,50	0
56	MG	CA	3062	1/1	0.96	0.23	13.55	44,44,44,44	0
56	MG	DA	3157	1/1	0.89	0.28	13.40	44,44,44,44	0
56	MG	BA	3053	1/1	0.99	0.27	13.38	22,22,22,22	0
56	MG	DA	3607	1/1	0.68	0.34	13.18	53,53,53,53	0
56	MG	DA	3172	1/1	0.89	0.32	13.13	51,51,51,51	0
56	MG	DA	3324	1/1	0.87	0.29	12.96	39,39,39,39	0
56	MG	DA	3402	1/1	0.91	0.27	12.77	65,65,65,65	0
56	MG	AA	3229	1/1	0.98	0.35	12.67	62,62,62,62	0
56	MG	BA	3043	1/1	0.97	0.30	12.53	39,39,39,39	0
56	MG	BA	3484	1/1	0.92	0.29	12.41	36,36,36,36	0
56	MG	BA	3182	1/1	0.92	0.31	12.24	41,41,41,41	0
56	MG	DV	3002	1/1	0.84	0.43	11.89	57,57,57,57	0
56	MG	BA	3724	1/1	0.90	0.34	11.81	44,44,44,44	0
56	MG	BU	206	1/1	0.95	0.34	11.23	43,43,43,43	0
56	MG	DA	3522	1/1	0.96	0.29	11.14	25,25,25,25	0
56	MG	DW	3002	1/1	0.78	0.39	11.10	65,65,65,65	0
56	MG	AA	3209	1/1	0.92	0.30	10.82	51,51,51,51	0
56	MG	CA	3059	1/1	0.86	0.41	10.56	67,67,67,67	0
56	MG	BA	3607	1/1	0.97	0.26	10.08	40,40,40,40	0
56	MG	BA	3101	1/1	0.82	0.25	9.70	60,60,60,60	0
56	MG	DA	3400	1/1	0.95	0.34	9.61	39,39,39,39	0
56	MG	BA	3048	1/1	0.97	0.25	9.35	28,28,28,28	0
56	MG	DA	3103	1/1	0.85	0.22	9.32	50,50,50,50	0
56	MG	CA	3119	1/1	0.92	0.26	9.27	58,58,58,58	0
56	MG	BA	3264	1/1	0.88	0.29	9.26	39,39,39,39	0
56	MG	DA	3350	1/1	0.99	0.30	9.24	29,29,29,29	0
56	MG	DA	3299	1/1	0.96	0.24	9.23	43,43,43,43	0
56	MG	DA	3538	1/1	0.73	0.27	8.88	56,56,56,56	0
56	MG	DB	3005	1/1	0.65	0.28	8.84	64,64,64,64	0
56	MG	DA	3030	1/1	0.93	0.28	8.83	40,40,40,40	0
56	MG	DE	301	1/1	0.95	0.29	8.76	45,45,45,45	0
56	MG	AA	3087	1/1	0.81	0.34	8.64	52,52,52,52	0
56	MG	BA	3242	1/1	0.96	0.33	8.60	42,42,42,42	0
56	MG	DA	3112	1/1	0.98	0.26	8.41	42,42,42,42	0
56	MG	CA	3037	1/1	0.83	0.25	8.41	55,55,55,55	0
56	MG	BA	3024	1/1	0.97	0.27	8.38	22,22,22,22	0
56	MG	AA	3161	1/1	0.84	0.26	8.38	46,46,46,46	0
56	MG	DA	3146	1/1	0.93	0.27	8.34	46,46,46,46	0
56	MG	BA	3770	1/1	0.88	0.30	8.27	37,37,37,37	0
56	MG	BA	3318	1/1	0.95	0.27	8.26	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3430	1/1	0.93	0.33	8.04	32,32,32,32	0
56	MG	BD	306	1/1	0.91	0.36	8.03	22,22,22,22	0
56	MG	DA	3165	1/1	0.98	0.29	8.00	33,33,33,33	0
56	MG	BA	3811	1/1	0.97	0.31	7.92	38,38,38,38	0
56	MG	DA	3416	1/1	0.96	0.34	7.92	40,40,40,40	0
56	MG	CA	3111	1/1	0.88	0.21	7.78	61,61,61,61	0
56	MG	BA	3441	1/1	0.91	0.27	7.74	46,46,46,46	0
56	MG	DA	3401	1/1	0.92	0.29	7.73	36,36,36,36	0
56	MG	DA	3171	1/1	0.98	0.28	7.57	38,38,38,38	0
56	MG	DA	3674	1/1	0.84	0.41	7.46	73,73,73,73	0
56	MG	CA	3121	1/1	0.84	0.23	7.35	75,75,75,75	0
56	MG	DA	3534	1/1	0.90	0.26	7.29	74,74,74,74	0
56	MG	BA	3452	1/1	0.96	0.30	7.28	27,27,27,27	0
56	MG	CA	3039	1/1	0.98	0.23	7.12	50,50,50,50	0
56	MG	AA	3029	1/1	0.94	0.27	7.00	53,53,53,53	0
56	MG	DA	3669	1/1	0.94	0.22	6.91	49,49,49,49	0
56	MG	BA	3083	1/1	0.92	0.29	6.79	47,47,47,47	0
56	MG	BX	102	1/1	0.94	0.31	6.78	41,41,41,41	0
56	MG	BA	3044	1/1	0.97	0.25	6.68	49,49,49,49	0
56	MG	BN	3005	1/1	0.93	0.39	6.58	51,51,51,51	0
56	MG	BA	3325	1/1	0.96	0.28	6.54	56,56,56,56	0
56	MG	BA	3227	1/1	0.83	0.26	6.46	57,57,57,57	0
56	MG	BA	3568	1/1	0.91	0.25	6.46	52,52,52,52	0
56	MG	AK	202	1/1	0.95	0.26	6.44	38,38,38,38	0
56	MG	BA	3450	1/1	0.97	0.28	6.43	34,34,34,34	0
56	MG	BA	3282	1/1	0.98	0.30	6.36	24,24,24,24	0
56	MG	DA	3100	1/1	0.93	0.24	6.33	36,36,36,36	0
56	MG	DA	3267	1/1	0.95	0.26	6.31	38,38,38,38	0
56	MG	BA	3555	1/1	0.96	0.29	6.26	33,33,33,33	0
56	MG	BA	3039	1/1	0.99	0.28	6.24	47,47,47,47	0
56	MG	BA	3240	1/1	0.91	0.26	6.24	45,45,45,45	0
56	MG	DA	3003	1/1	0.97	0.26	6.22	20,20,20,20	0
56	MG	DA	3233	1/1	0.93	0.25	6.18	43,43,43,43	0
56	MG	BA	3133	1/1	0.87	0.30	6.16	47,47,47,47	0
56	MG	CA	3047	1/1	0.98	0.24	6.12	35,35,35,35	0
56	MG	BA	3022	1/1	0.81	0.26	6.10	40,40,40,40	0
56	MG	AA	3073	1/1	0.83	0.24	6.10	58,58,58,58	0
56	MG	BA	3245	1/1	0.96	0.28	6.04	29,29,29,29	0
56	MG	BA	3440	1/1	0.99	0.27	6.03	29,29,29,29	0
56	MG	AA	3218	1/1	0.93	0.25	5.96	53,53,53,53	0
56	MG	DA	3015	1/1	0.98	0.26	5.88	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3152	1/1	0.94	0.25	5.80	42,42,42,42	0
56	MG	DA	3310	1/1	0.90	0.22	5.75	55,55,55,55	0
56	MG	BA	3596	1/1	0.96	0.32	5.68	45,45,45,45	0
56	MG	DA	3148	1/1	0.95	0.23	5.66	29,29,29,29	0
56	MG	BA	3109	1/1	0.95	0.28	5.66	42,42,42,42	0
56	MG	DA	3122	1/1	0.92	0.22	5.60	36,36,36,36	0
56	MG	BA	3347	1/1	0.79	0.26	5.57	48,48,48,48	0
56	MG	BF	310	1/1	0.94	0.25	5.53	38,38,38,38	0
56	MG	AA	3104	1/1	0.96	0.20	5.51	50,50,50,50	0
56	MG	DD	304	1/1	0.98	0.39	5.50	31,31,31,31	0
56	MG	DA	3050	1/1	0.99	0.23	5.43	40,40,40,40	0
56	MG	BA	3272	1/1	1.00	0.28	5.38	11,11,11,11	0
56	MG	AA	3162	1/1	0.94	0.28	5.36	59,59,59,59	0
56	MG	BA	3041	1/1	0.98	0.25	5.35	18,18,18,18	0
56	MG	DA	3084	1/1	0.95	0.27	5.35	27,27,27,27	0
56	MG	BA	3126	1/1	0.95	0.25	5.34	43,43,43,43	0
56	MG	DA	3115	1/1	0.81	0.18	5.32	41,41,41,41	0
56	MG	BA	3013	1/1	0.97	0.28	5.19	34,34,34,34	0
56	MG	BA	3007	1/1	0.93	0.25	5.18	51,51,51,51	0
56	MG	DA	3468	1/1	0.81	0.20	5.18	44,44,44,44	0
56	MG	DA	3108	1/1	0.97	0.22	5.13	30,30,30,30	0
56	MG	BA	3534	1/1	0.96	0.30	5.11	31,31,31,31	0
56	MG	DA	3278	1/1	0.94	0.21	5.08	53,53,53,53	0
56	MG	DA	3158	1/1	0.98	0.26	5.07	40,40,40,40	0
56	MG	BA	3552	1/1	0.96	0.25	5.05	34,34,34,34	0
56	MG	AA	3009	1/1	0.95	0.26	5.03	46,46,46,46	0
56	MG	BA	3609	1/1	0.99	0.26	4.97	20,20,20,20	0
56	MG	DA	3257	1/1	0.96	0.20	4.96	34,34,34,34	0
56	MG	AF	3001	1/1	0.98	0.26	4.95	40,40,40,40	0
56	MG	BA	3247	1/1	0.96	0.30	4.91	28,28,28,28	0
56	MG	BA	3431	1/1	0.71	0.27	4.90	55,55,55,55	0
56	MG	DA	3453	1/1	0.86	0.23	4.87	45,45,45,45	0
56	MG	BF	306	1/1	0.94	0.31	4.87	40,40,40,40	0
56	MG	DA	3033	1/1	0.93	0.22	4.82	31,31,31,31	0
56	MG	AA	3223	1/1	0.91	0.30	4.74	59,59,59,59	0
56	MG	BA	3572	1/1	0.98	0.27	4.67	63,63,63,63	0
56	MG	DA	3343	1/1	0.84	0.20	4.65	40,40,40,40	0
56	MG	DA	3209	1/1	0.76	0.24	4.63	52,52,52,52	0
56	MG	DA	3404	1/1	0.78	0.20	4.58	51,51,51,51	0
56	MG	DA	3593	1/1	0.95	0.24	4.41	39,39,39,39	0
56	MG	DA	3383	1/1	0.93	0.24	4.38	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3425	1/1	0.94	0.27	4.38	29,29,29,29	0
56	MG	DA	3035	1/1	0.94	0.24	4.37	38,38,38,38	0
56	MG	DA	3424	1/1	0.86	0.24	4.37	63,63,63,63	0
56	MG	BA	3512	1/1	0.88	0.28	4.33	27,27,27,27	0
56	MG	BA	3740	1/1	0.92	0.21	4.32	51,51,51,51	0
56	MG	DA	3068	1/1	0.87	0.17	4.31	58,58,58,58	0
56	MG	AA	3219	1/1	0.95	0.21	4.22	65,65,65,65	0
56	MG	BA	3211	1/1	0.97	0.28	4.20	36,36,36,36	0
56	MG	BF	305	1/1	0.92	0.26	4.17	47,47,47,47	0
56	MG	BA	3814	1/1	0.94	0.28	4.17	26,26,26,26	0
56	MG	DV	3001	1/1	0.95	0.35	4.03	71,71,71,71	0
56	MG	AA	3012	1/1	0.95	0.23	4.01	33,33,33,33	0
56	MG	BA	3403	1/1	0.95	0.28	4.00	31,31,31,31	0
56	MG	BN	3001	1/1	0.89	0.33	3.97	51,51,51,51	0
56	MG	DA	3362	1/1	0.95	0.22	3.88	43,43,43,43	0
56	MG	BA	3181	1/1	0.84	0.24	3.85	41,41,41,41	0
56	MG	BA	3545	1/1	0.94	0.25	3.81	41,41,41,41	0
56	MG	BA	3386	1/1	0.96	0.22	3.76	42,42,42,42	0
56	MG	BA	3117	1/1	0.92	0.23	3.73	42,42,42,42	0
56	MG	AA	3164	1/1	0.97	0.24	3.70	50,50,50,50	0
56	MG	DA	3356	1/1	0.98	0.26	3.70	20,20,20,20	0
56	MG	DA	3254	1/1	0.99	0.25	3.68	21,21,21,21	0
56	MG	BA	3151	1/1	0.92	0.28	3.65	42,42,42,42	0
56	MG	DA	3022	1/1	0.97	0.21	3.64	40,40,40,40	0
56	MG	DD	306	1/1	0.99	0.26	3.63	44,44,44,44	0
56	MG	CF	3001	1/1	0.94	0.26	3.61	38,38,38,38	0
56	MG	DA	3322	1/1	0.97	0.29	3.59	43,43,43,43	0
56	MG	BA	3148	1/1	0.96	0.27	3.59	15,15,15,15	0
56	MG	DA	3201	1/1	0.88	0.23	3.53	52,52,52,52	0
56	MG	CA	3174	1/1	0.96	0.25	3.44	46,46,46,46	0
56	MG	DA	3070	1/1	0.93	0.23	3.39	48,48,48,48	0
56	MG	DA	3270	1/1	0.94	0.22	3.38	49,49,49,49	0
56	MG	BA	3008	1/1	0.94	0.22	3.36	27,27,27,27	0
56	MG	BA	3205	1/1	0.88	0.24	3.33	41,41,41,41	0
56	MG	DA	3340	1/1	0.97	0.21	3.33	42,42,42,42	0
56	MG	AX	3013	1/1	0.96	0.30	3.31	39,39,39,39	0
56	MG	DD	303	1/1	0.87	0.25	3.27	49,49,49,49	0
56	MG	BA	3051	1/1	0.95	0.23	3.22	25,25,25,25	0
56	MG	BA	3334	1/1	0.99	0.25	3.22	30,30,30,30	0
56	MG	DA	3634	1/1	0.95	0.14	3.20	53,53,53,53	0
56	MG	DA	3647	1/1	0.94	0.22	3.16	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3835	1/1	0.89	0.20	3.15	46,46,46,46	0
56	MG	BA	3487	1/1	0.98	0.24	3.11	25,25,25,25	0
56	MG	DA	3097	1/1	0.94	0.21	3.11	43,43,43,43	0
56	MG	BA	3412	1/1	0.93	0.20	3.10	41,41,41,41	0
56	MG	BA	3417	1/1	0.96	0.22	3.10	33,33,33,33	0
56	MG	BA	3763	1/1	0.91	0.27	3.09	34,34,34,34	0
56	MG	BA	3372	1/1	0.97	0.22	3.08	24,24,24,24	0
56	MG	DA	3241	1/1	0.64	0.20	3.07	50,50,50,50	0
56	MG	DA	3354	1/1	0.90	0.24	3.05	46,46,46,46	0
56	MG	AA	3043	1/1	0.94	0.27	3.00	26,26,26,26	0
56	MG	DE	302	1/1	0.93	0.20	3.00	39,39,39,39	0
56	MG	BB	3001	1/1	0.89	0.20	2.99	50,50,50,50	0
56	MG	BA	3161	1/1	0.96	0.23	2.87	37,37,37,37	0
56	MG	DA	3098	1/1	0.74	0.21	2.78	43,43,43,43	0
56	MG	BA	3546	1/1	0.97	0.26	2.78	30,30,30,30	0
56	MG	BA	3514	1/1	0.84	0.25	2.77	41,41,41,41	0
56	MG	BA	3615	1/1	0.97	0.28	2.72	35,35,35,35	0
56	MG	BA	3533	1/1	0.94	0.23	2.70	50,50,50,50	0
56	MG	BA	3294	1/1	0.92	0.20	2.65	45,45,45,45	0
56	MG	AA	3072	1/1	0.79	0.19	2.64	68,68,68,68	0
56	MG	CA	3007	1/1	0.86	0.18	2.58	69,69,69,69	0
56	MG	CA	3142	1/1	0.86	0.18	2.54	61,61,61,61	0
56	MG	BA	3414	1/1	0.91	0.22	2.54	29,29,29,29	0
56	MG	BA	3001	1/1	0.92	0.20	2.44	43,43,43,43	0
56	MG	BA	3016	1/1	0.91	0.20	2.43	44,44,44,44	0
56	MG	BA	3352	1/1	0.91	0.26	2.43	29,29,29,29	0
56	MG	BA	3384	1/1	0.97	0.23	2.39	30,30,30,30	0
56	MG	DB	3006	1/1	0.90	0.18	2.39	62,62,62,62	0
56	MG	BD	308	1/1	0.94	0.28	2.38	39,39,39,39	0
56	MG	BA	3584	1/1	0.95	0.24	2.33	27,27,27,27	0
56	MG	AA	3133	1/1	0.96	0.23	2.32	30,30,30,30	0
56	MG	AA	3113	1/1	0.84	0.20	2.30	59,59,59,59	0
56	MG	DA	3332	1/1	0.96	0.20	2.28	41,41,41,41	0
56	MG	AA	3086	1/1	0.90	0.20	2.28	52,52,52,52	0
56	MG	CA	3098	1/1	0.92	0.22	2.23	43,43,43,43	0
56	MG	AA	3092	1/1	0.94	0.20	2.21	39,39,39,39	0
56	MG	DU	3002	1/1	0.93	0.22	2.13	50,50,50,50	0
56	MG	DA	3374	1/1	0.93	0.18	2.05	37,37,37,37	0
56	MG	BA	3362	1/1	0.95	0.25	2.02	19,19,19,19	0
56	MG	CA	3158	1/1	0.97	0.19	2.00	53,53,53,53	0
56	MG	DD	305	1/1	0.94	0.24	2.00	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3650	1/1	0.90	0.27	1.99	44,44,44,44	0
56	MG	BW	201	1/1	0.87	0.21	1.98	46,46,46,46	0
56	MG	CA	3177	1/1	0.88	0.21	1.97	62,62,62,62	0
56	MG	CA	3018	1/1	0.86	0.18	1.90	45,45,45,45	0
56	MG	BA	3820	1/1	0.89	0.20	1.90	45,45,45,45	0
56	MG	CA	3101	1/1	0.90	0.22	1.90	54,54,54,54	0
56	MG	DA	3449	1/1	0.94	0.19	1.89	47,47,47,47	0
56	MG	AX	3002	1/1	0.86	0.24	1.89	53,53,53,53	0
56	MG	BA	3704	1/1	0.93	0.23	1.84	55,55,55,55	0
56	MG	BV	203	1/1	0.94	0.24	1.82	32,32,32,32	0
56	MG	BA	3608	1/1	0.95	0.21	1.76	60,60,60,60	0
56	MG	DA	3666	1/1	0.96	0.22	1.72	41,41,41,41	0
56	MG	BA	3818	1/1	0.93	0.26	1.70	32,32,32,32	0
56	MG	BA	3172	1/1	0.90	0.23	1.65	45,45,45,45	0
56	MG	BA	3447	1/1	0.90	0.23	1.65	26,26,26,26	0
56	MG	BA	3535	1/1	0.97	0.25	1.63	18,18,18,18	0
56	MG	BA	3075	1/1	0.96	0.20	1.62	27,27,27,27	0
56	MG	BA	3460	1/1	0.98	0.23	1.59	35,35,35,35	0
56	MG	BA	3837	1/1	0.92	0.20	1.57	40,40,40,40	0
56	MG	BA	3175	1/1	0.94	0.21	1.57	35,35,35,35	0
56	MG	DA	3285	1/1	0.95	0.20	1.46	28,28,28,28	0
56	MG	DA	3490	1/1	0.96	0.18	1.44	39,39,39,39	0
56	MG	DA	3418	1/1	0.91	0.22	1.43	37,37,37,37	0
56	MG	BX	101	1/1	0.93	0.26	1.43	65,65,65,65	0
56	MG	DA	3345	1/1	0.97	0.18	1.42	35,35,35,35	0
56	MG	DF	304	1/1	0.96	0.22	1.39	39,39,39,39	0
56	MG	DA	3284	1/1	0.96	0.18	1.38	40,40,40,40	0
56	MG	BW	203	1/1	0.93	0.23	1.36	34,34,34,34	0
56	MG	DA	3331	1/1	0.94	0.25	1.35	39,39,39,39	0
56	MG	DA	3311	1/1	0.94	0.18	1.33	42,42,42,42	0
56	MG	DA	3549	1/1	0.84	0.18	1.33	57,57,57,57	0
56	MG	BA	3670	1/1	0.86	0.20	1.25	47,47,47,47	0
56	MG	BA	3691	1/1	0.94	0.25	1.25	38,38,38,38	0
56	MG	BF	301	1/1	0.95	0.26	1.25	38,38,38,38	0
56	MG	BA	3156	1/1	0.93	0.23	1.20	41,41,41,41	0
56	MG	DU	3001	1/1	0.97	0.25	1.19	50,50,50,50	0
56	MG	BB	3017	1/1	0.98	0.20	1.18	33,33,33,33	0
56	MG	BQ	3005	1/1	0.80	0.30	1.11	50,50,50,50	0
56	MG	BE	305	1/1	0.91	0.22	1.07	59,59,59,59	0
56	MG	BU	205	1/1	0.95	0.22	1.07	38,38,38,38	0
56	MG	DA	3588	1/1	0.97	0.16	1.06	39,39,39,39	0
56	MG	BA	3713	1/1	0.96	0.23	1.05	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3398	1/1	0.96	0.20	1.02	42,42,42,42	0
56	MG	DA	3444	1/1	0.98	0.18	1.00	30,30,30,30	0
56	MG	BA	3212	1/1	0.98	0.20	0.99	42,42,42,42	0
56	MG	DA	3455	1/1	0.96	0.18	0.97	27,27,27,27	0
56	MG	BV	201	1/1	0.99	0.22	0.91	29,29,29,29	0
56	MG	BA	3826	1/1	0.96	0.22	0.91	33,33,33,33	0
56	MG	BA	3326	1/1	0.87	0.23	0.91	38,38,38,38	0
56	MG	DA	3315	1/1	0.96	0.17	0.91	41,41,41,41	0
56	MG	BA	3383	1/1	0.98	0.23	0.88	24,24,24,24	0
56	MG	BA	3153	1/1	0.91	0.22	0.86	39,39,39,39	0
56	MG	BA	3217	1/1	0.97	0.21	0.82	20,20,20,20	0
56	MG	AA	3001	1/1	0.96	0.18	0.81	34,34,34,34	0
56	MG	BA	3132	1/1	0.94	0.21	0.77	42,42,42,42	0
56	MG	BA	3565	1/1	0.97	0.24	0.77	42,42,42,42	0
56	MG	DA	3673	1/1	0.89	0.16	0.75	61,61,61,61	0
56	MG	DA	3419	1/1	0.60	0.17	0.75	44,44,44,44	0
56	MG	DA	3017	1/1	0.99	0.21	0.73	28,28,28,28	0
56	MG	DA	3004	1/1	0.96	0.19	0.72	42,42,42,42	0
56	MG	DA	3086	1/1	0.85	0.19	0.72	62,62,62,62	0
56	MG	BQ	3001	1/1	0.96	0.23	0.71	40,40,40,40	0
56	MG	D7	102	1/1	0.97	0.22	0.71	43,43,43,43	0
56	MG	DA	3620	1/1	0.83	0.17	0.70	62,62,62,62	0
56	MG	DA	3166	1/1	0.96	0.17	0.64	46,46,46,46	0
56	MG	CA	3061	1/1	0.80	0.22	0.64	56,56,56,56	0
56	MG	D7	101	1/1	0.94	0.19	0.62	39,39,39,39	0
56	MG	BA	3632	1/1	0.98	0.17	0.61	55,55,55,55	0
56	MG	AA	3107	1/1	0.94	0.25	0.58	51,51,51,51	0
56	MG	AA	3120	1/1	0.92	0.16	0.57	59,59,59,59	0
56	MG	DA	3329	1/1	0.98	0.21	0.54	29,29,29,29	0
56	MG	BF	303	1/1	0.98	0.22	0.50	42,42,42,42	0
56	MG	DA	3313	1/1	0.97	0.20	0.48	23,23,23,23	0
56	MG	BA	3590	1/1	0.82	0.23	0.43	32,32,32,32	0
56	MG	BA	3178	1/1	0.97	0.25	0.41	38,38,38,38	0
56	MG	BA	3279	1/1	0.93	0.22	0.37	43,43,43,43	0
56	MG	DA	3440	1/1	0.94	0.18	0.37	39,39,39,39	0
57	PCY	AA	3231	40/40	0.92	0.33	0.37	45,69,81,87	0
56	MG	BA	3206	1/1	0.95	0.21	0.36	29,29,29,29	0
56	MG	BU	204	1/1	0.98	0.20	0.35	38,38,38,38	0
57	PCY	CA	3178	40/40	0.85	0.35	0.32	58,78,89,91	0
56	MG	CA	3093	1/1	0.96	0.17	0.31	34,34,34,34	0
56	MG	DD	302	1/1	0.88	0.23	0.30	49,49,49,49	0
56	MG	BA	3827	1/1	0.95	0.20	0.24	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3406	1/1	0.91	0.15	0.22	40,40,40,40	0
59	ZN	D5	501	1/1	0.99	0.15	0.21	53,53,53,53	0
56	MG	CA	3141	1/1	0.96	0.17	0.21	49,49,49,49	0
56	MG	B0	101	1/1	0.94	0.20	0.20	39,39,39,39	0
56	MG	CA	3131	1/1	0.97	0.18	0.20	55,55,55,55	0
56	MG	BD	307	1/1	0.98	0.21	0.19	35,35,35,35	0
56	MG	BA	3119	1/1	0.97	0.19	0.17	36,36,36,36	0
56	MG	DA	3124	1/1	0.97	0.19	0.17	34,34,34,34	0
56	MG	BA	3012	1/1	0.97	0.21	0.12	26,26,26,26	0
56	MG	CA	3140	1/1	0.95	0.16	0.12	79,79,79,79	0
56	MG	DA	3334	1/1	0.97	0.17	0.12	32,32,32,32	0
56	MG	DA	3320	1/1	0.88	0.16	0.11	40,40,40,40	0
56	MG	BA	3421	1/1	0.97	0.22	0.11	33,33,33,33	0
56	MG	DA	3671	1/1	0.85	0.22	0.09	59,59,59,59	0
56	MG	DA	3291	1/1	0.98	0.18	0.05	42,42,42,42	0
56	MG	BA	3108	1/1	0.97	0.19	0.04	24,24,24,24	0
56	MG	BF	302	1/1	0.96	0.22	0.02	39,39,39,39	0
56	MG	B6	101	1/1	0.93	0.18	0.01	48,48,48,48	0
56	MG	DA	3482	1/1	0.98	0.17	0.01	50,50,50,50	0
56	MG	DA	3243	1/1	0.94	0.17	0.01	54,54,54,54	0
56	MG	DQ	3003	1/1	0.90	0.19	0.00	58,58,58,58	0
56	MG	DA	3360	1/1	0.95	0.16	-0.03	51,51,51,51	0
56	MG	BN	3004	1/1	0.98	0.21	-0.04	50,50,50,50	0
56	MG	AA	3182	1/1	0.96	0.20	-0.05	52,52,52,52	0
56	MG	BA	3566	1/1	0.90	0.23	-0.05	30,30,30,30	0
56	MG	DA	3410	1/1	0.82	0.15	-0.07	62,62,62,62	0
56	MG	AA	3021	1/1	0.91	0.17	-0.10	45,45,45,45	0
56	MG	BA	3798	1/1	0.85	0.14	-0.15	61,61,61,61	0
56	MG	BA	3678	1/1	0.97	0.22	-0.17	58,58,58,58	0
56	MG	BD	311	1/1	0.96	0.21	-0.18	51,51,51,51	0
56	MG	DA	3430	1/1	0.98	0.21	-0.19	28,28,28,28	0
56	MG	BA	3637	1/1	0.86	0.20	-0.20	59,59,59,59	0
56	MG	DA	3314	1/1	0.97	0.18	-0.21	33,33,33,33	0
56	MG	DA	3226	1/1	0.95	0.15	-0.23	54,54,54,54	0
56	MG	BO	5001	1/1	0.90	0.17	-0.27	55,55,55,55	0
56	MG	BU	209	1/1	0.99	0.19	-0.27	27,27,27,27	0
56	MG	BA	3606	1/1	0.87	0.20	-0.27	34,34,34,34	0
56	MG	DA	3042	1/1	0.95	0.15	-0.28	41,41,41,41	0
56	MG	BB	3018	1/1	0.92	0.15	-0.30	77,77,77,77	0
56	MG	BD	309	1/1	0.98	0.20	-0.31	37,37,37,37	0
56	MG	DF	305	1/1	0.96	0.17	-0.31	43,43,43,43	0
56	MG	BA	3544	1/1	0.89	0.20	-0.32	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3407	1/1	0.83	0.19	-0.35	37,37,37,37	0
56	MG	BA	3027	1/1	0.96	0.20	-0.36	42,42,42,42	0
56	MG	DA	3665	1/1	0.85	0.17	-0.36	58,58,58,58	0
56	MG	BA	3756	1/1	0.91	0.21	-0.39	27,27,27,27	0
56	MG	AA	3056	1/1	0.93	0.19	-0.40	46,46,46,46	0
56	MG	DA	3515	1/1	0.90	0.14	-0.45	57,57,57,57	0
56	MG	AA	3105	1/1	0.93	0.20	-0.45	49,49,49,49	0
56	MG	AA	3153	1/1	0.81	0.17	-0.46	55,55,55,55	0
56	MG	DA	3338	1/1	0.93	0.19	-0.47	40,40,40,40	0
56	MG	DA	3420	1/1	0.93	0.16	-0.47	46,46,46,46	0
59	ZN	B4	501	1/1	0.95	0.12	-0.48	73,73,73,73	0
56	MG	DA	3012	1/1	0.97	0.18	-0.48	39,39,39,39	0
56	MG	DA	3489	1/1	0.95	0.16	-0.48	37,37,37,37	0
56	MG	CA	3153	1/1	0.88	0.16	-0.48	61,61,61,61	0
59	ZN	B5	104	1/1	1.00	0.15	-0.52	38,38,38,38	0
56	MG	BA	3392	1/1	0.86	0.19	-0.52	46,46,46,46	0
56	MG	BA	3404	1/1	0.95	0.18	-0.54	36,36,36,36	0
56	MG	DA	3250	1/1	0.92	0.13	-0.55	61,61,61,61	0
56	MG	AA	3030	1/1	0.89	0.16	-0.56	57,57,57,57	0
56	MG	DQ	3004	1/1	0.98	0.16	-0.58	51,51,51,51	0
56	MG	CA	3155	1/1	0.96	0.14	-0.59	50,50,50,50	0
56	MG	BR	201	1/1	0.94	0.17	-0.60	44,44,44,44	0
56	MG	DA	3006	1/1	0.97	0.15	-0.60	43,43,43,43	0
56	MG	BA	3302	1/1	0.93	0.16	-0.61	35,35,35,35	0
56	MG	D0	102	1/1	0.93	0.17	-0.66	62,62,62,62	0
56	MG	BA	3789	1/1	0.91	0.17	-0.66	39,39,39,39	0
56	MG	BA	3794	1/1	0.95	0.20	-0.66	33,33,33,33	0
56	MG	AA	3084	1/1	0.94	0.17	-0.67	49,49,49,49	0
56	MG	DA	3295	1/1	0.92	0.16	-0.69	58,58,58,58	0
56	MG	BA	3530	1/1	0.92	0.20	-0.69	51,51,51,51	0
56	MG	AA	3227	1/1	0.97	0.18	-0.73	48,48,48,48	0
56	MG	BA	3045	1/1	0.98	0.20	-0.76	42,42,42,42	0
56	MG	DA	3566	1/1	0.81	0.17	-0.76	48,48,48,48	0
56	MG	D3	3001	1/1	0.99	0.16	-0.77	58,58,58,58	0
56	MG	CA	3034	1/1	0.80	0.13	-0.81	61,61,61,61	0
56	MG	BA	3793	1/1	0.97	0.20	-0.84	38,38,38,38	0
59	ZN	B9	501	1/1	0.98	0.17	-0.84	49,49,49,49	0
56	MG	BP	202	1/1	0.91	0.20	-0.84	34,34,34,34	0
56	MG	BA	3104	1/1	0.98	0.19	-0.85	27,27,27,27	0
56	MG	BA	3646	1/1	0.98	0.19	-0.85	38,38,38,38	0
56	MG	CA	3072	1/1	0.85	0.14	-0.85	62,62,62,62	0
56	MG	CA	3078	1/1	0.97	0.16	-0.87	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
58	SF4	AD	501	8/8	0.99	0.14	-0.88	56,62,64,76	0
56	MG	BA	3342	1/1	0.91	0.18	-0.90	51,51,51,51	0
56	MG	BA	3453	1/1	0.91	0.21	-0.93	42,42,42,42	0
56	MG	BA	3476	1/1	0.98	0.21	-0.94	24,24,24,24	0
56	MG	BA	3124	1/1	0.91	0.20	-0.95	38,38,38,38	0
56	MG	AA	3186	1/1	0.99	0.16	-0.95	52,52,52,52	0
56	MG	BA	3050	1/1	0.99	0.17	-0.96	31,31,31,31	0
56	MG	AA	3016	1/1	0.92	0.16	-0.98	46,46,46,46	0
56	MG	DA	3554	1/1	0.98	0.18	-0.99	23,23,23,23	0
56	MG	BA	3131	1/1	0.92	0.18	-1.01	38,38,38,38	0
59	ZN	B6	103	1/1	0.98	0.13	-1.02	29,29,29,29	0
56	MG	DA	3481	1/1	0.96	0.18	-1.03	30,30,30,30	0
56	MG	CA	3014	1/1	0.94	0.14	-1.04	47,47,47,47	0
56	MG	BA	3467	1/1	0.84	0.20	-1.04	39,39,39,39	0
56	MG	BE	301	1/1	0.97	0.20	-1.05	23,23,23,23	0
56	MG	BA	3515	1/1	0.96	0.21	-1.06	20,20,20,20	0
56	MG	BA	3415	1/1	0.97	0.20	-1.07	29,29,29,29	0
56	MG	DA	3123	1/1	0.95	0.12	-1.08	47,47,47,47	0
56	MG	AA	3128	1/1	0.94	0.17	-1.09	41,41,41,41	0
56	MG	BA	3122	1/1	0.97	0.18	-1.09	26,26,26,26	0
56	MG	DA	3023	1/1	0.95	0.14	-1.10	30,30,30,30	0
56	MG	CA	3041	1/1	0.94	0.16	-1.12	58,58,58,58	0
56	MG	BA	3187	1/1	0.95	0.16	-1.12	36,36,36,36	0
56	MG	DA	3504	1/1	0.69	0.13	-1.12	60,60,60,60	0
56	MG	DA	3236	1/1	0.91	0.13	-1.15	48,48,48,48	0
56	MG	BA	3438	1/1	0.91	0.19	-1.16	47,47,47,47	0
56	MG	DA	3303	1/1	0.89	0.15	-1.17	42,42,42,42	0
56	MG	DA	3448	1/1	0.73	0.14	-1.19	41,41,41,41	0
56	MG	DA	3463	1/1	0.96	0.15	-1.20	37,37,37,37	0
56	MG	BA	3069	1/1	0.97	0.14	-1.22	31,31,31,31	0
59	ZN	BY	501	1/1	0.98	0.11	-1.24	58,58,58,58	0
56	MG	DA	3668	1/1	0.97	0.15	-1.25	79,79,79,79	0
56	MG	BA	3536	1/1	0.95	0.18	-1.26	48,48,48,48	0
56	MG	BA	3822	1/1	0.97	0.20	-1.26	21,21,21,21	0
56	MG	DA	3652	1/1	0.94	0.12	-1.27	49,49,49,49	0
56	MG	CA	3070	1/1	0.81	0.14	-1.28	71,71,71,71	0
56	MG	DA	3432	1/1	0.91	0.15	-1.28	56,56,56,56	0
56	MG	BA	3359	1/1	0.94	0.14	-1.29	46,46,46,46	0
56	MG	DA	3144	1/1	0.85	0.14	-1.30	63,63,63,63	0
56	MG	DA	3353	1/1	0.95	0.14	-1.32	37,37,37,37	0
59	ZN	D6	501	1/1	0.96	0.11	-1.33	73,73,73,73	0
56	MG	BA	3332	1/1	0.97	0.17	-1.34	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	CA	3051	1/1	0.64	0.11	-1.35	66,66,66,66	0
56	MG	DA	3388	1/1	0.98	0.14	-1.36	35,35,35,35	0
56	MG	BA	3201	1/1	0.91	0.17	-1.36	40,40,40,40	0
56	MG	AA	3003	1/1	0.87	0.16	-1.37	66,66,66,66	0
56	MG	DA	3260	1/1	0.94	0.13	-1.37	41,41,41,41	0
56	MG	DA	3230	1/1	0.96	0.15	-1.38	33,33,33,33	0
56	MG	BA	3696	1/1	0.95	0.16	-1.39	33,33,33,33	0
56	MG	DA	3104	1/1	0.98	0.15	-1.40	46,46,46,46	0
56	MG	AX	3005	1/1	0.92	0.15	-1.42	44,44,44,44	0
59	ZN	DY	501	1/1	0.92	0.09	-1.44	106,106,106,106	0
56	MG	AA	3130	1/1	0.86	0.16	-1.44	43,43,43,43	0
56	MG	AA	3074	1/1	0.95	0.17	-1.44	47,47,47,47	0
56	MG	DA	3366	1/1	0.86	0.13	-1.50	50,50,50,50	0
56	MG	BQ	3002	1/1	0.89	0.16	-1.53	37,37,37,37	0
56	MG	CA	3176	1/1	0.90	0.13	-1.56	43,43,43,43	0
56	MG	DA	3179	1/1	0.86	0.08	-1.56	46,46,46,46	0
56	MG	BA	3710	1/1	0.96	0.19	-1.57	28,28,28,28	0
56	MG	CA	3126	1/1	0.90	0.17	-1.59	72,72,72,72	0
56	MG	B4	502	1/1	0.88	0.12	-1.59	72,72,72,72	0
56	MG	BA	3805	1/1	0.93	0.16	-1.61	21,21,21,21	0
56	MG	DA	3318	1/1	0.91	0.18	-1.63	42,42,42,42	0
56	MG	CA	3036	1/1	0.90	0.09	-1.64	60,60,60,60	0
56	MG	AA	3154	1/1	0.98	0.14	-1.64	59,59,59,59	0
56	MG	BA	3587	1/1	0.95	0.20	-1.64	44,44,44,44	0
56	MG	BD	304	1/1	0.97	0.20	-1.67	48,48,48,48	0
56	MG	BE	308	1/1	0.96	0.17	-1.67	21,21,21,21	0
56	MG	DA	3175	1/1	0.97	0.08	-1.69	53,53,53,53	0
56	MG	DA	3016	1/1	0.96	0.12	-1.71	53,53,53,53	0
56	MG	CA	3066	1/1	0.98	0.14	-1.73	66,66,66,66	0
56	MG	AA	3228	1/1	0.86	0.10	-1.74	68,68,68,68	0
56	MG	BA	3219	1/1	0.91	0.19	-1.79	29,29,29,29	0
56	MG	DA	3595	1/1	0.91	0.18	-1.80	61,61,61,61	0
56	MG	DQ	3001	1/1	0.97	0.11	-1.81	48,48,48,48	0
56	MG	AA	3093	1/1	0.94	0.14	-1.86	50,50,50,50	0
56	MG	AA	3019	1/1	0.95	0.15	-1.87	48,48,48,48	0
56	MG	BA	3743	1/1	0.88	0.18	-1.89	21,21,21,21	0
59	ZN	AN	501	1/1	0.98	0.12	-1.89	58,58,58,58	0
56	MG	AK	201	1/1	0.95	0.14	-1.89	61,61,61,61	0
56	MG	BA	3434	1/1	0.74	0.20	-1.89	34,34,34,34	0
56	MG	BV	202	1/1	0.99	0.13	-1.89	26,26,26,26	0
56	MG	AA	3224	1/1	0.98	0.15	-1.90	33,33,33,33	0
56	MG	DA	3528	1/1	0.97	0.09	-1.91	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	3099	1/1	0.91	0.11	-1.93	62,62,62,62	0
58	SF4	CD	501	8/8	0.98	0.10	-1.96	54,64,76,87	0
59	ZN	D4	501	1/1	0.85	0.08	-1.96	119,119,119,119	0
56	MG	BA	3061	1/1	0.92	0.17	-1.98	40,40,40,40	0
56	MG	BA	3551	1/1	0.97	0.19	-1.98	33,33,33,33	0
56	MG	DA	3256	1/1	0.93	0.12	-1.98	47,47,47,47	0
56	MG	BU	201	1/1	0.94	0.14	-1.99	39,39,39,39	0
56	MG	AA	3077	1/1	0.93	0.14	-1.99	49,49,49,49	0
56	MG	BA	3185	1/1	0.98	0.20	-2.00	32,32,32,32	0
56	MG	BA	3643	1/1	0.96	0.20	-2.01	30,30,30,30	0
56	MG	DA	3494	1/1	0.96	0.18	-2.01	30,30,30,30	0
56	MG	BA	3190	1/1	0.94	0.16	-2.02	45,45,45,45	0
56	MG	BA	3817	1/1	0.98	0.17	-2.03	47,47,47,47	0
56	MG	BA	3357	1/1	0.86	0.19	-2.03	46,46,46,46	0
56	MG	BA	3420	1/1	0.94	0.19	-2.05	22,22,22,22	0
56	MG	DA	3586	1/1	0.92	0.09	-2.08	44,44,44,44	0
56	MG	BA	3501	1/1	0.94	0.18	-2.08	20,20,20,20	0
56	MG	CA	3031	1/1	0.85	0.14	-2.08	53,53,53,53	0
59	ZN	D9	501	1/1	0.91	0.07	-2.08	63,63,63,63	0
56	MG	DA	3176	1/1	0.85	0.12	-2.09	52,52,52,52	0
56	MG	B5	101	1/1	0.96	0.14	-2.09	31,31,31,31	0
56	MG	BA	3437	1/1	0.89	0.20	-2.09	28,28,28,28	0
56	MG	AA	3125	1/1	0.82	0.11	-2.10	71,71,71,71	0
56	MG	AA	3144	1/1	0.92	0.12	-2.14	50,50,50,50	0
56	MG	BA	3622	1/1	0.91	0.19	-2.16	31,31,31,31	0
56	MG	BA	3597	1/1	0.92	0.20	-2.21	44,44,44,44	0
56	MG	CA	3089	1/1	0.97	0.07	-2.22	58,58,58,58	0
56	MG	BV	205	1/1	0.99	0.12	-2.24	32,32,32,32	0
56	MG	CA	3075	1/1	0.95	0.10	-2.25	44,44,44,44	0
56	MG	DA	3643	1/1	0.89	0.10	-2.26	60,60,60,60	0
56	MG	DB	3002	1/1	0.90	0.15	-2.27	56,56,56,56	0
56	MG	AA	3115	1/1	0.90	0.11	-2.28	51,51,51,51	0
56	MG	DA	3570	1/1	0.97	0.10	-2.29	49,49,49,49	0
56	MG	CA	3063	1/1	0.94	0.14	-2.30	59,59,59,59	0
56	MG	AW	3004	1/1	0.95	0.12	-2.33	51,51,51,51	0
56	MG	B7	101	1/1	0.98	0.14	-2.34	33,33,33,33	0
56	MG	AA	3014	1/1	0.95	0.12	-2.34	69,69,69,69	0
56	MG	AA	3064	1/1	0.94	0.13	-2.34	61,61,61,61	0
56	MG	BA	3813	1/1	0.98	0.19	-2.36	4,4,4,4	0
56	MG	DA	3613	1/1	0.93	0.14	-2.37	50,50,50,50	0
56	MG	DA	3052	1/1	0.95	0.12	-2.38	38,38,38,38	0
56	MG	CA	3095	1/1	0.94	0.10	-2.38	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3816	1/1	0.97	0.19	-2.39	21,21,21,21	0
56	MG	DA	3328	1/1	0.91	0.14	-2.40	47,47,47,47	0
56	MG	BF	304	1/1	0.95	0.15	-2.44	32,32,32,32	0
56	MG	AA	3038	1/1	0.76	0.14	-2.45	51,51,51,51	0
56	MG	AM	201	1/1	0.96	0.05	-2.46	50,50,50,50	0
56	MG	DA	3409	1/1	0.93	0.09	-2.46	47,47,47,47	0
56	MG	DA	3670	1/1	0.98	0.13	-2.47	38,38,38,38	0
56	MG	BU	207	1/1	0.98	0.14	-2.47	29,29,29,29	0
56	MG	AN	502	1/1	0.83	0.13	-2.50	52,52,52,52	0
56	MG	AA	3008	1/1	0.93	0.15	-2.51	54,54,54,54	0
56	MG	BA	3400	1/1	0.99	0.17	-2.51	25,25,25,25	0
56	MG	AA	3146	1/1	0.96	0.11	-2.53	53,53,53,53	0
56	MG	BA	3445	1/1	0.91	0.20	-2.54	32,32,32,32	0
56	MG	BA	3381	1/1	0.94	0.14	-2.54	43,43,43,43	0
56	MG	DA	3032	1/1	0.87	0.15	-2.54	40,40,40,40	0
56	MG	DA	3517	1/1	0.96	0.10	-2.56	47,47,47,47	0
56	MG	DG	3001	1/1	0.97	0.04	-2.57	56,56,56,56	0
56	MG	BA	3589	1/1	0.98	0.18	-2.60	17,17,17,17	0
56	MG	CA	3120	1/1	0.93	0.12	-2.61	64,64,64,64	0
56	MG	DA	3480	1/1	0.87	0.13	-2.64	48,48,48,48	0
56	MG	B3	102	1/1	0.92	0.11	-2.67	35,35,35,35	0
56	MG	BA	3617	1/1	0.92	0.13	-2.71	64,64,64,64	0
56	MG	CA	3108	1/1	0.97	0.14	-2.75	51,51,51,51	0
56	MG	DA	3206	1/1	0.94	0.10	-2.76	39,39,39,39	0
56	MG	BA	3745	1/1	0.94	0.17	-2.77	30,30,30,30	0
56	MG	DF	303	1/1	0.95	0.07	-2.83	46,46,46,46	0
56	MG	DA	3582	1/1	0.97	0.11	-2.83	39,39,39,39	0
56	MG	BA	3539	1/1	0.95	0.21	-2.84	23,23,23,23	0
56	MG	BA	3354	1/1	0.92	0.17	-2.84	31,31,31,31	0
56	MG	CA	3065	1/1	0.79	0.07	-2.84	65,65,65,65	0
56	MG	BA	3337	1/1	0.93	0.17	-2.84	35,35,35,35	0
56	MG	AA	3138	1/1	0.92	0.17	-2.85	34,34,34,34	0
56	MG	DA	3364	1/1	0.96	0.14	-2.86	38,38,38,38	0
56	MG	DA	3245	1/1	0.95	0.10	-2.86	62,62,62,62	0
56	MG	BR	205	1/1	0.97	0.15	-2.90	29,29,29,29	0
56	MG	DA	3514	1/1	0.88	0.12	-2.91	41,41,41,41	0
56	MG	BA	3699	1/1	0.79	0.18	-2.92	42,42,42,42	0
56	MG	BA	3330	1/1	0.98	0.17	-2.93	29,29,29,29	0
56	MG	BA	3422	1/1	0.93	0.18	-2.95	32,32,32,32	0
56	MG	DA	3304	1/1	0.93	0.12	-2.95	40,40,40,40	0
56	MG	BA	3199	1/1	0.93	0.09	-2.99	53,53,53,53	0
56	MG	AA	3067	1/1	0.92	0.09	-2.99	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3306	1/1	0.86	0.13	-3.01	42,42,42,42	0
56	MG	BA	3254	1/1	0.88	0.16	-3.02	30,30,30,30	0
56	MG	AA	3205	1/1	0.83	0.12	-3.02	51,51,51,51	0
56	MG	DA	3045	1/1	0.97	0.12	-3.09	47,47,47,47	0
56	MG	BA	3303	1/1	0.97	0.17	-3.09	35,35,35,35	0
56	MG	DA	3391	1/1	0.92	0.09	-3.12	44,44,44,44	0
56	MG	BD	302	1/1	0.97	0.16	-3.13	23,23,23,23	0
56	MG	DA	3443	1/1	0.89	0.10	-3.15	51,51,51,51	0
56	MG	BA	3416	1/1	0.94	0.17	-3.17	21,21,21,21	0
56	MG	B8	101	1/1	0.73	0.14	-3.19	42,42,42,42	0
56	MG	CT	3001	1/1	0.94	0.07	-3.20	47,47,47,47	0
56	MG	BD	310	1/1	0.95	0.15	-3.22	31,31,31,31	0
56	MG	CA	3170	1/1	0.92	0.12	-3.22	64,64,64,64	0
56	MG	BA	3370	1/1	0.93	0.12	-3.23	60,60,60,60	0
56	MG	BF	309	1/1	0.98	0.16	-3.24	30,30,30,30	0
56	MG	DA	3010	1/1	0.96	0.07	-3.24	43,43,43,43	0
56	MG	DA	3594	1/1	0.96	0.07	-3.25	44,44,44,44	0
56	MG	BG	202	1/1	0.95	0.07	-3.25	46,46,46,46	0
56	MG	BE	303	1/1	0.96	0.16	-3.27	27,27,27,27	0
56	MG	BA	3072	1/1	0.97	0.14	-3.29	30,30,30,30	0
56	MG	B5	102	1/1	0.89	0.18	-3.29	45,45,45,45	0
56	MG	AA	3023	1/1	0.92	0.15	-3.34	37,37,37,37	0
56	MG	CE	202	1/1	0.93	0.05	-3.37	66,66,66,66	0
56	MG	DR	5001	1/1	0.87	0.08	-3.38	58,58,58,58	0
56	MG	BA	3774	1/1	0.91	0.19	-3.38	43,43,43,43	0
56	MG	BA	3731	1/1	0.99	0.12	-3.39	23,23,23,23	0
56	MG	BA	3832	1/1	0.89	0.09	-3.40	37,37,37,37	0
56	MG	BA	3142	1/1	0.98	0.14	-3.41	34,34,34,34	0
56	MG	DA	3485	1/1	0.92	0.11	-3.42	44,44,44,44	0
56	MG	CA	3030	1/1	0.94	0.08	-3.44	59,59,59,59	0
56	MG	BA	3423	1/1	0.93	0.18	-3.44	23,23,23,23	0
56	MG	BF	308	1/1	0.98	0.11	-3.45	36,36,36,36	0
56	MG	DA	3516	1/1	0.89	0.09	-3.46	59,59,59,59	0
56	MG	BA	3042	1/1	0.97	0.18	-3.52	40,40,40,40	0
56	MG	BA	3134	1/1	0.95	0.15	-3.52	35,35,35,35	0
56	MG	BA	3411	1/1	0.92	0.13	-3.57	36,36,36,36	0
56	MG	AA	3225	1/1	0.99	0.11	-3.58	26,26,26,26	0
56	MG	AA	3017	1/1	0.90	0.11	-3.60	62,62,62,62	0
56	MG	DA	3057	1/1	0.86	0.08	-3.64	47,47,47,47	0
56	MG	DA	3259	1/1	0.93	0.12	-3.64	34,34,34,34	0
56	MG	BU	203	1/1	0.99	0.14	-3.65	31,31,31,31	0
56	MG	BA	3210	1/1	0.98	0.20	-3.66	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
59	ZN	CN	501	1/1	0.91	0.04	-3.69	92,92,92,92	0
56	MG	BA	3054	1/1	0.97	0.17	-3.73	30,30,30,30	0
56	MG	DA	3664	1/1	0.94	0.08	-3.84	38,38,38,38	0
56	MG	BB	3023	1/1	0.97	0.11	-3.89	46,46,46,46	0
56	MG	DA	3275	1/1	0.97	0.09	-3.91	52,52,52,52	0
56	MG	AA	3013	1/1	0.97	0.07	-3.92	51,51,51,51	0
56	MG	DA	3011	1/1	0.98	0.09	-4.03	40,40,40,40	0
56	MG	BA	3758	1/1	0.83	0.14	-4.04	34,34,34,34	0
56	MG	BA	3116	1/1	0.93	0.15	-4.04	29,29,29,29	0
56	MG	BA	3336	1/1	0.97	0.13	-4.06	35,35,35,35	0
56	MG	BU	208	1/1	0.94	0.13	-4.10	41,41,41,41	0
56	MG	BA	3647	1/1	0.95	0.16	-4.11	45,45,45,45	0
56	MG	CA	3083	1/1	0.87	0.09	-4.12	58,58,58,58	0
56	MG	BA	3757	1/1	0.86	0.16	-4.22	25,25,25,25	0
56	MG	CA	3015	1/1	0.89	0.12	-4.22	58,58,58,58	0
56	MG	BB	3007	1/1	0.97	0.09	-4.23	36,36,36,36	0
56	MG	BA	3184	1/1	0.96	0.12	-4.28	30,30,30,30	0
56	MG	BD	303	1/1	0.98	0.15	-4.31	44,44,44,44	0
56	MG	BA	3339	1/1	0.95	0.15	-4.33	40,40,40,40	0
56	MG	BA	3834	1/1	0.95	0.13	-4.37	35,35,35,35	0
56	MG	BA	3232	1/1	0.92	0.14	-4.39	37,37,37,37	0
56	MG	BA	3150	1/1	0.90	0.12	-4.43	48,48,48,48	0
56	MG	DA	3228	1/1	0.99	0.05	-4.44	42,42,42,42	0
56	MG	DA	3128	1/1	0.96	0.07	-4.48	45,45,45,45	0
56	MG	BA	3355	1/1	0.99	0.15	-4.49	24,24,24,24	0
56	MG	CA	3055	1/1	0.76	0.12	-4.59	53,53,53,53	0
56	MG	DA	3149	1/1	0.87	0.10	-4.66	48,48,48,48	0
56	MG	BN	3003	1/1	0.98	0.15	-4.79	38,38,38,38	0
56	MG	BD	305	1/1	0.96	0.14	-4.83	37,37,37,37	0
56	MG	BA	3541	1/1	0.96	0.14	-4.83	29,29,29,29	0
56	MG	BA	3839	1/1	0.93	0.11	-4.87	38,38,38,38	0
56	MG	BA	3611	1/1	0.95	0.13	-4.92	42,42,42,42	0
56	MG	DA	3261	1/1	0.98	0.07	-4.92	44,44,44,44	0
56	MG	BA	3123	1/1	0.97	0.16	-4.92	35,35,35,35	0
56	MG	BA	3180	1/1	0.86	0.11	-4.93	58,58,58,58	0
56	MG	BA	3085	1/1	0.96	0.13	-4.95	31,31,31,31	0
56	MG	BB	3003	1/1	0.91	0.12	-4.98	40,40,40,40	0
56	MG	DA	3474	1/1	0.93	0.07	-5.13	53,53,53,53	0
56	MG	BA	3640	1/1	0.98	0.19	-5.14	39,39,39,39	0
56	MG	BA	3727	1/1	0.88	0.14	-5.19	39,39,39,39	0
56	MG	BA	3809	1/1	0.98	0.14	-5.25	29,29,29,29	0
56	MG	AA	3078	1/1	0.89	0.06	-5.27	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3302	1/1	0.95	0.12	-5.40	33,33,33,33	0
56	MG	BN	3002	1/1	0.89	0.12	-5.45	46,46,46,46	0
56	MG	BA	3649	1/1	0.98	0.10	-5.47	43,43,43,43	0
56	MG	BA	3037	1/1	0.95	0.16	-5.47	37,37,37,37	0
56	MG	BA	3735	1/1	0.98	0.14	-5.49	35,35,35,35	0
56	MG	BA	3365	1/1	0.83	0.13	-5.54	49,49,49,49	0
56	MG	BA	3025	1/1	0.96	0.15	-5.57	38,38,38,38	0
56	MG	BA	3561	1/1	0.97	0.15	-5.63	27,27,27,27	0
56	MG	DA	3375	1/1	0.89	0.11	-5.68	40,40,40,40	0
56	MG	AE	3001	1/1	0.96	0.06	-5.71	66,66,66,66	0
56	MG	BA	3250	1/1	0.89	0.19	-5.71	40,40,40,40	0
56	MG	BA	3380	1/1	0.95	0.12	-5.75	60,60,60,60	0
56	MG	BA	3697	1/1	0.99	0.12	-5.83	35,35,35,35	0
56	MG	BA	3374	1/1	0.93	0.08	-5.90	37,37,37,37	0
56	MG	BA	3410	1/1	0.90	0.10	-5.93	46,46,46,46	0
56	MG	BA	3513	1/1	0.97	0.15	-5.96	34,34,34,34	0
56	MG	BA	3792	1/1	0.95	0.16	-6.00	32,32,32,32	0
56	MG	BA	3583	1/1	0.80	0.12	-6.02	45,45,45,45	0
56	MG	BA	3661	1/1	0.94	0.09	-6.09	53,53,53,53	0
56	MG	DA	3273	1/1	0.87	0.11	-6.10	45,45,45,45	0
56	MG	DA	3425	1/1	0.98	0.07	-6.11	45,45,45,45	0
56	MG	BA	3115	1/1	0.89	0.08	-6.19	67,67,67,67	0
56	MG	DA	3553	1/1	0.95	0.14	-6.29	54,54,54,54	0
56	MG	DA	3135	1/1	0.93	0.11	-6.38	50,50,50,50	0
56	MG	AA	3129	1/1	0.94	0.08	-6.51	73,73,73,73	0
56	MG	BA	3313	1/1	0.87	0.15	-6.53	46,46,46,46	0
56	MG	CA	3077	1/1	0.99	0.06	-6.58	48,48,48,48	0
56	MG	DA	3431	1/1	0.96	0.17	-6.58	25,25,25,25	0
56	MG	CA	3004	1/1	0.92	0.07	-6.92	71,71,71,71	0
56	MG	BA	3462	1/1	0.99	0.13	-6.94	11,11,11,11	0
56	MG	AA	3047	1/1	0.88	0.09	-7.07	47,47,47,47	0
56	MG	BA	3213	1/1	0.94	0.09	-7.11	45,45,45,45	0
56	MG	DA	3307	1/1	0.96	0.08	-7.15	45,45,45,45	0
56	MG	BA	3553	1/1	0.83	0.16	-7.30	42,42,42,42	0
56	MG	BA	3026	1/1	0.97	0.14	-7.38	19,19,19,19	0
56	MG	BA	3737	1/1	0.97	0.11	-7.41	36,36,36,36	0
56	MG	BA	3741	1/1	0.93	0.11	-7.49	28,28,28,28	0
56	MG	AA	3048	1/1	0.89	0.08	-7.54	51,51,51,51	0
56	MG	AA	3002	1/1	0.93	0.08	-7.66	62,62,62,62	0
56	MG	BA	3324	1/1	0.95	0.17	-7.98	34,34,34,34	0
56	MG	AA	3035	1/1	0.90	0.07	-8.16	46,46,46,46	0
56	MG	DA	3662	1/1	0.96	0.09	-8.20	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	3021	1/1	0.92	0.13	-8.33	42,42,42,42	0
56	MG	BE	302	1/1	0.89	0.17	-8.72	34,34,34,34	0
56	MG	BA	3322	1/1	0.83	0.16	-9.05	32,32,32,32	0
56	MG	DA	3268	1/1	0.95	0.04	-9.15	60,60,60,60	0
56	MG	BA	3644	1/1	0.97	0.10	-9.49	36,36,36,36	0
56	MG	BA	3305	1/1	0.92	0.12	-9.82	33,33,33,33	0
56	MG	BA	3776	1/1	0.97	0.14	-9.85	49,49,49,49	0
56	MG	BA	3523	1/1	0.87	0.15	-9.88	64,64,64,64	0
56	MG	BA	3376	1/1	0.92	0.11	-10.13	34,34,34,34	0
56	MG	BA	3573	1/1	0.96	0.09	-10.26	32,32,32,32	0
56	MG	DA	3276	1/1	0.96	0.08	-10.45	33,33,33,33	0
56	MG	BA	3526	1/1	0.91	0.09	-11.19	32,32,32,32	0
56	MG	BA	3767	1/1	0.97	0.11	-11.20	29,29,29,29	0
56	MG	BA	3246	1/1	0.99	0.10	-13.28	27,27,27,27	0
56	MG	BA	3521	1/1	0.96	0.13	-15.07	36,36,36,36	0
56	MG	BA	3630	1/1	0.96	0.08	-22.64	30,30,30,30	0
56	MG	DA	3090	1/1	0.93	0.21	-	45,45,45,45	0
56	MG	AA	3027	1/1	0.94	0.24	-	54,54,54,54	0
56	MG	DA	3499	1/1	0.89	0.10	-	60,60,60,60	0
56	MG	DA	3625	1/1	0.95	0.20	-	53,53,53,53	0
56	MG	B5	105	1/1	0.94	0.10	-	49,49,49,49	0
56	MG	BA	3128	1/1	0.98	0.24	-	27,27,27,27	0
56	MG	BA	3084	1/1	0.96	0.18	-	45,45,45,45	0
56	MG	CA	3144	1/1	0.98	0.18	-	59,59,59,59	0
56	MG	DA	3198	1/1	0.96	0.08	-	51,51,51,51	0
56	MG	BA	3474	1/1	0.93	0.09	-	61,61,61,61	0
56	MG	CA	3104	1/1	0.92	0.11	-	64,64,64,64	0
56	MG	DA	3452	1/1	0.75	0.24	-	61,61,61,61	0
56	MG	DA	3513	1/1	0.80	0.17	-	50,50,50,50	0
56	MG	BA	3338	1/1	0.96	0.16	-	41,41,41,41	0
56	MG	CW	3001	1/1	0.91	0.32	-	63,63,63,63	0
56	MG	DA	3441	1/1	0.92	0.09	-	43,43,43,43	0
56	MG	DA	3639	1/1	0.95	0.14	-	64,64,64,64	0
56	MG	AA	3103	1/1	0.91	0.14	-	59,59,59,59	0
56	MG	DA	3029	1/1	0.90	0.21	-	51,51,51,51	0
56	MG	BA	3796	1/1	0.95	0.13	-	40,40,40,40	0
56	MG	DA	3317	1/1	0.97	0.15	-	55,55,55,55	0
56	MG	AD	502	1/1	0.90	0.29	-	56,56,56,56	0
56	MG	BA	3183	1/1	0.94	0.22	-	40,40,40,40	0
56	MG	DA	3246	1/1	0.86	0.12	-	39,39,39,39	0
56	MG	DA	3363	1/1	0.98	0.38	-	54,54,54,54	0
56	MG	DA	3529	1/1	0.95	0.09	-	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3173	1/1	0.95	0.30	-	36,36,36,36	0
56	MG	BA	3522	1/1	0.92	0.28	-	36,36,36,36	0
56	MG	DA	3281	1/1	0.98	0.23	-	33,33,33,33	0
56	MG	BA	3780	1/1	0.98	0.12	-	41,41,41,41	0
56	MG	DA	3587	1/1	0.89	0.09	-	61,61,61,61	0
56	MG	BA	3283	1/1	0.90	0.12	-	36,36,36,36	0
56	MG	DA	3358	1/1	0.89	0.32	-	45,45,45,45	0
56	MG	DA	3608	1/1	0.98	0.13	-	53,53,53,53	0
56	MG	BA	3520	1/1	0.92	0.32	-	47,47,47,47	0
56	MG	DA	3062	1/1	0.96	0.17	-	53,53,53,53	0
56	MG	BA	3481	1/1	0.84	0.29	-	45,45,45,45	0
56	MG	DA	3126	1/1	0.95	0.15	-	44,44,44,44	0
56	MG	DA	3651	1/1	0.97	0.16	-	47,47,47,47	0
56	MG	BA	3290	1/1	0.87	0.30	-	58,58,58,58	0
56	MG	DA	3160	1/1	0.94	0.19	-	59,59,59,59	0
56	MG	BA	3328	1/1	0.89	0.16	-	60,60,60,60	0
56	MG	DA	3021	1/1	0.95	0.30	-	48,48,48,48	0
56	MG	CA	3097	1/1	0.91	0.23	-	57,57,57,57	0
56	MG	DA	3255	1/1	0.93	0.05	-	59,59,59,59	0
56	MG	BA	3102	1/1	0.86	0.27	-	54,54,54,54	0
56	MG	AW	3006	1/1	0.91	0.16	-	50,50,50,50	0
56	MG	AA	3207	1/1	0.95	0.14	-	68,68,68,68	0
56	MG	DA	3208	1/1	0.92	0.10	-	59,59,59,59	0
56	MG	DA	3162	1/1	0.94	0.34	-	43,43,43,43	0
56	MG	CA	3134	1/1	0.91	0.14	-	70,70,70,70	0
56	MG	BA	3063	1/1	0.92	0.17	-	47,47,47,47	0
56	MG	BA	3171	1/1	0.85	0.33	-	53,53,53,53	0
56	MG	DA	3451	1/1	0.83	0.29	-	56,56,56,56	0
56	MG	CA	3044	1/1	0.98	0.23	-	55,55,55,55	0
56	MG	CX	3005	1/1	0.94	0.45	-	58,58,58,58	0
56	MG	DA	3051	1/1	0.68	0.20	-	56,56,56,56	0
56	MG	DA	3191	1/1	0.90	0.32	-	44,44,44,44	0
56	MG	BA	3059	1/1	0.87	0.11	-	55,55,55,55	0
56	MG	BA	3021	1/1	0.94	0.17	-	60,60,60,60	0
56	MG	DA	3523	1/1	0.92	0.14	-	57,57,57,57	0
56	MG	BA	3236	1/1	0.91	0.15	-	43,43,43,43	0
56	MG	BA	3186	1/1	0.87	0.19	-	51,51,51,51	0
56	MG	AA	3088	1/1	0.97	0.30	-	56,56,56,56	0
56	MG	BA	3098	1/1	0.94	0.35	-	26,26,26,26	0
56	MG	DA	3479	1/1	0.97	0.17	-	50,50,50,50	0
56	MG	AA	3127	1/1	0.92	0.18	-	48,48,48,48	0
56	MG	BA	3216	1/1	0.95	0.21	-	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3014	1/1	0.86	0.23	-	33,33,33,33	0
56	MG	DA	3464	1/1	0.95	0.11	-	44,44,44,44	0
56	MG	AA	3214	1/1	0.97	0.15	-	44,44,44,44	0
56	MG	DA	3483	1/1	0.92	0.38	-	48,48,48,48	0
56	MG	DA	3074	1/1	0.95	0.22	-	50,50,50,50	0
56	MG	AA	3071	1/1	0.85	0.25	-	62,62,62,62	0
56	MG	CA	3038	1/1	0.93	0.19	-	46,46,46,46	0
56	MG	AX	3008	1/1	0.89	0.36	-	57,57,57,57	0
56	MG	BA	3446	1/1	0.70	0.27	-	52,52,52,52	0
56	MG	DF	301	1/1	0.92	0.15	-	47,47,47,47	0
56	MG	BA	3169	1/1	0.95	0.25	-	47,47,47,47	0
56	MG	DA	3186	1/1	0.86	0.23	-	40,40,40,40	0
56	MG	D8	5001	1/1	0.88	0.23	-	55,55,55,55	0
56	MG	CA	3050	1/1	0.97	0.14	-	60,60,60,60	0
56	MG	BA	3802	1/1	0.85	0.13	-	56,56,56,56	0
56	MG	DA	3539	1/1	0.91	0.14	-	46,46,46,46	0
56	MG	BA	3391	1/1	0.97	0.14	-	41,41,41,41	0
56	MG	BA	3198	1/1	0.88	0.17	-	55,55,55,55	0
56	MG	BA	3113	1/1	0.87	0.32	-	58,58,58,58	0
56	MG	AA	3028	1/1	0.94	0.38	-	56,56,56,56	0
56	MG	AA	3126	1/1	0.94	0.17	-	46,46,46,46	0
56	MG	DA	3456	1/1	0.97	0.20	-	49,49,49,49	0
56	MG	DA	3286	1/1	0.77	0.14	-	64,64,64,64	0
56	MG	DA	3058	1/1	0.95	0.21	-	46,46,46,46	0
56	MG	BA	3458	1/1	0.99	0.25	-	19,19,19,19	0
56	MG	AA	3057	1/1	0.90	0.20	-	61,61,61,61	0
56	MG	CA	3149	1/1	0.95	0.27	-	65,65,65,65	0
56	MG	AX	3011	1/1	0.96	0.16	-	50,50,50,50	0
56	MG	DA	3476	1/1	0.98	0.24	-	45,45,45,45	0
56	MG	DA	3309	1/1	0.81	0.14	-	42,42,42,42	0
56	MG	BA	3095	1/1	0.80	0.30	-	53,53,53,53	0
56	MG	BA	3650	1/1	0.91	0.12	-	57,57,57,57	0
56	MG	DA	3054	1/1	0.94	0.15	-	43,43,43,43	0
56	MG	BA	3176	1/1	0.96	0.29	-	55,55,55,55	0
56	MG	AW	3002	1/1	0.81	0.17	-	69,69,69,69	0
56	MG	AA	3061	1/1	0.92	0.08	-	54,54,54,54	0
56	MG	DA	3498	1/1	0.93	0.09	-	57,57,57,57	0
56	MG	DA	3292	1/1	0.98	0.12	-	37,37,37,37	0
56	MG	BA	3017	1/1	0.85	0.22	-	50,50,50,50	0
56	MG	CA	3032	1/1	0.93	0.23	-	52,52,52,52	0
56	MG	AA	3112	1/1	0.85	0.14	-	57,57,57,57	0
56	MG	BA	3778	1/1	0.89	0.13	-	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3139	1/1	0.90	0.09	-	61,61,61,61	0
56	MG	DA	3056	1/1	0.97	0.25	-	44,44,44,44	0
56	MG	DA	3486	1/1	0.96	0.21	-	44,44,44,44	0
56	MG	BA	3532	1/1	0.95	0.27	-	49,49,49,49	0
56	MG	BA	3499	1/1	0.95	0.24	-	33,33,33,33	0
56	MG	AA	3123	1/1	0.97	0.17	-	57,57,57,57	0
56	MG	BA	3351	1/1	0.92	0.17	-	34,34,34,34	0
56	MG	BA	3154	1/1	0.97	0.28	-	29,29,29,29	0
56	MG	BA	3046	1/1	0.89	0.18	-	43,43,43,43	0
56	MG	DA	3336	1/1	0.97	0.09	-	47,47,47,47	0
56	MG	BA	3353	1/1	0.98	0.10	-	49,49,49,49	0
56	MG	BA	3255	1/1	0.89	0.26	-	58,58,58,58	0
56	MG	DA	3396	1/1	0.89	0.13	-	45,45,45,45	0
56	MG	BA	3418	1/1	0.98	0.16	-	32,32,32,32	0
56	MG	CA	3088	1/1	0.99	0.41	-	53,53,53,53	0
56	MG	DA	3231	1/1	0.84	0.32	-	57,57,57,57	0
56	MG	AA	3155	1/1	0.88	0.18	-	53,53,53,53	0
56	MG	DA	3169	1/1	0.96	0.14	-	49,49,49,49	0
56	MG	BA	3111	1/1	0.97	0.23	-	47,47,47,47	0
56	MG	DA	3488	1/1	0.95	0.13	-	37,37,37,37	0
56	MG	BA	3706	1/1	0.83	0.23	-	50,50,50,50	0
56	MG	DA	3253	1/1	0.97	0.22	-	38,38,38,38	0
56	MG	BA	3624	1/1	0.97	0.18	-	29,29,29,29	0
56	MG	BE	304	1/1	0.94	0.26	-	40,40,40,40	0
56	MG	AA	3025	1/1	0.96	0.12	-	43,43,43,43	0
56	MG	BA	3442	1/1	0.83	0.11	-	59,59,59,59	0
56	MG	BA	3777	1/1	0.88	0.23	-	49,49,49,49	0
56	MG	DA	3065	1/1	0.94	0.08	-	56,56,56,56	0
56	MG	BP	203	1/1	0.95	0.12	-	32,32,32,32	0
56	MG	BA	3810	1/1	0.93	0.25	-	50,50,50,50	0
56	MG	DA	3580	1/1	0.84	0.19	-	64,64,64,64	0
56	MG	BA	3808	1/1	0.92	0.14	-	34,34,34,34	0
56	MG	BA	3368	1/1	0.99	0.19	-	12,12,12,12	0
56	MG	BA	3479	1/1	0.98	0.14	-	37,37,37,37	0
56	MG	BA	3003	1/1	0.99	0.26	-	20,20,20,20	0
56	MG	DA	3106	1/1	0.86	0.27	-	61,61,61,61	0
56	MG	AA	3140	1/1	0.93	0.11	-	71,71,71,71	0
56	MG	BA	3145	1/1	0.93	0.27	-	32,32,32,32	0
56	MG	BA	3089	1/1	0.90	0.29	-	45,45,45,45	0
56	MG	DA	3475	1/1	0.95	0.13	-	42,42,42,42	0
56	MG	BA	3143	1/1	0.90	0.25	-	42,42,42,42	0
56	MG	BA	3711	1/1	0.93	0.26	-	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3043	1/1	0.91	0.17	-	48,48,48,48	0
56	MG	AA	3156	1/1	0.91	0.14	-	52,52,52,52	0
56	MG	BA	3726	1/1	0.65	0.23	-	70,70,70,70	0
56	MG	DA	3339	1/1	0.98	0.10	-	52,52,52,52	0
56	MG	BA	3717	1/1	0.86	0.19	-	58,58,58,58	0
56	MG	DD	301	1/1	0.97	0.37	-	39,39,39,39	0
56	MG	DA	3408	1/1	0.88	0.22	-	48,48,48,48	0
56	MG	DA	3386	1/1	0.96	0.17	-	48,48,48,48	0
56	MG	BA	3274	1/1	0.86	0.16	-	49,49,49,49	0
56	MG	BA	3455	1/1	0.87	0.17	-	39,39,39,39	0
56	MG	DA	3433	1/1	0.98	0.20	-	61,61,61,61	0
56	MG	CA	3164	1/1	0.90	0.07	-	54,54,54,54	0
56	MG	B9	502	1/1	0.92	0.10	-	57,57,57,57	0
56	MG	CJ	5001	1/1	0.53	0.14	-	76,76,76,76	0
56	MG	DA	3073	1/1	0.94	0.16	-	54,54,54,54	0
56	MG	CA	3001	1/1	0.94	0.25	-	73,73,73,73	0
56	MG	BA	3654	1/1	0.94	0.15	-	55,55,55,55	0
56	MG	BA	3557	1/1	0.87	0.22	-	56,56,56,56	0
56	MG	DA	3381	1/1	0.94	0.11	-	60,60,60,60	0
56	MG	DA	3458	1/1	0.94	0.11	-	42,42,42,42	0
56	MG	DA	3076	1/1	0.95	0.22	-	43,43,43,43	0
56	MG	BA	3683	1/1	0.64	0.15	-	61,61,61,61	0
56	MG	BA	3629	1/1	0.84	0.14	-	56,56,56,56	0
56	MG	BA	3505	1/1	0.94	0.12	-	54,54,54,54	0
56	MG	DA	3574	1/1	0.90	0.20	-	51,51,51,51	0
56	MG	DA	3426	1/1	0.95	0.17	-	41,41,41,41	0
56	MG	DA	3177	1/1	0.96	0.17	-	54,54,54,54	0
56	MG	DA	3648	1/1	0.90	0.12	-	60,60,60,60	0
56	MG	DA	3283	1/1	0.94	0.25	-	46,46,46,46	0
56	MG	DA	3027	1/1	0.92	0.21	-	53,53,53,53	0
56	MG	DA	3524	1/1	0.98	0.06	-	38,38,38,38	0
56	MG	CA	3024	1/1	0.90	0.14	-	63,63,63,63	0
56	MG	BA	3241	1/1	0.78	0.23	-	52,52,52,52	0
56	MG	BA	3265	1/1	0.98	0.27	-	29,29,29,29	0
56	MG	DA	3034	1/1	0.88	0.15	-	43,43,43,43	0
56	MG	DA	3579	1/1	0.96	0.07	-	55,55,55,55	0
56	MG	BA	3432	1/1	0.95	0.10	-	52,52,52,52	0
56	MG	BA	3267	1/1	0.94	0.14	-	37,37,37,37	0
56	MG	DA	3417	1/1	0.95	0.22	-	33,33,33,33	0
56	MG	BA	3028	1/1	0.79	0.14	-	59,59,59,59	0
56	MG	DA	3145	1/1	0.89	0.32	-	49,49,49,49	0
56	MG	DA	3369	1/1	0.93	0.05	-	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	3159	1/1	0.92	0.13	-	57,57,57,57	0
56	MG	AA	3166	1/1	0.93	0.13	-	65,65,65,65	0
56	MG	AX	3006	1/1	0.93	0.18	-	74,74,74,74	0
56	MG	DA	3367	1/1	0.92	0.08	-	51,51,51,51	0
56	MG	BA	3668	1/1	0.87	0.18	-	56,56,56,56	0
56	MG	BA	3100	1/1	0.85	0.14	-	45,45,45,45	0
56	MG	BA	3750	1/1	0.94	0.21	-	49,49,49,49	0
56	MG	BE	306	1/1	0.88	0.23	-	25,25,25,25	0
56	MG	DA	3659	1/1	0.94	0.48	-	67,67,67,67	0
56	MG	DA	3025	1/1	0.92	0.16	-	44,44,44,44	0
56	MG	BA	3137	1/1	0.94	0.24	-	45,45,45,45	0
56	MG	DA	3234	1/1	0.83	0.19	-	45,45,45,45	0
56	MG	DA	3365	1/1	0.91	0.34	-	57,57,57,57	0
56	MG	BA	3087	1/1	0.97	0.12	-	37,37,37,37	0
56	MG	DA	3558	1/1	0.96	0.25	-	34,34,34,34	0
56	MG	DA	3154	1/1	0.95	0.32	-	52,52,52,52	0
56	MG	DA	3532	1/1	0.98	0.14	-	57,57,57,57	0
56	MG	BA	3599	1/1	0.98	0.20	-	23,23,23,23	0
56	MG	DA	3469	1/1	0.97	0.13	-	54,54,54,54	0
56	MG	AA	3197	1/1	0.89	0.14	-	56,56,56,56	0
56	MG	BA	3427	1/1	0.89	0.25	-	32,32,32,32	0
56	MG	DA	3001	1/1	0.91	0.26	-	58,58,58,58	0
56	MG	BA	3556	1/1	0.97	0.11	-	45,45,45,45	0
56	MG	DA	3105	1/1	0.79	0.19	-	60,60,60,60	0
56	MG	BA	3721	1/1	0.93	0.18	-	47,47,47,47	0
56	MG	BA	3591	1/1	0.97	0.21	-	23,23,23,23	0
56	MG	BA	3695	1/1	0.86	0.22	-	48,48,48,48	0
56	MG	BA	3773	1/1	0.93	0.22	-	49,49,49,49	0
56	MG	AA	3159	1/1	0.86	0.09	-	59,59,59,59	0
56	MG	AW	3007	1/1	0.97	0.05	-	64,64,64,64	0
56	MG	DA	3147	1/1	0.92	0.09	-	44,44,44,44	0
56	MG	AA	3165	1/1	0.84	0.25	-	60,60,60,60	0
56	MG	BA	3473	1/1	0.96	0.27	-	57,57,57,57	0
56	MG	AA	3046	1/1	0.95	0.16	-	56,56,56,56	0
56	MG	AA	3119	1/1	0.94	0.10	-	58,58,58,58	0
56	MG	BA	3360	1/1	0.91	0.09	-	50,50,50,50	0
56	MG	DA	3346	1/1	0.97	0.15	-	35,35,35,35	0
56	MG	CA	3135	1/1	0.95	0.11	-	53,53,53,53	0
56	MG	DA	3195	1/1	0.92	0.19	-	57,57,57,57	0
56	MG	BA	3065	1/1	0.91	0.12	-	37,37,37,37	0
56	MG	BA	3093	1/1	0.90	0.32	-	38,38,38,38	0
56	MG	DA	3577	1/1	0.93	0.14	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3465	1/1	0.97	0.19	-	42,42,42,42	0
56	MG	DA	3087	1/1	0.90	0.21	-	49,49,49,49	0
56	MG	DA	3323	1/1	0.89	0.32	-	53,53,53,53	0
56	MG	BA	3730	1/1	0.98	0.13	-	27,27,27,27	0
56	MG	DA	3459	1/1	0.97	0.07	-	57,57,57,57	0
56	MG	BR	204	1/1	0.97	0.36	-	42,42,42,42	0
56	MG	DA	3569	1/1	0.85	0.21	-	57,57,57,57	0
56	MG	BA	3575	1/1	0.94	0.09	-	64,64,64,64	0
56	MG	CA	3113	1/1	0.94	0.11	-	55,55,55,55	0
56	MG	CA	3086	1/1	0.91	0.12	-	61,61,61,61	0
56	MG	AA	3085	1/1	0.83	0.15	-	55,55,55,55	0
56	MG	BA	3577	1/1	0.95	0.19	-	60,60,60,60	0
56	MG	DA	3130	1/1	0.95	0.25	-	47,47,47,47	0
56	MG	BA	3224	1/1	0.60	0.18	-	64,64,64,64	0
56	MG	DA	3216	1/1	0.94	0.29	-	46,46,46,46	0
56	MG	DA	3427	1/1	0.97	0.08	-	38,38,38,38	0
56	MG	CA	3169	1/1	0.79	0.21	-	65,65,65,65	0
56	MG	DA	3378	1/1	0.92	0.13	-	45,45,45,45	0
56	MG	AA	3010	1/1	0.95	0.14	-	59,59,59,59	0
56	MG	BA	3734	1/1	0.72	0.35	-	60,60,60,60	0
56	MG	BA	3558	1/1	0.95	0.19	-	29,29,29,29	0
56	MG	DA	3101	1/1	0.90	0.12	-	53,53,53,53	0
56	MG	AA	3177	1/1	0.96	0.14	-	57,57,57,57	0
56	MG	BA	3208	1/1	0.96	0.32	-	48,48,48,48	0
56	MG	BA	3141	1/1	0.94	0.23	-	38,38,38,38	0
56	MG	AA	3058	1/1	0.90	0.21	-	57,57,57,57	0
56	MG	DA	3213	1/1	0.81	0.23	-	61,61,61,61	0
56	MG	BA	3193	1/1	0.98	0.28	-	57,57,57,57	0
56	MG	BA	3281	1/1	0.94	0.17	-	49,49,49,49	0
56	MG	B2	3001	1/1	0.89	0.17	-	45,45,45,45	0
56	MG	DA	3215	1/1	0.98	0.20	-	37,37,37,37	0
56	MG	DA	3621	1/1	0.90	0.29	-	45,45,45,45	0
56	MG	BA	3457	1/1	0.94	0.21	-	44,44,44,44	0
56	MG	DA	3637	1/1	0.98	0.06	-	44,44,44,44	0
56	MG	B3	103	1/1	0.96	0.07	-	45,45,45,45	0
56	MG	AA	3039	1/1	0.94	0.15	-	61,61,61,61	0
56	MG	BA	3795	1/1	0.97	0.16	-	53,53,53,53	0
56	MG	BA	3804	1/1	0.66	0.10	-	58,58,58,58	0
56	MG	DA	3645	1/1	0.80	0.20	-	44,44,44,44	0
56	MG	BA	3364	1/1	0.90	0.15	-	42,42,42,42	0
56	MG	BA	3406	1/1	0.95	0.19	-	32,32,32,32	0
56	MG	DA	3197	1/1	0.88	0.15	-	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3736	1/1	0.84	0.17	-	56,56,56,56	0
56	MG	DA	3061	1/1	0.90	0.21	-	56,56,56,56	0
56	MG	DA	3347	1/1	0.95	0.16	-	44,44,44,44	0
56	MG	BA	3023	1/1	0.90	0.27	-	55,55,55,55	0
56	MG	BA	3682	1/1	0.99	0.13	-	50,50,50,50	0
56	MG	BA	3716	1/1	0.84	0.23	-	54,54,54,54	0
56	MG	DA	3337	1/1	0.95	0.09	-	43,43,43,43	0
56	MG	BA	3399	1/1	0.94	0.16	-	25,25,25,25	0
56	MG	CA	3150	1/1	0.95	0.16	-	62,62,62,62	0
56	MG	AA	3101	1/1	0.92	0.17	-	54,54,54,54	0
56	MG	BA	3483	1/1	0.95	0.28	-	38,38,38,38	0
56	MG	DA	3573	1/1	0.97	0.31	-	46,46,46,46	0
56	MG	BA	3569	1/1	0.90	0.32	-	57,57,57,57	0
56	MG	DA	3398	1/1	0.94	0.18	-	57,57,57,57	0
56	MG	DA	3357	1/1	0.95	0.14	-	44,44,44,44	0
56	MG	DA	3561	1/1	0.93	0.22	-	48,48,48,48	0
56	MG	DA	3429	1/1	0.82	0.26	-	40,40,40,40	0
56	MG	BA	3226	1/1	0.98	0.24	-	41,41,41,41	0
56	MG	BA	3489	1/1	0.97	0.11	-	44,44,44,44	0
56	MG	B3	101	1/1	0.89	0.31	-	48,48,48,48	0
56	MG	DA	3540	1/1	0.81	0.18	-	67,67,67,67	0
56	MG	BA	3031	1/1	0.91	0.23	-	56,56,56,56	0
56	MG	BA	3203	1/1	0.86	0.15	-	39,39,39,39	0
56	MG	BA	3146	1/1	0.96	0.19	-	42,42,42,42	0
56	MG	BA	3378	1/1	0.94	0.10	-	34,34,34,34	0
56	MG	BA	3631	1/1	0.95	0.14	-	43,43,43,43	0
56	MG	DA	3251	1/1	0.75	0.27	-	51,51,51,51	0
56	MG	BA	3189	1/1	0.96	0.16	-	30,30,30,30	0
56	MG	DA	3465	1/1	0.98	0.07	-	55,55,55,55	0
56	MG	BA	3344	1/1	0.92	0.14	-	37,37,37,37	0
56	MG	BA	3323	1/1	0.93	0.22	-	39,39,39,39	0
56	MG	AA	3034	1/1	0.95	0.26	-	48,48,48,48	0
56	MG	BA	3491	1/1	0.89	0.23	-	47,47,47,47	0
56	MG	DA	3185	1/1	0.95	0.24	-	54,54,54,54	0
56	MG	BA	3049	1/1	0.90	0.27	-	37,37,37,37	0
56	MG	BA	3688	1/1	0.94	0.20	-	45,45,45,45	0
56	MG	DA	3585	1/1	0.91	0.10	-	51,51,51,51	0
56	MG	DA	3373	1/1	0.96	0.10	-	31,31,31,31	0
56	MG	BA	3560	1/1	0.75	0.23	-	35,35,35,35	0
56	MG	AA	3032	1/1	0.87	0.09	-	75,75,75,75	0
56	MG	BA	3238	1/1	0.83	0.25	-	43,43,43,43	0
56	MG	DA	3487	1/1	0.78	0.24	-	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3622	1/1	0.97	0.18	-	53,53,53,53	0
56	MG	BA	3492	1/1	0.90	0.12	-	55,55,55,55	0
56	MG	DA	3301	1/1	0.98	0.23	-	48,48,48,48	0
56	MG	AA	3055	1/1	0.90	0.22	-	58,58,58,58	0
56	MG	CA	3016	1/1	0.86	0.10	-	61,61,61,61	0
56	MG	DA	3658	1/1	0.96	0.39	-	37,37,37,37	0
56	MG	BA	3244	1/1	0.93	0.10	-	63,63,63,63	0
56	MG	DA	3258	1/1	0.94	0.18	-	59,59,59,59	0
56	MG	BG	201	1/1	0.97	0.09	-	57,57,57,57	0
56	MG	BA	3068	1/1	0.96	0.26	-	51,51,51,51	0
56	MG	DA	3392	1/1	0.97	0.15	-	36,36,36,36	0
56	MG	B0	102	1/1	0.96	0.12	-	68,68,68,68	0
56	MG	DB	3011	1/1	0.91	0.09	-	52,52,52,52	0
56	MG	BA	3563	1/1	0.95	0.08	-	60,60,60,60	0
56	MG	BA	3586	1/1	0.87	0.16	-	65,65,65,65	0
56	MG	BA	3603	1/1	0.82	0.11	-	54,54,54,54	0
56	MG	BA	3666	1/1	0.91	0.12	-	58,58,58,58	0
56	MG	BA	3496	1/1	0.98	0.24	-	39,39,39,39	0
56	MG	AA	3191	1/1	0.95	0.24	-	48,48,48,48	0
56	MG	AA	3220	1/1	0.95	0.07	-	64,64,64,64	0
56	MG	CA	3100	1/1	0.95	0.23	-	62,62,62,62	0
56	MG	CA	3116	1/1	0.96	0.07	-	55,55,55,55	0
56	MG	BA	3060	1/1	0.87	0.20	-	56,56,56,56	0
56	MG	CA	3046	1/1	0.91	0.09	-	56,56,56,56	0
56	MG	CA	3130	1/1	0.96	0.12	-	60,60,60,60	0
56	MG	DA	3059	1/1	0.94	0.45	-	53,53,53,53	0
56	MG	BA	3701	1/1	0.91	0.14	-	51,51,51,51	0
56	MG	BA	3508	1/1	0.89	0.09	-	54,54,54,54	0
56	MG	DA	3654	1/1	0.97	0.11	-	55,55,55,55	0
56	MG	BA	3221	1/1	0.74	0.20	-	54,54,54,54	0
56	MG	BB	3006	1/1	0.97	0.14	-	38,38,38,38	0
56	MG	BA	3239	1/1	0.96	0.14	-	31,31,31,31	0
56	MG	CA	3163	1/1	0.96	0.17	-	53,53,53,53	0
56	MG	AA	3059	1/1	0.85	0.29	-	59,59,59,59	0
56	MG	CA	3013	1/1	0.90	0.10	-	63,63,63,63	0
56	MG	BA	3486	1/1	0.95	0.23	-	48,48,48,48	0
56	MG	DA	3110	1/1	0.83	0.13	-	50,50,50,50	0
56	MG	BA	3029	1/1	0.97	0.30	-	46,46,46,46	0
56	MG	DA	3136	1/1	0.96	0.22	-	44,44,44,44	0
56	MG	DA	3590	1/1	0.96	0.19	-	60,60,60,60	0
56	MG	CA	3064	1/1	0.67	0.11	-	57,57,57,57	0
56	MG	BA	3529	1/1	0.93	0.16	-	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3344	1/1	0.97	0.09	-	44,44,44,44	0
56	MG	DA	3341	1/1	0.96	0.21	-	31,31,31,31	0
56	MG	AA	3053	1/1	0.94	0.37	-	49,49,49,49	0
56	MG	DA	3235	1/1	0.87	0.28	-	61,61,61,61	0
56	MG	DA	3361	1/1	0.98	0.36	-	55,55,55,55	0
56	MG	CA	3114	1/1	0.92	0.20	-	56,56,56,56	0
56	MG	DA	3161	1/1	0.98	0.20	-	49,49,49,49	0
56	MG	BA	3395	1/1	0.97	0.19	-	44,44,44,44	0
56	MG	CA	3148	1/1	0.92	0.11	-	67,67,67,67	0
56	MG	BA	3309	1/1	0.95	0.06	-	55,55,55,55	0
56	MG	AA	3210	1/1	0.92	0.19	-	69,69,69,69	0
56	MG	DA	3395	1/1	0.88	0.19	-	42,42,42,42	0
56	MG	BA	3091	1/1	0.98	0.32	-	38,38,38,38	0
56	MG	BB	3021	1/1	0.95	0.12	-	54,54,54,54	0
56	MG	BA	3036	1/1	0.97	0.18	-	26,26,26,26	0
56	MG	DA	3630	1/1	0.89	0.17	-	49,49,49,49	0
56	MG	DA	3511	1/1	0.94	0.11	-	45,45,45,45	0
56	MG	CA	3152	1/1	0.84	0.36	-	79,79,79,79	0
56	MG	BA	3828	1/1	0.90	0.20	-	37,37,37,37	0
56	MG	DA	3618	1/1	0.92	0.26	-	54,54,54,54	0
56	MG	CA	3092	1/1	0.92	0.15	-	44,44,44,44	0
56	MG	BA	3388	1/1	0.95	0.13	-	52,52,52,52	0
56	MG	BA	3006	1/1	0.96	0.15	-	52,52,52,52	0
56	MG	DA	3037	1/1	0.81	0.16	-	54,54,54,54	0
56	MG	AA	3188	1/1	0.94	0.16	-	56,56,56,56	0
56	MG	AA	3062	1/1	0.81	0.14	-	60,60,60,60	0
56	MG	DA	3316	1/1	0.98	0.06	-	44,44,44,44	0
56	MG	CA	3008	1/1	0.97	0.12	-	50,50,50,50	0
56	MG	CA	3133	1/1	0.85	0.20	-	65,65,65,65	0
56	MG	BA	3638	1/1	0.87	0.26	-	38,38,38,38	0
56	MG	BA	3510	1/1	0.98	0.08	-	48,48,48,48	0
56	MG	BA	3314	1/1	0.91	0.15	-	47,47,47,47	0
56	MG	BF	311	1/1	0.94	0.18	-	43,43,43,43	0
56	MG	BA	3791	1/1	0.89	0.13	-	47,47,47,47	0
56	MG	AA	3110	1/1	0.65	0.22	-	61,61,61,61	0
56	MG	DA	3461	1/1	0.93	0.13	-	56,56,56,56	0
56	MG	BA	3524	1/1	0.88	0.13	-	53,53,53,53	0
56	MG	BD	301	1/1	0.93	0.20	-	49,49,49,49	0
56	MG	AA	3158	1/1	0.90	0.27	-	59,59,59,59	0
56	MG	BA	3223	1/1	0.94	0.16	-	29,29,29,29	0
56	MG	BA	3705	1/1	0.83	0.17	-	54,54,54,54	0
56	MG	DA	3009	1/1	0.97	0.19	-	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3192	1/1	0.84	0.25	-	48,48,48,48	0
56	MG	CX	3004	1/1	0.89	0.33	-	54,54,54,54	0
56	MG	AA	3096	1/1	0.94	0.27	-	48,48,48,48	0
56	MG	CA	3125	1/1	0.89	0.14	-	64,64,64,64	0
56	MG	AY	3001	1/1	0.96	0.31	-	70,70,70,70	0
56	MG	BA	3468	1/1	0.96	0.23	-	49,49,49,49	0
56	MG	AA	3083	1/1	0.93	0.15	-	52,52,52,52	0
56	MG	DE	304	1/1	0.92	0.22	-	47,47,47,47	0
56	MG	BW	202	1/1	0.90	0.31	-	49,49,49,49	0
56	MG	DA	3238	1/1	0.73	0.24	-	61,61,61,61	0
56	MG	DA	3018	1/1	0.99	0.18	-	41,41,41,41	0
56	MG	DB	3007	1/1	0.95	0.09	-	59,59,59,59	0
56	MG	DA	3393	1/1	0.81	0.10	-	52,52,52,52	0
56	MG	BA	3273	1/1	0.90	0.29	-	53,53,53,53	0
56	MG	CY	3001	1/1	0.96	0.26	-	58,58,58,58	0
56	MG	DA	3478	1/1	0.94	0.18	-	47,47,47,47	0
56	MG	AA	3215	1/1	0.92	0.19	-	57,57,57,57	0
56	MG	DA	3512	1/1	0.96	0.22	-	46,46,46,46	0
56	MG	BA	3275	1/1	0.88	0.13	-	46,46,46,46	0
56	MG	DA	3544	1/1	0.98	0.14	-	37,37,37,37	0
56	MG	CA	3045	1/1	0.97	0.36	-	58,58,58,58	0
56	MG	BA	3728	1/1	0.70	0.10	-	72,72,72,72	0
56	MG	BA	3092	1/1	0.93	0.27	-	41,41,41,41	0
56	MG	BA	3642	1/1	0.95	0.09	-	37,37,37,37	0
56	MG	CA	3019	1/1	0.86	0.39	-	58,58,58,58	0
56	MG	AA	3033	1/1	0.90	0.15	-	57,57,57,57	0
56	MG	AA	3054	1/1	0.93	0.43	-	52,52,52,52	0
56	MG	DA	3578	1/1	0.93	0.10	-	55,55,55,55	0
56	MG	BA	3179	1/1	0.88	0.19	-	39,39,39,39	0
56	MG	DA	3525	1/1	0.95	0.17	-	41,41,41,41	0
56	MG	DA	3394	1/1	0.92	0.14	-	49,49,49,49	0
56	MG	AA	3200	1/1	0.97	0.22	-	45,45,45,45	0
56	MG	DA	3596	1/1	0.66	0.44	-	63,63,63,63	0
56	MG	BA	3067	1/1	0.95	0.23	-	49,49,49,49	0
56	MG	CA	3146	1/1	0.89	0.05	-	69,69,69,69	0
56	MG	BA	3064	1/1	0.83	0.36	-	61,61,61,61	0
56	MG	DA	3342	1/1	0.94	0.10	-	56,56,56,56	0
56	MG	DN	5001	1/1	0.95	0.07	-	62,62,62,62	0
56	MG	DA	3520	1/1	0.97	0.05	-	48,48,48,48	0
56	MG	BA	3509	1/1	0.92	0.25	-	39,39,39,39	0
56	MG	BA	3308	1/1	0.96	0.21	-	39,39,39,39	0
56	MG	DA	3442	1/1	0.93	0.15	-	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3390	1/1	0.95	0.21	-	52,52,52,52	0
56	MG	DA	3178	1/1	0.90	0.12	-	54,54,54,54	0
56	MG	BA	3549	1/1	0.97	0.19	-	37,37,37,37	0
56	MG	BA	3742	1/1	0.83	0.17	-	51,51,51,51	0
56	MG	DA	3205	1/1	0.93	0.21	-	47,47,47,47	0
56	MG	BA	3397	1/1	0.96	0.23	-	53,53,53,53	0
56	MG	CA	3109	1/1	0.93	0.24	-	68,68,68,68	0
56	MG	DA	3657	1/1	0.87	0.10	-	67,67,67,67	0
56	MG	BA	3429	1/1	0.91	0.24	-	47,47,47,47	0
56	MG	BA	3078	1/1	0.98	0.19	-	17,17,17,17	0
56	MG	DA	3129	1/1	0.96	0.12	-	45,45,45,45	0
56	MG	BA	3287	1/1	0.92	0.29	-	54,54,54,54	0
56	MG	DA	3505	1/1	0.68	0.12	-	66,66,66,66	0
56	MG	AA	3141	1/1	0.95	0.10	-	55,55,55,55	0
56	MG	BA	3747	1/1	0.86	0.27	-	42,42,42,42	0
56	MG	BB	3020	1/1	0.92	0.16	-	54,54,54,54	0
56	MG	BA	3821	1/1	0.98	0.17	-	50,50,50,50	0
56	MG	CA	3042	1/1	0.97	0.12	-	58,58,58,58	0
56	MG	BA	3259	1/1	0.92	0.40	-	52,52,52,52	0
56	MG	AA	3121	1/1	0.96	0.15	-	66,66,66,66	0
56	MG	CA	3115	1/1	0.89	0.18	-	62,62,62,62	0
56	MG	BA	3207	1/1	0.89	0.18	-	38,38,38,38	0
56	MG	DA	3217	1/1	0.96	0.14	-	50,50,50,50	0
56	MG	DA	3457	1/1	0.88	0.23	-	47,47,47,47	0
56	MG	AA	3075	1/1	0.95	0.22	-	33,33,33,33	0
56	MG	DA	3510	1/1	0.97	0.24	-	50,50,50,50	0
56	MG	AA	3201	1/1	0.97	0.07	-	59,59,59,59	0
56	MG	AA	3193	1/1	0.98	0.09	-	43,43,43,43	0
56	MG	CA	3117	1/1	0.91	0.10	-	48,48,48,48	0
56	MG	DA	3038	1/1	0.97	0.43	-	47,47,47,47	0
56	MG	CA	3127	1/1	0.97	0.17	-	44,44,44,44	0
56	MG	CA	3085	1/1	0.88	0.20	-	71,71,71,71	0
56	MG	DA	3635	1/1	0.92	0.15	-	52,52,52,52	0
56	MG	BA	3358	1/1	0.89	0.42	-	64,64,64,64	0
56	MG	CA	3106	1/1	0.98	0.16	-	50,50,50,50	0
56	MG	CA	3145	1/1	0.95	0.13	-	63,63,63,63	0
56	MG	BA	3485	1/1	0.95	0.23	-	46,46,46,46	0
56	MG	AA	3213	1/1	0.90	0.08	-	69,69,69,69	0
56	MG	DA	3266	1/1	0.96	0.10	-	47,47,47,47	0
56	MG	DA	3174	1/1	0.95	0.17	-	48,48,48,48	0
56	MG	BR	203	1/1	0.82	0.20	-	44,44,44,44	0
56	MG	AA	3170	1/1	0.83	0.13	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3508	1/1	0.79	0.10	-	59,59,59,59	0
56	MG	BB	3008	1/1	0.83	0.30	-	54,54,54,54	0
56	MG	CA	3162	1/1	0.92	0.14	-	67,67,67,67	0
56	MG	DA	3559	1/1	0.93	0.18	-	48,48,48,48	0
56	MG	BA	3125	1/1	0.93	0.14	-	42,42,42,42	0
56	MG	DY	502	1/1	0.97	0.12	-	52,52,52,52	0
56	MG	DA	3667	1/1	0.92	0.96	-	73,73,73,73	0
56	MG	CX	3002	1/1	0.83	0.20	-	81,81,81,81	0
56	MG	BA	3621	1/1	0.99	0.23	-	52,52,52,52	0
56	MG	BA	3673	1/1	0.85	0.16	-	47,47,47,47	0
56	MG	DA	3467	1/1	0.94	0.31	-	43,43,43,43	0
56	MG	BZ	3001	1/1	0.88	0.22	-	52,52,52,52	0
56	MG	DA	3556	1/1	0.92	0.19	-	64,64,64,64	0
56	MG	BA	3135	1/1	0.95	0.21	-	35,35,35,35	0
56	MG	AA	3202	1/1	0.86	0.15	-	57,57,57,57	0
56	MG	AA	3183	1/1	0.91	0.14	-	71,71,71,71	0
56	MG	BA	3764	1/1	0.96	0.12	-	58,58,58,58	0
56	MG	BA	3761	1/1	0.94	0.19	-	54,54,54,54	0
56	MG	CA	3118	1/1	0.94	0.18	-	47,47,47,47	0
56	MG	BA	3749	1/1	0.90	0.25	-	45,45,45,45	0
56	MG	BA	3517	1/1	0.95	0.12	-	51,51,51,51	0
56	MG	BA	3377	1/1	0.78	0.23	-	30,30,30,30	0
56	MG	BA	3623	1/1	0.92	0.13	-	52,52,52,52	0
56	MG	BE	307	1/1	0.86	0.20	-	70,70,70,70	0
56	MG	DA	3114	1/1	0.97	0.13	-	28,28,28,28	0
56	MG	BA	3147	1/1	0.96	0.13	-	30,30,30,30	0
56	MG	CA	3160	1/1	0.95	0.16	-	65,65,65,65	0
56	MG	BA	3803	1/1	0.93	0.09	-	47,47,47,47	0
56	MG	DA	3502	1/1	0.92	0.20	-	64,64,64,64	0
56	MG	BA	3812	1/1	0.91	0.18	-	52,52,52,52	0
56	MG	DA	3617	1/1	0.95	0.36	-	53,53,53,53	0
56	MG	AA	3217	1/1	0.96	0.16	-	55,55,55,55	0
56	MG	DA	3560	1/1	0.98	0.19	-	34,34,34,34	0
56	MG	CW	3002	1/1	0.95	0.16	-	74,74,74,74	0
56	MG	AA	3171	1/1	0.93	0.10	-	48,48,48,48	0
56	MG	DA	3371	1/1	0.97	0.17	-	55,55,55,55	0
56	MG	BQ	3004	1/1	0.95	0.24	-	35,35,35,35	0
56	MG	DA	3200	1/1	0.97	0.35	-	43,43,43,43	0
56	MG	CA	3107	1/1	0.95	0.10	-	66,66,66,66	0
56	MG	DA	3445	1/1	0.78	0.23	-	72,72,72,72	0
56	MG	DA	3120	1/1	0.97	0.19	-	45,45,45,45	0
56	MG	CA	3009	1/1	0.96	0.22	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	3132	1/1	0.95	0.13	-	22,22,22,22	0
56	MG	AA	3142	1/1	0.85	0.23	-	62,62,62,62	0
56	MG	BA	3703	1/1	0.89	0.23	-	48,48,48,48	0
56	MG	BA	3733	1/1	0.96	0.26	-	41,41,41,41	0
56	MG	DA	3150	1/1	0.93	0.06	-	41,41,41,41	0
56	MG	BA	3306	1/1	0.94	0.18	-	31,31,31,31	0
56	MG	BB	3015	1/1	0.75	0.10	-	51,51,51,51	0
56	MG	DB	3009	1/1	0.96	0.19	-	47,47,47,47	0
56	MG	DA	3399	1/1	0.88	0.18	-	47,47,47,47	0
56	MG	BA	3497	1/1	0.97	0.21	-	41,41,41,41	0
56	MG	DA	3121	1/1	0.81	0.28	-	41,41,41,41	0
56	MG	BA	3684	1/1	0.96	0.20	-	49,49,49,49	0
56	MG	CA	3168	1/1	0.94	0.19	-	72,72,72,72	0
56	MG	BA	3079	1/1	0.72	0.32	-	57,57,57,57	0
56	MG	AA	3082	1/1	0.72	0.26	-	68,68,68,68	0
56	MG	DA	3094	1/1	0.92	0.19	-	52,52,52,52	0
56	MG	BA	3229	1/1	0.78	0.31	-	51,51,51,51	0
56	MG	DA	3194	1/1	0.88	0.23	-	35,35,35,35	0
56	MG	AA	3090	1/1	0.93	0.35	-	53,53,53,53	0
56	MG	AA	3004	1/1	0.73	0.14	-	67,67,67,67	0
56	MG	DA	3298	1/1	0.96	0.17	-	33,33,33,33	0
56	MG	BA	3559	1/1	0.94	0.20	-	30,30,30,30	0
56	MG	BA	3463	1/1	0.95	0.20	-	37,37,37,37	0
56	MG	DA	3503	1/1	0.92	0.14	-	37,37,37,37	0
56	MG	BA	3782	1/1	0.86	0.11	-	51,51,51,51	0
56	MG	BA	3504	1/1	0.90	0.19	-	58,58,58,58	0
56	MG	BA	3547	1/1	0.97	0.19	-	41,41,41,41	0
56	MG	DA	3583	1/1	0.82	0.25	-	60,60,60,60	0
56	MG	BA	3576	1/1	0.93	0.17	-	48,48,48,48	0
56	MG	DA	3183	1/1	0.90	0.22	-	58,58,58,58	0
56	MG	DA	3423	1/1	0.84	0.14	-	51,51,51,51	0
56	MG	D0	101	1/1	0.94	0.08	-	56,56,56,56	0
56	MG	DA	3646	1/1	0.98	0.08	-	49,49,49,49	0
56	MG	DA	3533	1/1	0.90	0.30	-	53,53,53,53	0
56	MG	BA	3658	1/1	0.94	0.23	-	45,45,45,45	0
56	MG	DA	3462	1/1	0.95	0.28	-	43,43,43,43	0
56	MG	CA	3091	1/1	0.98	0.15	-	48,48,48,48	0
56	MG	BA	3598	1/1	0.95	0.15	-	47,47,47,47	0
56	MG	DA	3300	1/1	0.92	0.26	-	60,60,60,60	0
56	MG	CX	3003	1/1	0.96	0.38	-	50,50,50,50	0
56	MG	AA	3172	1/1	0.97	0.16	-	47,47,47,47	0
56	MG	BA	3482	1/1	0.88	0.22	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3230	1/1	0.95	0.14	-	62,62,62,62	0
56	MG	CA	3105	1/1	0.94	0.14	-	49,49,49,49	0
56	MG	AA	3184	1/1	0.94	0.12	-	55,55,55,55	0
56	MG	BA	3518	1/1	0.97	0.20	-	43,43,43,43	0
56	MG	BA	3034	1/1	0.94	0.21	-	28,28,28,28	0
56	MG	BA	3080	1/1	0.98	0.10	-	24,24,24,24	0
56	MG	DA	3282	1/1	0.94	0.10	-	42,42,42,42	0
56	MG	AA	3045	1/1	0.92	0.32	-	59,59,59,59	0
56	MG	BA	3270	1/1	0.92	0.24	-	57,57,57,57	0
56	MG	AA	3080	1/1	0.90	0.21	-	47,47,47,47	0
56	MG	AA	3005	1/1	0.91	0.07	-	53,53,53,53	0
56	MG	BA	3019	1/1	0.92	0.32	-	42,42,42,42	0
56	MG	AA	3137	1/1	0.99	0.19	-	42,42,42,42	0
56	MG	DA	3496	1/1	0.95	0.06	-	48,48,48,48	0
56	MG	BA	3714	1/1	0.89	0.06	-	47,47,47,47	0
56	MG	BA	3436	1/1	0.91	0.22	-	46,46,46,46	0
56	MG	DA	3359	1/1	0.85	0.13	-	57,57,57,57	0
56	MG	BA	3195	1/1	0.97	0.27	-	50,50,50,50	0
56	MG	BA	3004	1/1	0.89	0.24	-	36,36,36,36	0
56	MG	BA	3341	1/1	0.91	0.16	-	57,57,57,57	0
56	MG	BA	3363	1/1	0.97	0.19	-	50,50,50,50	0
56	MG	CA	3076	1/1	0.93	0.19	-	56,56,56,56	0
56	MG	CA	3058	1/1	0.98	0.14	-	70,70,70,70	0
56	MG	DW	3003	1/1	0.96	0.34	-	47,47,47,47	0
56	MG	CA	3025	1/1	0.77	0.14	-	61,61,61,61	0
56	MG	BA	3593	1/1	0.92	0.14	-	42,42,42,42	0
56	MG	DA	3242	1/1	0.94	0.07	-	43,43,43,43	0
56	MG	BA	3729	1/1	0.87	0.11	-	52,52,52,52	0
56	MG	CA	3094	1/1	0.94	0.18	-	72,72,72,72	0
56	MG	DA	3500	1/1	0.89	0.12	-	45,45,45,45	0
56	MG	AA	3102	1/1	0.89	0.34	-	51,51,51,51	0
56	MG	BA	3228	1/1	0.90	0.22	-	50,50,50,50	0
56	MG	DA	3188	1/1	0.95	0.38	-	50,50,50,50	0
56	MG	BA	3346	1/1	0.90	0.14	-	32,32,32,32	0
56	MG	BA	3296	1/1	0.94	0.19	-	31,31,31,31	0
56	MG	BA	3278	1/1	0.86	0.10	-	55,55,55,55	0
56	MG	DA	3168	1/1	0.85	0.29	-	53,53,53,53	0
56	MG	AA	3181	1/1	0.85	0.19	-	75,75,75,75	0
56	MG	DA	3610	1/1	0.86	0.22	-	48,48,48,48	0
56	MG	DA	3325	1/1	0.79	0.25	-	57,57,57,57	0
56	MG	AA	3189	1/1	0.91	0.17	-	59,59,59,59	0
56	MG	BA	3331	1/1	0.97	0.15	-	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3330	1/1	0.95	0.17	-	46,46,46,46	0
56	MG	BA	3723	1/1	0.89	0.16	-	47,47,47,47	0
56	MG	BA	3830	1/1	0.98	0.18	-	21,21,21,21	0
56	MG	BA	3753	1/1	0.86	0.29	-	44,44,44,44	0
56	MG	BA	3459	1/1	0.96	0.17	-	48,48,48,48	0
56	MG	BA	3612	1/1	0.96	0.10	-	62,62,62,62	0
56	MG	DF	302	1/1	0.90	0.18	-	43,43,43,43	0
56	MG	BA	3815	1/1	0.91	0.28	-	50,50,50,50	0
56	MG	BA	3570	1/1	0.94	0.35	-	30,30,30,30	0
56	MG	BA	3494	1/1	0.95	0.13	-	57,57,57,57	0
56	MG	DA	3531	1/1	0.90	0.33	-	54,54,54,54	0
56	MG	BA	3472	1/1	0.81	0.23	-	70,70,70,70	0
56	MG	BA	3401	1/1	0.96	0.14	-	48,48,48,48	0
56	MG	BA	3304	1/1	0.93	0.20	-	39,39,39,39	0
56	MG	CA	3056	1/1	0.95	0.23	-	60,60,60,60	0
56	MG	DA	3436	1/1	0.77	0.13	-	54,54,54,54	0
56	MG	BA	3297	1/1	0.96	0.55	-	55,55,55,55	0
56	MG	DA	3142	1/1	0.90	0.11	-	45,45,45,45	0
56	MG	BA	3554	1/1	0.93	0.21	-	37,37,37,37	0
56	MG	BA	3097	1/1	0.93	0.17	-	52,52,52,52	0
56	MG	CA	3138	1/1	0.98	0.14	-	59,59,59,59	0
56	MG	BA	3197	1/1	0.86	0.30	-	36,36,36,36	0
56	MG	BA	3677	1/1	0.61	0.12	-	62,62,62,62	0
56	MG	BA	3057	1/1	0.98	0.20	-	53,53,53,53	0
56	MG	BA	3783	1/1	0.95	0.19	-	53,53,53,53	0
56	MG	DA	3599	1/1	0.97	0.24	-	38,38,38,38	0
56	MG	DA	3294	1/1	0.98	0.26	-	42,42,42,42	0
56	MG	BA	3574	1/1	0.88	0.12	-	63,63,63,63	0
56	MG	CA	3167	1/1	0.90	0.17	-	48,48,48,48	0
56	MG	DA	3641	1/1	0.94	0.09	-	44,44,44,44	0
56	MG	CA	3132	1/1	0.88	0.37	-	70,70,70,70	0
56	MG	DA	3495	1/1	0.88	0.09	-	62,62,62,62	0
56	MG	DA	3040	1/1	0.95	0.10	-	53,53,53,53	0
56	MG	DA	3240	1/1	0.95	0.17	-	51,51,51,51	0
56	MG	DB	3008	1/1	0.95	0.14	-	68,68,68,68	0
56	MG	BA	3266	1/1	0.86	0.24	-	64,64,64,64	0
56	MG	CA	3012	1/1	0.94	0.20	-	68,68,68,68	0
56	MG	BQ	3003	1/1	0.83	0.15	-	54,54,54,54	0
56	MG	BA	3771	1/1	0.98	0.20	-	41,41,41,41	0
56	MG	DA	3288	1/1	0.92	0.16	-	61,61,61,61	0
56	MG	DA	3277	1/1	0.96	0.10	-	56,56,56,56	0
56	MG	AA	3173	1/1	0.94	0.11	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3588	1/1	0.87	0.17	-	47,47,47,47	0
56	MG	DA	3053	1/1	0.86	0.09	-	45,45,45,45	0
56	MG	DA	3312	1/1	0.74	0.14	-	52,52,52,52	0
56	MG	DA	3491	1/1	0.92	0.17	-	45,45,45,45	0
56	MG	BA	3819	1/1	0.93	0.24	-	32,32,32,32	0
56	MG	DA	3604	1/1	0.77	0.13	-	57,57,57,57	0
56	MG	BA	3672	1/1	0.88	0.21	-	61,61,61,61	0
56	MG	BA	3094	1/1	0.89	0.24	-	43,43,43,43	0
56	MG	DA	3598	1/1	0.94	0.11	-	63,63,63,63	0
56	MG	BA	3656	1/1	0.97	0.18	-	45,45,45,45	0
56	MG	CA	3023	1/1	0.83	0.22	-	55,55,55,55	0
56	MG	BA	3651	1/1	0.92	0.18	-	56,56,56,56	0
56	MG	BA	3725	1/1	0.69	0.22	-	67,67,67,67	0
56	MG	CA	3033	1/1	0.94	0.15	-	56,56,56,56	0
56	MG	BA	3788	1/1	0.94	0.17	-	41,41,41,41	0
56	MG	AX	3003	1/1	0.70	0.16	-	66,66,66,66	0
56	MG	BA	3760	1/1	0.86	0.26	-	68,68,68,68	0
56	MG	BA	3118	1/1	0.97	0.34	-	38,38,38,38	0
56	MG	BA	3722	1/1	0.95	0.12	-	50,50,50,50	0
56	MG	BB	3012	1/1	0.88	0.08	-	59,59,59,59	0
56	MG	DA	3541	1/1	0.73	0.07	-	54,54,54,54	0
56	MG	BA	3379	1/1	0.94	0.18	-	45,45,45,45	0
56	MG	BB	3022	1/1	0.91	0.14	-	62,62,62,62	0
56	MG	BA	3249	1/1	0.70	0.29	-	74,74,74,74	0
56	MG	CA	3017	1/1	0.90	0.17	-	49,49,49,49	0
56	MG	BA	3679	1/1	0.88	0.23	-	61,61,61,61	0
56	MG	CA	3161	1/1	0.89	0.10	-	70,70,70,70	0
56	MG	AA	3208	1/1	0.93	0.16	-	45,45,45,45	0
56	MG	BA	3645	1/1	0.93	0.18	-	32,32,32,32	0
56	MG	BA	3329	1/1	0.93	0.19	-	29,29,29,29	0
56	MG	BA	3639	1/1	0.70	0.30	-	59,59,59,59	0
56	MG	DA	3385	1/1	0.97	0.14	-	55,55,55,55	0
56	MG	DA	3007	1/1	0.95	0.39	-	54,54,54,54	0
56	MG	AA	3199	1/1	0.85	0.24	-	59,59,59,59	0
56	MG	BA	3321	1/1	0.98	0.08	-	54,54,54,54	0
56	MG	DA	3072	1/1	0.91	0.09	-	36,36,36,36	0
56	MG	CA	3053	1/1	0.86	0.07	-	74,74,74,74	0
56	MG	BA	3627	1/1	0.96	0.17	-	45,45,45,45	0
56	MG	BA	3120	1/1	0.93	0.23	-	32,32,32,32	0
56	MG	BA	3475	1/1	0.90	0.15	-	53,53,53,53	0
56	MG	CA	3010	1/1	0.88	0.12	-	53,53,53,53	0
56	MG	DA	3271	1/1	0.90	0.14	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3801	1/1	0.98	0.10	-	53,53,53,53	0
56	MG	BA	3824	1/1	0.97	0.12	-	43,43,43,43	0
56	MG	BA	3348	1/1	0.90	0.13	-	54,54,54,54	0
56	MG	DA	3229	1/1	0.89	0.12	-	55,55,55,55	0
56	MG	BA	3507	1/1	0.96	0.12	-	39,39,39,39	0
56	MG	DA	3571	1/1	0.97	0.16	-	57,57,57,57	0
56	MG	DA	3602	1/1	0.89	0.34	-	51,51,51,51	0
56	MG	BA	3681	1/1	0.92	0.22	-	53,53,53,53	0
56	MG	CA	3080	1/1	0.94	0.28	-	52,52,52,52	0
56	MG	BA	3466	1/1	0.98	0.17	-	28,28,28,28	0
56	MG	BA	3136	1/1	0.93	0.12	-	58,58,58,58	0
56	MG	DA	3527	1/1	0.94	0.17	-	53,53,53,53	0
56	MG	BA	3200	1/1	0.94	0.28	-	56,56,56,56	0
56	MG	DA	3212	1/1	0.93	0.29	-	44,44,44,44	0
56	MG	BA	3413	1/1	0.82	0.19	-	41,41,41,41	0
56	MG	DA	3563	1/1	0.90	0.15	-	42,42,42,42	0
56	MG	DA	3132	1/1	0.89	0.43	-	41,41,41,41	0
56	MG	BA	3720	1/1	0.79	0.23	-	46,46,46,46	0
56	MG	BA	3675	1/1	0.98	0.17	-	37,37,37,37	0
56	MG	BA	3744	1/1	0.96	0.13	-	20,20,20,20	0
56	MG	DA	3044	1/1	0.87	0.10	-	58,58,58,58	0
56	MG	DA	3089	1/1	0.90	0.23	-	46,46,46,46	0
56	MG	DA	3092	1/1	0.93	0.26	-	48,48,48,48	0
56	MG	DE	303	1/1	0.94	0.26	-	44,44,44,44	0
56	MG	AA	3079	1/1	0.90	0.22	-	47,47,47,47	0
56	MG	BA	3262	1/1	0.95	0.31	-	47,47,47,47	0
56	MG	BA	3160	1/1	0.98	0.17	-	32,32,32,32	0
56	MG	DA	3550	1/1	0.93	0.08	-	51,51,51,51	0
56	MG	DA	3078	1/1	0.83	0.11	-	45,45,45,45	0
56	MG	DA	3605	1/1	0.79	0.15	-	52,52,52,52	0
56	MG	BA	3349	1/1	0.96	0.19	-	34,34,34,34	0
56	MG	DA	3091	1/1	0.96	0.18	-	43,43,43,43	0
56	MG	BA	3073	1/1	0.96	0.17	-	41,41,41,41	0
56	MG	BA	3488	1/1	0.95	0.10	-	50,50,50,50	0
56	MG	BA	3191	1/1	0.95	0.26	-	40,40,40,40	0
56	MG	AA	3118	1/1	0.95	0.20	-	53,53,53,53	0
56	MG	AW	3001	1/1	0.79	0.09	-	55,55,55,55	0
56	MG	CA	3003	1/1	0.93	0.24	-	58,58,58,58	0
56	MG	BA	3152	1/1	0.84	0.18	-	43,43,43,43	0
56	MG	BA	3698	1/1	0.93	0.13	-	48,48,48,48	0
56	MG	BA	3408	1/1	0.82	0.20	-	55,55,55,55	0
56	MG	BA	3286	1/1	0.94	0.33	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3222	1/1	0.88	0.18	-	54,54,54,54	0
56	MG	BA	3010	1/1	0.97	0.13	-	29,29,29,29	0
56	MG	AA	3011	1/1	0.88	0.20	-	64,64,64,64	0
56	MG	AA	3020	1/1	0.90	0.15	-	59,59,59,59	0
56	MG	BA	3838	1/1	0.90	0.19	-	50,50,50,50	0
56	MG	AA	3097	1/1	0.94	0.13	-	50,50,50,50	0
56	MG	DA	3153	1/1	0.96	0.15	-	44,44,44,44	0
56	MG	DA	3125	1/1	0.95	0.26	-	45,45,45,45	0
56	MG	BA	3005	1/1	0.82	0.21	-	51,51,51,51	0
56	MG	BA	3662	1/1	0.94	0.32	-	50,50,50,50	0
56	MG	BA	3222	1/1	0.96	0.36	-	27,27,27,27	0
56	MG	BA	3538	1/1	0.96	0.20	-	45,45,45,45	0
56	MG	BA	3055	1/1	0.94	0.23	-	31,31,31,31	0
56	MG	AA	3044	1/1	0.92	0.31	-	71,71,71,71	0
56	MG	BA	3618	1/1	0.86	0.18	-	63,63,63,63	0
56	MG	DA	3349	1/1	0.96	0.11	-	44,44,44,44	0
56	MG	BA	3464	1/1	0.90	0.21	-	56,56,56,56	0
56	MG	DA	3184	1/1	0.86	0.30	-	49,49,49,49	0
56	MG	DA	3113	1/1	0.97	0.29	-	44,44,44,44	0
56	MG	BA	3433	1/1	0.90	0.19	-	57,57,57,57	0
56	MG	AA	3106	1/1	0.91	0.17	-	51,51,51,51	0
56	MG	DA	3210	1/1	0.91	0.11	-	44,44,44,44	0
56	MG	DA	3274	1/1	0.94	0.22	-	33,33,33,33	0
56	MG	BA	3035	1/1	0.97	0.14	-	31,31,31,31	0
56	MG	DA	3407	1/1	0.90	0.08	-	46,46,46,46	0
56	MG	AA	3194	1/1	0.91	0.17	-	58,58,58,58	0
56	MG	CA	3147	1/1	0.84	0.18	-	72,72,72,72	0
56	MG	BA	3032	1/1	0.97	0.21	-	38,38,38,38	0
56	MG	AA	3124	1/1	0.95	0.20	-	53,53,53,53	0
56	MG	DA	3192	1/1	0.84	0.18	-	51,51,51,51	0
56	MG	AA	3230	1/1	0.89	0.18	-	68,68,68,68	0
56	MG	DA	3219	1/1	0.98	0.27	-	54,54,54,54	0
56	MG	BA	3052	1/1	0.89	0.31	-	43,43,43,43	0
56	MG	AA	3150	1/1	0.92	0.44	-	55,55,55,55	0
56	MG	BA	3271	1/1	0.92	0.11	-	26,26,26,26	0
56	MG	DV	3003	1/1	0.96	0.12	-	52,52,52,52	0
56	MG	DA	3244	1/1	0.95	0.13	-	48,48,48,48	0
56	MG	AA	3049	1/1	0.91	0.22	-	52,52,52,52	0
56	MG	DA	3428	1/1	0.97	0.10	-	61,61,61,61	0
56	MG	DA	3633	1/1	0.94	0.14	-	61,61,61,61	0
56	MG	AA	3163	1/1	0.96	0.15	-	37,37,37,37	0
56	MG	BA	3718	1/1	0.90	0.20	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	3149	1/1	0.95	0.21	-	41,41,41,41	0
56	MG	AA	3024	1/1	0.93	0.15	-	58,58,58,58	0
56	MG	DA	3521	1/1	0.76	0.17	-	51,51,51,51	0
56	MG	AA	3111	1/1	0.93	0.17	-	52,52,52,52	0
56	MG	BA	3537	1/1	0.91	0.13	-	49,49,49,49	0
56	MG	DA	3041	1/1	0.72	0.18	-	55,55,55,55	0
56	MG	AA	3089	1/1	0.90	0.26	-	57,57,57,57	0
56	MG	DA	3067	1/1	0.95	0.25	-	49,49,49,49	0
56	MG	BA	3700	1/1	0.89	0.20	-	54,54,54,54	0
56	MG	DA	3247	1/1	0.88	0.38	-	57,57,57,57	0
56	MG	BA	3040	1/1	0.96	0.14	-	47,47,47,47	0
56	MG	BA	3382	1/1	0.94	0.21	-	55,55,55,55	0
56	MG	AX	3007	1/1	0.94	0.24	-	72,72,72,72	0
56	MG	DA	3484	1/1	0.94	0.05	-	45,45,45,45	0
56	MG	AA	3196	1/1	0.97	0.13	-	32,32,32,32	0
56	MG	BA	3626	1/1	0.92	0.18	-	49,49,49,49	0
56	MG	BR	202	1/1	0.68	0.41	-	53,53,53,53	0
56	MG	BA	3797	1/1	0.90	0.20	-	52,52,52,52	0
56	MG	AX	3010	1/1	0.87	0.10	-	62,62,62,62	0
56	MG	DA	3156	1/1	0.94	0.12	-	43,43,43,43	0
56	MG	DA	3262	1/1	0.96	0.12	-	43,43,43,43	0
56	MG	BA	3799	1/1	0.95	0.22	-	47,47,47,47	0
56	MG	AA	3179	1/1	0.97	0.35	-	79,79,79,79	0
56	MG	BA	3387	1/1	0.91	0.06	-	65,65,65,65	0
56	MG	CA	3102	1/1	0.96	0.09	-	54,54,54,54	0
56	MG	DA	3131	1/1	0.91	0.15	-	52,52,52,52	0
56	MG	BF	312	1/1	0.96	0.14	-	47,47,47,47	0
56	MG	BA	3327	1/1	0.94	0.25	-	25,25,25,25	0
56	MG	CV	3001	1/1	0.95	0.19	-	58,58,58,58	0
56	MG	AA	3226	1/1	0.85	0.25	-	58,58,58,58	0
56	MG	BA	3751	1/1	0.90	0.14	-	45,45,45,45	0
56	MG	AA	3094	1/1	0.88	0.23	-	44,44,44,44	0
56	MG	AA	3204	1/1	0.73	0.19	-	71,71,71,71	0
56	MG	DA	3249	1/1	0.97	0.27	-	41,41,41,41	0
56	MG	AA	3095	1/1	0.73	0.28	-	68,68,68,68	0
56	MG	BA	3009	1/1	0.97	0.17	-	25,25,25,25	0
56	MG	BA	3209	1/1	0.96	0.12	-	41,41,41,41	0
56	MG	BA	3493	1/1	0.93	0.13	-	46,46,46,46	0
56	MG	DA	3031	1/1	0.94	0.41	-	51,51,51,51	0
56	MG	BA	3299	1/1	0.96	0.15	-	32,32,32,32	0
56	MG	DA	3189	1/1	0.97	0.25	-	48,48,48,48	0
56	MG	BA	3076	1/1	0.97	0.29	-	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	3070	1/1	0.97	0.22	-	49,49,49,49	0
56	MG	DB	3003	1/1	0.87	0.15	-	68,68,68,68	0
56	MG	CA	3020	1/1	0.80	0.13	-	73,73,73,73	0
56	MG	BA	3162	1/1	0.79	0.26	-	46,46,46,46	0
56	MG	DA	3653	1/1	0.98	0.15	-	58,58,58,58	0
56	MG	DA	3548	1/1	0.92	0.17	-	65,65,65,65	0
56	MG	DA	3077	1/1	0.95	0.18	-	43,43,43,43	0
56	MG	AA	3050	1/1	0.92	0.10	-	70,70,70,70	0
56	MG	BA	3738	1/1	0.90	0.11	-	58,58,58,58	0
56	MG	BF	307	1/1	0.87	0.23	-	39,39,39,39	0
56	MG	AA	3037	1/1	0.97	0.24	-	44,44,44,44	0
56	MG	DA	3252	1/1	0.98	0.20	-	29,29,29,29	0
56	MG	BA	3263	1/1	0.95	0.18	-	32,32,32,32	0
56	MG	AA	3069	1/1	0.95	0.21	-	67,67,67,67	0
56	MG	BA	3251	1/1	0.91	0.32	-	52,52,52,52	0
56	MG	BB	3011	1/1	0.81	0.06	-	59,59,59,59	0
56	MG	DW	3001	1/1	0.94	0.24	-	43,43,43,43	0
56	MG	BA	3317	1/1	0.82	0.19	-	64,64,64,64	0
56	MG	CA	3068	1/1	0.94	0.40	-	55,55,55,55	0
56	MG	BA	3578	1/1	0.93	0.25	-	47,47,47,47	0
56	MG	DA	3565	1/1	0.51	0.18	-	70,70,70,70	0
56	MG	CA	3151	1/1	0.92	0.08	-	65,65,65,65	0
56	MG	BA	3062	1/1	0.91	0.25	-	57,57,57,57	0
56	MG	BA	3707	1/1	0.91	0.14	-	66,66,66,66	0
56	MG	CA	3005	1/1	0.86	0.10	-	58,58,58,58	0
56	MG	DA	3333	1/1	0.90	0.07	-	50,50,50,50	0
56	MG	CA	3048	1/1	0.96	0.27	-	52,52,52,52	0
56	MG	BA	3361	1/1	0.94	0.16	-	35,35,35,35	0
56	MG	DA	3379	1/1	0.95	0.20	-	59,59,59,59	0
56	MG	BA	3471	1/1	0.95	0.06	-	45,45,45,45	0
56	MG	BA	3096	1/1	0.91	0.30	-	41,41,41,41	0
56	MG	BA	3261	1/1	0.88	0.26	-	44,44,44,44	0
56	MG	B8	103	1/1	0.97	0.22	-	48,48,48,48	0
56	MG	DA	3207	1/1	0.97	0.28	-	57,57,57,57	0
56	MG	BA	3664	1/1	0.98	0.14	-	43,43,43,43	0
56	MG	CA	3090	1/1	0.88	0.17	-	62,62,62,62	0
56	MG	DA	3471	1/1	0.96	0.15	-	50,50,50,50	0
56	MG	BA	3385	1/1	0.95	0.15	-	39,39,39,39	0
56	MG	BA	3748	1/1	0.86	0.17	-	63,63,63,63	0
56	MG	AA	3098	1/1	0.57	0.16	-	68,68,68,68	0
56	MG	CA	3052	1/1	0.94	0.09	-	65,65,65,65	0
56	MG	BB	3002	1/1	0.93	0.18	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AX	3004	1/1	0.92	0.21	-	70,70,70,70	0
56	MG	DA	3413	1/1	0.95	0.20	-	36,36,36,36	0
56	MG	BA	3167	1/1	0.96	0.19	-	50,50,50,50	0
56	MG	DA	3075	1/1	0.93	0.12	-	39,39,39,39	0
56	MG	BA	3641	1/1	0.90	0.18	-	49,49,49,49	0
56	MG	BA	3234	1/1	0.97	0.25	-	48,48,48,48	0
56	MG	DA	3305	1/1	0.82	0.18	-	28,28,28,28	0
56	MG	BA	3311	1/1	0.86	0.20	-	37,37,37,37	0
56	MG	AA	3190	1/1	0.82	0.11	-	65,65,65,65	0
56	MG	BA	3480	1/1	0.95	0.15	-	56,56,56,56	0
56	MG	B7	102	1/1	0.87	0.24	-	58,58,58,58	0
56	MG	DA	3619	1/1	0.98	0.03	-	58,58,58,58	0
56	MG	B1	102	1/1	0.79	0.41	-	68,68,68,68	0
56	MG	CA	3081	1/1	0.82	0.18	-	58,58,58,58	0
56	MG	DA	3083	1/1	0.95	0.18	-	51,51,51,51	0
56	MG	AA	3099	1/1	0.94	0.25	-	63,63,63,63	0
56	MG	DA	3173	1/1	0.98	0.17	-	30,30,30,30	0
56	MG	AA	3198	1/1	0.87	0.39	-	70,70,70,70	0
56	MG	BA	3077	1/1	0.95	0.20	-	34,34,34,34	0
56	MG	BA	3307	1/1	0.91	0.17	-	37,37,37,37	0
56	MG	DA	3079	1/1	0.86	0.17	-	48,48,48,48	0
56	MG	BA	3765	1/1	0.92	0.17	-	33,33,33,33	0
56	MG	DA	3005	1/1	0.94	0.20	-	58,58,58,58	0
56	MG	BA	3456	1/1	0.94	0.39	-	41,41,41,41	0
56	MG	BA	3439	1/1	0.88	0.17	-	58,58,58,58	0
56	MG	CA	3087	1/1	0.84	0.15	-	63,63,63,63	0
56	MG	AA	3135	1/1	0.93	0.10	-	65,65,65,65	0
56	MG	BA	3088	1/1	0.89	0.16	-	50,50,50,50	0
56	MG	DA	3564	1/1	0.94	0.31	-	53,53,53,53	0
56	MG	CA	3123	1/1	0.90	0.12	-	80,80,80,80	0
56	MG	DA	3109	1/1	0.65	0.20	-	66,66,66,66	0
56	MG	DA	3008	1/1	0.95	0.21	-	33,33,33,33	0
60	K	AX	3001	1/1	0.97	0.22	-	57,57,57,57	0
56	MG	AY	3003	1/1	0.91	0.14	-	48,48,48,48	0
56	MG	CA	3166	1/1	0.96	0.13	-	66,66,66,66	0
56	MG	BA	3292	1/1	0.89	0.15	-	42,42,42,42	0
56	MG	BY	502	1/1	0.94	0.13	-	50,50,50,50	0
56	MG	BA	3424	1/1	0.87	0.25	-	24,24,24,24	0
56	MG	BA	3070	1/1	0.80	0.26	-	55,55,55,55	0
56	MG	DA	3649	1/1	0.91	0.07	-	64,64,64,64	0
56	MG	AA	3147	1/1	0.94	0.11	-	55,55,55,55	0
56	MG	B5	103	1/1	0.92	0.18	-	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	3049	1/1	0.70	0.23	-	68,68,68,68	0
56	MG	DA	3134	1/1	0.95	0.13	-	49,49,49,49	0
56	MG	BA	3708	1/1	0.88	0.24	-	63,63,63,63	0
56	MG	AA	3131	1/1	0.98	0.32	-	63,63,63,63	0
56	MG	DA	3279	1/1	0.95	0.07	-	48,48,48,48	0
56	MG	BA	3663	1/1	0.77	0.14	-	50,50,50,50	0
56	MG	CA	3022	1/1	0.95	0.10	-	53,53,53,53	0
56	MG	AA	3136	1/1	0.85	0.08	-	53,53,53,53	0
56	MG	BA	3409	1/1	0.81	0.23	-	62,62,62,62	0
56	MG	CA	3171	1/1	0.94	0.19	-	63,63,63,63	0
56	MG	BB	3014	1/1	0.96	0.14	-	69,69,69,69	0
56	MG	BA	3562	1/1	0.96	0.18	-	35,35,35,35	0
56	MG	BA	3519	1/1	0.93	0.12	-	44,44,44,44	0
56	MG	AA	3151	1/1	0.98	0.16	-	41,41,41,41	0
56	MG	BA	3277	1/1	0.80	0.19	-	54,54,54,54	0
56	MG	DA	3581	1/1	0.91	0.19	-	63,63,63,63	0
56	MG	BA	3825	1/1	0.92	0.18	-	65,65,65,65	0
56	MG	BA	3396	1/1	0.92	0.22	-	55,55,55,55	0
56	MG	BA	3066	1/1	0.95	0.39	-	51,51,51,51	0
56	MG	DA	3421	1/1	0.96	0.21	-	53,53,53,53	0
56	MG	BA	3127	1/1	0.88	0.17	-	41,41,41,41	0
56	MG	DA	3297	1/1	0.87	0.12	-	66,66,66,66	0
56	MG	DA	3049	1/1	0.96	0.22	-	24,24,24,24	0
56	MG	DA	3661	1/1	0.92	0.20	-	42,42,42,42	0
56	MG	B0	103	1/1	0.97	0.06	-	54,54,54,54	0
56	MG	BA	3402	1/1	0.84	0.19	-	30,30,30,30	0
56	MG	AA	3041	1/1	0.94	0.26	-	52,52,52,52	0
56	MG	BA	3807	1/1	0.74	0.11	-	67,67,67,67	0
56	MG	DA	3435	1/1	0.97	0.16	-	44,44,44,44	0
56	MG	BA	3571	1/1	0.29	0.10	-	66,66,66,66	0
56	MG	BA	3419	1/1	0.89	0.17	-	39,39,39,39	0
56	MG	BA	3614	1/1	0.94	0.15	-	26,26,26,26	0
56	MG	DA	3460	1/1	0.90	0.17	-	65,65,65,65	0
56	MG	AW	3005	1/1	0.85	0.39	-	68,68,68,68	0
56	MG	BA	3667	1/1	0.89	0.11	-	52,52,52,52	0
56	MG	AA	3108	1/1	0.95	0.20	-	55,55,55,55	0
56	MG	AA	3169	1/1	0.90	0.18	-	64,64,64,64	0
56	MG	BA	3786	1/1	0.93	0.10	-	37,37,37,37	0
56	MG	BA	3086	1/1	0.96	0.28	-	41,41,41,41	0
56	MG	DA	3372	1/1	0.95	0.15	-	47,47,47,47	0
56	MG	BA	3543	1/1	0.94	0.25	-	26,26,26,26	0
56	MG	AA	3185	1/1	0.90	0.26	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3495	1/1	0.97	0.24	-	34,34,34,34	0
56	MG	DA	3143	1/1	0.96	0.23	-	50,50,50,50	0
56	MG	BA	3056	1/1	0.97	0.28	-	33,33,33,33	0
56	MG	BA	3312	1/1	0.88	0.18	-	33,33,33,33	0
56	MG	BA	3769	1/1	0.87	0.17	-	56,56,56,56	0
56	MG	DA	3477	1/1	0.88	0.08	-	55,55,55,55	0
56	MG	BA	3781	1/1	0.97	0.21	-	52,52,52,52	0
56	MG	DA	3081	1/1	0.91	0.27	-	45,45,45,45	0
56	MG	BA	3243	1/1	0.95	0.18	-	44,44,44,44	0
56	MG	DA	3537	1/1	0.91	0.17	-	55,55,55,55	0
56	MG	DA	3368	1/1	0.90	0.19	-	50,50,50,50	0
56	MG	DA	3308	1/1	0.97	0.16	-	45,45,45,45	0
56	MG	DA	3389	1/1	0.98	0.06	-	53,53,53,53	0
56	MG	BA	3252	1/1	0.93	0.24	-	45,45,45,45	0
56	MG	DA	3170	1/1	0.80	0.09	-	50,50,50,50	0
56	MG	BA	3366	1/1	0.93	0.17	-	45,45,45,45	0
56	MG	BA	3215	1/1	0.96	0.30	-	45,45,45,45	0
56	MG	CA	3079	1/1	0.96	0.15	-	54,54,54,54	0
56	MG	DA	3013	1/1	0.95	0.17	-	40,40,40,40	0
56	MG	BA	3371	1/1	0.85	0.13	-	54,54,54,54	0
56	MG	DA	3438	1/1	0.99	0.10	-	60,60,60,60	0
56	MG	DA	3384	1/1	0.91	0.10	-	52,52,52,52	0
56	MG	BA	3823	1/1	0.97	0.08	-	53,53,53,53	0
56	MG	BA	3235	1/1	0.93	0.15	-	37,37,37,37	0
56	MG	DA	3163	1/1	0.95	0.27	-	49,49,49,49	0
56	MG	DA	3265	1/1	0.95	0.31	-	52,52,52,52	0
56	MG	BA	3755	1/1	0.96	0.19	-	52,52,52,52	0
56	MG	DA	3085	1/1	0.86	0.19	-	52,52,52,52	0
56	MG	DA	3575	1/1	0.95	0.10	-	47,47,47,47	0
56	MG	BA	3310	1/1	0.93	0.20	-	57,57,57,57	0
56	MG	DA	3099	1/1	0.95	0.09	-	60,60,60,60	0
56	MG	AV	101	1/1	0.88	0.28	-	59,59,59,59	0
56	MG	DA	3039	1/1	0.90	0.22	-	56,56,56,56	0
56	MG	BA	3634	1/1	0.85	0.16	-	64,64,64,64	0
56	MG	BA	3157	1/1	0.98	0.17	-	36,36,36,36	0
56	MG	BA	3739	1/1	0.89	0.19	-	46,46,46,46	0
56	MG	DA	3382	1/1	0.97	0.12	-	44,44,44,44	0
56	MG	BA	3257	1/1	0.94	0.21	-	41,41,41,41	0
56	MG	DA	3321	1/1	0.86	0.27	-	35,35,35,35	0
56	MG	BA	3759	1/1	0.98	0.15	-	9,9,9,9	0
56	MG	CA	3124	1/1	0.90	0.16	-	79,79,79,79	0
56	MG	CA	3057	1/1	0.96	0.17	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3580	1/1	0.95	0.22	-	42,42,42,42	0
56	MG	BA	3130	1/1	0.93	0.26	-	48,48,48,48	0
56	MG	DA	3327	1/1	0.95	0.19	-	59,59,59,59	0
56	MG	BA	3625	1/1	0.91	0.14	-	57,57,57,57	0
56	MG	BU	202	1/1	0.97	0.22	-	40,40,40,40	0
56	MG	BA	3676	1/1	0.94	0.28	-	53,53,53,53	0
56	MG	CA	3067	1/1	0.90	0.10	-	79,79,79,79	0
56	MG	DA	3093	1/1	0.90	0.10	-	57,57,57,57	0
56	MG	AA	3174	1/1	0.92	0.13	-	60,60,60,60	0
56	MG	BA	3604	1/1	0.87	0.28	-	72,72,72,72	0
56	MG	DA	3080	1/1	0.95	0.22	-	45,45,45,45	0
56	MG	BA	3140	1/1	0.86	0.23	-	46,46,46,46	0
56	MG	BB	3013	1/1	0.94	0.14	-	42,42,42,42	0
56	MG	BA	3237	1/1	0.92	0.14	-	36,36,36,36	0
56	MG	BA	3686	1/1	0.90	0.24	-	30,30,30,30	0
56	MG	AA	3060	1/1	0.96	0.21	-	59,59,59,59	0
56	MG	DA	3180	1/1	0.94	0.14	-	51,51,51,51	0
56	MG	DA	3139	1/1	0.93	0.10	-	40,40,40,40	0
56	MG	DA	3466	1/1	0.72	0.17	-	62,62,62,62	0
56	MG	CA	3011	1/1	0.83	0.17	-	63,63,63,63	0
56	MG	DA	3060	1/1	0.86	0.23	-	47,47,47,47	0
56	MG	BA	3284	1/1	0.92	0.26	-	51,51,51,51	0
56	MG	CA	3028	1/1	0.86	0.19	-	60,60,60,60	0
56	MG	DA	3672	1/1	0.92	0.28	-	52,52,52,52	0
56	MG	DA	3626	1/1	0.94	0.06	-	54,54,54,54	0
56	MG	AA	3206	1/1	0.94	0.17	-	47,47,47,47	0
56	MG	BA	3754	1/1	0.93	0.17	-	60,60,60,60	0
56	MG	CA	3110	1/1	0.96	0.11	-	48,48,48,48	0
56	MG	BA	3373	1/1	0.97	0.18	-	38,38,38,38	0
56	MG	BA	3389	1/1	0.96	0.28	-	37,37,37,37	0
56	MG	BA	3498	1/1	0.96	0.07	-	54,54,54,54	0
56	MG	AA	3076	1/1	0.97	0.17	-	55,55,55,55	0
56	MG	BA	3692	1/1	0.84	0.28	-	57,57,57,57	0
56	MG	DA	3584	1/1	0.95	0.40	-	58,58,58,58	0
56	MG	BA	3620	1/1	0.90	0.15	-	47,47,47,47	0
56	MG	CA	3006	1/1	0.87	0.30	-	53,53,53,53	0
56	MG	DA	3644	1/1	0.97	0.49	-	55,55,55,55	0
56	MG	AA	3022	1/1	0.89	0.28	-	55,55,55,55	0
56	MG	BA	3448	1/1	0.94	0.22	-	28,28,28,28	0
56	MG	CA	3043	1/1	0.91	0.26	-	54,54,54,54	0
56	MG	DA	3326	1/1	0.95	0.18	-	46,46,46,46	0
56	MG	AA	3066	1/1	0.91	0.12	-	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	3136	1/1	0.95	0.18	-	65,65,65,65	0
56	MG	BA	3011	1/1	0.94	0.20	-	40,40,40,40	0
56	MG	BA	3188	1/1	0.99	0.24	-	19,19,19,19	0
56	MG	BA	3268	1/1	0.95	0.28	-	58,58,58,58	0
56	MG	BA	3655	1/1	0.87	0.12	-	50,50,50,50	0
56	MG	CA	3071	1/1	0.94	0.09	-	50,50,50,50	0
56	MG	AA	3006	1/1	0.96	0.14	-	37,37,37,37	0
56	MG	DA	3047	1/1	0.97	0.21	-	49,49,49,49	0
56	MG	DA	3551	1/1	0.93	0.16	-	55,55,55,55	0
56	MG	BA	3356	1/1	0.89	0.13	-	55,55,55,55	0
56	MG	BA	3542	1/1	0.92	0.16	-	48,48,48,48	0
56	MG	BA	3018	1/1	0.98	0.25	-	34,34,34,34	0
56	MG	DA	3624	1/1	0.97	0.07	-	47,47,47,47	0
56	MG	DA	3088	1/1	0.96	0.18	-	42,42,42,42	0
56	MG	BA	3074	1/1	0.97	0.24	-	32,32,32,32	0
56	MG	BA	3687	1/1	0.95	0.23	-	36,36,36,36	0
56	MG	DA	3535	1/1	0.94	0.35	-	54,54,54,54	0
56	MG	BA	3047	1/1	0.88	0.15	-	27,27,27,27	0
56	MG	BA	3602	1/1	0.94	0.17	-	46,46,46,46	0
56	MG	AA	3212	1/1	0.89	0.30	-	59,59,59,59	0
56	MG	BA	3470	1/1	0.72	0.16	-	48,48,48,48	0
56	MG	DA	3227	1/1	0.98	0.21	-	38,38,38,38	0
56	MG	BA	3790	1/1	0.94	0.21	-	32,32,32,32	0
56	MG	AA	3081	1/1	0.92	0.26	-	58,58,58,58	0
56	MG	BA	3746	1/1	0.96	0.33	-	25,25,25,25	0
56	MG	DA	3221	1/1	0.90	0.17	-	49,49,49,49	0
56	MG	CA	3128	1/1	0.92	0.10	-	63,63,63,63	0
56	MG	DA	3214	1/1	0.82	0.34	-	47,47,47,47	0
56	MG	BA	3628	1/1	0.93	0.17	-	30,30,30,30	0
56	MG	DA	3287	1/1	0.85	0.16	-	47,47,47,47	0
56	MG	BA	3833	1/1	0.95	0.20	-	43,43,43,43	0
56	MG	DA	3290	1/1	0.97	0.17	-	44,44,44,44	0
56	MG	BA	3260	1/1	0.93	0.56	-	57,57,57,57	0
56	MG	BA	3671	1/1	0.95	0.14	-	45,45,45,45	0
56	MG	DA	3609	1/1	0.93	0.16	-	60,60,60,60	0
56	MG	BA	3478	1/1	0.87	0.20	-	59,59,59,59	0
56	MG	AA	3114	1/1	0.79	0.34	-	51,51,51,51	0
56	MG	DA	3405	1/1	0.90	0.13	-	52,52,52,52	0
56	MG	DA	3380	1/1	0.90	0.09	-	55,55,55,55	0
56	MG	AA	3157	1/1	0.99	0.19	-	46,46,46,46	0
56	MG	BA	3177	1/1	0.95	0.30	-	44,44,44,44	0
56	MG	AA	3192	1/1	0.55	0.30	-	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	3154	1/1	0.93	0.17	-	62,62,62,62	0
56	MG	AA	3211	1/1	0.94	0.09	-	59,59,59,59	0
56	MG	BA	3369	1/1	0.98	0.17	-	55,55,55,55	0
56	MG	BA	3500	1/1	0.91	0.18	-	26,26,26,26	0
56	MG	BA	3158	1/1	0.92	0.19	-	44,44,44,44	0
56	MG	DA	3547	1/1	0.79	0.17	-	65,65,65,65	0
56	MG	DA	3612	1/1	0.89	0.23	-	56,56,56,56	0
56	MG	DA	3473	1/1	0.98	0.06	-	49,49,49,49	0
56	MG	DA	3591	1/1	0.84	0.20	-	56,56,56,56	0
56	MG	DA	3280	1/1	0.99	0.14	-	43,43,43,43	0
56	MG	CA	3060	1/1	0.87	0.24	-	68,68,68,68	0
56	MG	BA	3595	1/1	0.80	0.21	-	32,32,32,32	0
56	MG	DA	3555	1/1	0.95	0.08	-	54,54,54,54	0
56	MG	BA	3784	1/1	0.96	0.22	-	52,52,52,52	0
56	MG	DA	3264	1/1	0.95	0.13	-	31,31,31,31	0
56	MG	AX	3012	1/1	0.90	0.23	-	59,59,59,59	0
56	MG	BA	3289	1/1	0.83	0.26	-	55,55,55,55	0
56	MG	DA	3036	1/1	0.99	0.15	-	29,29,29,29	0
56	MG	DA	3116	1/1	0.98	0.10	-	57,57,57,57	0
56	MG	BA	3768	1/1	0.91	0.06	-	56,56,56,56	0
56	MG	BA	3582	1/1	0.93	0.16	-	44,44,44,44	0
56	MG	DA	3064	1/1	0.98	0.10	-	64,64,64,64	0
56	MG	BA	3081	1/1	0.93	0.19	-	49,49,49,49	0
56	MG	BA	3685	1/1	0.93	0.17	-	59,59,59,59	0
56	MG	DA	3493	1/1	0.82	0.27	-	58,58,58,58	0
56	MG	BA	3567	1/1	0.86	0.18	-	50,50,50,50	0
56	MG	DA	3232	1/1	0.95	0.28	-	53,53,53,53	0
56	MG	DA	3181	1/1	0.90	0.30	-	45,45,45,45	0
56	MG	CA	3137	1/1	0.85	0.19	-	52,52,52,52	0
56	MG	BB	3016	1/1	0.99	0.16	-	43,43,43,43	0
56	MG	DA	3589	1/1	0.91	0.15	-	63,63,63,63	0
56	MG	AA	3145	1/1	0.82	0.16	-	58,58,58,58	0
56	MG	DA	3082	1/1	0.95	0.22	-	34,34,34,34	0
56	MG	BA	3114	1/1	0.88	0.36	-	52,52,52,52	0
56	MG	BA	3732	1/1	0.93	0.26	-	40,40,40,40	0
56	MG	BA	3170	1/1	0.85	0.23	-	48,48,48,48	0
56	MG	DA	3655	1/1	0.89	0.17	-	57,57,57,57	0
56	MG	DA	3203	1/1	0.92	0.28	-	37,37,37,37	0
56	MG	DO	5001	1/1	0.98	0.16	-	51,51,51,51	0
56	MG	DA	3454	1/1	0.89	0.28	-	54,54,54,54	0
56	MG	DA	3545	1/1	0.89	0.16	-	37,37,37,37	0
56	MG	BA	3600	1/1	0.95	0.10	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3659	1/1	0.83	0.27	-	53,53,53,53	0
60	K	CX	3001	1/1	0.92	0.17	-	74,74,74,74	0
56	MG	DA	3642	1/1	0.84	0.15	-	49,49,49,49	0
56	MG	BA	3540	1/1	0.96	0.17	-	44,44,44,44	0
56	MG	BA	3301	1/1	0.96	0.14	-	26,26,26,26	0
56	MG	CE	201	1/1	0.96	0.19	-	50,50,50,50	0
56	MG	BA	3293	1/1	0.90	0.25	-	52,52,52,52	0
56	MG	DA	3518	1/1	0.93	0.18	-	50,50,50,50	0
56	MG	BA	3204	1/1	0.78	0.33	-	66,66,66,66	0
56	MG	DA	3111	1/1	0.92	0.14	-	33,33,33,33	0
56	MG	DA	3628	1/1	0.86	0.14	-	56,56,56,56	0
56	MG	BA	3090	1/1	0.91	0.20	-	37,37,37,37	0
56	MG	BA	3295	1/1	0.83	0.26	-	42,42,42,42	0
56	MG	CA	3084	1/1	0.85	0.31	-	69,69,69,69	0
56	MG	BA	3106	1/1	0.93	0.46	-	50,50,50,50	0
56	MG	CA	3026	1/1	0.79	0.29	-	64,64,64,64	0
56	MG	BA	3516	1/1	0.81	0.22	-	65,65,65,65	0
56	MG	CA	3156	1/1	0.95	0.10	-	68,68,68,68	0
56	MG	DA	3096	1/1	0.87	0.22	-	51,51,51,51	0
56	MG	DA	3119	1/1	0.92	0.20	-	62,62,62,62	0
56	MG	DA	3211	1/1	0.88	0.20	-	48,48,48,48	0
56	MG	BA	3454	1/1	0.94	0.15	-	31,31,31,31	0
56	MG	DA	3597	1/1	0.90	0.10	-	51,51,51,51	0
56	MG	DA	3552	1/1	0.97	0.07	-	43,43,43,43	0
56	MG	BA	3345	1/1	0.91	0.13	-	44,44,44,44	0
56	MG	CA	3175	1/1	0.90	0.16	-	39,39,39,39	0
56	MG	AA	3178	1/1	0.95	0.12	-	54,54,54,54	0
56	MG	BA	3477	1/1	0.87	0.20	-	55,55,55,55	0
56	MG	DA	3675	1/1	0.93	0.28	-	44,44,44,44	0
56	MG	DA	3218	1/1	0.99	0.16	-	47,47,47,47	0
56	MG	BA	3163	1/1	0.95	0.22	-	45,45,45,45	0
56	MG	BA	3002	1/1	0.83	0.37	-	62,62,62,62	0
56	MG	BA	3616	1/1	0.93	0.12	-	53,53,53,53	0
56	MG	B6	102	1/1	0.88	0.31	-	55,55,55,55	0
56	MG	DA	3151	1/1	0.96	0.26	-	44,44,44,44	0
56	MG	BA	3138	1/1	0.85	0.16	-	48,48,48,48	0
56	MG	DA	3117	1/1	0.94	0.28	-	60,60,60,60	0
56	MG	AA	3040	1/1	0.80	0.16	-	59,59,59,59	0
56	MG	B8	102	1/1	0.97	0.08	-	50,50,50,50	0
56	MG	DA	3020	1/1	0.90	0.14	-	50,50,50,50	0
56	MG	CA	3027	1/1	0.71	0.51	-	70,70,70,70	0
56	MG	AA	3139	1/1	0.88	0.14	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3444	1/1	0.86	0.18	-	48,48,48,48	0
56	MG	DA	3319	1/1	0.84	0.30	-	43,43,43,43	0
56	MG	AA	3195	1/1	0.98	0.14	-	59,59,59,59	0
56	MG	DA	3632	1/1	0.75	0.16	-	58,58,58,58	0
56	MG	BA	3752	1/1	0.87	0.18	-	19,19,19,19	0
56	MG	CA	3074	1/1	0.92	0.39	-	55,55,55,55	0
56	MG	BA	3015	1/1	0.90	0.23	-	47,47,47,47	0
56	MG	DA	3348	1/1	0.94	0.27	-	38,38,38,38	0
56	MG	DA	3606	1/1	0.91	0.22	-	54,54,54,54	0
56	MG	CA	3143	1/1	0.92	0.15	-	62,62,62,62	0
56	MG	AA	3221	1/1	0.87	0.14	-	49,49,49,49	0
56	MG	BA	3107	1/1	0.98	0.19	-	20,20,20,20	0
56	MG	BA	3350	1/1	0.94	0.24	-	27,27,27,27	0
56	MG	BA	3174	1/1	0.98	0.16	-	34,34,34,34	0
56	MG	BA	3288	1/1	0.98	0.38	-	40,40,40,40	0
56	MG	DA	3355	1/1	0.90	0.10	-	50,50,50,50	0
56	MG	BA	3511	1/1	0.87	0.23	-	54,54,54,54	0
56	MG	DA	3352	1/1	0.96	0.15	-	35,35,35,35	0
56	MG	AA	3175	1/1	0.83	0.20	-	54,54,54,54	0
56	MG	BA	3657	1/1	0.98	0.20	-	47,47,47,47	0
56	MG	DA	3447	1/1	0.97	0.27	-	35,35,35,35	0
56	MG	CA	3165	1/1	0.95	0.08	-	56,56,56,56	0
56	MG	DA	3501	1/1	0.96	0.15	-	59,59,59,59	0
56	MG	DA	3237	1/1	0.97	0.07	-	51,51,51,51	0
56	MG	AA	3168	1/1	0.96	0.08	-	62,62,62,62	0
56	MG	DA	3542	1/1	0.78	0.20	-	63,63,63,63	0
56	MG	BA	3166	1/1	0.97	0.22	-	40,40,40,40	0
56	MG	BA	3202	1/1	0.95	0.13	-	46,46,46,46	0
56	MG	DA	3026	1/1	0.91	0.14	-	42,42,42,42	0
56	MG	BA	3218	1/1	0.86	0.18	-	44,44,44,44	0
56	MG	CA	3103	1/1	0.95	0.10	-	75,75,75,75	0
56	MG	AA	3007	1/1	0.96	0.26	-	65,65,65,65	0
56	MG	BA	3071	1/1	0.99	0.33	-	42,42,42,42	0
56	MG	DA	3167	1/1	0.92	0.25	-	47,47,47,47	0
56	MG	DA	3220	1/1	0.92	0.19	-	46,46,46,46	0
56	MG	BA	3461	1/1	0.96	0.19	-	31,31,31,31	0
56	MG	BA	3256	1/1	0.94	0.32	-	49,49,49,49	0
56	MG	BA	3636	1/1	0.93	0.09	-	53,53,53,53	0
56	MG	AA	3117	1/1	0.97	0.16	-	48,48,48,48	0
56	MG	BA	3276	1/1	0.94	0.29	-	41,41,41,41	0
56	MG	BB	3009	1/1	0.79	0.27	-	58,58,58,58	0
56	MG	CA	3035	1/1	0.94	0.10	-	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3712	1/1	0.63	0.13	-	64,64,64,64	0
56	MG	DA	3601	1/1	0.96	0.19	-	54,54,54,54	0
56	MG	DA	3164	1/1	0.96	0.26	-	33,33,33,33	0
56	MG	B1	101	1/1	0.92	0.38	-	44,44,44,44	0
56	MG	DA	3118	1/1	0.97	0.25	-	52,52,52,52	0
56	MG	BA	3633	1/1	0.87	0.17	-	45,45,45,45	0
56	MG	DA	3603	1/1	0.94	0.14	-	52,52,52,52	0
56	MG	AA	3052	1/1	0.94	0.32	-	68,68,68,68	0
56	MG	BA	3058	1/1	0.91	0.20	-	36,36,36,36	0
56	MG	BA	3099	1/1	0.92	0.16	-	50,50,50,50	0
56	MG	AA	3222	1/1	0.93	0.24	-	67,67,67,67	0
56	MG	DA	3397	1/1	0.86	0.17	-	49,49,49,49	0
56	MG	DA	3376	1/1	0.90	0.24	-	54,54,54,54	0
56	MG	DA	3519	1/1	0.96	0.17	-	24,24,24,24	0
56	MG	BA	3030	1/1	0.71	0.19	-	50,50,50,50	0
56	MG	AX	3009	1/1	0.84	0.25	-	71,71,71,71	0
56	MG	DA	3002	1/1	0.86	0.17	-	68,68,68,68	0
56	MG	CA	3172	1/1	0.88	0.15	-	64,64,64,64	0
56	MG	BB	3010	1/1	0.94	0.11	-	48,48,48,48	0
56	MG	DA	3543	1/1	0.97	0.23	-	55,55,55,55	0
56	MG	CA	3139	1/1	0.90	0.15	-	61,61,61,61	0
56	MG	AA	3134	1/1	0.88	0.22	-	69,69,69,69	0
56	MG	BA	3231	1/1	0.99	0.24	-	37,37,37,37	0
56	MG	BV	204	1/1	0.95	0.21	-	50,50,50,50	0
56	MG	AA	3180	1/1	0.95	0.14	-	57,57,57,57	0
56	MG	BA	3121	1/1	0.97	0.36	-	41,41,41,41	0
56	MG	DA	3159	1/1	0.94	0.30	-	41,41,41,41	0
56	MG	DA	3526	1/1	0.92	0.22	-	47,47,47,47	0
56	MG	DB	3010	1/1	0.87	0.17	-	55,55,55,55	0
56	MG	AA	3167	1/1	0.97	0.21	-	47,47,47,47	0
56	MG	BA	3168	1/1	0.97	0.19	-	27,27,27,27	0
56	MG	AW	3003	1/1	0.91	0.31	-	59,59,59,59	0
56	MG	CA	3082	1/1	0.92	0.13	-	63,63,63,63	0
56	MG	BA	3340	1/1	0.97	0.13	-	45,45,45,45	0
56	MG	AA	3068	1/1	0.82	0.17	-	60,60,60,60	0
56	MG	BA	3155	1/1	0.97	0.12	-	54,54,54,54	0
56	MG	DA	3223	1/1	0.91	0.29	-	54,54,54,54	0
56	MG	DA	3048	1/1	0.94	0.15	-	45,45,45,45	0
56	MG	BA	3610	1/1	0.97	0.16	-	64,64,64,64	0
56	MG	DA	3616	1/1	0.90	0.07	-	45,45,45,45	0
56	MG	AA	3160	1/1	0.97	0.14	-	57,57,57,57	0
56	MG	DA	3289	1/1	0.96	0.36	-	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3225	1/1	0.89	0.23	-	54,54,54,54	0
56	MG	BA	3648	1/1	0.93	0.37	-	53,53,53,53	0
56	MG	DA	3572	1/1	0.93	0.25	-	28,28,28,28	0
56	MG	DA	3422	1/1	0.90	0.36	-	43,43,43,43	0
56	MG	DA	3439	1/1	0.87	0.14	-	50,50,50,50	0
56	MG	AA	3176	1/1	0.94	0.09	-	54,54,54,54	0
56	MG	BA	3443	1/1	0.97	0.12	-	25,25,25,25	0
56	MG	DA	3631	1/1	0.94	0.13	-	56,56,56,56	0
56	MG	BA	3291	1/1	0.83	0.21	-	71,71,71,71	0
56	MG	BA	3258	1/1	0.96	0.28	-	41,41,41,41	0
56	MG	DA	3028	1/1	0.74	0.17	-	70,70,70,70	0
56	MG	BA	3194	1/1	0.92	0.20	-	37,37,37,37	0
56	MG	CA	3122	1/1	0.82	0.15	-	70,70,70,70	0
56	MG	CA	3073	1/1	0.92	0.32	-	48,48,48,48	0
56	MG	BA	3319	1/1	0.97	0.29	-	20,20,20,20	0
56	MG	CA	3173	1/1	0.88	0.08	-	69,69,69,69	0
56	MG	AA	3091	1/1	0.80	0.10	-	70,70,70,70	0
56	MG	BA	3367	1/1	0.79	0.33	-	53,53,53,53	0
56	MG	DA	3403	1/1	0.85	0.15	-	57,57,57,57	0
56	MG	DA	3370	1/1	0.89	0.08	-	46,46,46,46	0
56	MG	BA	3449	1/1	0.92	0.29	-	60,60,60,60	0
56	MG	BA	3112	1/1	0.88	0.34	-	57,57,57,57	0
56	MG	AY	3002	1/1	0.93	0.12	-	68,68,68,68	0
56	MG	DA	3567	1/1	0.87	0.16	-	46,46,46,46	0
56	MG	DA	3614	1/1	0.78	0.14	-	50,50,50,50	0
56	MG	CA	3157	1/1	0.91	0.28	-	64,64,64,64	0
56	MG	BA	3594	1/1	0.87	0.23	-	24,24,24,24	0
56	MG	DA	3272	1/1	0.87	0.16	-	44,44,44,44	0
56	MG	BA	3159	1/1	0.96	0.22	-	30,30,30,30	0
56	MG	DA	3660	1/1	0.97	0.19	-	40,40,40,40	0
56	MG	BA	3775	1/1	0.97	0.17	-	43,43,43,43	0
56	MG	BA	3253	1/1	0.92	0.21	-	40,40,40,40	0
56	MG	DA	3390	1/1	0.92	0.07	-	54,54,54,54	0
56	MG	DA	3470	1/1	0.89	0.16	-	42,42,42,42	0
56	MG	BA	3660	1/1	0.96	0.18	-	51,51,51,51	0
56	MG	BA	3525	1/1	0.97	0.18	-	52,52,52,52	0
56	MG	BA	3787	1/1	0.90	0.22	-	59,59,59,59	0
56	MG	AA	3018	1/1	0.88	0.10	-	51,51,51,51	0
56	MG	BA	3581	1/1	0.91	0.11	-	38,38,38,38	0
56	MG	DD	307	1/1	0.90	0.14	-	56,56,56,56	0
56	MG	BA	3225	1/1	0.85	0.35	-	42,42,42,42	0
56	MG	DA	3411	1/1	0.96	0.17	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	3051	1/1	0.89	0.17	-	62,62,62,62	0
56	MG	AA	3116	1/1	0.85	0.27	-	61,61,61,61	0
56	MG	AA	3216	1/1	0.91	0.13	-	72,72,72,72	0
56	MG	DA	3066	1/1	0.75	0.13	-	65,65,65,65	0
56	MG	BA	3435	1/1	0.87	0.16	-	57,57,57,57	0
56	MG	BA	3619	1/1	0.93	0.39	-	51,51,51,51	0
56	MG	BA	3033	1/1	0.93	0.26	-	33,33,33,33	0
56	MG	BA	3680	1/1	0.94	0.15	-	52,52,52,52	0
56	MG	DA	3187	1/1	0.89	0.12	-	56,56,56,56	0
56	MG	DA	3196	1/1	0.88	0.09	-	53,53,53,53	0
56	MG	CA	3129	1/1	0.94	0.19	-	61,61,61,61	0
56	MG	BB	3005	1/1	0.93	0.19	-	64,64,64,64	0
56	MG	BA	3502	1/1	0.94	0.31	-	45,45,45,45	0
56	MG	BA	3709	1/1	0.95	0.29	-	44,44,44,44	0
56	MG	DQ	3002	1/1	0.97	0.17	-	42,42,42,42	0
56	MG	BA	3269	1/1	0.89	0.38	-	53,53,53,53	0
56	MG	BA	3653	1/1	0.97	0.28	-	49,49,49,49	0
56	MG	DA	3506	1/1	0.90	0.10	-	48,48,48,48	0
56	MG	BA	3800	1/1	0.95	0.15	-	39,39,39,39	0
56	MG	DA	3127	1/1	0.78	0.27	-	38,38,38,38	0
56	MG	DA	3640	1/1	0.94	0.14	-	52,52,52,52	0
56	MG	DA	3046	1/1	0.93	0.37	-	57,57,57,57	0
56	MG	BA	3564	1/1	0.88	0.18	-	41,41,41,41	0
56	MG	DA	3509	1/1	0.80	0.18	-	53,53,53,53	0
56	MG	DA	3141	1/1	0.94	0.21	-	56,56,56,56	0
56	MG	DA	3576	1/1	0.96	0.16	-	37,37,37,37	0
56	MG	BA	3613	1/1	0.91	0.13	-	45,45,45,45	0
56	MG	AA	3143	1/1	0.91	0.16	-	73,73,73,73	0
56	MG	BA	3689	1/1	0.75	0.22	-	57,57,57,57	0
56	MG	BA	3652	1/1	0.95	0.13	-	46,46,46,46	0
56	MG	DA	3239	1/1	0.92	0.20	-	54,54,54,54	0
56	MG	BA	3214	1/1	0.94	0.20	-	49,49,49,49	0
56	MG	DA	3269	1/1	0.89	0.20	-	32,32,32,32	0
56	MG	DA	3204	1/1	0.92	0.31	-	51,51,51,51	0
56	MG	DA	3351	1/1	0.91	0.12	-	39,39,39,39	0
56	MG	BA	3110	1/1	0.94	0.25	-	41,41,41,41	0
56	MG	BA	3144	1/1	0.91	0.09	-	43,43,43,43	0
56	MG	BA	3503	1/1	0.91	0.23	-	58,58,58,58	0
56	MG	BA	3601	1/1	0.92	0.16	-	42,42,42,42	0
56	MG	DA	3335	1/1	0.92	0.19	-	32,32,32,32	0
56	MG	BA	3315	1/1	0.76	0.14	-	56,56,56,56	0
56	MG	BA	3665	1/1	0.94	0.29	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CX	3006	1/1	0.70	0.50	-	70,70,70,70	0
56	MG	DA	3014	1/1	0.94	0.14	-	50,50,50,50	0
56	MG	BA	3690	1/1	0.88	0.21	-	63,63,63,63	0
56	MG	BA	3020	1/1	0.75	0.20	-	61,61,61,61	0
56	MG	BA	3248	1/1	0.90	0.15	-	45,45,45,45	0
56	MG	BA	3405	1/1	0.98	0.18	-	33,33,33,33	0
56	MG	BA	3693	1/1	0.84	0.13	-	70,70,70,70	0
56	MG	DA	3623	1/1	0.87	0.15	-	70,70,70,70	0
56	MG	DA	3377	1/1	0.94	0.07	-	42,42,42,42	0
56	MG	DB	3001	1/1	0.96	0.04	-	73,73,73,73	0
56	MG	BG	203	1/1	0.91	0.07	-	36,36,36,36	0
56	MG	CA	3002	1/1	0.89	0.07	-	51,51,51,51	0
56	MG	BA	3149	1/1	0.90	0.13	-	53,53,53,53	0
56	MG	DA	3248	1/1	0.88	0.31	-	33,33,33,33	0
56	MG	BA	3394	1/1	0.92	0.20	-	52,52,52,52	0
56	MG	BA	3316	1/1	0.94	0.25	-	23,23,23,23	0
56	MG	DA	3437	1/1	0.88	0.25	-	39,39,39,39	0
56	MG	CA	3112	1/1	0.95	0.15	-	59,59,59,59	0
56	MG	DA	3199	1/1	0.78	0.41	-	52,52,52,52	0
56	MG	BA	3233	1/1	0.90	0.33	-	48,48,48,48	0
56	MG	DA	3507	1/1	0.86	0.22	-	60,60,60,60	0
56	MG	BA	3335	1/1	0.97	0.17	-	50,50,50,50	0
56	MG	BA	3785	1/1	0.96	0.16	-	41,41,41,41	0
56	MG	DA	3472	1/1	0.96	0.06	-	33,33,33,33	0
56	MG	BA	3528	1/1	0.94	0.11	-	43,43,43,43	0
56	MG	BB	3004	1/1	0.86	0.11	-	47,47,47,47	0
56	MG	BA	3550	1/1	0.94	0.20	-	34,34,34,34	0
56	MG	DA	3636	1/1	0.92	0.24	-	56,56,56,56	0
56	MG	BA	3592	1/1	0.91	0.14	-	29,29,29,29	0
56	MG	BA	3674	1/1	0.86	0.11	-	47,47,47,47	0
56	MG	DA	3412	1/1	0.96	0.16	-	63,63,63,63	0
56	MG	BA	3285	1/1	0.96	0.37	-	49,49,49,49	0
56	MG	AA	3122	1/1	0.96	0.19	-	60,60,60,60	0
56	MG	AA	3152	1/1	0.94	0.13	-	45,45,45,45	0
56	MG	AA	3203	1/1	0.96	0.34	-	57,57,57,57	0
56	MG	DA	3629	1/1	0.96	0.22	-	52,52,52,52	0
56	MG	BA	3082	1/1	0.96	0.11	-	59,59,59,59	0
56	MG	DA	3627	1/1	0.96	0.04	-	48,48,48,48	0
56	MG	DA	3530	1/1	0.97	0.23	-	55,55,55,55	0
56	MG	DA	3568	1/1	0.82	0.13	-	54,54,54,54	0
56	MG	BA	3451	1/1	0.88	0.11	-	64,64,64,64	0
56	MG	DA	3224	1/1	0.79	0.35	-	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3140	1/1	0.90	0.11	-	34,34,34,34	0
56	MG	DA	3536	1/1	0.89	0.32	-	54,54,54,54	0
56	MG	DA	3071	1/1	0.97	0.37	-	44,44,44,44	0
56	MG	AA	3148	1/1	0.92	0.15	-	63,63,63,63	0
56	MG	DA	3190	1/1	0.92	0.26	-	45,45,45,45	0
56	MG	DA	3055	1/1	0.97	0.24	-	36,36,36,36	0
56	MG	DA	3615	1/1	0.86	0.33	-	47,47,47,47	0
56	MG	BA	3836	1/1	0.97	0.29	-	45,45,45,45	0
56	MG	BA	3490	1/1	0.96	0.22	-	44,44,44,44	0
56	MG	BA	3426	1/1	0.93	0.21	-	22,22,22,22	0
56	MG	CA	3040	1/1	0.90	0.12	-	58,58,58,58	0
56	MG	DA	3102	1/1	0.85	0.12	-	57,57,57,57	0
56	MG	BA	3196	1/1	0.84	0.23	-	51,51,51,51	0
56	MG	AA	3042	1/1	0.77	0.21	-	57,57,57,57	0
56	MG	BA	3635	1/1	0.95	0.28	-	62,62,62,62	0
56	MG	BA	3531	1/1	0.94	0.39	-	61,61,61,61	0
56	MG	AA	3109	1/1	0.92	0.32	-	64,64,64,64	0
56	MG	DA	3107	1/1	0.89	0.19	-	49,49,49,49	0
56	MG	BA	3772	1/1	0.98	0.17	-	31,31,31,31	0
56	MG	BA	3220	1/1	0.83	0.20	-	55,55,55,55	0
56	MG	DA	3638	1/1	0.91	0.25	-	60,60,60,60	0
56	MG	DA	3450	1/1	0.95	0.16	-	36,36,36,36	0
56	MG	AA	3100	1/1	0.85	0.08	-	68,68,68,68	0
56	MG	DA	3293	1/1	0.91	0.11	-	60,60,60,60	0
56	MG	DA	3592	1/1	0.94	0.17	-	52,52,52,52	0
56	MG	AA	3187	1/1	0.94	0.12	-	62,62,62,62	0
56	MG	DA	3414	1/1	0.95	0.16	-	41,41,41,41	0
56	MG	AA	3015	1/1	0.91	0.16	-	60,60,60,60	0
56	MG	BA	3719	1/1	0.93	0.13	-	42,42,42,42	0
56	MG	BB	3019	1/1	0.86	0.16	-	49,49,49,49	0
56	MG	AA	3036	1/1	0.95	0.12	-	52,52,52,52	0
56	MG	DA	3600	1/1	0.88	0.08	-	53,53,53,53	0
56	MG	BA	3506	1/1	0.94	0.26	-	51,51,51,51	0
56	MG	DA	3557	1/1	0.93	0.23	-	34,34,34,34	0
56	MG	BA	3605	1/1	0.74	0.13	-	61,61,61,61	0
56	MG	DA	3137	1/1	0.93	0.13	-	54,54,54,54	0
56	MG	DA	3492	1/1	0.96	0.12	-	47,47,47,47	0
56	MG	DA	3019	1/1	0.90	0.15	-	57,57,57,57	0
56	MG	BA	3164	1/1	0.93	0.28	-	43,43,43,43	0
56	MG	BA	3298	1/1	0.86	0.18	-	68,68,68,68	0
56	MG	AA	3065	1/1	0.98	0.17	-	58,58,58,58	0
56	MG	DA	3069	1/1	0.89	0.39	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	3054	1/1	0.86	0.16	-	71,71,71,71	0
56	MG	DA	3263	1/1	0.93	0.10	-	61,61,61,61	0
56	MG	CA	3029	1/1	0.88	0.38	-	61,61,61,61	0
56	MG	AA	3063	1/1	0.97	0.07	-	63,63,63,63	0
56	MG	DA	3546	1/1	0.88	0.11	-	53,53,53,53	0
56	MG	DA	3296	1/1	0.94	0.18	-	48,48,48,48	0
56	MG	BA	3806	1/1	0.97	0.17	-	51,51,51,51	0
56	MG	BA	3375	1/1	0.92	0.15	-	35,35,35,35	0
56	MG	DB	3004	1/1	0.88	0.15	-	51,51,51,51	0
56	MG	BA	3779	1/1	0.87	0.12	-	59,59,59,59	0
56	MG	BA	3548	1/1	0.90	0.28	-	48,48,48,48	0
56	MG	AA	3026	1/1	0.93	0.22	-	53,53,53,53	0
56	MG	CA	3069	1/1	0.77	0.12	-	68,68,68,68	0
56	MG	BA	3669	1/1	0.92	0.13	-	42,42,42,42	0
56	MG	BA	3343	1/1	0.95	0.18	-	33,33,33,33	0
56	MG	BA	3300	1/1	0.94	0.18	-	22,22,22,22	0
56	MG	BA	3702	1/1	0.91	0.07	-	51,51,51,51	0
56	MG	DA	3063	1/1	0.95	0.14	-	46,46,46,46	0
56	MG	AA	3031	1/1	0.94	0.09	-	44,44,44,44	0
56	MG	DA	3387	1/1	0.83	0.22	-	56,56,56,56	0
56	MG	BA	3333	1/1	0.74	0.11	-	61,61,61,61	0
56	MG	BA	3280	1/1	0.91	0.24	-	49,49,49,49	0
56	MG	CA	3096	1/1	0.96	0.15	-	61,61,61,61	0
56	MG	BA	3165	1/1	0.97	0.26	-	40,40,40,40	0
56	MG	BA	3579	1/1	0.90	0.08	-	47,47,47,47	0
56	MG	BA	3694	1/1	0.97	0.23	-	27,27,27,27	0
56	MG	BA	3129	1/1	0.99	0.22	-	36,36,36,36	0
56	MG	BA	3527	1/1	0.68	0.11	-	52,52,52,52	0
56	MG	BA	3766	1/1	0.93	0.19	-	31,31,31,31	0
56	MG	DA	3611	1/1	0.83	0.32	-	55,55,55,55	0
56	MG	DA	3656	1/1	0.99	0.17	-	62,62,62,62	0
56	MG	BA	3715	1/1	0.95	0.24	-	53,53,53,53	0
56	MG	DA	3133	1/1	0.92	0.29	-	40,40,40,40	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.