



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:31 PM GMT

PDB ID : 4W2I  
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with  
negamycin, mRNA and three deacylated tRNAs in the A, P and E sites  
Authors : Polikanov, Y.S.; Szal, T.; Jiang, F.; Gupta, P.; Matsuda, R.; Shiozuka, M.;  
Steitz, T.A.; Vazquez-Laslop, Nora; Mankin, A.S.  
Deposited on : 2014-09-12  
Resolution : 2.70 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

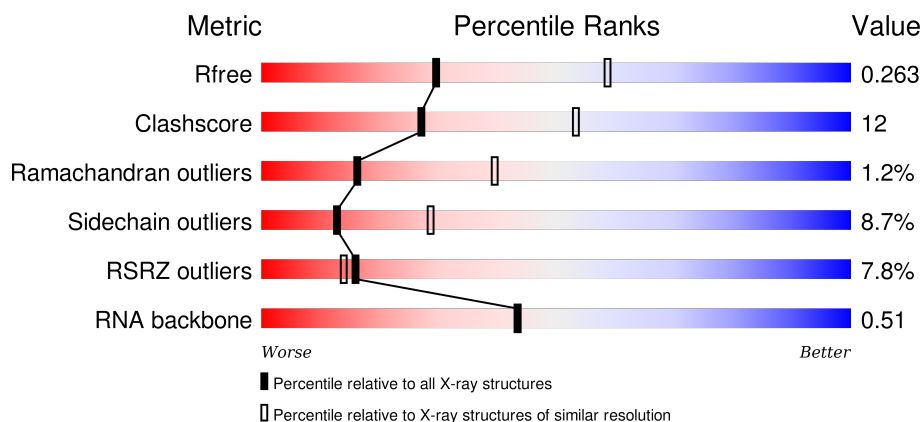
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)
RNA backbone	2183	1069 (3.10-2.30)

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	
1	CA	1521	
2	AB	256	
2	CB	256	

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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	






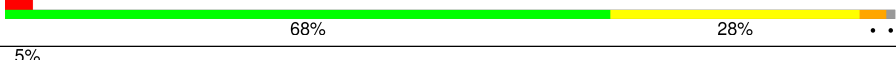

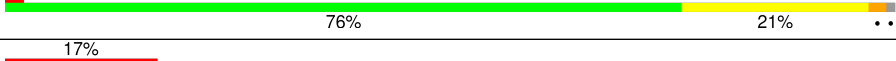

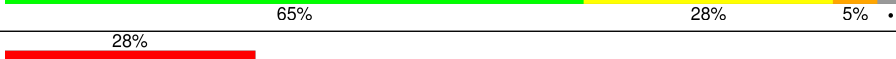
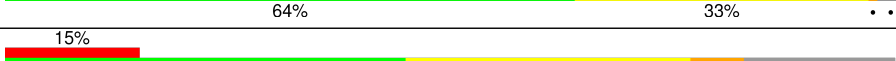
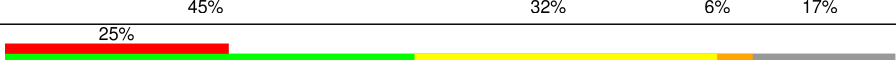
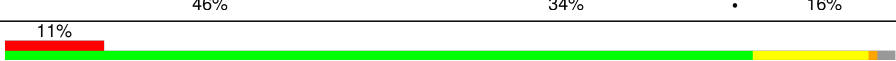
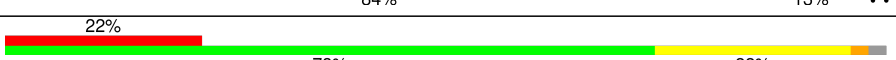
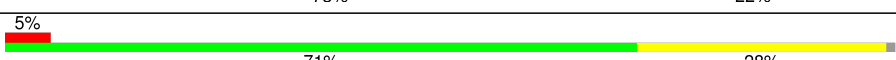
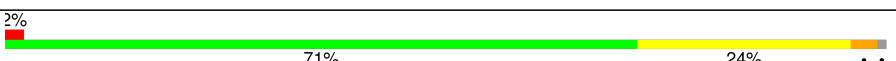
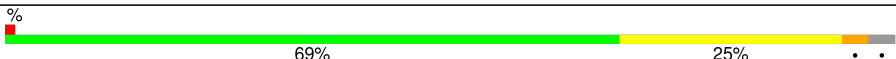
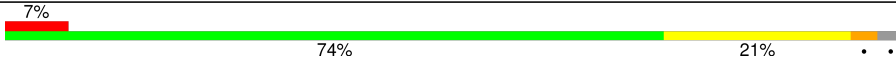



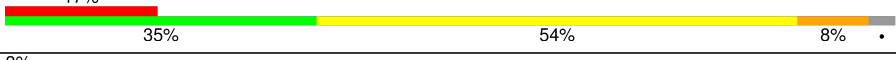
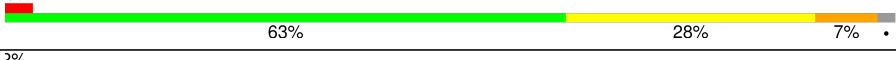


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Mol	Chain	Length	Quality of chain
27	BD	276	
27	DD	276	
28	BE	206	
28	DE	206	
29	BF	210	
29	DF	210	
30	BG	182	
30	DG	182	
31	BH	180	
31	DH	180	
32	BI	148	
32	DI	148	
33	BN	140	
33	DN	140	
34	BO	122	
34	DO	122	
35	BP	150	
35	DP	150	
36	BQ	141	
36	DQ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

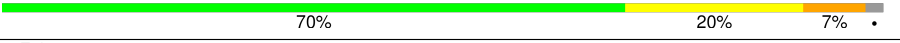







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Mol	Chain	Length	Quality of chain
39	DT	146	
40	BU	118	
40	DU	118	
41	BV	101	
41	DV	101	
42	BW	113	
42	DW	113	
43	BX	96	
43	DX	96	
44	BY	110	
44	DY	110	
45	BZ	206	
45	DZ	206	
46	B0	85	
46	D0	85	
47	B1	98	
47	D1	98	
48	B2	72	
48	D2	72	
49	B3	60	
49	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	3034	-	-	-	X
56	MG	AA	3052	-	-	-	X
56	MG	AA	3094	-	-	-	X
56	MG	AA	3127	-	-	-	X
56	MG	AA	3130	-	-	-	X
56	MG	AA	3172	-	-	-	X
56	MG	AE	3002	-	-	-	X
56	MG	AX	3002	-	-	-	X
56	MG	AX	3010	-	-	-	X
56	MG	B0	101	-	-	-	X
56	MG	B5	101	-	-	-	X
56	MG	B5	102	-	-	-	X
56	MG	B5	103	-	-	-	X
56	MG	B7	102	-	-	-	X
56	MG	BA	3007	-	-	-	X
56	MG	BA	3018	-	-	-	X
56	MG	BA	3022	-	-	-	X
56	MG	BA	3025	-	-	-	X
56	MG	BA	3026	-	-	-	X
56	MG	BA	3027	-	-	-	X
56	MG	BA	3028	-	-	-	X
56	MG	BA	3029	-	-	-	X
56	MG	BA	3061	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	BA	3089	-	-	-	X
56	MG	BA	3091	-	-	-	X
56	MG	BA	3094	-	-	-	X
56	MG	BA	3105	-	-	-	X
56	MG	BA	3106	-	-	-	X
56	MG	BA	3110	-	-	-	X
56	MG	BA	3116	-	-	-	X
56	MG	BA	3127	-	-	-	X
56	MG	BA	3131	-	-	-	X
56	MG	BA	3132	-	-	-	X
56	MG	BA	3136	-	-	-	X
56	MG	BA	3141	-	-	-	X
56	MG	BA	3143	-	-	-	X
56	MG	BA	3160	-	-	-	X
56	MG	BA	3164	-	-	-	X
56	MG	BA	3182	-	-	-	X
56	MG	BA	3188	-	-	-	X
56	MG	BA	3190	-	-	-	X
56	MG	BA	3194	-	-	-	X
56	MG	BA	3203	-	-	-	X
56	MG	BA	3209	-	-	-	X
56	MG	BA	3220	-	-	-	X
56	MG	BA	3237	-	-	-	X
56	MG	BA	3238	-	-	-	X
56	MG	BA	3244	-	-	-	X
56	MG	BA	3271	-	-	-	X
56	MG	BA	3327	-	-	-	X
56	MG	BA	3354	-	-	-	X
56	MG	BA	3399	-	-	-	X
56	MG	BA	3440	-	-	-	X
56	MG	BA	3460	-	-	-	X
56	MG	BA	3472	-	-	-	X
56	MG	BA	3479	-	-	-	X
56	MG	BA	3495	-	-	-	X
56	MG	BA	3541	-	-	-	X
56	MG	BA	3562	-	-	-	X
56	MG	BA	3615	-	-	-	X
56	MG	BA	3642	-	-	-	X
56	MG	BA	3649	-	-	-	X
56	MG	BA	3668	-	-	-	X
56	MG	BA	3672	-	-	-	X
56	MG	BA	3757	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	BA	3769	-	-	-	X
56	MG	BA	3773	-	-	-	X
56	MG	BA	3774	-	-	-	X
56	MG	BA	3776	-	-	-	X
56	MG	BA	3777	-	-	-	X
56	MG	BA	3782	-	-	-	X
56	MG	BA	3783	-	-	-	X
56	MG	BA	3785	-	-	-	X
56	MG	BD	304	-	-	-	X
56	MG	BD	305	-	-	-	X
56	MG	BD	307	-	-	-	X
56	MG	BD	308	-	-	-	X
56	MG	BD	309	-	-	-	X
56	MG	BD	311	-	-	-	X
56	MG	BE	304	-	-	-	X
56	MG	BF	301	-	-	-	X
56	MG	BF	302	-	-	-	X
56	MG	BF	304	-	-	-	X
56	MG	BF	305	-	-	-	X
56	MG	BF	306	-	-	-	X
56	MG	BF	308	-	-	-	X
56	MG	BF	309	-	-	-	X
56	MG	BN	3001	-	-	-	X
56	MG	BN	3004	-	-	-	X
56	MG	BN	3006	-	-	-	X
56	MG	BP	201	-	-	-	X
56	MG	BP	202	-	-	-	X
56	MG	BQ	3001	-	-	-	X
56	MG	BQ	3005	-	-	-	X
56	MG	BR	201	-	-	-	X
56	MG	BR	202	-	-	-	X
56	MG	BU	201	-	-	-	X
56	MG	BU	202	-	-	-	X
56	MG	BU	205	-	-	-	X
56	MG	BU	206	-	-	-	X
56	MG	BU	207	-	-	-	X
56	MG	BU	208	-	-	-	X
56	MG	BU	209	-	-	-	X
56	MG	BV	202	-	-	-	X
56	MG	BV	205	-	-	-	X
56	MG	BV	207	-	-	-	X
56	MG	BX	102	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	CA	3032	-	-	-	X
56	MG	CA	3035	-	-	-	X
56	MG	CA	3048	-	-	-	X
56	MG	CA	3055	-	-	-	X
56	MG	CA	3092	-	-	-	X
56	MG	CA	3140	-	-	-	X
56	MG	D3	3001	-	-	-	X
56	MG	D7	101	-	-	-	X
56	MG	DA	3006	-	-	-	X
56	MG	DA	3015	-	-	-	X
56	MG	DA	3023	-	-	-	X
56	MG	DA	3024	-	-	-	X
56	MG	DA	3025	-	-	-	X
56	MG	DA	3037	-	-	-	X
56	MG	DA	3065	-	-	-	X
56	MG	DA	3071	-	-	-	X
56	MG	DA	3078	-	-	-	X
56	MG	DA	3086	-	-	-	X
56	MG	DA	3125	-	-	-	X
56	MG	DA	3156	-	-	-	X
56	MG	DA	3160	-	-	-	X
56	MG	DA	3168	-	-	-	X
56	MG	DA	3186	-	-	-	X
56	MG	DA	3233	-	-	-	X
56	MG	DA	3244	-	-	-	X
56	MG	DA	3251	-	-	-	X
56	MG	DA	3284	-	-	-	X
56	MG	DA	3316	-	-	-	X
56	MG	DA	3361	-	-	-	X
56	MG	DA	3415	-	-	-	X
56	MG	DA	3449	-	-	-	X
56	MG	DA	3471	-	-	-	X
56	MG	DA	3553	-	-	-	X
56	MG	DA	3556	-	-	-	X
56	MG	DA	3558	-	-	-	X
56	MG	DA	3617	-	-	-	X
56	MG	DA	3621	-	-	-	X
56	MG	DD	304	-	-	-	X
56	MG	DD	306	-	-	-	X
56	MG	DD	307	-	-	-	X
56	MG	DD	308	-	-	-	X
56	MG	DE	301	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	DF	305	-	-	-	X
56	MG	DF	306	-	-	-	X
56	MG	DQ	3003	-	-	-	X
56	MG	DR	3001	-	-	-	X
56	MG	DU	3001	-	-	-	X
56	MG	DV	3001	-	-	-	X
56	MG	DV	3002	-	-	-	X
56	MG	DW	3002	-	-	-	X
57	NEG	AA	3216	-	-	X	X
57	NEG	AA	3219	-	-	-	X
57	NEG	AA	3221	-	-	-	X
57	NEG	AA	3222	-	-	-	X
57	NEG	AW	3004	-	-	-	X
57	NEG	CA	3170	-	-	-	X
57	NEG	CA	3173	-	-	-	X
57	NEG	CA	3174	-	-	-	X
57	NEG	CA	3175	-	-	-	X
57	NEG	CA	3177	-	-	-	X
57	NEG	CX	3004	-	-	-	X
59	ZN	B5	105	-	-	-	X

## 2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 297376 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	1496	Total	C	N	O	P	0	0	0
			32163	14314	5963	10390	1496			
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	12	Total	C	N	O	P	0	0	0
			252	115	46	80	11			

- 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	2822	Total	C	N	O	P	0	0	0
			60792	27054	11380	19537	2821			
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
			517	331	102	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	785	Total	Mg	0	0
			785	785		
56	CA	172	Total	Mg	0	0
			172	172		
56	DQ	4	Total	Mg	0	0
			4	4		
56	D3	1	Total	Mg	0	0
			1	1		
56	DF	6	Total	Mg	0	0
			6	6		
56	CV	1	Total	Mg	0	0
			1	1		
56	B8	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	BE	8	Total 8	Mg 8	0	0
56	AW	4	Total 4	Mg 4	0	0
56	DU	3	Total 3	Mg 3	0	0
56	B1	1	Total 1	Mg 1	0	0
56	AN	3	Total 3	Mg 3	0	0
56	BP	4	Total 4	Mg 4	0	0
56	AX	11	Total 11	Mg 11	0	0
56	CN	1	Total 1	Mg 1	0	0
56	DN	1	Total 1	Mg 1	0	0
56	CY	1	Total 1	Mg 1	0	0
56	DD	9	Total 9	Mg 9	0	0
56	B5	5	Total 5	Mg 5	0	0
56	BB	18	Total 18	Mg 18	0	0
56	BT	1	Total 1	Mg 1	0	0
56	D8	1	Total 1	Mg 1	0	0
56	AE	2	Total 2	Mg 2	0	0
56	DG	1	Total 1	Mg 1	0	0
56	B9	1	Total 1	Mg 1	0	0
56	BF	11	Total 11	Mg 11	0	0
56	AV	3	Total 3	Mg 3	0	0
56	BX	2	Total 2	Mg 2	0	0

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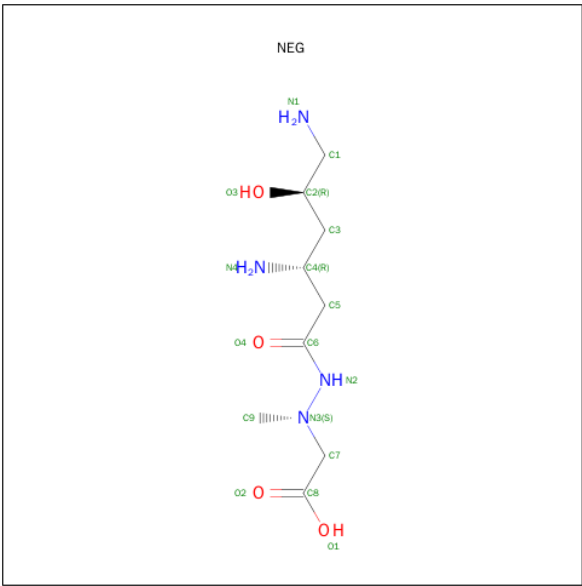
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	B2	1	Total 1	Mg 1	0	0
56	AA	218	Total 218	Mg 218	0	0
56	BQ	5	Total 5	Mg 5	0	0
56	D7	1	Total 1	Mg 1	0	0
56	CX	2	Total 2	Mg 2	0	0
56	DV	3	Total 3	Mg 3	0	0
56	B6	1	Total 1	Mg 1	0	0
56	AM	1	Total 1	Mg 1	0	0
56	BU	9	Total 9	Mg 9	0	0
56	DR	2	Total 2	Mg 2	0	0
56	AD	1	Total 1	Mg 1	0	0
56	BN	6	Total 6	Mg 6	0	0
56	CT	1	Total 1	Mg 1	0	0
56	D0	1	Total 1	Mg 1	0	0
56	BG	2	Total 2	Mg 2	0	0
56	BY	1	Total 1	Mg 1	0	0
56	DE	4	Total 4	Mg 4	0	0
56	B3	2	Total 2	Mg 2	0	0
56	CJ	1	Total 1	Mg 1	0	0
56	BR	3	Total 3	Mg 3	0	0
56	DA	623	Total 623	Mg 623	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	CE	1	Total 1	Mg 1	0	0
56	DW	4	Total 4	Mg 4	0	0
56	D5	1	Total 1	Mg 1	0	0
56	B7	4	Total 4	Mg 4	0	0
56	CF	1	Total 1	Mg 1	0	0
56	BV	7	Total 7	Mg 7	0	0
56	DP	1	Total 1	Mg 1	0	0
56	DO	2	Total 2	Mg 2	0	0
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	CD	1	Total 1	Mg 1	0	0
56	BD	11	Total 11	Mg 11	0	0
56	B0	3	Total 3	Mg 3	0	0
56	AO	1	Total 1	Mg 1	0	0
56	BW	4	Total 4	Mg 4	0	0
56	AY	3	Total 3	Mg 3	0	0
56	CK	1	Total 1	Mg 1	0	0
56	AF	1	Total 1	Mg 1	0	0
56	DB	12	Total 12	Mg 12	0	0

- Molecule 57 is NEGAMYCIN (three-letter code: NEG) (formula: C<sub>9</sub>H<sub>20</sub>N<sub>4</sub>O<sub>4</sub>).



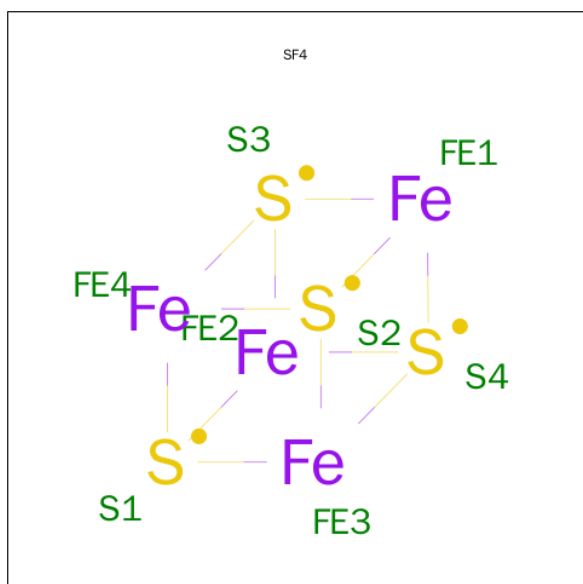
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
57	AA	1	Total	C	N	O	0	0
			17	9	4	4		
57	AA	1	Total	C	N	O	0	0
			17	9	4	4		
57	AA	1	Total	C	N	O	0	0
			17	9	4	4		
57	AA	1	Total	C	N	O	0	0
			17	9	4	4		
57	AA	1	Total	C	N	O	0	0
			17	9	4	4		
57	AA	1	Total	C	N	O	0	0
			17	9	4	4		
57	AW	1	Total	C	N	O	0	0
			17	9	4	4		
57	AX	1	Total	C	N	O	0	0
			17	9	4	4		
57	CA	1	Total	C	N	O	0	0
			17	9	4	4		
57	CA	1	Total	C	N	O	0	0
			17	9	4	4		
57	CA	1	Total	C	N	O	0	0
			17	9	4	4		
57	CA	1	Total	C	N	O	0	0
			17	9	4	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
57	CA	1	Total	C	N	O	0	0
			17	9	4	4		
57	CA	1	Total	C	N	O	0	0
			17	9	4	4		
57	CA	1	Total	C	N	O	0	0
			17	9	4	4		
57	CA	1	Total	C	N	O	0	0
			17	9	4	4		
57	CW	1	Total	C	N	O	0	0
			17	9	4	4		
57	CX	1	Total	C	N	O	0	0
			17	9	4	4		

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



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:  $\text{Zn}$ ).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	B5	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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	247	Total 247	O 247	0	0
61	AD	1	Total 1	O 1	0	0
61	AE	2	Total 2	O 2	0	0
61	AL	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	AM	2	Total 2	O 2	0	0
61	AO	1	Total 1	O 1	0	0
61	AV	3	Total 3	O 3	0	0
61	AW	13	Total 13	O 13	0	0
61	AX	11	Total 11	O 11	0	0
61	AY	1	Total 1	O 1	0	0
61	BA	1396	Total 1396	O 1396	0	0
61	BB	34	Total 34	O 34	0	0
61	BD	12	Total 12	O 12	0	0
61	BE	11	Total 11	O 11	0	0
61	BF	5	Total 5	O 5	0	0
61	BG	3	Total 3	O 3	0	0
61	BI	1	Total 1	O 1	0	0
61	BN	1	Total 1	O 1	0	0
61	BO	2	Total 2	O 2	0	0
61	BP	23	Total 23	O 23	0	0
61	BQ	3	Total 3	O 3	0	0
61	BR	1	Total 1	O 1	0	0
61	BT	2	Total 2	O 2	0	0
61	BU	3	Total 3	O 3	0	0
61	BV	2	Total 2	O 2	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	BW	1	Total 1	O 1	0	0
61	BX	2	Total 2	O 2	0	0
61	BZ	1	Total 1	O 1	0	0
61	B0	8	Total 8	O 8	0	0
61	B3	1	Total 1	O 1	0	0
61	B5	6	Total 6	O 6	0	0
61	B6	1	Total 1	O 1	0	0
61	B7	2	Total 2	O 2	0	0
61	B8	7	Total 7	O 7	0	0
61	CA	184	Total 184	O 184	0	0
61	CJ	2	Total 2	O 2	0	0
61	CP	1	Total 1	O 1	0	0
61	CV	2	Total 2	O 2	0	0
61	CW	3	Total 3	O 3	0	0
61	CX	6	Total 6	O 6	0	0
61	DA	960	Total 960	O 960	0	0
61	DB	8	Total 8	O 8	0	0
61	DD	16	Total 16	O 16	0	0
61	DE	9	Total 9	O 9	0	0
61	DF	5	Total 5	O 5	0	0
61	DN	3	Total 3	O 3	0	0

*Continued on next page...*

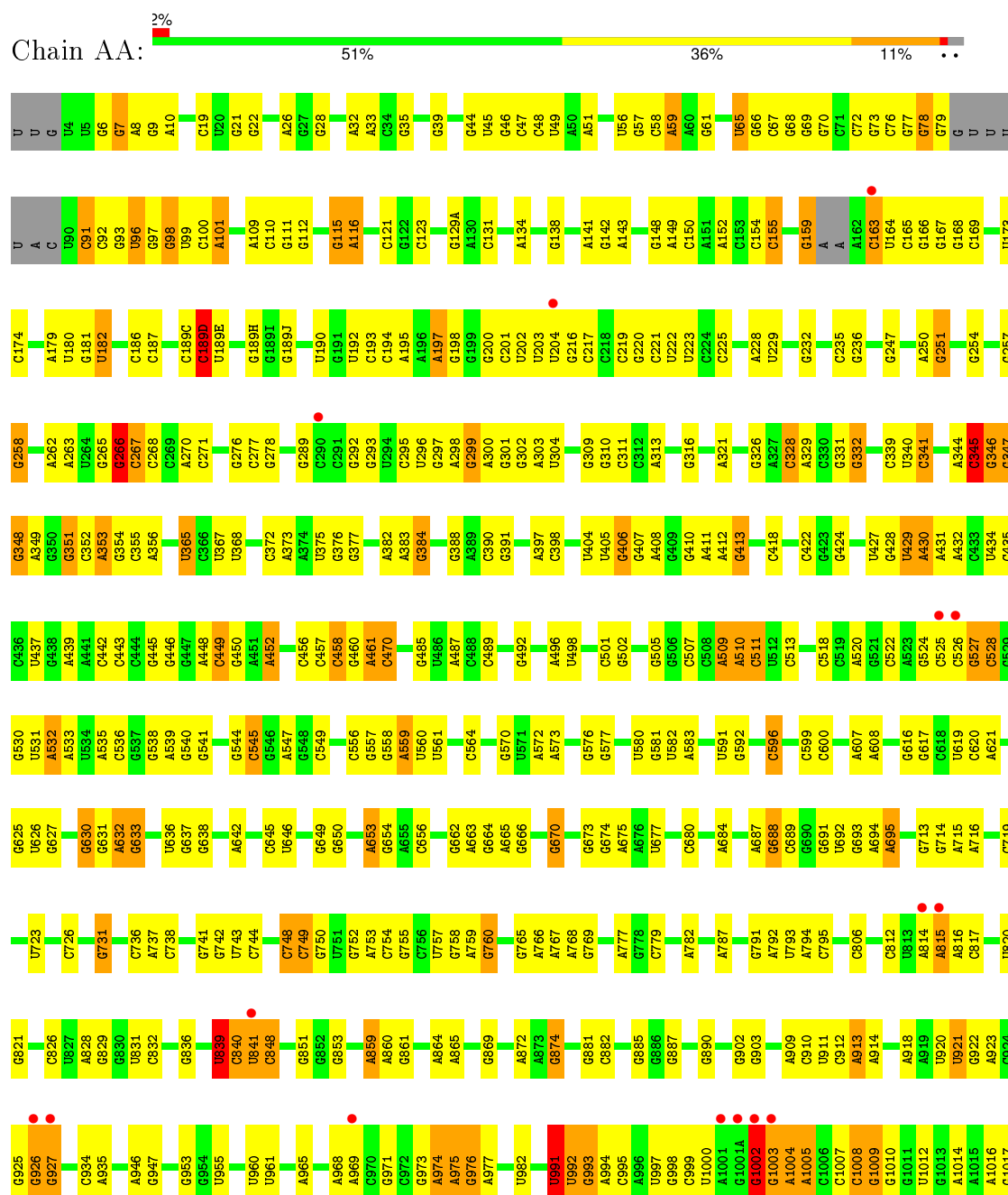
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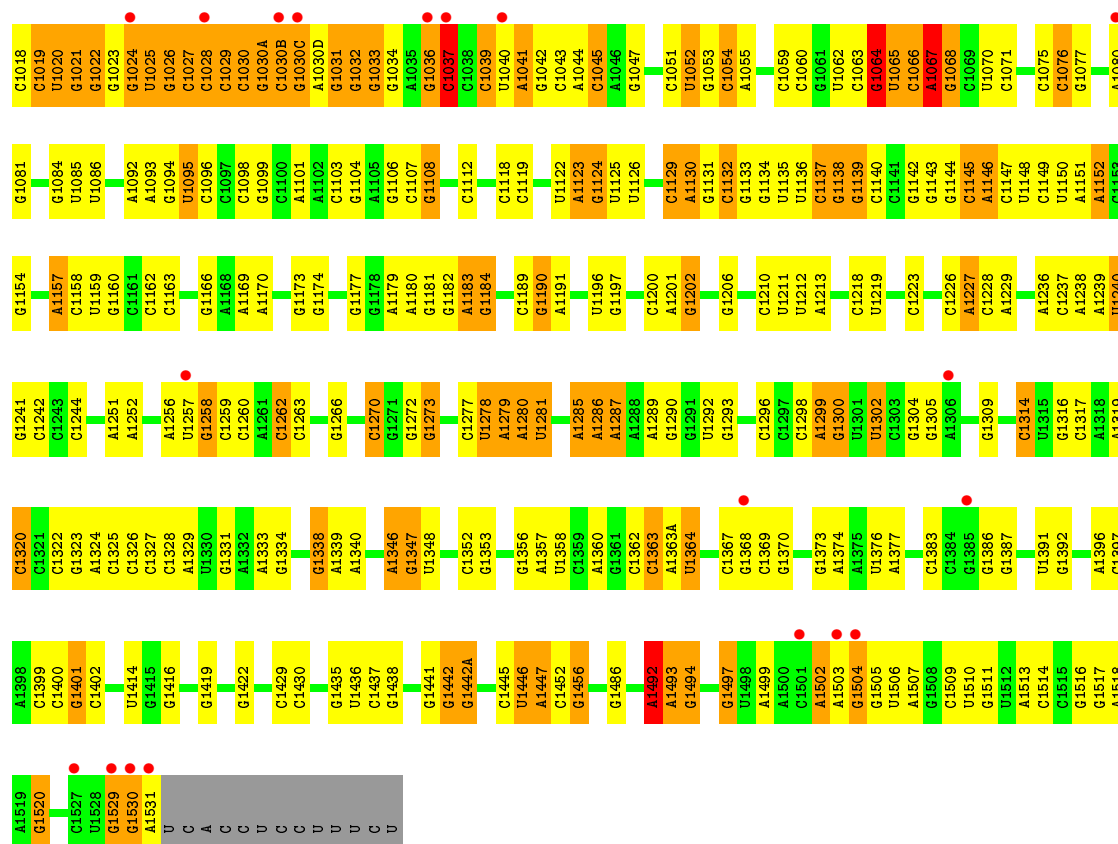
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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			2	2		
61	DP	15	Total	O	0	0
			15	15		
61	DQ	1	Total	O	0	0
			1	1		
61	DR	1	Total	O	0	0
			1	1		
61	DU	1	Total	O	0	0
			1	1		
61	DW	1	Total	O	0	0
			1	1		
61	DX	1	Total	O	0	0
			1	1		
61	DY	2	Total	O	0	0
			2	2		
61	D0	8	Total	O	0	0
			8	8		
61	D1	4	Total	O	0	0
			4	4		
61	D7	2	Total	O	0	0
			2	2		
61	D8	1	Total	O	0	0
			1	1		

### 3 Residue-property plots

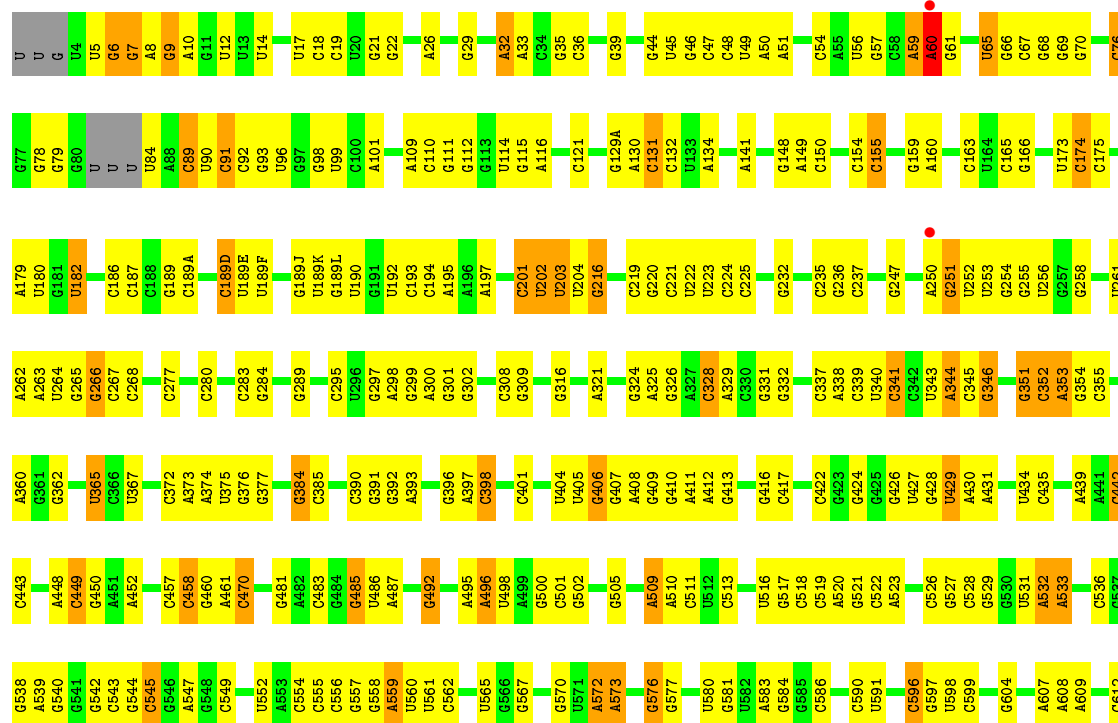
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

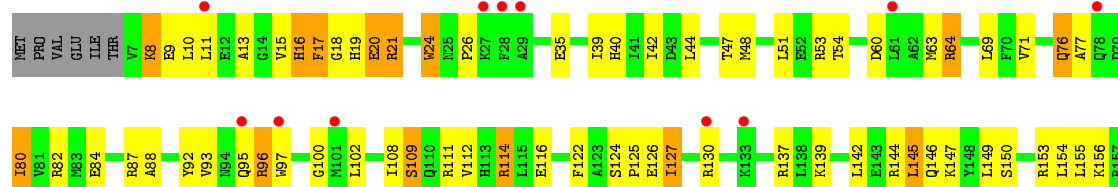
#### • Molecule 1: 16S Ribosomal RNA

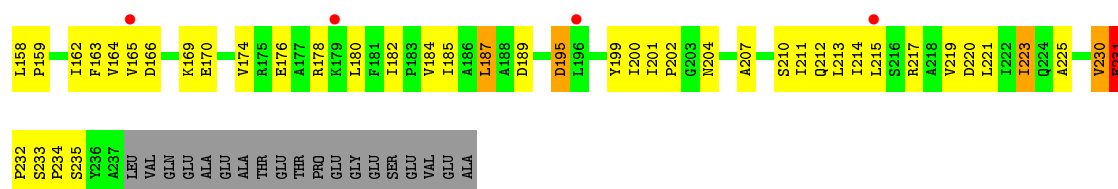




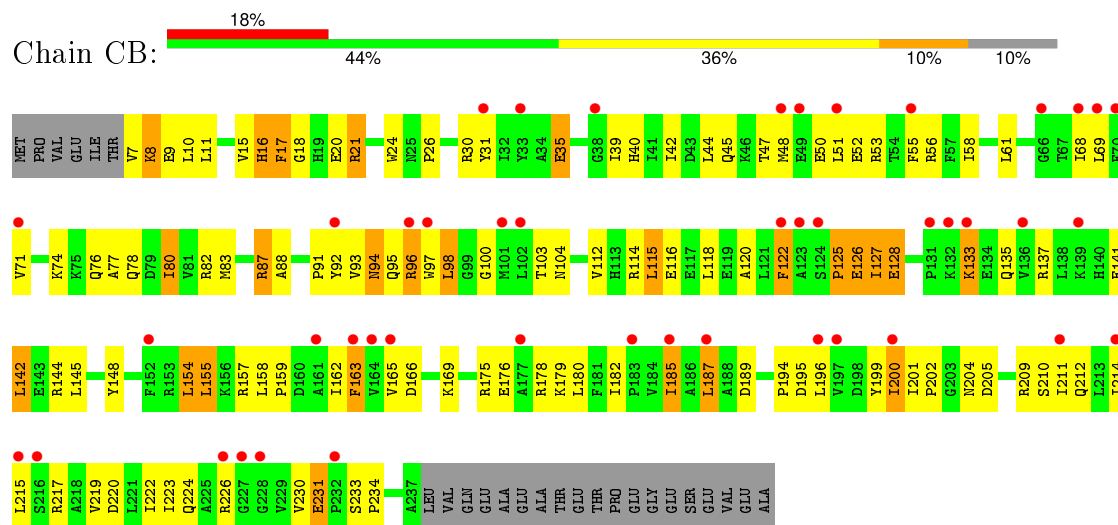
- Molecule 1: 16S Ribosomal RNA



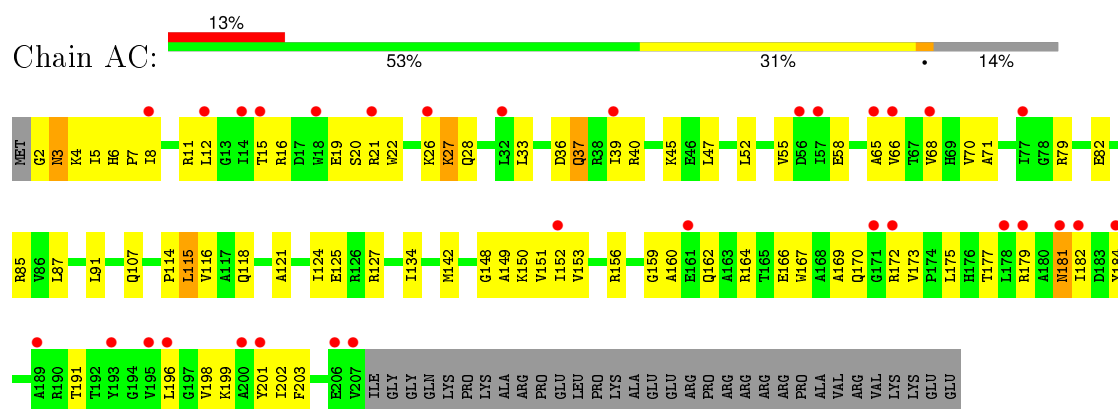




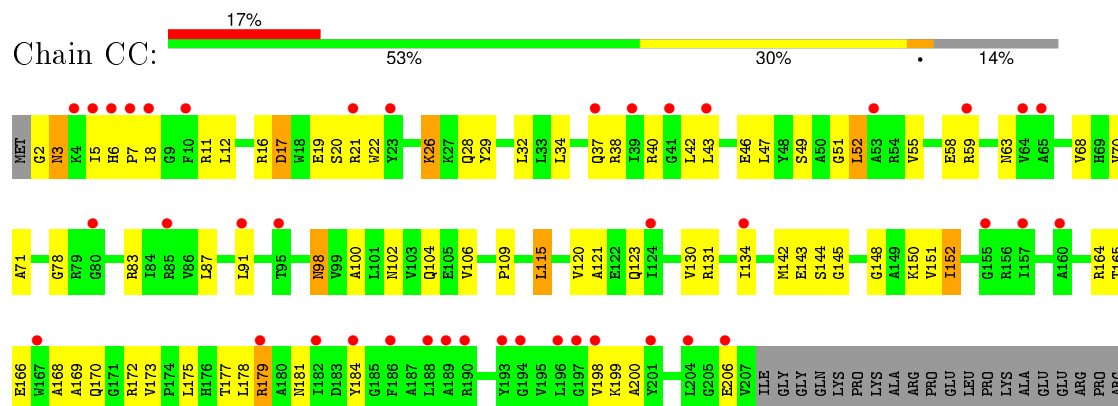
• Molecule 2: 30S Ribosomal Protein S2



• Molecule 3: 30S Ribosomal Protein S3

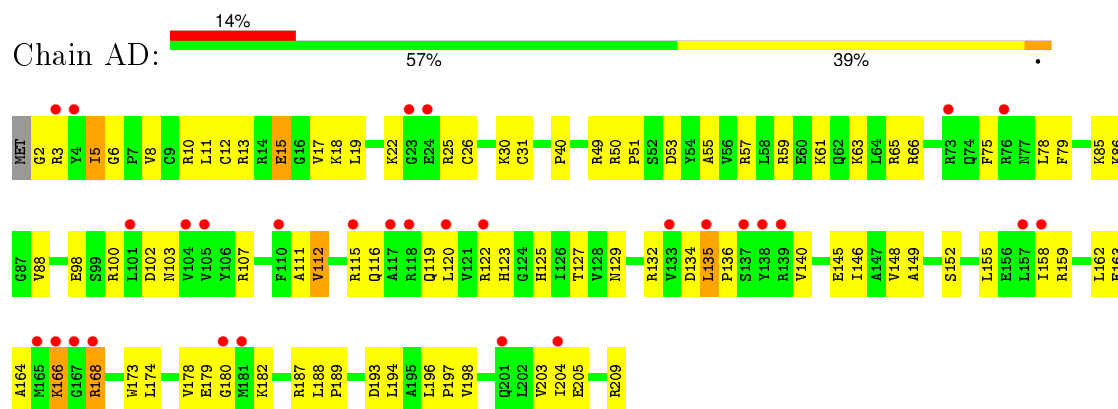


• Molecule 3: 30S Ribosomal Protein S3

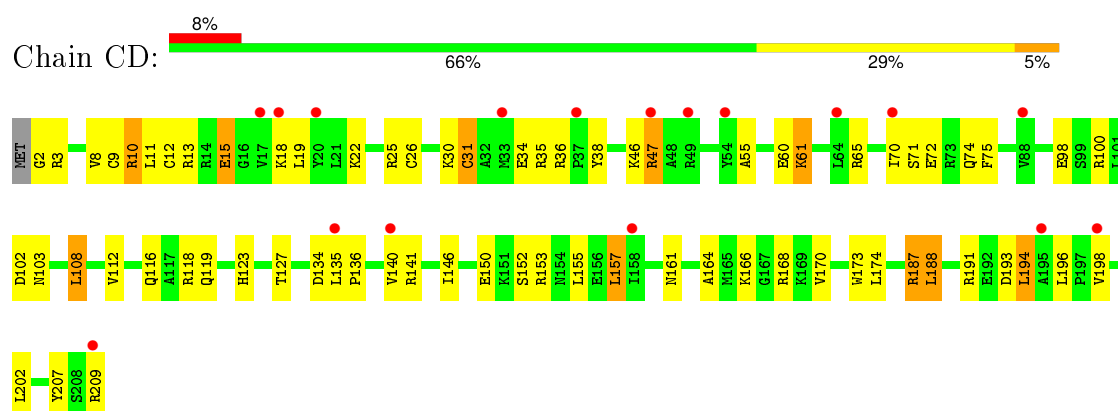


ARG  
ARG  
ARG  
PRO  
ALA  
VAL  
ARG  
VAL  
LYS  
LYS  
GLU  
GLU

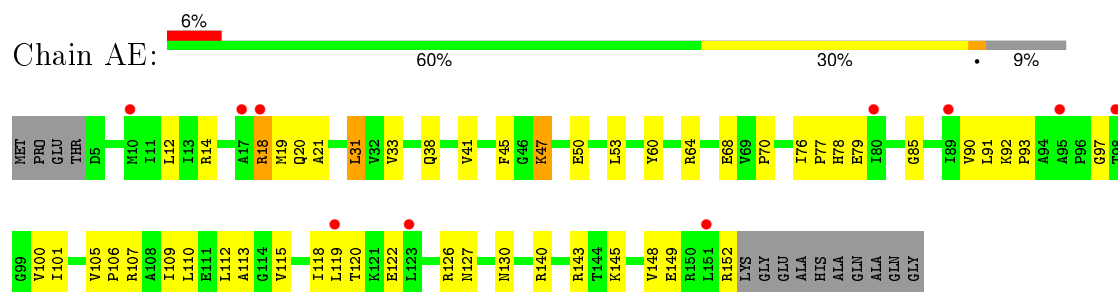
• Molecule 4: 30S Ribosomal Protein S4



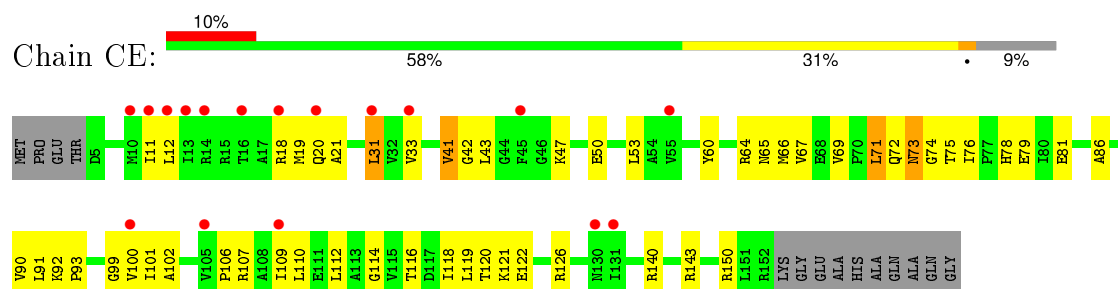
• Molecule 4: 30S Ribosomal Protein S4



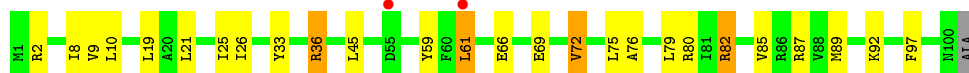
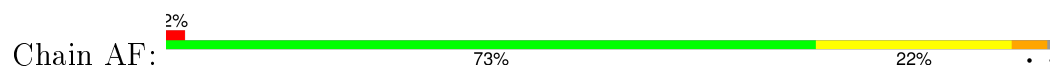
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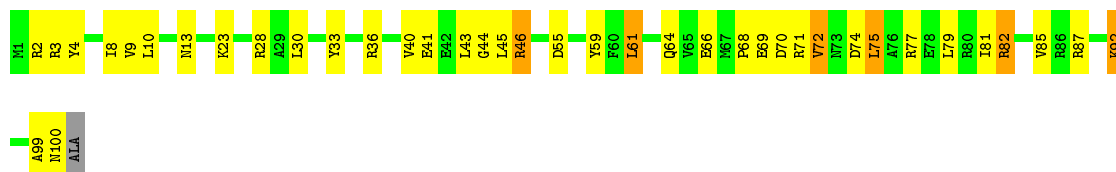
• Molecule 5: 30S Ribosomal Protein S5



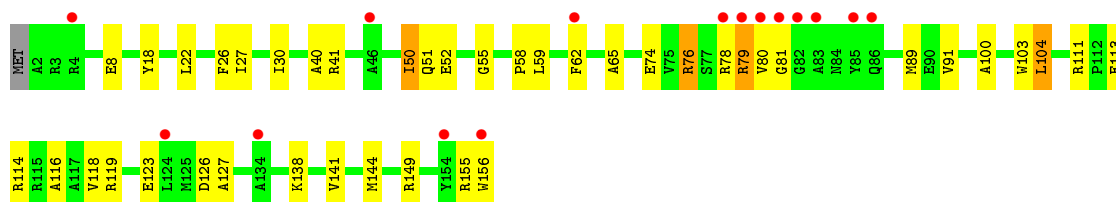
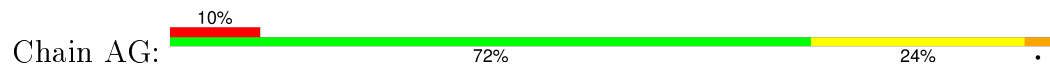
- Molecule 6: 30S Ribosomal Protein S6



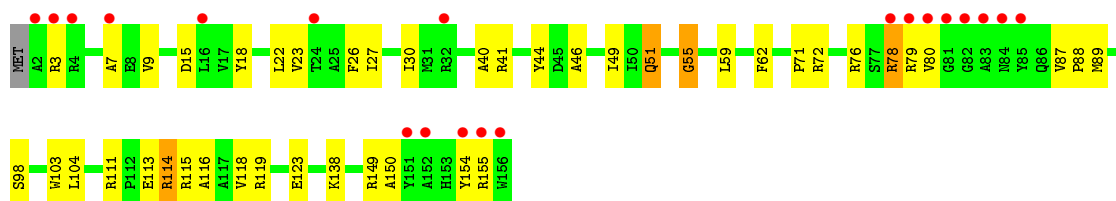
- Molecule 6: 30S Ribosomal Protein S6



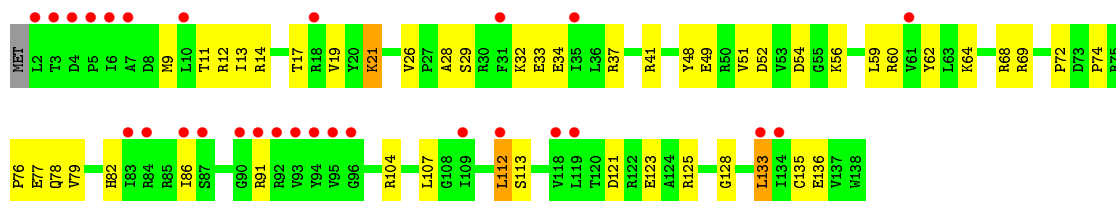
- Molecule 7: 30S Ribosomal Protein S7



- Molecule 7: 30S Ribosomal Protein S7

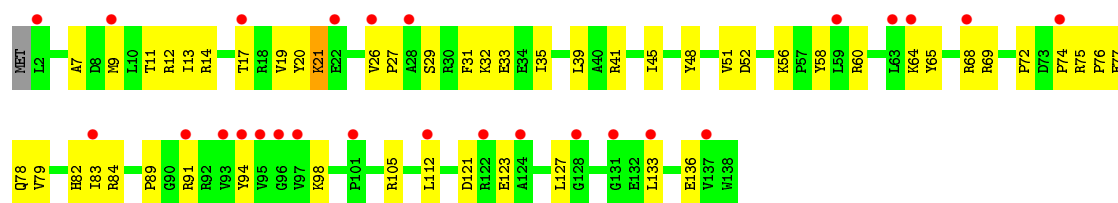


- Molecule 8: 30S Ribosomal Protein S8

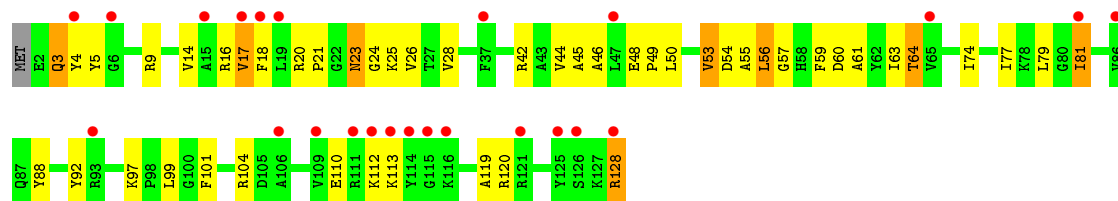


- Molecule 8: 30S Ribosomal Protein S8

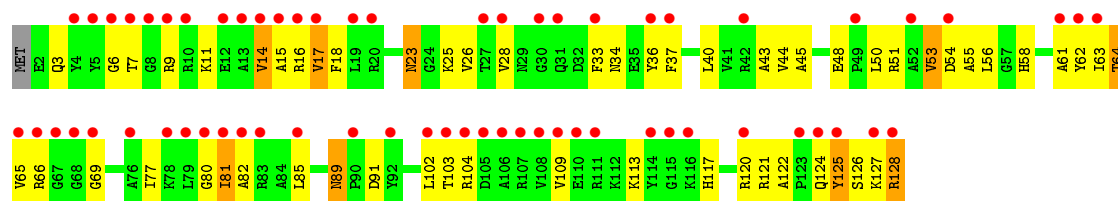




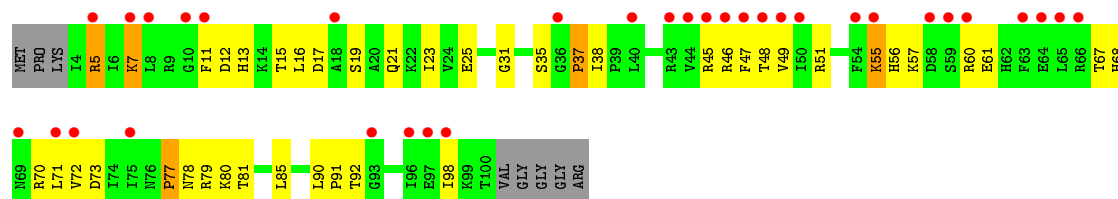
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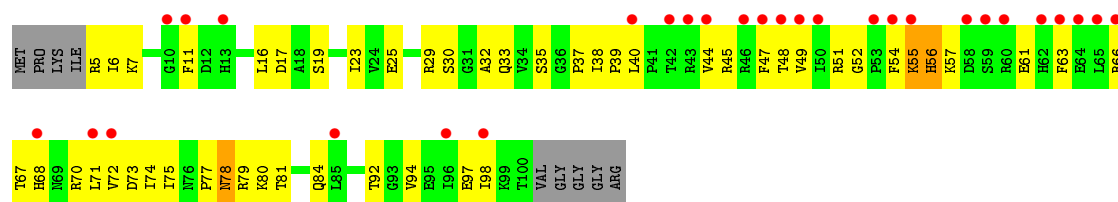
• Molecule 9: 30S Ribosomal Protein S9



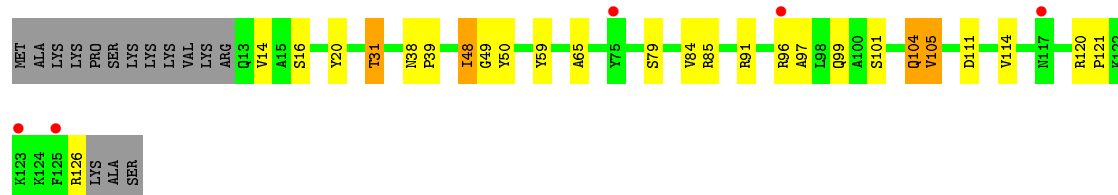
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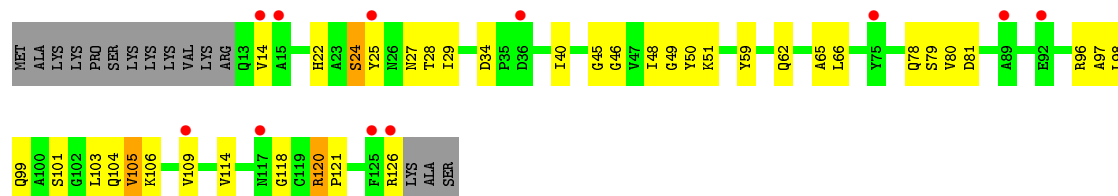
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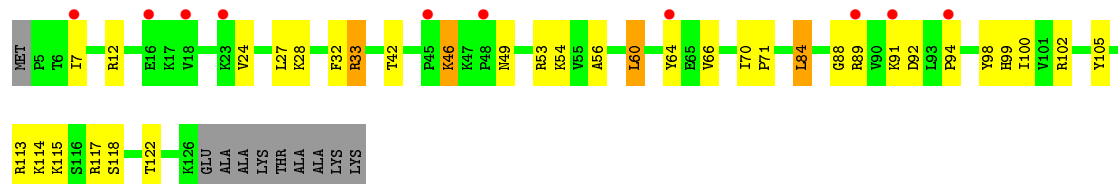
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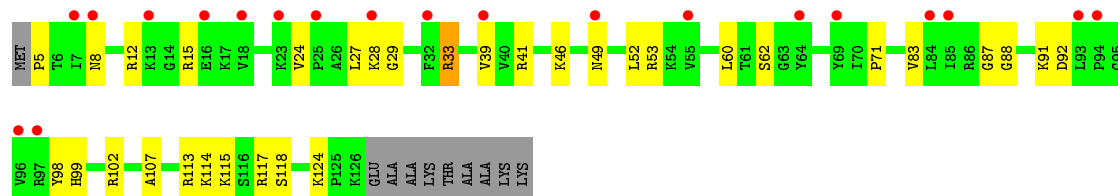
- Molecule 11: 30S Ribosomal Protein S11



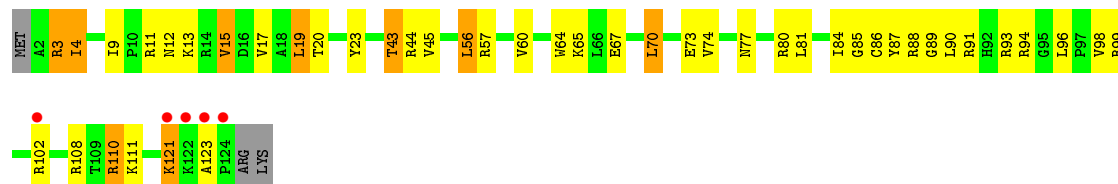
- Molecule 12: 30S Ribosomal Protein S12



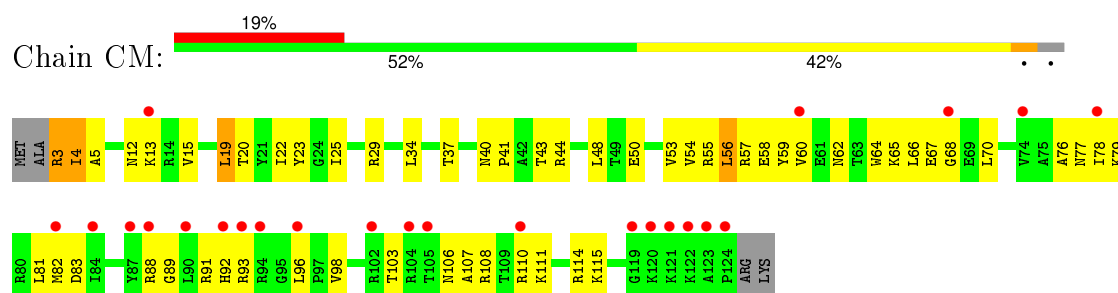
- Molecule 12: 30S Ribosomal Protein S12



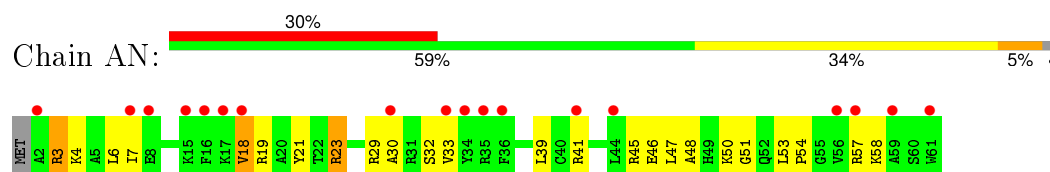
- Molecule 13: 30S Ribosomal Protein S13



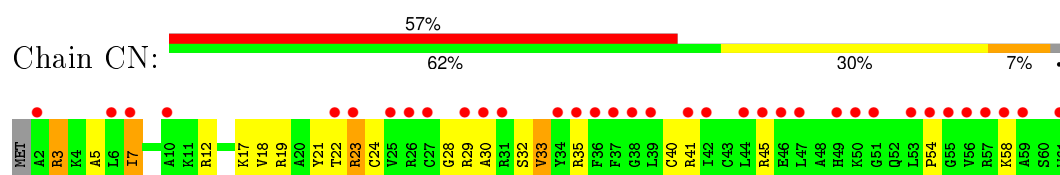
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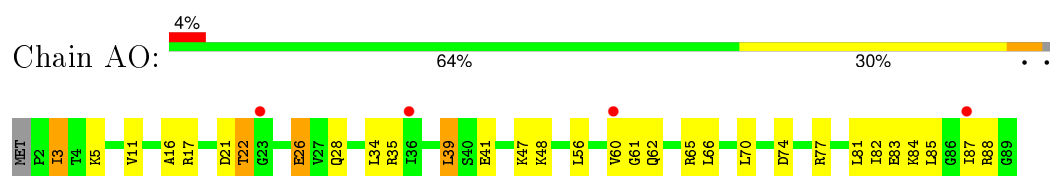
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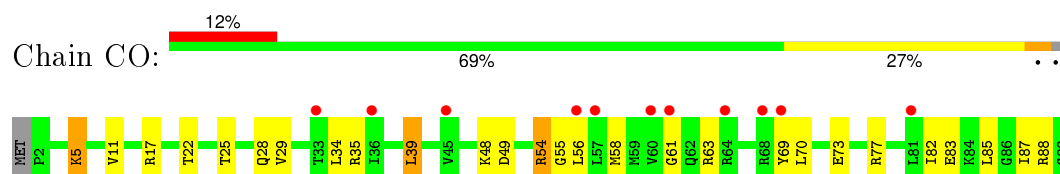
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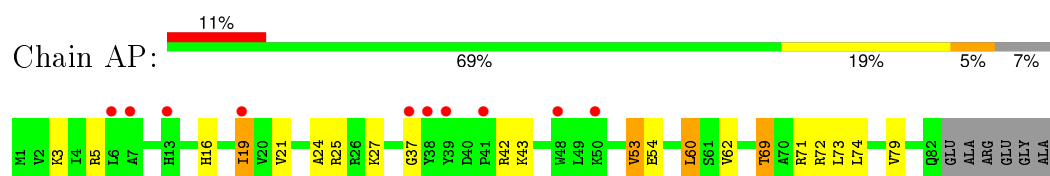
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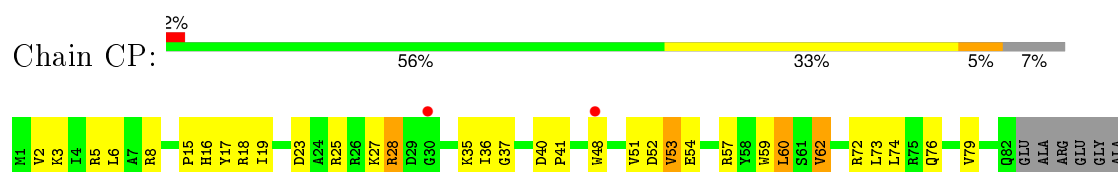
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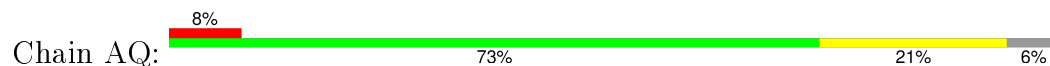
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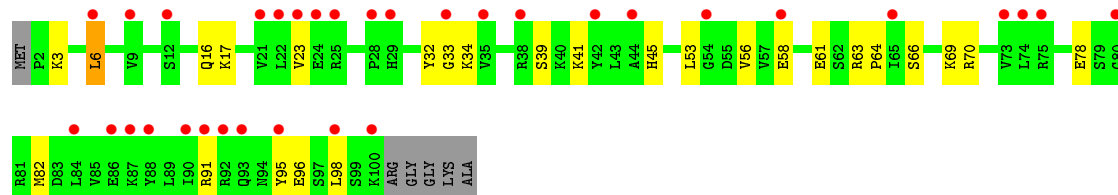
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- Molecule 17: 30S Ribosomal Protein S17



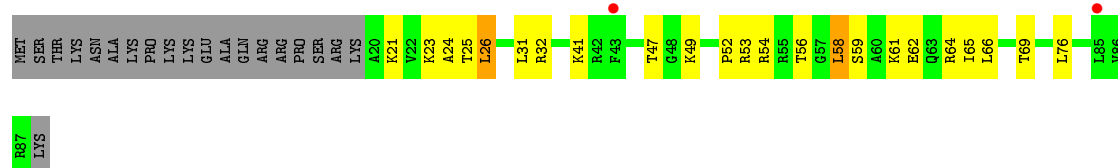
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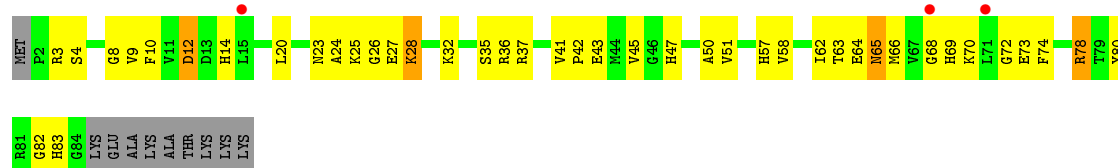
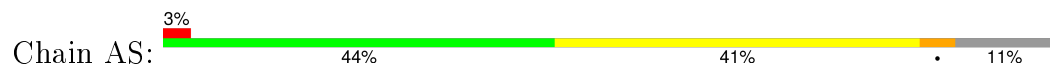
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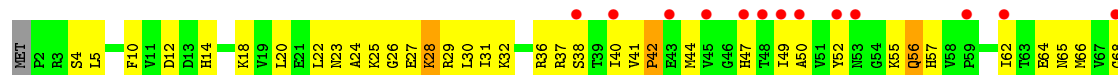
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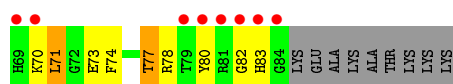


- Molecule 19: 30S Ribosomal Protein S19

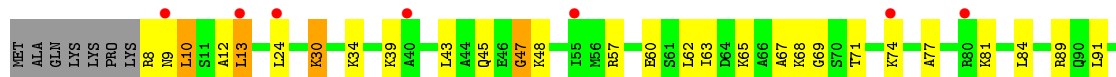


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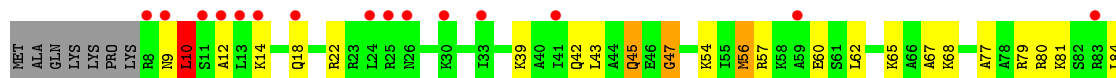




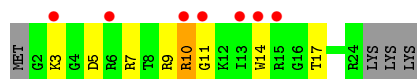
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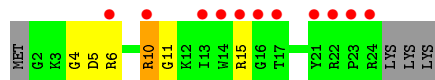
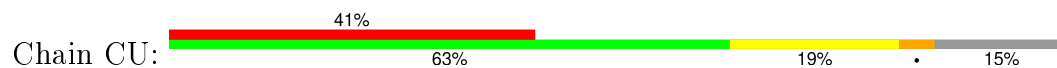
- Molecule 20: 30S Ribosomal Protein S20



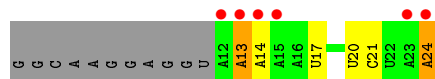
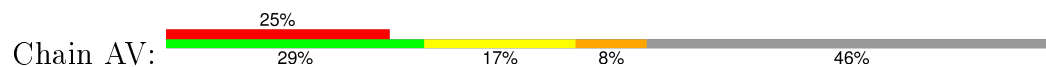
- Molecule 21: 30S Ribosomal Protein THX



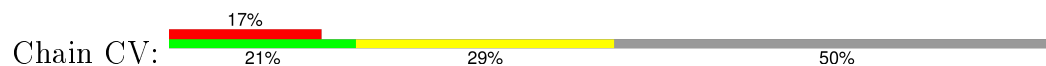
- Molecule 21: 30S Ribosomal Protein THX



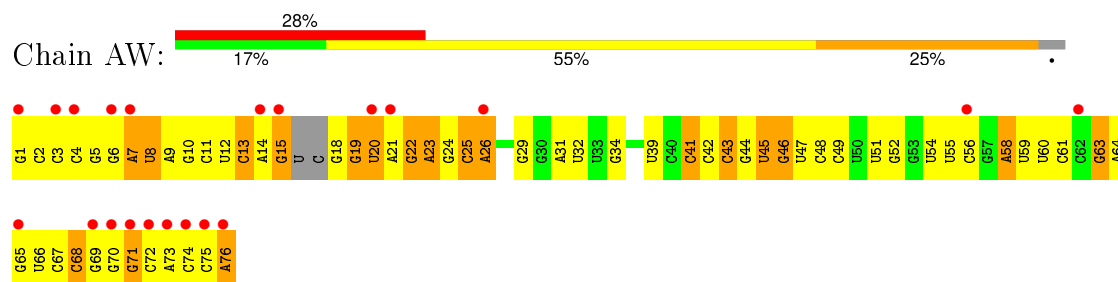
- Molecule 22: mRNA



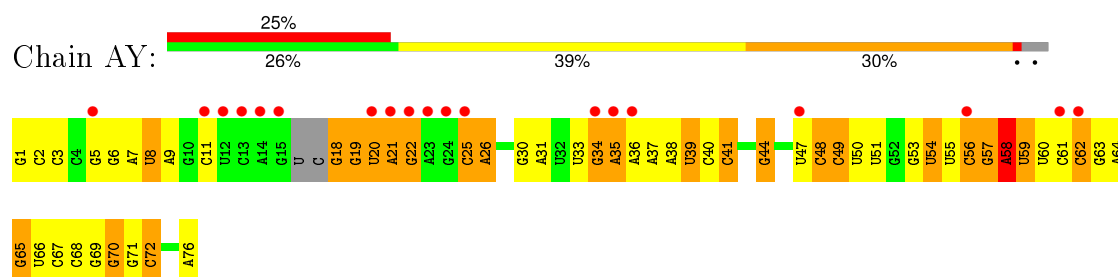
- Molecule 22: mRNA



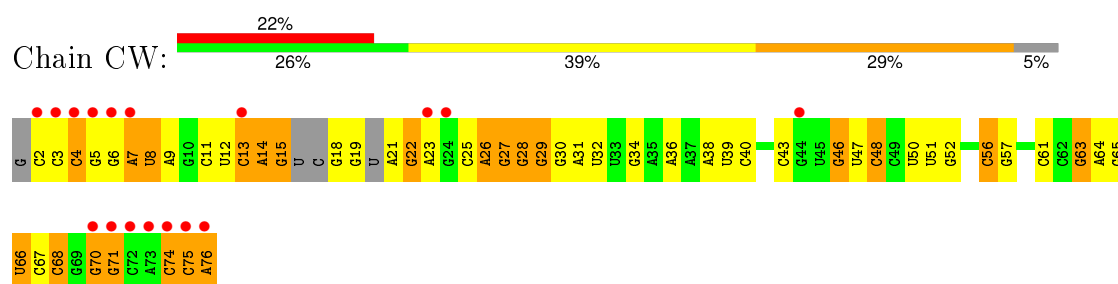
- Molecule 23: A/P-site tRNA



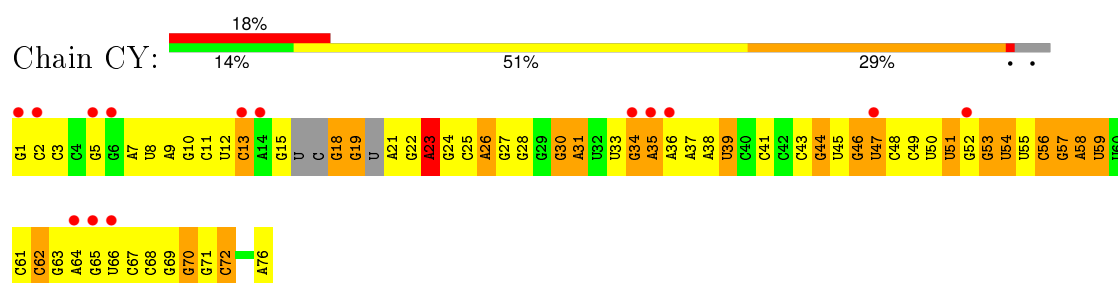
- Molecule 23: A/P-site tRNA



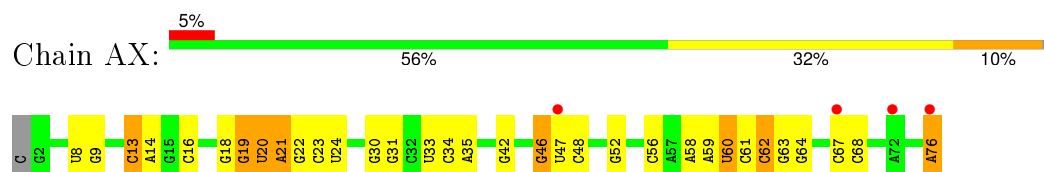
- Molecule 23: A/P-site tRNA



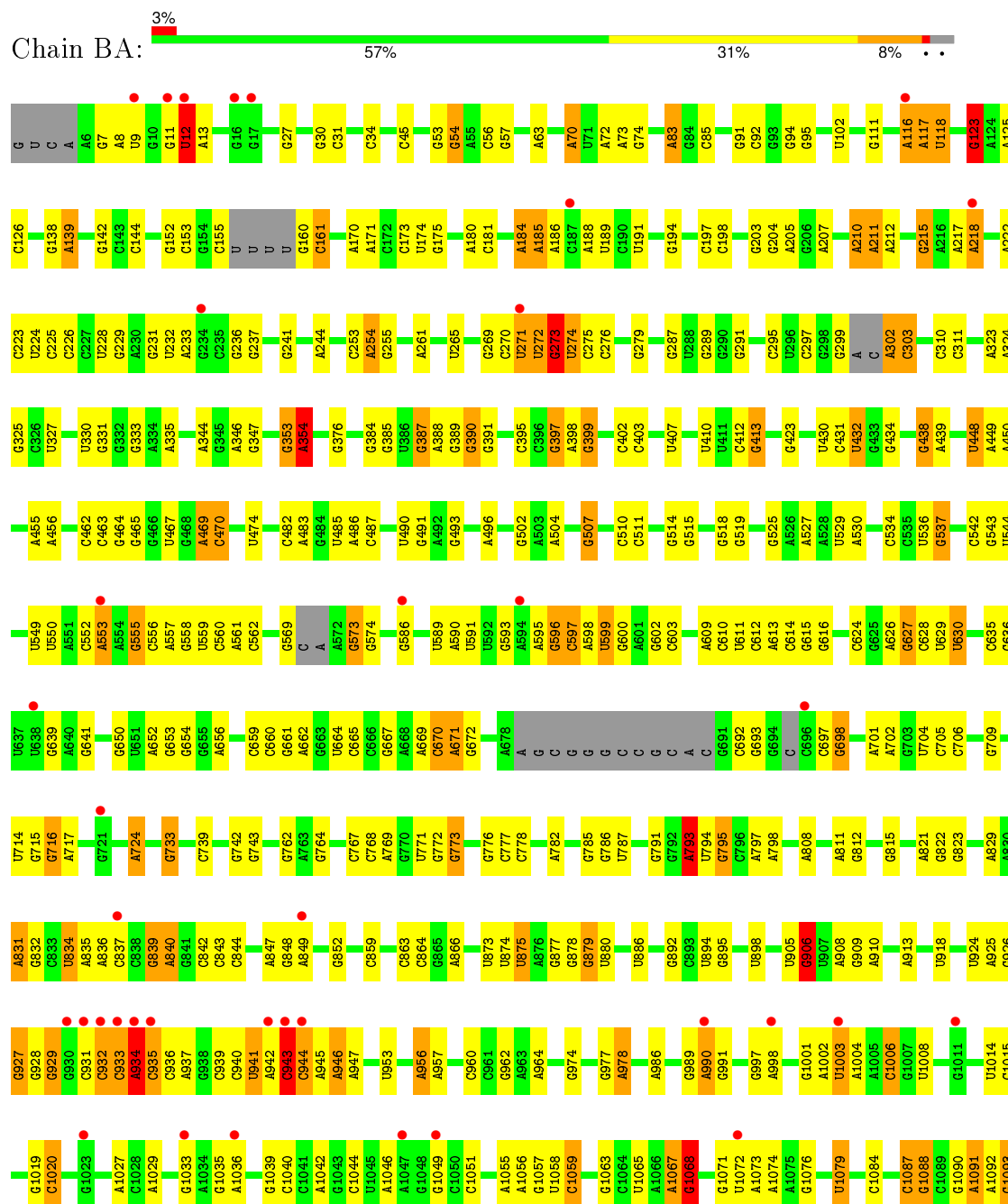
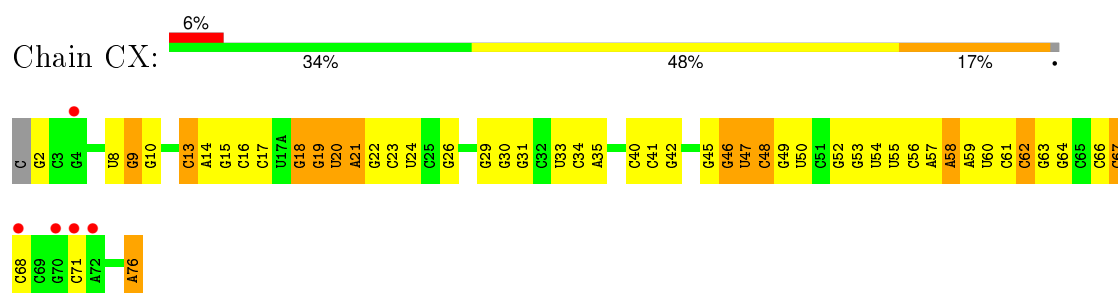
- Molecule 23: A/P-site tRNA



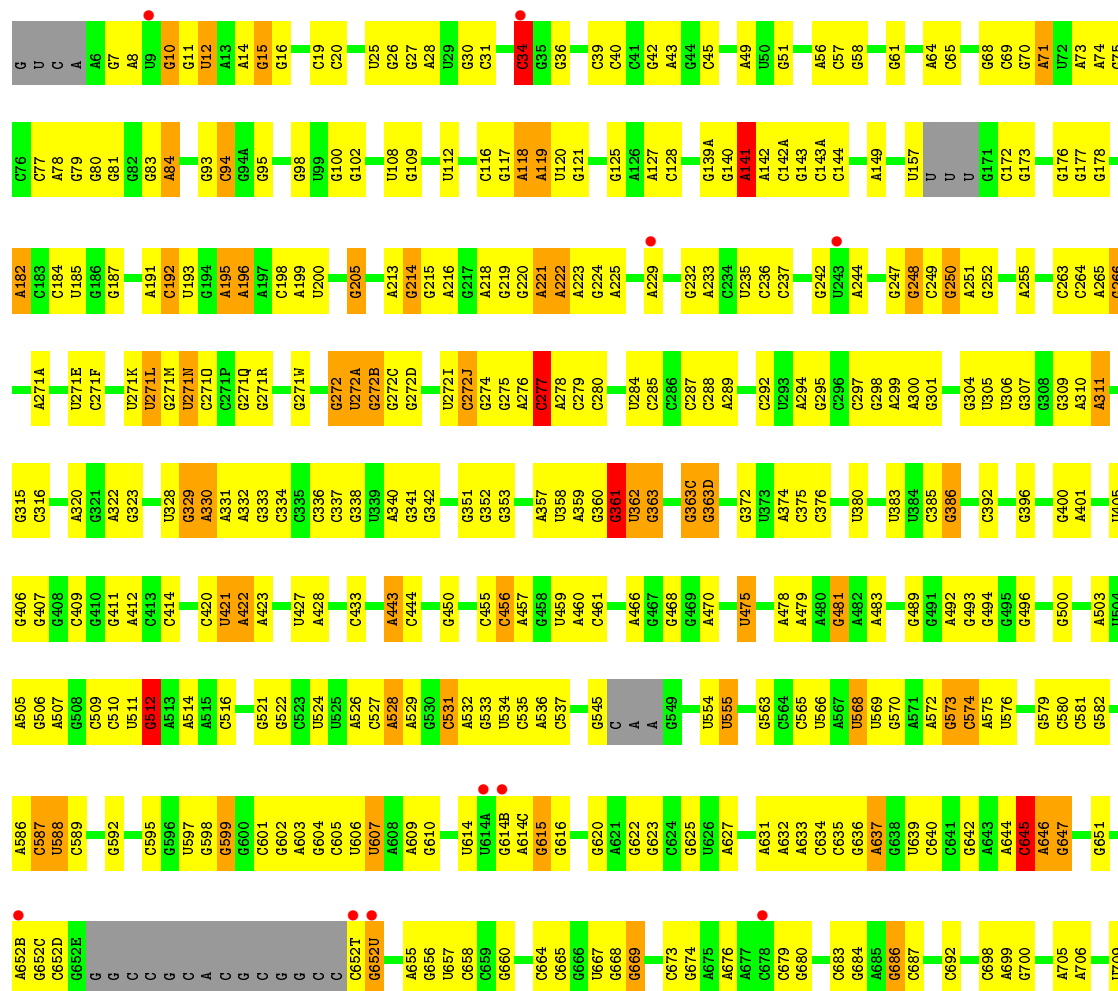
- Molecule 24: E-site tRNA



- Molecule 24: E-site tRNA



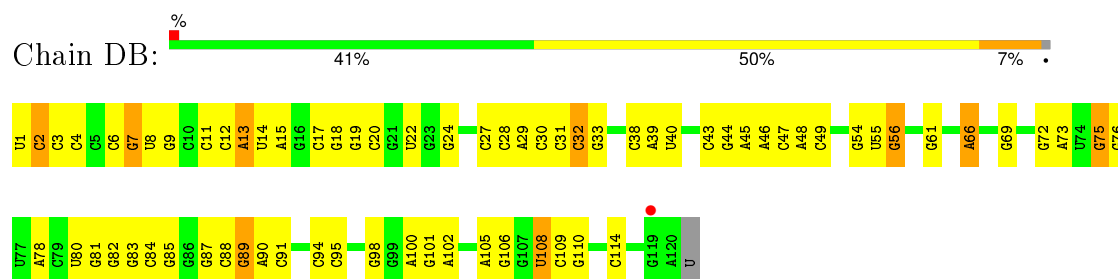




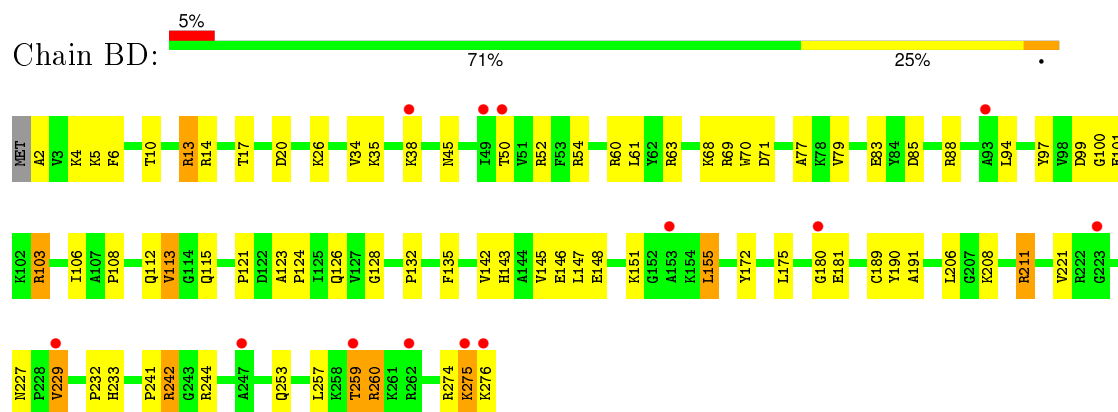
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G1816	G1816	G1817		G1822	G1823	G1824	G1825	G1826	G1827	G1828	G1829	C1830	U1833	U1834	U1835	C1836	C1837	C1838	G1839		G1842	C1843	A1848	U1851	A1854	G1855	G1856	G1857	G1858	C1866	A1876	A1877	G1878	A1878	C1880	C1881	A1885	C1886	A1889	A1890	C1894	C1895	G1896	G1897	U1898	G1899	A1900	G1906	A1943							
G1593	G1594	G1595	A1596	U1597	C1598	A1608	A1609	A1610	A1614	A1618	G1626	G1627	G1628	U1629	A1632	A1637	U1638	U1639	C1640	G1645	C1646	G1647	C1648	G1651	A1652	G1653	A1654	A1665	G1666	G1667	A1668	A1669	C1670	G1674	C1675	U1676	U1677	C1686	G1687	U1688	A1689	U1693	G1696	G1697	A1698	A1699	A1812	G1813	G1814							
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G1325	U1326	C1327	U1328	U1329	C1330	A1331	G1337	G1338	G1339	U1341	G1344	U1352	A1353	A1354	G1355	U1357	A1358	A1359	A1360	G1364	A1365	G1368	G1369	G1374	C1375	A1378	A1379	G1380	A1384	A1384	G1385	C1386	C1387	U1394	A1395	U1396	U1397	G1400	G1401	U1405	U1406	C1407	C1408	C1409	C1411	A1321										
U1142	A1142A	A1143	C1147	A1148	G1149	C1150	G1151	C1152	C1153	A1154	A1155	A1156	C1157	C1158	U1159	A1160	G1164	U1165	C1166	G1169	G1170	G1171	G	A	U	U	A	C1178	A1182	G1183	G1184	U1188	A1189	G1190	G1191	U1198	U1199	C1200	C1201	A1204	U1205	G1206	G1209	A1210	U1211	G1212	A1213	A1220								
C	C	U	U	U	U	A	A	G	A	U	C	G	G	U	A	A	G	U	G	U	U	U	A	A	U	U	C	C	A	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U								
U1014	G1015	U1019	A1020	A1021	G1022	U1023	G1024	A1025	U1026	A1027	A1028	A1029	G1030	C1031	A1032	U1033	C1038	G1039	C1040	C1041	G1042	C1043	G	A	A	G	A	C	C	A	G	A	G	A	G	U	U	U	U	U	U	U	U	U	U	U	U	U								
G946	G947	G948	C949	G950	C951	G952	A953	C954	C955	G956	G957	U958	A959	A960	G962	U963	C964	C965	G966	C971	G972	A973	G974	C975	G977	A980	A981	C982	G983	A984	G987	A988	G989	A990	C991	C992	G993	C994	C995	A996	G997	C998	U999	A1000	A1001	G1002	G1003	C1004	C1005	A1006	C1007	U1012	C1013			
G881	G882	C883	C884	C885	U886	U887	C888	C889	A890	G892	C893	C894	U895	A896	C897	C898	A899	A900	A901	C902	C903	C904	U905	G906	U907	A910	A911	C912	U913	C914	G915	G916	A917	A918	G919	G920	G921	U922	C923	C924	C925	A926	G927	G928	G932	A933	C936	U937	G938	G939	G873	G874	G875	A878	G879	G880
G806	U807	G808	G809	U810	U811	C812	U813	C814	C817	G818	A819	A820	A821	C825	U826	U827	U828	G831	G832	U833	C834	U839	C840	C845	C846	U847	A981	C914	G915	G916	A917	A918	G919	G920	G921	U922	C923	C924	C925	A926	G927	G928	G932	A933	C936	U937	G938	G939	G873	G874	G875	A878	G879	G880		
G710	G711	G717	C720	G726	G729	C730	C731	A734	G739	U740	G744	G745	G746	U747	G748	C749	A752	C753	C754	C755	G760	A761	U762	G763	G765	G771	A774	G775	G776	A782	A783	A784	G785	A788	G792	C795	G796	C797	G798	G801	A805															



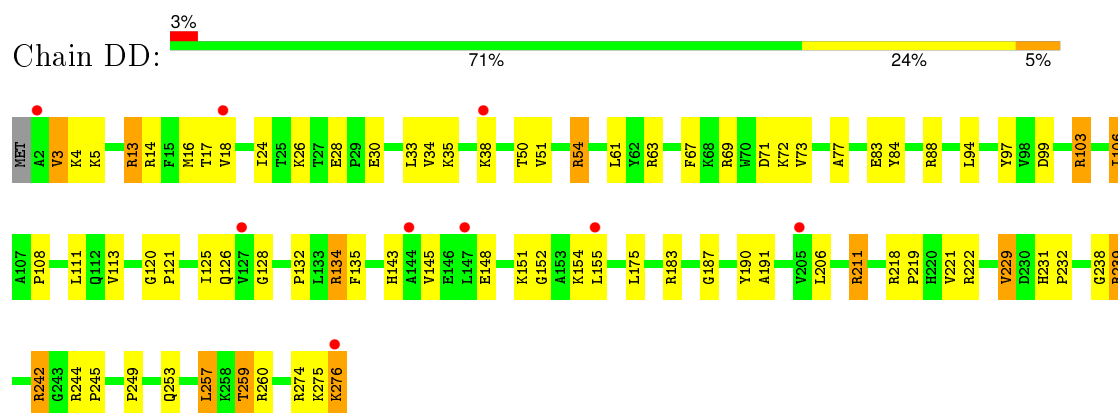
- Molecule 26: 5S Ribosomal RNA

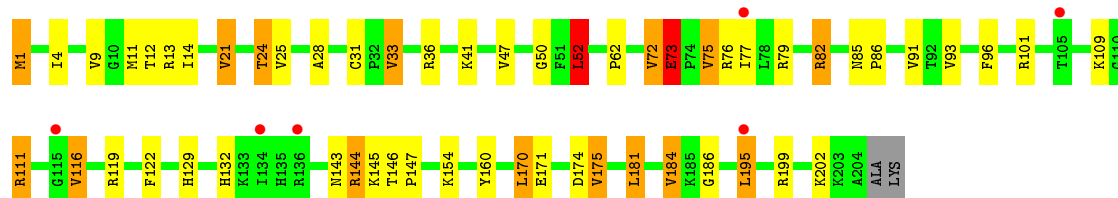


- Molecule 27: 50S Ribosomal Protein L2

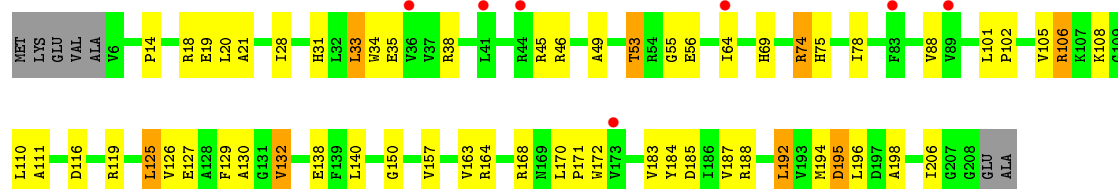


- Molecule 27: 50S Ribosomal Protein L2

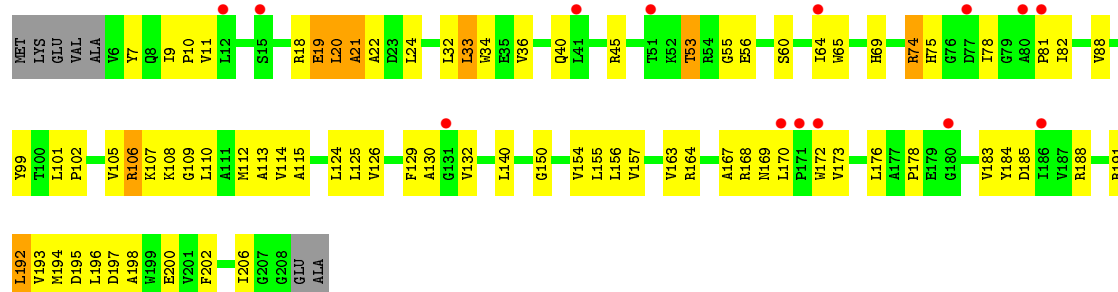




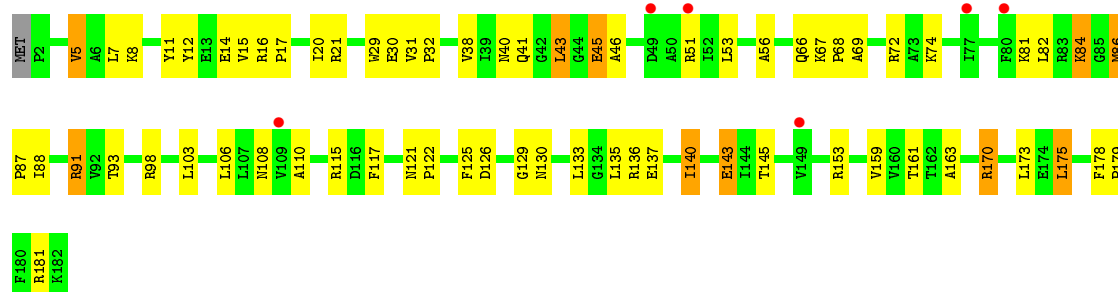
• Molecule 29: 50S Ribosomal Protein L4



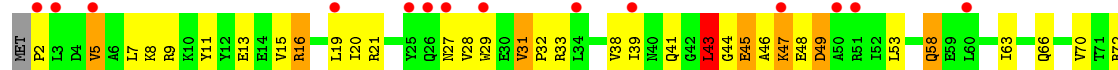
• Molecule 29: 50S Ribosomal Protein L4

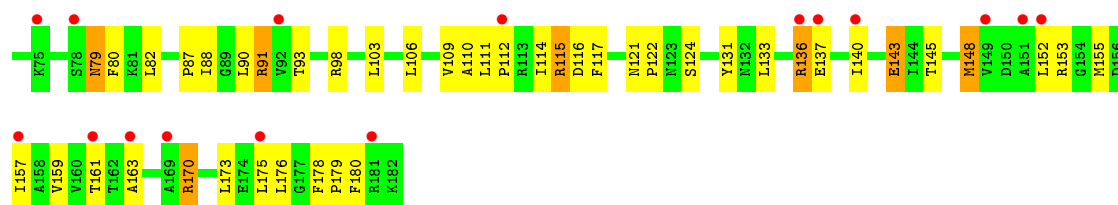


• Molecule 30: 50S Ribosomal Protein L5

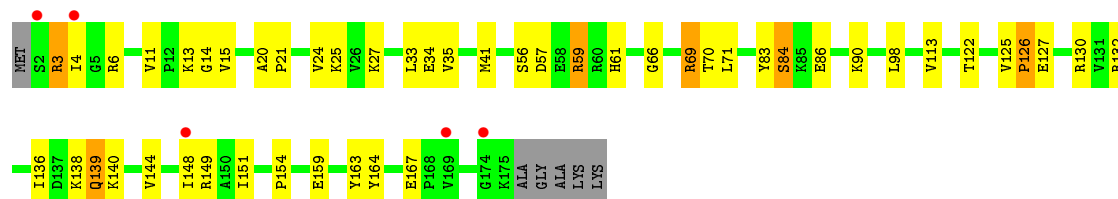
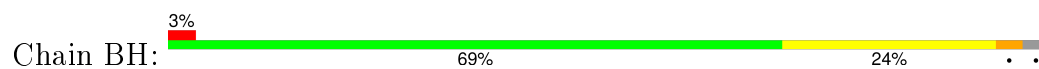


• Molecule 30: 50S Ribosomal Protein L5

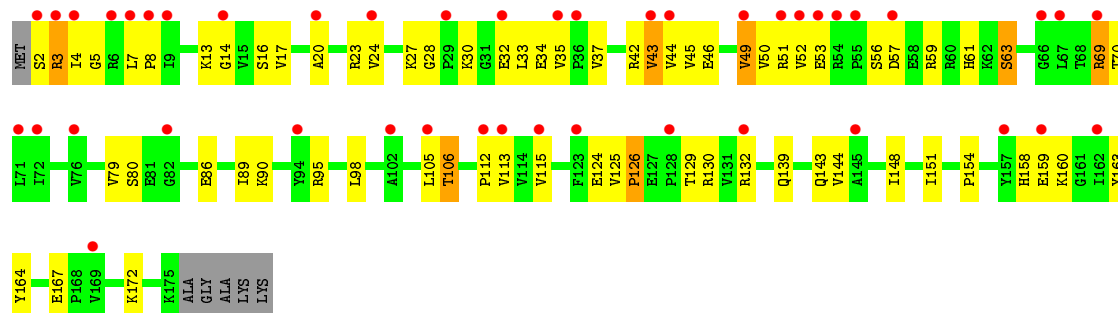




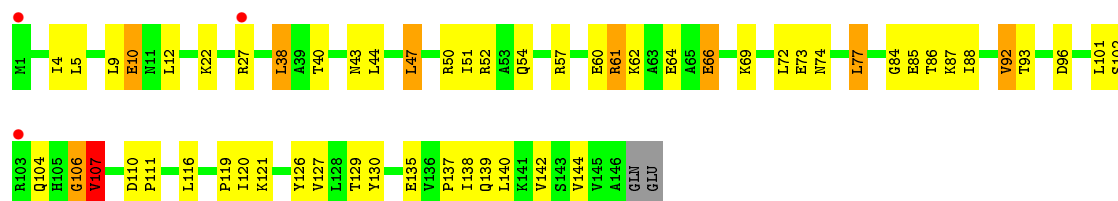
• Molecule 31: 50S Ribosomal Protein L6



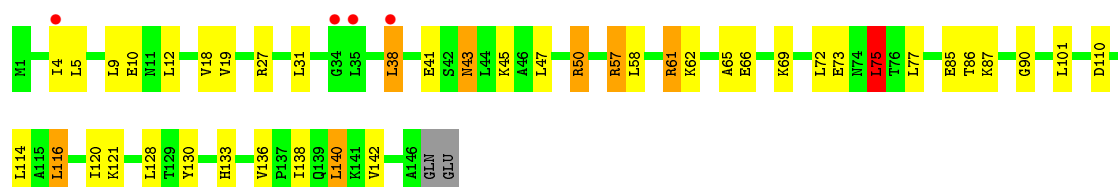
• Molecule 31: 50S Ribosomal Protein L6



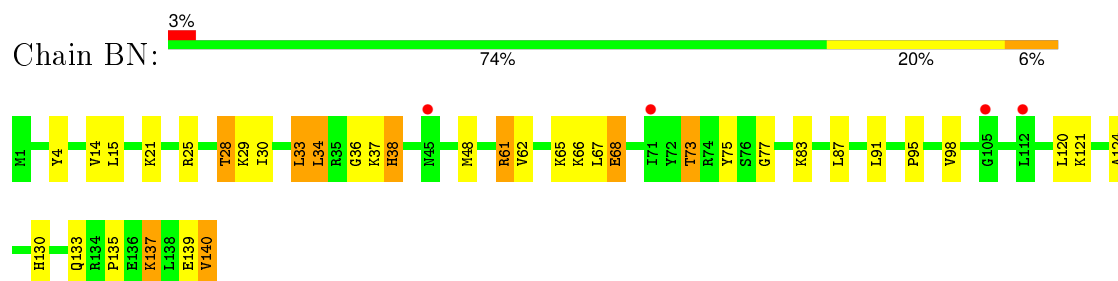
• Molecule 32: 50S Ribosomal Protein L9



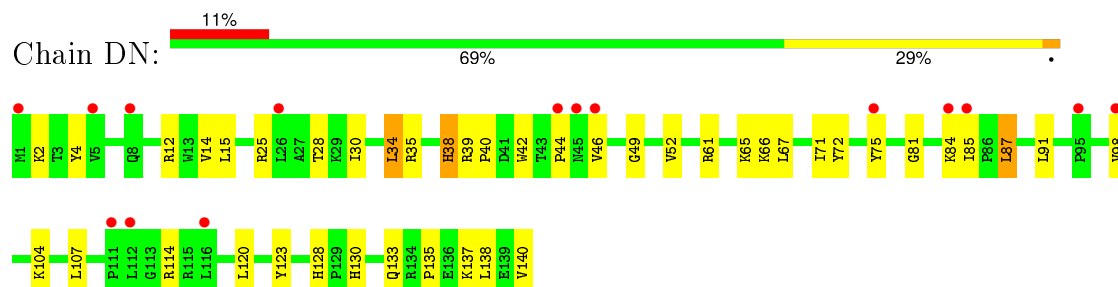
• Molecule 32: 50S Ribosomal Protein L9



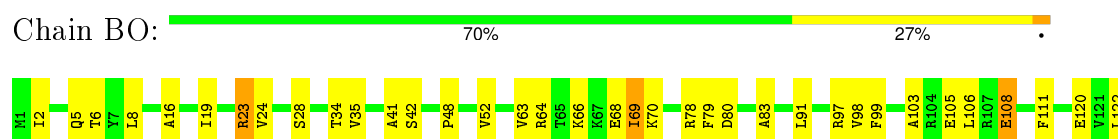
- Molecule 33: 50S Ribosomal Protein L13



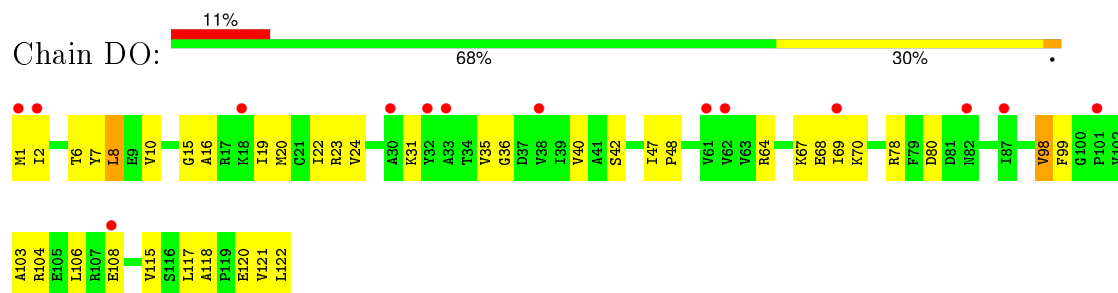
- Molecule 33: 50S Ribosomal Protein L13



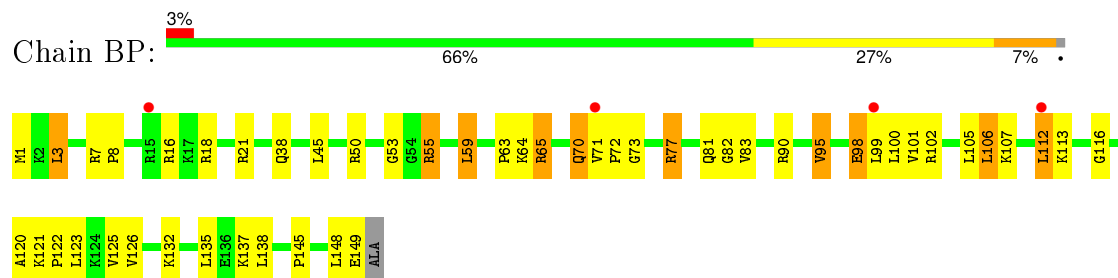
- Molecule 34: 50S Ribosomal Protein L14



- Molecule 34: 50S Ribosomal Protein L14

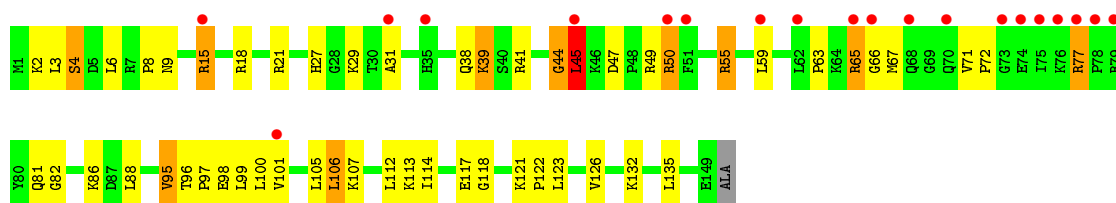


- Molecule 35: 50S Ribosomal Protein L15

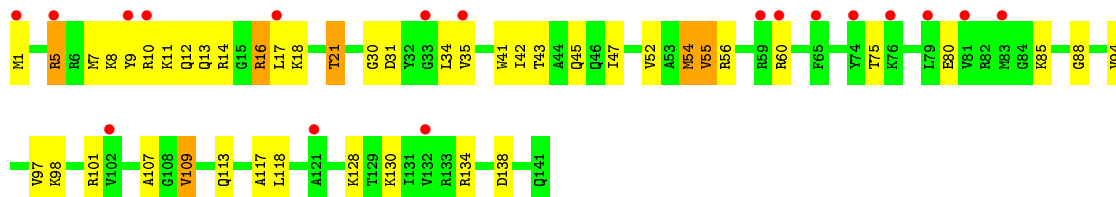


- Molecule 35: 50S Ribosomal Protein L15

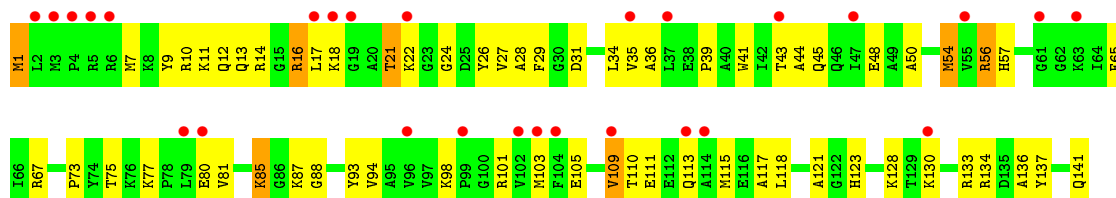




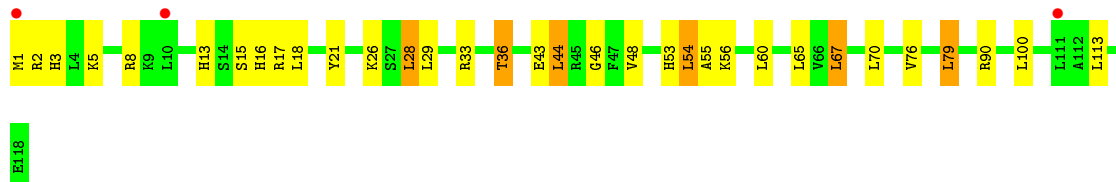
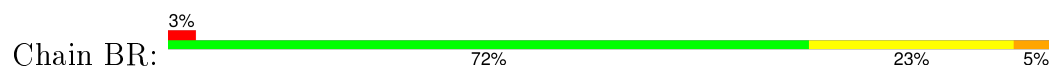
• Molecule 36: 50S Ribosomal Protein L16



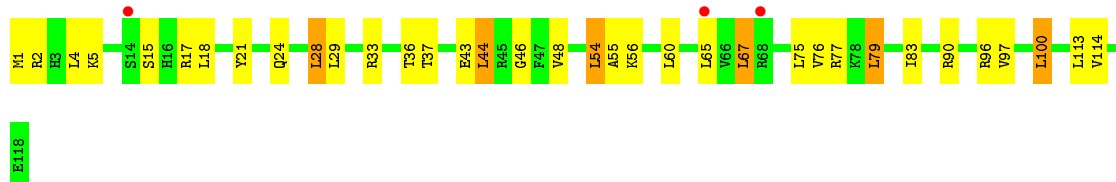
• Molecule 36: 50S Ribosomal Protein L16



• Molecule 37: 50S Ribosomal Protein L17

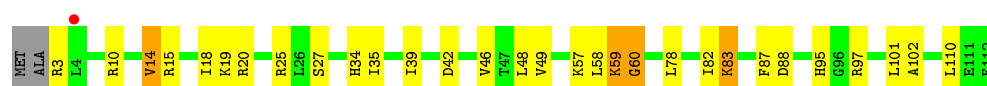


• Molecule 37: 50S Ribosomal Protein L17

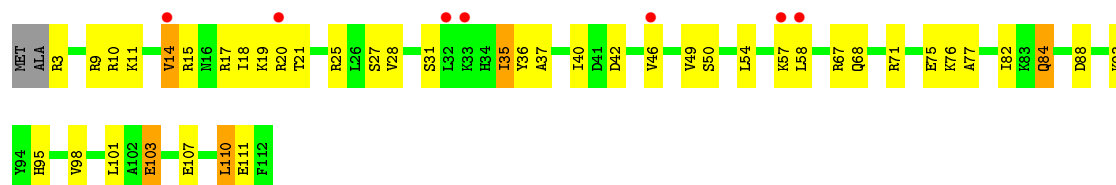


• Molecule 38: 50S Ribosomal Protein L18

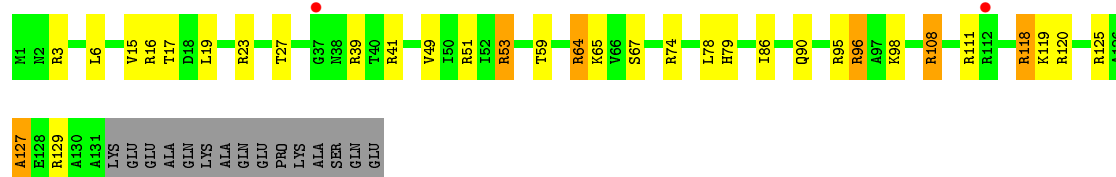




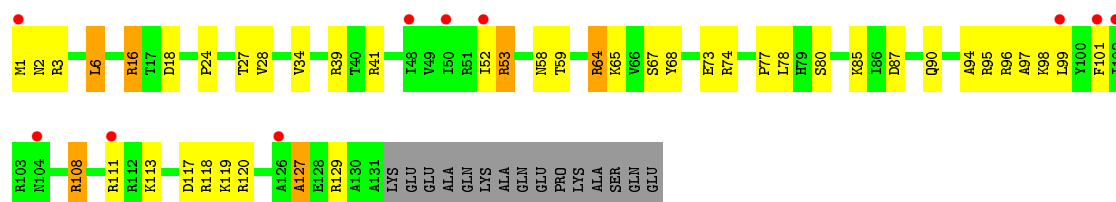
• Molecule 38: 50S Ribosomal Protein L18



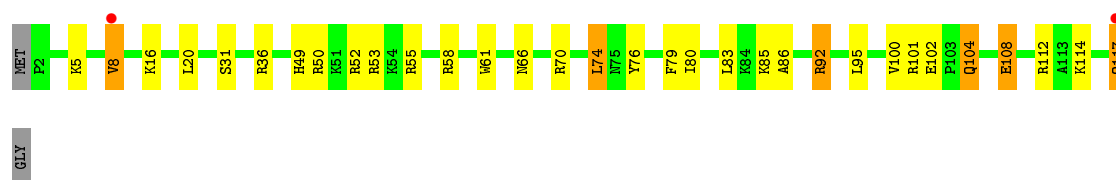
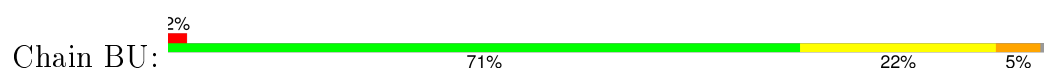
• Molecule 39: 50S Ribosomal Protein L19



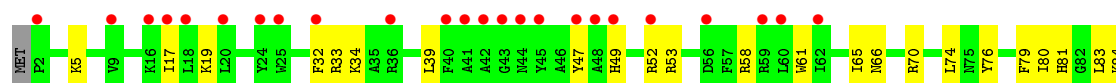
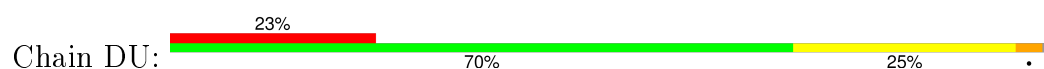
• Molecule 39: 50S Ribosomal Protein L19

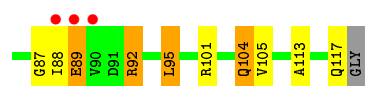


• Molecule 40: 50S Ribosomal Protein L20



• Molecule 40: 50S Ribosomal Protein L20

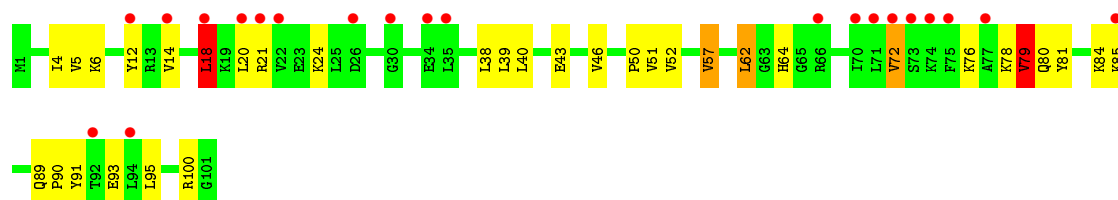




• Molecule 41: 50S Ribosomal Protein L21



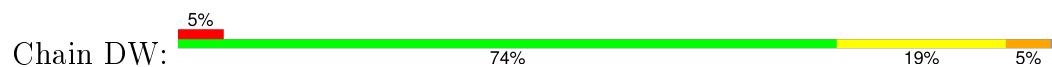
• Molecule 41: 50S Ribosomal Protein L21



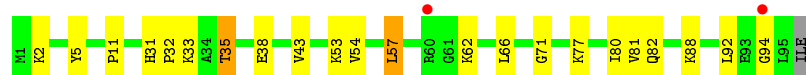
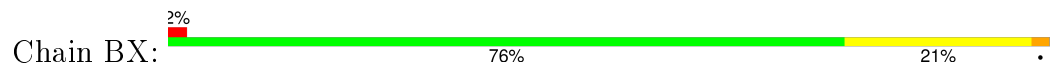
• Molecule 42: 50S Ribosomal Protein L22



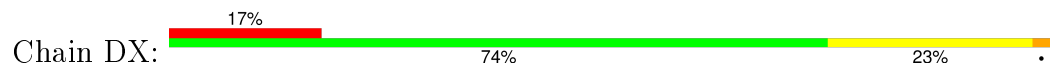
• Molecule 42: 50S Ribosomal Protein L22



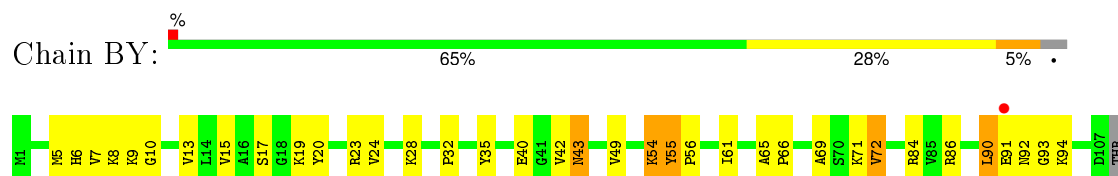
• Molecule 43: 50S Ribosomal Protein L23



• Molecule 43: 50S Ribosomal Protein L23

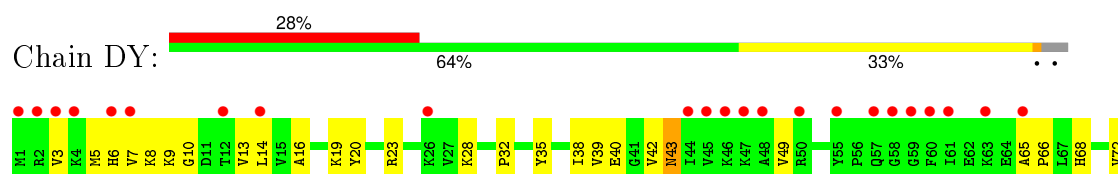


• Molecule 44: 50S Ribosomal Protein L24



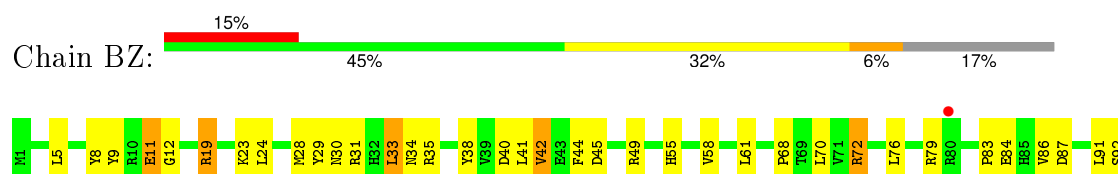
GLU  
GLU

• Molecule 44: 50S Ribosomal Protein L24



R73  
F74  
F75  
F76  
F77  
G80  
R84  
R85  
R86  
R87  
R88  
R89  
L90  
E91  
N92  
G93  
K94  
K95  
V98  
L106  
D107  
THR  
GLU  
GLU

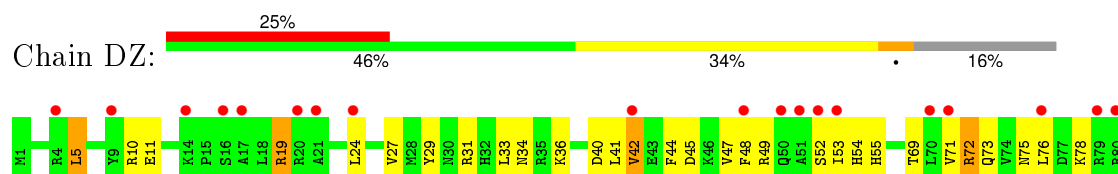
• Molecule 45: 50S Ribosomal Protein L25



D93  
E97  
V100  
P101  
L102  
L103  
F104  
V105  
G106  
T107  
P108  
A109  
G110  
V111  
R112  
A113  
G114  
G115  
V116  
Q118  
E119  
H120  
R122  
V126  
K127  
V128  
S129  
P130  
R131  
M132  
I133  
P134  
E135  
F136  
I137  
E138  
V139  
D140  
V141  
G142  
G143  
L144  
E145  
I146  
G147  
D148  
P149  
S150  
H151  
A152  
S153  
D154  
L155  
K156

L157  
G160  
V161  
E162  
L163  
A164  
V165  
S166  
P167  
E168  
E169  
T170  
T171  
I171  
ALA  
ALA  
VAL  
VAL  
PRO  
PRO  
GLU  
ASP  
VAL  
VAL  
GLU  
LEU  
ALA  
GLU  
GLU  
ALA  
ALA  
ALA  
GLU  
VAL  
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LYS  
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GLY  
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GLU

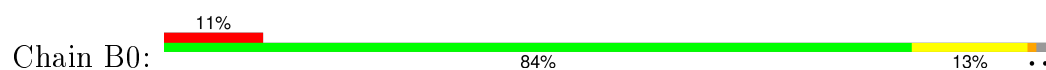
• Molecule 45: 50S Ribosomal Protein L25

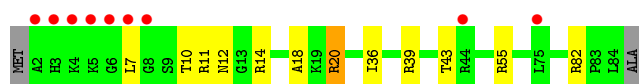


P83  
E84  
R85  
R86  
D87  
R88  
F89  
V90  
S92  
D93  
E94  
P95  
V96  
E97  
P98  
Y99  
V100  
F104  
V105  
G106  
P107  
T108  
A109  
G110  
V111  
R112  
A113  
G114  
G115  
V116  
Q118  
E119  
H120  
R122  
V126  
K127  
V128  
S129  
P130  
R131  
M132  
I133  
P134  
E135  
F136  
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L144  
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I146  
G147  
D148

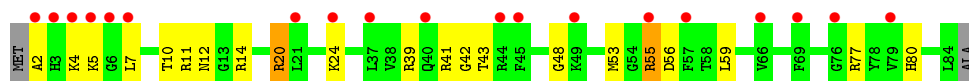
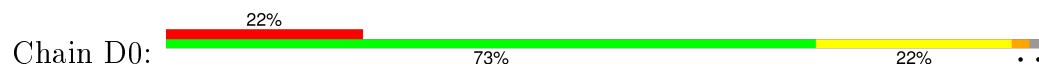
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D154  
L155  
K156  
L157  
P158  
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G160  
V161  
P167  
E168  
E169  
T170  
T171  
I171  
A172  
A173  
V174  
VAL  
PRO  
PRO  
GLU  
ASP  
VAL  
VAL  
GLU  
LEU  
ALA  
GLU  
GLU  
ALA  
ALA  
ALA  
GLU  
VAL  
VAL  
ILE  
LYS  
LYS  
LYS  
GLY  
GLY  
GLU  
GLU  
GLU  
GLU  
GLU

• Molecule 46: 50S Ribosomal Protein L27

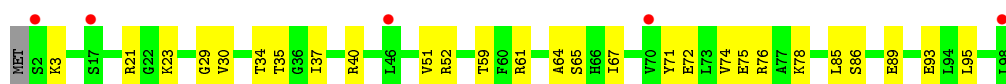
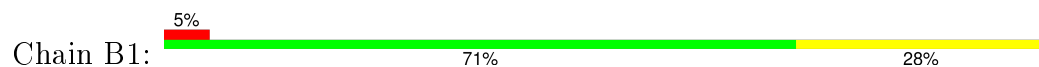




• Molecule 46: 50S Ribosomal Protein L27



• Molecule 47: 50S Ribosomal Protein L28



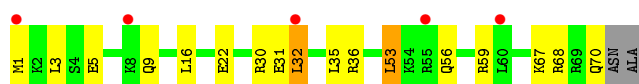
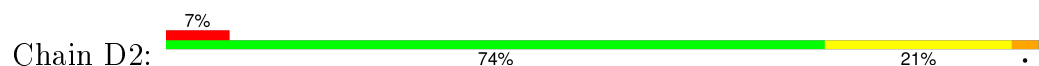
• Molecule 47: 50S Ribosomal Protein L28



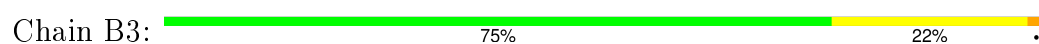
• Molecule 48: 50S Ribosomal Protein L29



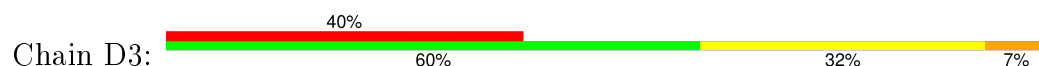
• Molecule 48: 50S Ribosomal Protein L29

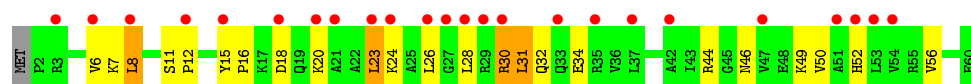


• Molecule 49: 50S Ribosomal Protein L30



• Molecule 49: 50S Ribosomal Protein L30

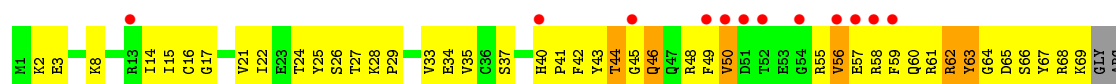




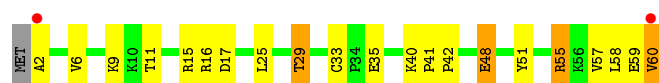
• Molecule 50: 50S Ribosomal Protein L31



• Molecule 50: 50S Ribosomal Protein L31



• Molecule 51: 50S Ribosomal Protein L32



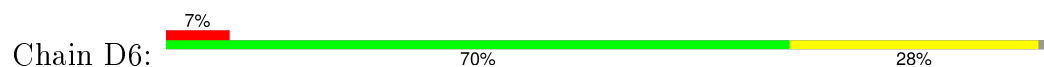
• Molecule 51: 50S Ribosomal Protein L32



• Molecule 52: 50S Ribosomal Protein L33

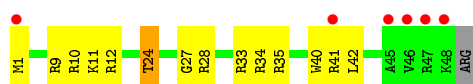


• Molecule 52: 50S Ribosomal Protein L33

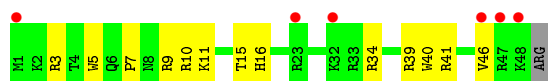
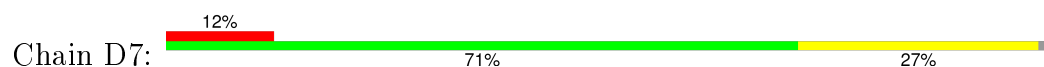


• Molecule 53: 50S Ribosomal Protein L34





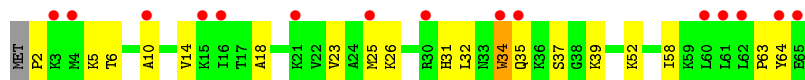
- Molecule 53: 50S Ribosomal Protein L34



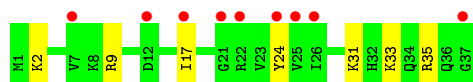
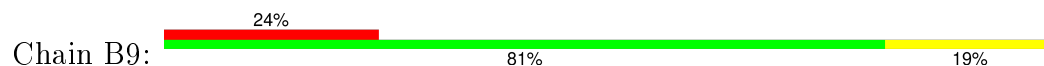
- Molecule 54: 50S Ribosomal Protein L35



- Molecule 54: 50S Ribosomal Protein L35



- Molecule 55: 50S Ribosomal Protein L36



- Molecule 55: 50S Ribosomal Protein L36



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	208.25Å 443.61Å 619.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	124.25 – 2.70 360.63 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.2 (124.25-2.70) 97.2 (360.63-2.70)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.28 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.210 , 0.257 0.218 , 0.263	Depositor DCC
$R_{free}$ test set	75600 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.2	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 56.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 1504988 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	297376	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.74% 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, MIA, NEG, 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	0.44	0/36002	0.92	46/56188 (0.1%)
1	CA	0.42	0/36170	0.94	42/56452 (0.1%)
2	AB	0.32	0/1881	0.59	0/2542
2	CB	0.32	0/1860	0.62	1/2518 (0.0%)
3	AC	0.30	0/1576	0.50	0/2130
3	CC	0.30	0/1566	0.53	0/2119
4	AD	0.31	0/1689	0.53	0/2267
4	CD	0.31	0/1704	0.55	1/2284 (0.0%)
5	AE	0.33	0/1145	0.53	0/1543
5	CE	0.33	0/1149	0.57	0/1548
6	AF	0.32	0/819	0.54	0/1111
6	CF	0.31	0/829	0.51	1/1123 (0.1%)
7	AG	0.30	0/1250	0.49	0/1679
7	CG	0.29	0/1254	0.52	0/1683
8	AH	0.29	0/1108	0.51	0/1494
8	CH	0.30	0/1108	0.52	0/1494
9	AI	0.30	0/1002	0.55	0/1346
9	CI	0.32	0/997	0.56	0/1343
10	AJ	0.29	0/722	0.56	0/982
10	CJ	0.31	0/727	0.58	0/988
11	AK	0.30	0/844	0.51	0/1145
11	CK	0.31	0/848	0.51	0/1149
12	AL	0.34	0/946	0.55	1/1274 (0.1%)
12	CL	0.33	0/946	0.58	0/1274
13	AM	0.32	0/969	0.59	0/1302
13	CM	0.29	0/961	0.54	0/1291
14	AN	0.30	0/501	0.50	0/664
14	CN	0.34	0/501	0.54	0/664
15	AO	0.34	0/739	0.53	0/985
15	CO	0.31	0/739	0.49	0/985
16	AP	0.32	0/697	0.57	0/939
16	CP	0.31	0/693	0.51	0/935

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AQ	0.31	0/836	0.52	0/1117
17	CQ	0.31	0/836	0.50	0/1117
18	AR	0.33	0/560	0.49	0/746
18	CR	0.28	0/560	0.51	0/746
19	AS	0.29	0/667	0.50	0/900
19	CS	0.32	0/661	0.63	0/893
20	AT	0.29	0/730	0.56	0/965
20	CT	0.29	0/729	0.52	0/965
21	AU	0.29	0/203	0.53	0/266
21	CU	0.34	0/203	0.52	0/266
22	AV	0.51	0/310	0.97	1/480 (0.2%)
22	CV	0.44	0/282	1.00	2/437 (0.5%)
23	AW	0.54	0/1602	1.16	6/2493 (0.2%)
23	AY	0.50	0/1602	1.09	2/2493 (0.1%)
23	CW	0.50	0/1556	1.10	2/2418 (0.1%)
23	CY	0.53	0/1579	1.15	2/2455 (0.1%)
24	AX	0.58	1/1725 (0.1%)	1.16	14/2689 (0.5%)
24	CX	0.52	0/1725	1.12	11/2689 (0.4%)
25	BA	0.65	6/68083 (0.0%)	1.00	128/106274 (0.1%)
25	DA	0.49	1/67542 (0.0%)	0.97	74/105428 (0.1%)
26	BB	0.51	0/2878	0.92	0/4490
26	DB	0.48	0/2878	0.91	2/4490 (0.0%)
27	BD	0.43	0/2186	0.62	0/2944
27	DD	0.39	0/2186	0.59	0/2944
28	BE	0.45	0/1592	0.58	0/2149
28	DE	0.37	0/1592	0.61	1/2149 (0.0%)
29	BF	0.39	0/1619	0.57	0/2193
29	DF	0.35	0/1615	0.58	0/2188
30	BG	0.32	0/1450	0.52	0/1959
30	DG	0.32	0/1449	0.55	0/1958
31	BH	0.36	0/1356	0.54	0/1834
31	DH	0.33	0/1356	0.53	0/1834
32	BI	0.32	0/1100	0.58	0/1501
32	DI	0.30	0/1076	0.56	1/1471 (0.1%)
33	BN	0.39	0/1144	0.53	0/1543
33	DN	0.33	0/1144	0.55	0/1543
34	BO	0.41	0/943	0.59	0/1269
34	DO	0.35	0/943	0.55	1/1269 (0.1%)
35	BP	0.39	0/1152	0.59	0/1533
35	DP	0.34	0/1152	0.64	1/1533 (0.1%)
36	BQ	0.41	0/1143	0.53	0/1527
36	DQ	0.35	0/1143	0.56	0/1527
37	BR	0.42	0/982	0.62	0/1312

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
37	DR	0.33	0/982	0.57	0/1312
38	BS	0.36	0/887	0.55	0/1180
38	DS	0.30	0/880	0.55	0/1172
39	BT	0.38	0/1105	0.58	0/1477
39	DT	0.32	0/1097	0.54	0/1468
40	BU	0.44	0/977	0.59	0/1301
40	DU	0.30	0/977	0.48	0/1301
41	BV	0.42	0/782	0.60	0/1049
41	DV	0.32	0/782	0.54	1/1049 (0.1%)
42	BW	0.44	0/897	0.57	0/1205
42	DW	0.34	0/897	0.52	0/1205
43	BX	0.43	0/764	0.61	1/1025 (0.1%)
43	DX	0.35	0/764	0.55	1/1025 (0.1%)
44	BY	0.40	0/819	0.59	0/1095
44	DY	0.33	0/819	0.53	0/1095
45	BZ	0.34	0/1379	0.59	0/1873
45	DZ	0.32	0/1390	0.56	0/1890
46	B0	0.42	0/662	0.63	0/881
46	D0	0.33	0/662	0.53	0/881
47	B1	0.41	0/762	0.56	0/1014
47	D1	0.35	0/762	0.54	0/1014
48	B2	0.38	0/590	0.58	0/781
48	D2	0.28	0/590	0.48	0/781
49	B3	0.37	0/474	0.58	0/635
49	D3	0.30	0/469	0.52	0/630
50	B4	0.37	0/571	0.71	0/768
50	D4	0.35	0/545	0.57	0/737
51	B5	0.43	0/469	0.64	0/635
51	D5	0.34	0/469	0.54	0/635
52	B6	0.41	0/460	0.57	0/613
52	D6	0.35	0/456	0.45	0/608
53	B7	0.44	0/426	0.60	0/561
53	D7	0.36	0/426	0.55	0/561
54	B8	0.43	0/525	0.61	0/691
54	D8	0.36	0/525	0.54	0/691
55	B9	0.42	0/310	0.50	0/407
55	D9	0.36	0/310	0.56	0/407
All	All	0.48	8/316673 (0.0%)	0.89	343/474091 (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
38	BS	0	1
All	All	0	4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	553	A	N9-C4	-8.54	1.32	1.37
25	BA	354	A	N9-C4	-8.21	1.32	1.37
25	BA	1188	A	N9-C4	-7.54	1.33	1.37
25	BA	990	A	N9-C4	-6.34	1.34	1.37
25	BA	2299	A	N9-C4	-6.34	1.34	1.37
25	DA	528	A	N9-C4	-6.24	1.34	1.37
25	BA	1067	A	N9-C4	-6.12	1.34	1.37
24	AX	14	A	C8-N7	-5.18	1.27	1.31

All (343) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BA	553	A	C2-N3-C4	-12.04	104.58	110.60
25	BA	354	A	C2-N3-C4	-11.68	104.76	110.60
1	AA	345	C	N1-C2-O2	11.09	125.55	118.90
25	BA	1686	U	O5'-P-OP2	-10.46	96.29	105.70
1	CA	1154	G	C5-C6-O6	10.31	134.78	128.60
24	AX	46	G	C6-N1-C2	-10.02	119.09	125.10
1	AA	1030(B)	C	N1-C2-O2	9.95	124.87	118.90
24	AX	14	A	C5-N7-C8	9.62	108.71	103.90
25	BA	2694	U	O5'-P-OP2	-9.53	97.13	105.70
24	AX	14	A	C4-C5-C6	9.43	121.72	117.00
1	AA	345	C	N3-C2-O2	-9.41	115.31	121.90
25	DA	801	G	O5'-P-OP2	-9.37	97.27	105.70
1	CA	1119	C	C2-N3-C4	9.30	124.55	119.90
25	BA	537	G	O4'-C1'-N9	8.90	115.32	108.20
25	BA	553	A	N3-C4-C5	8.60	132.82	126.80
25	BA	139	A	N7-C8-N9	8.57	118.09	113.80
25	DA	2248	C	O5'-P-OP2	-8.55	98.01	105.70
25	DA	34	C	N1-C2-O2	8.51	124.01	118.90
1	AA	345	C	C2-N1-C1'	8.49	128.14	118.80
25	BA	1067	A	C2-N3-C4	-8.48	106.36	110.60
25	BA	990	A	C2-N3-C4	-8.46	106.37	110.60
25	BA	2163	G	N3-C4-N9	8.40	131.04	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1030(B)	C	N3-C2-O2	-8.39	116.03	121.90
25	BA	1020	C	O5'-P-OP1	-8.31	98.22	105.70
25	BA	1188	A	C2-N3-C4	-8.26	106.47	110.60
24	CX	46	G	C6-N1-C2	-8.06	120.26	125.10
25	BA	139	A	C5-N7-C8	-8.05	99.87	103.90
25	BA	553	A	N3-C4-N9	-8.03	120.98	127.40
25	BA	31	C	O5'-P-OP1	-7.95	98.55	105.70
25	DA	34	C	C2-N1-C1'	7.93	127.52	118.80
25	DA	2136	C	N1-C2-O2	7.87	123.62	118.90
24	AX	22	G	C5-N7-C8	-7.85	100.37	104.30
24	CX	14	A	C5-N7-C8	7.84	107.82	103.90
1	AA	1030(B)	C	C2-N1-C1'	7.83	127.41	118.80
25	DA	2061	G	O5'-P-OP2	-7.82	98.67	105.70
1	CA	1029	C	N1-C2-O2	7.80	123.58	118.90
25	DA	362	U	C2-N1-C1'	7.75	127.00	117.70
25	BA	2163	G	N3-C4-C5	-7.66	124.77	128.60
1	AA	365	U	C5-C6-N1	-7.65	118.87	122.70
25	DA	2152	G	C5-C6-O6	-7.58	124.05	128.60
25	DA	1614	A	O5'-P-OP1	-7.57	98.89	105.70
25	BA	354	A	N3-C4-C5	7.56	132.09	126.80
25	DA	748	G	C4-N9-C1'	-7.28	117.04	126.50
23	AW	25	C	C5-C4-N4	7.27	125.29	120.20
1	AA	1036	G	C4-N9-C1'	7.14	135.78	126.50
25	BA	1807	G	O5'-P-OP2	-7.12	99.29	105.70
25	BA	2299	A	C2-N3-C4	-7.12	107.04	110.60
25	DA	362	U	N1-C2-O2	7.08	127.76	122.80
25	BA	12	U	C2-N1-C1'	7.07	126.19	117.70
1	AA	1002	G	N3-C4-N9	7.06	130.23	126.00
1	CA	1003	G	C4-N9-C1'	7.05	135.67	126.50
25	BA	934	A	O4'-C1'-N9	7.05	113.84	108.20
1	AA	345	C	C6-N1-C2	-7.04	117.48	120.30
1	AA	839	U	P-O3'-C3'	7.03	128.13	119.70
25	BA	2163	G	C8-N9-C1'	-7.01	117.89	127.00
1	CA	754	C	C2-N1-C1'	7.00	126.50	118.80
25	BA	990	A	C5-N7-C8	-6.98	100.41	103.90
25	BA	2163	G	C4-N9-C1'	6.98	135.57	126.50
1	CA	754	C	N1-C2-O2	6.95	123.07	118.90
25	BA	2163	G	C4-C5-C6	6.94	122.97	118.80
25	DA	2152	G	N1-C6-O6	6.94	124.06	119.90
25	DA	1204	A	O4'-C1'-N9	6.92	113.73	108.20
25	BA	2163	G	C5-N7-C8	6.86	107.73	104.30
24	CX	14	A	C4-C5-C6	6.83	120.42	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	DA	205	G	C8-N9-C4	6.83	109.13	106.40
25	BA	1249	A	O4'-C1'-N9	6.82	113.66	108.20
24	AX	14	A	C5-C6-N1	-6.79	114.31	117.70
1	AA	299	G	C5-C6-O6	-6.78	124.53	128.60
25	DA	141	A	N7-C8-N9	6.75	117.17	113.80
25	DA	362	U	C6-N1-C1'	-6.73	111.78	121.20
1	CA	1119	C	N3-C4-C5	-6.73	119.21	121.90
25	BA	1067	A	N1-C2-N3	6.71	132.66	129.30
25	BA	139	A	C8-N9-C4	-6.69	103.12	105.80
25	DA	528	A	C2-N3-C4	-6.68	107.26	110.60
25	BA	354	A	N1-C2-N3	6.66	132.63	129.30
23	AW	25	C	N3-C4-N4	-6.62	113.36	118.00
1	AA	254	G	O5'-P-OP1	-6.62	99.74	105.70
25	DA	1698	A	O4'-C1'-N9	6.62	113.50	108.20
25	BA	215	G	O4'-C1'-N9	6.61	113.49	108.20
25	BA	354	A	N3-C4-N9	-6.60	122.12	127.40
25	DA	645	C	C2-N1-C1'	6.58	126.04	118.80
1	AA	365	U	C2-N1-C1'	-6.56	109.82	117.70
24	AX	46	G	C5-C6-N1	6.55	114.78	111.50
1	CA	1003	G	C8-N9-C4	-6.54	103.78	106.40
25	DA	361	G	C8-N9-C4	-6.52	103.79	106.40
25	DA	34	C	N3-C2-O2	-6.51	117.34	121.90
25	DA	2554	U	O5'-P-OP1	-6.51	99.84	105.70
24	CX	22	G	C5-N7-C8	-6.46	101.07	104.30
25	BA	1188	A	N3-C4-C5	6.45	131.32	126.80
25	DA	748	G	C8-N9-C1'	6.45	135.38	127.00
25	BA	2014	G	P-O3'-C3'	6.42	127.41	119.70
1	CA	1158	C	N1-C2-O2	6.42	122.75	118.90
1	AA	1002	G	N3-C4-C5	-6.41	125.39	128.60
25	BA	848	G	O5'-P-OP2	-6.41	99.93	105.70
1	AA	1030(B)	C	C6-N1-C2	-6.40	117.74	120.30
25	BA	793	A	O4'-C1'-N9	6.39	113.31	108.20
1	CA	1064	G	P-O3'-C3'	6.39	127.36	119.70
1	AA	163	C	C2-N1-C1'	6.38	125.82	118.80
1	CA	1001(A)	G	N3-C4-N9	6.34	129.81	126.00
1	AA	558	G	O5'-P-OP1	-6.34	100.00	105.70
1	CA	1003	G	N3-C4-C5	-6.33	125.43	128.60
1	AA	1502	A	N1-C2-N3	6.33	132.46	129.30
1	AA	1396	A	C6-N1-C2	6.31	122.39	118.60
25	DA	645	C	N1-C2-O2	6.28	122.67	118.90
25	DA	362	U	C5-C6-N1	6.27	125.84	122.70
43	BX	57	LEU	CA-CB-CG	6.27	129.73	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BA	990	A	N1-C6-N6	6.23	122.34	118.60
1	CA	1003	G	N7-C8-N9	6.22	116.21	113.10
25	DA	2155	G	C6-N1-C2	6.22	128.83	125.10
25	BA	273	G	OP1-P-O3'	6.22	118.89	105.20
25	DA	2155	G	N3-C2-N2	6.19	124.23	119.90
25	DA	2243	U	O5'-P-OP1	-6.18	100.14	105.70
25	BA	1068	G	N3-C4-N9	-6.15	122.31	126.00
1	CA	79	G	C5-C6-O6	6.15	132.29	128.60
25	BA	1188	A	N3-C4-N9	-6.15	122.48	127.40
25	DA	2152	G	C6-C5-N7	-6.14	126.72	130.40
26	DB	1	U	C2-N1-C1'	6.13	125.05	117.70
1	CA	1154	G	N1-C6-O6	-6.12	116.23	119.90
1	AA	299	G	N1-C6-O6	6.11	123.57	119.90
25	DA	2143	C	C2-N3-C4	6.10	122.95	119.90
25	BA	1068	G	N3-C2-N2	-6.10	115.63	119.90
23	AY	58	A	OP1-P-O3'	6.09	118.59	105.20
1	AA	1036	G	C8-N9-C1'	-6.09	119.09	127.00
1	CA	1492	A	P-O3'-C3'	6.08	127.00	119.70
1	CA	1154	G	C6-N1-C2	6.07	128.74	125.10
1	CA	1004	A	N1-C6-N6	-6.06	114.96	118.60
25	BA	12	U	N1-C2-O2	6.05	127.03	122.80
24	AX	46	G	N3-C2-N2	-6.03	115.68	119.90
25	BA	1359	U	C2-N1-C1'	6.03	124.94	117.70
1	CA	1158	C	C2-N1-C1'	6.03	125.43	118.80
25	BA	1067	A	N3-C4-N9	-6.00	122.60	127.40
25	DA	2152	G	N3-C4-N9	6.00	129.60	126.00
25	BA	254	A	N1-C6-N6	5.99	122.19	118.60
25	DA	361	G	N3-C4-C5	-5.99	125.61	128.60
22	CV	19	U	C2-N3-C4	5.98	130.59	127.00
25	BA	184	A	N7-C8-N9	-5.97	110.82	113.80
25	DA	1021	A	C2-N3-C4	-5.96	107.62	110.60
25	BA	2173	G	C2-N3-C4	5.95	114.88	111.90
1	AA	1021	G	N3-C2-N2	5.94	124.06	119.90
25	BA	798	A	OP1-P-OP2	-5.94	110.70	119.60
1	CA	992	U	P-O3'-C3'	5.94	126.82	119.70
25	DA	1131	G	O4'-C1'-N9	5.92	112.94	108.20
25	DA	528	A	N3-C4-N9	-5.92	122.66	127.40
25	DA	2136	C	N3-C2-O2	-5.91	117.76	121.90
25	BA	943	C	C5-C6-N1	5.89	123.94	121.00
25	BA	123	G	O4'-C1'-N9	-5.89	103.49	108.20
1	CA	997	U	C5-C4-O4	5.89	129.43	125.90
25	BA	2210	C	N1-C2-O2	5.88	122.43	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BA	2299	A	N3-C4-C5	5.87	130.91	126.80
25	DA	2167	U	N1-C2-O2	5.86	126.90	122.80
25	BA	1745	A	C5-N7-C8	-5.85	100.98	103.90
25	BA	834	U	O5'-P-OP1	-5.84	100.44	105.70
25	BA	797	A	OP1-P-O3'	5.84	118.04	105.20
24	AX	14	A	C8-N9-C1'	-5.83	117.22	127.70
25	BA	2883	A	O4'-C1'-N9	5.82	112.86	108.20
1	AA	1492	A	P-O3'-C3'	5.82	126.68	119.70
25	BA	2858	G	O4'-C1'-N9	5.81	112.85	108.20
2	CB	115	LEU	CA-CB-CG	5.81	128.65	115.30
25	DA	192	C	O5'-P-OP1	-5.79	100.48	105.70
1	AA	754	C	C2-N1-C1'	5.79	125.17	118.80
25	BA	989	G	C4-N9-C1'	5.76	133.99	126.50
25	DA	2321	G	C4-N9-C1'	5.76	133.98	126.50
25	BA	1359	U	N1-C2-O2	5.75	126.82	122.80
25	BA	184	A	C5-N7-C8	5.74	106.77	103.90
43	DX	57	LEU	CA-CB-CG	5.74	128.50	115.30
25	DA	214	G	O4'-C1'-N9	5.74	112.79	108.20
24	AX	22	G	C4-C5-C6	-5.73	115.36	118.80
25	DA	383	U	O4'-C1'-N1	5.73	112.79	108.20
25	BA	2331	G	N3-C4-N9	-5.73	122.56	126.00
25	BA	2238	C	C6-N1-C2	5.72	122.59	120.30
24	AX	22	G	C5-C6-N1	5.71	114.36	111.50
25	DA	141	A	C8-N9-C4	-5.68	103.53	105.80
25	BA	1462	G	O4'-C1'-N9	5.68	112.74	108.20
25	BA	2459	G	C8-N9-C4	5.67	108.67	106.40
25	BA	2566	U	O5'-P-OP1	-5.67	100.59	105.70
25	BA	1006	C	O5'-P-OP2	-5.67	100.60	105.70
1	CA	754	C	C6-N1-C1'	-5.66	114.01	120.80
25	DA	192	C	OP1-P-OP2	5.65	128.08	119.60
23	AW	13	C	C2-N1-C1'	5.65	125.02	118.80
25	BA	2383	G	C5-C6-N1	5.65	114.32	111.50
25	BA	2054	G	N7-C8-N9	-5.65	110.28	113.10
25	BA	2331	G	N3-C4-C5	5.64	131.42	128.60
1	AA	839	U	OP1-P-O3'	5.63	117.58	105.20
1	AA	670	G	O5'-P-OP2	-5.62	100.64	105.70
25	BA	2515	A	N1-C2-N3	-5.61	126.49	129.30
24	CX	46	G	C5-C6-N1	5.61	114.31	111.50
25	BA	990	A	C4-C5-N7	5.60	113.50	110.70
25	BA	2220	A	OP1-P-O3'	5.59	117.51	105.20
25	BA	2250	G	N3-C4-N9	5.58	129.35	126.00
1	AA	754	C	N1-C2-O2	5.58	122.25	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	913	A	P-O3'-C3'	5.58	126.40	119.70
25	BA	2264	G	N3-C4-N9	-5.56	122.66	126.00
41	DV	18	LEU	CA-CB-CG	5.56	128.09	115.30
25	BA	2054	G	C5-N7-C8	5.56	107.08	104.30
23	CY	23	A	N1-C6-N6	5.55	121.93	118.60
25	BA	989	G	C8-N9-C1'	-5.54	119.79	127.00
22	AV	17	U	C5-C4-O4	5.54	129.22	125.90
25	BA	12	U	N3-C2-O2	-5.54	118.32	122.20
25	BA	1249	A	C2-N3-C4	-5.54	107.83	110.60
26	DB	1	U	N1-C2-O2	5.54	126.68	122.80
22	CV	19	U	C5-C4-O4	5.54	129.22	125.90
28	DE	72	VAL	C-N-CA	5.54	135.55	121.70
25	DA	362	U	N1-C2-N3	-5.53	111.58	114.90
1	CA	1502	A	N1-C2-N3	5.52	132.06	129.30
25	DA	1531	C	C5-C6-N1	5.52	123.76	121.00
25	BA	1745	A	C2-N3-C4	-5.52	107.84	110.60
1	CA	1029	C	C2-N3-C4	5.50	122.65	119.90
25	DA	746	A	O4'-C1'-N9	5.50	112.60	108.20
25	DA	34	C	C6-N1-C1'	-5.50	114.21	120.80
25	DA	1313	U	C2-N1-C1'	5.50	124.29	117.70
25	DA	2150	U	N1-C2-N3	5.49	118.20	114.90
1	CA	1030	C	N1-C2-O2	5.48	122.19	118.90
25	BA	254	A	C5-N7-C8	-5.48	101.16	103.90
25	DA	277	C	N1-C2-O2	5.48	122.19	118.90
25	BA	1067	A	C8-N9-C4	-5.48	103.61	105.80
25	BA	2513	C	C2-N1-C1'	-5.47	112.78	118.80
1	AA	1067	A	P-O3'-C3'	5.47	126.27	119.70
24	CX	35	A	O5'-P-OP1	-5.47	100.78	105.70
24	CX	46	G	N3-C2-N2	-5.47	116.07	119.90
1	AA	782	A	O5'-P-OP1	-5.46	100.79	105.70
25	BA	892	G	O4'-C1'-N9	5.46	112.57	108.20
25	BA	273	G	P-O3'-C3'	5.45	126.25	119.70
1	CA	1012	U	C2-N3-C4	-5.45	123.73	127.00
25	BA	1068	G	N3-C4-C5	5.45	131.32	128.60
25	BA	1221	G	P-O3'-C3'	5.45	126.23	119.70
25	BA	989	G	N3-C4-N9	5.44	129.27	126.00
24	CX	14	A	C5-C6-N1	-5.44	114.98	117.70
1	AA	1064	G	P-O3'-C3'	5.44	126.22	119.70
23	CW	36	A	C6-N1-C2	5.43	121.86	118.60
25	BA	1068	G	C4-N9-C1'	-5.43	119.44	126.50
25	BA	616	G	N1-C6-O6	-5.43	116.64	119.90
25	BA	1220	U	P-O3'-C3'	5.42	126.21	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BA	2258	G	C8-N9-C4	5.42	108.57	106.40
32	DI	75	LEU	CA-CB-CG	5.42	127.76	115.30
25	BA	1589	A	O5'-P-OP1	-5.41	100.83	105.70
1	AA	189(D)	C	N1-C2-O2	-5.40	115.66	118.90
25	BA	1743	G	O5'-P-OP2	-5.40	100.84	105.70
1	CA	1119	C	C5-C4-N4	5.40	123.98	120.20
24	CX	14	A	C8-N9-C1'	-5.38	118.01	127.70
25	BA	2802	C	N1-C2-O2	-5.38	115.67	118.90
25	DA	1022	G	N3-C4-N9	-5.38	122.77	126.00
25	DA	915	C	C6-N1-C2	-5.37	118.15	120.30
23	CY	23	A	C5-C6-N6	-5.37	119.40	123.70
25	DA	141	A	C5-N7-C8	-5.37	101.22	103.90
1	AA	345	C	C6-N1-C1'	-5.36	114.36	120.80
25	BA	111	G	N3-C4-N9	-5.36	122.78	126.00
1	AA	163	C	C6-N1-C1'	-5.35	114.38	120.80
1	CA	1390	U	N1-C2-O2	-5.35	119.06	122.80
1	CA	1030	C	C2-N1-C1'	5.35	124.69	118.80
25	BA	2210	C	C2-N1-C1'	5.34	124.68	118.80
25	DA	2139	C	N1-C2-O2	5.33	122.10	118.90
25	BA	399	G	O4'-C1'-N9	5.33	112.46	108.20
25	BA	2701	U	N3-C2-O2	-5.33	118.47	122.20
25	DA	1368	G	O5'-P-OP2	-5.31	100.92	105.70
25	DA	2143	C	C5-C6-N1	5.31	123.66	121.00
1	AA	1285	A	P-O3'-C3'	5.31	126.07	119.70
1	CA	365	U	C5-C6-N1	-5.31	120.05	122.70
25	BA	1177	G	O4'-C1'-N9	5.30	112.44	108.20
23	AW	15	G	N3-C2-N2	5.30	123.61	119.90
25	BA	410	U	O4'-C1'-N1	5.30	112.44	108.20
25	DA	748	G	C6-C5-N7	5.29	133.57	130.40
1	CA	1502	A	N7-C8-N9	5.28	116.44	113.80
23	AW	25	C	C2-N1-C1'	-5.27	113.00	118.80
25	DA	1992	G	P-O3'-C3'	5.27	126.03	119.70
24	AX	14	A	C4-N9-C1'	5.27	135.79	126.30
25	BA	184	A	P-O3'-C3'	5.27	126.03	119.70
25	BA	1745	A	N7-C8-N9	5.27	116.44	113.80
25	BA	2045	G	O5'-P-OP1	-5.26	100.96	105.70
24	CX	14	A	C4-N9-C1'	5.26	135.77	126.30
25	BA	795	G	O4'-C1'-N9	5.26	112.40	108.20
24	AX	35	A	C6-N1-C2	5.25	121.75	118.60
25	BA	2082	A	C8-N9-C4	5.25	107.90	105.80
24	AX	22	G	N7-C8-N9	5.23	115.72	113.10
25	BA	597	C	C6-N1-C2	5.23	122.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1012	U	N1-C2-O2	-5.21	119.15	122.80
25	DA	2167	U	C2-N1-C1'	5.21	123.95	117.70
12	AL	84	LEU	CA-CB-CG	5.21	127.28	115.30
1	AA	921	U	C2-N3-C4	5.21	130.12	127.00
25	BA	1450	C	O5'-P-OP2	-5.21	101.02	105.70
1	CA	1505	G	N3-C4-N9	-5.20	122.88	126.00
1	AA	1064	G	OP1-P-O3'	5.20	116.63	105.20
1	AA	890	G	O4'-C1'-N9	5.18	112.35	108.20
25	BA	507	G	O4'-C1'-N9	5.18	112.34	108.20
1	CA	997	U	C2-N1-C1'	-5.17	111.49	117.70
1	CA	1012	U	N1-C2-N3	5.17	118.00	114.90
25	DA	512	G	O4'-C1'-N9	5.17	112.34	108.20
25	DA	2139	C	C2-N1-C1'	5.17	124.49	118.80
25	DA	2167	U	N3-C2-O2	-5.17	118.58	122.20
25	DA	1300	U	P-O3'-C3'	5.16	125.89	119.70
24	CX	67	C	C2-N1-C1'	5.16	124.47	118.80
1	CA	1003	G	N3-C4-N9	5.16	129.09	126.00
25	DA	2152	G	N9-C4-C5	-5.15	103.34	105.40
25	DA	34	C	C6-N1-C2	-5.15	118.24	120.30
25	BA	2899	C	N1-C2-O2	5.15	121.99	118.90
23	CW	7	A	N1-C6-N6	5.14	121.69	118.60
25	BA	553	A	C5-C6-N1	-5.14	115.13	117.70
25	DA	912	C	N1-C2-O2	5.13	121.98	118.90
35	DP	44	GLY	C-N-CA	5.13	134.53	121.70
25	DA	2152	G	C4-C5-N7	5.13	112.85	110.80
25	BA	724	A	O5'-P-OP2	-5.13	101.08	105.70
25	BA	2163	G	C6-C5-N7	-5.13	127.32	130.40
25	DA	1558	A	P-O3'-C3'	5.12	125.85	119.70
25	BA	2802	C	C2-N1-C1'	-5.12	113.17	118.80
25	DA	574	C	N1-C2-O2	-5.12	115.83	118.90
1	CA	913	A	P-O3'-C3'	5.11	125.83	119.70
25	BA	2009	G	O5'-P-OP2	-5.09	101.11	105.70
24	AX	46	G	C5-C6-O6	-5.09	125.55	128.60
1	CA	1126	U	C5-C6-N1	5.09	125.25	122.70
25	BA	2605	U	N3-C4-O4	-5.09	115.84	119.40
6	CF	75	LEU	CA-CB-CG	5.09	127.00	115.30
1	CA	1126	U	C2-N1-C1'	5.08	123.80	117.70
1	CA	1331	G	O4'-C1'-N9	5.08	112.26	108.20
25	BA	1154	U	N3-C2-O2	-5.08	118.65	122.20
25	BA	1431	G	O4'-C1'-N9	5.07	112.26	108.20
23	AY	58	A	P-O3'-C3'	5.07	125.78	119.70
1	AA	1030(B)	C	C6-N1-C1'	-5.07	114.72	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	DA	2321	G	C8-N9-C1'	-5.07	120.42	127.00
25	BA	599	U	O5'-P-OP1	-5.06	101.14	105.70
25	DA	1786	A	O4'-C1'-N9	5.06	112.25	108.20
23	AW	25	C	C6-N1-C1'	5.06	126.87	120.80
1	AA	997	U	C5-C4-O4	5.05	128.93	125.90
25	BA	2162	C	N1-C2-O2	5.05	121.93	118.90
25	BA	2210	C	C6-N1-C1'	-5.05	114.74	120.80
25	BA	840	A	O5'-P-OP2	-5.05	101.16	105.70
1	CA	1158	C	C6-N1-C2	-5.05	118.28	120.30
25	BA	1359	U	N3-C2-O2	-5.05	118.67	122.20
25	DA	1653	G	P-O3'-C3'	5.05	125.75	119.70
34	DO	8	LEU	CA-CB-CG	5.04	126.89	115.30
1	AA	397	A	O4'-C1'-N9	5.04	112.23	108.20
25	BA	906	G	C4-N9-C1'	-5.04	119.95	126.50
25	BA	2162	C	C2-N1-C1'	5.04	124.34	118.80
25	BA	2173	G	C4-C5-N7	-5.04	108.78	110.80
1	CA	1154	G	C5-C6-N1	-5.04	108.98	111.50
25	DA	614	U	N3-C2-O2	-5.03	118.68	122.20
1	AA	991	U	P-O3'-C3'	5.02	125.73	119.70
1	CA	60	A	P-O3'-C3'	5.02	125.72	119.70
1	AA	266	G	P-O3'-C3'	5.01	125.71	119.70
25	BA	111	G	N3-C4-C5	5.01	131.10	128.60
25	BA	978	A	O4'-C1'-N9	5.01	112.21	108.20
25	BA	1700	G	C8-N9-C4	-5.01	104.40	106.40
4	CD	188	LEU	CA-CB-CG	5.00	126.81	115.30
25	DA	1266	G	C8-N9-C4	5.00	108.40	106.40
1	AA	1037	C	N1-C2-O2	5.00	121.90	118.90

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	8	LYS	Peptide
7	AG	79	ARG	Peptide
38	BS	58	LEU	Peptide
7	CG	78	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	32163	0	16234	552	0
1	CA	32312	0	16308	628	0
2	AB	1846	0	1867	78	0
2	CB	1825	0	1828	97	0
3	AC	1552	0	1546	55	0
3	CC	1542	0	1517	57	0
4	AD	1659	0	1676	64	0
4	CD	1674	0	1714	46	0
5	AE	1129	0	1185	36	0
5	CE	1133	0	1191	38	0
6	AF	806	0	793	20	0
6	CF	816	0	808	29	0
7	AG	1231	0	1238	27	0
7	CG	1235	0	1249	37	0
8	AH	1088	0	1126	35	0
8	CH	1088	0	1126	39	0
9	AI	983	0	986	41	0
9	CI	978	0	966	45	0
10	AJ	709	0	650	32	0
10	CJ	714	0	672	46	0
11	AK	829	0	825	14	0
11	CK	833	0	836	20	0
12	AL	930	0	980	28	0
12	CL	930	0	980	31	0
13	AM	958	0	1002	41	0
13	CM	950	0	988	43	0
14	AN	492	0	529	22	0
14	CN	492	0	529	24	0
15	AO	728	0	760	20	0
15	CO	728	0	760	23	0
16	AP	681	0	697	21	0
16	CP	677	0	686	22	0
17	AQ	823	0	891	17	0
17	CQ	823	0	891	20	0
18	AR	555	0	618	16	0
18	CR	555	0	618	17	0
19	AS	652	0	662	38	0
19	CS	646	0	644	35	0
20	AT	728	0	798	21	0
20	CT	727	0	796	18	0
21	AU	199	0	208	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	CU	199	0	208	4	0
22	AV	277	0	140	7	0
22	CV	252	0	130	6	0
23	AW	1588	0	820	66	0
23	AY	1581	0	805	62	0
23	CW	1541	0	784	47	0
23	CY	1561	0	796	65	0
24	AX	1625	0	828	13	0
24	CX	1625	0	828	31	0
25	BA	60792	0	30654	800	0
25	DA	60311	0	30412	1121	0
26	BB	2573	0	1306	23	0
26	DB	2573	0	1306	63	0
27	BD	2136	0	2218	67	0
27	DD	2136	0	2218	69	0
28	BE	1559	0	1618	35	0
28	DE	1559	0	1618	52	0
29	BF	1584	0	1625	41	0
29	DF	1580	0	1619	61	0
30	BG	1425	0	1443	41	0
30	DG	1424	0	1434	57	0
31	BH	1330	0	1407	30	0
31	DH	1330	0	1407	42	0
32	BI	1085	0	1114	38	0
32	DI	1061	0	1080	20	0
33	BN	1117	0	1184	24	0
33	DN	1117	0	1184	29	0
34	BO	933	0	996	22	0
34	DO	933	0	996	27	0
35	BP	1135	0	1212	44	0
35	DP	1135	0	1212	48	0
36	BQ	1122	0	1179	37	0
36	DQ	1122	0	1179	62	0
37	BR	968	0	1033	20	0
37	DR	968	0	1033	27	0
38	BS	877	0	938	20	0
38	DS	870	0	923	28	0
39	BT	1091	0	1151	22	0
39	DT	1083	0	1136	32	0
40	BU	959	0	1019	27	0
40	DU	959	0	1019	29	0
41	BV	771	0	830	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	DV	771	0	830	20	0
42	BW	886	0	940	21	0
42	DW	886	0	939	17	0
43	BX	750	0	814	18	0
43	DX	750	0	814	17	0
44	BY	806	0	881	26	0
44	DY	806	0	881	29	0
45	BZ	1349	0	1355	51	0
45	DZ	1360	0	1363	64	0
46	B0	653	0	674	13	0
46	D0	653	0	674	22	0
47	B1	755	0	826	17	0
47	D1	755	0	826	18	0
48	B2	588	0	643	11	0
48	D2	588	0	643	10	0
49	B3	469	0	518	6	0
49	D3	464	0	514	17	0
50	B4	558	0	544	27	0
50	D4	532	0	503	30	0
51	B5	455	0	465	15	0
51	D5	455	0	465	13	0
52	B6	453	0	473	10	0
52	D6	449	0	469	10	0
53	B7	418	0	467	18	0
53	D7	418	0	467	13	0
54	B8	517	0	582	25	0
54	D8	517	0	582	15	0
55	B9	307	0	335	4	0
55	D9	307	0	335	13	0
56	AA	218	0	0	0	0
56	AD	1	0	0	0	0
56	AE	2	0	0	0	0
56	AF	1	0	0	0	0
56	AM	1	0	0	0	0
56	AN	3	0	0	0	0
56	AO	1	0	0	0	0
56	AV	3	0	0	0	0
56	AW	4	0	0	0	0
56	AX	11	0	0	0	0
56	AY	3	0	0	0	0
56	B0	3	0	0	0	0
56	B1	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	B2	1	0	0	0	0
56	B3	2	0	0	0	0
56	B4	1	0	0	0	0
56	B5	5	0	0	0	0
56	B6	1	0	0	0	0
56	B7	4	0	0	0	0
56	B8	1	0	0	0	0
56	B9	1	0	0	0	0
56	BA	785	0	0	0	0
56	BB	18	0	0	0	0
56	BD	11	0	0	0	0
56	BE	8	0	0	0	0
56	BF	11	0	0	0	0
56	BG	2	0	0	0	0
56	BN	6	0	0	0	0
56	BO	1	0	0	0	0
56	BP	4	0	0	0	0
56	BQ	5	0	0	0	0
56	BR	3	0	0	0	0
56	BT	1	0	0	0	0
56	BU	9	0	0	0	0
56	BV	7	0	0	0	0
56	BW	4	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	172	0	0	0	0
56	CD	1	0	0	0	0
56	CE	1	0	0	0	0
56	CF	1	0	0	0	0
56	CJ	1	0	0	0	0
56	CK	1	0	0	0	0
56	CN	1	0	0	0	0
56	CT	1	0	0	0	0
56	CV	1	0	0	0	0
56	CW	2	0	0	0	0
56	CX	2	0	0	0	0
56	CY	1	0	0	0	0
56	D0	1	0	0	0	0
56	D3	1	0	0	0	0
56	D5	1	0	0	0	0
56	D7	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	D8	1	0	0	0	0
56	DA	623	0	0	0	0
56	DB	12	0	0	0	0
56	DD	9	0	0	0	0
56	DE	4	0	0	0	0
56	DF	6	0	0	0	0
56	DG	1	0	0	0	0
56	DN	1	0	0	0	0
56	DO	2	0	0	0	0
56	DP	1	0	0	0	0
56	DQ	4	0	0	0	0
56	DR	2	0	0	0	0
56	DU	3	0	0	0	0
56	DV	3	0	0	0	0
56	DW	4	0	0	0	0
56	DY	1	0	0	0	0
57	AA	119	0	133	18	0
57	AW	17	0	19	2	0
57	AX	17	0	19	3	0
57	CA	136	0	152	13	0
57	CW	17	0	19	1	0
57	CX	17	0	19	5	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	247	0	0	9	0
61	AD	1	0	0	0	0
61	AE	2	0	0	0	0
61	AL	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	AM	2	0	0	0	0
61	AO	1	0	0	0	0
61	AV	3	0	0	0	0
61	AW	13	0	0	2	0
61	AX	11	0	0	2	0
61	AY	1	0	0	0	0
61	B0	8	0	0	0	0
61	B3	1	0	0	0	0
61	B5	6	0	0	1	0
61	B6	1	0	0	0	0
61	B7	2	0	0	1	0
61	B8	7	0	0	1	0
61	BA	1396	0	0	65	0
61	BB	34	0	0	1	0
61	BD	12	0	0	2	0
61	BE	11	0	0	3	0
61	BF	5	0	0	0	0
61	BG	3	0	0	0	0
61	BI	1	0	0	0	0
61	BN	1	0	0	0	0
61	BO	2	0	0	0	0
61	BP	23	0	0	1	0
61	BQ	3	0	0	0	0
61	BR	1	0	0	0	0
61	BT	2	0	0	0	0
61	BU	3	0	0	0	0
61	BV	2	0	0	0	0
61	BW	1	0	0	1	0
61	BX	2	0	0	0	0
61	BZ	1	0	0	1	0
61	CA	184	0	0	14	0
61	CJ	2	0	0	2	0
61	CP	1	0	0	0	0
61	CV	2	0	0	0	0
61	CW	3	0	0	1	0
61	CX	6	0	0	0	0
61	D0	8	0	0	1	0
61	D1	4	0	0	0	0
61	D7	2	0	0	0	0
61	D8	1	0	0	0	0
61	DA	960	0	0	63	0
61	DB	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	DD	16	0	0	2	0
61	DE	9	0	0	0	0
61	DF	5	0	0	0	0
61	DN	3	0	0	0	0
61	DO	2	0	0	0	0
61	DP	15	0	0	0	0
61	DQ	1	0	0	1	0
61	DR	1	0	0	0	0
61	DU	1	0	0	0	0
61	DW	1	0	0	0	0
61	DX	1	0	0	0	0
61	DY	2	0	0	1	0
All	All	297376	0	196603	5587	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 12.

All (5587) 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)
23:CW:27:G:H1	23:CW:43:C:N4	1.53	1.07
23:CY:7:A:N6	23:CY:66:U:H3	1.50	1.07
23:AY:49:C:N4	23:AY:65:G:H1	1.56	1.03
23:CY:15:G:N2	23:CY:48:C:H42	1.55	1.03
53:B7:24:THR:HG22	53:B7:27:GLY:H	1.24	1.02
23:AW:7:A:N6	23:AW:66:U:H3	1.56	1.01
1:AA:1028:C:H42	1:AA:1033:G:H1	1.09	1.00
1:AA:72:C:H42	1:AA:97:G:H1	1.05	1.00
1:AA:999:C:N4	1:AA:1042:G:H1	1.58	1.00
43:BX:31:HIS:HD2	43:BX:33:LYS:H	1.10	0.99
1:CA:1002:G:H1	1:CA:1038:C:H42	0.99	0.99
23:CY:15:G:H22	23:CY:48:C:N4	1.60	0.99
38:DS:35:ILE:HD11	38:DS:101:LEU:HD12	1.43	0.98
1:CA:1000:U:H3	1:CA:1041:A:N6	1.62	0.98
23:CY:19:G:H1	23:CY:56:C:H42	0.98	0.98
25:DA:1798:U:H5'	27:DD:259:THR:HG22	1.47	0.97
2:CB:16:HIS:HB2	2:CB:204:ASN:HB3	1.46	0.97
1:AA:78:G:H1	1:AA:91:C:H42	1.09	0.96
1:CA:1002:G:H1	1:CA:1038:C:N4	1.64	0.96
25:BA:2158:C:N4	25:BA:2177:G:H1	1.63	0.96
1:CA:1422:G:H5''	34:DO:48:PRO:HB3	1.46	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:AA:3221:NEG:H71	25:BA:786:G:H1	1.28	0.95
1:CA:201:C:H42	1:CA:216:G:H1	1.04	0.95
1:AA:376:G:H5'	16:AP:5:ARG:HG2	1.50	0.94
25:BA:1829:U:H5'	27:BD:259:THR:HG22	1.48	0.94
46:B0:11:ARG:O	46:B0:14:ARG:NH2	2.02	0.93
25:DA:2123:G:H1	25:DA:2175:C:H42	0.95	0.93
46:B0:10:THR:HG22	46:B0:12:ASN:H	1.31	0.93
25:BA:2122:G:H1	25:BA:2211:U:H3	1.17	0.93
2:CB:87:ARG:HE	2:CB:233:SER:HB3	1.30	0.93
25:DA:2318:G:H21	38:DS:3:ARG:HH12	1.17	0.93
23:AY:7:A:H61	23:AY:66:U:H3	1.05	0.92
25:DA:2096:U:H3	25:DA:2193:G:H1	1.17	0.92
1:CA:1162:C:H42	1:CA:1174:G:H1	1.17	0.92
23:AY:19:G:H1	23:AY:56:C:H42	1.17	0.92
1:AA:998:G:H1	1:AA:1043:C:H42	1.17	0.92
25:BA:2146:G:H1	25:BA:2196:C:H42	0.97	0.91
1:CA:1000:U:H3	1:CA:1041:A:H61	0.93	0.91
25:BA:2146:G:H1	25:BA:2196:C:N4	1.67	0.91
23:CY:19:G:H1	23:CY:56:C:N4	1.69	0.91
25:DA:2123:G:H1	25:DA:2175:C:N4	1.69	0.91
25:DA:2130:U:H4'	25:DA:2133:G:H4'	1.50	0.91
1:AA:953:G:H5'	1:AA:965:A:H61	1.34	0.91
25:BA:1736:A:H62	25:BA:1745:A:H2	1.15	0.91
23:AY:26:A:H61	23:AY:44:G:H1	0.92	0.91
1:CA:1086:U:H3	1:CA:1099:G:H22	1.17	0.90
23:AW:11:C:N4	23:AW:24:G:H1	1.68	0.90
25:BA:1405:A:N1	25:BA:1418:U:N3	2.19	0.90
23:AW:29:G:H1	23:AW:41:C:H42	1.15	0.90
23:AY:26:A:N6	23:AY:44:G:H1	1.68	0.90
23:AW:11:C:H42	23:AW:24:G:H1	0.96	0.90
25:BA:2128:G:H1	25:BA:2205:C:H42	1.19	0.90
25:BA:537:G:N7	61:BA:4902:HOH:O	2.05	0.89
23:AW:7:A:H61	23:AW:66:U:H3	0.96	0.89
25:DA:2138:C:H42	25:DA:2153:G:H1	1.21	0.89
1:CA:1003:G:N2	1:CA:1025:U:O4	2.06	0.88
1:AA:406:G:H5'	4:AD:5:ILE:HD11	1.55	0.88
25:DA:2139:C:H42	25:DA:2152:G:H1	1.19	0.88
25:DA:740:U:OP2	61:DA:4494:HOH:O	1.91	0.88
33:DN:123:TYR:HH	33:DN:130:HIS:HE2	1.17	0.88
1:AA:1003:G:N2	1:AA:1004:A:N3	2.22	0.88
25:DA:2689:U:H4'	25:DA:2690:C:H5'	1.53	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2123:G:H1	25:BA:2210:C:H42	1.16	0.88
1:CA:770:C:OP1	61:CA:4102:HOH:O	1.91	0.88
23:AY:49:C:H42	23:AY:65:G:H1	0.91	0.88
46:D0:11:ARG:O	46:D0:14:ARG:NH2	2.08	0.87
25:BA:656:A:OP1	35:BP:65:ARG:NH1	2.07	0.87
1:AA:538:G:H5''	12:AL:114:LYS:HB2	1.56	0.87
2:AB:17:PHE:HB2	2:AB:44:LEU:HD21	1.56	0.87
1:AA:999:C:H42	1:AA:1042:G:H1	0.87	0.87
23:CY:15:G:H22	23:CY:48:C:H42	0.88	0.86
1:AA:1158:C:H5	1:AA:1181:G:H1	1.20	0.86
25:DA:880:G:N2	25:DA:898:C:O2	2.08	0.86
25:BA:2163:G:O6	25:BA:2172:U:O2	1.94	0.86
23:CY:43:C:H2'	23:CY:44:G:H8	1.39	0.86
34:DO:35:VAL:HG11	34:DO:103:ALA:HB3	1.56	0.86
25:DA:2046:G:H5'	51:D5:19:ARG:HA	1.57	0.86
1:CA:1024:G:H2'	1:CA:1025:U:H5''	1.58	0.86
1:AA:975:A:H4'	1:AA:976:G:H5''	1.57	0.86
3:AC:52:LEU:HD21	3:AC:55:VAL:HG23	1.58	0.86
23:CW:27:G:H1	23:CW:43:C:H42	0.90	0.85
25:BA:2695:C:O2	34:BO:70:LYS:NZ	2.09	0.85
2:AB:185:ILE:HG22	2:AB:199:TYR:HB2	1.58	0.85
36:DQ:21:THR:HG21	36:DQ:101:ARG:HD3	1.57	0.85
27:DD:238:GLY:O	61:DD:408:HOH:O	1.93	0.85
25:BA:615:G:O6	61:BA:4976:HOH:O	1.94	0.85
2:AB:16:HIS:HB2	2:AB:204:ASN:HB3	1.59	0.85
10:AJ:35:SER:HB3	10:AJ:73:ASP:HB2	1.57	0.85
1:CA:1030(A):G:N2	1:CA:1030(D):A:OP2	2.10	0.85
39:BT:65:LYS:HE2	39:BT:67:SER:HB2	1.59	0.85
25:DA:1204:A:H2	25:DA:1241:A:H62	1.21	0.84
1:AA:559:A:OP1	5:AE:126:ARG:NH2	2.10	0.84
23:CW:27:G:N2	23:CW:43:C:N3	2.25	0.84
25:DA:1670:C:OP1	61:DA:4090:HOH:O	1.93	0.84
1:CA:999:C:H42	1:CA:1042:G:H1	1.22	0.84
2:CB:18:GLY:HA2	2:CB:42:ILE:HG13	1.60	0.83
25:BA:2123:G:H1	25:BA:2210:C:N4	1.74	0.83
1:AA:664:G:H22	1:AA:741:G:H1	1.25	0.83
1:AA:1502:A:H2	1:AA:1505:G:H1	1.24	0.83
25:DA:2100:G:H1	25:DA:2189:U:H3	1.27	0.83
23:CW:7:A:N1	23:CW:66:U:O4	2.12	0.83
25:BA:1221:G:H1'	25:BA:1222:A:H5'	1.60	0.83
1:CA:953:G:H5'	1:CA:965:A:H61	1.43	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:CE:100:VAL:O	5:CE:107:ARG:NH2	2.12	0.82
25:DA:198:C:OP2	61:DA:4556:HOH:O	1.97	0.82
1:CA:1502:A:H2	1:CA:1505:G:H1	1.25	0.82
23:CY:50:U:H3	23:CY:64:A:N6	1.77	0.82
25:BA:325:G:OP2	44:BY:84:ARG:NH2	2.13	0.82
39:DT:65:LYS:HE2	39:DT:67:SER:HB2	1.61	0.82
23:AW:6:G:H1	23:AW:67:C:H42	1.27	0.82
1:AA:72:C:N4	1:AA:97:G:H1	1.76	0.82
25:DA:962:G:OP1	61:DA:4554:HOH:O	1.98	0.82
1:CA:975:A:H4'	1:CA:976:G:H5''	1.62	0.82
25:DA:1689:A:H62	25:DA:1698:A:H2	1.23	0.82
43:DX:31:HIS:HD2	43:DX:33:LYS:H	1.25	0.82
48:B2:22:GLU:OE2	48:B2:68:ARG:NH2	2.13	0.82
23:AY:49:C:N3	23:AY:65:G:N2	2.28	0.81
23:AY:7:A:N6	23:AY:66:U:H3	1.76	0.81
3:AC:40:ARG:NH2	3:AC:55:VAL:O	2.13	0.81
25:BA:739:C:O2'	27:BD:38:LYS:NZ	2.14	0.81
25:BA:1378:G:OP1	61:BA:4738:HOH:O	1.98	0.81
44:BY:92:ASN:HB3	44:BY:94:LYS:H	1.45	0.81
1:CA:1089:G:H1	1:CA:1096:C:H42	1.28	0.81
35:BP:98:GLU:OE1	35:BP:102:ARG:NH1	2.12	0.81
25:BA:1577:C:O2'	25:BA:1578:C:O5'	1.98	0.81
23:AW:19:G:H1	23:AW:56:C:H42	1.25	0.81
32:BI:92:VAL:HG13	32:BI:120:ILE:HB	1.60	0.81
25:DA:2807:G:N1	25:DA:2893:G:O6	2.13	0.81
27:BD:17:THR:O	27:BD:211:ARG:NH2	2.13	0.81
10:CJ:32:ALA:HB1	10:CJ:33:GLN:HA	1.61	0.81
27:BD:180:GLY:HA3	27:BD:275:LYS:HG3	1.61	0.81
1:AA:1422:G:H5''	34:BO:48:PRO:HB3	1.61	0.81
36:DQ:27:VAL:O	36:DQ:29:PHE:N	2.13	0.81
25:DA:994:C:OP1	40:DU:53:ARG:NH2	2.12	0.80
46:D0:10:THR:HG22	46:D0:12:ASN:H	1.44	0.80
25:DA:2683:C:O2	34:DO:70:LYS:NZ	2.15	0.80
25:DA:2683:C:OP1	39:DT:53:ARG:NH2	2.13	0.80
20:CT:10:LEU:HB3	20:CT:12:ALA:H	1.44	0.80
25:DA:2162:G:H4'	25:DA:2172:U:H2'	1.63	0.80
1:CA:26:A:N6	1:CA:558:G:O2'	2.14	0.80
25:DA:2148:G:H2'	25:DA:2149:G:H8	1.44	0.80
25:BA:2158:C:N3	25:BA:2177:G:N2	2.28	0.80
61:BA:5365:HOH:O	37:BR:3:HIS:NE2	2.15	0.80
1:CA:670:G:OP2	57:CA:3173:NEG:N2	2.14	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:999:C:N3	1:AA:1042:G:N2	2.28	0.80
43:BX:31:HIS:CD2	43:BX:33:LYS:H	1.98	0.80
1:CA:559:A:OP1	5:CE:126:ARG:NH2	2.15	0.80
25:DA:568:U:O4	61:DA:4175:HOH:O	1.99	0.79
1:AA:677:U:H3	1:AA:713:G:H22	1.29	0.79
25:BA:2146:G:N2	25:BA:2196:C:N3	2.28	0.79
45:BZ:72:ARG:NH2	45:BZ:97:GLU:O	2.15	0.79
25:DA:948:G:OP1	61:DA:4554:HOH:O	2.01	0.79
25:BA:1249:A:H2	25:BA:1287:A:H62	1.28	0.79
51:D5:16:ARG:NH1	51:D5:17:ASP:OD1	2.16	0.79
23:AY:50:U:O4	23:AY:64:A:N1	2.15	0.79
1:AA:1086:U:H3	1:AA:1099:G:H22	1.30	0.79
1:CA:1162:C:N4	1:CA:1174:G:H1	1.78	0.79
25:DA:2287:A:H62	25:DA:2344:U:H3	1.28	0.79
43:BX:35:THR:HG22	43:BX:38:GLU:H	1.48	0.79
1:AA:1189:C:OP1	10:AJ:51:ARG:NH2	2.15	0.79
1:CA:1166:G:N2	1:CA:1170:A:OP2	2.16	0.79
29:DF:185:ASP:HA	29:DF:188:ARG:HD3	1.64	0.79
25:BA:431:C:H4'	25:BA:432:U:H5'	1.65	0.79
3:CC:179:ARG:NH1	3:CC:206:GLU:OE1	2.16	0.78
25:DA:1019:U:H3	25:DA:1142(A):A:H62	1.30	0.78
25:DA:2789:C:O2	25:DA:2894:G:N1	2.15	0.78
27:BD:71:ASP:HB3	27:BD:103:ARG:HH22	1.46	0.78
23:AY:25:C:O2'	23:AY:26:A:O5'	2.00	0.78
25:DA:1147:C:H2'	25:DA:1148:A:H8	1.49	0.78
25:DA:847:U:O4	25:DA:933:A:N6	2.17	0.78
2:CB:187:LEU:HA	2:CB:201:ILE:HB	1.65	0.78
25:DA:831:G:O2'	35:DP:38:GLN:NE2	2.17	0.78
23:CY:51:U:H3	23:CY:63:G:H1	1.32	0.78
23:AY:26:A:N1	23:AY:44:G:N2	2.29	0.78
2:AB:15:VAL:O	2:AB:16:HIS:ND1	2.17	0.78
25:BA:2164:C:N3	25:BA:2171:G:O6	2.17	0.78
2:AB:201:ILE:HG21	2:AB:214:ILE:HG21	1.65	0.78
23:AW:19:G:N2	23:AW:56:C:N3	2.32	0.78
25:DA:2805:G:H2'	25:DA:2807:G:C8	2.18	0.78
42:BW:14:PRO:HG2	42:BW:78:GLU:HG2	1.65	0.78
38:BS:25:ARG:NH1	38:BS:42:ASP:OD1	2.16	0.77
13:CM:58:GLU:O	13:CM:62:ASN:ND2	2.17	0.77
25:BA:1361:C:OP2	61:BA:4738:HOH:O	2.01	0.77
1:AA:427:U:OP1	4:AD:13:ARG:NH2	2.17	0.77
1:CA:922:G:H4'	5:CE:20:GLN:HA	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AG:50:ILE:HD11	7:AG:58:PRO:HA	1.66	0.77
1:AA:316:G:OP2	1:AA:351:G:O2'	2.03	0.77
1:AA:1028:C:N4	1:AA:1033:G:H1	1.80	0.77
25:BA:2158:C:N4	25:BA:2177:G:N1	2.30	0.77
25:BA:297:C:O2	25:BA:387:G:N2	2.18	0.77
1:AA:310:G:OP2	16:AP:27:LYS:NZ	2.15	0.77
52:D6:10:LEU:HG	52:D6:54:ILE:HG13	1.66	0.77
1:AA:1007:C:N3	1:AA:1022:G:O6	2.16	0.77
25:BA:1313:U:OP1	61:BA:5106:HOH:O	2.02	0.77
25:DA:1783:A:OP1	61:DA:4494:HOH:O	2.02	0.77
25:BA:2188:G:N7	25:BA:2190:G:N2	2.33	0.77
1:CA:742:G:OP2	15:CO:35:ARG:NH2	2.17	0.77
1:AA:1183:A:H3'	1:AA:1184:G:H5''	1.67	0.77
2:AB:18:GLY:HA2	2:AB:42:ILE:HG13	1.67	0.76
25:DA:2355:C:H1'	46:D0:39:ARG:HH21	1.49	0.76
5:CE:33:VAL:HG21	5:CE:109:ILE:HA	1.65	0.76
30:BG:161:THR:HG22	30:BG:163:ALA:H	1.49	0.76
8:CH:69:ARG:NH2	8:CH:75:ARG:O	2.19	0.76
25:BA:1500:A:OP2	61:BA:4166:HOH:O	2.03	0.76
20:AT:10:LEU:HB3	20:AT:12:ALA:H	1.50	0.76
23:AW:67:C:O2'	23:AW:68:C:O4'	2.03	0.76
25:DA:792:G:O6	61:DA:4447:HOH:O	2.03	0.76
1:CA:1075:C:OP1	2:CB:179:LYS:NZ	2.19	0.76
36:BQ:21:THR:HG21	36:BQ:101:ARG:HD3	1.66	0.76
26:BB:8:U:O3'	38:BS:25:ARG:NH2	2.18	0.76
25:DA:1171:G:N2	25:DA:1178:C:N3	2.34	0.76
25:BA:2831:A:OP2	61:BA:5365:HOH:O	2.04	0.76
25:BA:1001:G:OP2	36:BQ:14:ARG:NH2	2.18	0.76
34:BO:35:VAL:HG11	34:BO:103:ALA:HB3	1.66	0.76
25:DA:631:A:OP1	35:DP:65:ARG:NH1	2.18	0.76
1:AA:78:G:H1	1:AA:91:C:N4	1.83	0.76
2:CB:178:ARG:HE	8:CH:74:PRO:HG3	1.50	0.76
13:AM:121:LYS:HE3	13:AM:121:LYS:H	1.50	0.76
45:DZ:72:ARG:NH2	45:DZ:97:GLU:O	2.18	0.76
7:CG:113:GLU:HG2	7:CG:119:ARG:HG2	1.68	0.76
25:DA:2142:C:N3	25:DA:2149:G:O6	2.18	0.76
2:CB:185:ILE:HG22	2:CB:199:TYR:HB2	1.66	0.76
23:CY:19:G:N2	23:CY:56:C:N3	2.28	0.76
23:AW:29:G:H1	23:AW:41:C:N4	1.83	0.76
11:AK:20:TYR:HB2	11:AK:31:THR:HG23	1.68	0.76
5:CE:102:ALA:HB1	5:CE:106:PRO:HG2	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:664:G:H22	1:CA:741:G:H1	1.34	0.75
1:AA:1029:C:O2	1:AA:1032:G:N1	2.19	0.75
25:BA:1189:A:OP2	61:BA:5287:HOH:O	2.04	0.75
1:AA:167:G:H2'	1:AA:168:G:H8	1.50	0.75
1:CA:522:C:H41	12:CL:53:ARG:HH22	1.30	0.75
1:AA:189(D):C:O2	1:AA:189(H):G:N1	2.19	0.75
1:CA:1004:A:N7	1:CA:1037:C:H2'	2.01	0.75
40:DU:76:TYR:OH	40:DU:92:ARG:NH1	2.20	0.75
1:AA:339:C:OP2	34:BO:97:ARG:NH1	2.20	0.75
25:DA:587:C:OP2	35:DP:21:ARG:NH2	2.18	0.75
1:CA:1083:U:OP2	61:CA:4096:HOH:O	2.04	0.75
2:CB:80:ILE:HD11	2:CB:212:GLN:HA	1.68	0.75
25:DA:1958:C:OP2	61:DA:4662:HOH:O	2.05	0.75
1:AA:1007:C:O2	1:AA:1022:G:N1	2.20	0.75
7:CG:111:ARG:NH1	7:CG:113:GLU:OE2	2.19	0.75
1:AA:347:G:O2'	1:AA:348:G:OP1	2.04	0.75
1:CA:677:U:H3	1:CA:713:G:H22	1.34	0.75
57:CA:3174:NEG:H72	25:DA:1945:G:OP1	1.86	0.75
25:BA:787:U:OP2	61:BA:4795:HOH:O	2.05	0.75
1:CA:1026:G:H5'	1:CA:1027:C:O5'	1.87	0.74
25:DA:1171:G:H1	25:DA:1178:C:H42	1.35	0.74
1:AA:1008:C:N3	1:AA:1021:G:O6	2.19	0.74
3:AC:15:THR:HG21	3:AC:181:ASN:HA	1.69	0.74
25:BA:388:A:H2'	25:BA:389:G:H8	1.51	0.74
13:CM:37:THR:O	13:CM:55:ARG:NH1	2.16	0.74
57:CA:3175:NEG:H72	25:DA:739:G:H1	1.52	0.74
12:CL:24:VAL:HG11	12:CL:27:LEU:HD22	1.70	0.74
57:AX:3013:NEG:N2	25:BA:2334:A:OP2	2.20	0.74
40:BU:76:TYR:OH	40:BU:92:ARG:NH1	2.20	0.74
25:DA:143:G:H4'	43:DX:35:THR:HG21	1.69	0.74
5:AE:33:VAL:HG21	5:AE:109:ILE:HA	1.70	0.74
47:D1:51:VAL:HG11	47:D1:74:VAL:HG21	1.70	0.74
43:DX:31:HIS:CD2	43:DX:33:LYS:H	2.05	0.74
1:AA:1348:U:H4'	9:AI:120:ARG:HD2	1.68	0.74
19:CS:50:ALA:HB1	19:CS:57:HIS:HB3	1.68	0.74
25:DA:2246:G:N7	61:DA:4073:HOH:O	2.21	0.74
25:BA:2169:G:H3'	25:BA:2170:G:H5''	1.67	0.74
1:AA:654:G:OP2	61:AA:4213:HOH:O	2.06	0.74
25:BA:30:G:OP2	40:BU:5:LYS:NZ	2.20	0.74
25:DA:309:G:N3	25:DA:329:G:O2'	2.19	0.74
25:DA:195:A:N7	61:DA:4556:HOH:O	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:CT:43:LEU:O	20:CT:47:GLY:N	2.21	0.73
45:BZ:151:HIS:O	45:BZ:153:SER:N	2.19	0.73
1:AA:345:C:OP2	39:BT:39:ARG:NH2	2.20	0.73
24:CX:21:A:H61	24:CX:46:G:H2'	1.50	0.73
25:DA:1762:A:N1	61:DA:4559:HOH:O	2.20	0.73
25:DA:2615:U:OP1	61:DA:4297:HOH:O	2.04	0.73
1:CA:1002:G:N2	1:CA:1038:C:N3	2.31	0.73
29:BF:185:ASP:OD1	29:BF:188:ARG:NH1	2.20	0.73
28:DE:72:VAL:HA	28:DE:73:GLU:HB3	1.69	0.73
1:AA:522:C:H41	12:AL:53:ARG:HH22	1.34	0.73
25:DA:323:G:HO2'	25:DA:1205:U:H3	1.35	0.73
38:DS:50:SER:O	38:DS:76:LYS:NZ	2.21	0.73
3:CC:34:LEU:HG	3:CC:38:ARG:HH12	1.53	0.73
25:DA:2143:C:H42	25:DA:2148:G:H1	1.34	0.73
2:AB:16:HIS:O	2:AB:18:GLY:N	2.21	0.73
25:DA:1271:G:OP2	61:DA:4489:HOH:O	2.06	0.73
42:BW:31:GLU:OE1	61:BW:4001:HOH:O	2.07	0.73
1:CA:1256:A:OP2	3:CC:26:LYS:NZ	2.21	0.73
23:CW:74:C:N4	25:DA:2507:C:O2'	2.21	0.73
25:DA:1310:G:OP2	53:D7:9:ARG:NH1	2.18	0.73
10:AJ:7:LYS:HG3	10:AJ:71:LEU:HD13	1.68	0.73
25:BA:2832:G:OP2	61:BA:5365:HOH:O	2.05	0.73
25:BA:692:C:N4	25:BA:698:G:O6	2.18	0.73
39:DT:16:ARG:NH1	39:DT:18:ASP:OD1	2.21	0.73
25:DA:2138:C:N4	25:DA:2153:G:H1	1.87	0.73
23:CY:43:C:H2'	23:CY:44:G:C8	2.23	0.73
27:BD:2:ALA:N	27:BD:20:ASP:OD2	2.21	0.73
19:AS:9:VAL:HG21	50:B4:61:ARG:HH12	1.53	0.73
1:AA:998:G:H1	1:AA:1043:C:N4	1.87	0.72
1:AA:266:G:H5''	1:AA:268:C:H41	1.54	0.72
45:BZ:117:LEU:HD11	45:BZ:144:LEU:HB3	1.70	0.72
1:CA:345:C:OP2	39:DT:39:ARG:NH2	2.22	0.72
25:DA:271(L):U:OP1	32:DI:50:ARG:NH2	2.23	0.72
2:CB:69:LEU:HB3	2:CB:162:ILE:HG22	1.69	0.72
28:BE:111:ARG:HG3	28:BE:160:TYR:CD2	2.23	0.72
23:CW:18:G:O2'	23:CW:57:G:N2	2.22	0.72
5:CE:122:GLU:O	5:CE:126:ARG:NH1	2.21	0.72
25:BA:139:A:H8	25:BA:1454:C:HO2'	1.38	0.72
25:DA:1971:A:OP2	27:DD:242:ARG:NH2	2.22	0.72
26:DB:15:A:OP2	26:DB:69:G:N2	2.21	0.72
23:AY:19:G:N2	23:AY:56:C:N3	2.33	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:953:G:H5'	1:AA:965:A:N6	2.05	0.72
25:DA:1937:A:OP1	61:DA:4724:HOH:O	2.07	0.72
25:DA:527:C:OP1	61:DA:4468:HOH:O	2.07	0.72
1:CA:1279:A:O2'	1:CA:1281:U:OP2	2.04	0.72
23:CY:76:A:H62	25:DA:2422:A:H5'	1.55	0.72
25:BA:303:C:H42	25:BA:385:G:H1	1.35	0.72
9:AI:16:ARG:HB2	9:AI:64:THR:HG22	1.71	0.72
25:BA:1044:C:OP1	61:BA:4747:HOH:O	2.06	0.72
25:DA:971:C:OP2	61:DA:4840:HOH:O	2.06	0.72
2:CB:30:ARG:HH21	2:CB:194:PRO:HB2	1.55	0.72
25:BA:1094:A:OP2	25:BA:1155:C:N4	2.18	0.72
25:DA:271(W):G:N7	61:DA:4937:HOH:O	2.23	0.72
4:CD:157:LEU:O	4:CD:161:ASN:ND2	2.23	0.72
25:DA:848:G:H2'	25:DA:849:A:C8	2.25	0.71
13:CM:23:TYR:HB3	13:CM:67:GLU:HA	1.72	0.71
23:AY:19:G:H1	23:AY:56:C:N4	1.88	0.71
29:DF:21:ALA:HB3	29:DF:22:ALA:HA	1.72	0.71
57:AA:3216:NEG:H11	57:AA:3216:NEG:HN42	1.55	0.71
1:CA:1125:U:O2'	1:CA:1126:U:H2'	1.89	0.71
25:DA:2589:A:OP1	61:DA:4444:HOH:O	2.08	0.71
1:CA:771:G:N7	61:CA:4043:HOH:O	2.22	0.71
1:CA:377:G:OP1	16:CP:3:LYS:HD2	1.91	0.71
1:CA:1157:A:H5'	1:CA:1158:C:C6	2.24	0.71
49:D3:8:LEU:HD13	49:D3:31:LEU:HD23	1.72	0.71
1:CA:1118:C:OP1	9:CI:104:ARG:NH1	2.23	0.71
25:DA:2308:G:O6	25:DA:2311:A:N6	2.20	0.71
1:AA:1064:G:N2	1:AA:1190:G:O2'	2.23	0.71
1:AA:1025:U:O2	1:AA:1036:G:O6	2.08	0.71
41:BV:95:LEU:HD13	41:BV:97:LYS:HD3	1.72	0.71
23:CW:2:C:N3	23:CW:71:G:O6	2.23	0.71
25:DA:2057:A:OP2	61:DA:4194:HOH:O	2.07	0.71
25:DA:2819:G:N7	61:DA:4367:HOH:O	2.23	0.71
25:BA:1740:U:O2'	27:BD:14:ARG:NH2	2.24	0.71
25:DA:2832:U:OP2	61:DA:4429:HOH:O	2.09	0.71
25:DA:2805:G:H2'	25:DA:2807:G:H8	1.54	0.71
6:CF:81:ILE:HD11	27:DD:125:ILE:HB	1.71	0.71
36:DQ:111:GLU:OE2	36:DQ:133:ARG:NH2	2.21	0.71
25:DA:2425:A:H4'	25:DA:2426:A:H5''	1.71	0.71
7:AG:111:ARG:NH1	7:AG:113:GLU:OE2	2.24	0.71
25:BA:2163:G:N7	25:BA:2173:G:N3	2.37	0.71
41:DV:40:LEU:HB2	41:DV:46:VAL:HG13	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:953:G:H5'	1:CA:965:A:N6	2.05	0.70
28:BE:105:THR:OG1	28:BE:199:ARG:NH2	2.24	0.70
2:AB:178:ARG:HH21	8:AH:74:PRO:HB3	1.55	0.70
25:DA:1816:G:O6	27:DD:35:LYS:NZ	2.22	0.70
25:BA:232:U:OP1	54:B8:6:THR:OG1	2.09	0.70
13:AM:84:ILE:HG13	13:AM:85:GLY:HA2	1.71	0.70
25:DA:2169:A:H2'	25:DA:2170:A:C8	2.26	0.70
25:DA:1153:C:OP1	40:DU:92:ARG:NH1	2.20	0.70
30:DG:161:THR:HG22	30:DG:163:ALA:H	1.57	0.70
2:CB:88:ALA:HB2	2:CB:219:VAL:HG13	1.71	0.70
25:BA:1814:A:N7	61:BA:5073:HOH:O	2.25	0.70
25:DA:2141:G:O6	25:DA:2150:U:O2	2.08	0.70
12:AL:24:VAL:HG11	12:AL:27:LEU:HD22	1.74	0.70
1:AA:1353:G:OP1	21:AU:10:ARG:NH1	2.18	0.70
25:DA:2139:C:N4	25:DA:2152:G:H1	1.88	0.70
23:CY:50:U:H3	23:CY:64:A:H61	1.37	0.70
1:AA:1182:G:H4'	1:AA:1183:A:H5'	1.71	0.70
1:AA:166:G:H2'	1:AA:167:G:H8	1.56	0.70
25:DA:783:A:OP2	61:DA:4444:HOH:O	2.10	0.70
52:B6:10:LEU:HG	52:B6:54:ILE:HG13	1.71	0.70
1:CA:14:U:OP2	61:CA:4074:HOH:O	2.09	0.70
1:AA:1456:G:O3'	20:AT:39:LYS:NZ	2.25	0.70
25:DA:2148:G:H2'	25:DA:2149:G:C8	2.27	0.70
1:CA:673:G:H2'	1:CA:674:G:C8	2.27	0.70
1:AA:1414:U:H3	1:AA:1486:G:H1	1.39	0.70
47:B1:85:LEU:HD22	47:B1:89:GLU:HG3	1.73	0.70
25:BA:2128:G:H1	25:BA:2205:C:N4	1.89	0.70
1:AA:1030(A):G:O2'	1:AA:1030(C):G:N7	2.24	0.70
1:AA:839:U:H3'	1:AA:840:C:H6	1.56	0.70
29:DF:53:THR:HG22	29:DF:56:GLU:HG3	1.72	0.70
1:AA:1320:C:O2	19:AS:36:ARG:NH2	2.25	0.70
25:DA:572:A:OP2	41:DV:78:LYS:NZ	2.24	0.70
45:DZ:117:LEU:HA	45:DZ:174:VAL:HA	1.71	0.70
1:AA:1003:G:H2'	1:AA:1004:A:H4'	1.73	0.70
2:CB:158:LEU:HD23	2:CB:182:ILE:HD11	1.74	0.70
25:BA:778:C:OP2	61:BA:4877:HOH:O	2.10	0.70
25:BA:591:U:O4	61:BA:4289:HOH:O	2.06	0.70
1:CA:1004:A:H8	1:CA:1005:A:H4'	1.56	0.69
25:DA:2124:G:N2	25:DA:2174:C:N3	2.39	0.69
47:B1:86:SER:OG	47:B1:89:GLU:OE1	2.08	0.69
1:CA:1278:U:H5'	1:CA:1279:A:O4'	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:AS:50:ALA:HB1	19:AS:57:HIS:HB3	1.72	0.69
25:DA:2317:C:N4	25:DA:2318:G:O6	2.25	0.69
15:CO:70:LEU:HD11	15:CO:77:ARG:HB2	1.73	0.69
25:BA:610:C:OP2	35:BP:21:ARG:NH2	2.25	0.69
25:BA:327:U:O4	61:BA:4758:HOH:O	2.07	0.69
2:CB:87:ARG:NH2	2:CB:220:ASP:OD1	2.26	0.69
25:DA:2120:G:H2'	25:DA:2121:G:H8	1.57	0.69
1:AA:353:A:H5'	1:AA:353:A:H8	1.57	0.69
1:AA:1005:A:H1'	1:AA:1036:G:H22	1.55	0.69
10:AJ:5:ARG:HD3	10:AJ:71:LEU:HD11	1.73	0.69
27:DD:71:ASP:HB3	27:DD:103:ARG:HH22	1.57	0.69
23:CY:62:C:H2'	23:CY:63:G:H8	1.58	0.69
1:CA:1029:C:N4	1:CA:1032:G:N1	2.41	0.69
10:CJ:74:ILE:HD11	10:CJ:81:THR:HG21	1.75	0.69
49:B3:3:ARG:NH1	49:B3:60:GLU:OE2	2.23	0.69
28:DE:47:VAL:HG11	28:DE:86:PRO:HD2	1.72	0.69
23:AW:19:G:H1	23:AW:56:C:N4	1.91	0.69
25:BA:1604:C:OP2	25:BA:1605:A:O2'	2.10	0.69
16:AP:53:VAL:HG13	16:AP:79:VAL:HG22	1.75	0.69
25:BA:934:A:O2'	25:BA:935:C:OP2	2.10	0.69
1:AA:109:A:N1	61:AA:4202:HOH:O	2.25	0.69
1:CA:1119:C:H42	1:CA:1154:G:H1	1.41	0.69
1:CA:839:U:H5''	1:CA:840:C:H5	1.57	0.69
25:DA:1798:U:OP2	27:DD:274:ARG:NH2	2.26	0.69
29:DF:101:LEU:O	29:DF:106:ARG:NH1	2.26	0.69
46:D0:2:ALA:N	61:D0:204:HOH:O	2.26	0.69
39:DT:64:ARG:HB2	39:DT:73:GLU:HG2	1.75	0.69
57:AA:3221:NEG:H71	25:BA:786:G:N1	2.05	0.68
25:BA:709:G:H5''	35:BP:16:ARG:HG2	1.74	0.68
45:DZ:111:VAL:HG21	45:DZ:117:LEU:HB2	1.75	0.68
10:CJ:17:ASP:OD1	10:CJ:70:ARG:NH1	2.25	0.68
25:BA:2320:G:O6	25:BA:2323:A:N6	2.18	0.68
25:DA:11:G:H2'	25:DA:12:U:H5''	1.75	0.68
25:BA:2649:U:H5''	28:BE:82:ARG:HH21	1.58	0.68
1:AA:1191:A:OP1	3:AC:4:LYS:NZ	2.25	0.68
45:DZ:144:LEU:HD22	45:DZ:174:VAL:HG23	1.73	0.68
1:CA:1128:C:H1'	1:CA:1147:C:H42	1.56	0.68
25:DA:468:G:N7	53:D7:39:ARG:NH2	2.41	0.68
30:DG:5:VAL:HG22	30:DG:8:LYS:H	1.57	0.68
25:DA:900:A:H2'	25:DA:901:A:H8	1.59	0.68
1:CA:656:C:O2'	15:CO:28:GLN:NE2	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:DS:84:GLN:H	38:DS:111:GLU:HB2	1.58	0.68
25:BA:2459:G:OP2	61:BA:4656:HOH:O	2.11	0.68
25:BA:650:G:N7	35:BP:107:LYS:NZ	2.41	0.68
25:BA:2460:A:OP1	61:BA:5152:HOH:O	2.11	0.68
1:AA:1124:G:N7	1:AA:1145:C:O2'	2.26	0.68
23:CY:21:A:H61	23:CY:46:7MG:H2'	1.59	0.68
1:CA:1305:G:H5'	21:CU:4:GLY:HA3	1.74	0.68
25:DA:1814:G:O3'	27:DD:54:ARG:NH2	2.27	0.68
1:AA:1029:C:N3	1:AA:1032:G:O6	2.27	0.68
1:AA:166:G:H2'	1:AA:167:G:C8	2.28	0.68
35:BP:116:GLY:O	35:BP:137:LYS:NZ	2.25	0.68
45:BZ:91:LEU:HD12	45:BZ:130:PRO:HG3	1.76	0.68
1:AA:656:C:O2'	15:AO:28:GLN:NE2	2.26	0.68
1:AA:1008:C:N3	1:AA:1021:G:C6	2.62	0.68
29:BF:185:ASP:HA	29:BF:188:ARG:HD3	1.75	0.68
7:AG:78:ARG:HH12	7:AG:79:ARG:HD2	1.58	0.68
25:DA:2049:G:N7	61:DA:4134:HOH:O	2.25	0.68
1:CA:1314:C:OP2	19:CS:4:SER:OG	2.09	0.68
1:AA:1036:G:H21	1:AA:1037:C:H1'	1.59	0.68
9:CI:9:ARG:HG2	9:CI:14:VAL:HG12	1.74	0.68
1:AA:596:C:OP2	61:AA:4080:HOH:O	2.12	0.68
31:DH:46:GLU:HB2	31:DH:49:VAL:HG12	1.75	0.68
25:DA:1721:G:N1	25:DA:1739:U:OP2	2.27	0.68
27:BD:69:ARG:NH2	27:BD:128:GLY:O	2.27	0.68
25:DA:2430:A:OP2	61:DA:4563:HOH:O	2.12	0.68
23:CY:76:A:N6	25:DA:2422:A:H5'	2.09	0.68
25:DA:1030:G:OP2	36:DQ:128:LYS:NZ	2.27	0.68
55:D9:25:VAL:HB	55:D9:34:GLN:HB2	1.76	0.68
25:DA:248:G:OP1	61:DA:4656:HOH:O	2.12	0.68
2:AB:178:ARG:HH22	8:AH:68:ARG:HH12	1.39	0.67
28:BE:127:ASP:OD2	61:BE:401:HOH:O	2.11	0.67
25:BA:1170:C:OP1	61:BA:4982:HOH:O	2.11	0.67
25:DA:607:U:OP1	29:DF:102:PRO:HA	1.94	0.67
9:CI:53:VAL:O	9:CI:55:ALA:N	2.27	0.67
1:CA:532:A:O2'	1:CA:533:A:OP1	2.12	0.67
1:AA:1008:C:C4	1:AA:1021:G:O6	2.47	0.67
25:BA:354:A:H2	25:BA:1255:A:HO2'	1.42	0.67
26:DB:54:G:H21	30:DG:29:TRP:HE1	1.41	0.67
27:DD:148:GLU:HB2	27:DD:151:LYS:HD2	1.76	0.67
1:CA:316:G:OP2	1:CA:351:G:O2'	2.13	0.67
1:AA:1026:G:H3'	1:AA:1027:C:H6	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2291:G:N7	46:B0:14:ARG:NH1	2.41	0.67
25:DA:1031:G:H21	55:D9:36:GLN:HE22	1.42	0.67
37:DR:56:LYS:NZ	37:DR:90:ARG:O	2.27	0.67
1:CA:999:C:N4	1:CA:1042:G:H1	1.92	0.67
39:BT:39:ARG:HH12	39:BT:41:ARG:HD3	1.59	0.67
1:AA:1320:C:H5'	19:AS:70:LYS:HG3	1.76	0.67
25:DA:1237:A:OP1	61:DA:4737:HOH:O	2.10	0.67
25:BA:932:C:H3'	25:BA:933:C:H5''	1.76	0.67
25:BA:1480:A:H61	25:BA:1605:A:H62	1.40	0.67
25:DA:2836:U:H2'	25:DA:2837:G:C8	2.30	0.67
25:DA:2584:U:H2'	25:DA:2585:U:H2'	1.77	0.67
29:BF:157:VAL:HB	29:BF:194:MET:HG2	1.75	0.67
29:DF:24:LEU:HD23	29:DF:115:ALA:HA	1.76	0.67
1:AA:1183:A:O2'	1:AA:1184:G:OP1	2.11	0.67
29:DF:64:ILE:HG21	29:DF:78:ILE:HG23	1.77	0.67
11:AK:79:SER:HA	11:AK:104:GLN:HB2	1.77	0.67
1:AA:1305:G:N2	1:AA:1331:G:H1'	2.10	0.67
25:DA:832:G:OP1	61:DA:4546:HOH:O	2.12	0.67
25:BA:2252:C:OP2	61:BA:4455:HOH:O	2.11	0.67
1:CA:1417:G:O6	61:CA:4052:HOH:O	2.11	0.67
1:CA:1089:G:H1	1:CA:1096:C:N4	1.92	0.67
25:DA:1647:G:OP1	61:DA:4489:HOH:O	2.11	0.67
29:DF:157:VAL:HB	29:DF:194:MET:HG2	1.77	0.67
37:DR:36:THR:HG22	37:DR:37:THR:H	1.58	0.67
1:AA:1492:A:O2'	1:AA:1493:A:O5'	2.12	0.67
57:CX:3004:NEG:N1	25:DA:2330:G:N7	2.43	0.67
1:CA:1277:C:HO2'	1:CA:1279:A:H8	1.41	0.67
9:AI:53:VAL:O	9:AI:55:ALA:N	2.28	0.67
25:DA:1183:G:H5''	49:D3:30:ARG:HH12	1.60	0.67
31:BH:86:GLU:OE2	31:BH:132:ARG:NH2	2.28	0.67
25:DA:2518:A:OP2	61:DA:4293:HOH:O	2.13	0.67
2:CB:78:GLN:NE2	2:CB:95:GLN:OE1	2.28	0.67
25:DA:2530:A:OP2	25:DA:2535:G:N2	2.28	0.67
25:DA:2472:G:H2'	25:DA:2475:C:H42	1.60	0.67
25:DA:361:G:H21	25:DA:362:U:H3	1.43	0.67
25:DA:2327:A:H2'	25:DA:2328:A:C8	2.30	0.67
25:BA:1067:A:H8	25:BA:1068:G:H5''	1.58	0.67
25:DA:2867:G:OP2	39:DT:119:LYS:NZ	2.27	0.67
25:BA:2307:C:OP1	38:BS:10:ARG:NH1	2.28	0.67
25:DA:2318:G:N2	38:DS:3:ARG:HH12	1.93	0.66
10:CJ:11:PHE:HE1	10:CJ:67:THR:HG22	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:653:A:OP1	8:AH:56:LYS:NZ	2.28	0.66
25:DA:1266:G:O5'	42:DW:15:ARG:NH2	2.28	0.66
7:AG:27:ILE:HD12	7:AG:40:ALA:HA	1.77	0.66
18:AR:32:ARG:HA	18:AR:69:THR:HG21	1.76	0.66
25:DA:1022:G:H22	25:DA:1142(A):A:H2	1.43	0.66
1:CA:1029:C:N3	1:CA:1032:G:N2	2.44	0.66
25:BA:2081:A:OP2	61:BA:4459:HOH:O	2.13	0.66
1:AA:993:G:O6	1:AA:1045:C:N4	2.28	0.66
25:BA:273:G:H4'	25:BA:274:U:OP1	1.94	0.66
25:DA:576:U:OP1	61:DA:4452:HOH:O	2.13	0.66
45:DZ:104:PHE:HA	45:DZ:139:VAL:HB	1.78	0.66
25:BA:542:C:OP1	51:B5:16:ARG:NH2	2.29	0.66
1:AA:347:G:H2'	1:AA:348:G:O4'	1.95	0.66
25:BA:2015:U:OP2	61:BA:5370:HOH:O	2.12	0.66
24:CX:64:G:O2'	36:DQ:10:ARG:NH2	2.28	0.66
1:CA:390:C:O3'	16:CP:28:ARG:NH2	2.27	0.66
37:DR:55:ALA:HB2	37:DR:79:LEU:HD13	1.76	0.66
29:DF:184:TYR:CE2	29:DF:188:ARG:HD2	2.31	0.66
25:DA:1508:A:H4'	25:DA:1509(A):A:C4	2.31	0.66
13:AM:3:ARG:HD2	13:AM:9:ILE:HG12	1.76	0.66
25:BA:2286:A:OP1	61:BA:5335:HOH:O	2.13	0.66
23:AW:10:G:N1	23:AW:25:C:O2	2.24	0.66
25:DA:1815:A:P	27:DD:54:ARG:HH22	2.18	0.66
3:AC:8:ILE:HG23	3:AC:16:ARG:HG2	1.78	0.66
2:AB:195:ASP:O	8:AH:68:ARG:NH2	2.28	0.66
25:BA:1065:U:HO2'	25:BA:1067:A:H2	1.42	0.66
1:CA:1129:C:H2'	1:CA:1139:G:N7	2.10	0.66
45:DZ:154:ASP:N	45:DZ:154:ASP:OD1	2.28	0.66
28:DE:73:GLU:HG3	28:DE:73:GLU:O	1.96	0.66
28:DE:36:ARG:HG2	28:DE:47:VAL:HG12	1.78	0.66
9:AI:50:LEU:HD13	9:AI:56:LEU:HA	1.78	0.66
25:DA:1796:U:H2'	25:DA:1797:C:C6	2.31	0.66
25:DA:223:A:O2'	25:DA:420:C:O2	2.13	0.66
28:BE:11:MET:HG2	28:BE:24:THR:HB	1.78	0.66
1:AA:1158:C:H5	1:AA:1181:G:N1	1.92	0.66
26:DB:13:A:N1	26:DB:69:G:O2'	2.25	0.66
7:AG:111:ARG:HD2	7:AG:123:GLU:HB2	1.78	0.66
25:BA:2299:A:H62	25:BA:2356:U:H3	1.42	0.66
36:DQ:1:MET:HG3	36:DQ:44:ALA:HB1	1.77	0.66
2:AB:63:MET:HB3	2:AB:225:ALA:HB1	1.78	0.66
32:DI:90:GLY:O	32:DI:121:LYS:NZ	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1229:A:OP2	13:CM:114:ARG:NH1	2.29	0.66
25:DA:304:G:O6	61:DA:4467:HOH:O	2.10	0.66
1:AA:346:G:OP1	39:BT:41:ARG:NH1	2.26	0.66
1:CA:35:G:O2'	12:CL:118:SER:O	2.13	0.66
1:AA:1118:C:H1'	1:AA:1179:A:C4	2.30	0.66
25:BA:2164:C:H2'	25:BA:2165:C:C6	2.31	0.65
57:AX:3013:NEG:O3	57:AX:3013:NEG:N4	2.29	0.65
5:AE:68:GLU:HG2	5:AE:70:PRO:HD3	1.78	0.65
13:CM:3:ARG:HA	50:D4:34:GLU:HG2	1.77	0.65
25:BA:185:A:H62	35:BP:38:GLN:HE22	1.44	0.65
25:DA:1190:G:H2'	25:DA:1191:G:H8	1.61	0.65
27:DD:67:PHE:HE1	27:DD:106:ILE:HD12	1.61	0.65
25:BA:2877:G:OP2	39:BT:119:LYS:NZ	2.27	0.65
9:AI:46:ALA:HB2	9:AI:74:ILE:HG23	1.77	0.65
1:CA:1309:G:O2'	13:CM:77:ASN:ND2	2.29	0.65
57:AW:3004:NEG:H91	25:BA:1965:U:H3'	1.77	0.65
7:CG:78:ARG:NH1	7:CG:154:TYR:O	2.29	0.65
25:BA:1424:A:OP1	53:B7:10:ARG:NH2	2.29	0.65
1:AA:742:G:OP2	15:AO:35:ARG:NH2	2.30	0.65
25:DA:71:A:N7	43:DX:31:HIS:HE1	1.94	0.65
25:DA:323:G:O2'	25:DA:1205:U:N3	2.25	0.65
27:DD:26:LYS:NZ	27:DD:30:GLU:OE1	2.30	0.65
26:BB:48:A:H4'	38:BS:95:HIS:HD2	1.61	0.65
13:CM:13:LYS:HA	13:CM:44:ARG:HH11	1.61	0.65
25:DA:857:C:OP2	46:D0:77:ARG:NH2	2.29	0.65
26:DB:66:A:H61	26:DB:109:C:H5'	1.61	0.65
1:CA:1521:G:N3	61:CA:4036:HOH:O	2.29	0.65
2:AB:69:LEU:HB3	2:AB:162:ILE:HG22	1.77	0.65
3:CC:142:MET:HG3	3:CC:170:GLN:HB3	1.78	0.65
25:DA:687:C:OP2	61:DA:4709:HOH:O	2.13	0.65
2:CB:24:TRP:CZ3	2:CB:26:PRO:HA	2.31	0.65
1:AA:922:G:H4'	5:AE:20:GLN:HA	1.78	0.65
25:DA:987:G:O2'	25:DA:1000:A:N3	2.25	0.65
25:DA:1300:U:H4'	25:DA:1301:A:H5''	1.78	0.65
1:CA:942:G:H21	9:CI:124:GLN:NE2	1.94	0.65
25:BA:70:A:N7	43:BX:31:HIS:HE1	1.94	0.65
24:CX:21:A:N6	24:CX:46:G:H2'	2.11	0.65
25:BA:1814:A:OP1	61:BA:4796:HOH:O	2.15	0.65
48:D2:16:LEU:O	48:D2:67:LYS:NZ	2.30	0.65
1:AA:96:U:H2'	1:AA:97:G:C8	2.32	0.65
25:DA:307:G:N2	25:DA:310:A:O5'	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:241:G:OP1	35:BP:50:ARG:NH1	2.29	0.65
44:BY:17:SER:OG	44:BY:71:LYS:NZ	2.28	0.65
10:AJ:17:ASP:OD1	10:AJ:70:ARG:NH1	2.30	0.65
45:DZ:92:SER:OG	45:DZ:93:ASP:N	2.29	0.65
54:D8:6:THR:HG22	54:D8:63:PRO:HD2	1.79	0.65
1:AA:1026:G:O6	1:AA:1034:G:N2	2.30	0.64
25:DA:144:C:H5'	43:DX:2:LYS:HE2	1.80	0.64
25:BA:743:G:N7	61:BA:4543:HOH:O	2.28	0.64
1:CA:405:U:O4	4:CD:2:GLY:N	2.31	0.64
27:BD:206:LEU:HD22	27:BD:211:ARG:HG2	1.79	0.64
57:CA:3173:NEG:H51	57:CA:3173:NEG:H11	1.78	0.64
10:AJ:16:LEU:HD21	10:AJ:70:ARG:HG2	1.79	0.64
16:CP:51:VAL:HG12	16:CP:53:VAL:H	1.62	0.64
25:BA:465:G:N7	61:BA:5330:HOH:O	2.29	0.64
25:BA:2121:U:H3	25:BA:2212:G:H1	1.44	0.64
1:AA:1132:C:H2'	1:AA:1133:G:H8	1.61	0.64
25:BA:2357:G:OP2	61:BA:4075:HOH:O	2.13	0.64
38:DS:15:ARG:O	38:DS:19:LYS:HG2	1.97	0.64
26:BB:87:G:N2	26:BB:90:A:OP2	2.28	0.64
36:BQ:18:LYS:O	36:BQ:98:LYS:NZ	2.25	0.64
3:AC:82:GLU:HG2	3:AC:85:ARG:HH21	1.60	0.64
10:CJ:78:ASN:O	10:CJ:80:LYS:N	2.30	0.64
45:DZ:24:LEU:HB2	45:DZ:41:LEU:HD23	1.80	0.64
27:BD:52:ARG:NH2	61:BD:411:HOH:O	2.30	0.64
25:BA:611:U:H2'	25:BA:612:C:C6	2.32	0.64
23:CY:7:A:H61	23:CY:66:U:H3	0.74	0.64
25:BA:1219:A:H4'	25:BA:1220:U:OP1	1.98	0.64
20:AT:9:ASN:O	20:AT:10:LEU:HB2	1.96	0.64
25:BA:1093:G:H2'	25:BA:1156:G:H22	1.63	0.64
29:DF:185:ASP:OD1	29:DF:188:ARG:NH1	2.30	0.64
1:AA:167:G:H2'	1:AA:168:G:C8	2.32	0.64
57:AA:3216:NEG:O1	61:AA:4240:HOH:O	2.13	0.64
27:DD:69:ARG:NH2	27:DD:128:GLY:O	2.31	0.64
50:D4:62:ARG:O	50:D4:64:GLY:N	2.30	0.64
2:AB:212:GLN:NE2	2:AB:234:PRO:O	2.30	0.64
5:CE:11:ILE:HB	5:CE:31:LEU:HB3	1.78	0.64
8:AH:29:SER:HB3	8:AH:32:LYS:HG3	1.78	0.64
13:CM:107:ALA:HB3	13:CM:111:LYS:HD2	1.79	0.64
4:AD:119:GLN:HG2	4:AD:123:HIS:CD2	2.33	0.64
25:DA:2123:G:N2	25:DA:2175:C:N3	2.42	0.64
1:AA:1002:G:H3'	1:AA:1003:G:C8	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:894:U:OP2	61:BA:4526:HOH:O	2.15	0.64
23:AY:2:C:H42	23:AY:71:G:H1	1.46	0.64
5:CE:92:LYS:HB3	5:CE:119:LEU:HB2	1.80	0.64
24:AX:21:A:H61	24:AX:46:G:H2'	1.63	0.64
9:AI:77:ILE:O	9:AI:81:ILE:HG22	1.98	0.64
25:DA:2031:A:N3	25:DA:2455:G:O2'	2.25	0.64
30:DG:39:ILE:HG12	30:DG:157:ILE:HG12	1.80	0.64
1:CA:538:G:H5''	12:CL:114:LYS:HB2	1.79	0.64
10:CJ:49:VAL:HG23	14:CN:41:ARG:HB2	1.80	0.64
25:DA:1159:U:H2'	25:DA:1160:G:H8	1.62	0.64
42:DW:18:ARG:NH1	42:DW:76:VAL:O	2.31	0.64
25:BA:2365:G:N7	61:BA:4567:HOH:O	2.30	0.64
25:BA:2149:G:H21	25:BA:2195:A:H1'	1.62	0.64
23:AW:10:G:O6	23:AW:25:C:N3	2.31	0.64
7:CG:113:GLU:HG3	7:CG:118:VAL:HG12	1.80	0.64
3:AC:12:LEU:HD23	3:AC:16:ARG:HB3	1.78	0.64
11:CK:98:LEU:O	11:CK:101:SER:OG	2.13	0.64
30:BG:108:ASN:HB3	50:B4:22:ILE:HD13	1.80	0.64
47:B1:51:VAL:HG11	47:B1:74:VAL:HG21	1.79	0.64
25:DA:1800:C:OP2	27:DD:183:ARG:NH2	2.30	0.64
1:CA:1132:C:H2'	1:CA:1133:G:H8	1.63	0.64
2:CB:96:ARG:HD2	2:CB:98:LEU:HD22	1.79	0.64
23:AW:7:A:N1	23:AW:66:U:O2	2.31	0.64
25:DA:1648:C:OP1	61:DA:4489:HOH:O	2.15	0.64
15:AO:39:LEU:HD13	15:AO:56:LEU:HB2	1.80	0.64
1:CA:1009:G:N2	1:CA:1021:G:H1'	2.13	0.64
25:BA:1189:A:OP1	33:BN:25:ARG:NH2	2.30	0.63
28:BE:47:VAL:HG21	28:BE:86:PRO:HD2	1.80	0.63
1:AA:1112:C:H1'	3:AC:179:ARG:HG2	1.80	0.63
27:DD:276:LYS:H	27:DD:276:LYS:HD3	1.61	0.63
32:DI:72:LEU:HA	32:DI:75:LEU:HD22	1.78	0.63
19:AS:27:GLU:HB3	19:AS:28:LYS:HB3	1.79	0.63
25:DA:2124:G:N1	25:DA:2174:C:N4	2.46	0.63
24:CX:47:U:H3'	24:CX:48:C:H5'	1.81	0.63
25:DA:811:U:O4	61:DA:4886:HOH:O	2.12	0.63
25:BA:671:A:H2'	25:BA:672:G:O4'	1.98	0.63
2:CB:47:THR:HA	2:CB:202:PRO:HG2	1.80	0.63
25:BA:2297:C:OP2	52:B6:6:ARG:NH1	2.29	0.63
50:B4:55:ARG:HB2	50:B4:56:VAL:O	1.99	0.63
5:AE:122:GLU:O	5:AE:126:ARG:NH1	2.31	0.63
23:CY:31:A:N1	23:CY:39:PSU:O2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:184:C:H2'	25:DA:185:U:C6	2.32	0.63
1:CA:1347:G:N2	1:CA:1373:G:H2'	2.14	0.63
20:AT:43:LEU:O	20:AT:47:GLY:N	2.31	0.63
19:AS:63:THR:OG1	19:AS:65:ASN:ND2	2.31	0.63
36:DQ:57:HIS:HD2	36:DQ:117:ALA:HB2	1.61	0.63
1:CA:148:G:H2'	1:CA:149:A:H8	1.63	0.63
25:DA:1149:G:H2'	25:DA:1150:C:C6	2.34	0.63
1:CA:1129:C:OP1	9:CI:16:ARG:NH1	2.31	0.63
53:D7:34:ARG:NH1	53:D7:41:ARG:O	2.31	0.63
25:DA:1470:G:N2	25:DA:1520:G:OP2	2.30	0.63
25:DA:1842:G:O2'	27:DD:253:GLN:NE2	2.31	0.63
2:CB:15:VAL:HG13	2:CB:209:ARG:HB3	1.81	0.63
1:AA:165:C:H2'	1:AA:166:G:C8	2.33	0.63
1:CA:1063:C:OP2	1:CA:1064:G:O2'	2.11	0.63
45:DZ:153:SER:HB3	45:DZ:167:PRO:HB3	1.79	0.63
61:CW:4001:HOH:O	25:DA:2602:A:N6	2.31	0.63
25:DA:2839:G:H5'	37:DR:46:GLY:HA2	1.80	0.63
25:DA:299:A:H5"	44:DY:86:ARG:HH21	1.64	0.63
25:BA:630:U:OP1	29:BF:102:PRO:HA	1.98	0.63
27:BD:148:GLU:HB2	27:BD:151:LYS:HD2	1.81	0.63
1:CA:1301:U:O2'	1:CA:1302:U:H5'	1.98	0.63
1:CA:1151:A:HO2'	1:CA:1152:A:H8	1.46	0.63
1:AA:511:C:OP2	4:AD:49:ARG:NH1	2.31	0.63
25:DA:2166:G:H3'	25:DA:2167:U:H5"	1.80	0.63
25:BA:1829:U:OP2	27:BD:274:ARG:NH2	2.29	0.63
25:BA:2210:C:H4'	25:BA:2210:C:OP1	1.97	0.63
7:AG:78:ARG:NH1	7:AG:79:ARG:HD2	2.14	0.63
1:CA:1292:U:OP2	7:CG:41:ARG:NH2	2.31	0.63
25:BA:1388:A:OP2	61:BA:4364:HOH:O	2.15	0.63
45:BZ:110:GLY:HA3	45:BZ:145:GLU:HA	1.81	0.63
2:CB:17:PHE:HB2	2:CB:44:LEU:HD11	1.79	0.63
25:DA:998:C:OP1	40:DU:92:ARG:NH2	2.32	0.63
20:AT:10:LEU:HD13	20:AT:12:ALA:HB2	1.81	0.63
1:AA:1292:U:OP2	7:AG:41:ARG:NH2	2.30	0.63
1:CA:920:U:H2'	1:CA:921:U:C6	2.33	0.63
35:DP:88:LEU:HD11	35:DP:114:ILE:HD12	1.80	0.63
45:BZ:92:SER:OG	45:BZ:93:ASP:N	2.32	0.63
25:BA:1039:G:OP1	40:BU:50:ARG:NH2	2.31	0.63
1:AA:26:A:O2'	4:AD:209:ARG:NH2	2.31	0.63
39:BT:95:ARG:HG2	39:BT:95:ARG:HH11	1.63	0.63
37:DR:97:VAL:HG22	37:DR:114:VAL:HG13	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1346:A:N1	1:CA:1374:A:H5''	2.14	0.63
42:DW:71:VAL:HA	42:DW:107:LEU:HD12	1.81	0.63
40:DU:49:HIS:HA	40:DU:52:ARG:HB3	1.81	0.63
50:D4:24:THR:OG1	50:D4:25:TYR:N	2.29	0.63
1:AA:1007:C:N3	1:AA:1022:G:C6	2.67	0.62
1:CA:1118:C:H1'	1:CA:1179:A:C5	2.34	0.62
25:DA:2357:U:OP1	46:D0:20:ARG:NH1	2.28	0.62
1:AA:70:G:H1	1:AA:99:U:H3	1.46	0.62
25:BA:2820:A:N6	25:BA:2900:G:O2'	2.31	0.62
23:AW:25:C:H2'	23:AW:26:A:H8	1.64	0.62
1:CA:1118:C:H2'	1:CA:1119:C:C6	2.34	0.62
25:DA:2472:G:N1	25:DA:2477:C:OP1	2.27	0.62
1:AA:59:A:N1	61:AA:4113:HOH:O	2.31	0.62
5:CE:143:ARG:NH1	8:CH:77:GLU:OE1	2.32	0.62
3:CC:52:LEU:HD21	3:CC:55:VAL:HG23	1.80	0.62
35:BP:16:ARG:NH1	61:BP:314:HOH:O	2.31	0.62
35:BP:50:ARG:HD3	54:B8:7:HIS:CD2	2.34	0.62
35:BP:63:PRO:HG2	54:B8:25:MET:HB2	1.82	0.62
1:AA:67:C:H2'	1:AA:68:G:C8	2.35	0.62
25:DA:2744:G:N2	31:DH:143:GLN:OE1	2.32	0.62
2:CB:45:GLN:HA	2:CB:48:MET:HE2	1.81	0.62
9:AI:17:VAL:HG23	9:AI:63:ILE:HG12	1.82	0.62
23:CY:25:C:H2'	23:CY:26:A:H8	1.62	0.62
23:AW:11:C:N3	23:AW:24:G:N2	2.41	0.62
23:CW:14:A:H61	23:CW:21:A:H2	1.48	0.62
25:DA:2297:C:O2	25:DA:2321:G:N2	2.33	0.62
5:AE:20:GLN:NE2	5:AE:21:ALA:O	2.32	0.62
1:CA:545:C:OP2	4:CD:65:ARG:NH2	2.31	0.62
25:BA:553:A:N1	25:BA:2064:A:H2'	2.15	0.62
1:CA:977:A:O2'	1:CA:981:U:N3	2.32	0.62
25:DA:1405:U:H2'	25:DA:1406:U:C6	2.34	0.62
1:AA:141:A:H1'	1:AA:182:U:O2	2.00	0.62
2:CB:74:LYS:HG3	2:CB:77:ALA:HB3	1.81	0.62
26:BB:13:A:N1	26:BB:69:G:O2'	2.31	0.62
3:AC:116:VAL:HG21	3:AC:202:ILE:HD11	1.81	0.62
44:DY:16:ALA:HB2	44:DY:73:ARG:HG3	1.82	0.62
1:AA:1173:G:H2'	1:AA:1174:G:H8	1.64	0.62
7:AG:113:GLU:HG2	7:AG:119:ARG:HG2	1.81	0.62
27:DD:132:PRO:HD3	27:DD:190:TYR:CZ	2.34	0.62
61:BA:5296:HOH:O	38:BS:3:ARG:HG2	1.99	0.62
25:BA:536:U:OP2	61:BA:4902:HOH:O	2.16	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:2506:U:OP1	28:DE:144:ARG:NH2	2.33	0.62
25:DA:1996:C:H4'	25:DA:1997:G:OP1	2.00	0.62
9:AI:49:PRO:HG3	9:AI:101:PHE:HD2	1.63	0.62
1:CA:411:A:OP2	4:CD:25:ARG:NH2	2.32	0.62
1:AA:532:A:N6	1:AA:1206:G:O2'	2.32	0.62
27:BD:71:ASP:HB3	27:BD:103:ARG:NH2	2.13	0.62
25:BA:1091:A:H1'	25:BA:1093:G:N3	2.13	0.62
25:DA:2120:G:H2'	25:DA:2121:G:C8	2.34	0.62
50:D4:44:THR:O	50:D4:46:GLN:N	2.32	0.62
1:CA:1010:G:N2	1:CA:1020:U:H1'	2.14	0.62
45:DZ:55:HIS:CE1	45:DZ:135:GLU:HG3	2.35	0.62
25:DA:2166:G:N7	25:DA:2168:G:N2	2.48	0.62
27:DD:132:PRO:HG2	27:DD:135:PHE:CD2	2.34	0.62
25:DA:796:C:H2'	25:DA:797:C:C6	2.35	0.62
47:D1:64:ALA:HA	47:D1:67:ILE:HG13	1.80	0.62
25:DA:2171:A:N3	25:DA:2172:U:N3	2.48	0.62
25:DA:196:A:H62	35:DP:38:GLN:HE22	1.47	0.62
26:DB:106:G:H5''	45:DZ:31:ARG:HG2	1.82	0.62
9:AI:53:VAL:HG11	9:AI:92:TYR:CE1	2.35	0.62
1:AA:1118:C:OP1	9:AI:104:ARG:NH1	2.32	0.62
1:AA:673:G:H2'	1:AA:674:G:C8	2.34	0.62
25:DA:582:G:OP2	61:DA:4953:HOH:O	2.16	0.62
32:BI:92:VAL:HG11	32:BI:144:VAL:HG11	1.82	0.61
1:AA:1305:G:H22	1:AA:1331:G:H1'	1.62	0.61
25:BA:2045:G:H5'	25:BA:2629:C:H4'	1.81	0.61
25:BA:2059:G:O6	61:BA:4774:HOH:O	2.13	0.61
38:BS:15:ARG:O	38:BS:19:LYS:HG2	2.00	0.61
45:BZ:138:GLU:H	45:BZ:156:LYS:NZ	1.98	0.61
23:CW:15:G:N2	23:CW:21:A:N3	2.48	0.61
25:BA:1613:A:OP1	27:BD:211:ARG:NH1	2.34	0.61
1:CA:1239:A:H62	1:CA:1299:A:H62	1.48	0.61
25:BA:709:G:OP1	61:BA:4752:HOH:O	2.16	0.61
25:DA:1250:G:N7	35:DP:18:ARG:NH2	2.48	0.61
25:DA:2103:C:N3	25:DA:2186:G:O6	2.33	0.61
1:CA:1317:C:N3	19:CS:37:ARG:NH2	2.45	0.61
23:CW:56:C:C5	25:DA:897:C:H1'	2.35	0.61
25:BA:1218:G:O2'	25:BA:1219:A:O5'	2.19	0.61
23:AW:54:5MU:OP2	36:BQ:60:ARG:NH1	2.34	0.61
47:D1:59:THR:O	47:D1:91:LYS:NZ	2.33	0.61
4:CD:152:SER:O	4:CD:155:LEU:HB2	2.00	0.61
25:DA:287:C:H2'	25:DA:288:C:H6	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CB:7:VAL:HG12	2:CB:8:LYS:HG2	1.80	0.61
11:CK:99:GLN:HG2	11:CK:105:VAL:HG21	1.83	0.61
25:DA:2193:G:H2'	25:DA:2194:G:H8	1.64	0.61
25:DA:2134:A:O2'	25:DA:2159:G:N3	2.33	0.61
25:BA:2164:C:O2	25:BA:2171:G:N1	2.25	0.61
53:B7:34:ARG:NH1	53:B7:41:ARG:O	2.34	0.61
1:CA:1360:A:OP2	14:CN:35:ARG:NH2	2.33	0.61
43:BX:11:PRO:HB3	43:BX:92:LEU:HD11	1.83	0.61
2:AB:211:ILE:HG22	2:AB:215:LEU:HD12	1.80	0.61
23:AY:21:A:O2'	23:AY:22:G:O4'	2.19	0.61
5:AE:50:GLU:HB2	5:AE:53:LEU:HD13	1.83	0.61
25:BA:794:U:O2'	42:BW:92:ARG:NH2	2.33	0.61
25:DA:2079:U:O3'	47:D1:35:THR:OG1	2.19	0.61
23:AW:6:G:H1	23:AW:67:C:N4	1.96	0.61
23:AW:68:C:H2'	23:AW:69:G:H8	1.65	0.61
3:CC:40:ARG:NH2	3:CC:55:VAL:O	2.33	0.61
57:CA:3177:NEG:N3	25:DA:15:G:OP2	2.33	0.61
37:DR:67:LEU:HD13	37:DR:76:VAL:HG21	1.81	0.61
25:BA:2367:C:H1'	46:B0:39:ARG:HH21	1.65	0.61
4:CD:119:GLN:HG2	4:CD:123:HIS:CD2	2.36	0.61
25:BA:2123:G:N2	25:BA:2210:C:N3	2.39	0.61
25:DA:299:A:H5"	44:DY:86:ARG:NH2	2.16	0.61
1:CA:410:G:OP1	4:CD:30:LYS:NZ	2.22	0.61
13:CM:79:LYS:NZ	13:CM:83:ASP:OD2	2.23	0.61
3:CC:134:ILE:HG23	3:CC:151:VAL:HB	1.82	0.61
3:CC:11:ARG:NH2	3:CC:177:THR:O	2.32	0.61
25:DA:1005:C:H2'	25:DA:1006:C:C6	2.36	0.61
25:DA:2445:G:OP1	29:DF:74:ARG:NH2	2.29	0.61
32:DI:110:ASP:N	32:DI:130:TYR:OH	2.27	0.61
2:AB:16:HIS:CG	2:AB:17:PHE:H	2.19	0.61
32:BI:72:LEU:C	32:BI:74:ASN:H	2.03	0.61
57:AA:3218:NEG:H51	57:AA:3218:NEG:H11	1.81	0.61
5:AE:92:LYS:HB3	5:AE:119:LEU:HB2	1.83	0.61
29:DF:53:THR:HG23	29:DF:55:GLY:H	1.66	0.61
19:AS:45:VAL:HA	19:AS:62:ILE:HG22	1.83	0.61
25:BA:1071:G:C4	25:BA:1180:C:H1'	2.35	0.61
6:CF:68:PRO:HB2	6:CF:71:ARG:HG3	1.83	0.61
25:DA:807:U:OP2	35:DP:41:ARG:NH2	2.33	0.61
16:CP:72:ARG:HH21	16:CP:73:LEU:HD21	1.64	0.61
25:DA:911:A:H2'	36:DQ:9:TYR:OH	2.00	0.61
2:AB:127:ILE:HG13	2:AB:130:ARG:HH11	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:CJ:47:PHE:N	10:CJ:63:PHE:O	2.32	0.61
1:CA:596:C:O2	1:CA:644:G:N2	2.19	0.61
38:DS:68:GLN:HE21	38:DS:71:ARG:HD3	1.66	0.61
25:BA:2825:C:H5'	51:B5:29:THR:HG21	1.81	0.61
12:CL:71:PRO:O	12:CL:102:ARG:NH1	2.34	0.61
29:BF:101:LEU:O	29:BF:106:ARG:NH1	2.33	0.61
23:CW:25:C:H2'	23:CW:26:A:C8	2.36	0.61
1:CA:1004:A:H3'	1:CA:1005:A:C5'	2.30	0.61
1:CA:523:A:H61	12:CL:92:ASP:HB2	1.66	0.61
25:DA:1165:U:H2'	25:DA:1166:C:C6	2.35	0.61
25:DA:361:G:N2	25:DA:362:U:H3	1.98	0.61
27:BD:147:LEU:HD13	27:BD:155:LEU:HD21	1.83	0.61
28:BE:31:CYS:HB3	28:BE:49:LEU:HG	1.82	0.61
25:DA:2646:C:OP2	25:DA:2732:G:O2'	2.15	0.61
17:CQ:6:LEU:HG	17:CQ:23:VAL:HG11	1.80	0.61
1:CA:8:A:H5'	5:CE:101:ILE:HG22	1.80	0.61
25:DA:2062:A:OP1	61:DA:4163:HOH:O	2.16	0.61
13:AM:84:ILE:HD12	19:AS:74:PHE:CE2	2.36	0.61
25:DA:279:C:N3	25:DA:361:G:N2	2.48	0.61
25:BA:2285:A:H2'	25:BA:2286:A:C8	2.34	0.61
1:AA:450:G:OP1	16:AP:43:LYS:NZ	2.32	0.61
1:CA:539:A:OP2	12:CL:115:LYS:NZ	2.34	0.61
23:CY:25:C:O2'	23:CY:26:A:O5'	2.16	0.61
9:AI:99:LEU:HB3	9:AI:101:PHE:CE1	2.35	0.61
1:AA:955:U:O2'	19:AS:83:HIS:HD2	1.83	0.61
1:CA:542:G:OP1	4:CD:10:ARG:NH2	2.32	0.61
29:DF:126:VAL:HG21	29:DF:129:PHE:CZ	2.35	0.61
1:AA:1416:G:N7	61:AA:4106:HOH:O	2.32	0.61
1:AA:1239:A:H62	1:AA:1299:A:N6	1.99	0.61
45:DZ:145:GLU:HG3	45:DZ:146:ILE:N	2.15	0.61
1:CA:815:A:N7	1:CA:1509:C:O2'	2.28	0.61
25:DA:2299:G:N1	25:DA:2318:G:N7	2.49	0.60
25:DA:2193:G:H2'	25:DA:2194:G:C8	2.36	0.60
1:AA:1505:G:O2'	22:AV:13:A:O2'	2.19	0.60
25:BA:1346:U:H4'	25:BA:1347:A:H5''	1.83	0.60
1:CA:1178:G:N2	1:CA:1181:G:OP2	2.32	0.60
4:AD:188:LEU:H	4:AD:188:LEU:HD23	1.65	0.60
23:CY:71:G:H4'	25:DA:1851:U:H4'	1.83	0.60
41:BV:40:LEU:HB2	41:BV:46:VAL:HG13	1.83	0.60
1:AA:1068:G:OP2	1:AA:1068:G:H8	1.85	0.60
1:AA:411:A:OP2	4:AD:25:ARG:NH2	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CB:16:HIS:CG	2:CB:17:PHE:H	2.19	0.60
5:CE:12:LEU:HB3	5:CE:31:LEU:HB2	1.84	0.60
1:AA:1510:U:H2'	1:AA:1511:G:C8	2.35	0.60
32:BI:40:THR:O	32:BI:44:LEU:HB2	2.02	0.60
25:BA:2804:C:H2'	25:BA:2805:G:H8	1.66	0.60
35:DP:95:VAL:HA	35:DP:99:LEU:HD21	1.83	0.60
1:CA:1492:A:O2'	1:CA:1493:A:O5'	2.11	0.60
25:BA:2339:A:H2'	25:BA:2340:A:C8	2.36	0.60
1:AA:96:U:H2'	1:AA:97:G:H8	1.66	0.60
1:AA:1030(C):G:N7	1:AA:1031:G:N2	2.49	0.60
25:DA:1188:U:H4'	41:DV:79:VAL:HG22	1.82	0.60
25:DA:531:C:N4	61:DA:4155:HOH:O	2.33	0.60
14:AN:3:ARG:HH21	14:AN:3:ARG:HB3	1.66	0.60
9:AI:5:TYR:HH	9:AI:16:ARG:HG2	1.67	0.60
2:AB:178:ARG:HG2	8:AH:72:PRO:HA	1.81	0.60
19:CS:14:HIS:O	19:CS:18:LYS:HG3	2.00	0.60
5:AE:60:TYR:CE1	5:AE:64:ARG:HD3	2.35	0.60
25:DA:625:G:N7	35:DP:107:LYS:NZ	2.44	0.60
25:BA:2139:A:O3'	25:BA:2140:U:H3'	2.01	0.60
1:CA:972:C:O2'	10:CJ:55:LYS:O	2.18	0.60
1:CA:353:A:H8	1:CA:353:A:H5'	1.65	0.60
49:D3:12:PRO:HB2	49:D3:20:LYS:HG2	1.82	0.60
15:CO:11:VAL:HG21	15:CO:34:LEU:HD22	1.83	0.60
25:DA:2133:G:N2	25:DA:2157:G:H1'	2.16	0.60
25:BA:1003:U:H5''	36:BQ:14:ARG:HD3	1.84	0.60
35:BP:126:VAL:HG12	35:BP:148:LEU:HD22	1.82	0.60
1:AA:1237:C:HO2'	1:AA:1300:G:H1	1.48	0.60
23:AW:5:G:H2'	23:AW:6:G:C8	2.36	0.60
25:DA:2298:A:H2'	25:DA:2299:G:O4'	2.02	0.60
25:DA:2727:G:O2'	34:DO:70:LYS:NZ	2.31	0.60
1:AA:1008:C:O2	1:AA:1021:G:N1	2.35	0.60
35:DP:59:LEU:HD21	54:D8:10:ALA:HA	1.84	0.60
25:DA:1532:C:N4	25:DA:1537:G:O6	2.34	0.60
25:BA:2348:A:H61	46:B0:43:THR:CG2	2.15	0.60
17:AQ:67:LYS:HA	17:AQ:70:ARG:HH12	1.67	0.60
25:BA:2331:G:H22	38:BS:3:ARG:NE	1.98	0.60
25:DA:2557:G:H2'	25:DA:2558:C:C6	2.37	0.60
1:CA:572:A:OP1	61:CA:4050:HOH:O	2.16	0.60
25:DA:588:U:H2'	25:DA:589:C:C6	2.36	0.60
1:AA:1356:G:H2'	1:AA:1357:A:C8	2.36	0.60
57:AA:3220:NEG:H71	25:BA:1967:G:OP1	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:2048:G:OP1	61:DA:4296:HOH:O	2.16	0.60
28:DE:116:VAL:HG13	28:DE:122:PHE:HB2	1.84	0.60
25:BA:1312:G:O5'	42:BW:15:ARG:NH2	2.35	0.60
25:DA:2273:A:H2'	25:DA:2274:A:C8	2.36	0.60
25:BA:1345:G:OP1	61:BA:4801:HOH:O	2.15	0.60
6:CF:45:LEU:HD12	6:CF:59:TYR:HD2	1.67	0.60
36:DQ:65:PHE:HB2	36:DQ:105:GLU:HB2	1.84	0.60
1:CA:1240:U:OP2	7:CG:116:ALA:N	2.35	0.60
1:CA:1148:U:O2'	9:CI:66:ARG:NH2	2.28	0.60
36:DQ:22:LYS:O	45:DZ:78:LYS:NZ	2.35	0.60
25:BA:1356:G:OP2	53:B7:9:ARG:NH1	2.28	0.60
19:CS:27:GLU:HG2	19:CS:47:HIS:NE2	2.16	0.60
12:AL:71:PRO:O	12:AL:102:ARG:NH1	2.33	0.60
25:DA:500:G:N1	25:DA:503:A:OP2	2.35	0.60
24:CX:23:C:H2'	24:CX:24:U:C6	2.37	0.60
45:DZ:138:GLU:HB2	45:DZ:156:LYS:HD2	1.83	0.60
30:DG:109:VAL:HG21	50:D4:14:ILE:HG21	1.83	0.60
25:BA:1232:G:H5''	41:BV:81:TYR:CE1	2.37	0.60
50:B4:57:GLU:HB3	50:B4:58:ARG:HG2	1.82	0.59
25:DA:2059:A:O2'	29:DF:69:HIS:HD2	1.84	0.59
1:AA:976:G:H5'	1:AA:1358:U:O2'	2.01	0.59
26:DB:66:A:N6	26:DB:108:U:H3'	2.17	0.59
10:CJ:61:GLU:OE2	14:CN:45:ARG:NE	2.33	0.59
1:AA:1240:U:OP2	7:AG:116:ALA:N	2.29	0.59
7:AG:76:ARG:HB3	7:AG:156:TRP:HH2	1.67	0.59
45:DZ:126:VAL:HG11	45:DZ:161:VAL:HG23	1.84	0.59
6:CF:100:ASN:HD21	18:CR:23:LYS:HG2	1.67	0.59
39:DT:27:THR:HB	39:DT:90:GLN:HB3	1.84	0.59
28:DE:111:ARG:HG3	28:DE:160:TYR:CD2	2.38	0.59
44:DY:94:LYS:NZ	61:DY:602:HOH:O	2.35	0.59
1:AA:1149:C:H2'	1:AA:1150:U:H6	1.67	0.59
40:BU:66:ASN:O	40:BU:70:ARG:HG3	2.02	0.59
4:AD:107:ARG:HH22	4:AD:194:LEU:HD13	1.67	0.59
33:DN:4:TYR:HB2	40:DU:101:ARG:NH1	2.16	0.59
24:CX:40:C:H2'	24:CX:41:C:H6	1.67	0.59
5:CE:20:GLN:NE2	5:CE:21:ALA:O	2.35	0.59
1:AA:1129:C:H5''	9:AI:16:ARG:HH12	1.67	0.59
25:DA:958:U:OP2	36:DQ:14:ARG:NH1	2.35	0.59
19:CS:22:LEU:HD22	19:CS:31:ILE:HD11	1.85	0.59
1:CA:1378:C:O2	7:CG:76:ARG:NH2	2.36	0.59
11:CK:48:ILE:O	11:CK:50:TYR:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:1700:G:H3'	37:BR:2:ARG:HD3	1.83	0.59
1:CA:664:G:P	18:CR:64:ARG:HH21	2.25	0.59
9:AI:3:GLN:OE1	9:AI:20:ARG:NH2	2.25	0.59
53:B7:34:ARG:NH2	61:B7:201:HOH:O	2.33	0.59
27:BD:108:PRO:HB3	27:BD:143:HIS:CE1	2.37	0.59
23:AW:51:U:H2'	23:AW:52:G:H8	1.67	0.59
30:DG:9:ARG:NH1	30:DG:13:GLU:OE1	2.35	0.59
25:DA:1021:A:H62	25:DA:1141:U:H3	1.50	0.59
25:DA:692:C:O2'	27:DD:38:LYS:NZ	2.35	0.59
25:DA:1998:G:HO2'	25:DA:2724:C:HO2'	1.49	0.59
25:DA:2771:C:H5''	28:DE:202:LYS:HD3	1.83	0.59
8:CH:7:ALA:O	8:CH:11:THR:OG1	2.14	0.59
36:DQ:109:VAL:HG13	36:DQ:113:GLN:HB3	1.84	0.59
25:DA:65:C:O2'	25:DA:456:C:N3	2.29	0.59
25:BA:1049:G:O2'	25:BA:1056:A:N1	2.28	0.59
7:CG:22:LEU:HG	7:CG:62:PHE:HE2	1.67	0.59
1:AA:1008:C:C2	1:AA:1021:G:N1	2.71	0.59
25:BA:1735:U:O2	25:BA:1747:A:H5'	2.03	0.59
25:DA:639:U:H2'	25:DA:640:C:C6	2.38	0.59
25:DA:1830:C:OP2	61:DA:4606:HOH:O	2.15	0.59
16:CP:23:ASP:OD1	16:CP:25:ARG:HD3	2.02	0.59
3:CC:29:TYR:OH	14:CN:54:PRO:O	2.17	0.59
1:AA:1003:G:C2'	1:AA:1004:A:H4'	2.32	0.59
25:DA:2497:A:OP1	61:DA:4078:HOH:O	2.17	0.59
1:AA:1064:G:H4'	1:AA:1065:U:OP1	2.02	0.59
3:AC:8:ILE:HD13	3:AC:184:TYR:HB3	1.85	0.59
1:AA:382:A:H2'	1:AA:383:A:C8	2.38	0.59
8:CH:51:VAL:HG11	8:CH:60:ARG:HH12	1.68	0.59
26:DB:11:C:H3'	26:DB:12:C:H6	1.66	0.59
25:BA:956:A:H62	36:BQ:12:GLN:HA	1.68	0.59
23:AW:1:G:H2'	23:AW:2:C:H6	1.68	0.59
17:AQ:26:GLN:HG2	17:AQ:37:LYS:HG2	1.83	0.59
8:AH:51:VAL:HG21	8:AH:60:ARG:HH11	1.68	0.59
27:BD:132:PRO:HG2	27:BD:135:PHE:CD2	2.38	0.59
1:CA:976:G:H5'	1:CA:1358:U:O2'	2.02	0.59
25:DA:1131:G:O6	25:DA:2040:C:H1'	2.03	0.59
4:CD:61:LYS:NZ	4:CD:207:TYR:OH	2.35	0.59
1:AA:920:U:H2'	1:AA:921:U:C6	2.38	0.59
3:AC:3:ASN:OD1	3:AC:3:ASN:N	2.35	0.59
25:DA:2701:C:OP1	61:DA:4911:HOH:O	2.16	0.59
27:DD:242:ARG:N	27:DD:242:ARG:HD3	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1119:C:N4	1:CA:1154:G:H1	2.00	0.59
1:CA:1053:G:N7	1:CA:1200:C:H5''	2.18	0.59
15:CO:39:LEU:HD13	15:CO:56:LEU:HB2	1.84	0.59
25:BA:1827:U:H2'	25:BA:1828:C:C6	2.38	0.59
25:DA:2787:C:H1'	28:DE:62:PRO:HG3	1.85	0.59
52:B6:13:CYS:SG	52:B6:47:THR:HG21	2.43	0.59
28:DE:28:ALA:HB3	28:DE:93:VAL:HG12	1.85	0.59
25:BA:2604:G:OP1	61:BA:4828:HOH:O	2.16	0.59
32:BI:130:TYR:HB3	32:BI:138:ILE:HB	1.84	0.59
45:DZ:100:VAL:HG21	45:DZ:134:PRO:HG2	1.83	0.59
50:B4:44:THR:O	50:B4:46:GLN:N	2.36	0.59
23:CW:39:PSU:H2'	23:CW:40:C:H6	1.66	0.59
23:CW:50:U:O4	23:CW:64:A:N1	2.36	0.59
25:BA:2511:C:OP1	61:BA:5152:HOH:O	2.16	0.59
1:CA:1305:G:O2'	1:CA:1331:G:N2	2.35	0.59
1:CA:1251:A:H2'	1:CA:1252:A:C8	2.37	0.59
5:AE:152:ARG:NH2	8:AH:107:LEU:O	2.35	0.59
13:CM:92:HIS:CE1	13:CM:98:VAL:HG21	2.37	0.59
3:CC:152:ILE:HG23	3:CC:199:LYS:HB2	1.85	0.59
31:DH:89:ILE:O	31:DH:129:THR:HG23	2.01	0.59
25:DA:2404:C:O3'	35:DP:77:ARG:NH2	2.35	0.59
10:AJ:21:GLN:NE2	10:AJ:25:GLU:OE2	2.34	0.59
13:CM:65:LYS:N	50:D4:50:VAL:HG21	2.18	0.59
39:DT:53:ARG:HB3	39:DT:53:ARG:HH11	1.67	0.58
23:CY:76:A:O2'	25:DA:2394:C:N3	2.30	0.58
5:CE:31:LEU:HD22	5:CE:43:LEU:HD11	1.85	0.58
32:BI:72:LEU:O	32:BI:74:ASN:N	2.34	0.58
25:DA:1012:U:H5	33:DN:28:THR:HG21	1.68	0.58
38:BS:34:HIS:O	38:BS:97:ARG:NH2	2.36	0.58
2:AB:16:HIS:CG	2:AB:17:PHE:N	2.70	0.58
25:BA:2132:G:O2'	25:BA:2142:G:OP2	2.21	0.58
25:BA:2190:G:C6	25:BA:2193:A:H8	2.20	0.58
1:CA:1052:U:H5''	1:CA:1053:G:OP2	2.03	0.58
25:BA:1648:U:O4	61:BA:4364:HOH:O	2.09	0.58
25:DA:2103:C:H2'	25:DA:2104:G:C8	2.38	0.58
25:BA:1546:G:N2	27:BD:99:ASP:O	2.32	0.58
23:CY:55:PSU:N3	23:CY:58:A:N7	2.51	0.58
25:DA:108:U:H2'	25:DA:109:G:C8	2.38	0.58
25:DA:1169:G:H1	25:DA:1180:C:H42	1.50	0.58
38:DS:103:GLU:O	38:DS:107:GLU:HG3	2.02	0.58
25:BA:927:G:H2'	25:BA:928:G:H8	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:345:C:O2	1:AA:345:C:H2'	2.01	0.58
23:CY:9:A:OP2	23:CY:13:C:N4	2.35	0.58
25:DA:361:G:N3	25:DA:362:U:N3	2.51	0.58
25:BA:2804:C:H2'	25:BA:2805:G:C8	2.38	0.58
26:DB:80:U:H2'	26:DB:81:G:C8	2.38	0.58
37:DR:33:ARG:HD2	37:DR:113:LEU:HD13	1.86	0.58
43:DX:43:VAL:HG21	43:DX:81:VAL:HG11	1.84	0.58
1:CA:864:A:H5'	5:CE:86:ALA:HB2	1.85	0.58
25:BA:661:G:OP1	35:BP:132:LYS:HE2	2.02	0.58
25:DA:376:C:OP1	61:DA:4657:HOH:O	2.17	0.58
26:DB:24:G:N2	26:DB:27:C:N3	2.39	0.58
57:CW:3002:NEG:N3	25:DA:1942:C:OP1	2.36	0.58
2:CB:120:ALA:O	2:CB:122:PHE:N	2.30	0.58
1:AA:946:A:O2'	1:AA:1333:A:N3	2.30	0.58
25:BA:11:G:H2'	25:BA:12:U:H5''	1.85	0.58
25:DA:1803:A:O2'	27:DD:259:THR:HG21	2.02	0.58
25:DA:2689:U:P	25:DA:2719:G:H22	2.26	0.58
25:BA:1220:U:O3'	25:BA:1221:G:H4'	2.03	0.58
1:CA:1323:G:H2'	1:CA:1324:A:C8	2.38	0.58
23:AW:51:U:H3	23:AW:63:G:H1	1.51	0.58
25:BA:908:A:OP2	61:BA:4344:HOH:O	2.17	0.58
30:DG:38:VAL:HG22	30:DG:93:THR:HG23	1.84	0.58
2:CB:21:ARG:HA	2:CB:39:ILE:HA	1.84	0.58
32:BI:129:THR:HG22	32:BI:139:GLN:HE22	1.68	0.58
33:BN:30:ILE:HG22	33:BN:34:LEU:HD22	1.84	0.58
47:D1:10:LYS:NZ	47:D1:65:SER:OG	2.37	0.58
23:CY:51:U:O2	23:CY:63:G:N2	2.34	0.58
25:DA:330:A:H2	25:DA:1210:A:HO2'	1.50	0.58
29:DF:7:TYR:O	29:DF:22:ALA:N	2.36	0.58
45:DZ:117:LEU:HD11	45:DZ:144:LEU:HD13	1.85	0.58
25:BA:331:G:H21	25:BA:354:A:H62	1.51	0.58
26:DB:33:G:H5'	30:DG:2:PRO:HD3	1.86	0.58
25:DA:2365:G:O6	54:D8:39:LYS:HE3	2.04	0.58
1:AA:731:G:H5'	1:AA:766:A:H4'	1.86	0.58
20:AT:60:GLU:HG3	20:AT:81:LYS:HD2	1.85	0.58
25:DA:2748:A:H5'	31:DH:4:ILE:HD12	1.85	0.58
1:AA:982:U:H5''	14:AN:6:LEU:HD21	1.85	0.58
25:DA:1025:G:C4	25:DA:1135:C:H1'	2.39	0.58
1:AA:78:G:N2	1:AA:91:C:N3	2.51	0.58
1:CA:1099:G:OP2	2:CB:144:ARG:NH2	2.37	0.58
25:DA:1713:U:H2'	25:DA:1714:G:H8	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:DW:11:ARG:HD2	42:DW:82:LEU:HD12	1.85	0.58
23:AW:76:A:H5''	25:BA:2614:A:H61	1.68	0.58
1:CA:1456:G:O3'	20:CT:39:LYS:NZ	2.37	0.58
25:DA:247:G:H4'	25:DA:386:G:C5	2.39	0.58
26:DB:3:C:H2'	26:DB:4:C:C6	2.39	0.58
25:DA:2612:C:OP2	51:D5:2:ALA:N	2.36	0.58
25:DA:400:G:N7	61:DA:4648:HOH:O	2.32	0.58
23:AY:26:A:N6	23:AY:44:G:N1	2.37	0.58
25:DA:997:G:OP1	40:DU:92:ARG:HG2	2.03	0.58
1:CA:662:G:H2'	1:CA:663:A:C8	2.39	0.58
2:CB:128:GLU:HG3	2:CB:135:GLN:HE22	1.68	0.58
25:BA:1441:A:OP1	61:BA:5091:HOH:O	2.17	0.58
2:AB:87:ARG:CZ	2:AB:233:SER:HB3	2.34	0.58
32:DI:31:LEU:HD21	32:DI:38:LEU:HG	1.85	0.58
45:DZ:45:ASP:OD1	45:DZ:49:ARG:NH1	2.35	0.58
34:DO:98:VAL:HG22	34:DO:118:ALA:HA	1.86	0.58
3:AC:19:GLU:HB3	3:AC:40:ARG:NH2	2.19	0.58
25:DA:1140:C:O3'	33:DN:25:ARG:NH1	2.37	0.58
25:BA:139:A:H8	25:BA:1454:C:O2'	1.87	0.58
25:DA:320:A:H4'	25:DA:322:A:C8	2.38	0.58
25:DA:2537:U:H2'	25:DA:2538:C:C6	2.38	0.58
1:CA:17:U:H2'	1:CA:18:C:C6	2.39	0.58
32:DI:4:ILE:HG12	32:DI:18:VAL:HG22	1.86	0.58
25:DA:1429:G:H2'	25:DA:1430:C:C6	2.38	0.58
45:BZ:24:LEU:HB2	45:BZ:41:LEU:HD23	1.85	0.58
1:AA:1039:C:H2'	1:AA:1040:U:C6	2.38	0.58
36:BQ:43:THR:HG22	36:BQ:94:VAL:HG12	1.86	0.58
6:AF:97:PHE:HD2	18:AR:31:LEU:HD12	1.69	0.58
45:DZ:105:VAL:N	45:DZ:139:VAL:O	2.36	0.58
24:AX:21:A:N6	24:AX:46:G:H2'	2.19	0.58
27:BD:132:PRO:HD3	27:BD:190:TYR:CZ	2.39	0.58
41:BV:5:VAL:HG21	41:BV:35:LEU:HD23	1.85	0.58
15:CO:54:ARG:NH1	15:CO:58:MET:SD	2.77	0.58
25:DA:1262:A:H2	51:D5:10:LYS:HD2	1.69	0.58
19:CS:49:ILE:HD13	19:CS:62:ILE:HD13	1.84	0.58
25:BA:2235:G:OP1	27:BD:172:TYR:OH	2.18	0.58
25:BA:1830:G:O2'	27:BD:181:GLU:OE2	2.18	0.58
1:AA:142:G:H2'	1:AA:143:A:H8	1.69	0.58
25:DA:2144:U:H1'	25:DA:2148:G:H22	1.69	0.58
25:DA:322:A:OP1	29:DF:168:ARG:HD2	2.04	0.58
4:CD:140:VAL:HG11	4:CD:146:ILE:HD11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:DP:2:LYS:NZ	35:DP:4:SER:OG	2.36	0.58
3:AC:134:ILE:HG23	3:AC:151:VAL:HB	1.84	0.58
25:DA:1434:A:H61	25:DA:1558:A:H62	1.50	0.58
25:BA:1201:A:OP1	40:BU:55:ARG:HD3	2.04	0.58
25:BA:596:G:OP2	41:BV:78:LYS:NZ	2.33	0.58
23:AW:8:4SU:H6	23:AW:8:4SU:O5'	2.04	0.58
25:DA:839:U:H2'	25:DA:840:C:C6	2.38	0.57
45:DZ:53:ILE:HD13	45:DZ:99:TYR:HB2	1.85	0.57
1:AA:222:U:H2'	1:AA:223:U:C6	2.38	0.57
25:DA:646:A:H2'	25:DA:647:G:O4'	2.03	0.57
9:AI:128:ARG:NH2	24:AX:33:U:OP2	2.25	0.57
25:DA:1773:A:H5''	61:DA:4621:HOH:O	2.03	0.57
25:DA:2125:G:N1	25:DA:2172:U:OP2	2.33	0.57
25:DA:2143:C:N4	25:DA:2148:G:H1	2.02	0.57
29:BF:184:TYR:CE2	29:BF:188:ARG:HD2	2.39	0.57
25:DA:2438:U:O2'	25:DA:2440:C:OP1	2.18	0.57
49:B3:19:GLN:OE1	49:B3:52:HIS:NE2	2.36	0.57
31:DH:17:VAL:HG11	31:DH:50:VAL:HG21	1.84	0.57
1:CA:1015:A:H1'	1:CA:1219:U:H5'	1.86	0.57
25:DA:193:U:OP1	61:DA:4562:HOH:O	2.17	0.57
33:DN:15:LEU:HB3	33:DN:137:LYS:HA	1.85	0.57
2:CB:178:ARG:NH2	8:CH:68:ARG:HH12	2.01	0.57
1:CA:1126:U:H3	10:CJ:40:LEU:HD11	1.67	0.57
1:AA:974:A:OP2	14:AN:41:ARG:NH1	2.36	0.57
4:CD:98:GLU:OE1	4:CD:103:ASN:ND2	2.27	0.57
1:CA:1222:G:OP1	19:CS:77:THR:HG21	2.05	0.57
25:BA:664:U:H2'	25:BA:665:C:C6	2.40	0.57
25:BA:236:G:H4'	25:BA:413:G:C5	2.38	0.57
25:DA:1038:C:H42	25:DA:1117:G:H1	1.51	0.57
25:DA:1866:C:H2'	25:DA:1876:A:O4'	2.04	0.57
23:AY:67:C:H2'	23:AY:68:C:C6	2.39	0.57
23:CW:27:G:H2'	23:CW:28:G:H8	1.69	0.57
25:DA:1358:G:O2'	25:DA:1359:A:H5''	2.03	0.57
25:BA:2348:A:H61	46:B0:43:THR:HG22	1.70	0.57
45:DZ:53:ILE:HG22	45:DZ:71:VAL:O	2.04	0.57
25:BA:2041:A:OP2	51:B5:9:LYS:NZ	2.38	0.57
47:D1:76:ARG:NH1	47:D1:97:LEU:O	2.37	0.57
25:DA:845:G:N2	25:DA:845:G:OP2	2.29	0.57
1:AA:859:A:OP2	1:AA:869:G:N1	2.31	0.57
1:AA:138:G:H1	1:AA:225:C:H42	1.50	0.57
50:D4:33:VAL:HG12	50:D4:35:VAL:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:2001:A:H4'	25:DA:2689:U:H2'	1.86	0.57
25:BA:672:G:N3	25:BA:2362:C:O2'	2.38	0.57
25:DA:652(T):C:H2'	25:DA:652(U):G:C8	2.40	0.57
25:DA:2638:G:OP1	28:DE:82:ARG:NH2	2.38	0.57
37:BR:28:LEU:HD12	37:BR:48:VAL:HG21	1.85	0.57
45:DZ:44:PHE:CZ	45:DZ:86:VAL:HG11	2.39	0.57
30:DG:136:ARG:HD2	30:DG:137:GLU:HG3	1.86	0.57
28:DE:12:THR:HG22	28:DE:13:ARG:H	1.69	0.57
25:DA:1593:G:H2'	25:DA:1594:G:C8	2.40	0.57
23:CY:7:A:N1	23:CY:66:U:O2	2.38	0.57
9:AI:20:ARG:O	9:AI:60:ASP:N	2.36	0.57
54:B8:62:LEU:HB3	54:B8:65:GLU:HG2	1.87	0.57
1:AA:1132:C:H2'	1:AA:1133:G:C8	2.39	0.57
1:CA:1151:A:O2'	1:CA:1152:A:H8	1.87	0.57
25:DA:1998:G:O2'	25:DA:2724:C:O2'	2.23	0.57
25:DA:2539:C:H4'	55:D9:35:ARG:HH22	1.70	0.57
17:AQ:45:HIS:NE2	17:AQ:47:PRO:HG3	2.19	0.57
9:AI:110:GLU:OE2	9:AI:113:LYS:NZ	2.36	0.57
42:DW:14:PRO:HG2	42:DW:78:GLU:HG2	1.85	0.57
5:AE:110:LEU:HD13	5:AE:118:ILE:HG21	1.87	0.57
50:B4:63:TYR:N	50:B4:64:GLY:HA2	2.19	0.57
1:AA:152:A:N6	1:AA:169:C:N3	2.52	0.57
25:DA:279:C:H2'	25:DA:280:C:H6	1.68	0.57
25:DA:1794:U:H2'	25:DA:1795:C:C6	2.40	0.57
45:BZ:111:VAL:C	45:BZ:113:ALA:H	2.08	0.57
1:AA:748:C:H4'	1:AA:749:C:O5'	2.05	0.57
1:CA:67:C:H2'	1:CA:68:G:C8	2.40	0.57
43:DX:88:LYS:NZ	43:DX:90:GLU:OE1	2.38	0.57
25:DA:602:G:O2'	25:DA:655:A:N6	2.37	0.57
36:DQ:85:LYS:HG2	46:D0:7:LEU:HB3	1.85	0.57
25:DA:492:A:H2'	25:DA:493:G:O4'	2.04	0.57
25:BA:1296:G:N7	35:BP:18:ARG:NH2	2.53	0.57
25:BA:997:G:OP1	36:BQ:16:ARG:NH2	2.38	0.57
1:CA:1059:C:OP2	3:CC:199:LYS:NZ	2.30	0.57
31:DH:27:LYS:NZ	31:DH:32:GLU:OE2	2.37	0.57
25:DA:1786:A:H1'	25:DA:1938:A:N6	2.19	0.57
32:DI:27:ARG:HD2	47:D1:71:TYR:CE1	2.39	0.57
29:DF:11:VAL:HG22	29:DF:125:LEU:HB2	1.87	0.57
10:CJ:38:ILE:HD11	10:CJ:71:LEU:HB3	1.86	0.57
25:DA:2336:A:H61	46:D0:43:THR:HG22	1.69	0.57
10:AJ:16:LEU:HD22	10:AJ:68:HIS:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AY:21:A:HO2'	23:AY:22:G:H8	1.53	0.57
10:AJ:55:LYS:O	10:AJ:57:LYS:N	2.38	0.57
25:DA:1352:U:OP1	61:DA:4149:HOH:O	2.18	0.57
18:CR:32:ARG:HA	18:CR:69:THR:HG21	1.86	0.57
39:DT:59:THR:HG23	39:DT:78:LEU:HB3	1.86	0.57
1:AA:1202:G:O4'	14:AN:29:ARG:NH1	2.38	0.57
25:BA:2761:A:H5'	31:BH:4:ILE:HD12	1.86	0.57
25:DA:644:A:H4'	25:DA:645:C:C5	2.40	0.57
1:CA:620:C:H2'	1:CA:621:A:O4'	2.05	0.57
36:DQ:31:ASP:OD1	36:DQ:134:ARG:NH1	2.38	0.57
25:DA:251:A:H2'	25:DA:252:G:O4'	2.05	0.57
30:DG:106:LEU:HA	30:DG:110:ALA:HB3	1.86	0.57
9:CI:28:VAL:HG22	9:CI:63:ILE:HB	1.86	0.57
34:DO:115:VAL:HG13	34:DO:121:VAL:HG21	1.87	0.57
1:AA:134:A:H61	16:AP:25:ARG:NH1	2.02	0.57
32:BI:93:THR:OG1	32:BI:96:ASP:OD1	2.22	0.57
1:CA:946:A:H2'	1:CA:947:G:C8	2.40	0.57
25:BA:602:G:H2'	25:BA:603:C:C6	2.40	0.57
1:CA:201:C:N4	1:CA:216:G:H1	1.87	0.56
25:BA:2122:G:H2'	25:BA:2123:G:C8	2.40	0.56
23:AW:25:C:H2'	23:AW:26:A:C8	2.39	0.56
1:AA:1002:G:O6	1:AA:1003:G:N2	2.38	0.56
25:DA:2142:C:H2'	25:DA:2143:C:C6	2.40	0.56
4:AD:88:VAL:HG22	5:AE:97:GLY:HA2	1.86	0.56
25:BA:1355:G:O6	61:BA:4959:HOH:O	2.18	0.56
18:CR:47:THR:HG23	18:CR:49:LYS:HG3	1.87	0.56
43:DX:53:LYS:HB3	43:DX:82:GLN:HB3	1.86	0.56
1:AA:1027:C:H2'	1:AA:1028:C:C5	2.41	0.56
24:CX:55:PSU:N3	24:CX:58:A:OP2	2.30	0.56
1:CA:570:G:OP2	57:CA:3171:NEG:H12	2.04	0.56
36:BQ:31:ASP:HA	36:BQ:134:ARG:HH11	1.69	0.56
26:DB:105:A:OP1	45:DZ:72:ARG:NH1	2.39	0.56
2:CB:74:LYS:NZ	2:CB:205:ASP:O	2.38	0.56
1:CA:1256:A:H61	1:CA:1278:U:H1'	1.71	0.56
25:DA:866:A:H2	25:DA:867:C:C4	2.23	0.56
23:CY:10:G:H1	23:CY:25:C:H42	1.51	0.56
25:DA:1406:U:H2'	25:DA:1407:C:C6	2.40	0.56
6:AF:82:ARG:HB3	6:AF:85:VAL:HG23	1.87	0.56
19:CS:42:PRO:HG3	50:D4:61:ARG:HG2	1.87	0.56
35:BP:121:LYS:O	35:BP:123:LEU:N	2.39	0.56
1:CA:757:U:H2'	1:CA:758:G:O4'	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:1055:A:OP2	33:BN:37:LYS:NZ	2.26	0.56
1:AA:356:A:N3	1:AA:368:U:O2'	2.33	0.56
13:AM:88:ARG:HG3	13:AM:98:VAL:HG11	1.86	0.56
55:B9:17:ILE:HG22	55:B9:24:TYR:HB2	1.88	0.56
38:BS:27:SER:HA	38:BS:88:ASP:HB3	1.87	0.56
25:DA:2183:C:H2'	25:DA:2184:G:H8	1.70	0.56
1:AA:662:G:H2'	1:AA:663:A:C8	2.39	0.56
3:CC:78:GLY:HA3	3:CC:83:ARG:H	1.69	0.56
26:DB:75:G:N2	45:DZ:73:GLN:OE1	2.36	0.56
53:B7:24:THR:HG22	53:B7:27:GLY:N	2.08	0.56
25:DA:2134:A:H3'	25:DA:2135:A:C8	2.41	0.56
25:DA:2153:G:H2'	25:DA:2154:G:C8	2.41	0.56
1:AA:1157:A:H4'	1:AA:1158:C:O5'	2.06	0.56
25:DA:864:G:H1	25:DA:912:C:H5	1.52	0.56
1:CA:1202:G:O4'	14:CN:29:ARG:NH1	2.38	0.56
28:BE:47:VAL:HG23	28:BE:84:PHE:O	2.04	0.56
52:B6:6:ARG:NH1	52:B6:26:ASN:HB2	2.20	0.56
25:DA:2815:C:H2'	25:DA:2816:C:H6	1.70	0.56
23:AW:51:U:H2'	23:AW:52:G:C8	2.41	0.56
25:DA:746:A:H2'	25:DA:2612:C:H5''	1.87	0.56
45:DZ:73:GLN:O	45:DZ:87:ASP:N	2.37	0.56
1:CA:1074:G:OP1	5:CE:64:ARG:NH2	2.39	0.56
1:CA:434:U:H2'	1:CA:435:C:C6	2.39	0.56
2:AB:231:GLU:HB3	2:AB:232:PRO:HD3	1.86	0.56
25:DA:1513:C:H2'	25:DA:1514:U:C6	2.41	0.56
1:AA:28:G:O2'	1:AA:296:U:OP1	2.22	0.56
7:CG:18:TYR:HB3	7:CG:59:LEU:HD13	1.88	0.56
47:D1:3:LYS:HB2	47:D1:61:ARG:HH12	1.70	0.56
28:DE:11:MET:HG2	28:DE:24:THR:HB	1.88	0.56
6:AF:2:ARG:NE	6:AF:69:GLU:HG2	2.20	0.56
25:DA:1007:C:OP1	33:DN:35:ARG:NH1	2.38	0.56
1:CA:1000:U:O2	1:CA:1041:A:N1	2.38	0.56
1:CA:1240:U:N3	7:CG:30:ILE:O	2.26	0.56
25:DA:1970:A:H4'	25:DA:1971:A:OP1	2.06	0.56
28:BE:24:THR:HG22	28:BE:186:GLY:O	2.05	0.56
25:BA:2389:A:H2'	25:BA:2390:A:C8	2.41	0.56
36:DQ:24:GLY:HA2	36:DQ:67:ARG:NH2	2.21	0.56
28:BE:174:ASP:OD1	28:BE:175:VAL:N	2.39	0.56
25:BA:1425:A:H4'	25:BA:1426:G:OP2	2.05	0.56
1:AA:1241:G:H2'	1:AA:1242:C:C6	2.41	0.56
23:AY:19:G:H3'	23:AY:20:U:H5'	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2132:G:OP1	25:BA:2167:C:N4	2.38	0.56
1:AA:1190:G:O2'	1:AA:1191:A:OP2	2.22	0.56
12:AL:24:VAL:HG12	12:AL:27:LEU:HB2	1.85	0.56
35:BP:50:ARG:HD3	54:B8:7:HIS:HD2	1.69	0.56
1:CA:1103:C:OP1	2:CB:96:ARG:NH2	2.38	0.56
1:CA:337:C:H2'	1:CA:338:A:C8	2.41	0.56
32:BI:106:GLY:HA2	32:BI:107:VAL:O	2.06	0.56
26:DB:55:U:O2'	30:DG:27:ASN:ND2	2.29	0.56
1:AA:489:C:OP1	4:AD:132:ARG:NH2	2.38	0.56
3:AC:156:ARG:NE	3:AC:160:ALA:O	2.37	0.56
1:AA:49:U:O4	1:AA:365:U:H5	1.89	0.56
25:DA:2590:A:O3'	27:DD:239:ARG:NH2	2.39	0.56
1:CA:10:A:OP2	5:CE:126:ARG:HD2	2.06	0.56
7:CG:111:ARG:HD2	7:CG:123:GLU:HB2	1.87	0.56
36:DQ:81:VAL:HB	46:D0:7:LEU:HD21	1.88	0.56
2:AB:35:GLU:HB2	2:AB:40:HIS:HD2	1.70	0.56
25:DA:2105:C:H2'	25:DA:2106:G:C8	2.41	0.56
3:AC:114:PRO:O	3:AC:118:GLN:NE2	2.36	0.56
8:CH:14:ARG:NH2	8:CH:83:ILE:O	2.36	0.56
25:DA:1400:G:H2'	25:DA:1401:G:C8	2.41	0.56
23:AW:18:G:H4'	23:AW:60:U:C5	2.41	0.56
25:DA:2602:A:H4'	25:DA:2603:G:O5'	2.06	0.56
3:CC:43:LEU:HD21	3:CC:91:LEU:HD13	1.86	0.56
25:DA:1805:U:O2	27:DD:50:THR:HB	2.05	0.56
8:CH:64:LYS:HG2	8:CH:79:VAL:HG21	1.88	0.56
1:CA:45:U:H2'	1:CA:46:G:C8	2.40	0.56
25:BA:1324:A:OP1	37:BR:36:THR:HG23	2.06	0.56
45:BZ:152:ALA:H	45:BZ:171:ILE:HG12	1.69	0.56
3:CC:109:PRO:HB3	3:CC:115:LEU:HD23	1.88	0.56
29:DF:167:ALA:HB1	29:DF:173:VAL:HG11	1.88	0.56
25:DA:2133:G:H22	25:DA:2157:G:H1'	1.69	0.56
35:DP:38:GLN:HG2	35:DP:45:LEU:HD23	1.87	0.56
13:AM:57:ARG:HH11	13:AM:57:ARG:HG3	1.70	0.56
25:DA:1796:U:H2'	25:DA:1797:C:H6	1.69	0.56
25:BA:553:A:C2	25:BA:2064:A:H2'	2.39	0.56
23:CY:1:G:H2'	23:CY:2:C:C6	2.41	0.56
8:AH:64:LYS:HG2	8:AH:79:VAL:HG21	1.88	0.56
30:DG:11:TYR:HA	30:DG:15:VAL:HB	1.87	0.56
25:BA:918:U:OP1	36:BQ:5:ARG:HD3	2.05	0.56
1:AA:692:U:O2'	1:AA:694:A:N7	2.31	0.56
4:CD:187:ARG:NH2	4:CD:193:ASP:OD2	2.32	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:BH:90:LYS:HD3	31:BH:159:GLU:HG2	1.88	0.56
28:BE:9:VAL:HB	39:BT:3:ARG:HG2	1.88	0.56
31:DH:154:PRO:HB3	31:DH:163:TYR:CZ	2.41	0.56
25:BA:1785:C:OP1	39:BT:96:ARG:NH1	2.39	0.56
1:CA:1144:G:N2	1:CA:1146:A:H62	2.04	0.56
1:AA:1027:C:N3	1:AA:1034:G:C6	2.74	0.56
25:DA:1190:G:H2'	25:DA:1191:G:C8	2.41	0.56
10:CJ:30:SER:O	10:CJ:81:THR:HG23	2.05	0.56
23:CY:18:G:N2	23:CY:55:PSU:N3	2.53	0.56
8:CH:9:MET:HG3	8:CH:26:VAL:HG11	1.87	0.56
25:BA:1475:G:H2'	25:BA:1476:C:C6	2.40	0.56
45:DZ:69:THR:HG22	45:DZ:90:VAL:HA	1.88	0.56
30:BG:15:VAL:HG22	30:BG:175:LEU:HB3	1.86	0.56
25:DA:2632:A:O2'	25:DA:2811:G:O2'	2.11	0.56
1:CA:1004:A:H62	1:CA:1037:C:H3'	1.69	0.55
13:AM:84:ILE:HD12	19:AS:74:PHE:HE2	1.71	0.55
27:DD:26:LYS:HE2	27:DD:28:GLU:O	2.05	0.55
25:BA:2044:U:O2'	25:BA:2629:C:H5'	2.06	0.55
29:DF:154:VAL:HG22	29:DF:191:ARG:HB2	1.87	0.55
3:CC:164:ARG:HG2	3:CC:165:THR:H	1.71	0.55
25:BA:1410:G:P	47:B1:3:LYS:HG3	2.46	0.55
25:BA:1059:C:OP2	61:BA:5284:HOH:O	2.18	0.55
1:AA:1103:C:OP1	2:AB:96:ARG:NH2	2.39	0.55
5:CE:42:GLY:HA2	5:CE:65:ASN:O	2.06	0.55
29:DF:150:GLY:HA2	29:DF:172:TRP:CD2	2.42	0.55
2:CB:77:ALA:HA	2:CB:80:ILE:HG22	1.88	0.55
1:AA:1142:G:H2'	1:AA:1143:G:O4'	2.06	0.55
32:DI:130:TYR:HB3	32:DI:138:ILE:HB	1.88	0.55
1:AA:736:C:H2'	1:AA:737:A:C8	2.42	0.55
38:DS:14:VAL:O	38:DS:18:ILE:HG12	2.06	0.55
25:DA:182:A:N3	25:DA:433:C:O2'	2.35	0.55
28:BE:29:GLY:HA3	61:BE:406:HOH:O	2.06	0.55
23:AY:76:A:N6	25:BA:2434:A:O4'	2.38	0.55
12:AL:49:ASN:ND2	12:AL:92:ASP:OD2	2.31	0.55
25:DA:2134:A:O2'	25:DA:2135:A:OP1	2.25	0.55
1:CA:160:A:H1'	1:CA:344:A:C5	2.41	0.55
1:AA:1129:C:O2'	1:AA:1139:G:N7	2.37	0.55
1:CA:674:G:H2'	1:CA:675:A:H8	1.70	0.55
23:CW:52:G:H5''	36:DQ:56:ARG:HH22	1.70	0.55
25:DA:2180:U:H2'	25:DA:2181:G:O4'	2.05	0.55
20:CT:18:GLN:O	20:CT:22:ARG:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:DX:65:ARG:HB2	43:DX:70:LEU:HD23	1.89	0.55
4:CD:108:LEU:HD13	4:CD:174:LEU:HD13	1.88	0.55
25:BA:847:A:OP1	25:BA:847:A:H8	1.89	0.55
30:DG:43:LEU:HD11	30:DG:153:ARG:HG2	1.89	0.55
1:CA:1131:G:H1	1:CA:1143:G:H21	1.54	0.55
26:DB:46:A:H2'	26:DB:47:C:H6	1.72	0.55
23:AY:6:G:O6	23:AY:7:A:N6	2.39	0.55
5:CE:33:VAL:HG13	5:CE:112:LEU:HD12	1.89	0.55
25:DA:1946:U:H2'	25:DA:1947:C:C6	2.41	0.55
1:CA:1179:A:H4'	9:CI:103:THR:HA	1.87	0.55
1:AA:1190:G:OP1	3:AC:5:ILE:N	2.36	0.55
37:DR:36:THR:HG22	37:DR:37:THR:N	2.20	0.55
1:AA:1173:G:H2'	1:AA:1174:G:C8	2.40	0.55
55:D9:22:ARG:NH1	55:D9:24:TYR:OH	2.40	0.55
19:AS:10:PHE:HE2	19:AS:37:ARG:HD3	1.71	0.55
25:DA:2378:A:H2'	38:DS:21:THR:HG21	1.88	0.55
25:BA:2303:U:H2'	25:BA:2304:C:C6	2.42	0.55
10:AJ:11:PHE:HE1	10:AJ:67:THR:HG22	1.71	0.55
12:AL:46:LYS:HD2	12:AL:94:PRO:HG3	1.89	0.55
25:BA:2457:G:OP1	29:BF:74:ARG:NH2	2.34	0.55
25:DA:1688:U:O2	25:DA:1700:A:H5'	2.06	0.55
2:CB:163:PHE:HA	2:CB:185:ILE:HG12	1.88	0.55
47:B1:89:GLU:O	47:B1:93:GLU:HG2	2.06	0.55
1:AA:839:U:H3'	1:AA:840:C:C6	2.40	0.55
25:BA:794:U:O2	25:BA:2036:A:H1'	2.06	0.55
10:CJ:55:LYS:O	10:CJ:57:LYS:N	2.39	0.55
36:DQ:18:LYS:O	36:DQ:98:LYS:NZ	2.27	0.55
25:DA:1020:A:N1	25:DA:1141:U:O2'	2.29	0.55
23:CW:52:G:H5''	36:DQ:56:ARG:NH2	2.21	0.55
1:CA:1218:C:H2'	1:CA:1219:U:C6	2.42	0.55
44:DY:87:LYS:HB3	44:DY:95:LYS:HD3	1.87	0.55
4:AD:173:TRP:HB2	4:AD:187:ARG:O	2.07	0.55
47:B1:23:LYS:HB3	47:B1:29:GLY:HA3	1.89	0.55
28:DE:77:ILE:HD13	28:DE:195:LEU:HD13	1.87	0.55
45:BZ:55:HIS:CE1	45:BZ:135:GLU:HG3	2.41	0.55
25:BA:346:A:OP1	29:BF:168:ARG:HD2	2.07	0.55
27:BD:242:ARG:HD3	27:BD:242:ARG:N	2.22	0.55
1:AA:1278:U:H5'	1:AA:1279:A:O4'	2.06	0.55
25:BA:1093:G:HO2'	25:BA:1094:A:H8	1.55	0.55
25:BA:1067:A:H62	25:BA:1186:U:H3	1.54	0.55
10:CJ:61:GLU:OE1	14:CN:58:LYS:NZ	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2568:C:H2'	25:BA:2569:G:O4'	2.07	0.55
1:AA:525:C:OP1	12:AL:89:ARG:NH1	2.39	0.55
31:DH:20:ALA:HB3	31:DH:23:ARG:HG3	1.88	0.55
39:DT:99:LEU:HD22	39:DT:101:PHE:HE1	1.71	0.55
25:BA:53:G:O2'	53:B7:35:ARG:HD3	2.06	0.55
25:DA:2291:U:H2'	25:DA:2292:C:C6	2.41	0.55
1:CA:1065:U:OP2	1:CA:1190:G:N2	2.39	0.55
45:DZ:54:HIS:NE2	45:DZ:123:ASP:OD2	2.39	0.55
39:BT:27:THR:HB	39:BT:90:GLN:HB3	1.89	0.55
25:DA:84:A:N1	25:DA:98:G:O2'	2.33	0.55
25:DA:2131:G:OP1	25:DA:2132:U:O2'	2.22	0.55
1:CA:1085:U:H3'	1:CA:1086:U:C5	2.42	0.55
23:AW:19:G:N1	23:AW:56:C:N4	2.47	0.55
25:DA:307:G:N1	25:DA:310:A:OP2	2.40	0.55
1:CA:344:A:H5'	1:CA:345:C:C5	2.41	0.55
25:DA:528:A:C2	25:DA:2042:A:H2'	2.42	0.55
25:BA:302:A:O2'	25:BA:303:C:OP1	2.19	0.55
25:BA:354:A:H2	25:BA:1255:A:O2'	1.88	0.55
25:DA:2114:A:N6	25:DA:2119:A:N7	2.54	0.55
23:CW:39:PSU:H2'	23:CW:40:C:C6	2.42	0.55
25:DA:142:A:N1	25:DA:1595:G:O2'	2.31	0.55
48:D2:22:GLU:OE2	48:D2:68:ARG:NH2	2.27	0.55
25:DA:819:A:C4	25:DA:1189:A:C2	2.94	0.55
1:AA:262:A:H2'	1:AA:263:A:C8	2.42	0.55
24:CX:2:G:O6	24:CX:71:C:N3	2.40	0.55
1:CA:328:C:H4'	1:CA:329:A:H5'	1.89	0.55
35:BP:64:LYS:HE3	54:B8:12:LYS:HD3	1.88	0.55
2:CB:16:HIS:O	2:CB:18:GLY:N	2.39	0.55
2:CB:16:HIS:CG	2:CB:17:PHE:N	2.74	0.55
1:CA:1162:C:N3	1:CA:1174:G:N2	2.48	0.55
12:CL:24:VAL:HG12	12:CL:27:LEU:HB2	1.88	0.55
26:DB:14:U:O3'	26:DB:108:U:O2'	2.25	0.55
25:BA:215:G:H21	25:BA:217:A:H62	1.53	0.55
9:CI:55:ALA:HA	9:CI:58:HIS:CD2	2.41	0.55
25:BA:2849:G:H5'	37:BR:46:GLY:HA2	1.89	0.55
25:BA:1040:C:OP1	40:BU:53:ARG:NH2	2.39	0.55
34:DO:1:MET:HG3	34:DO:67:LYS:HG2	1.88	0.55
25:DA:1264:G:H2'	25:DA:2014:A:N6	2.22	0.55
1:CA:999:C:H2'	1:CA:1000:U:C6	2.42	0.55
1:CA:1503:A:C4	22:CV:13:A:N6	2.74	0.55
1:CA:9:G:H2'	1:CA:10:A:H8	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:DZ:108:PRO:HB2	45:DZ:111:VAL:HG23	1.89	0.55
25:BA:1065:U:O2'	25:BA:1067:A:H2	1.89	0.55
1:CA:1132:C:H2'	1:CA:1133:G:C8	2.42	0.55
21:AU:5:ASP:O	21:AU:11:GLY:HA3	2.07	0.55
9:CI:125:TYR:HD1	9:CI:126:SER:N	2.05	0.55
4:AD:140:VAL:HG11	4:AD:146:ILE:HD11	1.89	0.55
31:BH:25:LYS:HG2	31:BH:34:GLU:HG2	1.88	0.55
25:BA:388:A:H2'	25:BA:389:G:C8	2.39	0.55
1:CA:1154:G:H2'	1:CA:1155:G:C8	2.42	0.55
1:CA:973:G:H3'	1:CA:974:A:H5''	1.88	0.55
1:AA:649:G:H2'	1:AA:650:G:H8	1.73	0.55
1:AA:181:G:H4'	1:AA:182:U:H5'	1.89	0.55
25:BA:2340:A:H2'	25:BA:2341:G:C8	2.41	0.55
5:AE:148:VAL:HG21	8:AH:107:LEU:HB3	1.88	0.55
25:DA:2136:C:O2'	25:DA:2137:C:O5'	2.24	0.55
25:BA:1269:G:N2	25:BA:1272:A:OP2	2.29	0.55
30:BG:115:ARG:HB3	30:BG:136:ARG:HH22	1.70	0.55
1:CA:1084:G:H5'	1:CA:1102:A:OP2	2.07	0.55
1:CA:1288:A:N3	1:CA:1352:C:O2'	2.36	0.55
20:CT:65:LYS:HA	20:CT:68:LYS:HD3	1.89	0.55
32:BI:77:LEU:HG	32:BI:101:LEU:HD23	1.89	0.55
20:CT:9:ASN:O	20:CT:10:LEU:HB2	2.06	0.54
25:BA:432:U:H6	25:BA:432:U:H5''	1.72	0.54
10:CJ:7:LYS:HG3	10:CJ:71:LEU:HD13	1.88	0.54
1:CA:1158:C:O2'	2:CB:133:LYS:NZ	2.40	0.54
25:DA:299:A:N1	25:DA:322:A:O2'	2.36	0.54
23:CY:1:G:H1	23:CY:72:C:H42	1.55	0.54
13:CM:88:ARG:HG3	13:CM:98:VAL:HG11	1.89	0.54
51:B5:58:LEU:HD23	51:B5:60:VAL:HG23	1.89	0.54
1:CA:1376:U:H2'	1:CA:1377:A:C8	2.43	0.54
1:AA:1223:C:OP2	19:AS:78:ARG:NH2	2.40	0.54
25:DA:2483:C:H2'	25:DA:2484:G:O4'	2.06	0.54
37:BR:67:LEU:HD13	37:BR:76:VAL:HG21	1.87	0.54
44:BY:28:LYS:HD2	44:BY:40:GLU:HG3	1.89	0.54
10:AJ:49:VAL:HG23	14:AN:41:ARG:HB2	1.87	0.54
41:DV:72:VAL:HG13	41:DV:85:LYS:HB3	1.89	0.54
25:BA:469:A:H1'	25:BA:1246:C:O4'	2.07	0.54
31:DH:42:ARG:NH1	31:DH:53:GLU:OE2	2.40	0.54
3:CC:20:SER:HB3	3:CC:22:TRP:HE1	1.72	0.54
39:BT:59:THR:HG23	39:BT:78:LEU:HB3	1.89	0.54
23:CW:27:G:H2'	23:CW:28:G:C8	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:2153:G:H2'	25:DA:2154:G:H8	1.72	0.54
25:DA:574:C:N3	28:DE:145:LYS:NZ	2.51	0.54
23:CY:9:A:O3'	23:CY:45:U:O2'	2.24	0.54
25:BA:1067:A:C8	25:BA:1068:G:H5''	2.40	0.54
1:AA:410:G:OP1	4:AD:30:LYS:NZ	2.24	0.54
25:DA:1429:G:H2'	25:DA:1430:C:H6	1.72	0.54
25:DA:2183:C:H2'	25:DA:2184:G:C8	2.43	0.54
25:DA:84:A:H5''	44:DY:8:LYS:HE3	1.90	0.54
27:DD:108:PRO:HB3	27:DD:143:HIS:CE1	2.42	0.54
5:CE:74:GLY:HA3	5:CE:116:THR:HG22	1.89	0.54
23:CY:5:G:H1	23:CY:68:C:H42	1.54	0.54
55:D9:14:CYS:HA	55:D9:27:CYS:HB2	1.87	0.54
2:AB:84:GLU:HB3	2:AB:219:VAL:HG21	1.90	0.54
8:AH:19:VAL:HG23	8:AH:21:LYS:HD3	1.89	0.54
25:DA:566:U:H5''	35:DP:29:LYS:HE3	1.89	0.54
24:AX:8:4SU:H6	24:AX:8:4SU:O5'	2.07	0.54
1:AA:630:G:H2'	1:AA:631:G:H8	1.72	0.54
1:AA:544:G:OP1	4:AD:59:ARG:NH2	2.32	0.54
23:CY:15:G:N1	23:CY:48:C:N3	2.45	0.54
25:BA:2162:C:O2	25:BA:2173:G:C2	2.61	0.54
1:AA:1052:U:H5''	1:AA:1053:G:OP2	2.08	0.54
33:BN:62:VAL:CG1	33:BN:66:LYS:HB2	2.38	0.54
13:AM:88:ARG:HG3	13:AM:98:VAL:CG1	2.37	0.54
47:D1:3:LYS:HB2	47:D1:61:ARG:NH1	2.23	0.54
25:BA:704:U:H2'	25:BA:705:C:C6	2.43	0.54
35:BP:83:VAL:HG13	35:BP:112:LEU:HD21	1.88	0.54
1:CA:340:U:H2'	1:CA:341:C:C6	2.42	0.54
1:AA:8:A:N6	4:AD:205:GLU:O	2.39	0.54
25:BA:714:U:O2	54:B8:2:PRO:HD2	2.07	0.54
25:BA:2812:A:N3	25:BA:2904:U:H1'	2.22	0.54
25:DA:2022:U:O2'	25:DA:2617:C:H5'	2.08	0.54
40:DU:66:ASN:O	40:DU:70:ARG:HG3	2.06	0.54
25:DA:2154:G:H2'	25:DA:2155:G:H5'	1.89	0.54
50:D4:14:ILE:HB	50:D4:22:ILE:HB	1.90	0.54
3:CC:164:ARG:NH1	3:CC:166:GLU:OE1	2.41	0.54
35:BP:100:LEU:HD12	35:BP:112:LEU:HD11	1.90	0.54
17:AQ:43:LEU:HD12	17:AQ:68:ARG:HG2	1.90	0.54
1:AA:461:A:O2'	1:AA:470:C:H5'	2.07	0.54
43:BX:43:VAL:HG21	43:BX:81:VAL:HG11	1.89	0.54
43:BX:53:LYS:HB3	43:BX:82:GLN:HB3	1.90	0.54
1:AA:100:C:H2'	1:AA:101:A:C8	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:2611:U:H5'	25:DA:2611:U:H6	1.72	0.54
1:AA:539:A:OP2	12:AL:115:LYS:NZ	2.40	0.54
23:CW:26:A:H2'	23:CW:27:G:C8	2.42	0.54
25:DA:2155:G:C5	25:DA:2156:G:H1'	2.43	0.54
25:BA:2162:C:N3	25:BA:2173:G:C6	2.76	0.54
28:DE:36:ARG:HD3	28:DE:85:ASN:HD21	1.73	0.54
38:BS:14:VAL:O	38:BS:18:ILE:HG12	2.07	0.54
45:BZ:145:GLU:H	45:BZ:148:ASP:HB2	1.73	0.54
10:CJ:63:PHE:HE1	14:CN:58:LYS:HG2	1.73	0.54
45:DZ:157:LEU:HB3	45:DZ:161:VAL:HG13	1.90	0.54
25:DA:882:G:O6	25:DA:893:C:N4	2.41	0.54
25:BA:2398:C:H2'	25:BA:2399:U:C6	2.43	0.54
4:AD:178:VAL:HG12	4:AD:179:GLU:H	1.72	0.54
9:CI:45:ALA:HA	9:CI:48:GLU:HB2	1.89	0.54
1:CA:736:C:H2'	1:CA:737:A:C8	2.41	0.54
25:BA:2416:C:O3'	35:BP:77:ARG:NH2	2.37	0.54
35:DP:121:LYS:O	35:DP:123:LEU:N	2.40	0.54
20:CT:57:ARG:HH22	20:CT:100:ILE:HD12	1.72	0.54
8:CH:121:ASP:OD1	8:CH:121:ASP:N	2.39	0.54
25:DA:2503:A:O2'	25:DA:2505:G:OP2	2.17	0.54
1:CA:997:U:H3	1:CA:1044:A:H61	1.53	0.54
23:CW:4:C:H42	23:CW:68:C:H42	1.55	0.54
25:DA:1693:U:O2'	27:DD:14:ARG:NH2	2.41	0.54
1:AA:664:G:N2	1:AA:741:G:H1	2.02	0.54
1:CA:664:G:N2	1:CA:741:G:H1	2.03	0.54
4:CD:112:VAL:HG13	4:CD:161:ASN:OD1	2.08	0.54
1:CA:1305:G:N2	1:CA:1331:G:H1'	2.23	0.54
25:BA:1065:U:H3	25:BA:1188:A:H62	1.56	0.54
33:DN:4:TYR:HB2	40:DU:101:ARG:HH12	1.72	0.54
33:DN:15:LEU:HB2	33:DN:135:PRO:HB2	1.89	0.54
30:DG:115:ARG:HG3	30:DG:136:ARG:HH21	1.73	0.54
9:CI:50:LEU:HD21	9:CI:81:ILE:HD11	1.90	0.54
25:DA:332:A:O2'	25:DA:334:C:OP2	2.20	0.54
25:DA:1802:A:N1	25:DA:1822:G:H1'	2.23	0.54
2:AB:102:LEU:HB3	2:AB:180:LEU:HD12	1.89	0.54
50:B4:33:VAL:HG12	50:B4:35:VAL:H	1.73	0.54
40:BU:79:PHE:CE2	40:BU:83:LEU:HD21	2.43	0.54
25:BA:1553:A:O2'	25:BA:1554:A:O4'	2.26	0.54
23:AY:7:A:O2'	23:AY:49:C:H5'	2.07	0.54
1:AA:1502:A:H2	1:AA:1505:G:N1	2.01	0.54
25:BA:1248:G:OP2	25:BA:1249:A:O2'	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AY:63:G:H2'	23:AY:64:A:O4'	2.08	0.54
36:BQ:14:ARG:HG2	36:BQ:41:TRP:HH2	1.73	0.54
1:CA:1299:A:H2'	1:CA:1299:A:N3	2.23	0.54
7:AG:113:GLU:HG3	7:AG:118:VAL:HG12	1.89	0.54
1:CA:1029:C:N4	1:CA:1032:G:C6	2.76	0.54
25:DA:10:G:H2'	25:DA:11:G:H8	1.72	0.54
1:CA:671:G:H5'	6:CF:77:ARG:HH22	1.73	0.54
34:BO:91:LEU:HB3	34:BO:111:PHE:CE1	2.43	0.54
25:BA:909:G:H2'	25:BA:910:A:O4'	2.08	0.54
7:CG:51:GLN:O	7:CG:55:GLY:HA2	2.08	0.54
1:CA:728:A:H2'	1:CA:729:A:C8	2.43	0.54
25:BA:397:G:OP1	25:BA:430:U:N3	2.23	0.54
1:CA:129(A):G:C6	1:CA:189(E):U:H4'	2.42	0.54
41:DV:43:GLU:OE2	41:DV:43:GLU:N	2.41	0.54
1:AA:991:U:O2'	1:AA:992:U:OP2	2.24	0.54
44:BY:5:MET:HE1	44:BY:32:PRO:HA	1.90	0.54
1:CA:1513:A:H2'	1:CA:1514:C:C6	2.42	0.54
1:CA:1002:G:C4	1:CA:1003:G:C8	2.96	0.54
23:AY:62:C:H2'	23:AY:63:G:H8	1.71	0.54
28:DE:72:VAL:HA	28:DE:73:GLU:CB	2.37	0.54
9:AI:26:VAL:HG22	9:AI:61:ALA:HB3	1.90	0.54
25:DA:1006:C:C2	25:DA:1138:G:N2	2.76	0.54
1:AA:382:A:H2'	1:AA:383:A:H8	1.73	0.54
25:DA:918:A:H5''	26:DB:98:G:O2'	2.08	0.54
52:D6:13:CYS:SG	52:D6:47:THR:HG21	2.47	0.54
12:CL:46:LYS:NZ	12:CL:91:LYS:O	2.40	0.54
37:BR:56:LYS:NZ	37:BR:90:ARG:O	2.41	0.54
42:DW:79:GLY:HA3	42:DW:100:THR:HG22	1.90	0.54
25:DA:1669:A:H5''	25:DA:2550:G:OP1	2.07	0.54
14:CN:21:TYR:HE2	14:CN:23:ARG:NE	2.05	0.54
23:AY:21:A:O2'	23:AY:22:G:OP1	2.26	0.54
6:AF:97:PHE:CD2	18:AR:31:LEU:HD12	2.43	0.54
13:AM:87:TYR:O	13:AM:91:ARG:HG2	2.08	0.54
41:DV:24:LYS:HG3	41:DV:64:HIS:HD2	1.73	0.54
54:B8:42:ARG:HD2	61:B8:206:HOH:O	2.08	0.54
25:BA:1314:A:H2'	25:BA:1315:A:O4'	2.08	0.54
25:BA:843:C:H2'	25:BA:844:C:C6	2.43	0.54
33:DN:67:LEU:HD13	33:DN:87:LEU:HD13	1.89	0.54
25:DA:2108:C:H2'	25:DA:2109:U:H5'	1.89	0.54
30:DG:49:ASP:N	30:DG:49:ASP:OD1	2.40	0.54
8:AH:34:GLU:OE1	8:AH:37:ARG:NH1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:84:U:H4'	1:CA:89:C:N3	2.23	0.54
29:BF:195:ASP:HB3	29:BF:198:ALA:H	1.70	0.54
50:D4:16:CYS:SG	50:D4:17:GLY:N	2.81	0.54
50:D4:26:SER:OG	50:D4:27:THR:N	2.41	0.54
23:AW:19:G:H4'	23:AW:20:U:OP1	2.08	0.53
23:CY:53:G:C8	23:CY:54:5MU:H72	2.43	0.53
19:AS:20:LEU:HD23	19:AS:23:ASN:HD22	1.74	0.53
1:AA:1509:C:H2'	1:AA:1510:U:O4'	2.08	0.53
25:DA:890:A:H2'	25:DA:892:G:H8	1.72	0.53
25:DA:2846:G:N7	61:DA:4362:HOH:O	2.33	0.53
27:DD:232:PRO:O	61:DD:404:HOH:O	2.19	0.53
14:AN:23:ARG:NH1	14:AN:30:ALA:HB2	2.23	0.53
1:AA:1399:C:C2	1:AA:1502:A:N6	2.76	0.53
1:AA:714:G:H2'	1:AA:715:A:C8	2.44	0.53
36:DQ:16:ARG:HG2	36:DQ:18:LYS:HE2	1.89	0.53
51:B5:48:GLU:O	51:B5:60:VAL:HG11	2.08	0.53
8:CH:41:ARG:NH2	8:CH:123:GLU:OE2	2.40	0.53
25:DA:2552:U:H2'	25:DA:2554:U:H5''	1.91	0.53
1:AA:527:G:O2'	1:AA:535:A:N1	2.29	0.53
25:DA:315:G:H2'	25:DA:316:C:C6	2.43	0.53
1:CA:1004:A:H5''	1:CA:1025:U:C5	2.42	0.53
10:AJ:38:ILE:HD11	10:AJ:71:LEU:HD23	1.90	0.53
19:CS:30:LEU:HD11	19:CS:50:ALA:HB2	1.90	0.53
28:DE:72:VAL:HG22	28:DE:73:GLU:HG2	1.91	0.53
27:DD:71:ASP:HB3	27:DD:103:ARG:NH2	2.23	0.53
51:B5:16:ARG:NH1	51:B5:17:ASP:OD1	2.42	0.53
23:AY:2:C:N4	23:AY:71:G:H1	2.05	0.53
30:DG:11:TYR:HB2	30:DG:176:LEU:HD21	1.90	0.53
1:AA:390:C:H2'	1:AA:391:G:C8	2.43	0.53
25:BA:272:U:H4'	32:BI:50:ARG:HH12	1.73	0.53
30:DG:46:ALA:HB2	30:DG:53:LEU:HD12	1.90	0.53
10:AJ:78:ASN:O	10:AJ:80:LYS:N	2.40	0.53
1:AA:1060:C:C5	3:AC:2:GLY:HA3	2.43	0.53
1:AA:194:C:O3'	20:AT:68:LYS:HD2	2.08	0.53
25:DA:30:G:H2'	25:DA:31:C:C6	2.43	0.53
34:BO:2:ILE:HD12	34:BO:6:THR:HG21	1.90	0.53
25:BA:1211:U:H2'	25:BA:1212:C:C6	2.44	0.53
25:BA:1033:G:O2'	25:BA:1046:A:N3	2.37	0.53
24:AX:64:G:O2'	36:BQ:10:ARG:NH2	2.41	0.53
6:CF:33:TYR:HE1	6:CF:74:ASP:HB3	1.74	0.53
2:AB:71:VAL:HB	2:AB:164:VAL:HG13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:BR:33:ARG:NH2	51:B5:57:VAL:O	2.38	0.53
25:BA:1834:A:O2'	27:BD:259:THR:HG21	2.08	0.53
2:CB:144:ARG:NH2	2:CB:148:TYR:OH	2.41	0.53
25:BA:1218:G:O2'	25:BA:1219:A:O4'	2.26	0.53
8:CH:19:VAL:HG23	8:CH:21:LYS:HD3	1.90	0.53
8:CH:68:ARG:NH1	8:CH:74:PRO:HB3	2.24	0.53
57:CA:3174:NEG:H2	25:DA:1954:G:H3'	1.91	0.53
25:DA:300:A:P	44:DY:86:ARG:HH22	2.32	0.53
25:DA:200:U:O2	25:DA:386:G:N2	2.41	0.53
25:DA:2693:A:H2'	25:DA:2694:G:H8	1.74	0.53
25:BA:2584:A:N7	28:BE:145:LYS:HB2	2.23	0.53
38:DS:27:SER:HA	38:DS:88:ASP:HB3	1.90	0.53
51:B5:11:THR:HG23	51:B5:15:ARG:HB3	1.90	0.53
3:AC:124:ILE:HD12	3:AC:196:LEU:HD12	1.90	0.53
25:BA:1874:C:H5'	27:BD:253:GLN:NE2	2.23	0.53
29:BF:53:THR:HG22	29:BF:55:GLY:H	1.73	0.53
1:CA:235:C:H5'	17:CQ:70:ARG:HG2	1.89	0.53
25:DA:1462:C:H4'	25:DA:2703:C:H5'	1.91	0.53
23:CY:36:A:H2'	23:CY:37:MIA:O4'	2.08	0.53
23:AW:58:A:O2'	23:AW:60:U:OP2	2.19	0.53
25:DA:568:U:H5'	25:DA:945:A:C6	2.44	0.53
17:AQ:66:SER:O	17:AQ:70:ARG:NH1	2.41	0.53
1:CA:1125:U:C2	10:CJ:38:ILE:HD13	2.44	0.53
45:DZ:117:LEU:HD23	45:DZ:119:GLU:HG2	1.91	0.53
13:AM:93:ARG:HB3	25:BA:935:C:OP1	2.08	0.53
25:BA:2320:G:O2'	25:BA:2322:A:N7	2.37	0.53
4:CD:25:ARG:NH1	4:CD:30:LYS:O	2.41	0.53
1:AA:1239:A:H4'	1:AA:1240:U:H5''	1.90	0.53
25:BA:1715:A:H4'	25:BA:1716:A:O5'	2.09	0.53
45:BZ:126:VAL:HG11	45:BZ:161:VAL:HG23	1.90	0.53
1:AA:757:U:H2'	1:AA:758:G:O4'	2.08	0.53
34:DO:120:GLU:HB2	39:DT:68:TYR:HE2	1.74	0.53
1:CA:1106:G:H5''	3:CC:172:ARG:HG2	1.90	0.53
1:AA:1323:G:H2'	1:AA:1324:A:C8	2.43	0.53
39:DT:117:ASP:OD2	39:DT:120:ARG:NE	2.29	0.53
25:BA:1076:G:OP2	36:BQ:128:LYS:NZ	2.42	0.53
1:CA:1157:A:H4'	1:CA:1158:C:O5'	2.09	0.53
1:AA:1352:C:OP1	21:AU:3:LYS:NZ	2.34	0.53
7:AG:78:ARG:NH1	7:AG:79:ARG:HH21	2.07	0.53
25:DA:2359:C:H2'	25:DA:2360:A:O4'	2.09	0.53
1:AA:973:G:H3'	1:AA:974:A:H5''	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:906:G:N2	25:DA:907:U:O2	2.41	0.53
1:CA:21:G:H2'	1:CA:22:G:C8	2.44	0.53
10:CJ:35:SER:HB3	10:CJ:73:ASP:HB2	1.89	0.53
25:BA:1846:A:OP2	27:BD:54:ARG:NH2	2.37	0.53
25:DA:2627:G:N2	25:DA:2777:G:OP2	2.41	0.53
25:DA:1653:G:H3'	37:DR:2:ARG:HD3	1.90	0.53
9:AI:24:GLY:HA2	9:AI:59:PHE:O	2.08	0.53
42:BW:25:ARG:NH2	42:BW:74:ALA:O	2.38	0.53
3:AC:33:LEU:HD12	3:AC:37:GLN:HE22	1.74	0.53
54:B8:63:PRO:HG2	54:B8:64:TYR:CE2	2.44	0.53
15:CO:25:THR:HG21	15:CO:70:LEU:HB2	1.91	0.53
50:B4:53:GLU:C	50:B4:55:ARG:H	2.10	0.53
25:DA:845:G:HO2'	25:DA:846:C:H5	1.54	0.53
5:CE:50:GLU:HB2	5:CE:53:LEU:HD13	1.90	0.53
25:BA:2407:C:O2'	47:B1:30:VAL:HG22	2.08	0.53
25:DA:2061:G:H5''	25:DA:2503:A:C2	2.44	0.53
1:CA:520:A:N1	1:CA:536:C:H1'	2.24	0.53
1:CA:1307:U:H2'	1:CA:1308:U:C6	2.44	0.53
25:DA:1550:C:H5'	25:DA:1742:G:N2	2.24	0.53
25:BA:2420:U:H2'	25:BA:2421:G:C8	2.43	0.53
8:AH:13:ILE:O	8:AH:17:THR:HG23	2.09	0.53
41:DV:6:LYS:HB2	41:DV:38:LEU:HD21	1.91	0.53
1:CA:427:U:OP1	4:CD:13:ARG:NH2	2.41	0.53
1:CA:1324:A:O4'	1:CA:1362:C:H4'	2.09	0.53
25:DA:331:A:OP1	25:DA:1209:G:N2	2.40	0.53
21:AU:3:LYS:HB3	21:AU:14:TRP:CG	2.43	0.53
25:DA:573:G:OP2	41:DV:78:LYS:NZ	2.40	0.53
29:DF:24:LEU:HD21	29:DF:114:VAL:HG12	1.91	0.53
24:CX:50:U:H3	24:CX:64:G:H1	1.56	0.53
25:DA:2808:U:C2'	25:DA:2809:A:H5'	2.39	0.53
9:AI:28:VAL:HA	9:AI:63:ILE:O	2.08	0.53
31:DH:90:LYS:HD2	31:DH:163:TYR:CD1	2.43	0.53
25:DA:566:U:P	41:DV:80:GLN:HE21	2.32	0.53
25:BA:1074:A:N6	25:BA:1171:G:H2'	2.24	0.53
36:BQ:109:VAL:HG13	36:BQ:113:GLN:HB3	1.90	0.53
1:CA:376:G:H5''	16:CP:5:ARG:HB2	1.90	0.53
23:CY:59:U:O5'	23:CY:59:U:H6	1.92	0.53
13:CM:3:ARG:HE	13:CM:4:ILE:HG22	1.74	0.53
25:DA:140:G:N2	25:DA:1596:A:H4'	2.24	0.53
25:DA:885:C:H2'	25:DA:886:C:H4'	1.90	0.53
25:DA:903:C:H2'	25:DA:904:C:C6	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:DT:85:LYS:NZ	39:DT:87:ASP:OD2	2.42	0.53
25:DA:1013:C:H2'	25:DA:1014:U:H6	1.74	0.53
3:CC:150:LYS:HG3	3:CC:169:ALA:HB2	1.91	0.53
29:DF:34:TRP:CE2	35:DP:8:PRO:HG3	2.44	0.53
52:B6:14:THR:HB	52:B6:48:VAL:O	2.09	0.53
43:BX:5:TYR:CZ	48:B2:30:ARG:HB2	2.44	0.53
5:AE:45:PHE:CD2	5:AE:47:LYS:HE2	2.44	0.53
3:CC:42:LEU:O	3:CC:46:GLU:HG2	2.09	0.53
25:DA:81:G:HO2'	25:DA:295:G:HO2'	1.57	0.53
1:CA:222:U:H2'	1:CA:223:U:C6	2.43	0.53
23:CW:28:G:C2	23:CW:29:G:H1'	2.44	0.53
2:CB:95:GLN:HB2	2:CB:148:TYR:HD1	1.74	0.53
44:BY:92:ASN:N	44:BY:93:GLY:HA2	2.24	0.53
57:CA:3174:NEG:H11	25:DA:1955:U:OP2	2.08	0.53
23:CY:9:A:H5'	23:CY:46:7MG:O4'	2.08	0.53
25:DA:375:C:H2'	25:DA:376:C:C6	2.44	0.53
30:DG:114:ILE:HG23	30:DG:136:ARG:NH2	2.24	0.53
37:DR:2:ARG:NH1	37:DR:5:LYS:O	2.42	0.53
1:CA:988:G:H2'	1:CA:989:C:O4'	2.09	0.53
1:AA:642:A:N3	8:AH:113:SER:OG	2.41	0.53
25:BA:2762:A:P	31:BH:3:ARG:HH21	2.32	0.53
40:BU:58:ARG:HA	40:BU:61:TRP:CE3	2.44	0.53
23:AY:40:C:H2'	23:AY:41:C:H6	1.73	0.53
17:CQ:95:TYR:HA	17:CQ:98:LEU:HD12	1.90	0.53
25:DA:2689:U:OP1	25:DA:2719:G:N1	2.37	0.52
57:CA:3175:NEG:C7	25:DA:739:G:H1	2.21	0.52
5:AE:33:VAL:HG13	5:AE:112:LEU:HD12	1.90	0.52
13:CM:23:TYR:O	13:CM:67:GLU:N	2.41	0.52
25:BA:1255:A:H5''	25:BA:1257:G:O4'	2.09	0.52
25:DA:1027:A:C2	25:DA:2488:A:H5'	2.45	0.52
25:DA:1300:U:H4'	25:DA:1301:A:C5'	2.39	0.52
28:DE:12:THR:HG23	39:DT:58:ASN:OD1	2.10	0.52
36:DQ:85:LYS:HB2	46:D0:7:LEU:HD12	1.91	0.52
18:AR:58:LEU:HB3	18:AR:62:GLU:HG3	1.91	0.52
4:AD:22:LYS:HB2	4:AD:26:CYS:SG	2.48	0.52
20:AT:57:ARG:HH12	20:AT:100:ILE:HD12	1.73	0.52
25:DA:272:G:H4'	25:DA:272(A):U:H5''	1.91	0.52
2:AB:76:GLN:H	2:AB:76:GLN:CD	2.13	0.52
11:AK:84:VAL:HG11	11:AK:91:ARG:HD2	1.91	0.52
23:AY:8:4SU:H4'	23:AY:48:C:H4'	1.91	0.52
25:BA:1787:G:H4'	25:BA:1789:G:O4'	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2162:C:H2'	25:BA:2173:G:N2	2.24	0.52
25:DA:1166:C:H1'	25:DA:1184:G:N2	2.23	0.52
25:DA:184:C:H2'	25:DA:185:U:H6	1.74	0.52
23:CW:76:A:H8	25:DA:2602:A:H61	1.56	0.52
2:AB:174:VAL:HG13	2:AB:184:VAL:HG11	1.91	0.52
20:AT:57:ARG:HH22	20:AT:100:ILE:HD12	1.75	0.52
1:AA:458:C:H2'	1:AA:460:G:O4'	2.08	0.52
25:DA:337:C:H2'	25:DA:338:G:O4'	2.09	0.52
25:DA:651:G:H4'	54:D8:18:ALA:HB3	1.91	0.52
8:CH:56:LYS:HB2	8:CH:58:TYR:HE1	1.74	0.52
19:CS:12:ASP:HB2	19:CS:38:SER:OG	2.09	0.52
25:DA:910:A:H62	36:DQ:12:GLN:HA	1.73	0.52
1:AA:1077:G:N2	1:AA:1080:A:OP2	2.40	0.52
25:DA:679:C:H2'	25:DA:680:G:H8	1.75	0.52
25:DA:2142:C:O2	25:DA:2149:G:N1	2.29	0.52
25:BA:139:A:C8	25:BA:1454:C:O2'	2.60	0.52
1:CA:1031:G:H2'	1:CA:1032:G:C8	2.45	0.52
25:DA:1278:A:OP1	37:DR:36:THR:HG23	2.08	0.52
25:DA:2472:G:H2'	25:DA:2475:C:N4	2.24	0.52
23:CY:25:C:H2'	23:CY:26:A:C8	2.44	0.52
25:BA:742:G:OP1	25:BA:1426:G:O2'	2.25	0.52
25:BA:2584:A:N7	28:BE:144:ARG:HD2	2.25	0.52
29:DF:34:TRP:CZ2	35:DP:8:PRO:HG3	2.45	0.52
12:AL:70:ILE:HG12	12:AL:100:ILE:HD12	1.91	0.52
25:DA:2055:C:H1'	28:DE:145:LYS:HE2	1.90	0.52
25:DA:2386:C:H4'	46:D0:56:ASP:HA	1.92	0.52
27:BD:121:PRO:HB3	27:BD:135:PHE:CE2	2.44	0.52
3:AC:164:ARG:HD2	3:AC:166:GLU:HG2	1.91	0.52
25:BA:63:A:O3'	43:BX:71:GLY:HA3	2.10	0.52
29:DF:178:PRO:HB3	29:DF:198:ALA:HA	1.91	0.52
25:DA:1151:G:H4'	40:DU:81:HIS:CG	2.45	0.52
25:BA:191:U:OP1	61:BA:4936:HOH:O	2.19	0.52
25:DA:1608:A:H1'	25:DA:1610:A:OP2	2.08	0.52
34:DO:2:ILE:HD12	34:DO:6:THR:HG21	1.90	0.52
25:BA:2236:G:H4'	25:BA:2238:C:C2	2.45	0.52
1:CA:748:C:H4'	1:CA:749:C:O5'	2.10	0.52
36:BQ:85:LYS:HG2	46:B0:7:LEU:HB3	1.92	0.52
25:DA:1374:G:H2'	25:DA:1375:C:C6	2.45	0.52
25:BA:2159:C:N3	25:BA:2176:G:O6	2.41	0.52
30:DG:72:ARG:NH1	30:DG:87:PRO:HG3	2.23	0.52
12:AL:117:ARG:HB3	12:AL:122:THR:HB	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:2882:A:OP1	37:DR:96:ARG:NE	2.31	0.52
16:CP:19:ILE:HG22	16:CP:36:ILE:HG13	1.91	0.52
2:CB:30:ARG:NH2	2:CB:195:ASP:OD1	2.43	0.52
25:BA:1093:G:H2'	25:BA:1156:G:N2	2.25	0.52
2:CB:158:LEU:HD21	2:CB:180:LEU:HD13	1.90	0.52
10:CJ:5:ARG:N	61:CJ:5101:HOH:O	2.42	0.52
34:DO:80:ASP:OD1	39:DT:64:ARG:NH2	2.43	0.52
26:DB:114:C:H4'	38:DS:46:VAL:HG22	1.90	0.52
1:CA:1317:C:OP1	14:CN:17:LYS:HG2	2.10	0.52
1:CA:1317:C:H42	14:CN:19:ARG:HH21	1.57	0.52
25:DA:108:U:H2'	25:DA:109:G:H8	1.75	0.52
25:DA:2625:G:H2'	25:DA:2626:C:O4'	2.10	0.52
25:DA:1427:A:H4'	25:DA:1428:C:O5'	2.08	0.52
25:DA:521:G:H2'	25:DA:522:G:H8	1.75	0.52
44:DY:90:LEU:HB3	44:DY:92:ASN:H	1.75	0.52
25:DA:1477:A:H2'	25:DA:1478:G:O4'	2.09	0.52
3:CC:3:ASN:N	3:CC:3:ASN:OD1	2.41	0.52
25:DA:117:G:OP2	25:DA:119:A:O2'	2.27	0.52
25:DA:2117:A:N6	25:DA:2171:A:N1	2.58	0.52
25:BA:2163:G:C4	25:BA:2164:C:H1'	2.44	0.52
1:CA:1239:A:H62	1:CA:1299:A:N6	2.07	0.52
26:DB:19:G:H2'	26:DB:20:C:O4'	2.10	0.52
41:BV:76:LYS:HB2	41:BV:81:TYR:HB3	1.92	0.52
3:CC:148:GLY:HA3	3:CC:172:ARG:O	2.10	0.52
1:AA:1080:A:H5'	5:AE:14:ARG:HH21	1.73	0.52
25:DA:1932:A:H2'	25:DA:1933:G:O4'	2.09	0.52
25:DA:516:C:OP1	51:D5:13:LYS:NZ	2.35	0.52
25:BA:223:C:H2'	25:BA:224:U:H6	1.74	0.52
40:BU:114:LYS:HA	40:BU:117:GLN:HE21	1.73	0.52
45:DZ:5:LEU:HD23	45:DZ:47:VAL:HG21	1.91	0.52
1:CA:554:C:H2'	1:CA:555:C:C6	2.44	0.52
13:AM:123:ALA:HB2	23:AW:39:PSU:H1'	1.91	0.52
25:BA:776:G:C6	27:BD:208:LYS:HB2	2.45	0.52
2:CB:137:ARG:HB3	2:CB:137:ARG:CZ	2.39	0.52
1:AA:1024:G:H2'	1:AA:1025:U:H5''	1.92	0.52
1:AA:1145:C:H4'	1:AA:1146:A:H5'	1.91	0.52
20:CT:10:LEU:HD22	20:CT:12:ALA:HB2	1.91	0.52
36:BQ:35:VAL:HG13	36:BQ:130:LYS:HB3	1.90	0.52
28:DE:72:VAL:HG13	28:DE:73:GLU:O	2.10	0.52
45:BZ:70:LEU:HG	45:BZ:91:LEU:HD21	1.91	0.52
10:AJ:13:HIS:HA	10:AJ:16:LEU:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1346:A:N6	1:CA:1375:A:OP2	2.43	0.52
36:DQ:16:ARG:HG3	36:DQ:17:LEU:H	1.75	0.52
5:AE:110:LEU:HD13	5:AE:118:ILE:HD13	1.90	0.52
30:DG:15:VAL:HG13	30:DG:175:LEU:HD23	1.91	0.52
25:DA:1665:A:H4'	34:DO:67:LYS:HB2	1.92	0.52
25:BA:2274:U:OP1	25:BA:2399:U:O2'	2.20	0.52
50:B4:16:CYS:SG	50:B4:17:GLY:N	2.83	0.52
25:BA:2262:G:OP1	36:BQ:85:LYS:NZ	2.37	0.52
44:DY:28:LYS:HD2	44:DY:40:GLU:HG3	1.92	0.52
25:DA:1341:U:OP1	25:DA:1397:U:N3	2.34	0.52
9:CI:51:ARG:HG2	9:CI:56:LEU:HD21	1.92	0.52
25:BA:1921:G:H2'	25:BA:1921:G:N3	2.23	0.52
1:AA:10:A:HO2'	1:AA:507:C:HO2'	1.58	0.52
25:BA:2021:C:H4'	25:BA:2736:C:O2	2.09	0.52
32:DI:140:LEU:HD13	32:DI:142:VAL:HG22	1.91	0.52
25:BA:1501:U:O2'	25:BA:1502:G:N7	2.37	0.52
2:CB:179:LYS:HA	8:CH:72:PRO:HG3	1.90	0.52
25:BA:1185:C:O3'	33:BN:25:ARG:NH1	2.43	0.52
57:AA:3216:NEG:N4	57:AA:3216:NEG:H11	2.24	0.52
1:CA:839:U:H5''	1:CA:840:C:C5	2.43	0.52
19:AS:20:LEU:HA	19:AS:23:ASN:HD22	1.75	0.52
31:BH:69:ARG:HG3	31:BH:70:THR:N	2.24	0.52
50:D4:59:PHE:HA	50:D4:61:ARG:N	2.24	0.52
25:BA:2846:U:H2'	25:BA:2847:G:C8	2.45	0.52
1:AA:1218:C:H2'	1:AA:1219:U:C6	2.45	0.52
39:DT:95:ARG:HG2	39:DT:95:ARG:HH11	1.75	0.52
8:AH:41:ARG:NH2	8:AH:123:GLU:OE2	2.43	0.52
1:CA:1004:A:C8	1:CA:1005:A:H4'	2.40	0.52
25:BA:927:G:H2'	25:BA:928:G:C8	2.44	0.52
1:AA:841:U:C5	1:AA:848:C:H1'	2.45	0.52
10:CJ:77:PRO:O	10:CJ:81:THR:OG1	2.16	0.52
36:BQ:16:ARG:HG3	36:BQ:17:LEU:H	1.75	0.52
2:CB:127:ILE:O	2:CB:128:GLU:HB2	2.09	0.52
25:DA:1991:U:H2'	25:DA:1992:G:H5''	1.91	0.52
25:DA:744:G:OP1	28:DE:132:HIS:ND1	2.35	0.52
1:CA:91:C:H2'	1:CA:92:C:C6	2.45	0.52
11:AK:99:GLN:HG2	11:AK:105:VAL:HG21	1.91	0.52
1:CA:309:G:O2'	1:CA:607:A:N1	2.40	0.52
23:CW:25:C:H2'	23:CW:26:A:H8	1.74	0.52
1:AA:72:C:N3	1:AA:97:G:N2	2.46	0.52
1:CA:1028:C:N3	1:CA:1033:G:C6	2.78	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:CG:26:PHE:CE1	7:CG:30:ILE:HD11	2.44	0.52
1:AA:1152:A:H5'	10:AJ:13:HIS:CG	2.45	0.52
2:CB:122:PHE:HA	2:CB:127:ILE:HD12	1.90	0.52
40:DU:79:PHE:HE2	40:DU:95:LEU:HD21	1.75	0.52
25:DA:601:C:OP1	29:DF:108:LYS:NZ	2.33	0.52
1:AA:56:U:H2'	1:AA:57:G:C8	2.45	0.52
34:BO:80:ASP:OD2	39:BT:64:ARG:NH2	2.42	0.52
19:CS:20:LEU:HA	19:CS:23:ASN:HD22	1.75	0.52
1:AA:292:G:C5	1:AA:293:G:H1'	2.44	0.52
1:CA:1401:G:C2	1:CA:1402:C:H1'	2.45	0.52
1:AA:636:U:H5''	17:AQ:2:PRO:HG3	1.91	0.52
1:CA:1027:C:H2'	1:CA:1028:C:C5	2.45	0.51
1:AA:741:G:H2'	1:AA:742:G:O4'	2.09	0.51
26:DB:66:A:H61	26:DB:108:U:H3'	1.75	0.51
25:DA:528:A:N1	25:DA:2042:A:H2'	2.25	0.51
29:DF:192:LEU:HD22	29:DF:194:MET:HG3	1.91	0.51
25:DA:2815:C:H2'	25:DA:2816:C:C6	2.45	0.51
1:CA:817:C:OP2	61:CA:4058:HOH:O	2.19	0.51
1:AA:1060:C:OP1	14:AN:45:ARG:NH2	2.39	0.51
25:BA:1809:U:H2'	25:BA:1815:A:N6	2.25	0.51
25:BA:2474:U:H1'	25:BA:2503:U:O4	2.10	0.51
1:AA:1302:U:C5	13:AM:17:VAL:HG21	2.45	0.51
1:AA:405:U:O4	4:AD:2:GLY:N	2.43	0.51
50:B4:26:SER:OG	50:B4:27:THR:N	2.43	0.51
47:B1:64:ALA:HA	47:B1:67:ILE:HG13	1.92	0.51
1:AA:1435:G:H2'	1:AA:1436:U:C6	2.45	0.51
25:BA:1320:A:N3	25:BA:1343:C:H1'	2.24	0.51
33:DN:38:HIS:CE1	33:DN:39:ARG:HG3	2.45	0.51
42:BW:14:PRO:HG2	42:BW:78:GLU:CG	2.38	0.51
1:AA:154:C:H2'	1:AA:155:C:H6	1.76	0.51
57:CA:3174:NEG:N3	25:DA:1946:U:OP2	2.44	0.51
31:BH:84:SER:OG	31:BH:132:ARG:NH1	2.43	0.51
23:AY:1:G:H2'	23:AY:2:C:C6	2.45	0.51
1:CA:1062:U:H2'	1:CA:1063:C:C6	2.45	0.51
3:CC:134:ILE:HG22	3:CC:168:ALA:HB3	1.93	0.51
1:AA:383:A:C5	1:AA:384:G:H1'	2.45	0.51
4:CD:61:LYS:HZ1	4:CD:72:GLU:CD	2.13	0.51
1:AA:921:U:O2	5:AE:19:MET:HB2	2.10	0.51
25:DA:890:A:H2'	25:DA:892:G:C8	2.44	0.51
25:DA:2343:C:HO2'	25:DA:2373:G:HO2'	1.59	0.51
45:DZ:29:TYR:HB3	45:DZ:34:ASN:HD22	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:1386:C:H2'	25:DA:1387:C:C6	2.45	0.51
25:DA:855:G:C6	25:DA:856:C:C4	2.98	0.51
28:DE:101:ARG:CZ	28:DE:171:GLU:HB2	2.40	0.51
8:AH:49:GLU:HG2	8:AH:62:TYR:HE1	1.75	0.51
25:DA:1220:A:OP2	40:DU:19:LYS:NZ	2.30	0.51
25:DA:1316:U:H2'	25:DA:1317:A:C8	2.45	0.51
23:AW:43:C:H2'	23:AW:44:G:C8	2.45	0.51
1:AA:1392:G:H21	1:AA:1502:A:H8	1.57	0.51
23:CY:62:C:H2'	23:CY:63:G:C8	2.42	0.51
25:DA:1815:A:H8	25:DA:1815:A:OP1	1.92	0.51
1:AA:449:C:H5''	1:AA:450:G:OP2	2.10	0.51
25:DA:252:G:P	35:DP:50:ARG:HH12	2.33	0.51
4:CD:173:TRP:HB2	4:CD:187:ARG:O	2.10	0.51
40:BU:79:PHE:O	40:BU:83:LEU:HD22	2.10	0.51
25:DA:2882:A:H5'	37:DR:96:ARG:HG3	1.90	0.51
25:BA:174:U:H4'	25:BA:207:A:H4'	1.91	0.51
25:BA:1431:G:O2'	25:BA:1442:U:O2	2.22	0.51
25:DA:1235:G:C6	25:DA:1236:G:N1	2.78	0.51
40:DU:83:LEU:HD12	40:DU:88:ILE:HD12	1.92	0.51
3:AC:162:GLN:NE2	22:AV:24:A:O2'	2.44	0.51
3:AC:153:VAL:HG22	3:AC:198:VAL:HG13	1.91	0.51
25:DA:265:A:H1'	25:DA:266:G:O4'	2.11	0.51
25:DA:19:C:H2'	25:DA:20:C:C6	2.45	0.51
25:BA:2255:U:H2'	25:BA:2256:U:C6	2.46	0.51
25:BA:2724:U:H2'	25:BA:2727:G:H5''	1.92	0.51
25:BA:514:G:O2'	42:BW:49:LYS:NZ	2.31	0.51
1:CA:324:G:OP2	61:CA:4084:HOH:O	2.19	0.51
25:DA:2124:G:H1	25:DA:2173:A:N6	2.08	0.51
37:DR:21:TYR:OH	37:DR:43:GLU:HG2	2.10	0.51
23:AY:34:G:H3'	23:AY:35:A:H8	1.75	0.51
25:BA:1221:G:H1'	25:BA:1222:A:C5'	2.34	0.51
23:AY:63:G:C2	23:AY:64:A:H1'	2.44	0.51
1:CA:663:A:O3'	18:CR:64:ARG:NH2	2.43	0.51
1:CA:1119:C:N3	1:CA:1154:G:N2	2.59	0.51
25:DA:2808:U:H2'	25:DA:2809:A:H5'	1.93	0.51
2:AB:80:ILE:HG13	2:AB:212:GLN:HG2	1.92	0.51
3:CC:87:LEU:O	3:CC:91:LEU:N	2.38	0.51
25:BA:2802:C:O2	25:BA:2903:G:N1	2.38	0.51
25:BA:2087:C:H2'	25:BA:2088:C:C6	2.45	0.51
32:BI:126:TYR:HB2	32:BI:142:VAL:HG23	1.91	0.51
3:CC:20:SER:HB3	3:CC:22:TRP:NE1	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:DD:108:PRO:HG2	27:DD:111:LEU:HB2	1.92	0.51
1:AA:452:A:H4'	16:AP:72:ARG:NH1	2.26	0.51
2:AB:71:VAL:HG12	2:AB:170:GLU:HG3	1.91	0.51
1:CA:374:A:C6	1:CA:375:U:C4	2.99	0.51
45:DZ:171:ILE:HD12	45:DZ:172:ALA:H	1.76	0.51
1:CA:266:G:H5''	1:CA:268:C:H41	1.75	0.51
31:BH:113:VAL:HG11	31:BH:151:ILE:HD13	1.92	0.51
25:DA:357:A:H2'	25:DA:358:U:C6	2.46	0.51
31:BH:98:LEU:HD13	31:BH:125:VAL:HG23	1.92	0.51
25:DA:80:G:O2'	25:DA:294:A:N1	2.41	0.51
15:AO:70:LEU:HD11	15:AO:77:ARG:HB2	1.92	0.51
25:DA:2252:G:H2'	25:DA:2253:G:C8	2.46	0.51
1:AA:278:G:OP2	17:AQ:41:LYS:NZ	2.30	0.51
9:AI:45:ALA:HA	9:AI:48:GLU:HB2	1.91	0.51
25:DA:2123:G:H2'	25:DA:2124:G:H8	1.75	0.51
1:AA:1053:G:N7	1:AA:1200:C:H5''	2.26	0.51
14:CN:23:ARG:NH1	14:CN:30:ALA:HB2	2.26	0.51
25:DA:2274:A:O2'	25:DA:2276:G:OP1	2.21	0.51
25:DA:2292:C:P	38:DS:17:ARG:HH12	2.33	0.51
25:DA:84:A:H5'	44:DY:8:LYS:HG2	1.92	0.51
25:BA:2574:U:O2'	34:BO:23:ARG:HD3	2.11	0.51
25:BA:211:A:H5''	25:BA:448:U:OP1	2.11	0.51
25:BA:2787:C:OP2	61:BA:4638:HOH:O	2.19	0.51
4:AD:53:ASP:O	4:AD:57:ARG:HG3	2.10	0.51
25:BA:599:U:O4	61:BA:4870:HOH:O	2.18	0.51
4:AD:129:ASN:OD1	4:AD:145:GLU:N	2.34	0.51
25:BA:1793:A:H2'	61:BA:5168:HOH:O	2.09	0.51
26:BB:57:A:H4'	30:BG:30:GLU:HG3	1.92	0.51
1:AA:1106:G:H5''	3:AC:172:ARG:HG2	1.92	0.51
25:DA:684:G:OP1	53:D7:16:HIS:ND1	2.41	0.51
25:BA:502:G:H4'	25:BA:527:A:N1	2.26	0.51
25:DA:821:A:H2'	25:DA:946:G:H5''	1.91	0.51
1:AA:632:A:H3'	1:AA:633:G:H8	1.74	0.51
1:AA:1054:C:C5	23:AW:34:G:H1'	2.46	0.51
23:CY:21:A:N6	23:CY:46:7MG:H81	2.25	0.51
19:AS:68:GLY:H	50:B4:58:ARG:NH1	2.09	0.51
38:DS:67:ARG:O	38:DS:71:ARG:HG3	2.10	0.51
9:CI:77:ILE:O	9:CI:81:ILE:HG22	2.10	0.51
25:DA:1337:G:H2'	25:DA:1338:G:O4'	2.11	0.51
25:BA:118:U:OP2	61:BA:4148:HOH:O	2.20	0.51
30:DG:80:PHE:O	30:DG:82:LEU:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:BH:59:ARG:HB2	31:BH:59:ARG:HH11	1.74	0.51
25:DA:2502:G:N7	61:DA:4672:HOH:O	2.34	0.51
1:AA:1177:G:OP2	9:AI:97:LYS:NZ	2.35	0.51
25:BA:2282:G:OP2	61:BA:4725:HOH:O	2.19	0.51
25:BA:2624:C:OP2	51:B5:2:ALA:N	2.44	0.51
25:DA:785:G:OP2	61:DA:4179:HOH:O	2.19	0.51
1:AA:1064:G:H1'	1:AA:1190:G:N2	2.25	0.51
1:AA:1190:G:HO2'	1:AA:1191:A:P	2.34	0.51
25:DA:11:G:N7	61:DA:4541:HOH:O	2.35	0.51
25:DA:2880:C:O3'	37:DR:90:ARG:NH1	2.44	0.51
25:DA:1012:U:C5	33:DN:28:THR:HG21	2.46	0.51
1:CA:1456:G:O6	20:CT:54:LYS:NZ	2.44	0.51
47:B1:3:LYS:HB2	47:B1:61:ARG:NH1	2.25	0.51
1:CA:738:C:OP1	6:CF:2:ARG:NH1	2.43	0.51
25:BA:561:A:H2'	25:BA:562:C:C6	2.46	0.51
1:CA:1189:C:OP1	10:CJ:51:ARG:NH2	2.44	0.51
45:BZ:132:ASN:ND2	45:BZ:160:GLY:HA3	2.26	0.51
25:BA:2639:G:O2'	25:BA:2794:A:N1	2.41	0.51
25:BA:906:G:O2'	25:BA:962:G:O6	2.17	0.51
25:BA:1823:G:O2'	25:BA:1861:C:OP1	2.25	0.51
25:BA:2707:C:H2'	25:BA:2708:U:C6	2.46	0.51
1:AA:65:U:H6	1:AA:65:U:H5'	1.75	0.51
25:DA:2123:G:H2'	25:DA:2124:G:C8	2.46	0.51
25:BA:2173:G:H2'	25:BA:2174:G:C8	2.46	0.51
1:CA:345:C:H4'	1:CA:346:G:C4	2.45	0.51
25:BA:302:A:H2'	25:BA:303:C:C6	2.46	0.51
1:CA:1149:C:O2'	1:CA:1280:A:N1	2.33	0.51
54:B8:6:THR:HG23	54:B8:63:PRO:HD2	1.92	0.51
10:CJ:11:PHE:CE1	10:CJ:67:THR:HG22	2.44	0.51
25:DA:987:G:H5''	25:DA:988:A:OP2	2.09	0.51
25:DA:1159:U:H2'	25:DA:1160:G:C8	2.45	0.51
23:AW:52:G:H5''	36:BQ:56:ARG:HH12	1.74	0.51
1:AA:750:G:H1'	15:AO:22:THR:HG23	1.92	0.51
3:AC:156:ARG:NH2	3:AC:159:GLY:O	2.37	0.51
25:DA:191:A:H2'	25:DA:192:C:C6	2.45	0.51
44:BY:6:HIS:HE1	44:BY:72:VAL:O	1.94	0.51
25:BA:261:A:N1	25:BA:291:G:O2'	2.38	0.51
12:AL:84:LEU:HB2	12:AL:105:TYR:CE2	2.45	0.51
3:AC:11:ARG:NH2	3:AC:177:THR:O	2.44	0.51
5:AE:143:ARG:NH1	8:AH:77:GLU:OE1	2.44	0.51
32:DI:12:LEU:HD22	32:DI:19:VAL:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:705:A:H2'	25:DA:706:A:O4'	2.11	0.51
1:CA:49:U:O4	1:CA:365:U:H5	1.93	0.51
1:CA:1122:U:C4	1:CA:1123:A:N7	2.78	0.51
27:DD:72:LYS:NZ	27:DD:99:ASP:OD2	2.32	0.51
25:DA:2206:G:H3'	25:DA:2207:G:C8	2.46	0.51
1:CA:866:C:C4	1:CA:867:G:H1'	2.45	0.51
1:AA:328:C:H4'	1:AA:329:A:H5'	1.92	0.51
1:AA:413:G:N2	1:AA:428:G:H1'	2.26	0.51
48:D2:9:GLN:HE22	48:D2:56:GLN:HB3	1.76	0.51
23:AW:66:U:H2'	23:AW:67:C:C6	2.46	0.51
23:AW:26:A:N1	23:AW:44:G:N2	2.59	0.51
25:BA:27:G:N2	25:BA:537:G:H1'	2.26	0.51
1:AA:1151:A:HO2'	1:AA:1152:A:H8	1.59	0.51
9:CI:18:PHE:HB2	9:CI:62:TYR:HB3	1.93	0.51
16:CP:52:ASP:O	16:CP:54:GLU:N	2.39	0.51
39:BT:23:ARG:HG3	39:BT:120:ARG:NH1	2.26	0.51
25:BA:2506:G:O2'	36:BQ:80:GLU:HA	2.11	0.51
1:AA:1000:U:O4	1:AA:1041:A:N1	2.43	0.51
26:BB:92:C:OP1	45:BZ:79:ARG:NH1	2.42	0.51
25:BA:1890:A:N6	25:BA:1905:G:O2'	2.42	0.51
27:BD:85:ASP:OD2	27:BD:88:ARG:NH1	2.40	0.51
25:BA:1223:C:H2'	25:BA:1224:C:H6	1.74	0.51
7:AG:78:ARG:HH12	7:AG:79:ARG:HH21	1.58	0.51
23:CY:71:G:H2'	23:CY:72:C:C6	2.46	0.51
8:CH:51:VAL:HG11	8:CH:60:ARG:NH1	2.26	0.51
26:DB:11:C:H3'	26:DB:12:C:C6	2.44	0.51
1:CA:1286:A:C8	1:CA:1287:A:H4'	2.45	0.51
25:DA:2849:U:H4'	25:DA:2868:A:C2	2.46	0.51
25:DA:2086:U:H2'	25:DA:2087:G:C8	2.46	0.51
25:DA:2285:C:OP2	52:D6:6:ARG:NH1	2.43	0.51
19:AS:51:VAL:O	19:AS:58:VAL:N	2.36	0.51
27:DD:145:VAL:HG13	27:DD:191:ALA:HB2	1.92	0.51
1:CA:637:G:H2'	1:CA:638:G:H8	1.75	0.51
1:CA:859:A:H2'	1:CA:860:A:O4'	2.10	0.51
35:DP:63:PRO:HG2	54:D8:25:MET:HB2	1.92	0.51
25:BA:2324:U:H5'	30:BG:88:ILE:HD11	1.93	0.51
1:CA:1388:C:H2'	1:CA:1389:C:C6	2.46	0.51
4:CD:191:ARG:NH1	4:CD:194:LEU:O	2.44	0.51
25:DA:698:C:O2'	25:DA:734:A:N6	2.43	0.51
1:AA:92:C:H2'	1:AA:93:G:C8	2.46	0.51
41:DV:14:VAL:HA	41:DV:18:LEU:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:DQ:43:THR:HA	36:DQ:94:VAL:HG12	1.93	0.51
23:AW:56:C:H5	25:BA:943:C:O4'	1.94	0.50
25:BA:927:G:N2	25:BA:944:C:N3	2.58	0.50
39:DT:16:ARG:HH11	39:DT:16:ARG:HB3	1.77	0.50
25:DA:2788:C:O2'	25:DA:2809:A:N3	2.43	0.50
25:BA:667:G:N2	25:BA:670:C:OP2	2.44	0.50
25:DA:2166:G:H3'	25:DA:2167:U:C5'	2.40	0.50
1:AA:1149:C:H2'	1:AA:1150:U:C6	2.46	0.50
45:BZ:152:ALA:HA	45:BZ:155:LEU:HD23	1.92	0.50
25:BA:1410:G:OP2	47:B1:3:LYS:HG3	2.11	0.50
35:BP:81:GLN:NE2	35:BP:105:LEU:O	2.44	0.50
25:DA:2019:A:H4'	40:DU:34:LYS:HD2	1.92	0.50
25:DA:642:G:H4'	25:DA:2349:G:H4'	1.93	0.50
25:BA:2060:G:H2'	25:BA:2061:C:O4'	2.11	0.50
25:BA:54:G:O2'	25:BA:125:A:N1	2.38	0.50
10:CJ:16:LEU:HD12	10:CJ:68:HIS:HB2	1.92	0.50
25:BA:310:C:H2'	25:BA:311:C:H6	1.75	0.50
7:CG:27:ILE:HD12	7:CG:40:ALA:HA	1.94	0.50
23:AY:37:MIA:H2'	23:AY:38:A:C8	2.46	0.50
23:AY:38:A:H2'	23:AY:39:PSU:O4'	2.12	0.50
1:CA:1502:A:H2	1:CA:1505:G:N1	2.01	0.50
25:BA:929:G:N2	25:BA:941:U:O2	2.44	0.50
25:BA:1153:G:H2'	25:BA:1153:G:N3	2.27	0.50
25:BA:1525:G:O2'	25:BA:1605:A:N1	2.40	0.50
38:BS:10:ARG:O	38:BS:14:VAL:HG13	2.11	0.50
24:CX:47:U:H3'	24:CX:48:C:C5'	2.41	0.50
7:CG:22:LEU:HG	7:CG:62:PHE:CE2	2.46	0.50
25:DA:2108:C:C2'	25:DA:2109:U:H5'	2.42	0.50
25:BA:2420:U:H2'	25:BA:2421:G:H8	1.76	0.50
25:BA:2130:C:H2'	25:BA:2131:U:C6	2.47	0.50
30:DG:145:THR:H	30:DG:148:MET:HE3	1.75	0.50
25:DA:1213:A:N3	25:DA:1238:G:O2'	2.37	0.50
25:DA:1779:U:H2'	61:DA:4904:HOH:O	2.10	0.50
25:DA:2224:G:H4'	25:DA:2226:C:C2	2.46	0.50
1:CA:1516:G:H2'	1:CA:1518:A:OP2	2.10	0.50
25:DA:71:A:H5''	25:DA:73:A:C8	2.45	0.50
13:AM:121:LYS:H	13:AM:121:LYS:CE	2.21	0.50
26:DB:66:A:N6	26:DB:109:C:H5'	2.25	0.50
1:AA:839:U:O2'	1:AA:840:C:H5'	2.11	0.50
12:CL:113:ARG:NE	12:CL:115:LYS:O	2.36	0.50
25:BA:667:G:H21	25:BA:671:A:H2	1.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1150:U:O2	10:CJ:39:PRO:HG2	2.12	0.50
42:BW:88:ARG:HG3	42:BW:92:ARG:HH21	1.75	0.50
30:DG:41:GLN:HG2	30:DG:155:MET:HB3	1.93	0.50
25:BA:1272:A:OP1	41:BV:84:LYS:HE2	2.12	0.50
25:BA:715:G:H5'	25:BA:716:G:OP2	2.11	0.50
16:CP:40:ASP:HB3	16:CP:48:TRP:HB2	1.93	0.50
44:DY:3:VAL:HB	44:DY:32:PRO:HB3	1.93	0.50
25:DA:2304:G:H22	25:DA:2312:U:H3	1.58	0.50
4:AD:111:ALA:HB2	4:AD:120:LEU:HD12	1.92	0.50
31:DH:28:GLY:HA3	31:DH:79:VAL:HB	1.94	0.50
25:DA:1899:G:N3	25:DA:1899:G:H2'	2.27	0.50
1:AA:620:C:C2	4:AD:135:LEU:HG	2.47	0.50
42:DW:35:ILE:HG23	51:D5:28:PRO:HD2	1.93	0.50
25:DA:2130:U:H3	25:DA:2159:G:N2	2.10	0.50
25:DA:2146:C:H4'	25:DA:2147:G:H5'	1.94	0.50
1:AA:418:C:H1'	1:AA:540:G:O2'	2.11	0.50
25:DA:307:G:N7	61:DA:4268:HOH:O	2.35	0.50
25:DA:1647:G:H3'	25:DA:1647:G:OP2	2.12	0.50
25:BA:934:A:HO2'	25:BA:935:C:P	2.33	0.50
25:DA:304:G:H2'	25:DA:305:U:C6	2.46	0.50
45:BZ:138:GLU:O	45:BZ:156:LYS:HD3	2.11	0.50
37:DR:100:LEU:HD11	37:DR:113:LEU:HD23	1.93	0.50
25:DA:1813:G:H1'	27:DD:50:THR:OG1	2.11	0.50
49:D3:23:LEU:HD13	49:D3:50:VAL:HG11	1.92	0.50
1:CA:431:A:OP1	61:CA:4124:HOH:O	2.19	0.50
25:DA:2097:C:H2'	25:DA:2098:U:O4'	2.11	0.50
1:AA:110:C:H2'	1:AA:111:G:O4'	2.12	0.50
25:DA:443:A:H1'	25:DA:1201:C:O4'	2.11	0.50
4:CD:8:VAL:HA	4:CD:11:LEU:HD13	1.93	0.50
1:CA:1068:G:OP2	1:CA:1068:G:H8	1.95	0.50
25:BA:1781:G:O2'	25:BA:2870:A:N1	2.37	0.50
1:CA:798:G:O6	61:CA:4041:HOH:O	2.17	0.50
25:DA:7:G:H2'	25:DA:8:A:C8	2.46	0.50
1:CA:1120:G:C5	1:CA:1154:G:N2	2.80	0.50
9:AI:99:LEU:HB3	9:AI:101:PHE:HE1	1.75	0.50
1:AA:815:A:N7	1:AA:1509:C:O2'	2.34	0.50
1:CA:947:G:H1	1:CA:1234:C:H42	1.58	0.50
25:DA:906:G:O3'	36:DQ:67:ARG:NH2	2.44	0.50
3:CC:131:ARG:NE	3:CC:166:GLU:OE2	2.44	0.50
23:AY:40:C:H2'	23:AY:41:C:C6	2.46	0.50
18:AR:56:THR:HB	18:AR:58:LEU:HD22	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:DF:197:ASP:O	29:DF:200:GLU:HB2	2.11	0.50
25:DA:2207:G:O2'	25:DA:2208:A:OP1	2.29	0.50
1:CA:828:A:N6	1:CA:858:G:O2'	2.44	0.50
49:D3:7:LYS:HE3	49:D3:32:GLN:NE2	2.27	0.50
4:AD:8:VAL:HA	4:AD:11:LEU:HD13	1.92	0.50
31:DH:30:LYS:HG3	31:DH:80:SER:O	2.11	0.50
19:CS:41:VAL:N	19:CS:44:MET:SD	2.76	0.50
25:DA:2854:G:H2'	25:DA:2855:C:C6	2.47	0.50
26:DB:38:C:O4'	38:DS:95:HIS:NE2	2.44	0.50
25:DA:924:C:H2'	25:DA:925:C:C6	2.46	0.50
3:CC:63:ASN:HB2	3:CC:98:ASN:HB2	1.92	0.50
47:D1:34:THR:HG21	47:D1:37:ILE:HG13	1.93	0.50
1:CA:1028:C:C4	1:CA:1033:G:O6	2.64	0.50
1:AA:1002:G:N3	1:AA:1003:G:H1'	2.27	0.50
2:AB:163:PHE:HA	2:AB:185:ILE:HG13	1.93	0.50
2:CB:103:THR:HA	2:CB:180:LEU:HD11	1.94	0.50
25:BA:1524:A:H2'	25:BA:1525:G:O4'	2.12	0.50
29:BF:192:LEU:HD22	29:BF:194:MET:HG3	1.92	0.50
33:BN:62:VAL:HG13	33:BN:66:LYS:HB2	1.92	0.50
25:DA:460:A:P	53:D7:41:ARG:HH22	2.34	0.50
1:CA:1494:G:H4'	25:DA:1913:A:N7	2.27	0.50
57:AA:3220:NEG:O4	57:AA:3220:NEG:H72	2.09	0.50
6:CF:69:GLU:H	6:CF:69:GLU:CD	2.15	0.50
1:AA:302:G:O2'	1:AA:556:C:H5''	2.12	0.50
27:BD:77:ALA:HB2	27:BD:97:TYR:CD1	2.47	0.50
34:BO:64:ARG:HB2	34:BO:83:ALA:HB3	1.94	0.50
25:BA:1014:U:H2'	25:BA:1015:C:C6	2.47	0.50
1:CA:833:U:H2'	1:CA:834:C:H6	1.76	0.50
7:AG:18:TYR:HB3	7:AG:59:LEU:HD13	1.93	0.50
1:CA:1187:G:H5'	9:CI:113:LYS:HE2	1.93	0.50
28:BE:179:GLU:HB3	28:BE:181:LEU:HD22	1.92	0.50
27:DD:17:THR:O	27:DD:211:ARG:NH2	2.38	0.50
25:DA:774:A:N3	25:DA:774:A:H2'	2.27	0.50
4:AD:134:ASP:O	4:AD:136:PRO:HD3	2.11	0.50
51:B5:35:GLU:HG3	51:B5:51:TYR:CB	2.42	0.50
2:AB:20:GLU:HA	2:AB:21:ARG:NH2	2.27	0.50
23:AW:65:G:H2'	23:AW:66:U:C6	2.47	0.50
25:DA:2127:G:H2'	25:DA:2128:C:H5'	1.93	0.50
1:AA:975:A:H8	1:AA:975:A:H5'	1.77	0.50
23:CW:7:A:H3'	23:CW:8:4SU:H6	1.94	0.50
25:DA:839:U:H2'	25:DA:840:C:H6	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:CY:76:A:N3	25:DA:2394:C:N4	2.56	0.50
25:BA:1067:A:H3'	25:BA:1067:A:C8	2.45	0.50
1:AA:993:G:H2'	1:AA:995:C:H41	1.77	0.50
28:BE:47:VAL:HG21	28:BE:86:PRO:CD	2.41	0.50
1:CA:983:A:N1	1:CA:1222:G:N2	2.60	0.50
28:DE:77:ILE:HG21	28:DE:195:LEU:HD13	1.94	0.50
1:CA:78:G:O6	1:CA:91:C:N3	2.44	0.50
25:BA:1343:C:OP2	61:BA:4481:HOH:O	2.19	0.50
25:BA:186:A:N6	25:BA:2442:A:H2'	2.25	0.50
6:CF:4:TYR:CE1	6:CF:92:LYS:HG3	2.46	0.50
25:BA:504:A:N1	25:BA:525:G:H4'	2.27	0.50
1:CA:865:A:H5'	1:CA:1078:U:C5	2.47	0.50
25:DA:289:A:N6	25:DA:351:G:O2'	2.44	0.50
25:DA:2774:C:H2'	25:DA:2775:A:O4'	2.10	0.50
2:AB:220:ASP:O	2:AB:223:ILE:HG12	2.12	0.50
25:DA:2876:G:H4'	39:DT:2:ASN:ND2	2.27	0.50
39:DT:108:ARG:HG2	39:DT:111:ARG:HH12	1.76	0.50
25:DA:2134:A:C2	25:DA:2159:G:H4'	2.47	0.50
8:CH:21:LYS:O	8:CH:65:TYR:OH	2.21	0.50
2:CB:178:ARG:NE	8:CH:74:PRO:HG3	2.25	0.50
1:AA:1008:C:O2'	1:AA:1009:G:OP1	2.23	0.50
25:DA:900:A:H2'	25:DA:901:A:C8	2.43	0.50
23:CW:75:C:H2'	23:CW:76:A:C4	2.47	0.50
25:DA:2557:G:H2'	25:DA:2558:C:H6	1.76	0.50
25:DA:478:A:N1	25:DA:500:G:H4'	2.27	0.50
1:AA:1202:G:N2	14:AN:46:GLU:OE1	2.44	0.50
25:BA:1993:A:OP2	27:BD:242:ARG:NH2	2.39	0.50
1:CA:769:G:H4'	1:CA:1513:A:H4'	1.93	0.50
34:DO:120:GLU:HG2	34:DO:122:LEU:HG	1.93	0.50
1:CA:554:C:H2'	1:CA:555:C:H6	1.77	0.50
10:CJ:16:LEU:HD23	10:CJ:94:VAL:HG22	1.94	0.50
30:BG:46:ALA:HB2	30:BG:53:LEU:HD12	1.93	0.50
30:DG:170:ARG:HH21	30:DG:180:PHE:HB2	1.76	0.50
25:BA:1452:U:H2'	25:BA:1453:C:C6	2.47	0.50
25:DA:2655:G:O2'	25:DA:2664:G:O6	2.25	0.50
25:DA:1639:U:H2'	25:DA:1640:C:H5''	1.93	0.50
36:DQ:50:ALA:HB1	36:DQ:121:ALA:HB1	1.94	0.50
25:BA:2051:G:H2'	25:BA:2053:A:OP1	2.11	0.50
23:AW:9:A:N3	23:AW:45:U:H2'	2.27	0.50
39:BT:19:LEU:HD22	39:BT:86:ILE:HG13	1.93	0.50
1:AA:1513:A:H2'	1:AA:1514:C:C6	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:219:C:H2'	1:CA:220:G:O4'	2.11	0.50
1:AA:1144:G:N2	1:AA:1146:A:H62	2.09	0.50
23:AY:34:G:H3'	23:AY:35:A:C8	2.47	0.50
23:CW:21:A:H1'	23:CW:48:C:N4	2.27	0.50
1:CA:1399:C:C2	1:CA:1502:A:N6	2.80	0.50
1:AA:1030(B):C:C3'	1:AA:1030(C):G:H5'	2.42	0.50
3:AC:15:THR:CG2	3:AC:181:ASN:HA	2.41	0.50
25:BA:2334:A:H2'	25:BA:2335:G:O4'	2.12	0.50
19:AS:36:ARG:HB3	19:AS:72:GLY:HA3	1.93	0.50
25:BA:469:A:C5	29:BF:45:ARG:HD2	2.46	0.50
3:CC:22:TRP:CD2	3:CC:59:ARG:HD2	2.46	0.50
29:DF:197:ASP:OD2	29:DF:198:ALA:N	2.45	0.50
26:BB:66:A:H61	26:BB:108:U:H2'	1.76	0.50
36:BQ:54:MET:HG3	36:BQ:117:ALA:HB1	1.92	0.50
25:BA:180:A:H2'	25:BA:181:C:C6	2.47	0.50
25:BA:2711:C:H2'	25:BA:2712:C:O4'	2.12	0.50
40:BU:108:GLU:O	40:BU:112:ARG:HG2	2.12	0.50
25:BA:1002:A:N1	25:BA:2470:G:H4'	2.27	0.50
1:CA:460:G:O6	1:CA:470:C:H5''	2.12	0.50
1:CA:1007:C:N3	1:CA:1022:G:O6	2.45	0.50
1:CA:1048:G:OP1	14:CN:3:ARG:NH2	2.45	0.50
1:CA:109:A:C6	1:CA:326:G:C6	3.00	0.50
1:CA:1304:G:C6	1:CA:1305:G:N1	2.80	0.49
25:BA:555:G:C5	25:BA:2044:U:H5''	2.46	0.49
50:D4:59:PHE:HA	50:D4:60:GLN:C	2.32	0.49
28:DE:170:LEU:HB3	28:DE:184:VAL:HG22	1.94	0.49
1:AA:691:G:H2'	1:AA:692:U:C6	2.47	0.49
2:AB:93:VAL:HG21	2:AB:97:TRP:CD1	2.46	0.49
52:D6:6:ARG:NH1	52:D6:26:ASN:HB2	2.27	0.49
35:BP:82:GLY:HA2	35:BP:113:LYS:O	2.11	0.49
25:DA:2692:C:OP2	61:DA:4608:HOH:O	2.20	0.49
13:AM:23:TYR:HB3	13:AM:67:GLU:HA	1.93	0.49
13:AM:80:ARG:HH22	19:AS:69:HIS:HE1	1.60	0.49
28:BE:14:ILE:HG13	28:BE:21:VAL:HG13	1.94	0.49
6:AF:21:LEU:O	6:AF:25:ILE:HG12	2.12	0.49
31:DH:8:PRO:HB3	31:DH:51:ARG:HG2	1.94	0.49
1:AA:625:G:H4'	16:AP:16:HIS:CD2	2.47	0.49
6:CF:46:ARG:HH11	6:CF:46:ARG:HB2	1.76	0.49
38:DS:37:ALA:HB2	38:DS:101:LEU:HD11	1.93	0.49
1:AA:1401:G:C2	1:AA:1402:C:H1'	2.47	0.49
25:DA:994:C:O2'	25:DA:996:A:OP1	2.16	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1182:G:C4'	1:AA:1183:A:H5'	2.41	0.49
25:DA:361:G:N3	25:DA:362:U:C4	2.80	0.49
25:DA:1843:C:H5'	27:DD:253:GLN:NE2	2.27	0.49
25:BA:553:A:C2	25:BA:2065:C:H4'	2.47	0.49
6:CF:45:LEU:HD12	6:CF:59:TYR:CD2	2.47	0.49
26:DB:46:A:H2'	26:DB:47:C:C6	2.46	0.49
51:B5:55:ARG:NH1	51:B5:57:VAL:HG22	2.27	0.49
2:AB:20:GLU:HA	2:AB:21:ARG:HH21	1.77	0.49
2:AB:223:ILE:HD12	2:AB:230:VAL:HG12	1.94	0.49
25:DA:489:G:N7	42:DW:49:LYS:NZ	2.60	0.49
25:DA:526:A:N3	25:DA:2044:C:H1'	2.28	0.49
25:BA:2863:C:H2'	25:BA:2864:G:C8	2.47	0.49
25:DA:1827:C:OP2	27:DD:222:ARG:NH1	2.44	0.49
25:BA:2221:A:OP2	25:BA:2222:C:H5	1.94	0.49
28:BE:12:THR:HG22	28:BE:13:ARG:H	1.76	0.49
25:DA:1254:A:C6	29:DF:82:ILE:HD11	2.47	0.49
36:DQ:35:VAL:HG13	36:DQ:130:LYS:HB3	1.93	0.49
1:CA:1226:C:H2'	13:CM:103:THR:HB	1.94	0.49
5:AE:127:ASN:HB3	5:AE:130:ASN:HB2	1.94	0.49
23:AW:67:C:O2'	23:AW:68:C:O5'	2.24	0.49
19:CS:52:TYR:HB2	19:CS:57:HIS:CE1	2.47	0.49
25:DA:866:A:H5''	25:DA:867:C:OP2	2.12	0.49
1:AA:922:G:H2'	1:AA:923:A:C8	2.47	0.49
1:CA:974:A:P	14:CN:29:ARG:HH21	2.35	0.49
31:DH:90:LYS:NZ	31:DH:159:GLU:OE1	2.38	0.49
1:AA:232:G:H1'	1:AA:262:A:N1	2.27	0.49
25:BA:1451:U:H2'	25:BA:1452:U:C6	2.47	0.49
25:BA:2402:U:P	54:B8:35:GLN:HE22	2.34	0.49
36:DQ:34:LEU:HB2	36:DQ:118:LEU:HD22	1.94	0.49
31:DH:69:ARG:HG3	31:DH:70:THR:N	2.27	0.49
25:DA:2307:G:H8	25:DA:2307:G:OP1	1.96	0.49
1:AA:1251:A:O2'	1:AA:1369:C:O2'	2.30	0.49
1:CA:779:C:O2'	11:CK:120:ARG:HD3	2.12	0.49
12:CL:117:ARG:NH2	12:CL:124:LYS:HB2	2.27	0.49
1:CA:881:G:OP1	12:CL:12:ARG:NH2	2.44	0.49
23:CY:7:A:N6	23:CY:66:U:N3	2.27	0.49
1:CA:1004:A:H2'	1:CA:1038:C:H1'	1.94	0.49
1:CA:1095:U:P	1:CA:1108:G:H1	2.35	0.49
23:AW:56:C:OP1	25:BA:943:C:H5'	2.12	0.49
35:DP:38:GLN:O	35:DP:39:LYS:CB	2.60	0.49
57:CA:3174:NEG:N1	25:DA:1949:G:O6	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:DQ:111:GLU:O	36:DQ:115:MET:HG2	2.12	0.49
1:AA:1239:A:H62	1:AA:1299:A:H62	1.60	0.49
1:CA:1509:C:H2'	1:CA:1510:U:O4'	2.13	0.49
4:AD:98:GLU:OE1	4:AD:103:ASN:ND2	2.44	0.49
25:DA:2364:C:H2'	25:DA:2365:G:O4'	2.12	0.49
14:AN:21:TYR:OH	14:AN:23:ARG:NH2	2.45	0.49
20:AT:65:LYS:HA	20:AT:68:LYS:HD3	1.94	0.49
30:DG:170:ARG:HH21	30:DG:180:PHE:CB	2.24	0.49
25:DA:2657:A:O3'	31:DH:160:LYS:NZ	2.44	0.49
17:AQ:62:SER:OG	17:AQ:72:ARG:HD3	2.12	0.49
25:DA:2848:G:C8	39:DT:97:ALA:HB2	2.48	0.49
15:CO:82:ILE:HB	15:CO:87:ILE:HB	1.94	0.49
31:BH:33:LEU:HD21	31:BH:136:ILE:HG13	1.94	0.49
4:CD:164:ALA:O	4:CD:168:ARG:NH2	2.46	0.49
6:AF:45:LEU:HD12	6:AF:59:TYR:HD2	1.77	0.49
9:CI:127:LYS:O	9:CI:128:ARG:HG2	2.12	0.49
12:CL:39:VAL:HG11	12:CL:41:ARG:HH11	1.78	0.49
1:AA:1499:A:H1'	1:AA:1520:G:H5'	1.95	0.49
25:DA:34:C:H2'	25:DA:34:C:O2	2.12	0.49
1:AA:250:A:H4'	1:AA:251:G:O5'	2.13	0.49
1:CA:141:A:H1'	1:CA:182:U:O2	2.13	0.49
52:B6:11:LEU:HB2	52:B6:21:TYR:HB2	1.93	0.49
1:AA:456:C:H2'	1:AA:457:C:C6	2.47	0.49
1:CA:1333:A:H2'	1:CA:1334:G:O4'	2.13	0.49
23:AY:53:G:H2'	23:AY:54:5MU:H71	1.93	0.49
1:AA:1005:A:H1'	1:AA:1036:G:N2	2.26	0.49
50:B4:59:PHE:C	50:B4:61:ARG:H	2.14	0.49
45:DZ:92:SER:O	45:DZ:130:PRO:HG2	2.12	0.49
44:DY:86:ARG:HB2	44:DY:98:VAL:HG23	1.94	0.49
2:AB:127:ILE:HG13	2:AB:130:ARG:NH1	2.27	0.49
13:AM:91:ARG:HB2	13:AM:98:VAL:HG13	1.92	0.49
1:AA:8:A:H5'	5:AE:101:ILE:HG22	1.94	0.49
25:DA:2846:G:H2'	25:DA:2847:U:O4'	2.13	0.49
25:DA:116:C:H2'	25:DA:117:G:O4'	2.12	0.49
25:DA:19:C:H2'	25:DA:20:C:H6	1.77	0.49
24:CX:17:C:OP1	24:CX:61:C:H5'	2.12	0.49
30:DG:179:PRO:HG3	50:D4:43:TYR:OH	2.12	0.49
25:BA:957:A:H2'	36:BQ:9:TYR:OH	2.12	0.49
7:AG:74:GLU:HG2	7:AG:91:VAL:HG22	1.95	0.49
35:DP:47:ASP:OD2	35:DP:49:ARG:NH2	2.46	0.49
1:CA:814:A:H2'	1:CA:816:A:H5''	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:653:G:H2'	25:BA:654:G:C8	2.48	0.49
25:BA:8:A:H2'	25:BA:9:U:C6	2.47	0.49
25:DA:1486:A:H2'	25:DA:1487:G:C8	2.47	0.49
25:BA:552:C:C5	25:BA:2792:U:H2'	2.48	0.49
3:CC:100:ALA:O	3:CC:102:ASN:ND2	2.42	0.49
26:DB:22:U:H3	26:DB:61:G:H1	1.59	0.49
25:DA:2405:G:O2'	25:DA:2411:A:N6	2.44	0.49
28:BE:116:VAL:HG13	28:BE:122:PHE:HB2	1.95	0.49
23:AY:58:A:H4'	23:AY:59:U:OP1	2.13	0.49
1:AA:1030(B):C:H2'	1:AA:1030(B):C:O2	2.11	0.49
1:CA:529:G:O6	12:CL:49:ASN:HA	2.12	0.49
1:CA:1256:A:N6	1:CA:1278:U:H1'	2.27	0.49
26:DB:17:C:H2'	26:DB:18:G:O4'	2.12	0.49
25:DA:2043:C:H1'	25:DA:2779:U:O4	2.11	0.49
29:DF:21:ALA:CB	29:DF:22:ALA:HA	2.41	0.49
19:AS:65:ASN:HD22	19:AS:66:MET:N	2.10	0.49
45:DZ:138:GLU:H	45:DZ:156:LYS:HD3	1.76	0.49
12:AL:56:ALA:HB2	12:AL:70:ILE:HD11	1.93	0.49
1:AA:309:G:H1'	1:AA:608:A:C2	2.47	0.49
25:BA:2470:G:O2'	25:BA:2472:U:O4	2.27	0.49
17:AQ:29:HIS:CE1	17:AQ:32:TYR:HD2	2.31	0.49
25:BA:2760:G:O6	25:BA:2768:C:H5''	2.12	0.49
8:AH:86:ILE:HG13	8:AH:133:LEU:HD22	1.94	0.49
61:BA:4092:HOH:O	36:BQ:75:THR:HG23	2.12	0.49
25:BA:1587:U:H2'	25:BA:1588:G:O4'	2.12	0.49
4:CD:18:LYS:NZ	4:CD:26:CYS:O	2.35	0.49
24:CX:10:G:N2	24:CX:26:G:H1'	2.27	0.49
1:CA:1220:G:O3'	19:CS:36:ARG:HD3	2.12	0.49
42:BW:68:ARG:HD3	42:BW:111:HIS:HA	1.94	0.49
25:DA:1686:C:H2'	25:DA:1687:G:O4'	2.12	0.49
43:BX:31:HIS:HD2	43:BX:33:LYS:N	1.94	0.49
1:CA:1154:G:H2'	1:CA:1155:G:H8	1.76	0.49
1:CA:404:U:H2'	1:CA:405:U:C6	2.48	0.49
1:AA:431:A:H2'	1:AA:432:A:O4'	2.13	0.49
9:CI:17:VAL:HG23	9:CI:63:ILE:HG12	1.94	0.49
3:CC:71:ALA:HA	3:CC:106:VAL:HB	1.95	0.49
45:DZ:171:ILE:HD12	45:DZ:172:ALA:N	2.28	0.49
44:DY:5:MET:HE1	44:DY:32:PRO:HA	1.93	0.49
1:AA:620:C:H2'	1:AA:621:A:O4'	2.13	0.49
8:AH:112:LEU:HB3	8:AH:133:LEU:HA	1.95	0.49
35:BP:101:VAL:HA	35:BP:106:LEU:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:CE:110:LEU:HD13	5:CE:118:ILE:HG21	1.95	0.49
8:AH:121:ASP:OD2	8:AH:121:ASP:N	2.44	0.49
1:AA:688:G:H2'	1:AA:689:C:H6	1.78	0.49
4:CD:12:CYS:SG	4:CD:19:LEU:HB2	2.52	0.49
3:CC:58:GLU:HB3	10:CJ:92:THR:HG21	1.95	0.49
1:AA:1442:G:O2'	1:AA:1442(A):G:OP1	2.19	0.49
11:CK:81:ASP:OD1	11:CK:106:LYS:HE2	2.13	0.49
25:BA:2556:G:H2'	25:BA:2557:G:O4'	2.13	0.49
35:BP:59:LEU:HD21	54:B8:10:ALA:HA	1.95	0.49
25:BA:2116:G:P	32:BI:22:LYS:HD2	2.53	0.49
25:BA:70:A:H5''	25:BA:72:A:C8	2.48	0.49
1:CA:976:G:H22	1:CA:1363:C:H5''	1.77	0.49
10:CJ:5:ARG:O	10:CJ:98:ILE:HA	2.13	0.49
25:BA:1068:G:OP2	33:BN:65:LYS:NZ	2.46	0.49
29:DF:129:PHE:CD2	29:DF:163:VAL:HG21	2.47	0.49
1:AA:1333:A:H2'	1:AA:1334:G:O4'	2.12	0.49
1:CA:576:G:O6	1:CA:880:C:O2'	2.23	0.49
36:DQ:26:TYR:O	36:DQ:67:ARG:NH1	2.46	0.49
29:BF:164:ARG:O	29:BF:168:ARG:HB2	2.12	0.49
1:CA:1121:U:C4	1:CA:1122:U:C4	3.00	0.49
25:BA:2859:U:O4	39:BT:23:ARG:NH2	2.38	0.49
27:DD:3:VAL:HG13	27:DD:17:THR:HB	1.95	0.49
25:DA:2177:C:H2'	25:DA:2178:C:O4'	2.13	0.49
12:AL:88:GLY:O	12:AL:99:HIS:HD2	1.95	0.49
28:DE:1:MET:HE1	28:DE:199:ARG:HB3	1.94	0.49
1:CA:993:G:O6	1:CA:1045:C:N4	2.39	0.49
25:DA:569:U:O2'	25:DA:983:A:N1	2.34	0.49
30:BG:126:ASP:OD2	30:BG:130:ASN:ND2	2.44	0.49
25:BA:733:G:C4	53:B7:11:LYS:HG2	2.47	0.49
29:DF:109:GLY:O	29:DF:113:ALA:N	2.46	0.49
1:AA:35:G:O2'	12:AL:118:SER:O	2.20	0.49
3:AC:71:ALA:HB2	3:AC:115:LEU:HD21	1.95	0.49
5:AE:78:HIS:HD1	8:AH:104:ARG:HD2	1.78	0.49
25:BA:2549:U:H2'	25:BA:2550:C:C6	2.47	0.49
31:BH:24:VAL:HG22	31:BH:35:VAL:HB	1.93	0.49
25:DA:861:A:N6	25:DA:916:G:O2'	2.46	0.49
53:B7:24:THR:O	53:B7:28:ARG:HG3	2.12	0.49
1:CA:1085:U:H3'	1:CA:1086:U:H5	1.77	0.49
1:CA:1227:A:N3	19:CS:83:HIS:HB3	2.28	0.49
25:DA:527:C:C4	25:DA:2779:U:H2'	2.47	0.49
1:AA:922:G:C6	1:AA:923:A:C6	3.01	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1016:A:H2'	1:CA:1017:G:O4'	2.12	0.49
25:DA:2453:A:N7	61:DA:4348:HOH:O	2.35	0.49
1:AA:946:A:H2'	1:AA:947:G:C8	2.48	0.49
25:DA:83:G:OP1	44:DY:95:LYS:NZ	2.44	0.49
4:AD:173:TRP:CE3	4:AD:174:LEU:HG	2.48	0.49
25:DA:2292:C:O2'	25:DA:2293:C:H5'	2.13	0.49
29:BF:53:THR:CG2	29:BF:55:GLY:H	2.25	0.49
1:CA:881:G:H2'	1:CA:882:C:O4'	2.12	0.49
25:BA:2116:G:OP1	32:BI:22:LYS:HD2	2.13	0.49
54:B8:23:VAL:HG11	54:B8:47:LYS:HD3	1.95	0.49
1:AA:116:A:H61	1:AA:313:A:H1'	1.76	0.49
3:CC:28:GLN:O	3:CC:32:LEU:HD23	2.12	0.49
25:BA:2150:C:H2'	25:BA:2151:C:C6	2.48	0.49
25:BA:407:U:OP1	61:BA:4340:HOH:O	2.20	0.49
25:DA:2320:A:N3	25:DA:2320:A:H2'	2.28	0.49
1:CA:597:G:N2	8:CH:94:TYR:OH	2.44	0.49
25:BA:1338:U:H2'	25:BA:1339:C:C6	2.48	0.49
25:BA:2096:U:H2'	25:BA:2097:U:C6	2.47	0.49
25:DA:597:U:H2'	25:DA:598:G:C8	2.48	0.49
25:BA:2143:G:H1	25:BA:2199:C:H42	1.61	0.49
2:AB:16:HIS:HB3	2:AB:210:SER:HB2	1.95	0.49
1:CA:1158:C:O3'	2:CB:133:LYS:NZ	2.45	0.49
26:DB:31:C:H4'	30:DG:29:TRP:CZ2	2.48	0.49
25:DA:1127:A:O2'	25:DA:2518:A:OP1	2.28	0.49
25:DA:185:U:H4'	25:DA:218:A:H4'	1.94	0.49
25:DA:952:G:OP1	36:DQ:16:ARG:NH2	2.46	0.49
25:DA:456:C:H4'	61:DA:4011:HOH:O	2.13	0.49
28:DE:170:LEU:HB3	28:DE:184:VAL:CG2	2.43	0.49
25:DA:586:A:N1	25:DA:809:G:O2'	2.39	0.49
42:DW:2:GLU:OE2	42:DW:72:LYS:NZ	2.27	0.49
25:DA:1939:U:OP1	25:DA:2604:U:O2'	2.30	0.49
37:BR:55:ALA:HB2	37:BR:79:LEU:HD13	1.95	0.49
25:DA:825:C:O2	35:DP:55:ARG:NH2	2.41	0.49
1:CA:1194:U:H2'	1:CA:1195:C:C6	2.47	0.49
1:CA:481:G:O2'	1:CA:483:C:N4	2.44	0.49
25:DA:1274:A:N3	25:DA:1297:C:H1'	2.28	0.49
27:BD:34:VAL:HG12	27:BD:63:ARG:HG3	1.95	0.49
42:BW:58:ALA:HB1	42:BW:64:MET:HB2	1.95	0.49
13:CM:68:GLY:HA3	30:DG:116:ASP:OD1	2.13	0.49
44:DY:7:VAL:HG21	44:DY:72:VAL:HG12	1.95	0.49
39:DT:77:PRO:HB2	39:DT:80:SER:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:879:G:H3'	25:DA:880:G:H8	1.77	0.48
1:AA:1009:G:H1'	1:AA:1021:G:C2	2.48	0.48
1:CA:532:A:H2	1:CA:1206:G:H21	1.60	0.48
51:B5:17:ASP:OD2	61:B5:4005:HOH:O	2.20	0.48
23:AY:2:C:N3	23:AY:71:G:N2	2.61	0.48
25:BA:2138:G:H2'	25:BA:2139:A:C5	2.48	0.48
1:AA:1149:C:OP2	9:AI:9:ARG:NH2	2.41	0.48
31:BH:4:ILE:O	31:BH:69:ARG:HG2	2.13	0.48
25:BA:1476:C:H2'	25:BA:1477:U:C6	2.48	0.48
45:BZ:132:ASN:HD22	45:BZ:160:GLY:HA3	1.78	0.48
25:BA:2053:A:C6	25:BA:2510:C:H1'	2.47	0.48
1:CA:500:G:O5'	12:CL:124:LYS:NZ	2.46	0.48
25:DA:700:G:O2'	25:DA:1632:A:N3	2.40	0.48
5:CE:41:VAL:O	5:CE:66:MET:HA	2.13	0.48
3:AC:142:MET:HG3	3:AC:170:GLN:HB3	1.94	0.48
31:DH:24:VAL:HG13	31:DH:37:VAL:HG21	1.94	0.48
25:BA:467:U:O2	29:BF:46:ARG:NH2	2.38	0.48
35:DP:101:VAL:HG23	35:DP:106:LEU:HD13	1.95	0.48
1:CA:29:G:O2'	1:CA:295:C:H4'	2.13	0.48
3:AC:58:GLU:HB3	10:AJ:92:THR:HG21	1.95	0.48
40:BU:49:HIS:HA	40:BU:52:ARG:HB3	1.95	0.48
40:BU:86:ALA:O	41:BV:49:THR:HG23	2.12	0.48
34:DO:64:ARG:NH2	34:DO:99:PHE:O	2.46	0.48
14:AN:48:ALA:HB2	14:AN:53:LEU:HD12	1.94	0.48
15:CO:5:LYS:HZ2	15:CO:5:LYS:H	1.61	0.48
25:DA:1114:G:H2'	25:DA:1115:G:H8	1.76	0.48
25:BA:1576:G:C6	25:BA:1577:C:N4	2.81	0.48
23:AY:50:U:H3	23:AY:64:A:H2	1.54	0.48
25:DA:1147:C:H2'	25:DA:1148:A:C8	2.39	0.48
1:CA:1298:C:H2'	7:CG:114:ARG:HH12	1.77	0.48
1:AA:235:C:H5'	17:AQ:70:ARG:HG2	1.94	0.48
25:BA:933:C:H4'	25:BA:933:C:OP1	2.12	0.48
25:BA:611:U:O4	25:BA:717:A:H1'	2.11	0.48
29:BF:102:PRO:HB2	29:BF:105:VAL:HG23	1.95	0.48
25:DA:2356:C:H2'	25:DA:2357:U:O4'	2.12	0.48
23:AW:76:A:H5''	25:BA:2614:A:N6	2.27	0.48
25:DA:1794:U:H2'	25:DA:1795:C:H6	1.77	0.48
25:BA:705:C:H2'	25:BA:706:C:C6	2.47	0.48
25:DA:2611:U:C4	51:D5:3:LYS:HG2	2.48	0.48
25:DA:30:G:OP2	40:DU:5:LYS:NZ	2.38	0.48
25:DA:910:A:C5	36:DQ:13:GLN:HG3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:173:C:H2'	25:BA:174:U:C6	2.48	0.48
25:DA:1667:G:O2'	25:DA:1991:U:O4	2.27	0.48
6:CF:43:LEU:HD23	6:CF:46:ARG:HH22	1.77	0.48
1:AA:570:G:H1'	1:AA:820:U:C4	2.48	0.48
2:CB:91:PRO:HG2	2:CB:155:LEU:HD23	1.94	0.48
1:CA:174:C:H2'	1:CA:175:C:H6	1.78	0.48
1:CA:179:A:H2'	1:CA:180:U:C6	2.48	0.48
25:DA:39:C:H2'	25:DA:40:C:C6	2.48	0.48
17:CQ:32:TYR:O	17:CQ:34:LYS:N	2.42	0.48
1:CA:975:A:N1	10:CJ:48:THR:HB	2.28	0.48
25:DA:784:A:C8	25:DA:792:G:C5	3.01	0.48
1:AA:1130:A:O3'	9:AI:20:ARG:NH2	2.46	0.48
1:CA:1236:A:O2'	1:CA:1304:G:H4'	2.13	0.48
1:CA:1291:G:C6	1:CA:1292:U:C4	3.01	0.48
2:CB:128:GLU:HG3	2:CB:135:GLN:NE2	2.28	0.48
25:DA:875:G:C2	25:DA:903:C:C2	3.02	0.48
5:AE:140:ARG:O	5:AE:143:ARG:NH2	2.47	0.48
25:DA:479:A:N3	25:DA:481:G:H5''	2.28	0.48
25:DA:1639:U:O2'	25:DA:2699:C:H4'	2.13	0.48
1:AA:1251:A:H2'	1:AA:1252:A:C8	2.47	0.48
28:DE:9:VAL:HG13	28:DE:25:VAL:O	2.13	0.48
13:AM:19:LEU:HD21	13:AM:56:LEU:HD11	1.95	0.48
41:DV:76:LYS:HB2	41:DV:81:TYR:HB3	1.95	0.48
25:BA:390:G:H2'	25:BA:391:G:C8	2.48	0.48
40:BU:102:GLU:HA	40:BU:104:GLN:HE22	1.79	0.48
2:CB:82:ARG:HG3	2:CB:92:TYR:OH	2.14	0.48
57:AA:3221:NEG:H71	25:BA:786:G:H22	1.78	0.48
23:AW:29:G:N2	23:AW:41:C:N3	2.49	0.48
1:AA:1183:A:HO2'	1:AA:1184:G:P	2.33	0.48
6:CF:44:GLY:HA2	6:CF:59:TYR:CZ	2.49	0.48
25:DA:64:A:O3'	43:DX:71:GLY:HA3	2.14	0.48
1:AA:445:G:H2'	1:AA:446:G:C8	2.48	0.48
25:DA:2105:C:H2'	25:DA:2106:G:H8	1.78	0.48
8:CH:56:LYS:HB2	8:CH:58:TYR:CE1	2.47	0.48
25:DA:684:G:N7	61:DA:4006:HOH:O	2.35	0.48
1:CA:1226:C:H4'	19:CS:80:TYR:OH	2.14	0.48
25:DA:833:U:O2	35:DP:55:ARG:NH2	2.47	0.48
2:CB:155:LEU:HD21	2:CB:159:PRO:HG3	1.95	0.48
5:AE:145:LYS:O	5:AE:149:GLU:HG2	2.14	0.48
1:AA:926:G:H5''	1:AA:927:G:O5'	2.13	0.48
1:CA:187:C:O2'	20:CT:89:ARG:NH2	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1122:U:H2'	1:AA:1123:A:O4'	2.14	0.48
44:DY:20:TYR:CE1	44:DY:43:ASN:HA	2.48	0.48
25:DA:36:G:N3	25:DA:450:G:O2'	2.43	0.48
12:AL:60:LEU:HD21	12:AL:66:VAL:HG22	1.95	0.48
3:AC:121:ALA:O	3:AC:125:GLU:HG3	2.13	0.48
25:BA:2094:G:H2'	25:BA:2095:C:O4'	2.13	0.48
25:BA:347:G:C8	29:BF:171:PRO:HG3	2.49	0.48
25:BA:1249:A:H2	25:BA:1287:A:N6	2.04	0.48
1:CA:1298:C:OP2	7:CG:114:ARG:NH2	2.44	0.48
25:DA:1165:U:H2'	25:DA:1166:C:H6	1.77	0.48
24:CX:64:G:H4'	36:DQ:10:ARG:NH1	2.29	0.48
45:DZ:145:GLU:H	45:DZ:148:ASP:HB2	1.79	0.48
25:DA:1262:A:C2	51:D5:10:LYS:HD2	2.48	0.48
25:DA:1316:U:H2'	25:DA:1317:A:H8	1.77	0.48
1:CA:814:A:N7	1:CA:816:A:C4	2.81	0.48
25:BA:2576:A:C2	25:BA:2659:U:H4'	2.49	0.48
26:DB:88:C:H2'	26:DB:89:G:O4'	2.14	0.48
25:DA:2785:C:OP1	28:DE:41:LYS:NZ	2.36	0.48
30:BG:106:LEU:HA	30:BG:110:ALA:HB3	1.96	0.48
26:BB:22:U:H2'	26:BB:23:G:C8	2.48	0.48
5:AE:100:VAL:O	5:AE:107:ARG:NH2	2.46	0.48
25:DA:2469:A:H2'	25:DA:2470:G:O4'	2.13	0.48
44:DY:9:LYS:HA	44:DY:10:GLY:HA2	1.55	0.48
25:DA:511:U:O4	25:DA:512:G:N1	2.46	0.48
25:BA:225:C:H2'	25:BA:226:C:C6	2.49	0.48
46:D0:53:MET:HG3	46:D0:59:LEU:HD23	1.95	0.48
9:AI:23:ASN:HD22	9:AI:25:LYS:HG2	1.77	0.48
26:DB:76:G:N2	26:DB:101:G:O6	2.36	0.48
8:CH:13:ILE:O	8:CH:17:THR:HG23	2.13	0.48
25:DA:2562:U:H1'	34:DO:23:ARG:HH11	1.78	0.48
25:BA:2132:G:H5"	25:BA:2167:C:H42	1.77	0.48
25:DA:2590:A:OP2	27:DD:238:GLY:HA2	2.13	0.48
25:BA:1223:C:H2'	25:BA:1224:C:C6	2.48	0.48
25:DA:962:G:H2'	25:DA:963:U:O4'	2.13	0.48
1:AA:164:U:H2'	1:AA:165:C:C6	2.49	0.48
27:DD:121:PRO:HB3	27:DD:135:PHE:CE2	2.48	0.48
25:DA:1005:C:H2'	25:DA:1006:C:H6	1.76	0.48
61:AX:3108:HOH:O	25:BA:2614:A:OP1	2.20	0.48
1:CA:958:A:N6	19:CS:77:THR:O	2.47	0.48
41:DV:24:LYS:CG	41:DV:64:HIS:HD2	2.27	0.48
25:BA:116:A:C8	25:BA:117:A:C8	3.01	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:109:A:H2'	1:CA:326:G:N2	2.28	0.48
15:CO:5:LYS:NZ	15:CO:5:LYS:H	2.11	0.48
6:AF:89:MET:HE1	18:AR:72:ARG:HB3	1.95	0.48
13:AM:13:LYS:HA	13:AM:44:ARG:HH11	1.79	0.48
25:DA:271(A):A:N1	25:DA:272(D):G:O2'	2.42	0.48
35:DP:82:GLY:HA2	35:DP:113:LYS:O	2.13	0.48
36:DQ:137:TYR:O	36:DQ:141:GLN:HG2	2.14	0.48
25:BA:898:U:O2'	49:B3:42:ALA:O	2.32	0.48
1:CA:501:C:H2'	1:CA:502:G:H8	1.79	0.48
1:CA:1003:G:H2'	1:CA:1004:A:O4'	2.14	0.48
25:DA:2139:C:N3	25:DA:2152:G:N2	2.58	0.48
3:AC:33:LEU:O	3:AC:37:GLN:NE2	2.46	0.48
2:AB:187:LEU:HA	2:AB:201:ILE:HB	1.95	0.48
1:AA:1030(A):G:H2'	1:AA:1030(C):G:OP2	2.14	0.48
25:DA:1950:G:N1	25:DA:1954:G:O2'	2.35	0.48
25:BA:1199:C:OP1	40:BU:92:ARG:NH1	2.46	0.48
10:CJ:6:ILE:HG12	10:CJ:98:ILE:HG13	1.96	0.48
25:DA:2472:G:H1	25:DA:2477:C:P	2.35	0.48
25:DA:322:A:OP2	29:DF:169:ASN:HB2	2.13	0.48
17:CQ:6:LEU:O	17:CQ:58:GLU:HA	2.13	0.48
25:DA:1169:G:H2'	25:DA:1170:G:C8	2.49	0.48
24:CX:2:G:OP1	46:D0:5:LYS:NZ	2.46	0.48
1:CA:737:A:H2'	1:CA:738:C:C6	2.49	0.48
25:DA:2265:U:H4'	36:DQ:13:GLN:HE22	1.78	0.48
25:DA:852:G:H2'	25:DA:853:G:H8	1.78	0.48
6:AF:9:VAL:HB	6:AF:87:ARG:HB2	1.95	0.48
46:D0:48:GLY:HA3	46:D0:80:HIS:ND1	2.29	0.48
1:AA:1066:C:O2'	1:AA:1067:A:H5'	2.13	0.48
1:AA:297:G:H4'	1:AA:557:G:H4'	1.95	0.48
2:AB:48:MET:HA	2:AB:51:LEU:HD12	1.95	0.48
1:AA:582:U:C2	1:AA:760:G:C6	3.01	0.48
1:CA:646:U:H2'	1:CA:647:C:C6	2.49	0.48
1:CA:193:C:H2'	1:CA:194:C:C6	2.48	0.48
25:DA:1452:A:O2'	25:DA:1453:U:H2'	2.13	0.48
37:BR:21:TYR:OH	37:BR:43:GLU:HG2	2.13	0.48
1:AA:1266:G:N2	1:AA:1270:C:N3	2.62	0.48
23:AY:53:G:C4	23:AY:54:5MU:H72	2.48	0.48
25:DA:2135:A:H61	25:DA:2157:G:N2	2.12	0.48
25:BA:2163:G:C5	25:BA:2164:C:H1'	2.48	0.48
25:BA:2172:U:C4	25:BA:2173:G:N7	2.82	0.48
25:DA:1301:A:H2	25:DA:1626:G:N3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:895:G:O6	25:BA:974:G:H2'	2.14	0.48
23:CY:10:G:H1	23:CY:25:C:N4	2.11	0.48
2:AB:77:ALA:HB2	2:AB:211:ILE:HD13	1.94	0.48
4:AD:107:ARG:NH2	4:AD:194:LEU:HD22	2.28	0.48
25:DA:1434:A:H61	25:DA:1558:A:N6	2.12	0.48
25:BA:1074:A:H61	25:BA:1171:G:H2'	1.79	0.48
31:BH:3:ARG:HG2	31:BH:6:ARG:HG2	1.95	0.48
1:AA:1014:A:C2	1:AA:1219:U:H1'	2.49	0.48
49:D3:26:LEU:HD21	49:D3:46:ASN:HB2	1.95	0.48
25:DA:1637:A:H4'	25:DA:2711:A:O2'	2.13	0.48
30:BG:66:GLN:OE1	30:BG:98:ARG:NE	2.39	0.48
22:AV:20:U:H2'	22:AV:21:C:C6	2.48	0.48
5:AE:12:LEU:HB3	5:AE:31:LEU:HB2	1.94	0.48
16:AP:19:ILE:HG22	16:AP:37:GLY:C	2.33	0.48
1:AA:509:A:O2'	1:AA:510:A:OP1	2.27	0.48
25:BA:2258:G:H2'	25:BA:2259:A:C8	2.48	0.48
6:CF:70:ASP:OD1	6:CF:70:ASP:N	2.45	0.48
39:DT:24:PRO:HD3	39:DT:52:ILE:HD12	1.95	0.48
1:CA:1320:C:O4'	19:CS:73:GLU:HG3	2.14	0.48
25:DA:2001:A:H2'	25:DA:2002:G:C8	2.49	0.48
25:DA:1124:C:H2'	25:DA:1125:G:O4'	2.14	0.48
26:BB:88:C:H2'	26:BB:89:G:O4'	2.14	0.48
33:DN:128:HIS:CE1	33:DN:135:PRO:HG2	2.48	0.48
1:CA:758:G:H4'	1:CA:880:C:H4'	1.95	0.48
17:CQ:66:SER:O	17:CQ:70:ARG:NH1	2.47	0.48
1:CA:637:G:H2'	1:CA:638:G:C8	2.49	0.48
34:BO:64:ARG:NH2	34:BO:99:PHE:O	2.47	0.48
1:AA:1346:A:N1	1:AA:1374:A:H5''	2.28	0.48
2:AB:158:LEU:HD12	2:AB:182:ILE:HD11	1.96	0.48
34:BO:120:GLU:HG2	34:BO:122:LEU:HG	1.95	0.48
25:BA:1195:G:H2'	25:BA:1196:C:C6	2.49	0.48
25:BA:2772:G:N7	61:BA:4272:HOH:O	2.35	0.48
1:AA:1309:G:O2'	13:AM:77:ASN:ND2	2.47	0.48
30:BG:45:GLU:HG2	30:BG:45:GLU:H	1.50	0.48
28:DE:31:CYS:HB2	28:DE:91:VAL:HB	1.96	0.48
23:CY:47:U:O2'	23:CY:48:C:H5'	2.13	0.48
23:AW:26:A:H61	23:AW:44:G:H1	1.61	0.48
44:BY:90:LEU:HB3	44:BY:92:ASN:H	1.79	0.48
25:DA:1003:G:N2	25:DA:1153:C:C2	2.81	0.48
36:DQ:111:GLU:CD	36:DQ:133:ARG:HH21	2.15	0.48
9:CI:16:ARG:N	9:CI:64:THR:O	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1510:U:H2'	1:CA:1511:G:C8	2.49	0.48
14:AN:3:ARG:NH2	14:AN:3:ARG:HB3	2.29	0.48
25:DA:989:G:H4'	25:DA:990:A:OP1	2.12	0.48
25:BA:207:A:C2	25:BA:224:U:H4'	2.49	0.48
25:DA:1639:U:C2'	25:DA:1640:C:H5''	2.44	0.48
25:BA:2658:C:OP2	25:BA:2745:G:O2'	2.19	0.48
35:DP:101:VAL:HA	35:DP:106:LEU:O	2.14	0.48
33:DN:42:TRP:CH2	33:DN:44:PRO:HB3	2.48	0.48
1:AA:911:U:H2'	1:AA:912:C:C6	2.49	0.48
25:DA:1711:C:H2'	25:DA:1712:C:C6	2.48	0.48
33:DN:12:ARG:HH21	33:DN:138:LEU:HD11	1.78	0.48
25:DA:2512:C:H2'	25:DA:2513:G:O4'	2.13	0.48
23:AW:72:C:H5'	61:AW:4009:HOH:O	2.13	0.48
2:AB:95:GLN:HG3	2:AB:147:LYS:HD3	1.95	0.48
1:CA:1412:C:H2'	1:CA:1413:A:C8	2.49	0.48
4:CD:60:GLU:HG2	4:CD:202:LEU:HB2	1.95	0.48
25:DA:2345:G:H4'	25:DA:2346:A:H5''	1.96	0.48
25:DA:784:A:C6	27:DD:229:VAL:HG11	2.49	0.47
1:CA:1240:U:OP2	7:CG:115:ARG:HA	2.13	0.47
27:DD:26:LYS:HB3	27:DD:83:GLU:HG2	1.95	0.47
1:CA:148:G:H2'	1:CA:149:A:C8	2.46	0.47
5:CE:140:ARG:O	5:CE:143:ARG:NH2	2.47	0.47
10:AJ:57:LYS:HE2	10:AJ:60:ARG:NH2	2.29	0.47
1:AA:625:G:H2'	1:AA:626:U:C6	2.49	0.47
1:CA:1226:C:H4'	19:CS:80:TYR:CZ	2.49	0.47
11:CK:79:SER:OG	11:CK:106:LYS:NZ	2.47	0.47
15:CO:5:LYS:HB2	15:CO:5:LYS:HZ3	1.79	0.47
25:BA:1547:C:O4'	27:BD:100:GLY:HA2	2.14	0.47
5:CE:81:GLU:HG2	5:CE:90:VAL:HG13	1.96	0.47
5:CE:90:VAL:O	5:CE:120:THR:HA	2.14	0.47
2:AB:145:LEU:HD12	2:AB:149:LEU:HD12	1.96	0.47
1:CA:1371:G:O3'	9:CI:69:GLY:HA3	2.14	0.47
1:CA:1069:C:O2'	1:CA:1192:C:H1'	2.14	0.47
36:BQ:42:ILE:HD13	36:BQ:97:VAL:HB	1.96	0.47
1:CA:1312:G:H5'	19:CS:5:LEU:HD21	1.96	0.47
1:CA:509:A:H5''	4:CD:55:ALA:HB2	1.95	0.47
2:AB:100:GLY:N	2:AB:176:GLU:OE2	2.38	0.47
23:CY:56:C:H2'	23:CY:57:G:H8	1.79	0.47
25:DA:2135:A:H61	25:DA:2157:G:H21	1.61	0.47
23:CW:7:A:N1	23:CW:66:U:C4	2.80	0.47
1:CA:953:G:C2	1:CA:954:G:H1'	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:2147:G:H2'	25:DA:2148:G:O4'	2.14	0.47
45:BZ:153:SER:HB3	45:BZ:167:PRO:HB3	1.96	0.47
25:BA:1152:G:H4'	25:BA:1153:G:OP2	2.14	0.47
25:DA:2025:C:H2'	25:DA:2026:C:C6	2.49	0.47
25:BA:2331:G:H4'	25:BA:2332:A:OP1	2.13	0.47
25:DA:287:C:H2'	25:DA:288:C:C6	2.47	0.47
1:CA:596:C:N3	1:CA:644:G:N1	2.47	0.47
4:AD:25:ARG:NH1	4:AD:30:LYS:HB3	2.30	0.47
25:BA:1553:A:O2'	25:BA:1554:A:O5'	2.27	0.47
1:CA:426:G:OP1	4:CD:36:ARG:HD2	2.14	0.47
25:DA:1013:C:H2'	25:DA:1014:U:C6	2.49	0.47
25:DA:2207:G:OP1	25:DA:2207:G:H8	1.96	0.47
26:BB:29:A:H2'	26:BB:30:C:C6	2.49	0.47
29:DF:65:TRP:CZ2	29:DF:75:HIS:HD2	2.32	0.47
29:BF:150:GLY:HA2	29:BF:172:TRP:CD2	2.49	0.47
25:BA:1580:G:N2	25:BA:1583:C:H41	2.11	0.47
4:AD:6:GLY:O	4:AD:115:ARG:NH1	2.45	0.47
1:AA:501:C:H2'	1:AA:502:G:C8	2.49	0.47
1:CA:486:U:H2'	1:CA:487:A:C8	2.49	0.47
4:AD:15:GLU:OE2	4:AD:66:ARG:NH1	2.47	0.47
35:DP:81:GLN:NE2	35:DP:105:LEU:O	2.47	0.47
23:AY:25:C:O2'	23:AY:26:A:O4'	2.32	0.47
25:BA:2169:G:C3'	25:BA:2170:G:H5''	2.42	0.47
23:CW:22:G:N7	23:CW:46:7MG:N2	2.60	0.47
25:DA:1153:C:H2'	25:DA:1154:G:O4'	2.14	0.47
26:DB:105:A:H2'	26:DB:106:G:O4'	2.14	0.47
57:CA:3175:NEG:H72	25:DA:739:G:N1	2.24	0.47
28:BE:24:THR:HG23	28:BE:184:VAL:HG12	1.96	0.47
57:AA:3220:NEG:N3	25:BA:1968:U:OP2	2.48	0.47
1:AA:142:G:H2'	1:AA:143:A:C8	2.49	0.47
45:BZ:111:VAL:HG12	45:BZ:112:ARG:H	1.79	0.47
32:BI:93:THR:H	32:BI:96:ASP:HB2	1.79	0.47
25:DA:565:C:H2'	25:DA:566:U:O4'	2.14	0.47
1:AA:452:A:O3'	16:AP:72:ARG:HD2	2.14	0.47
25:DA:1158:C:H4'	49:D3:32:GLN:HB2	1.97	0.47
1:AA:1280:A:O2'	1:AA:1281:U:H5''	2.14	0.47
45:BZ:58:VAL:HG12	45:BZ:68:PRO:HA	1.95	0.47
11:CK:24:SER:OG	11:CK:25:TYR:N	2.46	0.47
11:CK:34:ASP:HB3	11:CK:40:ILE:HD11	1.96	0.47
25:DA:1181:C:H2'	25:DA:1182:A:C8	2.50	0.47
1:AA:404:U:H5'	4:AD:122:ARG:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:DO:104:ARG:CZ	39:DT:34:VAL:HG11	2.44	0.47
25:DA:1033:U:OP1	55:D9:9:ARG:NH2	2.47	0.47
25:BA:1073:A:C2	25:BA:2500:A:H5'	2.49	0.47
3:CC:120:VAL:HA	3:CC:123:GLN:HB2	1.96	0.47
23:AY:19:G:H5''	23:AY:20:U:C5	2.49	0.47
25:DA:1697:G:OP2	25:DA:1698:A:O2'	2.22	0.47
26:DB:72:G:O2'	26:DB:105:A:N6	2.48	0.47
45:BZ:163:LEU:HD23	45:BZ:167:PRO:HG3	1.96	0.47
45:DZ:141:VAL:HG12	45:DZ:144:LEU:HD12	1.96	0.47
57:CX:3004:NEG:H71	25:DA:2323:G:N7	2.29	0.47
1:AA:993:G:O2'	1:AA:994:A:N7	2.47	0.47
25:BA:878:G:O2'	35:BP:38:GLN:NE2	2.47	0.47
25:DA:1300:U:C2	25:DA:1626:G:C6	3.01	0.47
9:AI:24:GLY:HA3	9:AI:57:GLY:HA2	1.95	0.47
25:BA:223:C:H2'	25:BA:224:U:C6	2.49	0.47
1:AA:545:C:OP1	4:AD:61:LYS:NZ	2.47	0.47
25:DA:570:G:H2'	25:DA:2030:A:C5	2.49	0.47
25:BA:390:G:H2'	25:BA:391:G:H8	1.78	0.47
1:CA:250:A:H4'	1:CA:251:G:O5'	2.12	0.47
37:DR:28:LEU:HD12	37:DR:48:VAL:HG21	1.96	0.47
22:CV:20:U:H2'	22:CV:21:C:C6	2.49	0.47
2:CB:52:GLU:HG2	2:CB:56:ARG:NH2	2.30	0.47
15:CO:17:ARG:HG3	15:CO:17:ARG:HH11	1.80	0.47
26:DB:40:U:C6	50:D4:2:LYS:HE3	2.49	0.47
25:DA:2315:G:H2'	25:DA:2316:C:C6	2.49	0.47
23:AY:58:A:H1'	23:AY:60:U:OP2	2.14	0.47
2:AB:16:HIS:HD2	2:AB:204:ASN:H	1.62	0.47
1:AA:1392:G:N2	1:AA:1502:A:H8	2.13	0.47
1:CA:976:G:OP1	14:CN:32:SER:N	2.42	0.47
1:AA:1130:A:H5'	9:AI:18:PHE:CE2	2.49	0.47
25:DA:2602:A:H4'	25:DA:2603:G:C5'	2.45	0.47
9:AI:49:PRO:HG3	9:AI:101:PHE:CD2	2.47	0.47
3:CC:130:VAL:O	3:CC:134:ILE:HG12	2.14	0.47
28:DE:24:THR:HG23	28:DE:184:VAL:HG12	1.96	0.47
1:AA:277:C:H5''	17:AQ:68:ARG:NH2	2.30	0.47
4:AD:178:VAL:O	4:AD:180:GLY:N	2.45	0.47
25:DA:2847:U:OP1	39:DT:98:LYS:HE2	2.14	0.47
25:DA:2693:A:H2'	25:DA:2694:G:C8	2.49	0.47
30:DG:179:PRO:HB2	50:D4:42:PHE:HE1	1.79	0.47
25:DA:1239:G:H2'	25:DA:1240:U:O4'	2.14	0.47
1:CA:1348:U:H4'	9:CI:120:ARG:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:47:THR:HA	2:AB:202:PRO:HG2	1.97	0.47
25:DA:2461:C:H2'	25:DA:2462:U:C6	2.50	0.47
30:BG:74:LYS:O	30:BG:84:LYS:NZ	2.47	0.47
25:DA:1354:A:H2'	25:DA:1355:G:O4'	2.14	0.47
2:AB:109:SER:O	2:AB:112:VAL:HG22	2.15	0.47
25:DA:272(B):G:H2'	25:DA:272(C):G:C8	2.50	0.47
25:DA:2494:G:O2'	36:DQ:80:GLU:HA	2.14	0.47
13:CM:50:GLU:O	13:CM:54:VAL:HG22	2.14	0.47
1:CA:1414:U:H3	1:CA:1486:G:H1	1.62	0.47
1:CA:1241:G:H2'	1:CA:1242:C:C6	2.49	0.47
19:AS:12:ASP:HB3	19:AS:14:HIS:CD2	2.50	0.47
1:AA:1004:A:C6	1:AA:1037:C:C4	3.03	0.47
25:BA:2162:C:C2	25:BA:2173:G:C2	3.03	0.47
1:AA:1125:U:H4'	10:AJ:5:ARG:NH2	2.29	0.47
1:CA:1392:G:N2	1:CA:1502:A:H8	2.12	0.47
1:CA:1090:U:H2'	1:CA:1091:U:C6	2.49	0.47
1:CA:9:G:H2'	1:CA:10:A:C8	2.48	0.47
1:CA:1075:C:C2'	1:CA:1076:C:H5'	2.44	0.47
10:CJ:45:ARG:HG2	10:CJ:47:PHE:CZ	2.49	0.47
36:BQ:31:ASP:HA	36:BQ:134:ARG:NH1	2.29	0.47
1:CA:1376:U:OP1	7:CG:98:SER:OG	2.25	0.47
29:BF:53:THR:HB	29:BF:56:GLU:OE2	2.14	0.47
25:BA:2159:C:O2	25:BA:2176:G:N1	2.36	0.47
16:CP:19:ILE:N	16:CP:37:GLY:O	2.46	0.47
25:DA:601:C:O2'	25:DA:605:C:H5''	2.14	0.47
27:DD:145:VAL:HG11	27:DD:175:LEU:HD11	1.97	0.47
5:AE:77:PRO:HG2	5:AE:78:HIS:HD2	1.78	0.47
8:CH:91:ARG:HD3	17:CQ:32:TYR:O	2.15	0.47
25:DA:2513:G:N2	28:DE:143:ASN:OD1	2.47	0.47
6:AF:76:ALA:O	6:AF:80:ARG:HG3	2.14	0.47
44:BY:54:LYS:H	44:BY:56:PRO:HD3	1.79	0.47
34:BO:68:GLU:HB3	34:BO:78:ARG:HB2	1.95	0.47
33:DN:34:LEU:O	33:DN:49:GLY:HA3	2.14	0.47
38:BS:35:ILE:HG12	38:BS:101:LEU:HD12	1.95	0.47
33:BN:91:LEU:HG	33:BN:98:VAL:HG21	1.97	0.47
1:CA:625:G:H2'	1:CA:626:U:C6	2.50	0.47
16:CP:59:TRP:HA	16:CP:62:VAL:HG12	1.95	0.47
6:CF:99:ALA:HB2	18:CR:31:LEU:HD21	1.97	0.47
32:DI:41:GLU:O	32:DI:45:LYS:HG3	2.14	0.47
19:AS:80:TYR:CZ	19:AS:82:GLY:HA2	2.49	0.47
25:DA:731:C:OP1	61:DA:4599:HOH:O	2.21	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AW:46:7MG:H5''	61:AW:4003:HOH:O	2.15	0.47
7:AG:26:PHE:O	7:AG:30:ILE:HG13	2.15	0.47
2:CB:55:PHE:HA	2:CB:58:ILE:HB	1.95	0.47
25:BA:1699:A:OP1	37:BR:8:ARG:NH1	2.47	0.47
25:BA:2158:C:H41	25:BA:2178:G:N2	2.12	0.47
25:BA:1405:A:H2'	25:BA:1406:A:H5'	1.96	0.47
25:BA:2168:C:O2'	25:BA:2169:G:OP2	2.29	0.47
25:BA:2190:G:C6	25:BA:2193:A:C8	3.02	0.47
25:BA:2141:A:O2'	25:BA:2142:G:H5'	2.14	0.47
27:BD:275:LYS:HB3	27:BD:276:LYS:H	1.24	0.47
35:DP:39:LYS:HB2	35:DP:45:LEU:HG	1.96	0.47
1:AA:632:A:H5'	1:AA:633:G:OP2	2.14	0.47
25:DA:1761:C:H3'	25:DA:1762:A:H5''	1.97	0.47
1:AA:345:C:H4'	1:AA:346:G:C4	2.50	0.47
25:DA:2572:A:C8	28:DE:144:ARG:HD2	2.50	0.47
25:DA:1127:A:H2'	25:DA:2518:A:H2	1.80	0.47
25:DA:359:A:H2'	25:DA:360:G:O4'	2.14	0.47
1:CA:974:A:OP2	14:CN:41:ARG:NH1	2.47	0.47
9:AI:26:VAL:HG13	9:AI:63:ILE:HD12	1.97	0.47
36:DQ:18:LYS:HE3	36:DQ:18:LYS:HB2	1.72	0.47
8:CH:51:VAL:HG12	8:CH:52:ASP:H	1.80	0.47
3:CC:70:VAL:N	3:CC:106:VAL:HG23	2.30	0.47
25:BA:560:C:O3'	40:BU:53:ARG:NH1	2.47	0.47
25:DA:747:U:O2	25:DA:2014:A:H1'	2.14	0.47
25:BA:1529:G:O6	25:BA:1553:A:N6	2.48	0.47
25:BA:397:G:H4'	25:BA:398:A:OP2	2.14	0.47
1:CA:779:C:H2'	1:CA:780:A:O4'	2.15	0.47
4:CD:22:LYS:HB2	4:CD:26:CYS:SG	2.55	0.47
25:DA:1114:G:H2'	25:DA:1115:G:C8	2.49	0.47
25:BA:2108:U:H2'	25:BA:2109:G:C8	2.50	0.47
31:BH:56:SER:OG	31:BH:57:ASP:N	2.47	0.47
25:BA:2376:C:H2'	25:BA:2377:G:O4'	2.15	0.47
8:CH:39:LEU:HB3	8:CH:45:ILE:HG12	1.95	0.47
25:BA:1559:C:H2'	25:BA:1560:U:O4'	2.15	0.47
25:BA:840:A:OP2	25:BA:2093:A:O2'	2.31	0.47
25:DA:632:A:H2'	25:DA:633:A:C8	2.49	0.47
26:DB:28:C:H2'	26:DB:29:A:C8	2.50	0.47
31:BH:13:LYS:HA	31:BH:14:GLY:HA2	1.67	0.47
24:CX:13:C:O2'	25:DA:1924:C:H4'	2.15	0.47
25:BA:2803:A:N3	25:BA:2803:A:H2'	2.28	0.47
35:DP:15:ARG:HD3	35:DP:15:ARG:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:434:U:H2'	1:AA:435:C:C6	2.50	0.47
25:DA:673:C:H5''	29:DF:81:PRO:HD2	1.96	0.47
1:CA:130:A:H1'	1:CA:263:A:O2'	2.14	0.47
25:BA:518:G:H2'	25:BA:519:G:O4'	2.14	0.47
1:AA:21:G:OP1	61:AA:4122:HOH:O	2.20	0.47
1:AA:765:G:N1	1:AA:812:C:O2'	2.38	0.47
1:AA:1286:A:C8	1:AA:1287:A:H4'	2.49	0.47
1:AA:1386:G:H2'	1:AA:1387:G:H8	1.79	0.47
13:CM:91:ARG:O	13:CM:96:LEU:N	2.44	0.47
1:CA:632:A:H5'	1:CA:633:G:OP2	2.15	0.47
25:BA:2124:U:H2'	25:BA:2125:C:C6	2.50	0.47
1:AA:1314:C:OP2	19:AS:4:SER:OG	2.14	0.47
6:AF:33:TYR:CD2	6:AF:75:LEU:HD23	2.50	0.47
48:B2:1:MET:N	48:B2:52:ASP:OD2	2.30	0.47
1:CA:949:A:N7	13:CM:106:ASN:ND2	2.63	0.47
28:DE:174:ASP:OD1	28:DE:175:VAL:N	2.48	0.47
1:CA:1028:C:C2	1:CA:1033:G:N1	2.82	0.47
2:CB:16:HIS:CB	2:CB:204:ASN:HB3	2.31	0.47
10:CJ:32:ALA:CB	10:CJ:33:GLN:HA	2.38	0.47
25:DA:873:G:H1'	36:DQ:29:PHE:HE2	1.79	0.47
25:DA:942:G:OP1	35:DP:39:LYS:NZ	2.48	0.47
1:CA:1239:A:H4'	1:CA:1240:U:H5''	1.97	0.47
1:AA:1030(C):G:H2'	1:AA:1030(D):A:C8	2.50	0.47
29:BF:125:LEU:HD12	29:BF:194:MET:HB2	1.97	0.47
54:D8:63:PRO:HG2	54:D8:64:TYR:CE2	2.50	0.47
1:AA:69:G:H2'	1:AA:70:G:C8	2.50	0.47
25:DA:919:G:C6	25:DA:2268:A:C6	3.03	0.47
25:DA:921:G:H2'	25:DA:922:U:C6	2.49	0.47
25:BA:2388:A:H2'	25:BA:2389:A:O4'	2.15	0.47
1:CA:396:G:O2'	1:CA:398:C:OP1	2.17	0.47
25:BA:1873:G:O2'	27:BD:253:GLN:NE2	2.47	0.47
25:BA:793:A:H2'	25:BA:2624:C:H5''	1.97	0.47
25:DA:2206:G:H8	25:DA:2207:G:N7	2.11	0.47
23:AY:36:A:H2'	23:AY:37:MIA:O4'	2.14	0.47
24:CX:9:G:O2'	24:CX:10:G:N7	2.42	0.47
25:DA:570:G:H2'	25:DA:2030:A:N7	2.30	0.47
1:CA:1262:C:H2'	1:CA:1263:C:C6	2.50	0.47
55:B9:2:LYS:HE2	55:B9:31:LYS:O	2.15	0.47
25:BA:1654:A:H1'	25:BA:1656:A:OP2	2.15	0.47
43:BX:32:PRO:HA	43:BX:77:LYS:HB2	1.96	0.47
1:CA:994:A:N7	1:CA:1216:G:H4'	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:CC:173:VAL:O	3:CC:175:LEU:HD12	2.15	0.47
31:DH:3:ARG:NH1	31:DH:5:GLY:H	2.13	0.47
1:CA:1109:C:H2'	1:CA:1110:A:O4'	2.15	0.47
23:CW:11:C:H2'	23:CW:12:U:H6	1.80	0.47
44:BY:19:LYS:HE2	44:BY:20:TYR:CE1	2.50	0.47
33:BN:4:TYR:CD2	40:BU:100:VAL:HG11	2.50	0.47
25:DA:2124:G:C6	25:DA:2174:C:N4	2.81	0.47
23:CW:8:4SU:H1'	23:CW:48:C:H1'	1.97	0.47
25:DA:932:G:H4'	25:DA:933:A:O5'	2.14	0.47
25:DA:828:U:H4'	25:DA:831:G:N1	2.29	0.47
1:CA:1298:C:H4'	1:CA:1299:A:H5'	1.96	0.47
57:AX:3013:NEG:H92	25:BA:2335:G:N7	2.30	0.47
52:B6:9:LEU:HA	52:B6:54:ILE:HB	1.96	0.47
57:CX:3004:NEG:N1	25:DA:2330:G:O6	2.47	0.47
25:DA:1126:A:OP1	25:DA:1126:A:H8	1.97	0.47
25:DA:1266:G:O2'	25:DA:2012:G:O6	2.23	0.47
1:CA:391:G:C6	1:CA:392:G:C5	3.03	0.47
16:CP:72:ARG:NH2	16:CP:73:LEU:HD21	2.29	0.47
25:DA:953:A:C2	25:DA:954:G:C8	3.03	0.47
25:DA:2811:G:N2	25:DA:2891:G:H1'	2.29	0.47
1:CA:1142:G:H2'	1:CA:1143:G:O4'	2.14	0.47
25:BA:323:A:N1	25:BA:346:A:O2'	2.46	0.47
2:AB:88:ALA:HB2	2:AB:219:VAL:HG13	1.97	0.47
25:DA:1486:A:H2'	25:DA:1487:G:H8	1.80	0.47
8:AH:121:ASP:HB2	8:AH:125:ARG:NH2	2.30	0.47
25:BA:834:U:H5''	25:BA:835:A:H5'	1.97	0.47
29:DF:113:ALA:HB2	29:DF:183:VAL:HB	1.97	0.47
16:AP:19:ILE:N	16:AP:37:GLY:O	2.48	0.47
26:DB:40:U:H2'	50:D4:2:LYS:HE3	1.97	0.47
5:CE:71:LEU:HG	5:CE:114:GLY:O	2.14	0.47
52:B6:4:GLU:HG3	52:B6:5:VAL:N	2.30	0.47
25:BA:1733:C:H2'	25:BA:1734:G:O4'	2.15	0.47
25:BA:2585:C:H3'	61:BA:5300:HOH:O	2.13	0.47
35:BP:95:VAL:HG13	35:BP:125:VAL:HG12	1.97	0.47
25:BA:2795:G:OP2	61:BA:4927:HOH:O	2.20	0.47
47:B1:72:GLU:O	47:B1:76:ARG:HG3	2.15	0.47
25:DA:752:A:P	53:D7:3:ARG:HH22	2.38	0.47
25:DA:1922:G:H2'	25:DA:1923:U:O4'	2.15	0.47
32:DI:66:GLU:OE2	32:DI:69:LYS:HD3	2.15	0.47
1:CA:69:G:H2'	1:CA:70:G:H8	1.79	0.47
25:DA:10:G:O2'	25:DA:2801(A):A:N6	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:CG:78:ARG:CZ	7:CG:79:ARG:HH12	2.28	0.47
19:AS:28:LYS:HZ2	19:AS:28:LYS:HB3	1.80	0.47
23:CY:23:A:H8	23:CY:23:A:O5'	1.98	0.47
45:BZ:121:HIS:HB3	45:BZ:123:ASP:O	2.14	0.47
39:DT:94:ALA:HB1	39:DT:99:LEU:HD21	1.97	0.47
1:CA:501:C:H2'	1:CA:502:G:C8	2.50	0.47
33:BN:95:PRO:HG2	33:BN:124:ALA:HB2	1.97	0.47
25:BA:1714:G:O2'	25:BA:2013:U:O4	2.27	0.47
1:AA:44:G:C2	1:AA:45:U:H1'	2.50	0.47
27:DD:34:VAL:HG12	27:DD:63:ARG:HG3	1.96	0.47
45:BZ:107:THR:HA	45:BZ:108:PRO:HD3	1.55	0.47
1:AA:1316:G:N1	1:AA:1319:A:OP2	2.44	0.47
25:DA:26:G:H1'	25:DA:514:A:N6	2.30	0.47
10:CJ:44:VAL:HG13	10:CJ:66:ARG:HG2	1.97	0.47
42:BW:18:ARG:NH1	42:BW:76:VAL:O	2.48	0.47
25:DA:459:U:H5''	53:D7:40:TRP:CD2	2.50	0.47
1:CA:926:G:H5''	1:CA:927:G:O5'	2.15	0.47
28:DE:14:ILE:HG13	28:DE:21:VAL:HG13	1.96	0.47
25:BA:2055:A:OP1	61:BA:4435:HOH:O	2.20	0.47
31:BH:154:PRO:HB3	31:BH:163:TYR:CZ	2.50	0.47
25:BA:1400:A:H2'	25:BA:1401:G:O4'	2.15	0.47
25:BA:886:U:H1'	25:BA:1236:G:H1'	1.96	0.47
1:CA:657:G:H21	15:CO:22:THR:HG1	1.63	0.47
25:BA:2170:G:C8	25:BA:2170:G:H5'	2.51	0.46
25:BA:2190:G:O6	25:BA:2193:A:H2'	2.16	0.46
10:AJ:5:ARG:NE	10:AJ:73:ASP:OD1	2.25	0.46
1:AA:148:G:H2'	1:AA:149:A:H8	1.81	0.46
26:DB:3:C:H2'	26:DB:4:C:H6	1.78	0.46
25:BA:1462:G:O2'	25:BA:1463:C:OP2	2.28	0.46
25:DA:888:C:H5''	25:DA:889:C:OP2	2.14	0.46
30:DG:15:VAL:HG22	30:DG:175:LEU:HB3	1.97	0.46
25:DA:2291:U:OP1	25:DA:2380:C:O2'	2.29	0.46
37:BR:67:LEU:CD1	37:BR:76:VAL:HG21	2.45	0.46
1:CA:997:U:H3	1:CA:1044:A:N6	2.13	0.46
4:CD:13:ARG:HB3	4:CD:38:TYR:O	2.15	0.46
1:AA:309:G:O2'	1:AA:607:A:N1	2.47	0.46
25:DA:2252:G:H2'	25:DA:2253:G:H8	1.80	0.46
44:BY:13:VAL:HB	44:BY:72:VAL:HG13	1.96	0.46
54:B8:23:VAL:HG13	54:B8:47:LYS:HB3	1.95	0.46
26:DB:87:G:N2	26:DB:90:A:OP2	2.47	0.46
45:BZ:45:ASP:O	45:BZ:49:ARG:HG3	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:BV:14:VAL:HB	41:BV:96:ILE:HG13	1.97	0.46
25:BA:231:G:C8	54:B8:5:LYS:HG2	2.50	0.46
55:D9:15:LYS:HE2	55:D9:17:ILE:HD13	1.97	0.46
25:DA:363(C):G:H2'	25:DA:363(D):G:H8	1.80	0.46
13:CM:34:LEU:HD13	13:CM:41:PRO:HA	1.97	0.46
1:AA:1070:U:H2'	1:AA:1071:C:C6	2.50	0.46
25:DA:949:C:H2'	25:DA:950:G:C8	2.50	0.46
25:DA:1032:A:H2	25:DA:1122:G:H22	1.62	0.46
20:CT:60:GLU:HG3	20:CT:81:LYS:HD2	1.97	0.46
1:AA:1026:G:O2'	1:AA:1027:C:OP1	2.27	0.46
1:AA:376:G:O3'	16:AP:5:ARG:HD2	2.15	0.46
25:BA:1834:A:H4'	27:BD:259:THR:HG23	1.97	0.46
23:AY:56:C:H2'	23:AY:57:G:O4'	2.14	0.46
19:AS:9:VAL:HG21	50:B4:61:ARG:NH1	2.27	0.46
25:DA:1826:G:H4'	27:DD:242:ARG:CZ	2.46	0.46
25:BA:1067:A:H3'	25:BA:1067:A:H8	1.79	0.46
25:BA:1068:G:N7	33:BN:66:LYS:HE2	2.30	0.46
10:CJ:49:VAL:HG23	14:CN:41:ARG:HD2	1.97	0.46
1:CA:1103:C:H5''	2:CB:98:LEU:HD13	1.97	0.46
1:CA:1014:A:C2	1:CA:1219:U:H1'	2.49	0.46
25:DA:81:G:O2'	25:DA:295:G:O2'	2.27	0.46
25:DA:338:G:O6	61:DA:4110:HOH:O	2.19	0.46
25:BA:2859:U:H4'	25:BA:2878:A:C2	2.50	0.46
25:DA:1484:G:H1	25:DA:1505:C:H42	1.63	0.46
45:DZ:158:PRO:HA	45:DZ:159:PRO:HD3	1.78	0.46
39:BT:118:ARG:HH22	39:BT:125:ARG:HH12	1.64	0.46
25:BA:2018:C:H4'	25:BA:2019:G:OP1	2.15	0.46
4:AD:12:CYS:SG	4:AD:19:LEU:HB2	2.55	0.46
25:BA:1079:U:OP1	55:B9:9:ARG:NH2	2.48	0.46
3:CC:47:LEU:O	3:CC:51:GLY:N	2.47	0.46
16:AP:60:LEU:HA	16:AP:60:LEU:HD12	1.80	0.46
42:BW:79:GLY:HA3	42:BW:100:THR:HG22	1.96	0.46
25:DA:2424:C:O2	25:DA:2429:G:O2'	2.26	0.46
25:DA:2243:U:H2'	25:DA:2244:U:C6	2.50	0.46
25:DA:1226:A:OP1	41:DV:84:LYS:HE2	2.15	0.46
1:CA:1025:U:H3	1:CA:1036:G:H1	1.63	0.46
24:CX:76:A:H3'	25:DA:2585:U:C5	2.49	0.46
25:BA:2148:A:N7	25:BA:2185:C:H1'	2.29	0.46
25:DA:981:A:N1	25:DA:2027:G:O2'	2.36	0.46
26:DB:24:G:N7	26:DB:56:G:H2'	2.30	0.46
1:AA:1277:C:O2'	1:AA:1279:A:H1'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:AO:74:ASP:CG	15:AO:77:ARG:HG3	2.36	0.46
1:AA:456:C:H2'	1:AA:457:C:H6	1.81	0.46
2:CB:92:TYR:CE2	2:CB:94:ASN:HB2	2.50	0.46
1:CA:449:C:H5''	1:CA:450:G:OP2	2.15	0.46
25:DA:2738:A:OP2	61:DA:4493:HOH:O	2.19	0.46
25:DA:1576:U:H2'	25:DA:1577:C:H6	1.79	0.46
26:BB:102:A:N7	61:BB:3117:HOH:O	2.35	0.46
26:BB:75:G:H5''	26:BB:75:G:H8	1.79	0.46
1:CA:768:A:OP2	61:CA:4023:HOH:O	2.21	0.46
32:BI:12:LEU:HD23	32:BI:12:LEU:HA	1.78	0.46
42:BW:46:PHE:O	42:BW:50:VAL:HG23	2.16	0.46
1:AA:1262:C:H2'	1:AA:1263:C:C6	2.50	0.46
25:DA:2060:A:N3	61:DA:4401:HOH:O	2.36	0.46
25:BA:2371:C:H2'	25:BA:2372:A:O4'	2.14	0.46
25:BA:160:G:O2'	25:BA:161:C:H5'	2.15	0.46
25:DA:2173:A:H2'	25:DA:2174:C:O4'	2.15	0.46
25:BA:1405:A:H2	25:BA:1418:U:O4	1.98	0.46
1:AA:1030:C:N3	1:AA:1031:G:C2	2.84	0.46
25:DA:468:G:H5''	29:DF:60:SER:HB2	1.96	0.46
29:DF:102:PRO:HB2	29:DF:105:VAL:HG23	1.97	0.46
25:DA:1278:A:H2'	25:DA:1279:G:C8	2.51	0.46
1:CA:826:C:H2'	1:CA:827:U:C6	2.51	0.46
25:DA:1130:U:O2	25:DA:2025:C:H5''	2.15	0.46
1:CA:1103:C:P	2:CB:96:ARG:HH22	2.38	0.46
15:AO:39:LEU:HB3	15:AO:56:LEU:HD13	1.96	0.46
25:DA:2104:G:H1	25:DA:2185:C:H42	1.63	0.46
1:CA:892:A:H2'	1:CA:893:C:C6	2.51	0.46
1:CA:375:U:C4	1:CA:376:G:N7	2.83	0.46
31:BH:56:SER:HB3	31:BH:61:HIS:ND1	2.31	0.46
4:CD:71:SER:OG	4:CD:74:GLN:HB2	2.15	0.46
29:BF:116:ASP:OD2	35:BP:1:MET:HB3	2.16	0.46
6:CF:9:VAL:HB	6:CF:87:ARG:HB2	1.97	0.46
36:BQ:52:VAL:O	36:BQ:55:VAL:HG12	2.16	0.46
25:DA:1889:A:H2'	25:DA:1890:A:C8	2.50	0.46
1:AA:1019:C:H2'	1:AA:1020:U:O4'	2.16	0.46
25:DA:2371:G:N3	52:D6:46:HIS:HE1	2.14	0.46
25:DA:2466:C:OP1	55:D9:4:ARG:HB2	2.16	0.46
25:DA:271(Q):G:H2'	25:DA:271(R):G:H8	1.80	0.46
26:BB:31:C:H4'	30:BG:29:TRP:CZ2	2.51	0.46
27:DD:152:GLY:O	27:DD:154:LYS:HG2	2.15	0.46
1:CA:933:G:OP2	7:CG:3:ARG:HB2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:573:A:N3	1:CA:883:C:O2'	2.41	0.46
30:DG:44:GLY:O	30:DG:47:LYS:HB2	2.16	0.46
25:DA:385:C:O2	35:DP:71:VAL:HG21	2.16	0.46
2:AB:169:LYS:HD3	2:AB:169:LYS:O	2.15	0.46
2:AB:189:ASP:OD1	2:AB:189:ASP:N	2.44	0.46
25:BA:1974:A:OP1	34:BO:42:SER:OG	2.26	0.46
30:DG:63:ILE:HA	30:DG:143:GLU:HG3	1.96	0.46
1:CA:716:A:N3	11:CK:118:GLY:HA2	2.29	0.46
23:CW:31:A:H2'	23:CW:32:PSU:O4'	2.15	0.46
25:DA:2740:A:N6	25:DA:2763:G:O2'	2.48	0.46
1:AA:1367:C:H4'	10:AJ:48:THR:HG21	1.98	0.46
1:CA:1027:C:OP1	1:CA:1027:C:H4'	2.15	0.46
1:AA:189(D):C:O2	1:AA:189(H):G:C6	2.68	0.46
25:BA:2357:G:N3	25:BA:2393:C:H2'	2.30	0.46
36:BQ:16:ARG:HG2	36:BQ:18:LYS:HE2	1.97	0.46
24:CX:23:C:H2'	24:CX:24:U:H6	1.79	0.46
50:B4:44:THR:OG1	50:B4:44:THR:O	2.25	0.46
25:DA:920:G:H2'	25:DA:921:G:H8	1.81	0.46
45:BZ:157:LEU:C	45:BZ:161:VAL:HG11	2.35	0.46
25:BA:287:G:N7	25:BA:448:U:H2'	2.30	0.46
25:BA:2639:G:N2	25:BA:2790:G:OP2	2.48	0.46
25:DA:42:G:H2'	25:DA:43:A:O4'	2.16	0.46
25:DA:597:U:H2'	25:DA:598:G:H8	1.80	0.46
1:AA:927:G:OP2	1:AA:927:G:H4'	2.15	0.46
1:AA:1104:G:H4'	2:AB:111:ARG:NH1	2.31	0.46
1:AA:501:C:H2'	1:AA:502:G:H8	1.81	0.46
25:DA:1916:A:H2'	25:DA:1917:U:O4'	2.16	0.46
1:CA:69:G:H2'	1:CA:70:G:C8	2.51	0.46
1:CA:986:A:H1'	19:CS:55:LYS:HA	1.97	0.46
18:CR:24:ALA:O	18:CR:26:LEU:N	2.41	0.46
1:CA:232:G:H1'	1:CA:262:A:N1	2.30	0.46
19:CS:24:ALA:O	19:CS:26:GLY:N	2.49	0.46
54:B8:52:LYS:N	54:B8:53:PRO:HD2	2.31	0.46
25:DA:1628:G:H2'	25:DA:1629:U:C6	2.50	0.46
29:DF:202:PHE:O	29:DF:206:ILE:HG12	2.15	0.46
25:BA:627:G:OP2	35:BP:90:ARG:NH1	2.48	0.46
40:DU:17:ILE:HG13	40:DU:32:PHE:HE1	1.80	0.46
4:CD:3:ARG:HD3	4:CD:118:ARG:CD	2.45	0.46
15:AO:62:GLN:HE21	15:AO:66:LEU:HD13	1.81	0.46
2:CB:16:HIS:HA	2:CB:204:ASN:HD22	1.80	0.46
1:AA:377:G:OP1	16:AP:3:LYS:HD2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:2154:G:C2	25:DA:2155:G:C8	3.03	0.46
25:DA:2277:G:OP2	46:D0:10:THR:HG21	2.16	0.46
35:BP:99:LEU:HD22	35:BP:102:ARG:HH22	1.80	0.46
25:DA:1127:A:H2'	25:DA:2518:A:C2	2.49	0.46
25:DA:1131:G:C2	25:DA:1132:A:C4	3.03	0.46
27:BD:145:VAL:HG11	27:BD:175:LEU:HD11	1.98	0.46
25:BA:12:U:O2	25:BA:12:U:H2'	2.14	0.46
45:DZ:48:PHE:HE1	45:DZ:71:VAL:HG11	1.81	0.46
1:AA:859:A:H2'	1:AA:860:A:O4'	2.15	0.46
32:BI:77:LEU:HB2	32:BI:142:VAL:HG12	1.98	0.46
1:AA:1223:C:P	19:AS:78:ARG:HH21	2.39	0.46
44:BY:6:HIS:CD2	44:BY:6:HIS:H	2.33	0.46
25:DA:853:G:H2'	25:DA:854:G:C8	2.51	0.46
1:CA:833:U:H2'	1:CA:834:C:C6	2.51	0.46
1:AA:1251:A:HO2'	1:AA:1369:C:HO2'	1.60	0.46
42:BW:68:ARG:HH11	42:BW:112:GLY:H	1.64	0.46
5:CE:41:VAL:HG23	5:CE:67:VAL:HG13	1.97	0.46
46:B0:18:ALA:HB3	46:B0:20:ARG:NH2	2.31	0.46
15:CO:69:TYR:CZ	15:CO:73:GLU:HG3	2.51	0.46
25:BA:1831:C:OP1	27:BD:260:ARG:NH2	2.48	0.46
8:AH:82:HIS:NE2	8:AH:136:GLU:OE2	2.47	0.46
7:CG:71:PRO:HG3	7:CG:103:TRP:CH2	2.51	0.46
45:DZ:40:ASP:OD2	45:DZ:42:VAL:HG13	2.15	0.46
25:DA:729:G:O2'	25:DA:763:G:H4'	2.14	0.46
1:AA:228:A:H2'	1:AA:229:U:O4'	2.16	0.46
25:DA:1467:C:C5	25:DA:1546:C:H2'	2.51	0.46
31:BH:11:VAL:HG13	31:BH:15:VAL:HG22	1.96	0.46
25:DA:1198:U:H2'	25:DA:1199:U:C6	2.50	0.46
7:CG:149:ARG:HD2	11:CK:59:TYR:CE1	2.50	0.46
1:CA:784:C:H4'	25:DA:1837:C:OP1	2.16	0.46
29:DF:155:LEU:HD11	29:DF:176:LEU:HD12	1.97	0.46
25:BA:210:A:N1	25:BA:254:A:O2'	2.41	0.46
5:AE:90:VAL:O	5:AE:120:THR:HA	2.15	0.46
1:AA:1391:U:H2'	1:AA:1392:G:C8	2.51	0.46
34:BO:34:THR:OG1	34:BO:35:VAL:N	2.48	0.46
1:AA:1031:G:H2'	1:AA:1032:G:C8	2.51	0.46
1:AA:155:C:N3	1:AA:167:G:N1	2.63	0.46
12:CL:53:ARG:NH1	12:CL:92:ASP:OD2	2.36	0.46
1:AA:632:A:H3'	1:AA:633:G:C8	2.50	0.46
25:DA:528:A:OP2	33:DN:114:ARG:NH1	2.48	0.46
3:AC:5:ILE:HG12	3:AC:6:HIS:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:1027:A:C6	25:DA:1126:A:C4	3.04	0.46
25:BA:895:G:N9	25:BA:978:A:H8	2.14	0.46
50:B4:54:GLY:C	50:B4:56:VAL:HA	2.36	0.46
23:CY:23:A:C6	23:CY:24:G:C6	3.04	0.46
8:CH:51:VAL:HG21	8:CH:60:ARG:HB2	1.97	0.46
23:CW:51:U:H2'	23:CW:52:G:C8	2.51	0.46
3:CC:131:ARG:NH1	5:CE:50:GLU:HG3	2.30	0.46
34:BO:2:ILE:HG13	34:BO:8:LEU:HD11	1.97	0.46
25:DA:2249:U:N3	25:DA:2253:G:OP2	2.45	0.46
25:BA:7:G:H2'	25:BA:8:A:O4'	2.15	0.46
25:BA:2556:G:H1'	25:BA:2658:C:H4'	1.96	0.46
2:AB:111:ARG:HH21	2:AB:114:ARG:HD2	1.80	0.46
1:CA:767:A:H2'	1:CA:768:A:O4'	2.16	0.46
44:BY:35:TYR:CE2	44:BY:69:ALA:HB3	2.51	0.46
15:CO:29:VAL:HG13	15:CO:63:ARG:HG3	1.97	0.46
1:AA:1016:A:H2'	1:AA:1017:G:O4'	2.16	0.46
25:DA:483:A:O2'	44:DY:49:VAL:O	2.30	0.46
4:CD:150:GLU:HA	4:CD:153:ARG:HE	1.80	0.46
18:CR:52:PRO:HB2	18:CR:54:ARG:HG2	1.98	0.46
18:CR:61:LYS:O	18:CR:65:ILE:HG12	2.15	0.46
25:BA:1035:G:H4'	25:BA:1036:A:OP1	2.16	0.46
25:DA:606:U:H4'	25:DA:658:C:H4'	1.96	0.46
27:DD:5:LYS:HE3	27:DD:5:LYS:HB3	1.58	0.46
18:AR:24:ALA:C	18:AR:26:LEU:H	2.19	0.46
25:DA:599:G:H5'	35:DP:9:ASN:ND2	2.31	0.46
1:AA:1027:C:O2	1:AA:1034:G:C2	2.69	0.46
25:BA:2160:C:H2'	25:BA:2161:C:C6	2.51	0.46
25:BA:2166:U:O2'	25:BA:2167:C:H2'	2.16	0.46
25:DA:1670:C:O2	28:DE:129:HIS:NE2	2.40	0.46
1:CA:26:A:O2'	4:CD:209:ARG:NH2	2.43	0.46
1:CA:346:G:OP1	39:DT:41:ARG:NH2	2.47	0.46
1:CA:1118:C:H1'	1:CA:1179:A:C4	2.51	0.46
23:AY:71:G:H2'	23:AY:72:C:C6	2.51	0.46
25:DA:2114:A:HO2'	25:DA:2167:U:H1'	1.81	0.46
1:CA:977:A:C2	1:CA:1224:G:C5	3.04	0.46
25:BA:1357:G:O6	53:B7:9:ARG:NH2	2.49	0.46
23:CW:51:U:H2'	23:CW:52:G:H8	1.80	0.46
25:DA:919:G:N2	25:DA:2269:A:OP2	2.48	0.46
45:BZ:111:VAL:O	45:BZ:113:ALA:N	2.46	0.46
1:AA:749:C:H2'	1:AA:750:G:H8	1.81	0.46
25:DA:31:C:OP1	61:DA:4533:HOH:O	2.20	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:BO:19:ILE:HB	34:BO:41:ALA:HB1	1.98	0.46
25:DA:1653:G:O3'	37:DR:2:ARG:HB2	2.16	0.46
25:BA:2021:C:H5''	25:BA:2736:C:O2'	2.16	0.46
25:DA:2206:G:C8	25:DA:2207:G:N7	2.84	0.46
25:BA:2753:A:C6	25:BA:2777:A:C8	3.04	0.46
2:AB:24:TRP:CZ3	2:AB:26:PRO:HA	2.50	0.46
2:CB:141:GLU:O	2:CB:145:LEU:HG	2.16	0.46
54:B8:17:THR:OG1	54:B8:21:LYS:HB2	2.16	0.46
25:BA:1548:C:H2'	25:BA:1549:U:C6	2.51	0.46
42:DW:33:ARG:NH2	42:DW:52:GLU:OE1	2.42	0.46
34:DO:36:GLY:HA2	34:DO:106:LEU:HD23	1.97	0.46
12:AL:28:LYS:HE2	12:AL:64:TYR:HE1	1.81	0.46
1:CA:56:U:H2'	1:CA:57:G:C8	2.51	0.46
1:CA:110:C:H2'	1:CA:111:G:O4'	2.16	0.46
32:DI:43:ASN:C	32:DI:43:ASN:HD22	2.19	0.46
25:BA:2541:G:H5''	25:BA:2542:A:H5''	1.96	0.46
47:D1:56:GLN:NE2	47:D1:87:PRO:HD3	2.31	0.46
9:CI:6:GLY:HA3	9:CI:80:GLY:O	2.16	0.46
31:DH:126:PRO:HB2	31:DH:130:ARG:HD2	1.96	0.46
10:AJ:37:PRO:HA	10:AJ:72:VAL:HG12	1.98	0.46
1:CA:1429:C:H2'	1:CA:1430:C:C6	2.51	0.46
1:AA:976:G:OP1	14:AN:32:SER:N	2.48	0.46
25:BA:1500:A:O2'	25:BA:1501:U:H2'	2.16	0.46
25:DA:573:G:O2'	25:DA:574:C:H3'	2.16	0.46
9:CI:55:ALA:HA	9:CI:58:HIS:HD2	1.81	0.46
6:AF:97:PHE:N	18:AR:30:ASP:OD1	2.40	0.46
32:BI:93:THR:HG22	32:BI:119:PRO:HB3	1.98	0.46
31:BH:3:ARG:CG	31:BH:6:ARG:HG2	2.46	0.46
1:CA:220:G:H2'	1:CA:221:C:H5'	1.98	0.46
1:CA:1320:C:OP1	19:CS:70:LYS:HE3	2.16	0.46
25:DA:1490:A:O2'	25:DA:1491:G:H5'	2.15	0.46
1:CA:693:G:H2'	1:CA:694:A:C8	2.51	0.46
25:BA:1813:C:H1'	25:BA:2621:U:H5''	1.97	0.46
28:BE:28:ALA:HB3	28:BE:93:VAL:HG12	1.98	0.46
6:CF:30:LEU:HD23	6:CF:75:LEU:HD21	1.98	0.46
25:BA:659:C:H2'	25:BA:660:C:C6	2.51	0.46
25:DA:2758:A:C2	25:DA:2759:G:H1'	2.51	0.46
1:AA:1227:A:OP2	13:AM:111:LYS:HE3	2.16	0.46
25:DA:1885:A:H2'	25:DA:1886:C:O4'	2.16	0.46
1:CA:667:G:O2'	15:CO:49:ASP:OD1	2.22	0.46
25:BA:2156:A:O2'	25:BA:2157:A:OP1	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:864:G:C6	25:DA:865:C:N4	2.84	0.46
13:AM:3:ARG:O	13:AM:57:ARG:NH1	2.49	0.46
25:DA:218:A:C2	25:DA:235:U:H4'	2.51	0.46
25:DA:674:G:O2'	29:DF:74:ARG:HD3	2.16	0.46
25:DA:2674:G:H2'	25:DA:2675:A:C8	2.51	0.46
50:B4:62:ARG:HA	50:B4:62:ARG:HD3	1.68	0.46
25:BA:324:A:P	44:BY:86:ARG:HH22	2.39	0.46
25:BA:629:U:H4'	25:BA:705:C:H4'	1.96	0.46
20:CT:56:MET:HG3	20:CT:57:ARG:N	2.31	0.46
25:DA:2019:A:C4'	40:DU:34:LYS:HD2	2.46	0.46
2:AB:48:MET:HA	2:AB:51:LEU:HB2	1.98	0.46
26:BB:74:U:H2'	26:BB:75:G:O4'	2.16	0.46
25:DA:271(Q):G:H2'	25:DA:271(R):G:C8	2.51	0.46
25:DA:1545:A:H2'	25:DA:1546:C:O4'	2.15	0.46
1:CA:1073:U:O2'	2:CB:104:ASN:OD1	2.25	0.46
25:BA:1095:C:H1'	25:BA:1159:U:H4'	1.98	0.46
19:AS:3:ARG:NH1	19:AS:8:GLY:O	2.49	0.46
9:CI:33:PHE:CE1	9:CI:43:ALA:HB1	2.51	0.46
1:CA:630:G:H2'	1:CA:631:G:H8	1.81	0.46
12:AL:42:THR:HG22	12:AL:54:LYS:HD2	1.98	0.46
25:BA:1843:A:O2'	27:BD:45:ASN:N	2.45	0.46
27:BD:26:LYS:HB3	27:BD:83:GLU:HG2	1.98	0.46
1:AA:865:A:C2	1:AA:918:A:H4'	2.50	0.46
25:DA:275:G:H2'	25:DA:276:A:O4'	2.16	0.46
45:BZ:136:PHE:O	45:BZ:137:ILE:HG13	2.16	0.46
25:BA:2302:G:C2	25:BA:2355:C:O2	2.69	0.46
31:DH:56:SER:HB3	31:DH:61:HIS:ND1	2.31	0.46
12:CL:33:ARG:HD3	12:CL:62:SER:HB3	1.98	0.46
20:CT:90:GLN:HB2	20:CT:90:GLN:HE21	1.48	0.46
24:AX:59:A:H2'	24:AX:60:U:H5'	1.98	0.46
1:AA:129(A):G:C6	1:AA:189(E):U:H4'	2.51	0.46
1:CA:516:U:O2'	1:CA:519:C:N3	2.43	0.46
25:BA:2156:A:OP2	25:BA:2178:G:N1	2.48	0.45
25:DA:7:G:H2'	25:DA:8:A:H8	1.81	0.45
25:BA:2162:C:H1'	25:BA:2174:G:N2	2.31	0.45
25:BA:943:C:C4	25:BA:944:C:N4	2.85	0.45
1:AA:1031:G:H2'	1:AA:1032:G:H8	1.81	0.45
19:AS:64:GLU:HB3	50:B4:59:PHE:HE2	1.80	0.45
25:BA:1154:U:O2'	25:BA:1155:C:O4'	2.34	0.45
19:AS:32:LYS:HA	19:AS:50:ALA:HB3	1.96	0.45
25:DA:2262:U:H4'	25:DA:2328:A:C2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:320:A:H4'	25:DA:322:A:N7	2.31	0.45
25:DA:1005:C:C2	25:DA:1143:A:C5	3.04	0.45
35:DP:59:LEU:HD23	54:D8:58:ILE:HD13	1.96	0.45
32:BI:129:THR:HG22	32:BI:139:GLN:NE2	2.31	0.45
50:B4:64:GLY:C	50:B4:66:SER:H	2.19	0.45
1:CA:892:A:O2'	1:CA:1415:G:H4'	2.16	0.45
30:DG:41:GLN:HB3	30:DG:43:LEU:HD22	1.97	0.45
25:BA:2724:U:OP1	25:BA:2727:G:H4'	2.15	0.45
25:BA:2151:C:N3	25:BA:2181:G:O6	2.49	0.45
2:CB:53:ARG:O	2:CB:56:ARG:HB3	2.15	0.45
1:AA:45:U:H2'	1:AA:46:G:C8	2.51	0.45
18:CR:53:ARG:HA	18:CR:56:THR:OG1	2.16	0.45
1:CA:692:U:O2'	1:CA:694:A:N7	2.39	0.45
1:CA:1071:C:H2'	1:CA:1072:G:H8	1.81	0.45
30:DG:173:LEU:HD22	30:DG:178:PHE:CE1	2.51	0.45
31:DH:13:LYS:HA	31:DH:14:GLY:HA2	1.69	0.45
9:CI:26:VAL:HG22	9:CI:61:ALA:HB3	1.97	0.45
33:BN:21:LYS:NZ	33:BN:140:VAL:OXT	2.38	0.45
25:DA:615:G:OP1	29:DF:40:GLN:HG2	2.16	0.45
30:BG:72:ARG:NH1	30:BG:87:PRO:HG3	2.32	0.45
2:CB:100:GLY:N	2:CB:176:GLU:OE2	2.38	0.45
25:BA:1841:A:H2'	25:BA:1842:G:O4'	2.16	0.45
24:AX:23:C:H2'	24:AX:24:U:C6	2.51	0.45
20:AT:30:LYS:HD2	20:AT:71:THR:HG23	1.98	0.45
25:DA:1446:C:H42	25:DA:1465:G:H1	1.63	0.45
13:CM:20:THR:HA	13:CM:25:ILE:HG22	1.98	0.45
13:CM:64:TRP:HB2	13:CM:66:LEU:HD21	1.98	0.45
26:DB:8:U:O2'	38:DS:40:ILE:HD13	2.16	0.45
25:BA:1594:C:H2'	25:BA:1595:C:C6	2.51	0.45
25:BA:2705:A:H2'	25:BA:2706:G:C8	2.50	0.45
25:DA:749:C:O2	25:DA:1618:A:H2'	2.16	0.45
25:DA:301:G:OP2	44:DY:84:ARG:NH2	2.48	0.45
32:BI:10:GLU:HG3	32:BI:10:GLU:H	1.56	0.45
2:CB:189:ASP:N	2:CB:189:ASP:OD1	2.45	0.45
36:DQ:54:MET:HG2	36:DQ:54:MET:H	1.55	0.45
36:DQ:136:ALA:HB1	45:DZ:52:SER:HB3	1.98	0.45
8:AH:33:GLU:HG2	8:AH:48:TYR:CE2	2.52	0.45
25:BA:2742:G:H2'	25:BA:2743:C:O4'	2.16	0.45
23:AY:18:G:C2	23:AY:58:A:C5	3.03	0.45
1:AA:975:A:H4'	1:AA:976:G:C5'	2.38	0.45
1:AA:715:A:H2'	1:AA:716:A:C8	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:839:U:H1'	25:DA:1191:G:H1'	1.97	0.45
1:AA:1007:C:C2	1:AA:1022:G:N1	2.84	0.45
1:AA:1151:A:O2'	1:AA:1152:A:H8	1.99	0.45
36:DQ:57:HIS:CD2	36:DQ:117:ALA:HB2	2.45	0.45
1:AA:149:A:H2'	1:AA:150:C:C6	2.51	0.45
47:D1:91:LYS:HG2	47:D1:95:LEU:HD22	1.98	0.45
25:DA:918:A:H1'	26:DB:80:U:H1'	1.98	0.45
2:AB:231:GLU:HB3	2:AB:232:PRO:CD	2.44	0.45
1:AA:528:C:H41	12:AL:49:ASN:CG	2.19	0.45
25:DA:2702:U:H4'	25:DA:2703:C:OP1	2.15	0.45
1:CA:863:U:H2'	1:CA:865:A:OP2	2.17	0.45
54:B8:23:VAL:CG1	54:B8:47:LYS:HD3	2.46	0.45
25:DA:1576:U:H2'	25:DA:1577:C:C6	2.50	0.45
1:AA:1010:G:N2	1:AA:1020:U:H1'	2.31	0.45
4:AD:155:LEU:O	4:AD:159:ARG:HG3	2.15	0.45
9:AI:4:TYR:CE2	9:AI:88:TYR:HA	2.51	0.45
25:BA:1634:C:H2'	25:BA:1635:C:C6	2.52	0.45
38:BS:39:ILE:HB	38:BS:49:VAL:HG13	1.98	0.45
12:AL:32:PHE:O	12:AL:33:ARG:HD2	2.16	0.45
2:CB:166:ASP:OD2	2:CB:169:LYS:HB2	2.16	0.45
25:BA:1749:G:N7	61:BA:5038:HOH:O	2.36	0.45
25:BA:1387:U:O2	43:BX:80:ILE:HD12	2.16	0.45
25:DA:536:A:H2'	25:DA:537:C:C6	2.51	0.45
25:BA:1847:G:O6	27:BD:35:LYS:NZ	2.38	0.45
38:DS:25:ARG:HD3	38:DS:42:ASP:OD2	2.15	0.45
25:DA:1270:C:O2'	25:DA:1325:G:H2'	2.16	0.45
1:CA:562:C:H1'	12:CL:15:ARG:HB3	1.98	0.45
25:DA:524:U:H4'	25:DA:555:U:H4'	1.97	0.45
28:BE:2:LYS:HG3	28:BE:200:GLU:HB2	1.97	0.45
1:CA:964:A:N3	1:CA:969:A:O2'	2.39	0.45
19:AS:24:ALA:O	19:AS:26:GLY:N	2.49	0.45
16:AP:3:LYS:HG3	16:AP:24:ALA:HB2	1.97	0.45
46:B0:10:THR:HG22	46:B0:12:ASN:N	2.14	0.45
2:AB:207:ALA:O	2:AB:210:SER:HB3	2.17	0.45
2:AB:54:THR:HG21	2:AB:201:ILE:HD11	1.97	0.45
1:CA:1095:U:H2'	1:CA:1096:C:C6	2.51	0.45
25:DA:940:G:N3	25:DA:1191:G:H4'	2.31	0.45
25:DA:1946:U:H2'	25:DA:1947:C:H6	1.80	0.45
25:BA:215:G:N2	25:BA:217:A:H62	2.13	0.45
1:AA:1062:U:H2'	1:AA:1063:C:C6	2.51	0.45
57:AA:3220:NEG:H71	25:BA:1967:G:P	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:595:A:OP2	41:BV:78:LYS:NZ	2.50	0.45
30:DG:137:GLU:HG2	30:DG:152:LEU:HD22	1.99	0.45
25:DA:2554:U:H2'	25:DA:2555:U:C6	2.51	0.45
1:AA:292:G:N7	1:AA:293:G:H1'	2.30	0.45
25:BA:125:A:H5''	25:BA:126:C:C6	2.50	0.45
6:AF:19:LEU:HD11	6:AF:59:TYR:CE2	2.52	0.45
1:CA:509:A:N3	1:CA:543:C:O2'	2.44	0.45
4:AD:63:LYS:HG3	4:AD:198:VAL:HG22	1.97	0.45
25:BA:1911:A:O2'	25:BA:2109:G:H5'	2.16	0.45
25:DA:2741:A:H2'	25:DA:2742:C:O4'	2.16	0.45
11:CK:65:ALA:HB3	11:CK:97:ALA:HB3	1.97	0.45
10:AJ:45:ARG:HG2	10:AJ:47:PHE:CZ	2.51	0.45
3:AC:22:TRP:CE2	14:AN:54:PRO:HG3	2.51	0.45
4:CD:134:ASP:O	4:CD:136:PRO:HD3	2.17	0.45
19:CS:66:MET:HB2	19:CS:74:PHE:CZ	2.52	0.45
25:DA:340:A:H2'	25:DA:341:G:O4'	2.17	0.45
23:CY:69:G:H2'	23:CY:70:G:O4'	2.16	0.45
1:AA:197:A:C5	1:AA:221:C:H4'	2.51	0.45
25:BA:1627:A:OP2	25:BA:1627:A:H8	1.99	0.45
10:CJ:23:ILE:HA	10:CJ:23:ILE:HD13	1.79	0.45
37:BR:54:LEU:HD12	37:BR:54:LEU:HA	1.84	0.45
25:BA:791:G:OP1	61:BA:4785:HOH:O	2.21	0.45
25:DA:937:U:H2'	25:DA:938:G:O4'	2.16	0.45
25:BA:1836:U:O2	27:BD:50:THR:HB	2.15	0.45
1:CA:1328:C:O2'	13:CM:29:ARG:NH2	2.47	0.45
25:DA:1778:U:H2'	25:DA:1784:A:N6	2.30	0.45
25:DA:7:G:OP1	33:DN:130:HIS:HE1	1.99	0.45
26:DB:106:G:C5'	45:DZ:31:ARG:HG2	2.47	0.45
40:BU:76:TYR:CE1	40:BU:80:ILE:HG13	2.52	0.45
1:AA:1147:C:HO2'	9:AI:5:TYR:HH	1.54	0.45
1:CA:1055:A:C5	1:CA:1206:G:C2	3.04	0.45
1:CA:1133:G:H2'	1:CA:1134:G:C8	2.51	0.45
3:CC:37:GLN:HA	3:CC:40:ARG:HG3	1.98	0.45
25:BA:559:U:H2'	25:BA:560:C:C6	2.51	0.45
4:AD:18:LYS:NZ	4:AD:26:CYS:O	2.26	0.45
1:CA:302:G:N3	1:CA:556:C:H4'	2.31	0.45
25:BA:2867:G:N2	25:BA:2870:A:OP2	2.38	0.45
2:CB:91:PRO:HG3	2:CB:154:LEU:HD12	1.99	0.45
33:DN:138:LEU:HA	33:DN:138:LEU:HD23	1.66	0.45
1:CA:131:C:H2'	1:CA:132:C:C6	2.52	0.45
13:CM:25:ILE:HD12	13:CM:66:LEU:HD22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:AO:85:LEU:HD23	15:AO:85:LEU:HA	1.84	0.45
25:BA:543:G:H2'	25:BA:544:U:C6	2.51	0.45
43:DX:4:ALA:HB1	43:DX:42:ALA:HA	1.98	0.45
25:DA:771:G:OP1	53:D7:10:ARG:HD3	2.16	0.45
25:BA:2856:G:H2'	25:BA:2857:U:O4'	2.16	0.45
40:DU:89:GLU:HB2	41:DV:50:PRO:HB2	1.97	0.45
25:BA:463:C:H2'	25:BA:464:G:C8	2.51	0.45
27:DD:218:ARG:HB3	27:DD:219:PRO:HD2	1.98	0.45
17:CQ:56:VAL:HB	17:CQ:78:GLU:HB3	1.99	0.45
25:DA:748:G:C8	42:DW:89:ALA:HB1	2.51	0.45
38:BS:59:LYS:HB2	38:BS:60:GLY:H	1.52	0.45
1:CA:59:A:H5''	1:CA:60:A:H5''	1.98	0.45
25:BA:1685:C:H5''	25:BA:2722:C:O2'	2.15	0.45
29:BF:20:LEU:HD22	29:BF:21:ALA:H	1.82	0.45
18:CR:21:LYS:HA	18:CR:21:LYS:HD3	1.72	0.45
5:CE:73:ASN:OD1	5:CE:73:ASN:N	2.50	0.45
32:BI:61:ARG:HA	32:BI:61:ARG:HH11	1.82	0.45
2:CB:223:ILE:HA	2:CB:226:ARG:HG2	1.99	0.45
1:AA:814:A:H2'	1:AA:816:A:H5''	1.99	0.45
31:DH:113:VAL:HG11	31:DH:151:ILE:HD13	1.99	0.45
25:DA:2074:U:H2'	25:DA:2075:U:C6	2.51	0.45
1:AA:1095:U:P	1:AA:1108:G:H1	2.39	0.45
23:CW:9:A:H4'	23:CW:46:7MG:O4'	2.16	0.45
1:CA:952:U:H2'	1:CA:953:G:H8	1.82	0.45
25:DA:2141:G:O4'	25:DA:2151:G:N2	2.50	0.45
25:BA:1296:G:OP2	35:BP:21:ARG:NH1	2.47	0.45
1:CA:840:C:H4'	1:CA:841:U:OP1	2.17	0.45
25:DA:1184:G:OP1	49:D3:30:ARG:HD2	2.16	0.45
57:AW:3004:NEG:N3	25:BA:1964:C:OP1	2.50	0.45
14:CN:24:CYS:HB3	14:CN:29:ARG:H	1.81	0.45
2:CB:98:LEU:H	2:CB:98:LEU:HD23	1.81	0.45
9:AI:99:LEU:HB3	9:AI:101:PHE:CD1	2.52	0.45
23:CY:18:G:C2	23:CY:55:PSU:O4	2.70	0.45
1:AA:692:U:H1'	1:AA:695:A:N7	2.32	0.45
25:DA:2283:C:H2'	25:DA:2284:C:O4'	2.16	0.45
1:AA:545:C:O2'	1:AA:549:C:OP1	2.21	0.45
31:DH:7:LEU:HA	31:DH:8:PRO:HD3	1.75	0.45
25:DA:554:U:O2'	25:DA:555:U:H5'	2.15	0.45
45:DZ:152:ALA:HB3	45:DZ:169:GLU:HB3	1.97	0.45
39:BT:15:VAL:HG13	39:BT:79:HIS:CE1	2.51	0.45
25:BA:2755:C:OP1	55:B9:35:ARG:NH1	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:DB:94:C:H2'	26:DB:95:C:C6	2.52	0.45
10:CJ:25:GLU:O	10:CJ:29:ARG:HG2	2.15	0.45
5:CE:93:PRO:HG2	8:CH:105:ARG:NE	2.31	0.45
35:BP:138:LEU:HD23	35:BP:145:PRO:HG3	1.97	0.45
25:BA:1938:A:H2'	25:BA:1939:U:O4'	2.17	0.45
30:BG:69:ALA:HB3	30:BG:91:ARG:HH21	1.82	0.45
36:BQ:11:LYS:HE2	36:BQ:88:GLY:O	2.16	0.45
25:BA:1679:A:OP2	61:BA:4905:HOH:O	2.21	0.45
29:BF:18:ARG:NH2	29:BF:127:GLU:OE1	2.50	0.45
1:AA:826:C:H4'	8:AH:12:ARG:HG2	1.97	0.45
4:AD:112:VAL:HG23	4:AD:116:GLN:OE1	2.16	0.45
25:BA:1725:G:N3	25:BA:1725:G:H5''	2.31	0.45
25:DA:2750:A:H8	25:DA:2750:A:OP1	2.00	0.45
1:CA:65:U:H6	1:CA:65:U:H5'	1.81	0.45
9:CI:89:ASN:HD22	9:CI:91:ASP:H	1.64	0.45
25:DA:1024:G:OP1	25:DA:1026:U:H5'	2.16	0.45
1:AA:179:A:H2'	1:AA:180:U:C6	2.51	0.45
1:AA:666:G:H5'	1:AA:726:C:H1'	1.98	0.45
49:B3:43:ILE:O	49:B3:47:VAL:HG23	2.16	0.45
44:BY:92:ASN:HB3	44:BY:94:LYS:N	2.23	0.45
25:BA:1537:G:O2'	27:BD:101:GLU:HB2	2.16	0.45
1:AA:189(C):C:H2'	1:AA:189(D):C:O4'	2.17	0.45
1:AA:522:C:H41	12:AL:53:ARG:NH2	2.06	0.45
1:CA:1277:C:HO2'	1:CA:1279:A:H1'	1.81	0.45
1:AA:1063:C:OP2	1:AA:1064:G:O2'	2.24	0.45
28:DE:33:VAL:HG21	28:DE:36:ARG:HE	1.82	0.45
25:BA:1186:U:H4'	25:BA:1188:A:O4'	2.17	0.45
3:AC:79:ARG:O	3:AC:82:GLU:HB2	2.17	0.45
11:CK:101:SER:OG	11:CK:103:LEU:HD23	2.17	0.45
1:CA:149:A:H2'	1:CA:150:C:C6	2.52	0.45
26:DB:91:C:OP2	36:DQ:16:ARG:NH1	2.49	0.45
1:CA:19:C:H5''	5:CE:86:ALA:HB3	1.97	0.45
34:DO:98:VAL:HG13	34:DO:117:LEU:HB3	1.99	0.45
18:AR:59:SER:OG	18:AR:62:GLU:HG2	2.17	0.45
25:DA:679:C:H2'	25:DA:680:G:C8	2.51	0.45
45:DZ:171:ILE:HG13	45:DZ:171:ILE:H	1.68	0.45
12:CL:88:GLY:O	12:CL:99:HIS:HD2	1.98	0.45
33:BN:15:LEU:HB2	33:BN:135:PRO:HB2	1.97	0.45
25:DA:1509(B):A:H2'	25:DA:1510:G:C8	2.52	0.45
9:CI:37:PHE:HD1	9:CI:40:LEU:HD12	1.81	0.45
32:BI:66:GLU:HA	32:BI:69:LYS:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:DP:97:PRO:HD3	35:DP:126:VAL:O	2.16	0.45
15:AO:3:ILE:HG12	15:AO:3:ILE:O	2.16	0.45
25:DA:2238:G:H2'	25:DA:2238:G:N3	2.32	0.45
7:AG:144:MET:HB3	7:AG:144:MET:HE2	1.89	0.45
25:BA:2418:U:H2'	25:BA:2418:U:OP2	2.17	0.45
2:CB:114:ARG:O	2:CB:118:LEU:HG	2.16	0.45
1:CA:1400:C:H4'	22:CV:18:G:C5	2.52	0.45
25:BA:1419:A:H2'	25:BA:1420:G:O4'	2.16	0.45
25:BA:2028:C:O2'	25:BA:2833:A:N3	2.48	0.45
2:CB:93:VAL:HG21	2:CB:97:TRP:HE1	1.80	0.45
25:BA:2174:G:H2'	25:BA:2175:G:O4'	2.17	0.45
25:BA:1218:G:H2'	25:BA:1218:G:OP2	2.17	0.45
25:DA:1022:G:N7	33:DN:66:LYS:HE2	2.32	0.45
1:CA:1149:C:OP1	9:CI:14:VAL:HG11	2.17	0.45
35:BP:63:PRO:HD3	54:B8:27:THR:HG22	1.99	0.45
27:BD:132:PRO:HG2	27:BD:135:PHE:HD2	1.79	0.45
23:CY:55:PSU:N3	23:CY:58:A:C8	2.85	0.45
1:AA:860:A:H2'	1:AA:861:G:O4'	2.17	0.45
25:BA:815:G:O2'	25:BA:1425:A:N1	2.41	0.45
23:AY:76:A:H4'	47:B1:30:VAL:HG21	1.98	0.45
34:BO:8:LEU:HB2	34:BO:19:ILE:HG13	1.99	0.45
40:DU:81:HIS:O	40:DU:84:LYS:HB3	2.16	0.45
1:AA:1309:G:OP2	13:AM:99:ARG:NH2	2.50	0.45
13:CM:50:GLU:HA	13:CM:53:VAL:HB	1.99	0.45
3:CC:47:LEU:HD12	3:CC:68:VAL:HG11	1.99	0.45
28:BE:121:ASN:ND2	61:BE:409:HOH:O	2.50	0.45
25:DA:2723:C:OP2	28:DE:109:LYS:NZ	2.47	0.45
25:BA:2588:G:H1'	61:BA:5252:HOH:O	2.17	0.45
19:CS:68:GLY:H	50:D4:58:ARG:HH11	1.64	0.45
27:DD:73:VAL:HG13	27:DD:120:GLY:HA3	1.99	0.45
25:DA:1614:A:C2	42:DW:93:ALA:HB2	2.52	0.45
42:BW:19:LEU:HB3	51:B5:25:LEU:HD11	1.99	0.45
6:CF:82:ARG:HA	6:CF:82:ARG:HD2	1.74	0.45
25:DA:2296:U:OP2	38:DS:9:ARG:NH2	2.40	0.45
38:DS:28:VAL:HG11	38:DS:98:VAL:HG13	1.98	0.45
1:AA:881:G:H2'	1:AA:882:C:O4'	2.16	0.45
2:CB:50:GLU:HB3	2:CB:200:ILE:O	2.17	0.45
27:DD:13:ARG:HA	27:DD:13:ARG:HD2	1.83	0.45
2:AB:146:GLN:O	2:AB:150:SER:HB3	2.17	0.45
25:DA:1854:A:H2'	25:DA:1855:G:O4'	2.17	0.45
10:AJ:19:SER:OG	10:AJ:91:PRO:HD2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:613:A:H2'	25:BA:614:C:O4'	2.17	0.45
25:BA:2651:A:H2'	25:BA:2652:G:O4'	2.16	0.45
7:CG:26:PHE:O	7:CG:30:ILE:HG13	2.17	0.45
1:CA:1255:G:H3'	3:CC:26:LYS:HZ3	1.82	0.45
25:BA:2081:A:O2'	29:BF:69:HIS:HD2	1.99	0.45
3:AC:12:LEU:HD11	14:AN:51:GLY:HA2	1.99	0.45
1:AA:449:C:O2	16:AP:42:ARG:HD2	2.17	0.45
25:BA:895:G:N3	25:BA:978:A:H1'	2.32	0.45
1:CA:539:A:H2'	1:CA:540:G:C8	2.51	0.45
27:BD:68:LYS:HD3	27:BD:70:TRP:CH2	2.52	0.45
32:BI:130:TYR:N	32:BI:138:ILE:O	2.43	0.45
50:B4:46:GLN:HA	50:B4:48:ARG:HH21	1.82	0.45
25:DA:251:A:C4	25:DA:252:G:H1'	2.51	0.45
47:B1:3:LYS:HB2	47:B1:61:ARG:HH12	1.81	0.45
25:BA:2902:G:H4'	25:BA:2903:G:O5'	2.17	0.45
25:BA:323:A:H5''	44:BY:86:ARG:HH21	1.82	0.45
1:CA:362:G:N2	1:CA:365:U:OP2	2.49	0.45
25:DA:861:A:C2	25:DA:917:A:C4	3.05	0.45
25:BA:2198:A:H2'	25:BA:2199:C:C6	2.52	0.45
25:BA:2013:U:H2'	25:BA:2014:G:H5''	1.98	0.45
1:CA:1259:C:C4	1:CA:1260:C:H1'	2.52	0.45
25:BA:463:C:H2'	25:BA:464:G:H8	1.81	0.45
25:BA:1456:G:H2'	25:BA:1457:C:C6	2.51	0.45
25:DA:222:A:H3'	25:DA:421:U:H5'	1.99	0.45
7:AG:149:ARG:HD2	11:AK:59:TYR:CZ	2.52	0.45
47:B1:34:THR:HG21	47:B1:37:ILE:HG13	1.99	0.45
41:DV:21:ARG:HG2	41:DV:91:TYR:CD2	2.52	0.45
25:DA:2390:U:P	54:D8:35:GLN:HE22	2.40	0.45
31:BH:83:TYR:CE2	31:BH:138:LYS:HB2	2.52	0.45
25:BA:768:C:H2'	25:BA:769:A:C8	2.52	0.45
1:CA:688:G:H5'	11:CK:46:GLY:C	2.37	0.45
4:CD:196:LEU:C	4:CD:198:VAL:H	2.20	0.45
25:DA:1379:A:H4'	25:DA:1380:G:OP2	2.16	0.45
23:CW:25:C:O2'	23:CW:26:A:H5'	2.16	0.45
16:AP:3:LYS:O	16:AP:21:VAL:HA	2.17	0.45
25:BA:1221:G:N2	25:BA:1223:C:OP1	2.50	0.45
1:AA:1131:G:P	9:AI:20:ARG:HH22	2.40	0.45
25:DA:866:A:N6	25:DA:914:C:C4	2.85	0.45
15:AO:56:LEU:O	15:AO:60:VAL:HG23	2.17	0.45
50:B4:56:VAL:O	50:B4:57:GLU:O	2.34	0.45
23:CY:25:C:O2'	23:CY:26:A:O4'	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:588:U:H6	25:DA:588:U:O5'	2.00	0.45
25:DA:2274:A:C5	25:DA:2276:G:C8	3.05	0.45
8:AH:51:VAL:HG11	8:AH:60:ARG:NH1	2.32	0.45
13:CM:78:ILE:HA	13:CM:81:LEU:HD12	1.99	0.45
25:DA:1364:G:P	47:D1:3:LYS:HG3	2.57	0.45
1:CA:309:G:H1'	1:CA:608:A:C2	2.52	0.45
49:D3:46:ASN:O	49:D3:50:VAL:HG22	2.17	0.45
25:DA:1181:C:H2'	25:DA:1182:A:H8	1.82	0.45
25:DA:2741:A:N6	25:DA:2763:G:O2'	2.47	0.45
25:BA:1177:G:N2	33:BN:73:THR:HG23	2.32	0.45
4:AD:163:GLU:O	4:AD:166:LYS:HG2	2.16	0.45
25:DA:977:G:N3	25:DA:1001:A:H2	2.15	0.45
25:BA:2860:A:OP2	25:BA:2876:U:H5	2.00	0.45
25:DA:2653:U:H5''	25:DA:2654:A:OP2	2.17	0.45
25:BA:573:G:H2'	25:BA:574:G:O4'	2.17	0.45
25:BA:85:C:H4'	25:BA:102:U:H1'	1.99	0.45
1:CA:850:U:H2'	1:CA:851:G:H5''	1.99	0.45
1:AA:340:U:H2'	1:AA:341:C:C6	2.52	0.45
6:CF:23:LYS:HG2	6:CF:61:LEU:HD21	1.99	0.45
25:DA:1039:G:C6	25:DA:1040:C:C4	3.05	0.45
2:CB:87:ARG:NH1	2:CB:219:VAL:HG12	2.32	0.45
40:DU:76:TYR:CZ	40:DU:80:ILE:HG13	2.52	0.45
1:CA:1179:A:H2'	1:CA:1180:A:O4'	2.17	0.45
2:CB:7:VAL:HB	2:CB:8:LYS:H	1.62	0.45
23:AW:75:C:H2'	23:AW:76:A:C4	2.52	0.45
30:DG:45:GLU:H	30:DG:45:GLU:HG2	1.39	0.45
39:BT:16:ARG:HH21	39:BT:19:LEU:HD11	1.81	0.45
44:DY:6:HIS:HE1	44:DY:72:VAL:O	2.00	0.45
25:DA:27:G:N2	25:DA:512:G:H1'	2.32	0.45
1:CA:192:U:H2'	1:CA:193:C:C6	2.52	0.45
25:DA:127:A:H5''	25:DA:128:C:C6	2.52	0.45
25:DA:2370:G:H2'	25:DA:2371:G:C8	2.51	0.45
4:AD:166:LYS:HB2	4:AD:168:ARG:NH2	2.32	0.45
32:DI:114:LEU:HD11	32:DI:128:LEU:HD13	1.98	0.45
8:CH:31:PHE:O	8:CH:35:ILE:HG13	2.17	0.45
25:BA:2661:U:H2'	25:BA:2662:U:C6	2.51	0.45
3:AC:173:VAL:O	3:AC:175:LEU:HD12	2.16	0.45
24:CX:49:G:C2	24:CX:66:C:C2	3.05	0.45
45:BZ:19:ARG:NH1	45:BZ:84:GLU:O	2.49	0.45
1:CA:299:G:H2'	1:CA:300:A:C8	2.52	0.45
34:BO:16:ALA:HB2	34:BO:52:VAL:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:586:C:O3'	8:CH:89:PRO:HB3	2.17	0.45
8:AH:11:THR:HG23	8:AH:14:ARG:NH1	2.32	0.45
25:DA:636:G:OP1	35:DP:132:LYS:HE2	2.17	0.45
7:CG:15:ASP:OD2	7:CG:44:TYR:OH	2.27	0.45
25:DA:1782:C:H1'	25:DA:2609:U:H5''	1.99	0.45
1:CA:742:G:P	15:CO:35:ARG:HH22	2.40	0.44
29:DF:192:LEU:HD13	29:DF:194:MET:HE2	1.98	0.44
25:DA:2475:C:H42	25:DA:2529:G:H22	1.65	0.44
1:CA:390:C:H2'	1:CA:391:G:C8	2.53	0.44
28:BE:170:LEU:HB3	28:BE:184:VAL:HG22	1.97	0.44
31:DH:44:VAL:O	31:DH:50:VAL:HA	2.17	0.44
25:DA:1038:C:N4	25:DA:1117:G:H1	2.14	0.44
28:DE:24:THR:HG22	28:DE:186:GLY:O	2.17	0.44
45:BZ:150:LEU:HB3	45:BZ:171:ILE:HD11	1.99	0.44
25:DA:30:G:C6	25:DA:31:C:C4	3.06	0.44
25:BA:254:A:H1'	25:BA:255:G:O4'	2.18	0.44
25:DA:936:C:H2'	25:DA:937:U:C6	2.52	0.44
25:DA:1378:A:OP1	53:D7:10:ARG:NH2	2.50	0.44
33:BN:15:LEU:HD12	33:BN:137:LYS:HG2	1.99	0.44
50:D4:56:VAL:HG13	50:D4:57:GLU:H	1.81	0.44
25:BA:1534:G:H2'	25:BA:1535:U:O4'	2.18	0.44
1:AA:1376:U:H2'	1:AA:1377:A:C8	2.53	0.44
24:CX:15:G:H2'	24:CX:59:A:N1	2.32	0.44
30:DG:70:VAL:HA	30:DG:90:LEU:HD23	1.98	0.44
25:DA:664:C:H2'	25:DA:665:C:C6	2.52	0.44
25:BA:1674:G:H2'	25:BA:1675:U:C6	2.52	0.44
36:DQ:36:ALA:HB2	36:DQ:103:MET:SD	2.57	0.44
25:DA:2850:A:C2	25:DA:2851:A:C4	3.05	0.44
4:AD:100:ARG:HB3	4:AD:102:ASP:OD1	2.17	0.44
43:DX:92:LEU:C	43:DX:94:GLY:H	2.21	0.44
20:CT:91:LEU:HD23	20:CT:91:LEU:HA	1.82	0.44
1:AA:1437:C:H2'	1:AA:1438:G:C8	2.52	0.44
24:CX:19:G:H4'	24:CX:20:U:OP2	2.17	0.44
25:DA:2427:C:H5''	25:DA:2428:G:OP1	2.17	0.44
25:DA:392:C:H5''	25:DA:409:C:H5''	2.00	0.44
23:AW:24:G:C6	23:AW:25:C:N3	2.85	0.44
1:CA:1505:G:H4'	22:CV:13:A:H2	1.82	0.44
25:DA:820:A:H1'	25:DA:943:U:H1'	1.99	0.44
1:CA:1256:A:N1	1:CA:1278:U:H1'	2.31	0.44
1:AA:839:U:O2'	1:AA:840:C:OP1	2.35	0.44
25:DA:2324:C:H5''	25:DA:2325:G:H5'	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:1419:A:C8	25:DA:1421:G:C6	3.06	0.44
45:BZ:109:ALA:HB3	45:BZ:145:GLU:OE2	2.17	0.44
3:CC:19:GLU:HB3	3:CC:40:ARG:HH22	1.82	0.44
1:AA:674:G:H2'	1:AA:675:A:C8	2.52	0.44
10:CJ:47:PHE:HB2	10:CJ:63:PHE:HB2	1.99	0.44
27:BD:145:VAL:HB	27:BD:155:LEU:HB2	1.99	0.44
28:BE:31:CYS:HA	28:BE:32:PRO:HD2	1.89	0.44
25:DA:919:G:C6	25:DA:920:G:C5	3.05	0.44
26:DB:2:C:H2'	26:DB:3:C:H6	1.82	0.44
30:BG:11:TYR:HA	30:BG:15:VAL:HB	1.99	0.44
31:DH:23:ARG:NH1	31:DH:34:GLU:OE2	2.50	0.44
25:BA:2707:C:H2'	25:BA:2708:U:H6	1.82	0.44
26:BB:14:U:O3'	26:BB:108:U:O2'	2.35	0.44
6:CF:46:ARG:NH1	6:CF:46:ARG:HB2	2.31	0.44
25:BA:2555:G:H2'	25:BA:2556:G:O4'	2.17	0.44
1:CA:598:U:H4'	8:CH:94:TYR:CG	2.53	0.44
37:DR:44:LEU:HD22	37:DR:48:VAL:HG23	1.98	0.44
33:BN:4:TYR:HB2	40:BU:101:ARG:NH1	2.31	0.44
25:BA:491:G:OP1	53:B7:12:ARG:NH2	2.50	0.44
6:CF:82:ARG:HB2	6:CF:85:VAL:HG23	1.98	0.44
1:AA:645:C:H2'	1:AA:646:U:C6	2.52	0.44
1:AA:600:C:H4'	8:AH:128:GLY:O	2.17	0.44
27:BD:232:PRO:HB3	27:BD:244:ARG:CZ	2.48	0.44
32:BI:47:LEU:O	32:BI:51:ILE:HG13	2.17	0.44
25:BA:1384:G:N7	43:BX:62:LYS:NZ	2.57	0.44
25:DA:711:G:H1	25:DA:720:C:H42	1.65	0.44
25:DA:620:G:H8	25:DA:622:G:O6	2.00	0.44
1:CA:567:G:O6	12:CL:5:PRO:HD3	2.17	0.44
25:DA:1651:G:C6	25:DA:1652:A:C5	3.05	0.44
35:DP:86:LYS:HB3	35:DP:118:GLY:HA3	1.97	0.44
30:BG:14:GLU:O	30:BG:17:PRO:HD2	2.18	0.44
30:BG:38:VAL:HG22	30:BG:93:THR:HG23	1.99	0.44
1:AA:903:G:OP1	61:AA:4042:HOH:O	2.21	0.44
25:BA:1952:G:O2'	25:BA:1990:G:O6	2.25	0.44
23:AY:18:G:H1	23:AY:55:PSU:H1'	1.82	0.44
46:D0:12:ASN:HA	46:D0:14:ARG:HH21	1.81	0.44
25:DA:898:C:C5	25:DA:899:A:C5	3.05	0.44
1:AA:1392:G:N2	1:AA:1502:A:C8	2.85	0.44
23:CY:50:U:O2	23:CY:64:A:N1	2.50	0.44
25:DA:2149:G:H5''	25:DA:2150:U:OP2	2.17	0.44
25:DA:942:G:H4'	25:DA:1190:G:H5'	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:BV:97:LYS:HA	41:BV:97:LYS:HD2	1.81	0.44
52:B6:9:LEU:HD13	52:B6:51:GLU:HG3	2.00	0.44
55:D9:7:VAL:HG12	55:D9:34:GLN:HB3	1.98	0.44
27:DD:67:PHE:CE1	27:DD:106:ILE:HD12	2.47	0.44
50:D4:46:GLN:HA	50:D4:48:ARG:NH1	2.33	0.44
25:DA:795:C:H2'	25:DA:796:C:C6	2.52	0.44
25:DA:639:U:H2'	25:DA:640:C:H6	1.82	0.44
25:BA:2130:C:H2'	25:BA:2131:U:H6	1.80	0.44
1:AA:626:U:C2	1:AA:627:G:C8	3.05	0.44
19:AS:12:ASP:OD1	19:AS:35:SER:HB3	2.17	0.44
31:DH:3:ARG:HH12	31:DH:5:GLY:HA3	1.82	0.44
25:BA:1447:G:H2'	25:BA:1448:C:O4'	2.18	0.44
30:BG:122:PRO:HD3	30:BG:181:ARG:HG2	1.99	0.44
25:BA:197:C:H2'	25:BA:198:C:C6	2.53	0.44
25:DA:668:G:H5'	25:DA:669:G:OP2	2.17	0.44
1:AA:219:C:H2'	1:AA:220:G:O4'	2.17	0.44
4:AD:50:ARG:HA	4:AD:51:PRO:HD3	1.76	0.44
11:AK:120:ARG:HA	11:AK:121:PRO:HD3	1.83	0.44
44:DY:14:LEU:HB2	44:DY:75:ILE:HD11	1.99	0.44
27:DD:4:LYS:HB3	27:DD:18:VAL:HG23	2.00	0.44
38:DS:110:LEU:HD12	38:DS:110:LEU:HA	1.82	0.44
32:BI:62:LYS:HE3	32:BI:62:LYS:HB2	1.78	0.44
14:CN:22:THR:HB	14:CN:33:VAL:HG11	1.99	0.44
1:AA:1075:C:C2'	1:AA:1076:C:H5'	2.48	0.44
23:CY:57:G:H2'	23:CY:57:G:N3	2.32	0.44
1:AA:1002:G:C6	1:AA:1003:G:C2	3.05	0.44
1:AA:1004:A:N1	1:AA:1037:C:N4	2.65	0.44
25:DA:879:G:C6	25:DA:899:A:H1'	2.53	0.44
35:BP:99:LEU:HD22	35:BP:102:ARG:NH2	2.32	0.44
25:DA:996:A:C2	25:DA:997:G:C8	3.05	0.44
25:DA:2363:C:O2	46:D0:39:ARG:NH2	2.42	0.44
1:AA:1008:C:C2	1:AA:1021:G:C6	3.06	0.44
9:CI:9:ARG:O	9:CI:104:ARG:HG3	2.17	0.44
1:AA:1236:A:H4'	1:AA:1304:G:H4'	1.99	0.44
35:BP:50:ARG:HH21	54:B8:7:HIS:HD2	1.63	0.44
25:BA:2331:G:H3'	25:BA:2331:G:OP1	2.17	0.44
1:AA:1298:C:OP2	7:AG:114:ARG:NH2	2.49	0.44
25:BA:956:A:N1	25:BA:2289:G:H1'	2.32	0.44
42:DW:82:LEU:HD22	42:DW:84:ARG:HH22	1.83	0.44
9:CI:17:VAL:HG11	9:CI:81:ILE:HA	1.99	0.44
1:CA:570:G:H1'	1:CA:820:U:C4	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:1476:C:H2'	25:BA:1477:U:H6	1.81	0.44
25:BA:344:A:H4'	25:BA:346:A:C8	2.52	0.44
14:AN:21:TYR:HE2	14:AN:23:ARG:NE	2.15	0.44
31:DH:2:SER:O	31:DH:3:ARG:HG2	2.17	0.44
45:DZ:159:PRO:HA	45:DZ:160:GLY:HA2	1.67	0.44
13:CM:19:LEU:HB3	13:CM:25:ILE:HG21	1.99	0.44
4:AD:152:SER:O	4:AD:155:LEU:HB2	2.17	0.44
25:BA:767:C:H2'	25:BA:768:C:H6	1.83	0.44
25:DA:141:A:C8	25:DA:1408:C:O2'	2.69	0.44
1:CA:991:U:HO2'	1:CA:992:U:C5'	2.30	0.44
26:BB:42:C:OP1	30:BG:67:LYS:NZ	2.48	0.44
51:D5:35:GLU:HG3	51:D5:51:TYR:CG	2.53	0.44
17:CQ:3:LYS:HB3	17:CQ:61:GLU:HB3	1.99	0.44
23:AW:22:G:HO2'	23:AW:23:A:P	2.41	0.44
1:CA:265:G:H5'	17:CQ:64:PRO:O	2.17	0.44
25:DA:1817:G:OP1	27:DD:88:ARG:NH2	2.43	0.44
31:DH:59:ARG:O	31:DH:63:SER:OG	2.35	0.44
6:AF:8:ILE:HD12	6:AF:26:ILE:HD13	1.99	0.44
54:D8:26:LYS:HZ2	54:D8:26:LYS:HB3	1.82	0.44
1:AA:1258:G:H2'	1:AA:1259:C:C6	2.52	0.44
4:CD:100:ARG:HB3	4:CD:102:ASP:OD1	2.18	0.44
25:DA:686:G:N2	25:DA:788:A:H61	2.16	0.44
6:CF:13:ASN:ND2	6:CF:55:ASP:OD2	2.51	0.44
25:BA:624:C:OP1	29:BF:108:LYS:HE3	2.18	0.44
57:AA:3216:NEG:H91	23:AW:34:G:H5'	1.99	0.44
23:CY:24:G:C6	23:CY:25:C:N4	2.85	0.44
25:DA:955:C:N4	25:DA:956:G:C6	2.86	0.44
25:DA:1169:G:H1	25:DA:1180:C:N4	2.13	0.44
45:DZ:45:ASP:CG	45:DZ:49:ARG:HH11	2.21	0.44
1:AA:138:G:H1	1:AA:225:C:N4	2.14	0.44
28:DE:170:LEU:HA	28:DE:170:LEU:HD12	1.81	0.44
30:DG:11:TYR:CZ	30:DG:16:ARG:HG2	2.53	0.44
6:CF:2:ARG:NE	6:CF:69:GLU:HG2	2.32	0.44
25:DA:30:G:C5	25:DA:31:C:C4	3.05	0.44
2:AB:71:VAL:HA	2:AB:93:VAL:HG23	2.00	0.44
14:CN:3:ARG:O	14:CN:7:ILE:HG23	2.17	0.44
8:CH:29:SER:HB3	8:CH:32:LYS:HG3	1.99	0.44
1:AA:192:U:H2'	1:AA:193:C:H6	1.83	0.44
1:AA:836:G:OP1	18:AR:61:LYS:NZ	2.40	0.44
53:D7:11:LYS:HE3	53:D7:15:THR:OG1	2.18	0.44
25:DA:2745:C:H2'	25:DA:2746:U:O4'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:47:LEU:HD12	3:AC:68:VAL:HG11	2.00	0.44
1:AA:1047:G:H5''	14:AN:4:LYS:HD2	1.99	0.44
10:CJ:54:PHE:O	10:CJ:56:HIS:N	2.46	0.44
9:CI:117:HIS:HB2	9:CI:121:ARG:HG3	2.00	0.44
27:BD:5:LYS:HE3	27:BD:5:LYS:HB3	1.63	0.44
41:BV:65:GLY:HA3	41:BV:91:TYR:CZ	2.53	0.44
6:AF:36:ARG:NH1	6:AF:66:GLU:OE1	2.51	0.44
7:AG:22:LEU:HG	7:AG:62:PHE:HE2	1.82	0.44
1:AA:1272:G:H2'	1:AA:1273:G:O4'	2.18	0.44
25:BA:831:A:C8	25:BA:839:G:C5	3.06	0.44
1:CA:1042:G:H2'	1:CA:1043:C:O4'	2.18	0.44
25:DA:1022:G:OP2	33:DN:65:LYS:NZ	2.45	0.44
25:DA:307:G:O2'	25:DA:309:G:N7	2.40	0.44
1:AA:353:A:C8	1:AA:353:A:H5'	2.44	0.44
36:BQ:18:LYS:HB2	36:BQ:18:LYS:HE3	1.71	0.44
10:CJ:52:GLY:O	14:CN:41:ARG:NH2	2.38	0.44
2:CB:15:VAL:CG1	2:CB:209:ARG:HB3	2.46	0.44
1:CA:1152:A:O2'	1:CA:1153:C:H5'	2.17	0.44
57:CA:3177:NEG:H32	25:DA:16:G:N7	2.33	0.44
1:CA:1014:A:N3	1:CA:1219:U:H1'	2.33	0.44
25:DA:2682:U:O2'	39:DT:58:ASN:ND2	2.50	0.44
36:DQ:31:ASP:HA	36:DQ:134:ARG:HH11	1.81	0.44
1:AA:446:G:N2	1:AA:489:C:N3	2.66	0.44
1:CA:375:U:O3'	16:CP:6:LEU:HB2	2.18	0.44
25:DA:2699:C:H2'	25:DA:2700:C:O4'	2.18	0.44
25:DA:2526:G:H5'	25:DA:2742:C:O2'	2.18	0.44
18:CR:58:LEU:HD23	18:CR:66:LEU:HD22	1.99	0.44
32:BI:4:ILE:HG21	32:BI:47:LEU:HG	2.00	0.44
1:CA:76:C:H42	1:CA:93:G:H1	1.66	0.44
32:DI:116:LEU:HD21	32:DI:120:ILE:HG13	2.00	0.44
25:BA:275:C:H2'	25:BA:276:C:C6	2.53	0.44
25:BA:1820:A:H2'	25:BA:1821:C:O4'	2.17	0.44
25:BA:412:C:O2	35:BP:71:VAL:HG21	2.17	0.44
25:DA:2468:G:C2	25:DA:2481:G:N3	2.86	0.44
31:BH:126:PRO:HB2	31:BH:127:GLU:H	1.64	0.44
1:CA:1468:A:H2'	1:CA:1469:G:O4'	2.18	0.44
24:AX:19:G:H4'	24:AX:20:U:OP2	2.18	0.44
25:DA:2769:C:H2'	25:DA:2770:G:O4'	2.18	0.44
45:BZ:146:ILE:HA	45:BZ:147:GLY:HA2	1.79	0.44
25:BA:771:U:H2'	25:BA:772:G:O4'	2.18	0.44
4:AD:162:LEU:HD23	4:AD:162:LEU:HA	1.74	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:DP:6:LEU:HA	35:DP:6:LEU:HD23	1.79	0.44
3:CC:17:ASP:N	3:CC:17:ASP:OD1	2.50	0.44
25:DA:2516:G:C6	25:DA:2517:C:C4	3.06	0.44
25:DA:2467:C:H4'	36:DQ:123:HIS:CG	2.53	0.44
23:AY:59:U:H3'	23:AY:60:U:H6	1.82	0.44
1:AA:998:G:N2	1:AA:1043:C:N3	2.55	0.44
25:BA:2136:A:C2	25:BA:2190:G:H1'	2.53	0.44
25:BA:2170:G:O2'	25:BA:2171:G:OP2	2.30	0.44
1:AA:664:G:P	18:AR:64:ARG:HH21	2.40	0.44
1:CA:527:G:O6	12:CL:49:ASN:ND2	2.51	0.44
25:BA:217:A:H8	25:BA:218:A:H5'	1.82	0.44
29:DF:20:LEU:HD12	29:DF:125:LEU:HD13	2.00	0.44
25:DA:2801(A):A:H1'	25:DA:2895:U:H1'	2.00	0.44
1:CA:1051:C:H2'	1:CA:1052:U:C6	2.53	0.44
25:DA:280:C:C2	25:DA:362:U:O4	2.71	0.44
26:DB:6:C:H2'	26:DB:7:G:O4'	2.18	0.44
9:CI:16:ARG:HB2	9:CI:64:THR:HB	2.00	0.44
54:D8:63:PRO:HG2	54:D8:64:TYR:CD2	2.53	0.44
3:AC:82:GLU:HG2	3:AC:85:ARG:NH2	2.30	0.44
1:CA:1009:G:H22	1:CA:1021:G:H1'	1.81	0.44
1:CA:921:U:O2	5:CE:19:MET:HB2	2.17	0.44
50:D4:15:ILE:O	50:D4:33:VAL:N	2.50	0.44
36:DQ:24:GLY:HA2	36:DQ:67:ARG:HH22	1.81	0.44
26:DB:39:A:O2'	26:DB:46:A:N1	2.46	0.44
25:DA:118:A:H1'	25:DA:178:G:O4'	2.18	0.44
25:BA:2403:G:O6	25:BA:2437:A:H8	2.00	0.44
1:AA:509:A:H5''	4:AD:55:ALA:HB2	2.00	0.44
24:AX:59:A:C2'	24:AX:60:U:H5'	2.47	0.44
25:BA:1822:A:H8	25:BA:1822:A:OP2	2.01	0.44
41:BV:1:MET:HB2	41:BV:43:GLU:OE2	2.18	0.44
1:CA:1249:C:H4'	9:CI:36:TYR:OH	2.18	0.44
19:AS:41:VAL:O	19:AS:43:GLU:N	2.50	0.44
25:BA:2023:A:H2'	25:BA:2024:G:C8	2.52	0.44
25:DA:1709:U:H2'	25:DA:1710:C:C6	2.52	0.44
25:DA:2659:G:OP1	31:DH:158:HIS:NE2	2.45	0.44
34:DO:68:GLU:HB3	34:DO:78:ARG:HB2	2.00	0.44
25:DA:1540:U:H2'	25:DA:1541:G:O4'	2.17	0.44
26:BB:106:G:H5'	45:BZ:31:ARG:HG2	1.99	0.44
1:CA:7:G:H21	5:CE:121:LYS:HG2	1.83	0.44
25:DA:1825:A:OP1	27:DD:249:PRO:HD3	2.17	0.44
25:DA:1645:G:H5''	25:DA:1646:C:O4'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:1302:G:O2'	29:BF:75:HIS:HE1	2.01	0.44
25:BA:1688:A:H2'	25:BA:1689:G:O4'	2.18	0.44
32:BI:38:LEU:HD12	32:BI:38:LEU:H	1.82	0.44
25:DA:2230:G:C6	25:DA:2231:C:C4	3.06	0.44
25:DA:760:G:H2'	25:DA:761:A:O4'	2.18	0.44
6:CF:36:ARG:NH2	6:CF:66:GLU:OE2	2.51	0.44
25:DA:297:C:H2'	25:DA:298:G:O4'	2.17	0.44
43:DX:12:VAL:HG22	43:DX:29:TRP:CE2	2.53	0.44
25:DA:2162:G:H4'	25:DA:2172:U:C2'	2.42	0.44
25:BA:2203:G:O2'	25:BA:2204:G:OP1	2.34	0.44
25:BA:2165:C:C2	25:BA:2171:G:C2	3.05	0.44
1:AA:976:G:N2	1:AA:1363:C:OP2	2.25	0.44
25:DA:848:G:C4	25:DA:933:A:H8	2.36	0.44
25:DA:817:C:H2'	25:DA:818:G:O4'	2.18	0.44
25:BA:692:C:H2'	25:BA:693:G:O4'	2.18	0.44
26:DB:32:C:H2'	26:DB:33:G:O4'	2.18	0.44
25:DA:2387:U:H1'	46:D0:41:ARG:HE	1.82	0.44
26:BB:89:G:H2'	26:BB:90:A:C8	2.52	0.44
25:DA:1596:A:H2'	25:DA:1597:A:O4'	2.17	0.44
27:BD:145:VAL:HG12	27:BD:146:GLU:O	2.18	0.44
27:BD:70:TRP:HB3	27:BD:190:TYR:CE1	2.53	0.44
28:BE:144:ARG:HB3	28:BE:145:LYS:H	1.52	0.44
25:BA:515:G:N7	42:BW:49:LYS:NZ	2.65	0.44
25:BA:181:C:O2'	25:BA:849:A:N3	2.38	0.44
25:DA:660:G:H5'	29:DF:99:TYR:CE2	2.52	0.44
25:BA:863:C:H2'	25:BA:864:C:H6	1.83	0.44
39:BT:118:ARG:HD2	39:BT:118:ARG:HA	1.49	0.44
5:CE:76:ILE:O	5:CE:93:PRO:HB3	2.17	0.44
25:DA:1510:G:H2'	25:DA:1511:C:O4'	2.18	0.44
4:AD:168:ARG:H	4:AD:168:ARG:CD	2.31	0.44
25:BA:2642:G:H2'	25:BA:2643:G:C8	2.53	0.44
6:AF:36:ARG:CB	6:AF:36:ARG:HH11	2.31	0.44
1:CA:255:G:H1'	17:CQ:16:GLN:NE2	2.32	0.44
38:BS:46:VAL:HG12	38:BS:48:LEU:HD12	1.99	0.44
25:DA:992:C:OP1	40:DU:47:TYR:OH	2.24	0.44
48:B2:11:GLU:O	48:B2:15:LYS:HG3	2.18	0.44
25:BA:486:A:H2'	25:BA:487:C:O4'	2.18	0.44
1:AA:591:U:H2'	1:AA:592:G:C8	2.52	0.44
1:CA:6:G:H4'	1:CA:298:A:H4'	1.99	0.44
3:AC:149:ALA:HA	3:AC:201:TYR:O	2.18	0.44
25:DA:2032:G:OP2	25:DA:2454:G:O2'	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:83:A:H5''	44:BY:8:LYS:HG2	1.99	0.44
38:DS:77:ALA:HB1	38:DS:82:ILE:HB	2.00	0.44
36:BQ:34:LEU:HB2	36:BQ:118:LEU:HD22	1.99	0.44
25:BA:1405:A:N3	25:BA:1405:A:H5'	2.33	0.44
25:DA:2153:G:C2	25:DA:2154:G:C5	3.06	0.44
25:BA:2169:G:N3	25:BA:2170:G:H5''	2.33	0.44
1:AA:1399:C:C2	1:AA:1401:G:C5	3.06	0.44
35:DP:65:ARG:HD3	35:DP:66:GLY:N	2.33	0.44
25:DA:1310:G:OP2	53:D7:9:ARG:HD2	2.17	0.44
1:CA:532:A:H2	1:CA:1206:G:N2	2.15	0.44
25:BA:932:C:H3'	25:BA:933:C:C5'	2.47	0.44
25:DA:2321:G:O2'	25:DA:2322:A:OP1	2.29	0.44
25:DA:2331:G:O2'	25:DA:2336:A:N1	2.30	0.44
1:CA:1347:G:H22	1:CA:1373:G:H2'	1.83	0.44
1:AA:59:A:H3'	1:AA:331:G:H22	1.82	0.44
14:CN:23:ARG:HG3	14:CN:28:GLY:O	2.18	0.44
2:AB:77:ALA:HB2	2:AB:165:VAL:HG11	1.99	0.44
1:CA:337:C:H2'	1:CA:338:A:H8	1.80	0.44
1:CA:1145:C:H4'	1:CA:1146:A:H5'	1.99	0.44
1:AA:738:C:OP2	6:AF:92:LYS:NZ	2.40	0.44
10:AJ:11:PHE:CE1	10:AJ:67:THR:HG22	2.52	0.44
53:B7:35:ARG:HG3	53:B7:42:LEU:HD11	2.00	0.44
23:AY:8:4SU:H1'	23:AY:48:C:O2	2.18	0.44
25:DA:466:A:N3	25:DA:683:C:H1'	2.33	0.44
1:CA:1069:C:H4'	1:CA:1192:C:O2	2.17	0.44
25:BA:2377:G:O6	54:B8:39:LYS:HE3	2.18	0.44
25:BA:1558:G:H2'	25:BA:1559:C:O4'	2.18	0.44
25:BA:1653:C:H4'	25:BA:1654:A:O5'	2.18	0.44
1:AA:1070:U:OP1	5:AE:18:ARG:NH1	2.51	0.44
25:BA:2369:U:OP1	46:B0:20:ARG:HD3	2.17	0.44
25:BA:791:G:OP1	28:BE:132:HIS:ND1	2.48	0.44
25:DA:506:G:O3'	25:DA:507:A:H8	2.01	0.44
16:CP:17:TYR:HE2	16:CP:41:PRO:HG3	1.83	0.44
7:CG:46:ALA:HA	7:CG:49:ILE:HD12	1.99	0.44
1:AA:831:U:H2'	1:AA:832:C:C6	2.52	0.44
25:BA:270:C:H4'	25:BA:271:U:OP1	2.18	0.44
1:CA:280:C:N3	17:CQ:39:SER:N	2.66	0.44
25:DA:272(J):C:H42	25:DA:363:G:H1	1.65	0.44
45:DZ:75:ASN:O	45:DZ:84:GLU:N	2.29	0.44
25:DA:1838:C:N4	25:DA:1898:U:H2'	2.33	0.44
25:BA:2077:C:O2	61:BA:4428:HOH:O	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:BF:196:LEU:HA	29:BF:196:LEU:HD23	1.76	0.44
25:DA:2051:A:H5'	25:DA:2578:G:O4'	2.18	0.44
1:CA:922:G:C6	1:CA:923:A:C6	3.06	0.43
45:DZ:110:GLY:HA3	45:DZ:174:VAL:HG21	1.99	0.43
25:DA:248:G:C2	25:DA:2431:U:H4'	2.53	0.43
26:DB:48:A:H2'	26:DB:49:C:C6	2.53	0.43
9:AI:79:LEU:HD22	9:AI:104:ARG:HB2	1.99	0.43
14:CN:24:CYS:HB2	14:CN:40:CYS:HB3	2.00	0.43
25:DA:236:C:H2'	25:DA:237:C:C6	2.53	0.43
45:BZ:145:GLU:O	45:BZ:148:ASP:N	2.39	0.43
25:DA:964:C:O2'	25:DA:2273:A:N3	2.41	0.43
23:CW:38:A:C6	23:CW:39:PSU:C2	3.05	0.43
25:DA:251:A:C5	25:DA:252:G:H1'	2.53	0.43
25:DA:2532:G:C6	25:DA:2533:A:C6	3.05	0.43
50:B4:16:CYS:HA	50:B4:33:VAL:O	2.18	0.43
16:AP:72:ARG:NH2	16:AP:73:LEU:HD21	2.33	0.43
25:DA:2705:A:H2'	25:DA:2706:G:O4'	2.18	0.43
40:DU:65:ILE:HD11	40:DU:95:LEU:HB3	2.00	0.43
25:BA:2787:C:H2'	25:BA:2788:A:O4'	2.18	0.43
25:DA:1417:C:H2'	25:DA:1418:G:O4'	2.18	0.43
28:DE:9:VAL:HG22	28:DE:25:VAL:HB	1.99	0.43
44:DY:19:LYS:HE2	44:DY:20:TYR:CE1	2.53	0.43
13:AM:11:ARG:O	13:AM:13:LYS:N	2.50	0.43
7:CG:150:ALA:HA	11:CK:59:TYR:HB3	1.99	0.43
25:BA:2705:A:H2'	25:BA:2706:G:H8	1.83	0.43
25:BA:2722:C:H2'	25:BA:2723:A:C8	2.53	0.43
1:AA:909:A:H2'	1:AA:910:C:O4'	2.18	0.43
25:BA:212:A:O4'	25:BA:449:A:H5'	2.18	0.43
52:D6:11:LEU:HB2	52:D6:21:TYR:HB2	2.00	0.43
50:D4:40:HIS:HA	50:D4:41:PRO:HD2	1.84	0.43
6:CF:8:ILE:HD11	6:CF:79:LEU:HD13	1.99	0.43
25:DA:2833:G:H4'	25:DA:2834:G:OP2	2.18	0.43
11:CK:22:HIS:HB3	11:CK:29:ILE:HB	1.99	0.43
49:D3:16:PRO:HB2	49:D3:18:ASP:OD1	2.16	0.43
2:CB:35:GLU:HB2	2:CB:40:HIS:HD2	1.83	0.43
25:DA:2820:A:O5'	37:DR:4:LEU:HD23	2.17	0.43
1:AA:1325:C:O2'	1:AA:1326:C:H5'	2.17	0.43
50:B4:24:THR:OG1	50:B4:25:TYR:N	2.50	0.43
26:BB:7:G:H5"	26:BB:7:G:H8	1.83	0.43
27:DD:134:ARG:HG3	27:DD:187:GLY:O	2.18	0.43
31:DH:98:LEU:HA	31:DH:98:LEU:HD12	1.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:CY:27:G:H2'	23:CY:28:G:C8	2.53	0.43
57:AA:3221:NEG:H11	25:BA:786:G:O6	2.17	0.43
1:AA:377:G:P	16:AP:5:ARG:HD2	2.58	0.43
25:DA:1357:U:H2'	25:DA:1358:G:O4'	2.18	0.43
1:CA:1075:C:H2'	1:CA:1076:C:H5'	1.99	0.43
23:CW:63:G:H2'	23:CW:64:A:C8	2.53	0.43
2:CB:125:PRO:O	2:CB:127:ILE:N	2.51	0.43
25:DA:1116:C:H2'	25:DA:1117:G:C8	2.53	0.43
1:CA:44:G:H2'	1:CA:45:U:O4'	2.18	0.43
5:CE:99:GLY:HA2	5:CE:116:THR:O	2.18	0.43
6:CF:69:GLU:O	6:CF:72:VAL:HG12	2.17	0.43
2:AB:166:ASP:O	2:AB:170:GLU:N	2.48	0.43
25:DA:2265:U:C4	25:DA:2266:A:C5	3.06	0.43
25:DA:118:A:H3'	25:DA:119:A:H5''	2.00	0.43
6:CF:4:TYR:HE1	6:CF:92:LYS:HG3	1.83	0.43
25:DA:2773:C:H2'	25:DA:2774:C:H6	1.83	0.43
15:CO:85:LEU:HB3	15:CO:87:ILE:HG13	2.00	0.43
42:BW:65:LEU:HD12	42:BW:68:ARG:HE	1.83	0.43
25:DA:1580:A:H5'	25:DA:1581:G:OP2	2.18	0.43
4:AD:196:LEU:C	4:AD:198:VAL:H	2.22	0.43
25:DA:1466:G:O3'	25:DA:1546:C:O2'	2.35	0.43
1:CA:1327:C:O2'	1:CA:1328:C:H5'	2.18	0.43
30:BG:16:ARG:O	30:BG:20:ILE:HG13	2.18	0.43
1:AA:779:C:O2'	11:AK:120:ARG:HD3	2.18	0.43
3:AC:150:LYS:HG3	3:AC:169:ALA:HB2	2.00	0.43
1:AA:1347:G:N2	1:AA:1373:G:H2'	2.33	0.43
25:DA:1894:C:C2'	25:DA:1895:C:H5'	2.48	0.43
1:CA:818:G:O2'	1:CA:819:A:H5'	2.18	0.43
1:CA:189(K):U:H2'	1:CA:189(L):G:C8	2.54	0.43
25:DA:1530:C:H42	25:DA:1539:G:H1	1.64	0.43
25:DA:176:G:O2'	25:DA:177:G:H5'	2.18	0.43
48:B2:25:VAL:HG11	48:B2:61:LEU:HD21	1.98	0.43
32:BI:27:ARG:HD2	47:B1:71:TYR:CE1	2.54	0.43
13:CM:5:ALA:CB	13:CM:22:ILE:HD12	2.48	0.43
1:AA:236:G:H5''	17:AQ:42:TYR:OH	2.17	0.43
33:BN:33:LEU:HD12	33:BN:33:LEU:HA	1.87	0.43
38:BS:83:LYS:HB2	38:BS:83:LYS:HE2	1.91	0.43
1:CA:495:A:H4'	1:CA:496:A:OP1	2.18	0.43
25:DA:70:G:H5''	25:DA:112:U:O2	2.18	0.43
1:CA:581:G:OP1	15:CO:61:GLY:HA3	2.18	0.43
8:CH:12:ARG:CZ	8:CH:27:PRO:HD3	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:DU:104:GLN:OE1	40:DU:105:VAL:HG23	2.18	0.43
25:BA:2560:G:H2'	25:BA:2561:G:O4'	2.17	0.43
1:AA:1028:C:N3	1:AA:1033:G:N2	2.53	0.43
23:AY:20:U:H3'	23:AY:20:U:OP2	2.17	0.43
25:BA:2132:G:N3	25:BA:2142:G:H1'	2.33	0.43
1:CA:1392:G:N2	1:CA:1502:A:C8	2.87	0.43
25:DA:2143:C:H2'	25:DA:2144:U:O4'	2.18	0.43
25:DA:972:G:C6	25:DA:973:A:C6	3.06	0.43
2:CB:211:ILE:O	2:CB:215:LEU:HB2	2.18	0.43
1:CA:1381:U:O2'	7:CG:79:ARG:HG3	2.18	0.43
1:CA:1010:G:H22	1:CA:1020:U:H1'	1.81	0.43
25:DA:93:G:H2'	25:DA:94:C:C6	2.53	0.43
26:DB:2:C:H2'	26:DB:3:C:C6	2.53	0.43
9:CI:50:LEU:HD23	9:CI:85:LEU:HD11	2.00	0.43
25:BA:1992:A:H4'	25:BA:1993:A:OP1	2.18	0.43
25:BA:1716:A:H5''	25:BA:2562:G:OP1	2.18	0.43
28:DE:101:ARG:NH2	28:DE:171:GLU:HB2	2.33	0.43
1:AA:1106:G:C6	1:AA:1107:C:C4	3.06	0.43
25:BA:2638:C:H2'	25:BA:2639:G:O4'	2.18	0.43
25:DA:853:G:H2'	25:DA:854:G:H8	1.82	0.43
25:DA:925:C:H2'	25:DA:926:A:H8	1.83	0.43
12:CL:8:ASN:O	12:CL:12:ARG:HG3	2.19	0.43
31:DH:24:VAL:HG22	31:DH:35:VAL:HB	2.00	0.43
1:CA:130:A:H5'	17:CQ:63:ARG:HE	1.84	0.43
25:DA:752:A:OP1	53:D7:3:ARG:NH2	2.45	0.43
2:CB:118:LEU:HD13	2:CB:142:LEU:HB2	2.01	0.43
25:BA:1821:C:H2'	25:BA:1822:A:C5	2.53	0.43
1:CA:984:C:H2'	1:CA:985:C:H6	1.83	0.43
25:DA:2228:G:C6	25:DA:2229:C:C4	3.06	0.43
29:BF:28:ILE:HD13	29:BF:119:ARG:HE	1.83	0.43
24:CX:53:G:H3'	24:CX:54:5MU:H71	1.98	0.43
1:CA:253:U:H2'	1:CA:254:G:C8	2.54	0.43
25:DA:336:C:HO2'	44:DY:35:TYR:HH	1.67	0.43
32:BI:54:GLN:HG3	32:BI:57:ARG:NH2	2.34	0.43
25:BA:91:G:H2'	25:BA:92:C:C6	2.53	0.43
25:DA:1445:A:OP2	25:DA:1445(A):C:N4	2.39	0.43
25:DA:1268:A:H2'	25:DA:1269:A:O4'	2.18	0.43
41:DV:12:TYR:CD2	41:DV:20:LEU:HD21	2.52	0.43
7:AG:89:MET:SD	7:AG:155:ARG:HB2	2.58	0.43
25:BA:1944:G:H2'	25:BA:1945:U:C6	2.53	0.43
1:AA:872:A:C8	1:AA:874:G:C8	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:2406:U:C2	35:DP:72:PRO:HG2	2.54	0.43
38:BS:87:PHE:CE1	38:BS:102:ALA:HB2	2.53	0.43
28:DE:181:LEU:HD21	39:DT:6:LEU:HD12	2.00	0.43
25:DA:311:A:C6	25:DA:328:U:C4	3.06	0.43
1:AA:97:G:H2'	1:AA:98:G:O4'	2.18	0.43
25:BA:1834:A:H2'	25:BA:1835:C:O4'	2.19	0.43
12:AL:113:ARG:O	12:AL:114:LYS:HD2	2.19	0.43
1:CA:953:G:H2'	1:CA:954:G:O4'	2.18	0.43
35:DP:44:GLY:CA	35:DP:45:LEU:HB2	2.48	0.43
8:CH:20:TYR:CE2	8:CH:75:ARG:HG2	2.54	0.43
43:DX:35:THR:HG22	43:DX:37:THR:H	1.83	0.43
1:AA:1139:G:N2	1:AA:1143:G:C6	2.87	0.43
4:CD:112:VAL:HG22	4:CD:116:GLN:OE1	2.19	0.43
10:CJ:38:ILE:HD11	10:CJ:71:LEU:HD23	2.00	0.43
1:AA:109:A:C6	1:AA:326:G:C6	3.06	0.43
1:AA:1239:A:C4	1:AA:1298:C:N4	2.86	0.43
25:DA:953:A:C6	25:DA:965:C:N3	2.86	0.43
25:DA:2364:C:OP1	46:D0:55:ARG:HD3	2.19	0.43
25:DA:889:C:O2'	25:DA:890:A:O5'	2.35	0.43
25:DA:182:A:H2	25:DA:433:C:O2	2.00	0.43
25:DA:479:A:O2'	25:DA:481:G:H5'	2.18	0.43
25:BA:9:U:O4	25:BA:2641:A:H2	2.02	0.43
11:CK:80:VAL:O	11:CK:106:LYS:N	2.50	0.43
5:AE:77:PRO:HG2	5:AE:78:HIS:CD2	2.52	0.43
25:BA:925:A:N6	25:BA:946:A:C8	2.87	0.43
25:DA:1857:G:C6	25:DA:1858:G:C6	3.06	0.43
25:DA:1857:G:O2'	25:DA:1885:A:N6	2.46	0.43
1:AA:865:A:H2	1:AA:918:A:H4'	1.83	0.43
25:DA:2870:C:H2'	25:DA:2871:C:O4'	2.19	0.43
29:DF:33:LEU:HD13	29:DF:112:MET:HE2	1.99	0.43
15:AO:82:ILE:HD12	15:AO:88:ARG:HB2	2.00	0.43
27:DD:77:ALA:HB2	27:DD:97:TYR:CD2	2.53	0.43
45:BZ:105:VAL:N	45:BZ:139:VAL:O	2.46	0.43
25:BA:1027:A:N1	25:BA:2049:G:O2'	2.45	0.43
1:CA:384:G:H2'	1:CA:385:C:C6	2.54	0.43
40:BU:74:LEU:H	40:BU:74:LEU:HD12	1.82	0.43
2:CB:196:LEU:HD12	2:CB:196:LEU:HA	1.86	0.43
48:B2:29:LYS:HG2	48:B2:57:ILE:HD13	1.99	0.43
16:CP:15:PRO:O	16:CP:16:HIS:ND1	2.51	0.43
1:AA:1429:C:H2'	1:AA:1430:C:C6	2.53	0.43
1:AA:375:U:OP1	16:AP:69:THR:HG21	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:DU:58:ARG:HA	40:DU:61:TRP:CE3	2.54	0.43
1:AA:1027:C:C2	1:AA:1034:G:N1	2.87	0.43
1:CA:1005:A:H1'	1:CA:1025:U:C2	2.53	0.43
37:DR:21:TYR:CZ	37:DR:43:GLU:HG2	2.52	0.43
12:CL:24:VAL:HG13	12:CL:98:TYR:CE1	2.53	0.43
12:CL:24:VAL:HG13	12:CL:98:TYR:HE1	1.84	0.43
26:DB:66:A:N6	26:DB:109:C:OP2	2.51	0.43
25:BA:384:G:H2'	25:BA:385:G:H8	1.82	0.43
1:CA:839:U:O2'	1:CA:840:C:OP1	2.29	0.43
1:AA:1304:G:C6	1:AA:1305:G:N1	2.86	0.43
57:CX:3004:NEG:N2	25:DA:2322:A:OP2	2.52	0.43
2:CB:96:ARG:HH11	2:CB:98:LEU:HA	1.82	0.43
35:DP:99:LEU:HD12	35:DP:100:LEU:HD23	2.00	0.43
25:BA:1968:U:H2'	25:BA:1969:C:C6	2.53	0.43
25:BA:2818:U:O2'	25:BA:2819:A:H5'	2.19	0.43
1:AA:524:G:H2'	1:AA:525:C:C6	2.52	0.43
25:DA:2107:C:H2'	25:DA:2108:C:O4'	2.18	0.43
25:BA:1874:C:H5'	27:BD:253:GLN:HE22	1.83	0.43
4:AD:61:LYS:HA	4:AD:203:VAL:HG22	2.00	0.43
1:CA:501:C:H1'	1:CA:549:C:H1'	2.01	0.43
2:AB:112:VAL:O	2:AB:116:GLU:HB2	2.19	0.43
25:BA:1698:G:H2'	25:BA:1699:A:O4'	2.18	0.43
25:BA:1911:A:N1	25:BA:2246:G:H1'	2.34	0.43
25:BA:2364:A:N6	25:BA:2377:G:O2'	2.51	0.43
1:AA:44:G:C6	1:AA:45:U:C2	3.07	0.43
25:DA:949:C:H2'	25:DA:950:G:H8	1.84	0.43
25:BA:2283:G:OP1	46:B0:18:ALA:HB1	2.19	0.43
18:AR:26:LEU:HD13	18:AR:26:LEU:HA	1.88	0.43
30:BG:12:TYR:HA	30:BG:16:ARG:HG3	1.99	0.43
25:BA:624:C:O2'	25:BA:628:C:OP1	2.28	0.43
25:DA:851:U:H5'	49:D3:49:LYS:HD2	1.99	0.43
1:CA:707:C:H2'	1:CA:708:C:C6	2.52	0.43
1:CA:811:C:H4'	1:CA:900:A:N6	2.34	0.43
28:DE:146:THR:HA	28:DE:147:PRO:HA	1.89	0.43
50:B4:40:HIS:HA	50:B4:41:PRO:HD2	1.76	0.43
25:DA:77:C:OP1	48:D2:59:ARG:HD3	2.18	0.43
1:CA:978:A:O2'	1:CA:1322:C:N3	2.46	0.43
23:AY:69:G:H2'	23:AY:70:G:O4'	2.18	0.43
1:CA:1004:A:C2	1:CA:1038:C:C4	3.06	0.43
25:DA:2126:A:H61	25:DA:2172:U:H5'	1.83	0.43
23:AW:26:A:N6	23:AW:44:G:H1	2.15	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:BY:92:ASN:OD1	44:BY:94:LYS:HG3	2.19	0.43
7:CG:113:GLU:CG	7:CG:119:ARG:HG2	2.45	0.43
50:B4:59:PHE:HA	50:B4:61:ARG:HG2	2.01	0.43
29:DF:20:LEU:HD22	29:DF:21:ALA:H	1.84	0.43
1:AA:1064:G:H1'	1:AA:1190:G:H21	1.83	0.43
2:AB:178:ARG:NH2	8:AH:74:PRO:HB3	2.27	0.43
45:DZ:108:PRO:HB3	45:DZ:144:LEU:HB3	2.00	0.43
36:DQ:22:LYS:HE2	36:DQ:22:LYS:HB3	1.81	0.43
50:D4:62:ARG:HD3	50:D4:62:ARG:HA	1.73	0.43
24:CX:8:4SU:H1'	24:CX:48:C:O2	2.18	0.43
2:CB:48:MET:HA	2:CB:51:LEU:HD12	2.01	0.43
27:DD:132:PRO:HG2	27:DD:135:PHE:HD2	1.80	0.43
1:AA:1299:A:H5''	1:AA:1299:A:N3	2.34	0.43
45:DZ:145:GLU:HG3	45:DZ:146:ILE:H	1.81	0.43
1:AA:411:A:OP2	4:AD:30:LYS:HD2	2.17	0.43
25:DA:372:G:H8	47:D1:65:SER:O	2.02	0.43
25:BA:596:G:O2'	25:BA:597:C:H3'	2.19	0.43
25:DA:2889:C:H3'	25:DA:2891:G:C8	2.53	0.43
10:AJ:61:GLU:OE1	14:AN:58:LYS:NZ	2.42	0.43
1:CA:1106:G:H2'	1:CA:1107:C:C6	2.54	0.43
25:DA:1151:G:C2	25:DA:1152:C:C2	3.07	0.43
1:AA:58:C:O2'	1:AA:388:G:N7	2.46	0.43
25:DA:2751:G:H8	31:DH:2:SER:HA	1.83	0.43
23:CW:11:C:H2'	23:CW:12:U:C6	2.53	0.43
25:DA:938:G:OP1	54:D8:52:LYS:HD2	2.18	0.43
15:AO:85:LEU:HB3	15:AO:87:ILE:HG13	1.99	0.43
6:AF:8:ILE:HD11	6:AF:79:LEU:HD13	2.01	0.43
38:BS:48:LEU:HD23	38:BS:82:ILE:HD11	2.00	0.43
42:DW:46:PHE:O	42:DW:50:VAL:HG23	2.18	0.43
29:BF:132:VAL:HA	29:BF:138:GLU:HB3	2.01	0.43
1:AA:767:A:H2'	1:AA:768:A:O4'	2.18	0.43
24:AX:13:C:O2'	25:BA:1946:C:H4'	2.18	0.43
25:DA:2203:U:O2'	25:DA:2205:C:H5'	2.18	0.43
25:BA:589:U:H2'	25:BA:590:A:O4'	2.19	0.43
1:AA:1360:A:OP1	1:AA:1360:A:H8	2.00	0.43
16:CP:60:LEU:HD13	16:CP:60:LEU:HA	1.80	0.43
2:AB:137:ARG:CZ	2:AB:137:ARG:HB3	2.48	0.43
1:AA:520:A:N1	1:AA:536:C:H1'	2.33	0.43
1:AA:1026:G:HO2'	1:AA:1027:C:P	2.41	0.43
25:BA:1576:G:O2'	25:BA:1577:C:H5'	2.18	0.43
25:DA:997:G:O2'	25:DA:998:C:H5'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:AP:74:LEU:HG	16:AP:79:VAL:HG21	1.99	0.43
25:DA:1131:G:H8	25:DA:2025:C:H4'	1.84	0.43
50:D4:46:GLN:C	50:D4:48:ARG:H	2.22	0.43
1:CA:1011:G:N2	1:CA:1019:C:H1'	2.34	0.43
25:BA:344:A:H4'	25:BA:346:A:N7	2.33	0.43
25:BA:599:U:H2'	25:BA:600:G:C8	2.54	0.43
25:DA:2206:G:H3'	25:DA:2207:G:N7	2.34	0.43
9:CI:127:LYS:HB2	9:CI:127:LYS:HE3	1.87	0.43
13:CM:91:ARG:HD2	13:CM:91:ARG:HA	1.92	0.43
1:CA:70:G:H1	1:CA:99:U:H3	1.67	0.43
1:CA:986:A:H2'	1:CA:987:G:O4'	2.18	0.43
7:CG:88:PRO:HG3	7:CG:149:ARG:HA	2.01	0.43
13:CM:19:LEU:HD12	13:CM:19:LEU:HA	1.90	0.43
4:AD:164:ALA:C	4:AD:168:ARG:HH11	2.22	0.43
24:CX:53:G:H2'	24:CX:54:5MU:C6	2.54	0.43
1:AA:1429:C:H2'	1:AA:1430:C:H6	1.83	0.43
7:CG:87:VAL:HG11	7:CG:155:ARG:HA	2.00	0.43
25:DA:676:A:H1'	25:DA:2443:C:H1'	2.00	0.43
2:CB:61:LEU:HD23	2:CB:68:ILE:HD11	2.00	0.43
36:BQ:30:GLY:HA2	36:BQ:107:ALA:HB2	2.00	0.43
4:AD:79:PHE:CE1	4:AD:204:ILE:HD13	2.53	0.43
25:DA:1756:G:H4'	25:DA:1758:G:O4'	2.19	0.43
1:CA:1366:C:H2'	1:CA:1367:C:C6	2.53	0.43
1:CA:32:A:C2	1:CA:33:A:C4	3.06	0.43
41:DV:62:LEU:HD23	41:DV:93:GLU:HG2	2.00	0.43
25:BA:1769:G:H2'	25:BA:1770:A:H8	1.84	0.43
33:BN:28:THR:HG22	33:BN:29:LYS:N	2.33	0.43
32:BI:88:ILE:O	32:BI:121:LYS:NZ	2.50	0.43
36:DQ:75:THR:HG21	36:DQ:87:LYS:NZ	2.34	0.43
13:AM:65:LYS:NZ	13:AM:73:GLU:HG3	2.34	0.43
36:DQ:77:LYS:HE2	61:DQ:3101:HOH:O	2.18	0.43
4:AD:78:LEU:HD23	4:AD:78:LEU:HA	1.84	0.43
34:BO:108:GLU:HG3	34:BO:108:GLU:H	1.48	0.43
48:D2:31:GLU:O	48:D2:35:LEU:HG	2.19	0.43
13:AM:86:CYS:HB2	19:AS:73:GLU:HB3	2.01	0.43
8:AH:28:ALA:HA	8:AH:59:LEU:HG	2.00	0.43
1:AA:1363(A):A:H4'	1:AA:1364:U:H2'	2.01	0.43
27:BD:101:GLU:OE1	27:BD:103:ARG:NH1	2.45	0.43
1:CA:741:G:H2'	1:CA:742:G:O4'	2.19	0.43
2:CB:211:ILE:HG13	2:CB:211:ILE:H	1.66	0.43
10:CJ:6:ILE:HA	10:CJ:97:GLU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:1823:G:OP1	27:DD:54:ARG:NH1	2.52	0.43
1:CA:1012:U:O2	1:CA:1017:G:O6	2.36	0.43
13:CM:82:MET:HE2	13:CM:92:HIS:HB3	2.01	0.43
1:CA:1015:A:N3	1:CA:1218:C:O2'	2.41	0.43
25:DA:644:A:C2	25:DA:2369:A:H1'	2.54	0.43
3:CC:71:ALA:HB1	3:CC:109:PRO:HG3	2.01	0.43
25:DA:2484:G:C2	25:DA:2485:G:C8	3.07	0.43
23:AY:8:4SU:H4'	23:AY:48:C:C4'	2.48	0.43
13:AM:80:ARG:HH22	19:AS:69:HIS:CE1	2.36	0.43
1:CA:993:G:H2'	1:CA:993:G:N3	2.34	0.43
3:CC:32:LEU:HD13	3:CC:32:LEU:HA	1.86	0.43
1:CA:1434:A:H2'	1:CA:1435:G:O4'	2.19	0.43
25:DA:1588:C:H2'	25:DA:1589:C:C6	2.54	0.43
25:DA:1711:C:H2'	25:DA:1712:C:H6	1.84	0.43
25:BA:864:C:O2'	25:BA:886:U:H5''	2.19	0.43
1:CA:59:A:H3'	1:CA:331:G:H22	1.83	0.43
2:CB:118:LEU:HB3	2:CB:142:LEU:HD12	2.01	0.43
25:BA:1701:A:C1'	25:BA:2833:A:H5'	2.49	0.43
1:AA:831:U:H2'	1:AA:832:C:H6	1.83	0.43
1:CA:253:U:H2'	1:CA:254:G:H8	1.83	0.43
15:AO:26:GLU:HB3	15:AO:81:LEU:HD13	2.01	0.43
25:BA:549:U:H2'	25:BA:550:U:C6	2.54	0.43
28:BE:143:ASN:HD22	28:BE:147:PRO:CD	2.32	0.43
25:BA:2032:G:O6	61:BA:4615:HOH:O	2.21	0.43
25:DA:813:U:H2'	25:DA:814:C:C6	2.54	0.43
3:CC:6:HIS:HA	3:CC:7:PRO:HD3	1.85	0.43
25:BA:1683:C:H2'	25:BA:1684:A:C8	2.54	0.43
1:AA:1329:A:N7	21:AU:7:ARG:NH2	2.65	0.43
33:BN:68:GLU:H	33:BN:68:GLU:HG2	1.65	0.43
20:AT:13:LEU:HG	20:AT:13:LEU:H	1.45	0.43
30:DG:79:ASN:OD1	30:DG:79:ASN:N	2.51	0.43
25:DA:928:G:O5'	25:DA:928:G:H8	2.01	0.43
1:CA:261:U:OP2	20:CT:79:ARG:NH2	2.52	0.43
36:DQ:73:PRO:HA	36:DQ:93:TYR:CD1	2.54	0.43
29:DF:9:ILE:HA	29:DF:10:PRO:HD3	1.85	0.43
15:AO:61:GLY:O	15:AO:65:ARG:HG3	2.19	0.43
2:CB:219:VAL:HA	2:CB:222:ILE:HG12	2.00	0.43
25:DA:2100:G:C6	25:DA:2190:G:C6	3.06	0.43
1:AA:713:G:H2'	1:AA:714:G:C8	2.53	0.43
36:BQ:35:VAL:HA	36:BQ:101:ARG:O	2.18	0.43
13:AM:93:ARG:HG2	25:BA:935:C:O4'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:BZ:130:PRO:HA	45:BZ:133:ILE:HG13	2.00	0.43
25:BA:274:U:H5	32:BI:52:ARG:HD3	1.84	0.43
25:DA:2031:A:C6	25:DA:2498:C:H1'	2.53	0.43
25:DA:460:A:H2'	25:DA:461:C:O4'	2.18	0.43
40:BU:50:ARG:HH12	41:BV:72:VAL:HA	1.83	0.43
3:CC:19:GLU:HB3	3:CC:40:ARG:NH2	2.33	0.43
43:BX:92:LEU:HA	43:BX:92:LEU:HD12	1.75	0.43
1:CA:1494:G:H4'	25:DA:1913:A:C8	2.54	0.43
11:CK:45:GLY:O	11:CK:50:TYR:HB2	2.18	0.43
15:CO:54:ARG:HH11	15:CO:58:MET:CE	2.32	0.43
32:DI:27:ARG:HD2	47:D1:71:TYR:CZ	2.54	0.43
25:DA:2881:C:H2'	25:DA:2882:A:O4'	2.19	0.43
1:CA:308:C:H2'	1:CA:309:G:C8	2.54	0.43
25:BA:552:C:C4	25:BA:2792:U:H2'	2.54	0.43
1:CA:1371:G:C6	1:CA:1372:U:C4	3.07	0.43
26:BB:29:A:H2'	26:BB:30:C:O4'	2.19	0.43
13:AM:94:ARG:CZ	19:AS:80:TYR:HD2	2.32	0.43
1:CA:927:G:OP2	1:CA:927:G:H4'	2.19	0.43
55:D9:17:ILE:HD12	55:D9:17:ILE:HA	1.94	0.43
20:AT:30:LYS:O	20:AT:34:LYS:HG3	2.19	0.43
25:DA:938:G:OP2	54:D8:52:LYS:NZ	2.44	0.43
25:BA:1769:G:H2'	25:BA:1770:A:C8	2.54	0.43
1:CA:154:C:H2'	1:CA:155:C:C6	2.54	0.43
25:DA:2716:U:O2'	25:DA:2717:G:H5'	2.18	0.43
42:BW:48:ALA:O	42:BW:52:GLU:HB2	2.19	0.43
25:DA:754:C:H2'	25:DA:755:C:C6	2.54	0.43
1:AA:299:G:H8	1:AA:299:G:O5'	2.02	0.43
11:AK:38:ASN:HA	11:AK:39:PRO:HD3	1.87	0.43
23:AW:31:A:H2'	23:AW:32:PSU:O4'	2.19	0.43
14:AN:39:LEU:HD11	14:AN:47:LEU:HD12	2.00	0.43
25:DA:1745(A):C:H5'	25:DA:1746:G:OP2	2.18	0.43
15:CO:48:LYS:HD3	15:CO:48:LYS:HA	1.60	0.43
45:DZ:19:ARG:HE	45:DZ:19:ARG:HB2	1.42	0.43
25:BA:1884:A:H2'	25:BA:1885:A:C8	2.53	0.43
25:DA:1422:G:H4'	25:DA:1493:C:OP1	2.18	0.43
24:AX:61:C:H2'	24:AX:62:C:H6	1.83	0.43
34:BO:69:ILE:HD11	34:BO:105:GLU:CD	2.38	0.43
16:CP:18:ARG:HG2	16:CP:35:LYS:HE3	2.00	0.43
25:BA:2156:A:OP2	25:BA:2178:G:N2	2.52	0.43
25:DA:1140:C:OP2	33:DN:66:LYS:NZ	2.40	0.43
2:CB:201:ILE:HG21	2:CB:214:ILE:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:662:G:H2'	1:CA:663:A:H8	1.82	0.43
29:DF:106:ARG:H	29:DF:106:ARG:HG2	1.51	0.43
25:DA:864:G:H4'	26:DB:102:A:H4'	2.00	0.43
25:BA:402:C:H2'	25:BA:403:C:C6	2.54	0.43
11:AK:104:GLN:HB3	11:AK:104:GLN:HE21	1.55	0.43
1:CA:392:G:H2'	1:CA:393:A:C8	2.54	0.43
25:DA:2114:A:H2'	25:DA:2114:A:N3	2.33	0.43
25:BA:2332:A:H2'	25:BA:2332:A:N3	2.34	0.43
9:AI:9:ARG:HG2	9:AI:14:VAL:HG13	2.01	0.43
45:DZ:45:ASP:O	45:DZ:49:ARG:HG3	2.19	0.43
25:DA:493:G:H2'	25:DA:494:G:O4'	2.18	0.43
1:CA:828:A:H5''	1:CA:859:A:N1	2.34	0.43
10:CJ:16:LEU:HD23	10:CJ:16:LEU:HA	1.87	0.43
25:BA:2221:A:H5''	25:BA:2222:C:OP2	2.19	0.43
2:CB:92:TYR:HE2	2:CB:94:ASN:HB2	1.83	0.43
24:CX:18:G:O2'	24:CX:19:G:H5'	2.18	0.43
25:DA:622:G:H2'	25:DA:623:G:H8	1.84	0.43
25:BA:1717:C:O2	28:BE:129:HIS:NE2	2.44	0.43
2:CB:230:VAL:HG22	2:CB:231:GLU:H	1.84	0.43
3:AC:87:LEU:O	3:AC:91:LEU:N	2.40	0.43
25:BA:1556:A:H5'	25:BA:1557:A:OP2	2.18	0.43
1:CA:604:G:C2	1:CA:635:G:C5	3.07	0.43
3:CC:8:ILE:HG23	3:CC:16:ARG:HG2	2.01	0.43
30:BG:117:PHE:HZ	30:BG:179:PRO:HG2	1.83	0.43
12:CL:28:LYS:N	12:CL:29:GLY:HA2	2.33	0.43
25:DA:271(E):U:H2'	25:DA:271(F):C:C6	2.53	0.43
1:AA:407:G:H2'	1:AA:408:A:C8	2.54	0.43
3:CC:184:TYR:HA	3:CC:200:ALA:O	2.19	0.43
25:BA:2230:U:O4'	47:B1:52:ARG:NH2	2.51	0.43
3:CC:121:ALA:HB2	3:CC:198:VAL:HG21	2.00	0.43
25:BA:2623:U:H6	25:BA:2623:U:H5'	1.84	0.43
13:CM:108:ARG:HD3	13:CM:108:ARG:HA	1.86	0.43
25:BA:1615:G:H5'	27:BD:60:ARG:HA	2.01	0.43
32:DI:133:HIS:HD2	32:DI:136:VAL:HG23	1.84	0.43
25:DA:2064:C:H2'	25:DA:2065:C:C6	2.53	0.43
1:CA:1028:C:O2	1:CA:1034:G:H1'	2.18	0.42
25:DA:2299:G:H2'	25:DA:2300:G:H8	1.84	0.42
1:AA:1002:G:C6	1:AA:1003:G:N3	2.87	0.42
25:DA:2689:U:C4'	25:DA:2690:C:H5'	2.37	0.42
25:BA:2166:U:C2	25:BA:2170:G:N1	2.88	0.42
25:DA:945:A:C4	25:DA:2448:A:C2	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:DZ:97:GLU:HG2	45:DZ:97:GLU:H	1.58	0.42
1:CA:343:U:O2'	1:CA:344:A:H2'	2.18	0.42
29:DF:11:VAL:HB	29:DF:18:ARG:HB3	2.01	0.42
25:DA:1469:A:H2'	25:DA:1470:G:O4'	2.19	0.42
25:DA:139(A):G:O2'	25:DA:140:G:H5'	2.18	0.42
25:DA:952:G:C4	25:DA:966:G:C2	3.07	0.42
25:DA:1430:C:H2'	25:DA:1431:U:C6	2.54	0.42
45:BZ:41:LEU:HD21	45:BZ:83:PRO:HG2	2.00	0.42
1:CA:892:A:C6	1:CA:893:C:C4	3.07	0.42
20:CT:14:LYS:O	20:CT:18:GLN:HG3	2.19	0.42
25:BA:1276:C:H2'	25:BA:1277:G:C8	2.54	0.42
7:CG:23:VAL:O	7:CG:27:ILE:HG12	2.19	0.42
1:AA:619:U:N3	4:AD:134:ASP:OD1	2.32	0.42
25:DA:1032:A:O3'	55:D9:16:VAL:HG11	2.19	0.42
25:DA:276:A:H5''	25:DA:277:C:H5'	2.01	0.42
25:BA:1701:A:O4'	25:BA:2833:A:H5'	2.19	0.42
1:AA:192:U:H2'	1:AA:193:C:C6	2.54	0.42
25:DA:676:A:H2	25:DA:2069:G:N3	2.17	0.42
42:DW:4:LYS:HB2	42:DW:106:ILE:HG12	2.00	0.42
29:BF:183:VAL:O	29:BF:187:VAL:HG23	2.19	0.42
1:CA:277:C:OP1	17:CQ:41:LYS:HE2	2.19	0.42
25:BA:95:G:OP1	48:B2:46:GLN:NE2	2.47	0.42
25:DA:637:A:H8	35:DP:117:GLU:HG3	1.84	0.42
25:BA:1207:C:O2'	41:BV:8:GLY:HA2	2.19	0.42
31:BH:164:TYR:HB2	31:BH:167:GLU:HB2	2.00	0.42
25:DA:1394:U:H2'	25:DA:1395:A:O4'	2.19	0.42
32:BI:84:GLY:O	32:BI:86:THR:N	2.51	0.42
4:AD:65:ARG:HG2	4:AD:75:PHE:CD2	2.54	0.42
36:DQ:11:LYS:HE3	36:DQ:88:GLY:O	2.19	0.42
25:BA:399:G:H8	47:B1:65:SER:O	2.02	0.42
13:AM:108:ARG:HD3	13:AM:108:ARG:HA	1.82	0.42
1:AA:616:G:O2'	1:AA:617:G:H5'	2.19	0.42
25:BA:1898:A:H2'	25:BA:1899:A:C8	2.54	0.42
25:DA:1952:A:OP1	34:DO:42:SER:OG	2.24	0.42
25:DA:224:G:H2'	25:DA:225:A:O4'	2.18	0.42
33:BN:75:TYR:CE2	33:BN:77:GLY:HA2	2.53	0.42
8:CH:69:ARG:HG3	8:CH:76:PRO:HA	2.01	0.42
25:BA:384:G:H2'	25:BA:385:G:C8	2.54	0.42
25:DA:1814:G:H4'	27:DD:51:VAL:HG21	2.00	0.42
42:DW:18:ARG:HG3	42:DW:76:VAL:HB	1.99	0.42
27:DD:245:PRO:HB2	27:DD:253:GLN:HG2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:CS:10:PHE:HE1	19:CS:37:ARG:HD3	1.84	0.42
26:DB:91:C:H5'	36:DQ:18:LYS:HA	2.01	0.42
46:D0:55:ARG:HE	46:D0:55:ARG:HB2	1.54	0.42
34:DO:120:GLU:HB2	39:DT:68:TYR:CE2	2.54	0.42
1:AA:405:U:OP2	4:AD:3:ARG:NH2	2.52	0.42
25:DA:443:A:N7	29:DF:45:ARG:HG2	2.34	0.42
27:DD:206:LEU:HD22	27:DD:211:ARG:HG2	2.01	0.42
33:DN:34:LEU:HD23	33:DN:107:LEU:HD21	2.01	0.42
25:DA:2258:C:O2'	25:DA:2427:C:OP2	2.30	0.42
25:BA:449:A:H2'	25:BA:450:A:C8	2.54	0.42
3:AC:39:ILE:HG23	3:AC:91:LEU:HD11	2.01	0.42
30:BG:179:PRO:HG3	50:B4:43:TYR:OH	2.19	0.42
25:BA:2564:U:H2'	25:BA:2566:U:H5''	2.00	0.42
41:BV:55:ALA:HB2	41:BV:101:GLY:HA2	2.01	0.42
26:DB:83:G:H4'	49:D3:52:HIS:CG	2.54	0.42
49:D3:6:VAL:HG13	49:D3:56:VAL:HG22	2.01	0.42
39:BT:127:ALA:O	39:BT:129:ARG:N	2.51	0.42
17:AQ:56:VAL:HB	17:AQ:78:GLU:HB3	2.01	0.42
1:CA:54:C:H2'	1:CA:352:C:H41	1.84	0.42
11:AK:48:ILE:O	11:AK:50:TYR:N	2.51	0.42
25:DA:172:C:H2'	25:DA:173:G:C8	2.55	0.42
33:DN:71:ILE:HG21	33:DN:84:LYS:HB3	2.01	0.42
25:DA:2662:A:H8	25:DA:2662:A:O5'	2.02	0.42
25:DA:2859:G:H2'	25:DA:2860:A:C8	2.55	0.42
25:BA:1231:G:OP1	61:BA:4357:HOH:O	2.22	0.42
40:BU:85:LYS:HE2	40:BU:85:LYS:HB3	1.82	0.42
1:CA:685:G:C2	1:CA:686:U:C4	3.07	0.42
35:BP:3:LEU:HA	35:BP:3:LEU:HD12	1.91	0.42
23:CW:70:G:H8	23:CW:70:G:OP2	2.02	0.42
25:BA:2250:G:H2'	25:BA:2250:G:N3	2.33	0.42
25:BA:2270:C:O2'	25:BA:2439:C:OP2	2.35	0.42
1:CA:416:G:C5	1:CA:417:C:C4	3.07	0.42
1:CA:971:G:H1'	1:CA:1365:G:O2'	2.19	0.42
33:DN:30:ILE:HG23	33:DN:52:VAL:HG11	2.01	0.42
25:BA:2162:C:H1'	25:BA:2174:G:H22	1.84	0.42
2:CB:77:ALA:HB2	2:CB:211:ILE:HD13	2.01	0.42
19:CS:32:LYS:HA	19:CS:50:ALA:HB3	2.01	0.42
3:AC:6:HIS:HA	3:AC:7:PRO:HD3	1.92	0.42
1:CA:841:U:C5	1:CA:848:C:H1'	2.55	0.42
28:BE:47:VAL:O	28:BE:80:GLU:HA	2.19	0.42
25:DA:2646:C:H2'	25:DA:2647:U:O4'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:CS:27:GLU:HB3	19:CS:28:LYS:HB3	2.01	0.42
25:BA:1057:G:OP2	40:BU:66:ASN:ND2	2.37	0.42
37:BR:44:LEU:HD22	37:BR:48:VAL:HG23	2.01	0.42
31:BH:4:ILE:HG22	31:BH:69:ARG:HG2	2.01	0.42
6:AF:69:GLU:O	6:AF:72:VAL:HG12	2.19	0.42
1:CA:340:U:H2'	1:CA:341:C:H6	1.85	0.42
25:BA:776:G:C5	27:BD:208:LYS:HB2	2.54	0.42
1:CA:608:A:H2'	1:CA:609:A:O4'	2.18	0.42
25:BA:287:G:O6	25:BA:448:U:O2'	2.25	0.42
25:DA:14:A:N1	25:DA:2044:C:O2'	2.43	0.42
25:DA:2469:A:C6	25:DA:2470:G:C4	3.08	0.42
25:DA:27:G:O2'	25:DA:28:A:OP2	2.35	0.42
13:AM:11:ARG:C	13:AM:13:LYS:H	2.21	0.42
13:AM:11:ARG:HA	13:AM:45:VAL:HB	2.01	0.42
1:AA:530:G:O6	22:AV:21:C:H1'	2.19	0.42
25:BA:946:A:H2'	25:BA:947:A:O4'	2.19	0.42
25:BA:1583:C:H2'	25:BA:1584:G:O4'	2.18	0.42
44:BY:43:ASN:HD22	44:BY:43:ASN:HA	1.68	0.42
50:D4:57:GLU:HA	50:D4:58:ARG:HA	1.75	0.42
25:DA:1614:A:H8	25:DA:1614:A:P	2.43	0.42
32:BI:54:GLN:HG3	32:BI:57:ARG:HH22	1.83	0.42
1:CA:154:C:C2'	1:CA:155:C:H5'	2.49	0.42
25:BA:1899:A:H3'	25:BA:1900:G:O4'	2.19	0.42
25:BA:879:G:N3	35:BP:53:GLY:HA3	2.35	0.42
44:BY:9:LYS:HA	44:BY:10:GLY:HA2	1.66	0.42
47:D1:83:GLU:HA	47:D1:84:GLY:HA2	1.67	0.42
10:AJ:81:THR:O	10:AJ:85:LEU:N	2.37	0.42
33:DN:91:LEU:HG	33:DN:98:VAL:HG21	1.99	0.42
31:BH:139:GLN:HG3	31:BH:140:LYS:N	2.34	0.42
15:AO:11:VAL:HG21	15:AO:34:LEU:HD22	2.00	0.42
13:AM:60:VAL:HG22	13:AM:64:TRP:HZ3	1.83	0.42
1:CA:1209:C:O2'	1:CA:1214:C:N4	2.52	0.42
27:BD:4:LYS:HE2	27:BD:6:PHE:CE1	2.55	0.42
1:AA:1338:G:C6	1:AA:1339:A:C6	3.07	0.42
1:AA:1092:A:H2'	1:AA:1093:A:C8	2.54	0.42
37:DR:17:ARG:HG2	37:DR:21:TYR:CE2	2.55	0.42
23:CW:7:A:C6	23:CW:66:U:O4	2.72	0.42
23:AW:56:C:C5	25:BA:943:C:O4'	2.72	0.42
25:DA:1022:G:C5	25:DA:1140:C:C4	3.08	0.42
1:AA:1007:C:O5'	1:AA:1007:C:H6	2.02	0.42
25:BA:2333:G:H5''	25:BA:2334:A:OP2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:528:A:H2	25:DA:2043:C:H5'	1.84	0.42
23:CY:76:A:H62	25:DA:2422:A:C5'	2.29	0.42
7:AG:111:ARG:HH11	7:AG:111:ARG:HB3	1.84	0.42
10:CJ:74:ILE:HG22	61:CJ:5101:HOH:O	2.19	0.42
13:AM:90:LEU:O	13:AM:93:ARG:HB2	2.18	0.42
1:AA:1493:A:H5''	1:AA:1494:G:OP2	2.19	0.42
25:BA:2298:A:H4'	25:BA:2299:A:O4'	2.19	0.42
1:AA:1179:A:H2'	1:AA:1180:A:O4'	2.19	0.42
25:DA:2815:C:H5'	51:D5:29:THR:HG21	2.02	0.42
1:CA:338:A:H2'	1:CA:339:C:O4'	2.20	0.42
43:BX:54:VAL:HG22	43:BX:81:VAL:HG12	2.02	0.42
27:DD:231:HIS:ND1	27:DD:232:PRO:HD2	2.34	0.42
25:DA:2849:U:OP2	39:DT:95:ARG:NH1	2.53	0.42
1:CA:607:A:H2'	1:CA:608:A:O4'	2.19	0.42
25:DA:601:C:O2	25:DA:605:C:H4'	2.20	0.42
25:BA:515:G:H8	25:BA:515:G:OP1	2.03	0.42
25:BA:310:C:H2'	25:BA:311:C:C6	2.53	0.42
1:CA:36:C:O2'	12:CL:117:ARG:NH2	2.51	0.42
8:AH:86:ILE:HG12	8:AH:135:CYS:HA	2.01	0.42
25:DA:569:U:C4	25:DA:570:G:C6	3.07	0.42
26:DB:89:G:C6	26:DB:90:A:C6	3.08	0.42
4:AD:15:GLU:HG2	4:AD:63:LYS:HB3	2.00	0.42
25:DA:2372:G:H1'	52:D6:46:HIS:CE1	2.54	0.42
1:AA:881:G:P	12:AL:12:ARG:HH22	2.42	0.42
25:DA:2746:U:O4	25:DA:2755:C:H4'	2.18	0.42
1:AA:872:A:C4	1:AA:874:G:N7	2.87	0.42
25:DA:2661:G:H2'	25:DA:2662:A:C8	2.55	0.42
31:DH:164:TYR:HB2	31:DH:167:GLU:HB2	2.01	0.42
8:CH:33:GLU:HG2	8:CH:48:TYR:CE1	2.54	0.42
54:B8:36:LYS:HB2	54:B8:41:ILE:CD1	2.49	0.42
11:CK:27:ASN:OD1	11:CK:28:THR:N	2.52	0.42
25:DA:2261:C:H1'	25:DA:2388:A:N3	2.34	0.42
4:AD:10:ARG:HB2	4:AD:40:PRO:HG3	2.02	0.42
25:BA:1495:G:H4'	25:BA:1589:A:OP1	2.19	0.42
25:BA:1817:A:H1'	25:BA:1960:A:N6	2.34	0.42
25:BA:1694:G:H3'	25:BA:1694:G:OP2	2.19	0.42
27:DD:33:LEU:HD23	27:DD:33:LEU:HA	1.85	0.42
34:DO:7:TYR:CE1	34:DO:20:MET:HB2	2.55	0.42
25:DA:1224:C:C4	25:DA:1225:G:C6	3.08	0.42
23:AY:7:A:HO2'	23:AY:49:C:H5'	1.85	0.42
1:AA:1003:G:N2	1:AA:1004:A:H1'	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:898:C:H3'	25:DA:899:A:C8	2.54	0.42
25:BA:2164:C:N3	25:BA:2171:G:C6	2.87	0.42
22:AV:13:A:H3'	22:AV:14:A:H5''	2.02	0.42
1:CA:1362:C:H2'	1:CA:1363:C:H5''	2.02	0.42
43:DX:31:HIS:HA	43:DX:32:PRO:HD3	1.91	0.42
25:DA:828:U:C5	25:DA:2247:A:H4'	2.54	0.42
1:CA:522:C:H41	12:CL:53:ARG:NH2	2.05	0.42
28:DE:144:ARG:HB3	28:DE:145:LYS:H	1.44	0.42
1:CA:517:G:N1	1:CA:533:A:OP2	2.42	0.42
20:AT:48:LYS:HA	20:AT:48:LYS:HD3	1.80	0.42
29:DF:164:ARG:O	29:DF:168:ARG:HB2	2.20	0.42
8:CH:77:GLU:HG3	8:CH:78:GLN:N	2.34	0.42
25:BA:2331:G:H22	38:BS:3:ARG:CZ	2.33	0.42
1:CA:1011:G:C6	1:CA:1012:U:C2	3.07	0.42
23:AW:52:G:H5''	36:BQ:56:ARG:NH1	2.34	0.42
23:AW:1:G:H2'	23:AW:2:C:C6	2.51	0.42
26:DB:81:G:C6	26:DB:82:G:C5	3.07	0.42
9:CI:82:ALA:HA	9:CI:85:LEU:HD12	2.01	0.42
1:CA:945:G:C2	1:CA:946:A:C8	3.07	0.42
37:BR:53:HIS:O	37:BR:56:LYS:HB2	2.19	0.42
37:BR:33:ARG:HD2	37:BR:113:LEU:HD13	2.01	0.42
1:AA:1080:A:H5'	5:AE:14:ARG:NH2	2.35	0.42
1:AA:292:G:O2'	1:AA:608:A:N6	2.51	0.42
40:DU:83:LEU:O	40:DU:87:GLY:N	2.52	0.42
25:DA:266:G:N2	25:DA:427:U:H1'	2.35	0.42
25:DA:983:A:C6	25:DA:984:A:N1	2.88	0.42
25:DA:833:U:H2'	25:DA:834:C:C6	2.54	0.42
25:BA:225:C:H2'	25:BA:226:C:H6	1.84	0.42
30:DG:47:LYS:HB3	30:DG:48:GLU:H	1.62	0.42
1:AA:1017:G:H2'	1:AA:1018:C:C6	2.54	0.42
25:DA:1422:G:H1'	25:DA:1496:A:N1	2.35	0.42
25:BA:1817:A:H8	61:BA:4001:HOH:O	2.02	0.42
41:DV:4:ILE:HD12	41:DV:39:LEU:HB3	2.02	0.42
25:DA:1328:G:O2'	25:DA:1329:U:H2'	2.19	0.42
45:DZ:27:VAL:HG12	45:DZ:85:HIS:HE1	1.83	0.42
25:BA:1825:U:H2'	25:BA:1826:C:C6	2.53	0.42
25:BA:1639:G:H2'	25:BA:1640:G:C8	2.54	0.42
52:D6:35:GLU:HG2	52:D6:50:ARG:HD3	2.00	0.42
44:DY:39:VAL:HB	44:DY:42:VAL:HB	2.02	0.42
25:BA:1756:U:H2'	25:BA:1757:C:C6	2.54	0.42
31:DH:106:THR:HG23	31:DH:112:PRO:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:BI:135:GLU:C	32:BI:137:PRO:HD3	2.40	0.42
27:DD:275:LYS:HD2	27:DD:275:LYS:HA	1.86	0.42
1:AA:437:U:O2'	4:AD:125:HIS:HE1	2.03	0.42
5:AE:105:VAL:HB	5:AE:106:PRO:HD3	2.01	0.42
1:CA:407:G:H2'	1:CA:408:A:C8	2.54	0.42
20:CT:67:ALA:HB2	20:CT:77:ALA:HB2	2.02	0.42
25:BA:964:A:H5''	26:BB:98:G:O2'	2.20	0.42
26:DB:43:C:H2'	26:DB:45:A:N7	2.34	0.42
1:CA:922:G:N3	1:CA:1398:A:H2	2.18	0.42
25:DA:142(A):C:H2'	25:DA:143:G:O4'	2.20	0.42
25:DA:1814:G:H5''	27:DD:54:ARG:HH21	1.84	0.42
19:AS:23:ASN:HA	19:AS:27:GLU:CD	2.40	0.42
23:CW:76:A:OP2	25:DA:2602:A:N6	2.53	0.42
1:CA:1346:A:H61	1:CA:1374:A:H3'	1.85	0.42
25:DA:2356:C:O3'	46:D0:20:ARG:HD3	2.19	0.42
1:CA:428:G:OP2	4:CD:10:ARG:NH1	2.52	0.42
13:CM:65:LYS:HA	50:D4:50:VAL:HG11	2.00	0.42
2:CB:125:PRO:C	2:CB:127:ILE:H	2.23	0.42
25:DA:892:G:C4	25:DA:893:C:H1'	2.54	0.42
1:CA:1289:A:H2'	1:CA:1290:G:H5'	2.02	0.42
25:DA:990:A:H5''	25:DA:991:C:OP1	2.19	0.42
25:DA:910:A:N3	25:DA:2264:C:O2'	2.44	0.42
1:AA:1441:G:H5''	1:AA:1442:G:O5'	2.19	0.42
25:DA:1453:U:OP1	37:DR:77:ARG:NH1	2.46	0.42
25:DA:2302:G:C6	25:DA:2315:G:C6	3.08	0.42
25:DA:2370:G:C6	25:DA:2371:G:C6	3.08	0.42
18:CR:52:PRO:O	18:CR:56:THR:HG23	2.20	0.42
35:BP:120:ALA:HB1	35:BP:138:LEU:HA	2.02	0.42
10:AJ:90:LEU:HA	10:AJ:91:PRO:HD3	1.92	0.42
25:BA:2152:U:H4'	25:BA:2155:G:H4'	2.02	0.42
25:BA:2566:U:H2'	25:BA:2567:U:C6	2.54	0.42
1:CA:1499:A:H1'	1:CA:1520:G:H5'	2.01	0.42
1:CA:612:C:O2	1:CA:629:G:N2	2.53	0.42
13:AM:15:VAL:HG22	13:AM:43:THR:O	2.20	0.42
1:AA:7:G:H5'	1:AA:298:A:O4'	2.17	0.42
1:CA:189:G:H2'	1:CA:189(A):C:C6	2.55	0.42
11:AK:97:ALA:O	11:AK:101:SER:HB3	2.19	0.42
52:D6:40:CYS:HA	52:D6:41:PRO:HD3	1.87	0.42
25:DA:263:C:H2'	25:DA:264:C:O4'	2.20	0.42
25:BA:2329:C:H2'	25:BA:2330:G:O4'	2.18	0.42
30:DG:111:LEU:HB2	30:DG:112:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:1949:A:C6	25:BA:1950:A:C6	3.08	0.42
13:CM:40:ASN:HB3	13:CM:43:THR:HG23	2.02	0.42
47:D1:23:LYS:HB3	47:D1:29:GLY:HA3	2.01	0.42
25:DA:656:G:H2'	25:DA:657:U:O4'	2.19	0.42
48:D2:53:LEU:HA	48:D2:53:LEU:HD23	1.67	0.42
1:AA:526:C:P	12:AL:91:LYS:HE3	2.60	0.42
31:DH:86:GLU:HG3	31:DH:132:ARG:NH2	2.34	0.42
31:DH:115:VAL:HG11	31:DH:148:ILE:HD13	2.01	0.42
1:CA:1025:U:O2'	1:CA:1026:G:C8	2.72	0.42
25:DA:2124:G:C2	25:DA:2174:C:N3	2.88	0.42
25:BA:2127:C:H2'	25:BA:2128:G:C8	2.55	0.42
3:AC:36:ASP:O	3:AC:40:ARG:HG3	2.19	0.42
30:DG:33:ARG:O	30:DG:161:THR:HG23	2.19	0.42
45:DZ:107:THR:HA	45:DZ:108:PRO:HD3	1.81	0.42
25:DA:1031:G:H5''	55:D9:8:LYS:HE3	2.01	0.42
25:BA:875:U:H4'	25:BA:878:G:N1	2.35	0.42
2:AB:80:ILE:HG13	2:AB:212:GLN:HA	2.01	0.42
25:DA:2027:G:H2'	25:DA:2028:U:O4'	2.19	0.42
15:AO:56:LEU:HD21	25:BA:762:G:C2	2.55	0.42
43:BX:92:LEU:C	43:BX:94:GLY:H	2.23	0.42
2:AB:77:ALA:CB	2:AB:165:VAL:HG11	2.50	0.42
38:DS:68:GLN:HE21	38:DS:68:GLN:HA	1.84	0.42
25:BA:1347:A:O2'	25:BA:1348:A:H3'	2.19	0.42
25:DA:1913:A:H4'	25:DA:1914:C:C5'	2.50	0.42
1:AA:1237:C:O2'	1:AA:1300:G:N1	2.36	0.42
26:DB:80:U:H2'	26:DB:81:G:H8	1.84	0.42
25:DA:247:G:H4'	25:DA:386:G:C6	2.55	0.42
45:BZ:152:ALA:H	45:BZ:171:ILE:CG1	2.33	0.42
3:CC:164:ARG:HG2	3:CC:165:THR:N	2.33	0.42
1:CA:1512:U:H2'	1:CA:1513:A:C8	2.54	0.42
45:DZ:29:TYR:HB3	45:DZ:34:ASN:ND2	2.35	0.42
25:DA:2018:G:H2'	25:DA:2019:A:O4'	2.20	0.42
16:CP:48:TRP:HH2	16:CP:76:GLN:HE22	1.67	0.42
25:DA:2526:G:C5	25:DA:2527:C:C5	3.07	0.42
18:CR:56:THR:HB	18:CR:58:LEU:HD22	2.01	0.42
25:DA:709:U:H2'	25:DA:710:G:H8	1.84	0.42
25:DA:328:U:H4'	44:DY:68:HIS:CG	2.54	0.42
25:BA:2665:U:H2'	25:BA:2666:A:C8	2.55	0.42
25:BA:485:U:H5''	53:B7:40:TRP:CD2	2.55	0.42
25:DA:475:U:H4'	25:DA:510:C:H5'	2.01	0.42
17:CQ:45:HIS:HA	17:CQ:69:LYS:HE3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:182:ILE:HD13	3:AC:203:PHE:HA	2.02	0.42
25:DA:244:A:C2	25:DA:255:A:C4	3.08	0.42
25:BA:1471:G:H2'	25:BA:1472:G:C8	2.54	0.42
25:DA:271(N):U:H3'	25:DA:271(O):C:H5'	2.02	0.42
1:CA:203:U:H2'	1:CA:203:U:OP2	2.20	0.42
25:DA:1675:C:O5'	25:DA:1675:C:H6	2.01	0.42
18:AR:42:ARG:HB3	18:AR:42:ARG:HH21	1.85	0.42
1:AA:1529:G:H4'	1:AA:1530:G:OP2	2.19	0.42
25:BA:701:A:O2'	25:BA:702:A:H5'	2.20	0.42
23:AW:68:C:C2	23:AW:69:G:C8	3.08	0.42
25:DA:2126:A:N3	25:DA:2127:G:H1'	2.35	0.42
1:CA:975:A:H4'	1:CA:976:G:C5'	2.41	0.42
25:DA:1002:G:N2	25:DA:1154:G:H1'	2.34	0.42
25:BA:142:G:O2'	43:BX:35:THR:HG21	2.19	0.42
1:AA:1148:U:O4'	9:AI:16:ARG:HD2	2.19	0.42
25:BA:1091:A:OP1	25:BA:1091:A:H4'	2.19	0.42
1:AA:1051:C:H2'	1:AA:1052:U:C6	2.55	0.42
57:AA:3216:NEG:H93	61:AA:4239:HOH:O	2.19	0.42
25:DA:2331:G:N3	25:DA:2336:A:C2	2.88	0.42
25:DA:988:A:O5'	49:D3:11:SER:HB2	2.20	0.42
25:DA:2026:C:H2'	25:DA:2027:G:O4'	2.20	0.42
3:CC:5:ILE:HD11	10:CJ:61:GLU:OE1	2.19	0.42
46:B0:43:THR:O	46:B0:43:THR:HG23	2.20	0.42
13:CM:81:LEU:HD13	13:CM:88:ARG:HG2	2.02	0.42
25:DA:1170:G:N2	25:DA:1179:C:O2	2.53	0.42
25:BA:1550:C:H2'	25:BA:1551:C:C6	2.54	0.42
31:DH:16:SER:OG	31:DH:27:LYS:HB2	2.20	0.42
25:DA:645:C:O2	25:DA:645:C:H2'	2.20	0.42
1:AA:737:A:H2'	1:AA:738:C:C6	2.54	0.42
1:CA:1529:G:H4'	1:CA:1530:G:OP2	2.20	0.42
1:CA:426:G:OP1	4:CD:38:TYR:OH	2.32	0.42
20:AT:100:ILE:HB	20:AT:101:GLY:H	1.69	0.42
19:CS:40:ILE:HA	19:CS:44:MET:SD	2.60	0.42
25:BA:2863:C:H2'	25:BA:2864:G:H8	1.85	0.42
25:BA:653:G:H2'	25:BA:654:G:H8	1.85	0.42
2:AB:158:LEU:HA	2:AB:159:PRO:HD3	1.84	0.42
1:CA:130:A:H5'	17:CQ:63:ARG:NE	2.34	0.42
30:BG:121:ASN:HA	30:BG:122:PRO:HD3	1.80	0.42
30:BG:67:LYS:HG2	30:BG:68:PRO:HD2	2.02	0.42
1:CA:154:C:H2'	1:CA:155:C:H6	1.84	0.42
34:BO:66:LYS:HA	34:BO:79:PHE:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:CL:83:VAL:HG23	12:CL:107:ALA:HB2	2.01	0.42
45:BZ:40:ASP:OD2	45:BZ:42:VAL:HG13	2.20	0.42
25:DA:1503:U:H2'	25:DA:1504:C:C6	2.55	0.42
27:BD:233:HIS:HA	61:BD:405:HOH:O	2.20	0.42
1:CA:165:C:H2'	1:CA:166:G:C8	2.54	0.42
1:CA:448:A:OP2	1:CA:485:G:N2	2.31	0.42
25:BA:1370:G:N7	61:BA:4365:HOH:O	2.36	0.42
11:CK:62:GLN:O	11:CK:66:LEU:HG	2.20	0.42
1:CA:909:A:H2'	1:CA:910:C:O4'	2.20	0.42
45:BZ:44:PHE:CZ	45:BZ:86:VAL:HG11	2.55	0.42
1:AA:787:A:N1	1:AA:795:C:N4	2.66	0.42
40:BU:20:LEU:HD23	40:BU:20:LEU:HA	1.83	0.42
25:BA:1660:A:P	25:BA:1660:A:H8	2.43	0.42
48:D2:32:LEU:HD13	48:D2:36:ARG:NH1	2.34	0.42
25:DA:2887:U:H2'	25:DA:2888:C:C6	2.55	0.42
1:CA:134:A:H1'	1:CA:325:A:C5	2.54	0.42
1:CA:967:C:H2'	1:CA:968:A:C8	2.55	0.42
45:BZ:23:LYS:HB3	45:BZ:38:TYR:CD1	2.55	0.42
25:DA:2510:C:C4	25:DA:2511:U:C4	3.08	0.42
25:DA:2126:A:N6	25:DA:2162:G:O2'	2.52	0.42
23:AY:25:C:O2'	23:AY:26:A:H8	2.02	0.42
30:BG:129:GLY:O	30:BG:161:THR:HB	2.19	0.42
8:CH:20:TYR:HA	8:CH:65:TYR:CE2	2.55	0.42
2:CB:31:TYR:HE2	2:CB:194:PRO:HB3	1.85	0.42
1:AA:840:C:H4'	1:AA:841:U:OP1	2.19	0.42
49:B3:3:ARG:CZ	49:B3:36:VAL:HG11	2.50	0.42
57:CX:3004:NEG:HN41	57:CX:3004:NEG:C8	2.33	0.42
25:DA:2323:G:H2'	25:DA:2324:C:O4'	2.20	0.42
25:DA:1164:G:C2	25:DA:1165:U:C2	3.07	0.42
25:DA:2037:G:H2'	25:DA:2038:G:C8	2.55	0.42
28:BE:33:VAL:HB	28:BE:47:VAL:CG1	2.50	0.42
1:CA:1318:A:H4'	19:CS:10:PHE:CE1	2.55	0.42
1:CA:406:G:H21	4:CD:119:GLN:HE22	1.68	0.42
13:CM:76:ALA:HA	13:CM:79:LYS:HB3	2.00	0.42
25:DA:954:G:C5	25:DA:955:C:C5	3.08	0.42
1:AA:1149:C:P	9:AI:9:ARG:HH21	2.42	0.42
8:AH:51:VAL:HG11	8:AH:60:ARG:HH12	1.84	0.42
25:BA:2901:A:C6	25:BA:2902:G:C6	3.08	0.42
1:CA:1288:A:H2'	1:CA:1289:A:O4'	2.20	0.42
27:DD:232:PRO:HB3	27:DD:244:ARG:CZ	2.49	0.42
1:CA:324:G:N7	61:CA:4083:HOH:O	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:219:G:C6	25:DA:220:G:C6	3.08	0.42
1:AA:769:G:H4'	1:AA:1513:A:H4'	2.02	0.42
36:DQ:35:VAL:HG12	36:DQ:130:LYS:O	2.19	0.42
24:CX:9:G:N3	24:CX:45:G:H2'	2.34	0.42
1:CA:993:G:H2'	1:CA:995:C:H41	1.85	0.42
1:CA:130:A:O2'	1:CA:131:C:O5'	2.30	0.42
30:DG:44:GLY:HA2	30:DG:88:ILE:HG22	2.01	0.42
25:BA:2418:U:H6	25:BA:2418:U:H2'	1.69	0.42
1:AA:1437:C:H2'	1:AA:1438:G:H8	1.84	0.42
25:BA:831:A:O4'	27:BD:227:ASN:ND2	2.52	0.42
27:DD:134:ARG:H	27:DD:134:ARG:HG3	1.49	0.42
3:CC:12:LEU:HD23	3:CC:16:ARG:HB3	2.02	0.42
2:CB:83:MET:HB3	2:CB:234:PRO:HG2	2.02	0.42
25:BA:1261:G:OP1	40:BU:8:VAL:HG22	2.20	0.42
1:CA:616:G:OP2	4:CD:141:ARG:NH2	2.43	0.42
9:CI:23:ASN:ND2	9:CI:25:LYS:HG2	2.35	0.42
25:DA:2635:C:OP1	28:DE:79:ARG:NH2	2.52	0.42
18:AR:40:LEU:HB3	18:AR:79:LEU:HD11	2.02	0.42
1:CA:457:C:H2'	1:CA:458:C:C6	2.55	0.42
1:CA:457:C:H2'	1:CA:458:C:H6	1.85	0.42
25:DA:2649:U:H2'	25:DA:2650:U:C6	2.55	0.42
1:CA:1060:C:N4	3:CC:2:GLY:HA2	2.35	0.42
31:BH:144:VAL:O	31:BH:148:ILE:HG13	2.20	0.42
29:BF:33:LEU:HD12	29:BF:33:LEU:HA	1.88	0.42
25:DA:1877:A:OP2	25:DA:1877:A:H8	2.03	0.42
25:BA:1360:C:H5'	25:BA:1360:C:H6	1.85	0.42
32:DI:61:ARG:HA	32:DI:61:ARG:HD3	1.64	0.42
25:DA:68:G:H2'	25:DA:69:C:O4'	2.20	0.42
28:BE:52:LEU:HD12	28:BE:77:ILE:HD11	2.01	0.42
25:DA:56:A:H2'	25:DA:57:C:O4'	2.19	0.42
25:BA:880:U:O2	35:BP:55:ARG:NH2	2.52	0.42
23:AW:70:G:H2'	23:AW:71:G:O4'	2.20	0.42
25:DA:2690:C:OP1	37:DR:17:ARG:NH1	2.31	0.42
25:BA:2161:C:C4	25:BA:2162:C:C5	3.08	0.42
25:BA:2163:G:C2	25:BA:2164:C:H1'	2.54	0.42
25:BA:1577:C:O2'	25:BA:1578:C:H6	2.03	0.42
25:BA:1577:C:O2'	25:BA:1578:C:P	2.78	0.42
1:CA:1256:A:H61	1:CA:1278:U:C2'	2.32	0.42
57:AA:3216:NEG:C9	23:AW:34:G:H5'	2.50	0.42
25:DA:863:A:P	36:DQ:22:LYS:HG3	2.59	0.42
1:AA:1044:A:C5	1:AA:1045:C:H1'	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:1028:A:H62	25:DA:1125:G:H2'	1.85	0.42
38:DS:11:LYS:O	38:DS:15:ARG:HG3	2.19	0.42
25:DA:2360:A:C2	25:DA:2361:A:H1'	2.55	0.42
25:DA:1996:C:P	34:DO:31:LYS:HZ1	2.42	0.42
45:DZ:146:ILE:H	45:DZ:146:ILE:HG13	1.66	0.42
25:BA:1356:G:OP2	53:B7:9:ARG:HD2	2.20	0.42
25:BA:956:A:C5	36:BQ:13:GLN:HG3	2.55	0.42
50:D4:15:ILE:HD13	50:D4:21:VAL:HG13	2.01	0.42
1:CA:719:C:O2'	18:CR:49:LYS:HB3	2.20	0.42
1:CA:1352:C:H2'	1:CA:1353:G:C8	2.55	0.42
1:CA:526:C:OP1	12:CL:91:LYS:HE3	2.19	0.42
1:AA:1445:C:C4	1:AA:1446:U:C4	3.08	0.42
25:DA:1741:A:H2'	25:DA:1742:G:O4'	2.20	0.42
45:BZ:128:VAL:HG23	45:BZ:160:GLY:O	2.19	0.42
25:BA:593:G:H2'	25:BA:2052:A:N7	2.35	0.42
19:CS:80:TYR:CZ	19:CS:82:GLY:HA2	2.55	0.42
25:DA:699:A:H4'	25:DA:1554:A:N6	2.34	0.42
1:CA:1435:G:H2'	1:CA:1436:U:C6	2.55	0.42
44:BY:20:TYR:CE1	44:BY:43:ASN:HA	2.55	0.42
25:BA:491:G:P	53:B7:12:ARG:HH22	2.43	0.42
25:DA:622:G:H2'	25:DA:623:G:C8	2.54	0.42
6:CF:3:ARG:HD3	6:CF:64:GLN:NE2	2.35	0.42
29:BF:64:ILE:HG21	29:BF:78:ILE:HG23	2.02	0.42
1:CA:714:G:H2'	1:CA:715:A:C8	2.55	0.42
1:AA:200:G:H1	1:AA:217:C:H42	1.67	0.42
25:BA:56:C:H2'	25:BA:57:G:O4'	2.20	0.42
33:DN:75:TYR:HA	33:DN:81:GLY:O	2.20	0.42
25:BA:1857:G:H2'	25:BA:1858:C:O4'	2.19	0.42
49:B3:26:LEU:O	49:B3:35:ARG:NE	2.51	0.42
38:DS:36:TYR:OH	38:DS:54:LEU:HD22	2.20	0.42
1:CA:590:C:H2'	1:CA:591:U:C6	2.55	0.42
26:BB:78:A:C2	26:BB:100:A:C4	3.07	0.42
25:BA:233:A:C2	25:BA:244:A:C4	3.08	0.42
25:BA:2732:G:OP2	61:BA:4924:HOH:O	2.22	0.42
25:BA:1432:C:H2'	25:BA:1433:C:C6	2.55	0.42
45:BZ:29:TYR:HB3	45:BZ:34:ASN:ND2	2.35	0.42
23:CW:21:A:N6	23:CW:46:7MG:N3	2.67	0.41
1:CA:1096:C:O2	1:CA:1170:A:O2'	2.35	0.41
25:DA:2287:A:C4	25:DA:2289:G:C8	3.08	0.41
25:DA:2287:A:N6	25:DA:2344:U:H3	2.06	0.41
1:AA:1129:C:C5'	9:AI:16:ARG:HH12	2.30	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:2330:G:H21	46:D0:42:GLY:N	2.18	0.41
1:CA:1129:C:H1'	1:CA:1130:A:N7	2.35	0.41
12:CL:113:ARG:O	12:CL:114:LYS:HD2	2.19	0.41
31:DH:129:THR:O	31:DH:129:THR:HG22	2.20	0.41
25:DA:1169:G:H22	25:DA:1180:C:H42	1.68	0.41
7:CG:51:GLN:HB3	7:CG:51:GLN:HE21	1.57	0.41
25:DA:2703:C:H2'	25:DA:2704:C:H6	1.84	0.41
25:BA:2658:C:H2'	25:BA:2659:U:O4'	2.20	0.41
1:CA:192:U:H2'	1:CA:193:C:H6	1.85	0.41
22:AV:20:U:H2'	22:AV:21:C:H6	1.84	0.41
1:AA:19:C:H4'	1:AA:864:A:O4'	2.20	0.41
1:CA:300:A:H1'	1:CA:565:U:O2	2.20	0.41
25:DA:709:U:H2'	25:DA:710:G:C8	2.55	0.41
8:AH:26:VAL:HG22	8:AH:59:LEU:HB2	2.01	0.41
28:DE:4:ILE:HG22	28:DE:96:PHE:HE2	1.85	0.41
25:DA:2548:G:H2'	25:DA:2549:G:O4'	2.20	0.41
25:DA:422:A:H2'	25:DA:423:A:C8	2.55	0.41
25:BA:1440:U:H4'	25:BA:1649:A:H4'	2.02	0.41
1:CA:904:C:OP2	61:CA:4139:HOH:O	2.21	0.41
32:BI:110:ASP:HA	32:BI:111:PRO:HD2	1.87	0.41
25:BA:2228:G:HO2'	25:BA:2229:A:P	2.43	0.41
1:CA:50:A:N1	1:CA:360:A:O2'	2.39	0.41
25:DA:2687:U:H2'	25:DA:2688:U:O4'	2.20	0.41
4:CD:31:CYS:O	4:CD:35:ARG:HG3	2.19	0.41
6:AF:61:LEU:HD12	6:AF:61:LEU:HA	1.85	0.41
42:BW:2:GLU:OE2	42:BW:72:LYS:NZ	2.34	0.41
1:AA:1516:G:H2'	1:AA:1518:A:OP2	2.20	0.41
27:BD:112:GLN:O	27:BD:115:GLN:HG2	2.20	0.41
1:CA:224:C:H2'	1:CA:225:C:C6	2.55	0.41
1:CA:1135:U:H2'	1:CA:1137:C:O2	2.20	0.41
25:BA:1616:A:H2'	25:BA:1617:A:O4'	2.19	0.41
23:AY:54:5MU:H73	23:AY:55:PSU:O2	2.20	0.41
25:BA:940:C:H2'	25:BA:941:U:O4'	2.20	0.41
25:DA:942:G:C6	25:DA:943:U:C4	3.08	0.41
25:DA:330:A:HO2'	25:DA:331:A:H8	1.68	0.41
1:CA:1120:G:N7	1:CA:1154:G:N2	2.68	0.41
3:AC:5:ILE:HG12	3:AC:6:HIS:N	2.34	0.41
23:CY:21:A:N6	23:CY:46:7MG:H2'	2.32	0.41
25:DA:360:G:H2'	25:DA:361:G:O4'	2.20	0.41
25:DA:1028:A:H2'	25:DA:1029:A:C8	2.55	0.41
8:AH:9:MET:SD	8:AH:32:LYS:HB3	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:981:U:H5'	14:CN:21:TYR:CZ	2.55	0.41
7:AG:76:ARG:HB3	7:AG:156:TRP:CH2	2.52	0.41
25:DA:250:G:C6	25:DA:251:A:C6	3.07	0.41
25:BA:2901:A:C2'	25:BA:2902:G:H5'	2.51	0.41
25:BA:469:A:C6	29:BF:45:ARG:HD2	2.55	0.41
1:AA:583:A:N6	1:AA:758:G:O2'	2.51	0.41
9:AI:21:PRO:HA	9:AI:59:PHE:HA	2.02	0.41
31:BH:3:ARG:HH22	31:BH:66:GLY:HA3	1.85	0.41
25:DA:117:G:C6	25:DA:119:A:C6	3.08	0.41
13:AM:17:VAL:O	13:AM:20:THR:OG1	2.26	0.41
25:BA:1792:C:C2'	25:BA:1793:A:H5'	2.50	0.41
25:DA:2018:G:P	51:D5:9:LYS:HZ1	2.42	0.41
44:DY:6:HIS:CD2	44:DY:6:HIS:H	2.37	0.41
2:AB:114:ARG:HG2	2:AB:145:LEU:HD21	2.02	0.41
1:CA:694:A:O2'	23:CY:38:A:O2'	2.32	0.41
9:CI:89:ASN:C	9:CI:89:ASN:HD22	2.23	0.41
1:AA:1258:G:H2'	1:AA:1259:C:H6	1.84	0.41
31:BH:149:ARG:NH1	31:BH:167:GLU:OE1	2.53	0.41
25:DA:57:C:H2'	25:DA:58:G:O4'	2.20	0.41
25:BA:873:U:H4'	35:BP:55:ARG:HB2	2.02	0.41
29:DF:32:LEU:O	29:DF:36:VAL:HG23	2.20	0.41
25:BA:1087:C:H5'	25:BA:1088:G:OP2	2.20	0.41
29:BF:31:HIS:NE2	29:BF:35:GLU:OE2	2.49	0.41
51:D5:41:PRO:HA	51:D5:42:PRO:HD2	1.86	0.41
13:AM:70:LEU:O	13:AM:74:VAL:HG23	2.20	0.41
1:CA:731:G:H5'	1:CA:766:A:H4'	2.02	0.41
1:CA:1370:G:N7	9:CI:109:VAL:HG11	2.36	0.41
25:DA:1368:G:C2	25:DA:1369:G:C8	3.08	0.41
25:DA:2250:G:O2'	25:DA:2496:C:OP1	2.31	0.41
25:DA:284:U:H2'	25:DA:285:C:C6	2.55	0.41
25:BA:821:A:H2'	25:BA:821:A:N3	2.35	0.41
45:BZ:11:GLU:HB3	45:BZ:12:GLY:H	1.77	0.41
30:DG:103:LEU:HA	30:DG:103:LEU:HD23	1.77	0.41
1:AA:1162:C:H2'	1:AA:1163:C:C6	2.55	0.41
24:CX:29:G:C6	24:CX:30:G:C5	3.08	0.41
1:CA:1140:C:H2'	1:CA:1141:C:H6	1.84	0.41
25:BA:144:C:H5'	43:BX:2:LYS:HE2	2.02	0.41
1:CA:1002:G:C4	1:CA:1003:G:H8	2.37	0.41
1:CA:1024:G:H2'	1:CA:1024:G:N3	2.36	0.41
23:CW:13:C:HO2'	23:CW:14:A:P	2.43	0.41
25:DA:993:G:C6	25:DA:994:C:C4	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AY:50:U:C4	23:AY:64:A:N1	2.88	0.41
25:DA:1015:G:O6	25:DA:1148:A:N6	2.53	0.41
25:BA:354:A:H2	25:BA:1255:A:C2'	2.33	0.41
13:CM:57:ARG:NH1	50:D4:34:GLU:HA	2.35	0.41
3:AC:82:GLU:HA	3:AC:85:ARG:HH21	1.84	0.41
50:D4:64:GLY:C	50:D4:66:SER:H	2.23	0.41
17:CQ:6:LEU:HD12	17:CQ:6:LEU:HA	1.86	0.41
1:CA:114:U:H1'	1:CA:353:A:H1'	2.02	0.41
25:BA:1477:U:H2'	25:BA:1478:C:C6	2.55	0.41
32:BI:77:LEU:CB	32:BI:142:VAL:HG12	2.50	0.41
25:BA:1715:A:O2'	25:BA:1721:G:N7	2.47	0.41
4:CD:11:LEU:O	4:CD:15:GLU:HB2	2.20	0.41
1:AA:115:G:H4'	1:AA:116:A:O5'	2.20	0.41
1:AA:33:A:N3	12:AL:32:PHE:HE2	2.19	0.41
1:CA:1328:C:O2'	13:CM:29:ARG:NE	2.52	0.41
1:CA:744:C:O2'	1:CA:851:G:N2	2.53	0.41
25:DA:1268:A:C2	25:DA:2013:A:C4	3.08	0.41
31:DH:164:TYR:N	31:DH:167:GLU:OE1	2.37	0.41
25:BA:1495:G:O2'	25:BA:1575:A:N1	2.42	0.41
1:AA:159:G:H3'	1:AA:344:A:C2	2.54	0.41
13:CM:89:GLY:O	13:CM:93:ARG:N	2.53	0.41
41:DV:89:GLN:HA	41:DV:90:PRO:HD3	1.87	0.41
29:BF:126:VAL:HG21	29:BF:129:PHE:CZ	2.55	0.41
15:AO:48:LYS:HD2	15:AO:48:LYS:HA	1.83	0.41
31:BH:27:LYS:HE2	31:BH:27:LYS:HB3	1.87	0.41
48:D2:3:LEU:HD23	48:D2:3:LEU:HA	1.81	0.41
37:DR:54:LEU:HD12	37:DR:54:LEU:HA	1.95	0.41
23:AW:5:G:C2	23:AW:6:G:C4	3.08	0.41
25:BA:785:G:H3'	25:BA:786:G:C8	2.55	0.41
25:BA:2290:A:OP2	46:B0:12:ASN:ND2	2.48	0.41
3:AC:33:LEU:O	3:AC:36:ASP:HB2	2.20	0.41
25:DA:963:U:H5''	61:DA:4078:HOH:O	2.20	0.41
25:DA:2147:G:N1	25:DA:2148:G:N3	2.69	0.41
25:DA:568:U:H5'	25:DA:945:A:N6	2.36	0.41
25:DA:2286:A:H4'	25:DA:2287:A:O4'	2.21	0.41
1:AA:332:G:OP2	20:AT:10:LEU:HD12	2.19	0.41
1:AA:168:G:O2'	1:AA:169:C:H5'	2.20	0.41
1:CA:1279:A:O2'	1:CA:1282:C:N4	2.54	0.41
1:AA:266:G:O2'	1:AA:267:C:OP2	2.32	0.41
25:BA:1094:A:N1	25:BA:1158:G:O2'	2.39	0.41
25:BA:1154:U:O2'	25:BA:1155:C:H6	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1063:C:H3'	1:AA:1064:G:H2'	2.02	0.41
45:DZ:111:VAL:HG22	45:DZ:174:VAL:HG13	2.03	0.41
23:CY:12:U:C2	23:CY:13:C:H1'	2.55	0.41
25:BA:1067:A:H61	25:BA:1188:A:N6	2.19	0.41
25:DA:2038:G:H2'	25:DA:2039:C:O4'	2.19	0.41
25:DA:2114:A:O2'	25:DA:2167:U:H1'	2.20	0.41
1:AA:674:G:H2'	1:AA:675:A:H8	1.85	0.41
32:BI:72:LEU:C	32:BI:74:ASN:N	2.72	0.41
35:DP:96:THR:H	35:DP:99:LEU:HG	1.85	0.41
27:BD:70:TRP:HB3	27:BD:190:TYR:CZ	2.55	0.41
30:DG:66:GLN:NE2	30:DG:93:THR:O	2.46	0.41
25:DA:1593:G:H2'	25:DA:1594:G:H8	1.85	0.41
1:AA:1055:A:H2'	3:AC:156:ARG:HD2	2.01	0.41
30:DG:19:LEU:HD22	30:DG:32:PRO:HG2	2.02	0.41
30:DG:43:LEU:HD12	30:DG:45:GLU:HG3	2.02	0.41
25:DA:974:G:N2	25:DA:989:G:H1'	2.35	0.41
1:CA:12:U:H4'	1:CA:526:C:O2'	2.20	0.41
1:AA:1219:U:OP1	14:AN:19:ARG:NH2	2.44	0.41
25:DA:265:A:C8	25:DA:266:G:H1'	2.55	0.41
25:BA:2786:C:H2'	25:BA:2787:C:H6	1.84	0.41
11:CK:120:ARG:HA	11:CK:121:PRO:HD3	1.76	0.41
25:BA:733:G:N2	25:BA:835:A:H61	2.18	0.41
25:DA:699:A:H2'	25:DA:700:G:O4'	2.21	0.41
25:DA:2562:U:O2'	34:DO:23:ARG:HD3	2.20	0.41
22:CV:20:U:H2'	22:CV:21:C:H6	1.84	0.41
4:CD:150:GLU:O	4:CD:153:ARG:HG2	2.20	0.41
30:BG:86:MET:HA	30:BG:87:PRO:HD3	1.94	0.41
24:CX:18:G:C5	24:CX:57:A:C6	3.09	0.41
1:AA:198:G:C5	1:AA:220:G:C2	3.08	0.41
1:CA:202:U:H3'	1:CA:203:U:C6	2.55	0.41
1:CA:1243:C:OP1	21:CU:10:ARG:HB3	2.21	0.41
1:CA:256:U:OP1	17:CQ:17:LYS:NZ	2.42	0.41
1:CA:1264:C:H2'	1:CA:1265:G:H8	1.86	0.41
25:DA:2313:C:H4'	30:DG:91:ARG:HG3	2.02	0.41
1:AA:719:C:N4	18:AR:71:LYS:HE2	2.35	0.41
1:CA:283:C:C2	1:CA:284:G:C8	3.09	0.41
4:AD:17:VAL:HG11	4:AD:197:PRO:HG3	2.02	0.41
11:AK:85:ARG:HG2	11:AK:111:ASP:O	2.20	0.41
25:BA:2702:C:OP1	37:BR:17:ARG:NH1	2.33	0.41
57:AA:3217:NEG:O4	57:AA:3217:NEG:N4	2.51	0.41
9:CI:34:ASN:N	9:CI:34:ASN:OD1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:CC:178:LEU:HD13	3:CC:178:LEU:HA	1.91	0.41
19:CS:56:GLN:HB3	19:CS:56:GLN:HE21	1.71	0.41
18:CR:76:LEU:HA	18:CR:76:LEU:HD12	1.85	0.41
4:AD:85:LYS:HG3	4:AD:86:LYS:H	1.86	0.41
1:AA:670:G:OP2	57:AA:3219:NEG:H91	2.21	0.41
25:DA:2139:C:C4	25:DA:2153:G:C2	3.08	0.41
25:DA:2144:U:N3	25:DA:2146:C:N3	2.69	0.41
25:DA:817:C:O2'	25:DA:839:U:OP1	2.26	0.41
1:AA:1352:C:H2'	1:AA:1353:G:C8	2.56	0.41
1:CA:1031:G:H2'	1:CA:1032:G:H8	1.84	0.41
1:CA:841:U:H6	1:CA:841:U:OP1	2.02	0.41
23:CY:22:G:N7	23:CY:46:7MG:C2	2.89	0.41
25:BA:330:U:H2'	25:BA:331:G:O4'	2.20	0.41
25:DA:305:U:H2'	25:DA:306:U:C6	2.55	0.41
54:B8:7:HIS:HB3	54:B8:61:LEU:HB3	2.02	0.41
25:DA:918:A:N3	26:DB:80:U:H4'	2.36	0.41
25:BA:1055:A:P	33:BN:37:LYS:HZ1	2.35	0.41
30:DG:16:ARG:NE	30:DG:31:VAL:HG11	2.35	0.41
10:AJ:77:PRO:HB2	10:AJ:78:ASN:H	1.63	0.41
23:AY:8:4SU:OP2	23:AY:8:4SU:H6	2.21	0.41
25:BA:2846:U:C4	25:BA:2893:A:N6	2.89	0.41
1:AA:1296:C:H4'	1:AA:1302:U:C5	2.56	0.41
25:DA:699:A:H4'	25:DA:1554:A:H61	1.85	0.41
25:DA:1589:C:H2'	25:DA:1590:U:C6	2.55	0.41
5:AE:31:LEU:HA	5:AE:31:LEU:HD23	1.65	0.41
29:BF:170:LEU:HD23	29:BF:172:TRP:CZ2	2.55	0.41
25:BA:1790:A:H1'	25:BA:2723:A:C2	2.54	0.41
2:CB:93:VAL:HG21	2:CB:97:TRP:NE1	2.35	0.41
30:BG:16:ARG:HB2	30:BG:17:PRO:HD3	2.02	0.41
9:CI:121:ARG:NH1	9:CI:122:ALA:O	2.53	0.41
1:CA:707:C:H2'	1:CA:708:C:H6	1.86	0.41
45:BZ:8:TYR:HB2	45:BZ:38:TYR:CE2	2.54	0.41
30:BG:5:VAL:HG22	30:BG:8:LYS:H	1.85	0.41
44:DY:38:ILE:HD13	44:DY:66:PRO:HA	2.02	0.41
25:BA:438:G:C5	35:BP:72:PRO:HB3	2.55	0.41
1:AA:1098:C:P	2:AB:144:ARG:HH21	2.44	0.41
34:DO:8:LEU:HB2	34:DO:19:ILE:HG13	2.01	0.41
25:DA:2295:C:OP1	38:DS:10:ARG:NH1	2.54	0.41
15:AO:16:ALA:HB1	15:AO:21:ASP:HB3	2.03	0.41
1:CA:1067:A:O5'	1:CA:1067:A:H8	2.03	0.41
1:AA:1169:A:C6	1:AA:1170:A:C6	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:BR:13:HIS:CE1	37:BR:16:HIS:HB2	2.55	0.41
13:AM:96:LEU:O	13:AM:110:ARG:NH1	2.46	0.41
1:AA:637:G:H2'	1:AA:638:G:C8	2.55	0.41
23:CW:27:G:O5'	23:CW:27:G:H8	2.04	0.41
1:CA:1023:G:C4	1:CA:1024:G:C8	3.09	0.41
25:DA:2127:G:C6	25:DA:2128:C:C5	3.08	0.41
43:DX:31:HIS:CD2	43:DX:33:LYS:HB2	2.56	0.41
25:DA:2118:U:N3	25:DA:2149:G:H1'	2.36	0.41
7:CG:115:ARG:HG2	7:CG:118:VAL:HG23	2.03	0.41
24:CX:64:G:H4'	36:DQ:10:ARG:CZ	2.51	0.41
25:DA:304:G:H2'	25:DA:305:U:H6	1.86	0.41
25:BA:998:A:OP2	36:BQ:16:ARG:NE	2.40	0.41
25:BA:669:A:H4'	25:BA:670:C:H5	1.85	0.41
25:DA:954:G:O2'	25:DA:2274:A:N1	2.49	0.41
1:AA:974:A:P	14:AN:29:ARG:HH21	2.44	0.41
30:DG:31:VAL:HA	30:DG:32:PRO:HD2	1.85	0.41
25:BA:2902:G:H5''	25:BA:2903:G:O4'	2.21	0.41
25:DA:974:G:C4	25:DA:989:G:C2	3.09	0.41
35:DP:121:LYS:HB3	35:DP:123:LEU:HG	2.02	0.41
26:DB:84:C:OP1	49:D3:15:TYR:OH	2.29	0.41
10:AJ:61:GLU:OE2	14:AN:45:ARG:NE	2.46	0.41
25:DA:2265:U:C4'	36:DQ:13:GLN:HE22	2.34	0.41
25:BA:2143:G:H2'	25:BA:2144:U:C6	2.56	0.41
1:CA:179:A:H2'	1:CA:180:U:H6	1.85	0.41
44:DY:43:ASN:CG	44:DY:65:ALA:HB3	2.41	0.41
1:CA:543:C:O2'	1:CA:544:G:H5'	2.20	0.41
26:DB:28:C:H2'	26:DB:29:A:H8	1.86	0.41
48:B2:48:HIS:O	48:B2:52:ASP:HB2	2.21	0.41
25:DA:1243:G:H2'	25:DA:1244:G:O4'	2.20	0.41
1:CA:264:U:H2'	1:CA:265:G:O4'	2.20	0.41
25:DA:2468:G:O2'	25:DA:2481:G:N2	2.51	0.41
25:BA:1640:G:H2'	25:BA:1641:G:O4'	2.21	0.41
31:DH:144:VAL:O	31:DH:148:ILE:HG12	2.21	0.41
9:CI:15:ALA:HB2	9:CI:65:VAL:HG23	2.02	0.41
25:DA:1790:C:H5''	25:DA:1791:A:OP1	2.19	0.41
25:BA:635:C:H2'	25:BA:636:G:O4'	2.21	0.41
7:AG:103:TRP:CH2	7:AG:141:VAL:HG21	2.56	0.41
1:CA:665:A:N3	1:CA:732:C:H2'	2.36	0.41
26:BB:113:G:H2'	26:BB:114:C:C6	2.56	0.41
30:BG:103:LEU:HD23	30:BG:103:LEU:HA	1.78	0.41
25:BA:1690:G:H2'	25:BA:1691:C:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1084:G:C5	1:AA:1085:U:C4	3.08	0.41
1:AA:429:U:H1'	1:AA:430:A:H5''	2.02	0.41
25:BA:2128:G:N2	25:BA:2205:C:N3	2.58	0.41
25:BA:1217:G:C5	25:BA:1218:G:C8	3.09	0.41
25:DA:848:G:C2	25:DA:933:A:H1'	2.55	0.41
25:DA:2415:G:O3'	35:DP:66:GLY:HA2	2.19	0.41
1:AA:347:G:HO2'	1:AA:348:G:P	2.36	0.41
25:DA:143:G:H2'	25:DA:143(A):C:C6	2.55	0.41
1:AA:266:G:O3'	17:AQ:67:LYS:HB2	2.21	0.41
25:BA:1188:A:C4	25:BA:1190:G:C8	3.09	0.41
13:AM:4:ILE:HD12	13:AM:57:ARG:HA	2.02	0.41
5:CE:31:LEU:HA	5:CE:31:LEU:HD23	1.77	0.41
25:BA:670:C:H5'	25:BA:671:A:OP2	2.21	0.41
1:CA:1493:A:H5''	1:CA:1494:G:OP2	2.21	0.41
25:DA:954:G:C6	25:DA:955:C:C4	3.09	0.41
15:CO:55:GLY:HA2	15:CO:58:MET:CE	2.50	0.41
28:DE:12:THR:HG22	28:DE:13:ARG:N	2.35	0.41
30:DG:16:ARG:O	30:DG:20:ILE:HG13	2.20	0.41
25:BA:174:U:H2'	25:BA:175:G:C8	2.56	0.41
1:CA:193:C:H2'	1:CA:194:C:H6	1.85	0.41
30:BG:84:LYS:HZ3	30:BG:84:LYS:HG3	1.75	0.41
1:AA:1316:G:H4'	14:AN:18:VAL:HG13	2.02	0.41
40:DU:17:ILE:HG23	40:DU:39:LEU:HD12	2.02	0.41
25:BA:1036:A:OP1	25:BA:1203:G:H5''	2.20	0.41
18:AR:24:ALA:O	18:AR:26:LEU:N	2.47	0.41
25:BA:1386:U:H4'	25:BA:1387:U:OP2	2.20	0.41
25:BA:490:U:H2'	25:BA:491:G:O4'	2.20	0.41
25:DA:2516:G:O6	25:DA:2517:C:N4	2.54	0.41
25:DA:414:C:H4'	25:DA:1879:C:O2	2.20	0.41
44:BY:65:ALA:HA	44:BY:66:PRO:HD3	1.90	0.41
25:DA:2271:G:C5	25:DA:2272:U:C5	3.09	0.41
25:DA:2366:A:H2'	25:DA:2367:G:O4'	2.21	0.41
30:BG:173:LEU:HD22	30:BG:178:PHE:CE1	2.55	0.41
30:DG:121:ASN:HA	30:DG:122:PRO:HD3	1.78	0.41
1:AA:1504:G:OP1	1:AA:1507:A:H4'	2.21	0.41
13:CM:56:LEU:O	13:CM:60:VAL:HG12	2.21	0.41
1:AA:448:A:C4	1:AA:487:A:C2	3.09	0.41
45:BZ:28:MET:HE2	45:BZ:35:ARG:HB2	2.02	0.41
34:BO:63:VAL:HG12	34:BO:106:LEU:HD11	2.03	0.41
1:AA:1003:G:C2	1:AA:1004:A:N3	2.89	0.41
2:AB:13:ALA:HA	2:AB:17:PHE:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:16:HIS:C	2:AB:18:GLY:H	2.20	0.41
22:AV:14:A:C2	23:AY:34:G:C2	3.09	0.41
23:AW:18:G:O6	23:AW:55:PSU:H1'	2.21	0.41
25:DA:820:A:C2	25:DA:821:A:C4	3.08	0.41
25:DA:2415:G:O2'	35:DP:67:MET:HG3	2.21	0.41
25:BA:1454:C:H2'	25:BA:1455:C:C6	2.55	0.41
25:BA:1814:A:H5'	25:BA:2620:G:H4'	2.03	0.41
25:DA:1797:C:H4'	27:DD:257:LEU:O	2.21	0.41
1:CA:1229:A:OP2	13:CM:114:ARG:HD3	2.20	0.41
25:BA:2148:A:H4'	25:BA:2149:G:OP1	2.21	0.41
1:CA:1019:C:H2'	1:CA:1020:U:O4'	2.21	0.41
17:AQ:45:HIS:O	17:AQ:73:VAL:HG23	2.21	0.41
1:CA:892:A:H2'	1:CA:893:C:H6	1.86	0.41
3:CC:71:ALA:CA	3:CC:106:VAL:HB	2.51	0.41
30:DG:16:ARG:HE	30:DG:31:VAL:HG11	1.85	0.41
30:DG:28:VAL:O	30:DG:31:VAL:HG12	2.21	0.41
25:BA:842:C:H2'	25:BA:843:C:C6	2.56	0.41
25:DA:2553:G:H5''	25:DA:2554:U:OP2	2.20	0.41
25:BA:2052:A:H4'	25:BA:2053:A:C8	2.56	0.41
24:CX:61:C:H2'	24:CX:62:C:H6	1.86	0.41
25:DA:860:U:O2'	25:DA:861:A:H5'	2.20	0.41
25:BA:1401:G:H2'	25:BA:1402:G:O4'	2.21	0.41
3:AC:20:SER:HB3	3:AC:22:TRP:NE1	2.36	0.41
6:CF:61:LEU:HD12	6:CF:61:LEU:HA	1.88	0.41
49:D3:6:VAL:HG12	49:D3:28:LEU:HD11	2.02	0.41
1:CA:448:A:P	1:CA:485:G:H22	2.43	0.41
25:BA:2294:G:OP1	25:BA:2295:C:H1'	2.21	0.41
35:DP:27:HIS:O	35:DP:31:ALA:HA	2.21	0.41
25:DA:2545:G:N3	25:DA:2565:A:H2	2.19	0.41
25:DA:2821:A:C2	25:DA:2822:G:C4	3.09	0.41
1:AA:580:U:H2'	1:AA:581:G:O4'	2.20	0.41
1:AA:123:C:OP1	1:AA:311:C:O2'	2.29	0.41
30:BG:143:GLU:O	50:B4:28:LYS:NZ	2.38	0.41
32:DI:57:ARG:HH22	32:DI:58:LEU:HD12	1.84	0.41
39:BT:108:ARG:HA	39:BT:111:ARG:NH1	2.36	0.41
25:DA:1839:G:C8	25:DA:1927:A:H1'	2.56	0.41
3:AC:27:LYS:HA	3:AC:27:LYS:HD2	1.72	0.41
25:BA:333:G:N3	25:BA:353:G:O2'	2.44	0.41
25:DA:121:G:H4'	25:DA:149:A:H5'	2.01	0.41
28:BE:78:LEU:O	28:BE:79:ARG:HG2	2.21	0.41
1:AA:377:G:OP1	16:AP:5:ARG:HD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AY:55:PSU:C2	23:AY:57:G:H5'	2.56	0.41
1:AA:1003:G:H2'	1:AA:1004:A:C4'	2.49	0.41
2:AB:17:PHE:HA	2:AB:44:LEU:HD11	2.03	0.41
1:AA:925:G:H1'	1:AA:1502:A:C4	2.56	0.41
23:CW:14:A:H2'	23:CW:15:G:O4'	2.21	0.41
23:AW:54:5MU:H2'	23:AW:55:PSU:O4'	2.21	0.41
36:DQ:29:PHE:HB2	36:DQ:105:GLU:OE2	2.20	0.41
1:AA:540:G:H2'	1:AA:541:G:O4'	2.21	0.41
7:CG:111:ARG:HH11	7:CG:111:ARG:HB3	1.86	0.41
1:AA:348:G:C2'	1:AA:349:A:H5'	2.51	0.41
25:DA:307:G:H22	25:DA:310:A:P	2.43	0.41
1:AA:265:G:H2'	1:AA:267:C:H5	1.85	0.41
25:DA:1900:A:N1	25:DA:1970:A:C6	2.89	0.41
1:CA:1126:U:N3	10:CJ:40:LEU:HD11	2.34	0.41
1:CA:1148:U:H2'	1:CA:1149:C:O4'	2.21	0.41
25:DA:2572:A:O5'	25:DA:2574:G:H4'	2.20	0.41
35:BP:38:GLN:HG2	35:BP:45:LEU:HD23	2.02	0.41
3:AC:82:GLU:HA	3:AC:85:ARG:HE	1.86	0.41
25:BA:672:G:H8	25:BA:672:G:O5'	2.04	0.41
25:DA:300:A:N1	25:DA:333:G:O2'	2.48	0.41
1:CA:1151:A:O4'	10:CJ:39:PRO:HB2	2.21	0.41
25:DA:2167:U:H2'	25:DA:2167:U:O2	2.20	0.41
1:AA:1292:U:H2'	1:AA:1293:G:C8	2.56	0.41
1:CA:977:A:H2	1:CA:1224:G:C6	2.38	0.41
2:CB:8:LYS:HG3	2:CB:9:GLU:H	1.85	0.41
27:BD:146:GLU:HB2	27:BD:189:CYS:HB3	2.02	0.41
4:AD:188:LEU:HA	4:AD:189:PRO:HD3	1.91	0.41
25:DA:956:G:H2'	25:DA:957:A:H2'	2.03	0.41
36:DQ:17:LEU:HB3	36:DQ:39:PRO:HB2	2.02	0.41
25:BA:123:G:N2	53:B7:9:ARG:HB3	2.36	0.41
25:DA:918:A:C5	25:DA:919:G:H1'	2.55	0.41
55:D9:22:ARG:NH1	55:D9:35:ARG:HD2	2.36	0.41
1:CA:1287:A:C6	1:CA:1288:A:C6	3.09	0.41
1:AA:276:G:O3'	17:AQ:68:ARG:NH1	2.54	0.41
1:CA:735:C:H2'	1:CA:736:C:C6	2.56	0.41
1:CA:189(D):C:H2'	1:CA:189(E):U:O4'	2.21	0.41
1:CA:89:C:H2'	1:CA:90:U:O4'	2.21	0.41
25:DA:2552:U:C2	25:DA:2554:U:H5'	2.56	0.41
25:BA:2584:A:O5'	25:BA:2586:G:H4'	2.21	0.41
5:AE:45:PHE:CE2	5:AE:47:LYS:HE2	2.56	0.41
1:AA:57:G:H2'	1:AA:58:C:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:B6:21:TYR:CD1	52:B6:38:LYS:HG2	2.56	0.41
15:CO:85:LEU:HA	15:CO:85:LEU:HD23	1.94	0.41
1:AA:564:C:H5'	17:AQ:32:TYR:CE1	2.56	0.41
1:CA:174:C:H2'	1:CA:175:C:C6	2.55	0.41
1:CA:1434:A:H61	1:CA:1467:G:H1'	1.86	0.41
25:DA:27:G:C2	25:DA:512:G:N3	2.88	0.41
33:DN:104:LYS:HA	33:DN:107:LEU:HD12	2.02	0.41
26:DB:28:C:H5''	38:DS:31:SER:HB3	2.03	0.41
25:DA:534:U:H2'	25:DA:535:C:C6	2.56	0.41
1:CA:1428:A:H2'	1:CA:1429:C:O4'	2.21	0.41
25:BA:1594:C:H2'	25:BA:1595:C:H6	1.84	0.41
1:CA:1400:C:H5'	22:CV:18:G:C6	2.56	0.41
1:AA:1325:C:H4'	21:AU:17:THR:HG21	2.02	0.41
31:DH:98:LEU:HB2	31:DH:125:VAL:HG23	2.02	0.41
49:D3:18:ASP:N	49:D3:18:ASP:OD1	2.54	0.41
29:DF:33:LEU:HA	29:DF:33:LEU:HD12	1.77	0.41
7:CG:89:MET:SD	7:CG:155:ARG:HB2	2.61	0.41
25:DA:2278:A:OP1	36:DQ:11:LYS:HD2	2.21	0.41
25:BA:2271:G:C8	25:BA:2439:C:C4	3.09	0.41
1:AA:526:C:OP1	12:AL:91:LYS:HE3	2.21	0.41
13:CM:43:THR:OG1	13:CM:48:LEU:HD21	2.21	0.41
1:CA:1137:C:H5''	1:CA:1138:G:OP1	2.21	0.41
29:BF:129:PHE:CD1	29:BF:163:VAL:HG21	2.55	0.41
25:BA:782:A:N7	25:BA:808:A:H2	2.19	0.41
41:DV:5:VAL:CG1	41:DV:57:VAL:HG21	2.50	0.41
25:DA:2712:U:H2'	25:DA:2714:G:H5''	2.03	0.41
28:DE:52:LEU:HB3	28:DE:76:ARG:HD3	2.02	0.41
33:BN:121:LYS:HG2	33:BN:130:HIS:NE2	2.36	0.41
8:AH:69:ARG:HG3	8:AH:76:PRO:HA	2.03	0.41
30:BG:125:PHE:CZ	30:BG:170:ARG:HA	2.56	0.41
25:DA:1999:C:H2'	25:DA:2000:G:O4'	2.20	0.41
1:AA:1210:C:N4	1:AA:1211:U:O4	2.54	0.41
39:BT:51:ARG:HG3	39:BT:98:LYS:HD2	2.02	0.41
43:DX:84:ALA:HB3	43:DX:87:GLN:NE2	2.36	0.41
1:AA:1229:A:O3'	24:AX:30:G:H5''	2.20	0.41
25:BA:1414:G:C2	25:BA:1415:G:C8	3.09	0.41
12:AL:7:ILE:HA	12:AL:7:ILE:HD13	1.85	0.41
25:BA:1321:A:O2'	25:BA:1692:G:N3	2.53	0.41
27:BD:79:VAL:HG12	27:BD:113:VAL:HA	2.03	0.41
30:BG:41:GLN:NE2	30:BG:153:ARG:HB3	2.36	0.41
26:DB:44:G:OP1	30:DG:98:ARG:NH2	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:1880:C:H2'	25:DA:1881:C:H6	1.86	0.41
25:BA:1541:A:C6	25:BA:1542:A:C6	3.09	0.41
3:CC:143:GLU:C	3:CC:145:GLY:H	2.24	0.41
25:DA:1330:C:O2'	25:DA:1331:A:H5'	2.21	0.41
25:DA:980:A:C4	25:DA:1136:G:O4'	2.74	0.41
25:DA:1668:A:C8	25:DA:1674:G:C6	3.09	0.41
16:CP:74:LEU:O	16:CP:79:VAL:HG23	2.20	0.41
1:CA:297:G:H4'	1:CA:557:G:H4'	2.03	0.41
48:B2:32:LEU:HD13	48:B2:36:ARG:NH1	2.35	0.41
25:DA:2110:G:H1'	25:DA:2111:C:OP1	2.21	0.41
18:CR:59:SER:OG	18:CR:62:GLU:HG2	2.20	0.41
20:CT:42:GLN:O	20:CT:45:GLN:HB3	2.21	0.41
17:CQ:53:LEU:HD23	17:CQ:82:MET:HE1	2.02	0.41
15:AO:17:ARG:HH11	15:AO:17:ARG:HG3	1.84	0.41
4:CD:166:LYS:HD3	4:CD:166:LYS:HA	1.91	0.41
34:DO:10:VAL:HG21	34:DO:16:ALA:HB3	2.03	0.41
25:DA:2607:G:H2'	25:DA:2608:G:O4'	2.21	0.41
27:BD:123:ALA:HA	27:BD:124:PRO:HD3	1.93	0.41
25:BA:905:U:O2	25:BA:2280:A:H2'	2.20	0.41
45:BZ:30:ASN:OD1	45:BZ:33:LEU:HD23	2.21	0.41
1:AA:270:A:H2'	1:AA:271:C:C6	2.56	0.41
23:CY:34:G:C6	23:CY:35:A:C6	3.08	0.41
2:CB:16:HIS:HB3	2:CB:210:SER:CB	2.51	0.41
25:BA:2128:G:H2'	25:BA:2129:C:C6	2.56	0.41
25:BA:2172:U:N3	25:BA:2173:G:N7	2.69	0.41
10:AJ:5:ARG:O	10:AJ:98:ILE:HA	2.21	0.41
25:DA:1002:G:H2'	25:DA:1003:G:O4'	2.21	0.41
25:BA:2650:G:P	28:BE:82:ARG:HH22	2.44	0.41
1:CA:1206:G:C6	1:CA:1207:G:C5	3.09	0.41
37:DR:79:LEU:HD23	37:DR:83:ILE:HD12	2.03	0.41
25:BA:2148:A:N3	25:BA:2149:G:H1'	2.36	0.41
25:DA:581:C:H2'	25:DA:582:G:C8	2.56	0.41
29:DF:156:LEU:HD21	29:DF:163:VAL:HG12	2.02	0.41
23:CY:18:G:N2	23:CY:55:PSU:C4	2.89	0.41
9:AI:113:LYS:HD2	9:AI:119:ALA:O	2.21	0.41
25:DA:83:G:N1	25:DA:102:G:O2'	2.44	0.41
1:AA:262:A:C6	1:AA:263:A:C6	3.08	0.41
25:DA:2704:C:H2'	25:DA:2705:A:O4'	2.21	0.41
48:B2:30:ARG:O	48:B2:34:GLU:HG3	2.20	0.41
33:DN:39:ARG:HA	33:DN:40:PRO:HD3	1.90	0.41
1:AA:1226:C:H4'	19:AS:80:TYR:OH	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:DB:78:A:C2	26:DB:100:A:C4	3.09	0.41
1:AA:1095:U:H2'	1:AA:1096:C:O4'	2.21	0.41
27:DD:13:ARG:HD2	27:DD:16:MET:HE3	2.03	0.41
1:CA:984:C:H2'	1:CA:985:C:C6	2.56	0.41
1:AA:684:A:H1'	11:AK:39:PRO:HD2	2.02	0.41
30:BG:56:ALA:HA	30:BG:153:ARG:HH21	1.86	0.41
40:DU:113:ALA:O	40:DU:117:GLN:HG2	2.21	0.41
28:DE:50:GLY:CA	28:DE:75:VAL:HG11	2.50	0.41
1:AA:743:U:H2'	1:AA:744:C:C6	2.55	0.41
5:CE:72:GLN:O	5:CE:75:THR:HG22	2.21	0.41
25:DA:1983:C:H4'	25:DA:2606:C:H4'	2.03	0.41
25:BA:2579:G:H2'	25:BA:2580:C:C6	2.56	0.41
1:CA:1272:G:H2'	1:CA:1273:G:O4'	2.21	0.41
27:BD:13:ARG:HD2	27:BD:13:ARG:HA	1.76	0.41
27:BD:10:THR:OG1	27:BD:13:ARG:HG2	2.21	0.41
25:DA:2651:C:C2'	25:DA:2652:C:H5'	2.51	0.41
1:CA:717:C:O2'	1:CA:734:G:O4'	2.28	0.41
33:DN:72:TYR:N	33:DN:85:ILE:O	2.52	0.41
25:DA:634:C:H2'	25:DA:635:C:C6	2.56	0.41
25:DA:187:G:N3	25:DA:1365:A:H2	2.19	0.41
25:DA:1344:G:C6	25:DA:1385:G:N7	2.89	0.41
2:CB:175:ARG:HB3	2:CB:175:ARG:NH1	2.36	0.41
30:DG:58:GLN:OE1	30:DG:58:GLN:HA	2.21	0.41
1:CA:442:C:H42	1:CA:492:G:H1	1.68	0.41
1:CA:401:C:H1'	1:CA:622:A:H1'	2.04	0.41
5:AE:76:ILE:O	5:AE:93:PRO:HB3	2.21	0.41
25:BA:2360:U:O4	25:BA:2394:G:N1	2.54	0.41
25:DA:374:A:C2	25:DA:401:A:C4	3.09	0.41
25:BA:2204:G:C2	25:BA:2205:C:C2	3.09	0.40
1:AA:1399:C:H4'	1:AA:1400:C:O5'	2.21	0.40
25:DA:1148:A:O2'	25:DA:1149:G:H5'	2.21	0.40
25:DA:805:G:C4'	35:DP:38:GLN:HB2	2.51	0.40
23:CY:52:G:C2	23:CY:53:G:H1'	2.55	0.40
1:AA:1053:G:H3'	57:AA:3216:NEG:H72	2.02	0.40
1:CA:1176:A:H2'	1:CA:1177:G:C8	2.56	0.40
54:B8:6:THR:HG22	54:B8:62:LEU:HA	2.03	0.40
1:CA:1055:A:OP2	1:CA:1055:A:H8	2.04	0.40
1:AA:649:G:H2'	1:AA:650:G:C8	2.55	0.40
37:BR:2:ARG:NH1	37:BR:5:LYS:O	2.54	0.40
23:AW:75:C:H2'	23:AW:76:A:N9	2.36	0.40
1:AA:295:C:H2'	1:AA:296:U:O4'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1144:G:H21	1:CA:1146:A:H62	1.69	0.40
4:AD:173:TRP:HE1	4:AD:193:ASP:HB3	1.86	0.40
1:CA:1065:U:H1'	1:CA:1066:C:OP2	2.21	0.40
1:AA:1446:U:O2'	1:AA:1447:A:O5'	2.40	0.40
25:DA:874:G:H2'	25:DA:875:G:O4'	2.21	0.40
45:DZ:29:TYR:O	45:DZ:89:PHE:HD1	2.04	0.40
3:AC:148:GLY:HA3	3:AC:172:ARG:O	2.20	0.40
48:D2:1:MET:SD	48:D2:56:GLN:NE2	2.94	0.40
25:BA:2324:U:O2'	30:BG:40:ASN:ND2	2.49	0.40
23:AW:9:A:H1'	23:AW:45:U:O2'	2.20	0.40
5:CE:41:VAL:O	5:CE:67:VAL:HG12	2.20	0.40
36:BQ:42:ILE:HG22	36:BQ:47:ILE:HG13	2.02	0.40
1:CA:1216:G:H5''	14:CN:5:ALA:HB2	2.03	0.40
25:BA:2368:C:H2'	25:BA:2369:U:O4'	2.21	0.40
41:BV:21:ARG:HG2	41:BV:91:TYR:CD1	2.56	0.40
25:BA:831:A:C6	27:BD:229:VAL:HG11	2.56	0.40
16:CP:8:ARG:HG3	16:CP:17:TYR:CE1	2.56	0.40
28:DE:181:LEU:HD12	28:DE:181:LEU:HA	1.84	0.40
25:BA:1541:A:H2'	25:BA:1542:A:C8	2.55	0.40
45:DZ:10:ARG:HG3	45:DZ:36:LYS:HB3	2.03	0.40
25:DA:1472:A:N6	25:DA:1519:G:H1'	2.36	0.40
1:AA:791:G:N2	1:AA:1497:G:O3'	2.54	0.40
1:CA:583:A:H2'	1:CA:584:G:O4'	2.21	0.40
25:BA:1572:G:C6	25:BA:1573:G:C2	3.09	0.40
53:D7:5:TRP:CD1	53:D7:7:PRO:HD3	2.56	0.40
1:AA:1327:C:O2'	1:AA:1328:C:H5'	2.21	0.40
1:AA:22:G:H4'	1:AA:885:G:C8	2.57	0.40
1:AA:1059:C:OP2	3:AC:199:LYS:NZ	2.42	0.40
33:BN:36:GLY:HA2	33:BN:38:HIS:CE1	2.56	0.40
2:CB:112:VAL:O	2:CB:116:GLU:N	2.34	0.40
25:BA:1727:U:O2	25:BA:1794:G:H3'	2.20	0.40
10:AJ:12:ASP:OD2	10:AJ:15:THR:HG23	2.21	0.40
30:BG:31:VAL:HA	30:BG:32:PRO:HD2	1.75	0.40
3:AC:152:ILE:HG23	3:AC:167:TRP:HB3	2.03	0.40
50:D4:28:LYS:HA	50:D4:29:PRO:HD3	1.89	0.40
4:AD:148:VAL:HG12	4:AD:149:ALA:O	2.21	0.40
1:CA:1004:A:N6	1:CA:1037:C:C2	2.89	0.40
1:AA:1003:G:C2	1:AA:1004:A:H1'	2.55	0.40
1:CA:976:G:C8	1:CA:1358:U:C2	3.08	0.40
1:CA:975:A:H5'	1:CA:975:A:H8	1.87	0.40
7:CG:114:ARG:H	7:CG:114:ARG:HG2	1.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:DF:20:LEU:HA	29:DF:20:LEU:HD23	1.76	0.40
12:AL:24:VAL:HG13	12:AL:98:TYR:CE1	2.56	0.40
10:CJ:6:ILE:HB	10:CJ:72:VAL:CG2	2.51	0.40
25:DA:2335:A:C8	25:DA:2337:G:C5	3.08	0.40
25:DA:2040:C:H2'	25:DA:2041:U:O4'	2.21	0.40
23:CY:30:G:H2'	23:CY:31:A:H8	1.86	0.40
25:DA:235:U:H2'	25:DA:236:C:C6	2.57	0.40
20:AT:47:GLY:HA2	20:AT:48:LYS:C	2.41	0.40
1:CA:353:A:C8	1:CA:353:A:H5'	2.52	0.40
19:CS:28:LYS:HB2	19:CS:29:ARG:CB	2.51	0.40
4:AD:103:ASN:O	4:AD:107:ARG:HG2	2.21	0.40
45:DZ:53:ILE:HG13	45:DZ:53:ILE:H	1.64	0.40
50:B4:62:ARG:C	50:B4:64:GLY:HA2	2.42	0.40
1:CA:946:A:C6	1:CA:947:G:C6	3.08	0.40
36:BQ:134:ARG:HA	36:BQ:138:ASP:OD2	2.21	0.40
25:DA:886:C:H3'	25:DA:887:A:H5''	2.02	0.40
51:B5:59:GLU:HG2	51:B5:60:VAL:N	2.36	0.40
1:AA:1324:A:O4'	1:AA:1362:C:H4'	2.22	0.40
40:DU:83:LEU:HB3	40:DU:88:ILE:HB	2.02	0.40
36:DQ:41:TRP:HB3	36:DQ:94:VAL:HG21	2.02	0.40
13:AM:80:ARG:NH2	19:AS:69:HIS:CE1	2.89	0.40
25:BA:2402:U:O2'	25:BA:2403:G:H5'	2.21	0.40
9:CI:128:ARG:NH2	24:CX:33:U:OP2	2.54	0.40
25:DA:1581:G:H2'	25:DA:1582:C:O4'	2.20	0.40
28:DE:9:VAL:HB	39:DT:3:ARG:HG2	2.04	0.40
25:BA:863:C:H2'	25:BA:864:C:C6	2.55	0.40
26:DB:94:C:H2'	26:DB:95:C:H6	1.85	0.40
25:BA:831:A:C5	27:BD:229:VAL:HG21	2.55	0.40
25:BA:2152:U:H2'	25:BA:2153:G:N2	2.35	0.40
25:DA:2820:A:C6	37:DR:4:LEU:HD11	2.57	0.40
25:BA:1684:A:H5'	25:BA:1791:A:O2'	2.21	0.40
25:BA:2564:U:C2	25:BA:2566:U:H5'	2.57	0.40
11:AK:65:ALA:HB3	11:AK:97:ALA:HB3	2.04	0.40
39:DT:127:ALA:C	39:DT:129:ARG:N	2.74	0.40
25:BA:493:G:OP1	53:B7:33:ARG:NH1	2.55	0.40
42:BW:86:LEU:HD22	42:BW:96:ILE:HD11	2.02	0.40
1:AA:1289:A:H2'	1:AA:1290:G:H5'	2.03	0.40
35:BP:70:GLN:O	35:BP:73:GLY:N	2.49	0.40
1:AA:303:A:H2'	1:AA:304:U:O4'	2.21	0.40
25:DA:49:A:H5''	25:DA:51:G:O4'	2.21	0.40
30:BG:137:GLU:HB2	30:BG:140:ILE:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:D6:8:LYS:HD3	54:D8:34:TRP:CD2	2.56	0.40
30:DG:124:SER:HB2	30:DG:131:TYR:CE1	2.57	0.40
21:CU:6:ARG:HG2	21:CU:15:ARG:HD2	2.03	0.40
25:BA:228:U:H2'	25:BA:229:G:O4'	2.21	0.40
25:BA:2186:C:H5	25:BA:2187:G:C4	2.39	0.40
20:AT:45:GLN:HB2	20:AT:91:LEU:HD13	2.03	0.40
44:BY:15:VAL:HG21	44:BY:42:VAL:HG11	2.02	0.40
37:BR:26:LYS:HE2	37:BR:70:LEU:O	2.21	0.40
23:AW:4:C:H2'	23:AW:5:G:H8	1.85	0.40
1:CA:1038:C:O2'	1:CA:1039:C:H5'	2.21	0.40
25:BA:2132:G:H5''	25:BA:2167:C:N4	2.36	0.40
2:AB:54:THR:HG23	2:AB:199:TYR:HB3	2.02	0.40
23:CW:66:U:C4	23:CW:67:C:C2	3.09	0.40
1:CA:1091:U:C2	1:CA:1093:A:OP2	2.75	0.40
1:AA:427:U:H1'	1:AA:541:G:OP1	2.21	0.40
25:DA:2615:U:N1	51:D5:7:PRO:HA	2.36	0.40
1:CA:1330:U:H4'	13:CM:23:TYR:CE1	2.56	0.40
29:DF:18:ARG:HG2	29:DF:19:GLU:H	1.86	0.40
1:CA:674:G:H2'	1:CA:675:A:C8	2.52	0.40
2:CB:180:LEU:HD23	2:CB:180:LEU:HA	1.89	0.40
1:AA:109:A:C8	1:AA:326:G:H2'	2.57	0.40
25:DA:1028:A:N6	25:DA:1125:G:H2'	2.37	0.40
23:CW:52:G:C6	23:CW:63:G:C6	3.10	0.40
9:CI:28:VAL:HA	9:CI:63:ILE:O	2.21	0.40
32:BI:102:SER:O	32:BI:106:GLY:HA3	2.21	0.40
45:BZ:121:HIS:HB2	45:BZ:171:ILE:HG22	2.04	0.40
25:DA:990:A:H1'	25:DA:1156:A:N3	2.36	0.40
25:BA:1314:A:C2	25:BA:2035:A:C4	3.10	0.40
2:AB:170:GLU:O	2:AB:174:VAL:HG23	2.22	0.40
16:CP:40:ASP:HB3	16:CP:48:TRP:CB	2.51	0.40
25:DA:861:A:H2'	25:DA:862:G:O4'	2.22	0.40
25:DA:1418:G:H2'	25:DA:1579:A:H62	1.85	0.40
13:AM:19:LEU:HA	13:AM:19:LEU:HD13	1.74	0.40
25:DA:2784:C:H2'	25:DA:2785:C:C6	2.57	0.40
44:BY:54:LYS:HA	44:BY:55:TYR:HA	1.79	0.40
8:CH:39:LEU:HA	8:CH:39:LEU:HD13	1.87	0.40
1:AA:1367:C:H2'	1:AA:1368:G:O4'	2.21	0.40
1:CA:1072:G:H2'	1:CA:1073:U:C6	2.56	0.40
29:BF:14:PRO:HD2	29:BF:127:GLU:OE2	2.21	0.40
1:AA:179:A:H2'	1:AA:180:U:H6	1.87	0.40
25:BA:772:G:C6	25:BA:773:G:N1	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:580:U:H2'	1:CA:581:G:O4'	2.20	0.40
25:DA:2715:C:H2'	25:DA:2716:U:C6	2.57	0.40
1:CA:971:G:P	1:CA:1231:G:H21	2.43	0.40
53:B7:33:ARG:HD2	53:B7:33:ARG:HH11	1.75	0.40
25:DA:667:U:O2	54:D8:2:PRO:HD2	2.20	0.40
1:CA:552:U:O3'	12:CL:87:GLY:HA3	2.21	0.40
27:BD:142:VAL:HG13	27:BD:191:ALA:HB1	2.03	0.40
34:DO:22:ILE:HG12	34:DO:40:VAL:O	2.22	0.40
34:DO:15:GLY:O	34:DO:47:ILE:HG12	2.22	0.40
2:AB:60:ASP:O	2:AB:64:ARG:HB2	2.22	0.40
25:BA:1570:G:H2'	25:BA:1571:G:O4'	2.21	0.40
20:AT:67:ALA:C	20:AT:69:GLY:H	2.25	0.40
45:BZ:87:ASP:OD2	61:BZ:3101:HOH:O	2.22	0.40
31:DH:43:VAL:HG13	31:DH:52:VAL:HG22	2.03	0.40
29:DF:124:LEU:HB3	29:DF:193:VAL:HG22	2.03	0.40
1:AA:1137:C:H5''	1:AA:1138:G:OP1	2.21	0.40
2:AB:122:PHE:HE1	2:AB:139:LYS:N	2.20	0.40
25:DA:242:G:C8	54:D8:5:LYS:HG2	2.56	0.40
8:CH:82:HIS:NE2	8:CH:136:GLU:OE2	2.53	0.40
5:AE:113:ALA:HB3	5:AE:115:VAL:HG23	2.03	0.40
25:BA:152:G:H2'	25:BA:153:C:C6	2.56	0.40
44:BY:49:VAL:HG21	44:BY:61:ILE:HG23	2.02	0.40
25:DA:2432:A:C6	25:DA:2433:A:C6	3.09	0.40
42:BW:71:VAL:HA	42:BW:107:LEU:HD12	2.03	0.40
23:AY:49:C:N4	23:AY:65:G:N1	2.38	0.40
25:DA:1803:A:H4'	27:DD:259:THR:HG23	2.02	0.40
1:CA:954:G:H21	1:CA:1227:A:H62	1.68	0.40
23:AW:55:PSU:O3'	25:BA:943:C:H4'	2.21	0.40
29:DF:184:TYR:O	29:DF:188:ARG:HG3	2.21	0.40
1:CA:521:G:O2'	1:CA:522:C:H5'	2.21	0.40
2:CB:77:ALA:CB	2:CB:165:VAL:HG11	2.51	0.40
40:BU:76:TYR:CZ	40:BU:80:ILE:HG13	2.56	0.40
1:AA:1118:C:H2'	1:AA:1119:C:C6	2.56	0.40
19:AS:27:GLU:HG2	19:AS:47:HIS:CE1	2.56	0.40
25:DA:581:C:OP2	40:DU:33:ARG:HD3	2.20	0.40
45:DZ:145:GLU:HB3	45:DZ:148:ASP:CG	2.41	0.40
25:DA:64:A:H2'	25:DA:65:C:O4'	2.20	0.40
25:DA:2617:C:C2'	25:DA:2618:G:H5'	2.51	0.40
54:B8:38:GLY:O	54:B8:42:ARG:HB2	2.21	0.40
1:CA:555:C:H2'	1:CA:556:C:C6	2.56	0.40
25:DA:221:A:N1	25:DA:265:A:O2'	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2573:A:H2'	25:BA:2574:U:O4'	2.21	0.40
48:D2:1:MET:HG2	48:D2:5:GLU:OE1	2.21	0.40
25:BA:1780:A:H2'	25:BA:1781:G:O4'	2.21	0.40
30:BG:126:ASP:HB2	30:BG:130:ASN:O	2.21	0.40
44:DY:13:VAL:HB	44:DY:72:VAL:HG13	2.02	0.40
25:DA:2784:C:H2'	25:DA:2785:C:H6	1.86	0.40
25:BA:2012:C:H2'	25:BA:2013:U:O4'	2.21	0.40
25:DA:25:U:C4	25:DA:26:G:C6	3.09	0.40
1:CA:836:G:C6	1:CA:851:G:C5	3.10	0.40
16:CP:57:ARG:HH21	16:CP:79:VAL:HA	1.87	0.40
8:CH:82:HIS:HE2	8:CH:136:GLU:HG3	1.85	0.40
1:CA:1338:G:C6	1:CA:1339:A:C6	3.10	0.40
29:BF:111:ALA:HB2	29:BF:206:ILE:HG21	2.04	0.40
28:BE:3:GLY:HA3	28:BE:81:ILE:HD12	2.03	0.40
1:CA:919:A:O2'	1:CA:1080:A:N1	2.38	0.40
29:BF:34:TRP:CH2	35:BP:8:PRO:HB3	2.56	0.40
25:DA:609:A:C8	25:DA:610:G:C8	3.09	0.40
25:BA:470:C:H4'	29:BF:49:ALA:HB2	2.03	0.40
25:BA:1752:G:C6	25:BA:1753:U:C4	3.10	0.40
20:AT:63:ILE:HG22	20:AT:77:ALA:HB1	2.03	0.40
29:DF:140:LEU:HD21	29:DF:170:LEU:HD11	2.03	0.40
32:DI:62:LYS:HA	32:DI:65:ALA:HB3	2.03	0.40
40:BU:16:LYS:HE2	40:BU:16:LYS:HB3	1.95	0.40
2:AB:108:ILE:HA	2:AB:108:ILE:HD13	1.92	0.40
1:AA:257:G:H2'	1:AA:258:G:O4'	2.21	0.40
25:DA:579:G:H2'	25:DA:580:C:C6	2.56	0.40
25:BA:1516:A:H2'	25:BA:1517:G:O4'	2.20	0.40
48:B2:9:GLN:HE22	48:B2:56:GLN:HB3	1.85	0.40
31:BH:20:ALA:HB1	31:BH:21:PRO:HD2	2.03	0.40
24:AX:76:A:H1'	61:AX:3101:HOH:O	2.21	0.40
7:AG:65:ALA:HB1	7:AG:127:ALA:HB3	2.03	0.40
1:AA:187:C:O2'	20:AT:89:ARG:NH2	2.53	0.40
25:DA:2318:G:H21	38:DS:3:ARG:NH1	2.00	0.40
25:DA:999:U:H5''	25:DA:1154:G:O6	2.22	0.40
1:CA:1118:C:OP1	9:CI:9:ARG:HD2	2.20	0.40
7:AG:111:ARG:NH2	7:AG:126:ASP:OD2	2.55	0.40
25:DA:864:G:OP2	36:DQ:22:LYS:HE3	2.21	0.40
33:BN:61:ARG:HG3	33:BN:62:VAL:H	1.87	0.40
25:BA:2331:G:N2	38:BS:3:ARG:HA	2.37	0.40
45:DZ:55:HIS:HE1	45:DZ:135:GLU:HG3	1.80	0.40
25:DA:797:C:H2'	25:DA:798:G:O4'	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:2078:C:C4	25:DA:2079:U:C4	3.10	0.40
25:DA:1665:A:H2'	25:DA:1666:G:O4'	2.21	0.40
39:BT:53:ARG:O	39:BT:59:THR:HA	2.22	0.40
19:CS:38:SER:HB2	19:CS:71:LEU:HD22	2.02	0.40
25:BA:117:A:H4'	25:BA:118:U:OP1	2.21	0.40
44:BY:7:VAL:HG21	44:BY:72:VAL:HG12	2.04	0.40
25:DA:2283:C:C2	25:DA:2389:G:C2	3.09	0.40
1:AA:864:A:H2'	1:AA:865:A:C8	2.57	0.40
25:BA:1383:G:H2'	25:BA:1384:G:O4'	2.20	0.40
6:AF:8:ILE:HG22	6:AF:10:LEU:HD22	2.03	0.40
1:AA:299:G:C6	1:AA:300:A:C6	3.10	0.40
25:DA:172:C:H2'	25:DA:173:G:H8	1.86	0.40
47:D1:54:ALA:HB1	47:D1:83:GLU:HG3	2.03	0.40
10:AJ:85:LEU:HD23	10:AJ:85:LEU:HA	1.97	0.40
1:CA:584:G:H5'	17:CQ:91:ARG:HH22	1.86	0.40
4:CD:70:ILE:HG23	4:CD:75:PHE:HB2	2.04	0.40
42:DW:43:GLY:O	42:DW:47:VAL:HG23	2.22	0.40
25:DA:1410:G:H2'	25:DA:1411:C:C6	2.56	0.40
29:DF:195:ASP:OD1	29:DF:196:LEU:N	2.54	0.40
45:BZ:9:TYR:OH	45:BZ:61:LEU:HD23	2.21	0.40
25:BA:1925:G:OP1	27:BD:241:PRO:HB2	2.22	0.40
27:DD:24:ILE:HD13	27:DD:84:TYR:HB2	2.03	0.40
21:CU:5:ASP:O	21:CU:11:GLY:HA3	2.21	0.40
13:AM:81:LEU:O	13:AM:89:GLY:HA3	2.22	0.40
2:AB:82:ARG:HG3	2:AB:92:TYR:CZ	2.57	0.40
25:BA:510:C:H2'	25:BA:511:C:C6	2.57	0.40
1:CA:429:U:H3'	4:CD:9:CYS:SG	2.61	0.40
7:AG:100:ALA:O	7:AG:104:LEU:HB2	2.22	0.40
51:B5:41:PRO:HA	51:B5:42:PRO:HD2	1.82	0.40
1:CA:1238:A:C2	1:CA:1303:C:H4'	2.57	0.40
1:CA:236:G:C6	1:CA:237:C:C4	3.09	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%)	196 (86%)	24 (10%)	9 (4%)	4	8
2	CB	229/256 (90%)	195 (85%)	24 (10%)	10 (4%)	3	6
3	AC	204/239 (85%)	182 (89%)	18 (9%)	4 (2%)	9	24
3	CC	204/239 (85%)	182 (89%)	19 (9%)	3 (2%)	13	32
4	AD	206/209 (99%)	193 (94%)	12 (6%)	1 (0%)	34	63
4	CD	206/209 (99%)	196 (95%)	8 (4%)	2 (1%)	19	45
5	AE	146/162 (90%)	135 (92%)	10 (7%)	1 (1%)	26	55
5	CE	146/162 (90%)	135 (92%)	10 (7%)	1 (1%)	26	55
6	AF	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
6	CF	98/101 (97%)	95 (97%)	2 (2%)	1 (1%)	19	45
7	AG	153/156 (98%)	141 (92%)	9 (6%)	3 (2%)	9	24
7	CG	153/156 (98%)	143 (94%)	7 (5%)	3 (2%)	9	24
8	AH	135/138 (98%)	130 (96%)	4 (3%)	1 (1%)	26	55
8	CH	135/138 (98%)	129 (96%)	5 (4%)	1 (1%)	26	55
9	AI	125/128 (98%)	113 (90%)	10 (8%)	2 (2%)	12	30
9	CI	125/128 (98%)	112 (90%)	10 (8%)	3 (2%)	7	19
10	AJ	95/105 (90%)	82 (86%)	7 (7%)	6 (6%)	2	2
10	CJ	94/105 (90%)	81 (86%)	7 (7%)	6 (6%)	2	2
11	AK	112/129 (87%)	106 (95%)	4 (4%)	2 (2%)	11	27
11	CK	112/129 (87%)	106 (95%)	4 (4%)	2 (2%)	11	27
12	AL	120/132 (91%)	117 (98%)	3 (2%)	0	100	100
12	CL	120/132 (91%)	116 (97%)	4 (3%)	0	100	100
13	AM	121/126 (96%)	109 (90%)	11 (9%)	1 (1%)	24	51
13	CM	120/126 (95%)	107 (89%)	11 (9%)	2 (2%)	11	29
14	AN	58/61 (95%)	57 (98%)	1 (2%)	0	100	100
14	CN	58/61 (95%)	57 (98%)	1 (2%)	0	100	100
15	AO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
15	CO	86/89 (97%)	82 (95%)	3 (4%)	1 (1%)	16	39
16	AP	80/88 (91%)	76 (95%)	3 (4%)	1 (1%)	15	37
16	CP	80/88 (91%)	76 (95%)	3 (4%)	1 (1%)	15	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	AQ	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
17	CQ	97/105 (92%)	93 (96%)	3 (3%)	1 (1%)	19	45
18	AR	66/88 (75%)	65 (98%)	0	1 (2%)	13	32
18	CR	66/88 (75%)	65 (98%)	0	1 (2%)	13	32
19	AS	81/93 (87%)	71 (88%)	8 (10%)	2 (2%)	7	18
19	CS	81/93 (87%)	69 (85%)	10 (12%)	2 (2%)	7	18
20	AT	94/106 (89%)	86 (92%)	2 (2%)	6 (6%)	2	2
20	CT	94/106 (89%)	87 (93%)	1 (1%)	6 (6%)	2	2
21	AU	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
21	CU	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
27	BD	273/276 (99%)	257 (94%)	15 (6%)	1 (0%)	39	69
27	DD	273/276 (99%)	255 (93%)	16 (6%)	2 (1%)	26	55
28	BE	202/206 (98%)	196 (97%)	5 (2%)	1 (0%)	34	63
28	DE	202/206 (98%)	195 (96%)	5 (2%)	2 (1%)	19	45
29	BF	201/210 (96%)	199 (99%)	1 (0%)	1 (0%)	34	63
29	DF	201/210 (96%)	197 (98%)	2 (1%)	2 (1%)	19	45
30	BG	179/182 (98%)	167 (93%)	10 (6%)	2 (1%)	17	42
30	DG	179/182 (98%)	166 (93%)	10 (6%)	3 (2%)	11	29
31	BH	172/180 (96%)	163 (95%)	8 (5%)	1 (1%)	30	59
31	DH	172/180 (96%)	162 (94%)	9 (5%)	1 (1%)	30	59
32	BI	144/148 (97%)	128 (89%)	12 (8%)	4 (3%)	6	15
32	DI	144/148 (97%)	130 (90%)	12 (8%)	2 (1%)	14	35
33	BN	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
33	DN	138/140 (99%)	133 (96%)	4 (3%)	1 (1%)	26	55
34	BO	120/122 (98%)	114 (95%)	5 (4%)	1 (1%)	24	51
34	DO	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
35	BP	147/150 (98%)	140 (95%)	6 (4%)	1 (1%)	26	55
35	DP	147/150 (98%)	137 (93%)	7 (5%)	3 (2%)	9	24
36	BQ	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
36	DQ	139/141 (99%)	133 (96%)	5 (4%)	1 (1%)	26	55
37	BR	116/118 (98%)	110 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	DR	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
38	BS	108/112 (96%)	102 (94%)	5 (5%)	1 (1%)	21	49
38	DS	108/112 (96%)	102 (94%)	5 (5%)	1 (1%)	21	49
39	BT	129/146 (88%)	121 (94%)	7 (5%)	1 (1%)	24	51
39	DT	129/146 (88%)	124 (96%)	4 (3%)	1 (1%)	24	51
40	BU	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
40	DU	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
41	BV	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	19	45
41	DV	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	19	45
42	BW	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
42	DW	110/113 (97%)	110 (100%)	0	0	100	100
43	BX	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
43	DX	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
44	BY	105/110 (96%)	98 (93%)	6 (6%)	1 (1%)	19	45
44	DY	105/110 (96%)	100 (95%)	5 (5%)	0	100	100
45	BZ	169/206 (82%)	145 (86%)	21 (12%)	3 (2%)	11	27
45	DZ	172/206 (84%)	153 (89%)	18 (10%)	1 (1%)	30	59
46	B0	81/85 (95%)	79 (98%)	2 (2%)	0	100	100
46	D0	81/85 (95%)	77 (95%)	3 (4%)	1 (1%)	16	39
47	B1	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
47	D1	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
48	B2	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
48	D2	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
49	B3	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
49	D3	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
50	B4	67/71 (94%)	50 (75%)	12 (18%)	5 (8%)	1	1
50	D4	67/71 (94%)	51 (76%)	8 (12%)	8 (12%)	0	0
51	B5	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
51	D5	57/60 (95%)	57 (100%)	0	0	100	100
52	B6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
52	D6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	B7	46/49 (94%)	46 (100%)	0	0	100	100
53	D7	46/49 (94%)	45 (98%)	0	1 (2%)	8	22
54	B8	62/65 (95%)	62 (100%)	0	0	100	100
54	D8	62/65 (95%)	62 (100%)	0	0	100	100
55	B9	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
55	D9	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
All	All	11409/12128 (94%)	10706 (94%)	562 (5%)	141 (1%)	16	39

All (141) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	16	HIS
2	AB	17	PHE
2	AB	231	GLU
7	AG	80	VAL
9	AI	44	VAL
9	AI	54	ASP
10	AJ	31	GLY
10	AJ	56	HIS
10	AJ	77	PRO
10	AJ	79	ARG
20	AT	10	LEU
27	BD	275	LYS
29	BF	130	ALA
30	BG	43	LEU
31	BH	126	PRO
32	BI	107	VAL
45	BZ	152	ALA
50	B4	45	GLY
50	B4	55	ARG
50	B4	57	GLU
50	B4	62	ARG
2	CB	10	LEU
2	CB	16	HIS
2	CB	17	PHE
2	CB	231	GLU
4	CD	46	LYS
7	CG	80	VAL
9	CI	54	ASP
10	CJ	55	LYS

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Mol	Chain	Res	Type
10	CJ	56	HIS
10	CJ	79	ARG
20	CT	95	ALA
20	CT	99	LEU
28	DE	73	GLU
29	DF	21	ALA
29	DF	130	ALA
30	DG	43	LEU
30	DG	47	LYS
31	DH	126	PRO
32	DI	10	GLU
36	DQ	28	ALA
50	D4	45	GLY
50	D4	62	ARG
50	D4	63	TYR
50	D4	68	ARG
53	D7	46	VAL
2	AB	126	GLU
3	AC	107	GLN
7	AG	55	GLY
7	AG	81	GLY
10	AJ	55	LYS
11	AK	49	GLY
13	AM	12	ASN
18	AR	25	THR
19	AS	42	PRO
20	AT	47	GLY
20	AT	96	GLY
32	BI	85	GLU
32	BI	106	GLY
39	BT	127	ALA
41	BV	79	VAL
45	BZ	163	LEU
2	CB	8	LYS
2	CB	20	GLU
2	CB	126	GLU
7	CG	7	ALA
7	CG	55	GLY
9	CI	44	VAL
10	CJ	75	ILE
10	CJ	78	ASN
11	CK	49	GLY

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Mol	Chain	Res	Type
19	CS	25	LYS
20	CT	10	LEU
20	CT	47	GLY
20	CT	100	ILE
27	DD	3	VAL
27	DD	239	ARG
35	DP	39	LYS
39	DT	127	ALA
41	DV	79	VAL
5	AE	85	GLY
19	AS	25	LYS
20	AT	95	ALA
20	AT	102	GLY
8	CH	133	LEU
9	CI	11	LYS
13	CM	59	TYR
19	CS	42	PRO
32	DI	85	GLU
50	D4	49	PHE
2	AB	213	LEU
3	AC	26	LYS
8	AH	133	LEU
28	BE	52	LEU
32	BI	73	GLU
50	B4	49	PHE
3	CC	26	LYS
4	CD	47	ARG
13	CM	12	ASN
15	CO	88	ARG
18	CR	25	THR
28	DE	52	LEU
33	DN	2	LYS
38	DS	84	GLN
46	D0	4	LYS
50	D4	55	ARG
2	AB	9	GLU
2	AB	10	LEU
3	AC	65	ALA
3	AC	66	VAL
4	AD	166	LYS
20	AT	100	ILE
30	BG	51	ARG

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Mol	Chain	Res	Type
34	BO	5	GLN
44	BY	54	LYS
3	CC	144	SER
3	CC	181	ASN
11	CK	105	VAL
50	D4	46	GLN
50	D4	65	ASP
10	AJ	37	PRO
35	BP	122	PRO
45	BZ	157	LEU
2	CB	21	ARG
2	CB	127	ILE
10	CJ	37	PRO
30	DG	117	PHE
35	DP	45	LEU
45	DZ	157	LEU
16	AP	53	VAL
2	CB	125	PRO
17	CQ	33	GLY
6	CF	40	VAL
20	CT	102	GLY
35	DP	122	PRO
11	AK	105	VAL
16	CP	53	VAL
38	BS	60	GLY
5	CE	69	VAL
2	AB	124	SER
2	AB	125	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	AB	192/220 (87%)	162 (84%)	30 (16%)	<b>3</b> <b>8</b>
2	CB	187/220 (85%)	163 (87%)	24 (13%)	<b>5</b> <b>12</b>
3	AC	143/188 (76%)	132 (92%)	11 (8%)	<b>16</b> <b>36</b>

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	CC	140/188 (74%)	130 (93%)	10 (7%)	18	41
4	AD	170/181 (94%)	161 (95%)	9 (5%)	28	57
4	CD	173/181 (96%)	159 (92%)	14 (8%)	15	33
5	AE	113/123 (92%)	106 (94%)	7 (6%)	23	49
5	CE	114/123 (93%)	103 (90%)	11 (10%)	10	24
6	AF	83/90 (92%)	79 (95%)	4 (5%)	31	62
6	CF	85/90 (94%)	77 (91%)	8 (9%)	11	25
7	AG	119/127 (94%)	112 (94%)	7 (6%)	24	51
7	CG	120/127 (94%)	114 (95%)	6 (5%)	30	60
8	AH	114/119 (96%)	108 (95%)	6 (5%)	28	57
8	CH	114/119 (96%)	109 (96%)	5 (4%)	35	65
9	AI	90/99 (91%)	80 (89%)	10 (11%)	8	17
9	CI	89/99 (90%)	77 (86%)	12 (14%)	5	11
10	AJ	66/92 (72%)	62 (94%)	4 (6%)	23	49
10	CJ	69/92 (75%)	67 (97%)	2 (3%)	50	80
11	AK	82/99 (83%)	74 (90%)	8 (10%)	10	23
11	CK	83/99 (84%)	73 (88%)	10 (12%)	6	14
12	AL	97/109 (89%)	94 (97%)	3 (3%)	47	78
12	CL	97/109 (89%)	94 (97%)	3 (3%)	47	78
13	AM	93/101 (92%)	83 (89%)	10 (11%)	8	18
13	CM	92/101 (91%)	84 (91%)	8 (9%)	13	29
14	AN	49/50 (98%)	42 (86%)	7 (14%)	4	10
14	CN	49/50 (98%)	43 (88%)	6 (12%)	6	14
15	AO	78/80 (98%)	69 (88%)	9 (12%)	7	16
15	CO	78/80 (98%)	74 (95%)	4 (5%)	29	59
16	AP	69/74 (93%)	63 (91%)	6 (9%)	13	29
16	CP	68/74 (92%)	63 (93%)	5 (7%)	17	39
17	AQ	94/97 (97%)	91 (97%)	3 (3%)	46	77
17	CQ	94/97 (97%)	92 (98%)	2 (2%)	61	87
18	AR	59/77 (77%)	54 (92%)	5 (8%)	13	30
18	CR	59/77 (77%)	56 (95%)	3 (5%)	29	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	AS	69/80 (86%)	65 (94%)	4 (6%)	25	52
19	CS	67/80 (84%)	60 (90%)	7 (10%)	9	20
20	AT	70/82 (85%)	63 (90%)	7 (10%)	9	22
20	CT	70/82 (85%)	63 (90%)	7 (10%)	9	22
21	AU	18/22 (82%)	16 (89%)	2 (11%)	8	17
21	CU	18/22 (82%)	17 (94%)	1 (6%)	26	54
27	BD	215/218 (99%)	200 (93%)	15 (7%)	19	42
27	DD	215/218 (99%)	197 (92%)	18 (8%)	14	30
28	BE	164/166 (99%)	147 (90%)	17 (10%)	9	20
28	DE	164/166 (99%)	146 (89%)	18 (11%)	8	18
29	BF	160/166 (96%)	147 (92%)	13 (8%)	15	33
29	DF	159/166 (96%)	148 (93%)	11 (7%)	19	43
30	BG	143/156 (92%)	125 (87%)	18 (13%)	5	13
30	DG	142/156 (91%)	123 (87%)	19 (13%)	5	11
31	BH	144/148 (97%)	135 (94%)	9 (6%)	22	48
31	DH	144/148 (97%)	130 (90%)	14 (10%)	10	23
32	BI	110/124 (89%)	92 (84%)	18 (16%)	3	7
32	DI	104/124 (84%)	88 (85%)	16 (15%)	3	8
33	BN	118/119 (99%)	101 (86%)	17 (14%)	4	10
33	DN	118/119 (99%)	109 (92%)	9 (8%)	16	37
34	BO	100/100 (100%)	94 (94%)	6 (6%)	24	50
34	DO	100/100 (100%)	96 (96%)	4 (4%)	38	69
35	BP	115/116 (99%)	102 (89%)	13 (11%)	7	16
35	DP	115/116 (99%)	102 (89%)	13 (11%)	7	16
36	BQ	111/111 (100%)	101 (91%)	10 (9%)	12	27
36	DQ	111/111 (100%)	100 (90%)	11 (10%)	10	22
37	BR	101/101 (100%)	88 (87%)	13 (13%)	5	12
37	DR	101/101 (100%)	87 (86%)	14 (14%)	4	10
38	BS	87/88 (99%)	80 (92%)	7 (8%)	15	33
38	DS	85/88 (97%)	75 (88%)	10 (12%)	6	15
39	BT	115/127 (91%)	106 (92%)	9 (8%)	16	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	DT	113/127 (89%)	102 (90%)	11 (10%)	10	23
40	BU	93/94 (99%)	84 (90%)	9 (10%)	10	23
40	DU	93/94 (99%)	88 (95%)	5 (5%)	27	56
41	BV	80/82 (98%)	72 (90%)	8 (10%)	9	22
41	DV	80/82 (98%)	71 (89%)	9 (11%)	7	16
42	BW	90/92 (98%)	82 (91%)	8 (9%)	12	27
42	DW	90/92 (98%)	82 (91%)	8 (9%)	12	27
43	BX	77/78 (99%)	73 (95%)	4 (5%)	29	58
43	DX	77/78 (99%)	75 (97%)	2 (3%)	54	83
44	BY	85/91 (93%)	78 (92%)	7 (8%)	14	32
44	DY	85/91 (93%)	82 (96%)	3 (4%)	43	74
45	BZ	145/179 (81%)	132 (91%)	13 (9%)	12	27
45	DZ	145/179 (81%)	130 (90%)	15 (10%)	9	20
46	B0	65/67 (97%)	61 (94%)	4 (6%)	23	49
46	D0	65/67 (97%)	62 (95%)	3 (5%)	33	64
47	B1	80/83 (96%)	73 (91%)	7 (9%)	12	28
47	D1	80/83 (96%)	74 (92%)	6 (8%)	17	38
48	B2	65/67 (97%)	61 (94%)	4 (6%)	23	49
48	D2	65/67 (97%)	61 (94%)	4 (6%)	23	49
49	B3	51/52 (98%)	46 (90%)	5 (10%)	10	23
49	D3	50/52 (96%)	43 (86%)	7 (14%)	4	10
50	B4	60/63 (95%)	50 (83%)	10 (17%)	3	7
50	D4	53/63 (84%)	44 (83%)	9 (17%)	2	6
51	B5	50/52 (96%)	43 (86%)	7 (14%)	4	10
51	D5	50/52 (96%)	45 (90%)	5 (10%)	9	22
52	B6	51/52 (98%)	47 (92%)	4 (8%)	16	35
52	D6	50/52 (96%)	49 (98%)	1 (2%)	63	87
53	B7	41/42 (98%)	39 (95%)	2 (5%)	31	61
53	D7	41/42 (98%)	41 (100%)	0	100	100
54	B8	54/55 (98%)	50 (93%)	4 (7%)	17	39
54	D8	54/55 (98%)	48 (89%)	6 (11%)	8	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	B9	34/34 (100%)	33 (97%)	1 (3%)	50	80
55	D9	34/34 (100%)	32 (94%)	2 (6%)	24	51
All	All	9321/10066 (93%)	8506 (91%)	815 (9%)	13	29

All (815) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AB	8	LYS
2	AB	11	LEU
2	AB	19	HIS
2	AB	20	GLU
2	AB	21	ARG
2	AB	24	TRP
2	AB	39	ILE
2	AB	53	ARG
2	AB	64	ARG
2	AB	76	GLN
2	AB	80	ILE
2	AB	96	ARG
2	AB	109	SER
2	AB	114	ARG
2	AB	127	ILE
2	AB	142	LEU
2	AB	145	LEU
2	AB	153	ARG
2	AB	154	LEU
2	AB	155	LEU
2	AB	156	LYS
2	AB	187	LEU
2	AB	195	ASP
2	AB	200	ILE
2	AB	217	ARG
2	AB	221	LEU
2	AB	223	ILE
2	AB	230	VAL
2	AB	231	GLU
2	AB	235	SER
3	AC	3	ASN
3	AC	21	ARG
3	AC	27	LYS
3	AC	28	GLN

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Mol	Chain	Res	Type
3	AC	37	GLN
3	AC	45	LYS
3	AC	70	VAL
3	AC	115	LEU
3	AC	127	ARG
3	AC	181	ASN
3	AC	191	THR
4	AD	5	ILE
4	AD	15	GLU
4	AD	31	CYS
4	AD	112	VAL
4	AD	127	THR
4	AD	135	LEU
4	AD	158	ILE
4	AD	168	ARG
4	AD	182	LYS
5	AE	18	ARG
5	AE	31	LEU
5	AE	38	GLN
5	AE	41	VAL
5	AE	47	LYS
5	AE	79	GLU
5	AE	91	LEU
6	AF	36	ARG
6	AF	61	LEU
6	AF	72	VAL
6	AF	82	ARG
7	AG	8	GLU
7	AG	50	ILE
7	AG	51	GLN
7	AG	52	GLU
7	AG	76	ARG
7	AG	104	LEU
7	AG	138	LYS
8	AH	21	LYS
8	AH	52	ASP
8	AH	54	ASP
8	AH	78	GLN
8	AH	91	ARG
8	AH	112	LEU
9	AI	3	GLN
9	AI	17	VAL

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Mol	Chain	Res	Type
9	AI	23	ASN
9	AI	42	ARG
9	AI	53	VAL
9	AI	56	LEU
9	AI	64	THR
9	AI	81	ILE
9	AI	112	LYS
9	AI	128	ARG
10	AJ	5	ARG
10	AJ	7	LYS
10	AJ	23	ILE
10	AJ	46	ARG
11	AK	14	VAL
11	AK	16	SER
11	AK	31	THR
11	AK	48	ILE
11	AK	96	ARG
11	AK	104	GLN
11	AK	114	VAL
11	AK	126	ARG
12	AL	33	ARG
12	AL	46	LYS
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	102	ARG
13	AM	110	ARG
13	AM	121	LYS
14	AN	3	ARG
14	AN	7	ILE
14	AN	18	VAL
14	AN	23	ARG
14	AN	33	VAL
14	AN	50	LYS
14	AN	57	ARG
15	AO	3	ILE
15	AO	5	LYS

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Mol	Chain	Res	Type
15	AO	22	THR
15	AO	26	GLU
15	AO	39	LEU
15	AO	41	GLU
15	AO	47	LYS
15	AO	83	GLU
15	AO	84	LYS
16	AP	19	ILE
16	AP	54	GLU
16	AP	60	LEU
16	AP	62	VAL
16	AP	69	THR
16	AP	71	ARG
17	AQ	6	LEU
17	AQ	60	ILE
17	AQ	98	LEU
18	AR	21	LYS
18	AR	26	LEU
18	AR	46	GLU
18	AR	58	LEU
18	AR	76	LEU
19	AS	12	ASP
19	AS	28	LYS
19	AS	65	ASN
19	AS	78	ARG
20	AT	8	ARG
20	AT	13	LEU
20	AT	24	LEU
20	AT	30	LYS
20	AT	62	LEU
20	AT	74	LYS
20	AT	84	LEU
21	AU	9	ARG
21	AU	10	ARG
27	BD	13	ARG
27	BD	61	LEU
27	BD	94	LEU
27	BD	103	ARG
27	BD	106	ILE
27	BD	113	VAL
27	BD	126	GLN
27	BD	155	LEU

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Mol	Chain	Res	Type
27	BD	211	ARG
27	BD	221	VAL
27	BD	229	VAL
27	BD	242	ARG
27	BD	257	LEU
27	BD	259	THR
27	BD	260	ARG
28	BE	1	MET
28	BE	21	VAL
28	BE	24	THR
28	BE	33	VAL
28	BE	49	LEU
28	BE	73	GLU
28	BE	77	ILE
28	BE	82	ARG
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	170	LEU
28	BE	175	VAL
28	BE	181	LEU
29	BF	19	GLU
29	BF	33	LEU
29	BF	38	ARG
29	BF	53	THR
29	BF	74	ARG
29	BF	88	VAL
29	BF	106	ARG
29	BF	110	LEU
29	BF	125	LEU
29	BF	132	VAL
29	BF	140	LEU
29	BF	192	LEU
29	BF	195	ASP
30	BG	5	VAL
30	BG	7	LEU
30	BG	21	ARG
30	BG	43	LEU
30	BG	45	GLU

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Mol	Chain	Res	Type
30	BG	81	LYS
30	BG	82	LEU
30	BG	84	LYS
30	BG	86	MET
30	BG	91	ARG
30	BG	133	LEU
30	BG	135	LEU
30	BG	140	ILE
30	BG	143	GLU
30	BG	145	THR
30	BG	159	VAL
30	BG	170	ARG
30	BG	175	LEU
31	BH	3	ARG
31	BH	41	MET
31	BH	59	ARG
31	BH	69	ARG
31	BH	71	LEU
31	BH	84	SER
31	BH	122	THR
31	BH	130	ARG
31	BH	139	GLN
32	BI	5	LEU
32	BI	9	LEU
32	BI	10	GLU
32	BI	38	LEU
32	BI	43	ASN
32	BI	47	LEU
32	BI	60	GLU
32	BI	61	ARG
32	BI	64	GLU
32	BI	66	GLU
32	BI	77	LEU
32	BI	87	LYS
32	BI	92	VAL
32	BI	104	GLN
32	BI	107	VAL
32	BI	116	LEU
32	BI	127	VAL
32	BI	140	LEU
33	BN	14	VAL
33	BN	28	THR

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Mol	Chain	Res	Type
33	BN	33	LEU
33	BN	34	LEU
33	BN	38	HIS
33	BN	48	MET
33	BN	61	ARG
33	BN	67	LEU
33	BN	68	GLU
33	BN	73	THR
33	BN	83	LYS
33	BN	87	LEU
33	BN	120	LEU
33	BN	133	GLN
33	BN	137	LYS
33	BN	139	GLU
33	BN	140	VAL
34	BO	23	ARG
34	BO	24	VAL
34	BO	28	SER
34	BO	69	ILE
34	BO	98	VAL
34	BO	108	GLU
35	BP	3	LEU
35	BP	7	ARG
35	BP	55	ARG
35	BP	59	LEU
35	BP	65	ARG
35	BP	70	GLN
35	BP	77	ARG
35	BP	95	VAL
35	BP	98	GLU
35	BP	106	LEU
35	BP	112	LEU
35	BP	135	LEU
35	BP	149	GLU
36	BQ	1	MET
36	BQ	5	ARG
36	BQ	7	MET
36	BQ	8	LYS
36	BQ	16	ARG
36	BQ	21	THR
36	BQ	45	GLN
36	BQ	54	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
36	BQ	55	VAL
36	BQ	109	VAL
37	BR	1	MET
37	BR	15	SER
37	BR	18	LEU
37	BR	28	LEU
37	BR	29	LEU
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
38	BS	14	VAL
38	BS	20	ARG
38	BS	57	LYS
38	BS	59	LYS
38	BS	78	LEU
38	BS	83	LYS
38	BS	110	LEU
39	BT	6	LEU
39	BT	17	THR
39	BT	49	VAL
39	BT	53	ARG
39	BT	64	ARG
39	BT	74	ARG
39	BT	96	ARG
39	BT	108	ARG
39	BT	118	ARG
40	BU	8	VAL
40	BU	31	SER
40	BU	36	ARG
40	BU	74	LEU
40	BU	92	ARG
40	BU	95	LEU
40	BU	104	GLN
40	BU	108	GLU
40	BU	117	GLN
41	BV	28	GLU
41	BV	43	GLU

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Mol	Chain	Res	Type
41	BV	52	VAL
41	BV	62	LEU
41	BV	72	VAL
41	BV	79	VAL
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	67	ASP
42	BW	100	THR
42	BW	107	LEU
43	BX	35	THR
43	BX	57	LEU
43	BX	66	LEU
43	BX	88	LYS
44	BY	23	ARG
44	BY	24	VAL
44	BY	43	ASN
44	BY	55	TYR
44	BY	72	VAL
44	BY	90	LEU
44	BY	91	GLU
45	BZ	5	LEU
45	BZ	11	GLU
45	BZ	19	ARG
45	BZ	33	LEU
45	BZ	42	VAL
45	BZ	72	ARG
45	BZ	76	LEU
45	BZ	97	GLU
45	BZ	136	PHE
45	BZ	154	ASP
45	BZ	155	LEU
45	BZ	156	LYS
45	BZ	170	THR
46	B0	20	ARG
46	B0	36	ILE
46	B0	55	ARG
46	B0	82	ARG

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Mol	Chain	Res	Type
47	B1	21	ARG
47	B1	35	THR
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	32	LEU
48	B2	53	LEU
48	B2	70	GLN
49	B3	8	LEU
49	B3	23	LEU
49	B3	31	LEU
49	B3	58	VAL
49	B3	60	GLU
50	B4	34	GLU
50	B4	46	GLN
50	B4	50	VAL
50	B4	56	VAL
50	B4	58	ARG
50	B4	59	PHE
50	B4	63	TYR
50	B4	66	SER
50	B4	68	ARG
50	B4	69	LYS
51	B5	6	VAL
51	B5	29	THR
51	B5	33	CYS
51	B5	40	LYS
51	B5	48	GLU
51	B5	55	ARG
51	B5	60	VAL
52	B6	4	GLU
52	B6	14	THR
52	B6	38	LYS
52	B6	48	VAL
53	B7	1	MET
53	B7	24	THR
54	B8	6	THR
54	B8	14	VAL
54	B8	31	HIS

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Mol	Chain	Res	Type
54	B8	32	LEU
55	B9	33	LYS
2	CB	11	LEU
2	CB	35	GLU
2	CB	71	VAL
2	CB	76	GLN
2	CB	80	ILE
2	CB	87	ARG
2	CB	94	ASN
2	CB	96	ARG
2	CB	98	LEU
2	CB	115	LEU
2	CB	122	PHE
2	CB	126	GLU
2	CB	128	GLU
2	CB	133	LYS
2	CB	142	LEU
2	CB	154	LEU
2	CB	155	LEU
2	CB	157	ARG
2	CB	163	PHE
2	CB	185	ILE
2	CB	187	LEU
2	CB	200	ILE
2	CB	217	ARG
2	CB	224	GLN
3	CC	3	ASN
3	CC	17	ASP
3	CC	21	ARG
3	CC	49	SER
3	CC	52	LEU
3	CC	98	ASN
3	CC	104	GLN
3	CC	115	LEU
3	CC	152	ILE
3	CC	179	ARG
4	CD	10	ARG
4	CD	15	GLU
4	CD	31	CYS
4	CD	34	GLU
4	CD	47	ARG
4	CD	61	LYS

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Mol	Chain	Res	Type
4	CD	108	LEU
4	CD	127	THR
4	CD	135	LEU
4	CD	157	LEU
4	CD	170	VAL
4	CD	187	ARG
4	CD	188	LEU
4	CD	194	LEU
5	CE	18	ARG
5	CE	31	LEU
5	CE	41	VAL
5	CE	47	LYS
5	CE	60	TYR
5	CE	71	LEU
5	CE	73	ASN
5	CE	78	HIS
5	CE	79	GLU
5	CE	91	LEU
5	CE	150	ARG
6	CF	10	LEU
6	CF	28	ARG
6	CF	41	GLU
6	CF	46	ARG
6	CF	61	LEU
6	CF	72	VAL
6	CF	82	ARG
6	CF	92	LYS
7	CG	9	VAL
7	CG	51	GLN
7	CG	72	ARG
7	CG	104	LEU
7	CG	114	ARG
7	CG	138	LYS
8	CH	21	LYS
8	CH	84	ARG
8	CH	98	LYS
8	CH	112	LEU
8	CH	127	LEU
9	CI	3	GLN
9	CI	7	THR
9	CI	14	VAL
9	CI	17	VAL

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Mol	Chain	Res	Type
9	CI	23	ASN
9	CI	53	VAL
9	CI	64	THR
9	CI	81	ILE
9	CI	89	ASN
9	CI	102	LEU
9	CI	125	TYR
9	CI	128	ARG
10	CJ	19	SER
10	CJ	84	GLN
11	CK	14	VAL
11	CK	24	SER
11	CK	51	LYS
11	CK	78	GLN
11	CK	96	ARG
11	CK	104	GLN
11	CK	109	VAL
11	CK	114	VAL
11	CK	120	ARG
11	CK	126	ARG
12	CL	33	ARG
12	CL	52	LEU
12	CL	60	LEU
13	CM	3	ARG
13	CM	4	ILE
13	CM	15	VAL
13	CM	19	LEU
13	CM	56	LEU
13	CM	70	LEU
13	CM	110	ARG
13	CM	115	LYS
14	CN	3	ARG
14	CN	7	ILE
14	CN	12	ARG
14	CN	18	VAL
14	CN	23	ARG
14	CN	33	VAL
15	CO	5	LYS
15	CO	39	LEU
15	CO	54	ARG
15	CO	83	GLU
16	CP	2	VAL

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Mol	Chain	Res	Type
16	CP	27	LYS
16	CP	28	ARG
16	CP	60	LEU
16	CP	62	VAL
17	CQ	6	LEU
17	CQ	96	GLU
18	CR	26	LEU
18	CR	41	LYS
18	CR	58	LEU
19	CS	28	LYS
19	CS	56	GLN
19	CS	64	GLU
19	CS	65	ASN
19	CS	71	LEU
19	CS	77	THR
19	CS	78	ARG
20	CT	10	LEU
20	CT	45	GLN
20	CT	56	MET
20	CT	62	LEU
20	CT	80	ARG
20	CT	84	LEU
20	CT	90	GLN
21	CU	10	ARG
27	DD	13	ARG
27	DD	54	ARG
27	DD	61	LEU
27	DD	94	LEU
27	DD	103	ARG
27	DD	106	ILE
27	DD	113	VAL
27	DD	126	GLN
27	DD	134	ARG
27	DD	155	LEU
27	DD	211	ARG
27	DD	221	VAL
27	DD	229	VAL
27	DD	242	ARG
27	DD	257	LEU
27	DD	259	THR
27	DD	260	ARG
27	DD	276	LYS

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Mol	Chain	Res	Type
28	DE	1	MET
28	DE	21	VAL
28	DE	24	THR
28	DE	33	VAL
28	DE	52	LEU
28	DE	73	GLU
28	DE	75	VAL
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	170	LEU
28	DE	175	VAL
28	DE	181	LEU
28	DE	184	VAL
28	DE	195	LEU
29	DF	19	GLU
29	DF	20	LEU
29	DF	33	LEU
29	DF	53	THR
29	DF	74	ARG
29	DF	88	VAL
29	DF	106	ARG
29	DF	107	LYS
29	DF	110	LEU
29	DF	132	VAL
29	DF	192	LEU
30	DG	5	VAL
30	DG	7	LEU
30	DG	16	ARG
30	DG	21	ARG
30	DG	31	VAL
30	DG	43	LEU
30	DG	45	GLU
30	DG	49	ASP
30	DG	58	GLN
30	DG	79	ASN
30	DG	91	ARG
30	DG	115	ARG
30	DG	133	LEU

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Mol	Chain	Res	Type
30	DG	136	ARG
30	DG	140	ILE
30	DG	143	GLU
30	DG	148	MET
30	DG	159	VAL
30	DG	170	ARG
31	DH	3	ARG
31	DH	33	LEU
31	DH	43	VAL
31	DH	45	VAL
31	DH	49	VAL
31	DH	57	ASP
31	DH	63	SER
31	DH	69	ARG
31	DH	95	ARG
31	DH	105	LEU
31	DH	106	THR
31	DH	124	GLU
31	DH	139	GLN
31	DH	172	LYS
32	DI	5	LEU
32	DI	9	LEU
32	DI	38	LEU
32	DI	43	ASN
32	DI	47	LEU
32	DI	50	ARG
32	DI	57	ARG
32	DI	61	ARG
32	DI	73	GLU
32	DI	75	LEU
32	DI	77	LEU
32	DI	86	THR
32	DI	87	LYS
32	DI	101	LEU
32	DI	116	LEU
32	DI	140	LEU
33	DN	14	VAL
33	DN	34	LEU
33	DN	38	HIS
33	DN	46	VAL
33	DN	61	ARG
33	DN	87	LEU

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Mol	Chain	Res	Type
33	DN	120	LEU
33	DN	133	GLN
33	DN	140	VAL
34	DO	24	VAL
34	DO	69	ILE
34	DO	98	VAL
34	DO	108	GLU
35	DP	3	LEU
35	DP	4	SER
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	95	VAL
35	DP	98	GLU
35	DP	106	LEU
35	DP	112	LEU
35	DP	135	LEU
36	DQ	1	MET
36	DQ	7	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	85	LYS
36	DQ	109	VAL
36	DQ	110	THR
37	DR	1	MET
37	DR	15	SER
37	DR	18	LEU
37	DR	24	GLN
37	DR	28	LEU
37	DR	29	LEU
37	DR	44	LEU
37	DR	54	LEU
37	DR	60	LEU
37	DR	65	LEU
37	DR	67	LEU

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Mol	Chain	Res	Type
37	DR	75	LEU
37	DR	79	LEU
37	DR	100	LEU
38	DS	14	VAL
38	DS	20	ARG
38	DS	35	ILE
38	DS	49	VAL
38	DS	57	LYS
38	DS	58	LEU
38	DS	75	GLU
38	DS	93	LYS
38	DS	103	GLU
38	DS	110	LEU
39	DT	1	MET
39	DT	6	LEU
39	DT	16	ARG
39	DT	28	VAL
39	DT	53	ARG
39	DT	64	ARG
39	DT	74	ARG
39	DT	96	ARG
39	DT	108	ARG
39	DT	113	LYS
39	DT	118	ARG
40	DU	74	LEU
40	DU	89	GLU
40	DU	92	ARG
40	DU	95	LEU
40	DU	104	GLN
41	DV	18	LEU
41	DV	51	VAL
41	DV	52	VAL
41	DV	57	VAL
41	DV	62	LEU
41	DV	72	VAL
41	DV	79	VAL
41	DV	95	LEU
41	DV	100	ARG
42	DW	4	LYS
42	DW	11	ARG
42	DW	15	ARG
42	DW	17	VAL

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Mol	Chain	Res	Type
42	DW	51	LEU
42	DW	52	GLU
42	DW	100	THR
42	DW	107	LEU
43	DX	57	LEU
43	DX	88	LYS
44	DY	23	ARG
44	DY	43	ASN
44	DY	91	GLU
45	DZ	5	LEU
45	DZ	11	GLU
45	DZ	19	ARG
45	DZ	33	LEU
45	DZ	42	VAL
45	DZ	72	ARG
45	DZ	76	LEU
45	DZ	86	VAL
45	DZ	97	GLU
45	DZ	119	GLU
45	DZ	131	ARG
45	DZ	136	PHE
45	DZ	154	ASP
45	DZ	155	LEU
45	DZ	170	THR
46	D0	20	ARG
46	D0	24	LYS
46	D0	55	ARG
47	D1	21	ARG
47	D1	35	THR
47	D1	40	ARG
47	D1	59	THR
47	D1	78	LYS
47	D1	95	LEU
48	D2	30	ARG
48	D2	32	LEU
48	D2	53	LEU
48	D2	70	GLN
49	D3	8	LEU
49	D3	23	LEU
49	D3	24	LYS
49	D3	30	ARG
49	D3	31	LEU

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Mol	Chain	Res	Type
49	D3	34	GLU
49	D3	44	ARG
50	D4	3	GLU
50	D4	8	LYS
50	D4	37	SER
50	D4	44	THR
50	D4	50	VAL
50	D4	56	VAL
50	D4	63	TYR
50	D4	67	TYR
50	D4	69	LYS
51	D5	6	VAL
51	D5	29	THR
51	D5	33	CYS
51	D5	40	LYS
51	D5	59	GLU
52	D6	28	ARG
54	D8	14	VAL
54	D8	23	VAL
54	D8	31	HIS
54	D8	32	LEU
54	D8	34	TRP
54	D8	37	SER
55	D9	13	LYS
55	D9	26	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (114) such sidechains are listed below:

Mol	Chain	Res	Type
2	AB	40	HIS
3	AC	37	GLN
3	AC	104	GLN
3	AC	136	GLN
3	AC	162	GLN
3	AC	181	ASN
4	AD	77	ASN
4	AD	123	HIS
4	AD	125	HIS
5	AE	38	GLN
5	AE	56	GLN
6	AF	73	ASN
6	AF	100	ASN

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Mol	Chain	Res	Type
7	AG	13	GLN
7	AG	28	ASN
7	AG	97	GLN
9	AI	23	ASN
9	AI	34	ASN
9	AI	58	HIS
9	AI	124	GLN
10	AJ	56	HIS
11	AK	93	GLN
11	AK	104	GLN
12	AL	78	GLN
12	AL	99	HIS
13	AM	62	ASN
13	AM	77	ASN
14	AN	49	HIS
15	AO	28	GLN
15	AO	62	GLN
19	AS	23	ASN
19	AS	65	ASN
19	AS	69	HIS
19	AS	83	HIS
20	AT	45	GLN
27	BD	87	ASN
27	BD	253	GLN
28	BE	85	ASN
29	BF	69	HIS
29	BF	169	ASN
29	BF	203	GLN
30	BG	40	ASN
32	BI	54	GLN
32	BI	74	ASN
35	BP	38	GLN
35	BP	70	GLN
36	BQ	57	HIS
39	BT	43	GLN
39	BT	58	ASN
39	BT	123	GLN
40	BU	81	HIS
40	BU	117	GLN
43	BX	31	HIS
43	BX	82	GLN
44	BY	6	HIS

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Mol	Chain	Res	Type
44	BY	43	ASN
45	BZ	55	HIS
48	B2	70	GLN
55	B9	36	GLN
2	CB	16	HIS
2	CB	40	HIS
2	CB	76	GLN
2	CB	135	GLN
3	CC	104	GLN
3	CC	123	GLN
3	CC	136	GLN
4	CD	74	GLN
4	CD	77	ASN
4	CD	123	HIS
4	CD	125	HIS
5	CE	38	GLN
6	CF	100	ASN
7	CG	11	GLN
7	CG	51	GLN
7	CG	97	GLN
9	CI	23	ASN
9	CI	58	HIS
9	CI	73	GLN
9	CI	89	ASN
9	CI	124	GLN
11	CK	93	GLN
12	CL	78	GLN
12	CL	99	HIS
13	CM	77	ASN
15	CO	28	GLN
15	CO	62	GLN
16	CP	76	GLN
19	CS	69	HIS
20	CT	45	GLN
20	CT	90	GLN
27	DD	253	GLN
28	DE	85	ASN
29	DF	69	HIS
29	DF	75	HIS
29	DF	169	ASN
29	DF	203	GLN
30	DG	40	ASN

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Mol	Chain	Res	Type
32	DI	43	ASN
32	DI	133	HIS
34	DO	89	ASN
35	DP	38	GLN
36	DQ	13	GLN
36	DQ	57	HIS
38	DS	68	GLN
39	DT	58	ASN
39	DT	123	GLN
40	DU	117	GLN
43	DX	31	HIS
43	DX	82	GLN
44	DY	43	ASN
45	DZ	34	ASN
45	DZ	55	HIS
50	D4	46	GLN
55	D9	36	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1493/1521 (98%)	280 (18%)	27 (1%)
1	CA	1501/1521 (98%)	280 (18%)	24 (1%)
22	AV	12/24 (50%)	2 (16%)	0
22	CV	11/24 (45%)	2 (18%)	0
23	AW	71/76 (93%)	31 (43%)	1 (1%)
23	AY	72/76 (94%)	33 (45%)	4 (5%)
23	CW	68/76 (89%)	30 (44%)	2 (2%)
23	CY	70/76 (92%)	31 (44%)	1 (1%)
24	AX	75/77 (97%)	21 (28%)	2 (2%)
24	CX	75/77 (97%)	21 (28%)	1 (1%)
25	BA	2814/2915 (96%)	455 (16%)	28 (0%)
25	DA	2791/2915 (95%)	518 (18%)	29 (1%)
26	BB	119/121 (98%)	13 (10%)	2 (1%)
26	DB	119/121 (98%)	14 (11%)	0
All	All	9291/9620 (96%)	1731 (18%)	121 (1%)

All (1731) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G

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Mol	Chain	Res	Type
1	AA	7	G
1	AA	9	G
1	AA	32	A
1	AA	39	G
1	AA	47	C
1	AA	48	C
1	AA	51	A
1	AA	59	A
1	AA	61	G
1	AA	65	U
1	AA	66	G
1	AA	73	G
1	AA	76	C
1	AA	77	G
1	AA	78	G
1	AA	79	G
1	AA	91	C
1	AA	96	U
1	AA	98	G
1	AA	101	A
1	AA	112	G
1	AA	116	A
1	AA	121	C
1	AA	131	C
1	AA	155	C
1	AA	159	G
1	AA	163	C
1	AA	173	U
1	AA	174	C
1	AA	182	U
1	AA	186	C
1	AA	189(D)	C
1	AA	189(J)	G
1	AA	190	U
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	247	G

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Mol	Chain	Res	Type
1	AA	251	G
1	AA	258	G
1	AA	266	G
1	AA	267	C
1	AA	289	G
1	AA	301	G
1	AA	321	A
1	AA	328	C
1	AA	332	G
1	AA	341	C
1	AA	345	C
1	AA	346	G
1	AA	347	G
1	AA	348	G
1	AA	351	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	384	G
1	AA	398	C
1	AA	406	G
1	AA	412	A
1	AA	413	G
1	AA	422	C
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	458	C
1	AA	461	A
1	AA	470	C
1	AA	485	G
1	AA	492	G
1	AA	496	A

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Mol	Chain	Res	Type
1	AA	498	U
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	527	G
1	AA	528	C
1	AA	531	U
1	AA	532	A
1	AA	533	A
1	AA	545	C
1	AA	547	A
1	AA	559	A
1	AA	560	U
1	AA	561	U
1	AA	572	A
1	AA	573	A
1	AA	576	G
1	AA	577	G
1	AA	596	C
1	AA	599	C
1	AA	630	G
1	AA	632	A
1	AA	633	G
1	AA	653	A
1	AA	665	A
1	AA	680	C
1	AA	687	A
1	AA	688	G
1	AA	693	G
1	AA	695	A
1	AA	723	U
1	AA	731	G
1	AA	749	C
1	AA	752	G
1	AA	753	A
1	AA	755	G
1	AA	759	A
1	AA	760	G
1	AA	777	A

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Mol	Chain	Res	Type
1	AA	792	A
1	AA	793	U
1	AA	794	A
1	AA	806	C
1	AA	815	A
1	AA	817	C
1	AA	821	G
1	AA	828	A
1	AA	829	G
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	887	G
1	AA	902	G
1	AA	914	A
1	AA	926	G
1	AA	927	G
1	AA	934	C
1	AA	935	A
1	AA	960	U
1	AA	961	U
1	AA	968	A
1	AA	969	A
1	AA	971	G
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	1002	G
1	AA	1003	G
1	AA	1004	A
1	AA	1005	A
1	AA	1009	G
1	AA	1019	C
1	AA	1020	U

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Mol	Chain	Res	Type
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	C
1	AA	1030(A)	G
1	AA	1030(C)	G
1	AA	1031	G
1	AA	1032	G
1	AA	1033	G
1	AA	1037	C
1	AA	1039	C
1	AA	1041	A
1	AA	1045	C
1	AA	1052	U
1	AA	1054	C
1	AA	1065	U
1	AA	1066	C
1	AA	1068	G
1	AA	1076	C
1	AA	1081	G
1	AA	1094	G
1	AA	1095	U
1	AA	1101	A
1	AA	1108	G
1	AA	1123	A
1	AA	1124	G
1	AA	1126	U
1	AA	1129	C
1	AA	1130	A
1	AA	1132	C
1	AA	1134	G
1	AA	1135	U
1	AA	1136	U
1	AA	1137	C
1	AA	1138	G
1	AA	1139	G
1	AA	1140	C

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Mol	Chain	Res	Type
1	AA	1145	C
1	AA	1146	A
1	AA	1152	A
1	AA	1154	G
1	AA	1157	A
1	AA	1159	U
1	AA	1160	G
1	AA	1166	G
1	AA	1183	A
1	AA	1184	G
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	1238	A
1	AA	1240	U
1	AA	1244	C
1	AA	1256	A
1	AA	1257	U
1	AA	1258	G
1	AA	1260	C
1	AA	1262	C
1	AA	1270	C
1	AA	1273	G
1	AA	1278	U
1	AA	1279	A
1	AA	1280	A
1	AA	1281	U
1	AA	1286	A
1	AA	1287	A
1	AA	1299	A
1	AA	1300	G
1	AA	1302	U
1	AA	1314	C
1	AA	1317	C
1	AA	1320	C
1	AA	1322	C
1	AA	1338	G
1	AA	1340	A

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Mol	Chain	Res	Type
1	AA	1346	A
1	AA	1347	G
1	AA	1363	C
1	AA	1364	U
1	AA	1370	G
1	AA	1383	C
1	AA	1397	C
1	AA	1401	G
1	AA	1419	G
1	AA	1442	G
1	AA	1442(A)	G
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	1494	G
1	AA	1497	G
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
22	AV	13	A
22	AV	24	A
23	AW	3	C
23	AW	7	A
23	AW	8	4SU
23	AW	12	U
23	AW	13	C
23	AW	14	A
23	AW	15	G
23	AW	19	G
23	AW	20	U
23	AW	21	A
23	AW	22	G
23	AW	23	A
23	AW	26	A

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Mol	Chain	Res	Type
23	AW	41	C
23	AW	42	C
23	AW	43	C
23	AW	45	U
23	AW	46	7MG
23	AW	47	U
23	AW	48	C
23	AW	49	C
23	AW	58	A
23	AW	59	U
23	AW	61	C
23	AW	63	G
23	AW	64	A
23	AW	68	C
23	AW	71	G
23	AW	73	A
23	AW	74	C
23	AW	76	A
24	AX	9	G
24	AX	13	C
24	AX	16	C
24	AX	18	G
24	AX	19	G
24	AX	20	U
24	AX	21	A
24	AX	31	G
24	AX	34	C
24	AX	42	G
24	AX	47	U
24	AX	48	C
24	AX	52	G
24	AX	56	C
24	AX	58	A
24	AX	60	U
24	AX	62	C
24	AX	63	G
24	AX	67	C
24	AX	68	C
24	AX	76	A
23	AY	3	C
23	AY	5	G
23	AY	8	4SU

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Mol	Chain	Res	Type
23	AY	9	A
23	AY	11	C
23	AY	19	G
23	AY	20	U
23	AY	21	A
23	AY	22	G
23	AY	25	C
23	AY	26	A
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	41	C
23	AY	44	G
23	AY	47	U
23	AY	48	C
23	AY	49	C
23	AY	51	U
23	AY	54	5MU
23	AY	56	C
23	AY	57	G
23	AY	58	A
23	AY	59	U
23	AY	61	C
23	AY	62	C
23	AY	65	G
23	AY	70	G
23	AY	72	C
25	BA	12	U
25	BA	13	A
25	BA	34	C
25	BA	45	C
25	BA	54	G
25	BA	70	A
25	BA	73	A
25	BA	74	G
25	BA	83	A
25	BA	94	G
25	BA	116	A
25	BA	117	A

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Mol	Chain	Res	Type
25	BA	118	U
25	BA	123	G
25	BA	138	G
25	BA	155	C
25	BA	161	C
25	BA	170	A
25	BA	171	A
25	BA	185	A
25	BA	188	A
25	BA	189	U
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	218	A
25	BA	222	A
25	BA	237	G
25	BA	253	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	279	G
25	BA	289	G
25	BA	295	C
25	BA	299	G
25	BA	303	C
25	BA	335	A
25	BA	353	G
25	BA	354	A
25	BA	376	G
25	BA	387	G
25	BA	390	G
25	BA	395	C
25	BA	397	G
25	BA	413	G
25	BA	423	G
25	BA	432	U

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Mol	Chain	Res	Type
25	BA	434	G
25	BA	438	G
25	BA	439	A
25	BA	448	U
25	BA	455	A
25	BA	456	A
25	BA	462	C
25	BA	469	A
25	BA	470	C
25	BA	474	U
25	BA	482	C
25	BA	483	A
25	BA	496	A
25	BA	507	G
25	BA	529	U
25	BA	530	A
25	BA	534	C
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	586	G
25	BA	596	G
25	BA	598	A
25	BA	609	A
25	BA	626	A
25	BA	627	G
25	BA	630	U
25	BA	639	G
25	BA	641	G
25	BA	652	A
25	BA	662	A
25	BA	670	C
25	BA	671	A
25	BA	697	C
25	BA	698	G
25	BA	716	G
25	BA	724	A
25	BA	733	G
25	BA	764	G

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Mol	Chain	Res	Type
25	BA	773	G
25	BA	777	C
25	BA	795	G
25	BA	811	A
25	BA	812	G
25	BA	822	G
25	BA	823	G
25	BA	829	A
25	BA	831	A
25	BA	832	G
25	BA	836	A
25	BA	837	C
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	879	G
25	BA	906	G
25	BA	913	A
25	BA	924	U
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	939	C
25	BA	941	U
25	BA	942	A
25	BA	943	C
25	BA	944	C
25	BA	945	A
25	BA	946	A
25	BA	953	U
25	BA	956	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
25	BA	960	C
25	BA	977	G
25	BA	986	A
25	BA	990	A
25	BA	991	G
25	BA	1003	U
25	BA	1004	A
25	BA	1006	C
25	BA	1008	U
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	1063	G
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	1090	G
25	BA	1091	A
25	BA	1092	A
25	BA	1093	G
25	BA	1094	A
25	BA	1097	G
25	BA	1153	G
25	BA	1156	G
25	BA	1158	G
25	BA	1163	G
25	BA	1175	A
25	BA	1176	U
25	BA	1180	C
25	BA	1181	G
25	BA	1201	A
25	BA	1217	G
25	BA	1218	G
25	BA	1219	A
25	BA	1220	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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	1265	A
25	BA	1290	G
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	1352	C
25	BA	1360	C
25	BA	1398	U
25	BA	1405	A
25	BA	1406	A
25	BA	1411	A
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	1474	C
25	BA	1491	A
25	BA	1496	A
25	BA	1497	G
25	BA	1501	U
25	BA	1502	G
25	BA	1514	C
25	BA	1518	A
25	BA	1525	G
25	BA	1529	G
25	BA	1536	A
25	BA	1539	C
25	BA	1554	A
25	BA	1555	C
25	BA	1556	A

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Mol	Chain	Res	Type
25	BA	1557	A
25	BA	1561	C
25	BA	1569	U
25	BA	1571	G
25	BA	1578	C
25	BA	1581	U
25	BA	1589	A
25	BA	1605	A
25	BA	1613	A
25	BA	1616	A
25	BA	1625	U
25	BA	1627	A
25	BA	1628	G
25	BA	1629	C
25	BA	1631	C
25	BA	1632	A
25	BA	1653	C
25	BA	1654	A
25	BA	1656	A
25	BA	1676	G
25	BA	1686	U
25	BA	1694	G
25	BA	1695	C
25	BA	1701	A
25	BA	1711	A
25	BA	1721	G
25	BA	1735	U
25	BA	1743	G
25	BA	1747	A
25	BA	1748	A
25	BA	1767	A
25	BA	1768	U
25	BA	1769	G
25	BA	1789	G
25	BA	1793	A
25	BA	1794	G
25	BA	1795	G
25	BA	1800	G
25	BA	1804	A
25	BA	1811	A
25	BA	1817	A
25	BA	1822	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
25	BA	1831	C
25	BA	1832	G
25	BA	1847	G
25	BA	1870	G
25	BA	1878	A
25	BA	1899	A
25	BA	1900	G
25	BA	1907	A
25	BA	1911	A
25	BA	1922	A
25	BA	1928	G
25	BA	1941	A
25	BA	1951	G
25	BA	1952	G
25	BA	1953	U
25	BA	1959	A
25	BA	1960	A
25	BA	1967	G
25	BA	1968	U
25	BA	1977	U
25	BA	1985	U
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
25	BA	2078	G
25	BA	2082	A
25	BA	2083	G
25	BA	2084	A
25	BA	2091	G
25	BA	2115	G

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Mol	Chain	Res	Type
25	BA	2124	U
25	BA	2132	G
25	BA	2133	C
25	BA	2138	G
25	BA	2140	U
25	BA	2141	A
25	BA	2142	G
25	BA	2143	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	2156	A
25	BA	2157	A
25	BA	2158	C
25	BA	2159	C
25	BA	2162	C
25	BA	2163	G
25	BA	2164	C
25	BA	2165	C
25	BA	2166	U
25	BA	2167	C
25	BA	2168	C
25	BA	2169	G
25	BA	2170	G
25	BA	2171	G
25	BA	2175	G
25	BA	2177	G
25	BA	2178	G
25	BA	2179	G
25	BA	2180	A
25	BA	2181	G
25	BA	2185	C
25	BA	2188	G
25	BA	2189	U
25	BA	2190	G
25	BA	2191	A
25	BA	2193	A
25	BA	2194	U
25	BA	2195	A

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Mol	Chain	Res	Type
25	BA	2196	C
25	BA	2200	C
25	BA	2203	G
25	BA	2204	G
25	BA	2206	G
25	BA	2207	C
25	BA	2208	G
25	BA	2209	G
25	BA	2210	C
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	2281	A
25	BA	2290	A
25	BA	2295	C
25	BA	2299	A
25	BA	2301	G
25	BA	2317	A
25	BA	2326	C
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	2362	C
25	BA	2366	G
25	BA	2384	G
25	BA	2391	G
25	BA	2395	G
25	BA	2397	C
25	BA	2408	G
25	BA	2418	U
25	BA	2436	C

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Mol	Chain	Res	Type
25	BA	2437	A
25	BA	2441	G
25	BA	2442	A
25	BA	2444	A
25	BA	2446	A
25	BA	2447	A
25	BA	2451	A
25	BA	2453	C
25	BA	2459	G
25	BA	2460	A
25	BA	2473	C
25	BA	2480	G
25	BA	2481	A
25	BA	2483	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	2547	G
25	BA	2566	U
25	BA	2578	A
25	BA	2579	G
25	BA	2585	C
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	2685	G
25	BA	2701	U
25	BA	2702	C
25	BA	2714	U
25	BA	2715	C
25	BA	2719	G
25	BA	2725	A
25	BA	2726	A
25	BA	2727	G

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Mol	Chain	Res	Type
25	BA	2734	A
25	BA	2739	U
25	BA	2746	A
25	BA	2770	A
25	BA	2771	A
25	BA	2777	A
25	BA	2778	A
25	BA	2779	G
25	BA	2791	A
25	BA	2803	A
25	BA	2804	C
25	BA	2806	G
25	BA	2813	G
25	BA	2815	C
25	BA	2828	G
25	BA	2830	A
25	BA	2831	A
25	BA	2845	A
25	BA	2882	G
25	BA	2890	C
25	BA	2902	G
25	BA	2903	G
25	BA	2906	U
26	BB	2	C
26	BB	7	G
26	BB	9	G
26	BB	24	G
26	BB	47	C
26	BB	56	G
26	BB	57	A
26	BB	73	A
26	BB	75	G
26	BB	85	G
26	BB	106	G
26	BB	109	C
26	BB	110	G
1	CA	5	U
1	CA	6	G
1	CA	7	G
1	CA	9	G
1	CA	32	A
1	CA	39	G

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Mol	Chain	Res	Type
1	CA	47	C
1	CA	48	C
1	CA	51	A
1	CA	59	A
1	CA	61	G
1	CA	65	U
1	CA	66	G
1	CA	76	C
1	CA	89	C
1	CA	91	C
1	CA	96	U
1	CA	98	G
1	CA	101	A
1	CA	112	G
1	CA	116	A
1	CA	121	C
1	CA	131	C
1	CA	155	C
1	CA	159	G
1	CA	163	C
1	CA	173	U
1	CA	174	C
1	CA	182	U
1	CA	186	C
1	CA	189(D)	C
1	CA	189(F)	U
1	CA	189(J)	G
1	CA	190	U
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	247	G
1	CA	251	G
1	CA	252	U
1	CA	258	G
1	CA	266	G
1	CA	267	C
1	CA	289	G

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Mol	Chain	Res	Type
1	CA	301	G
1	CA	321	A
1	CA	328	C
1	CA	332	G
1	CA	341	C
1	CA	344	A
1	CA	346	G
1	CA	351	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	384	G
1	CA	397	A
1	CA	398	C
1	CA	406	G
1	CA	409	G
1	CA	412	A
1	CA	413	G
1	CA	422	C
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	458	C
1	CA	461	A
1	CA	470	C
1	CA	485	G
1	CA	492	G
1	CA	496	A
1	CA	498	U
1	CA	505	G
1	CA	510	A
1	CA	511	C
1	CA	513	C

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Mol	Chain	Res	Type
1	CA	518	C
1	CA	528	C
1	CA	531	U
1	CA	532	A
1	CA	533	A
1	CA	545	C
1	CA	547	A
1	CA	559	A
1	CA	560	U
1	CA	561	U
1	CA	572	A
1	CA	573	A
1	CA	576	G
1	CA	577	G
1	CA	596	C
1	CA	599	C
1	CA	630	G
1	CA	632	A
1	CA	633	G
1	CA	650	G
1	CA	653	A
1	CA	665	A
1	CA	680	C
1	CA	687	A
1	CA	688	G
1	CA	693	G
1	CA	695	A
1	CA	723	U
1	CA	731	G
1	CA	749	C
1	CA	752	G
1	CA	753	A
1	CA	755	G
1	CA	759	A
1	CA	760	G
1	CA	777	A
1	CA	792	A
1	CA	793	U
1	CA	794	A
1	CA	806	C
1	CA	815	A
1	CA	817	C

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Mol	Chain	Res	Type
1	CA	821	G
1	CA	828	A
1	CA	829	G
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	887	G
1	CA	902	G
1	CA	914	A
1	CA	926	G
1	CA	927	G
1	CA	934	C
1	CA	935	A
1	CA	960	U
1	CA	961	U
1	CA	968	A
1	CA	969	A
1	CA	971	G
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	999	C
1	CA	1002	G
1	CA	1003	G
1	CA	1005	A
1	CA	1019	C
1	CA	1020	U
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

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Mol	Chain	Res	Type
1	CA	1030	C
1	CA	1030(A)	G
1	CA	1030(C)	G
1	CA	1031	G
1	CA	1033	G
1	CA	1037	C
1	CA	1038	C
1	CA	1039	C
1	CA	1041	A
1	CA	1045	C
1	CA	1052	U
1	CA	1054	C
1	CA	1055	A
1	CA	1065	U
1	CA	1066	C
1	CA	1068	G
1	CA	1076	C
1	CA	1081	G
1	CA	1087	G
1	CA	1094	G
1	CA	1095	U
1	CA	1101	A
1	CA	1108	G
1	CA	1117	G
1	CA	1124	G
1	CA	1125	U
1	CA	1126	U
1	CA	1129	C
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	1145	C
1	CA	1146	A
1	CA	1147	C
1	CA	1152	A
1	CA	1154	G
1	CA	1157	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	CA	1159	U
1	CA	1160	G
1	CA	1166	G
1	CA	1183	A
1	CA	1184	G
1	CA	1196	U
1	CA	1197	G
1	CA	1202	G
1	CA	1211	U
1	CA	1212	U
1	CA	1213	A
1	CA	1227	A
1	CA	1228	C
1	CA	1238	A
1	CA	1240	U
1	CA	1244	C
1	CA	1256	A
1	CA	1257	U
1	CA	1258	G
1	CA	1260	C
1	CA	1262	C
1	CA	1270	C
1	CA	1273	G
1	CA	1278	U
1	CA	1279	A
1	CA	1280	A
1	CA	1281	U
1	CA	1282	C
1	CA	1287	A
1	CA	1299	A
1	CA	1300	G
1	CA	1305	G
1	CA	1314	C
1	CA	1317	C
1	CA	1320	C
1	CA	1322	C
1	CA	1340	A
1	CA	1346	A
1	CA	1347	G
1	CA	1363	C
1	CA	1364	U
1	CA	1370	G

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Mol	Chain	Res	Type
1	CA	1383	C
1	CA	1397	C
1	CA	1401	G
1	CA	1419	G
1	CA	1442	G
1	CA	1442(A)	G
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	1494	G
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	14	A
22	CV	24	A
23	CW	3	C
23	CW	5	G
23	CW	6	G
23	CW	8	4SU
23	CW	13	C
23	CW	14	A
23	CW	15	G
23	CW	19	G
23	CW	22	G
23	CW	23	A
23	CW	26	A
23	CW	27	G
23	CW	28	G
23	CW	29	G
23	CW	30	G
23	CW	34	G
23	CW	46	7MG
23	CW	47	U

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Mol	Chain	Res	Type
23	CW	48	C
23	CW	56	C
23	CW	61	C
23	CW	63	G
23	CW	65	G
23	CW	66	U
23	CW	68	C
23	CW	70	G
23	CW	71	G
23	CW	74	C
23	CW	75	C
23	CW	76	A
24	CX	9	G
24	CX	13	C
24	CX	16	C
24	CX	18	G
24	CX	19	G
24	CX	20	U
24	CX	21	A
24	CX	31	G
24	CX	34	C
24	CX	42	G
24	CX	47	U
24	CX	48	C
24	CX	52	G
24	CX	56	C
24	CX	58	A
24	CX	60	U
24	CX	62	C
24	CX	63	G
24	CX	67	C
24	CX	68	C
24	CX	76	A
23	CY	3	C
23	CY	8	4SU
23	CY	11	C
23	CY	13	C
23	CY	19	G
23	CY	23	A
23	CY	26	A
23	CY	30	G
23	CY	31	A

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Mol	Chain	Res	Type
23	CY	33	U
23	CY	34	G
23	CY	35	A
23	CY	39	PSU
23	CY	41	C
23	CY	44	G
23	CY	46	7MG
23	CY	47	U
23	CY	49	C
23	CY	51	U
23	CY	53	G
23	CY	54	5MU
23	CY	56	C
23	CY	57	G
23	CY	58	A
23	CY	59	U
23	CY	61	C
23	CY	62	C
23	CY	65	G
23	CY	67	C
23	CY	70	G
23	CY	72	C
25	DA	10	G
25	DA	12	U
25	DA	15	G
25	DA	34	C
25	DA	45	C
25	DA	61	G
25	DA	71	A
25	DA	74	A
25	DA	75	G
25	DA	78	A
25	DA	79	G
25	DA	84	A
25	DA	94	C
25	DA	95	G
25	DA	100	G
25	DA	118	A
25	DA	119	A
25	DA	120	U
25	DA	125	G
25	DA	141	A

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Mol	Chain	Res	Type
25	DA	157	U
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	232	G
25	DA	233	A
25	DA	248	G
25	DA	250	G
25	DA	266	G
25	DA	271(K)	U
25	DA	271(L)	U
25	DA	271(M)	G
25	DA	271(N)	U
25	DA	272	G
25	DA	272(A)	U
25	DA	272(B)	G
25	DA	272(I)	U
25	DA	272(J)	C
25	DA	274	G
25	DA	277	C
25	DA	278	A
25	DA	292	C
25	DA	311	A
25	DA	329	G
25	DA	330	A
25	DA	342	G
25	DA	352	G
25	DA	353	G
25	DA	361	G
25	DA	363	G
25	DA	363(C)	G
25	DA	363(D)	G
25	DA	380	U
25	DA	386	G

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Mol	Chain	Res	Type
25	DA	396	G
25	DA	405	U
25	DA	406	G
25	DA	407	G
25	DA	411	G
25	DA	412	A
25	DA	421	U
25	DA	422	A
25	DA	428	A
25	DA	443	A
25	DA	444	C
25	DA	455	C
25	DA	456	C
25	DA	457	A
25	DA	470	A
25	DA	475	U
25	DA	481	G
25	DA	496	G
25	DA	505	A
25	DA	509	C
25	DA	512	G
25	DA	529	A
25	DA	531	C
25	DA	532	A
25	DA	533	G
25	DA	545	G
25	DA	555	U
25	DA	563	G
25	DA	568	U
25	DA	573	G
25	DA	575	A
25	DA	587	C
25	DA	588	U
25	DA	592	G
25	DA	595	C
25	DA	599	G
25	DA	603	A
25	DA	604	G
25	DA	607	U
25	DA	614(B)	G
25	DA	614(C)	A
25	DA	615	G

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Mol	Chain	Res	Type
25	DA	616	G
25	DA	627	A
25	DA	637	A
25	DA	645	C
25	DA	646	A
25	DA	647	G
25	DA	652(B)	A
25	DA	652(C)	G
25	DA	652(D)	C
25	DA	652(U)	G
25	DA	669	G
25	DA	686	G
25	DA	717	G
25	DA	726	G
25	DA	730	C
25	DA	752	A
25	DA	753	C
25	DA	765	G
25	DA	775	G
25	DA	776	G
25	DA	782	A
25	DA	784	A
25	DA	785	G
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	857	C
25	DA	859	G
25	DA	866	A
25	DA	867	C
25	DA	874	G
25	DA	878	A
25	DA	879	G
25	DA	880	G
25	DA	882	G
25	DA	884	C
25	DA	886	C
25	DA	887	A
25	DA	888	C

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Mol	Chain	Res	Type
25	DA	889	C
25	DA	890	A
25	DA	893	C
25	DA	894	C
25	DA	896	A
25	DA	897	C
25	DA	900	A
25	DA	901	A
25	DA	903	C
25	DA	910	A
25	DA	915	C
25	DA	917	A
25	DA	932	G
25	DA	933	A
25	DA	938	G
25	DA	941	A
25	DA	944	G
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	980	A
25	DA	983	A
25	DA	987	G
25	DA	996	A
25	DA	1005	C
25	DA	1012	U
25	DA	1013	C
25	DA	1022	G
25	DA	1025	G
25	DA	1026	U
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

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Mol	Chain	Res	Type
25	DA	1118	C
25	DA	1127	A
25	DA	1128	A
25	DA	1129	A
25	DA	1133	U
25	DA	1135	C
25	DA	1136	G
25	DA	1139	G
25	DA	1142(A)	A
25	DA	1157	G
25	DA	1170	G
25	DA	1171	G
25	DA	1188	U
25	DA	1206	G
25	DA	1210	A
25	DA	1211	U
25	DA	1220	A
25	DA	1247	A
25	DA	1253	A
25	DA	1256	G
25	DA	1262	A
25	DA	1271	G
25	DA	1272	A
25	DA	1273	U
25	DA	1300	U
25	DA	1301	A
25	DA	1303	G
25	DA	1314	C
25	DA	1319	G
25	DA	1320	C
25	DA	1321	A
25	DA	1327	C
25	DA	1352	U
25	DA	1359	A
25	DA	1360	A
25	DA	1365	A
25	DA	1368	G
25	DA	1379	A
25	DA	1384	A
25	DA	1385	G
25	DA	1386	C
25	DA	1416	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
25	DA	1417	C
25	DA	1419	A
25	DA	1420	U
25	DA	1421	G
25	DA	1428	C
25	DA	1437	C
25	DA	1445	A
25	DA	1449	A
25	DA	1450	G
25	DA	1460	A
25	DA	1471	A
25	DA	1482	G
25	DA	1490	A
25	DA	1493	C
25	DA	1494	A
25	DA	1497	U
25	DA	1504	C
25	DA	1505	C
25	DA	1508	A
25	DA	1509	C
25	DA	1509(A)	A
25	DA	1512	U
25	DA	1531	C
25	DA	1532	C
25	DA	1533	G
25	DA	1542	A
25	DA	1547	C
25	DA	1554	A
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	1582	C
25	DA	1584	C
25	DA	1586	A
25	DA	1594	G
25	DA	1598	C
25	DA	1608	A
25	DA	1609	A
25	DA	1610	A

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Mol	Chain	Res	Type
25	DA	1640	C
25	DA	1648	C
25	DA	1654	A
25	DA	1674	G
25	DA	1696	G
25	DA	1700	A
25	DA	1701	A
25	DA	1703	G
25	DA	1721	G
25	DA	1722	A
25	DA	1746	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	1800	C
25	DA	1801	G
25	DA	1812	A
25	DA	1816	G
25	DA	1828	G
25	DA	1829	A
25	DA	1833	U
25	DA	1835	G
25	DA	1848	A
25	DA	1877	A
25	DA	1878	G
25	DA	1895	C
25	DA	1896	G
25	DA	1900	A
25	DA	1906	G
25	DA	1913	A
25	DA	1914	C
25	DA	1927	A
25	DA	1929	G
25	DA	1930	G
25	DA	1937	A
25	DA	1938	A
25	DA	1945	G

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Mol	Chain	Res	Type
25	DA	1955	U
25	DA	1963	U
25	DA	1966	A
25	DA	1967	C
25	DA	1970	A
25	DA	1971	A
25	DA	1972	A
25	DA	1993	U
25	DA	1997	G
25	DA	2020	A
25	DA	2023	G
25	DA	2031	A
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	2097	C
25	DA	2101	G
25	DA	2104	G
25	DA	2109	U
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	2120	G
25	DA	2122	U
25	DA	2124	G
25	DA	2126	A
25	DA	2127	G
25	DA	2128	C
25	DA	2129	C
25	DA	2130	U
25	DA	2131	G
25	DA	2132	U
25	DA	2133	G

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Mol	Chain	Res	Type
25	DA	2134	A
25	DA	2135	A
25	DA	2136	C
25	DA	2137	C
25	DA	2139	C
25	DA	2142	C
25	DA	2143	C
25	DA	2144	U
25	DA	2145	C
25	DA	2146	C
25	DA	2147	G
25	DA	2148	G
25	DA	2150	U
25	DA	2155	G
25	DA	2156	G
25	DA	2157	G
25	DA	2158	A
25	DA	2159	G
25	DA	2160	G
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	2174	C
25	DA	2177	C
25	DA	2178	C
25	DA	2181	G
25	DA	2185	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	2219	G
25	DA	2225	A
25	DA	2238	G
25	DA	2239	G

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Mol	Chain	Res	Type
25	DA	2268	A
25	DA	2269	A
25	DA	2273	A
25	DA	2275	C
25	DA	2278	A
25	DA	2280	G
25	DA	2283	C
25	DA	2287	A
25	DA	2293	C
25	DA	2305	A
25	DA	2308	G
25	DA	2309	A
25	DA	2312	U
25	DA	2319	G
25	DA	2320	A
25	DA	2321	G
25	DA	2322	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	2352	A
25	DA	2376	A
25	DA	2379	G
25	DA	2383	G
25	DA	2385	C
25	DA	2399	G
25	DA	2406	U
25	DA	2410	G
25	DA	2422	A
25	DA	2423	U
25	DA	2425	A
25	DA	2426	A
25	DA	2429	G
25	DA	2430	A
25	DA	2434	A
25	DA	2435	A
25	DA	2439	A
25	DA	2441	C

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Mol	Chain	Res	Type
25	DA	2445	G
25	DA	2448	A
25	DA	2459	A
25	DA	2468	G
25	DA	2476	A
25	DA	2484	G
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	2518	A
25	DA	2520	C
25	DA	2525	G
25	DA	2536	G
25	DA	2542	A
25	DA	2554	U
25	DA	2555	U
25	DA	2566	A
25	DA	2567	G
25	DA	2573	C
25	DA	2579	C
25	DA	2584	U
25	DA	2585	U
25	DA	2586	C
25	DA	2602	A
25	DA	2603	G
25	DA	2609	U
25	DA	2611	U
25	DA	2612	C
25	DA	2615	U
25	DA	2629	A
25	DA	2630	G
25	DA	2632	A
25	DA	2646	C
25	DA	2652	C
25	DA	2654	A
25	DA	2663	G
25	DA	2673	G
25	DA	2689	U
25	DA	2690	C

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Mol	Chain	Res	Type
25	DA	2691	C
25	DA	2702	U
25	DA	2712(A)	A
25	DA	2713	A
25	DA	2714	G
25	DA	2718	G
25	DA	2726	U
25	DA	2732	G
25	DA	2733	A
25	DA	2739	U
25	DA	2751	G
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	2793	G
25	DA	2794	C
25	DA	2802	G
25	DA	2809	A
25	DA	2818	G
25	DA	2820	A
25	DA	2821	A
25	DA	2833	G
25	DA	2835	A
25	DA	2836	U
25	DA	2872	G
25	DA	2879	C
25	DA	2880	C
25	DA	2892	A
25	DA	2893	G
25	DA	2894	G
25	DA	2895	U
25	DA	2897	U
26	DB	2	C
26	DB	7	G
26	DB	9	G
26	DB	13	A
26	DB	30	C
26	DB	32	C

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Mol	Chain	Res	Type
26	DB	56	G
26	DB	66	A
26	DB	73	A
26	DB	75	G
26	DB	85	G
26	DB	89	G
26	DB	108	U
26	DB	110	G

All (121) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	115	G
1	AA	266	G
1	AA	345	C
1	AA	347	G
1	AA	429	U
1	AA	509	A
1	AA	560	U
1	AA	687	A
1	AA	748	C
1	AA	793	U
1	AA	839	U
1	AA	913	A
1	AA	991	U
1	AA	1008	C
1	AA	1026	G
1	AA	1027	C
1	AA	1029	C
1	AA	1064	G
1	AA	1065	U
1	AA	1067	A
1	AA	1190	G
1	AA	1201	A
1	AA	1212	U
1	AA	1256	A
1	AA	1285	A
1	AA	1442	G
1	AA	1492	A
23	AW	22	G
24	AX	20	U
24	AX	47	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
23	AY	18	G
23	AY	21	A
23	AY	25	C
23	AY	58	A
25	BA	184	A
25	BA	185	A
25	BA	273	G
25	BA	302	A
25	BA	793	A
25	BA	811	A
25	BA	1019	G
25	BA	1093	G
25	BA	1219	A
25	BA	1220	U
25	BA	1221	G
25	BA	1255	A
25	BA	1425	A
25	BA	1577	C
25	BA	1700	G
25	BA	2014	G
25	BA	2140	U
25	BA	2148	A
25	BA	2156	A
25	BA	2166	U
25	BA	2170	G
25	BA	2203	G
25	BA	2347	A
25	BA	2418	U
25	BA	2613	C
25	BA	2701	U
25	BA	2769	U
25	BA	2902	G
26	BB	56	G
26	BB	109	C
1	CA	60	A
1	CA	115	G
1	CA	251	G
1	CA	266	G
1	CA	429	U
1	CA	509	A
1	CA	532	A
1	CA	560	U

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Mol	Chain	Res	Type
1	CA	687	A
1	CA	748	C
1	CA	793	U
1	CA	913	A
1	CA	991	U
1	CA	992	U
1	CA	1027	C
1	CA	1064	G
1	CA	1065	U
1	CA	1067	A
1	CA	1128	C
1	CA	1183	A
1	CA	1201	A
1	CA	1256	A
1	CA	1442	G
1	CA	1492	A
23	CW	4	C
23	CW	13	C
24	CX	20	U
23	CY	18	G
25	DA	195	A
25	DA	196	A
25	DA	249	C
25	DA	271(K)	U
25	DA	277	C
25	DA	587	C
25	DA	752	A
25	DA	774	A
25	DA	827	U
25	DA	856	C
25	DA	900	A
25	DA	1210	A
25	DA	1300	U
25	DA	1301	A
25	DA	1427	A
25	DA	1493	C
25	DA	1558	A
25	DA	1653	G
25	DA	1913	A
25	DA	1992	G
25	DA	2110	G
25	DA	2126	A

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Mol	Chain	Res	Type
25	DA	2134	A
25	DA	2321	G
25	DA	2351	G
25	DA	2422	A
25	DA	2602	A
25	DA	2689	U
25	DA	2756	U

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

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	23	13,21,22	1.21	1 (7%)	18,30,33	3.54	6 (33%)
23	MIA	AW	37	23	21,31,32	1.79	3 (14%)	26,44,47	1.57	7 (26%)
23	PSU	AW	39	23	13,21,22	1.39	1 (7%)	18,30,33	3.82	6 (33%)
23	7MG	AW	46	23	19,26,27	1.05	1 (5%)	24,39,42	2.85	6 (25%)
23	5MU	AW	54	23	12,22,23	0.31	0	14,32,35	2.53	2 (14%)
23	PSU	AW	55	23	13,21,22	1.14	1 (7%)	18,30,33	3.88	6 (33%)
23	4SU	AW	8	23	11,21,22	1.12	1 (9%)	13,30,33	1.37	1 (7%)
24	5MC	AX	32	24	13,22,23	1.30	1 (7%)	15,32,35	1.05	1 (6%)
24	5MU	AX	54	24	12,22,23	0.34	0	14,32,35	2.42	2 (14%)
24	PSU	AX	55	24	13,21,22	1.48	1 (7%)	18,30,33	3.34	6 (33%)
24	4SU	AX	8	24	11,21,22	1.17	1 (9%)	13,30,33	1.86	1 (7%)
23	PSU	AY	32	23	13,21,22	1.35	1 (7%)	18,30,33	3.23	6 (33%)
23	MIA	AY	37	23	15,24,32	1.24	2 (13%)	16,35,47	2.22	2 (12%)
23	PSU	AY	39	23	13,21,22	1.12	2 (15%)	18,30,33	3.30	5 (27%)
23	7MG	AY	46	23	19,26,27	1.12	1 (5%)	24,39,42	3.09	7 (29%)
23	5MU	AY	54	23	12,22,23	0.30	0	14,32,35	2.93	2 (14%)
23	PSU	AY	55	23	13,21,22	1.18	1 (7%)	18,30,33	3.18	5 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	4SU	AY	8	23	11,21,22	1.12	1 (9%)	13,30,33	1.47	1 (7%)
23	PSU	CW	32	23	13,21,22	1.22	1 (7%)	18,30,33	3.37	6 (33%)
23	MIA	CW	37	23	15,24,32	1.19	2 (13%)	16,35,47	2.34	2 (12%)
23	PSU	CW	39	23	13,21,22	1.29	1 (7%)	18,30,33	3.28	6 (33%)
23	7MG	CW	46	23	19,26,27	1.05	1 (5%)	24,39,42	3.03	7 (29%)
23	5MU	CW	54	23	12,22,23	0.43	0	14,32,35	2.88	2 (14%)
23	PSU	CW	55	23	13,21,22	1.03	1 (7%)	18,30,33	3.61	6 (33%)
23	4SU	CW	8	23	11,21,22	1.20	1 (9%)	13,30,33	1.23	1 (7%)
24	5MC	CX	32	24	13,22,23	1.38	1 (7%)	15,32,35	0.96	1 (6%)
24	5MU	CX	54	24	12,22,23	0.42	0	14,32,35	2.07	2 (14%)
24	PSU	CX	55	24	13,21,22	1.18	1 (7%)	18,30,33	3.42	6 (33%)
24	4SU	CX	8	24	11,21,22	1.15	1 (9%)	13,30,33	1.76	1 (7%)
23	PSU	CY	32	23	13,21,22	0.97	1 (7%)	18,30,33	3.45	5 (27%)
23	MIA	CY	37	23	15,24,32	1.26	2 (13%)	16,35,47	2.18	2 (12%)
23	PSU	CY	39	23	13,21,22	1.39	2 (15%)	18,30,33	2.93	6 (33%)
23	7MG	CY	46	23	19,26,27	1.12	1 (5%)	24,39,42	2.89	6 (25%)
23	5MU	CY	54	23	12,22,23	0.37	0	14,32,35	2.21	2 (14%)
23	PSU	CY	55	23	13,21,22	0.88	1 (7%)	18,30,33	3.64	6 (33%)
23	4SU	CY	8	23	11,21,22	1.20	1 (9%)	13,30,33	1.36	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	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	-	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	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
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	-6.81	1.70	1.75
24	AX	55	PSU	C5-C1'	-4.77	1.48	1.52
23	AW	39	PSU	C5-C1'	-4.58	1.48	1.52
23	AY	32	PSU	C5-C1'	-4.40	1.48	1.52
23	CW	39	PSU	C5-C1'	-4.19	1.48	1.52
23	CY	39	PSU	C5-C1'	-4.12	1.48	1.52
23	AW	32	PSU	C5-C1'	-3.85	1.48	1.52
23	CW	32	PSU	C5-C1'	-3.84	1.48	1.52
24	CX	55	PSU	C5-C1'	-3.72	1.49	1.52
23	AY	55	PSU	C5-C1'	-3.69	1.49	1.52
24	AX	8	4SU	C4-S4	-3.64	1.60	1.67
23	CW	8	4SU	C4-S4	-3.63	1.60	1.67
23	CY	8	4SU	C4-S4	-3.60	1.60	1.67
24	CX	8	4SU	C4-S4	-3.53	1.60	1.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AW	55	PSU	C5-C1'	-3.50	1.49	1.52
23	AW	8	4SU	C4-S4	-3.47	1.60	1.67
23	AY	8	4SU	C4-S4	-3.35	1.61	1.67
23	CW	55	PSU	C5-C1'	-3.06	1.49	1.52
23	CY	32	PSU	C5-C1'	-2.82	1.49	1.52
23	AY	39	PSU	C5-C1'	-2.76	1.49	1.52
23	CY	55	PSU	C5-C1'	-2.68	1.49	1.52
23	AY	39	PSU	O4'-C1'	-2.60	1.40	1.44
23	CY	39	PSU	O4'-C1'	-2.11	1.41	1.44
23	AW	37	MIA	C6-N1	2.14	1.36	1.33
23	CW	37	MIA	C2-N3	2.32	1.36	1.32
23	CY	37	MIA	C2-N3	2.34	1.36	1.32
23	AY	37	MIA	C2-N3	2.37	1.36	1.32
23	AW	37	MIA	C5-C4	3.00	1.47	1.40
23	CW	46	7MG	C5-C4	3.10	1.47	1.39
23	AW	46	7MG	C5-C4	3.14	1.48	1.39
23	CY	46	7MG	C5-C4	3.19	1.48	1.39
23	CW	37	MIA	C5-C4	3.25	1.47	1.40
23	AY	46	7MG	C5-C4	3.30	1.48	1.39
23	AY	37	MIA	C5-C4	3.43	1.48	1.40
23	CY	37	MIA	C5-C4	3.56	1.48	1.40
24	AX	32	5MC	C5-C4	4.49	1.48	1.41
24	CX	32	5MC	C5-C4	4.79	1.48	1.41

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	AW	55	PSU	N1-C2-N3	-12.34	120.46	128.33
23	AW	39	PSU	N1-C2-N3	-11.99	120.68	128.33
23	CY	32	PSU	N1-C2-N3	-11.22	121.17	128.33
23	AW	32	PSU	N1-C2-N3	-11.12	121.24	128.33
24	CX	55	PSU	N1-C2-N3	-10.85	121.41	128.33
23	CW	55	PSU	N1-C2-N3	-10.74	121.48	128.33
23	CW	32	PSU	N1-C2-N3	-10.65	121.54	128.33
23	CY	55	PSU	N1-C2-N3	-10.50	121.63	128.33
23	AY	39	PSU	N1-C2-N3	-10.19	121.83	128.33
24	AX	55	PSU	N1-C2-N3	-10.15	121.86	128.33
23	CW	39	PSU	N1-C2-N3	-10.11	121.88	128.33
23	AY	32	PSU	N1-C2-N3	-10.05	121.92	128.33
23	AY	55	PSU	N1-C2-N3	-10.01	121.95	128.33
23	CW	46	7MG	C5-C4-N3	-10.00	117.08	126.82
23	AY	46	7MG	C5-C4-N3	-9.20	117.85	126.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	CY	39	PSU	N1-C2-N3	-8.96	122.62	128.33
23	AW	46	7MG	C5-C4-N3	-8.25	118.78	126.82
23	CW	37	MIA	N3-C2-N1	-8.14	122.66	128.89
23	CY	46	7MG	C5-C4-N3	-7.93	119.09	126.82
23	AY	37	MIA	N3-C2-N1	-7.59	123.08	128.89
23	CY	37	MIA	N3-C2-N1	-7.52	123.13	128.89
24	AX	8	4SU	C5-C4-N3	-6.33	117.43	123.63
23	CY	55	PSU	C5-C1'-C2'	-6.03	104.82	115.52
24	CX	8	4SU	C5-C4-N3	-6.01	117.75	123.63
23	AW	54	5MU	C5-C4-N3	-5.96	118.50	125.14
23	CW	54	5MU	C5-C4-N3	-5.90	118.56	125.14
23	AY	54	5MU	C5-C4-N3	-5.84	118.64	125.14
24	AX	54	5MU	C5-C4-N3	-5.48	119.03	125.14
23	CY	46	7MG	C5-C6-N1	-5.39	115.17	123.46
24	CX	54	5MU	C5-C4-N3	-5.30	119.23	125.14
23	CW	55	PSU	C5-C1'-C2'	-5.27	106.16	115.52
23	AY	46	7MG	C5-C6-N1	-5.15	115.54	123.46
23	CY	54	5MU	C5-C4-N3	-5.00	119.57	125.14
23	AW	46	7MG	C5-C6-N1	-4.98	115.81	123.46
23	AY	8	4SU	C5-C4-N3	-4.97	118.77	123.63
23	AW	55	PSU	C5-C1'-C2'	-4.93	106.77	115.52
23	AW	8	4SU	C5-C4-N3	-4.45	119.27	123.63
23	CW	46	7MG	C5-C6-N1	-4.40	116.69	123.46
23	CY	8	4SU	C5-C4-N3	-4.05	119.67	123.63
24	AX	55	PSU	C5-C6-N1	-3.93	118.85	124.39
24	CX	55	PSU	C5-C6-N1	-3.87	118.93	124.39
23	CW	8	4SU	C5-C4-N3	-3.81	119.90	123.63
23	CW	39	PSU	C5-C6-N1	-3.80	119.03	124.39
23	AW	32	PSU	C5-C1'-C2'	-3.76	108.85	115.52
23	AY	32	PSU	C5-C6-N1	-3.71	119.15	124.39
23	AW	39	PSU	C5-C6-N1	-3.56	119.36	124.39
23	CW	32	PSU	C5-C6-N1	-3.46	119.50	124.39
23	AW	37	MIA	C12-N6-C6	-3.43	119.15	123.42
23	AY	55	PSU	C5-C6-N1	-3.42	119.56	124.39
24	AX	55	PSU	C5-C1'-C2'	-3.35	109.57	115.52
23	AW	55	PSU	C5-C6-N1	-3.30	119.74	124.39
23	CW	37	MIA	C4-C5-N7	-3.24	106.50	109.48
23	AW	32	PSU	C5-C6-N1	-3.20	119.88	124.39
23	CW	55	PSU	C5-C6-N1	-3.16	119.93	124.39
23	CY	39	PSU	C5-C6-N1	-3.12	119.99	124.39
23	AY	37	MIA	C4-C5-N7	-3.11	106.61	109.48
23	CY	37	MIA	C4-C5-N7	-3.08	106.65	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	AW	37	MIA	C4-C5-N7	-3.04	106.69	109.48
23	CW	46	7MG	CM7-N7-C8	-3.00	112.01	120.52
23	CY	32	PSU	C5-C6-N1	-2.99	120.17	124.39
23	AW	46	7MG	CM7-N7-C8	-2.91	112.28	120.52
23	CY	55	PSU	C5-C6-N1	-2.79	120.45	124.39
23	AW	37	MIA	C5-C6-N1	-2.75	117.64	120.48
23	CY	46	7MG	CM7-N7-C8	-2.66	112.97	120.52
23	AW	39	PSU	C5-C1'-C2'	-2.66	110.80	115.52
23	AY	46	7MG	CM7-N7-C8	-2.62	113.09	120.52
23	CW	39	PSU	C5-C1'-C2'	-2.61	110.89	115.52
23	CY	39	PSU	C5-C1'-C2'	-2.48	111.11	115.52
23	CW	32	PSU	C5-C1'-C2'	-2.38	111.30	115.52
24	CX	55	PSU	C5-C1'-C2'	-2.34	111.36	115.52
23	AW	37	MIA	N3-C2-N1	-2.34	122.31	126.79
23	AY	32	PSU	C5-C1'-C2'	-2.12	111.75	115.52
23	AW	37	MIA	N6-C6-N1	2.01	121.12	118.52
23	AY	46	7MG	C2-N3-C4	2.01	120.41	114.53
23	AW	37	MIA	C11-S10-C2	2.02	103.55	102.26
23	AY	39	PSU	C5-C1'-C2'	2.04	119.14	115.52
23	AY	46	7MG	CM7-N7-C5	2.16	131.31	124.09
23	CY	46	7MG	CM7-N7-C5	2.18	131.37	124.09
23	CW	46	7MG	C2-N3-C4	2.25	121.10	114.53
23	AW	46	7MG	CM7-N7-C5	2.26	131.64	124.09
23	CW	46	7MG	CM7-N7-C5	2.26	131.64	124.09
23	AW	32	PSU	O4'-C1'-C2'	2.38	107.15	104.73
23	AW	55	PSU	O4'-C1'-C2'	2.38	107.16	104.73
24	AX	32	5MC	N4-C4-N3	2.39	120.41	116.95
24	CX	32	5MC	N4-C4-N3	2.45	120.50	116.95
23	CW	55	PSU	O4'-C1'-C2'	2.53	107.31	104.73
23	CY	39	PSU	O4'-C1'-C2'	2.57	107.34	104.73
23	AY	39	PSU	O4'-C1'-C2'	2.70	107.48	104.73
24	AX	55	PSU	O4'-C1'-C2'	2.72	107.50	104.73
23	CY	55	PSU	O4'-C1'-C2'	2.74	107.52	104.73
23	CY	32	PSU	O4'-C1'-C2'	2.82	107.61	104.73
23	CW	32	PSU	O4'-C1'-C2'	2.84	107.63	104.73
24	CX	55	PSU	O4'-C1'-C2'	2.87	107.66	104.73
23	AW	39	PSU	O4'-C1'-C2'	2.92	107.71	104.73
23	AY	32	PSU	O4'-C1'-C2'	3.00	107.79	104.73
23	AW	37	MIA	C2-N1-C6	3.06	122.33	113.35
23	CW	39	PSU	O4'-C1'-C2'	3.07	107.86	104.73
23	AY	39	PSU	C6-N1-C2	3.11	120.47	115.47
23	AY	55	PSU	O4'-C1'-C2'	3.27	108.06	104.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	CY	39	PSU	C6-N1-C2	3.65	121.34	115.47
23	CY	55	PSU	C6-N1-C2	3.66	121.36	115.47
23	CW	46	7MG	C6-N1-C2	3.86	121.30	115.94
23	CW	55	PSU	C6-N1-C2	3.94	121.80	115.47
23	AY	55	PSU	C6-N1-C2	3.95	121.82	115.47
23	AW	32	PSU	C6-N1-C2	4.05	121.99	115.47
23	AY	32	PSU	C6-N1-C2	4.06	122.00	115.47
24	AX	55	PSU	C6-N1-C2	4.10	122.06	115.47
23	CW	32	PSU	C6-N1-C2	4.12	122.09	115.47
23	CY	32	PSU	C6-N1-C2	4.14	122.12	115.47
23	AW	39	PSU	C6-N1-C2	4.15	122.14	115.47
23	CW	39	PSU	C6-N1-C2	4.17	122.18	115.47
23	AW	55	PSU	C6-N1-C2	4.46	122.64	115.47
24	CX	55	PSU	C6-N1-C2	4.49	122.68	115.47
23	AW	46	7MG	C6-N1-C2	4.99	122.86	115.94
24	CX	54	5MU	C4-N3-C2	5.32	119.84	115.25
23	AY	46	7MG	C6-N1-C2	5.36	123.37	115.94
23	CY	46	7MG	C6-N1-C2	5.61	123.72	115.94
23	CY	39	PSU	C4-N3-C2	5.73	120.20	115.25
23	AY	32	PSU	C4-N3-C2	6.18	120.59	115.25
23	AY	55	PSU	C4-N3-C2	6.21	120.61	115.25
23	CW	39	PSU	C4-N3-C2	6.26	120.66	115.25
23	CY	54	5MU	C4-N3-C2	6.30	120.70	115.25
24	CX	55	PSU	C4-N3-C2	6.32	120.71	115.25
24	AX	55	PSU	C4-N3-C2	6.39	120.77	115.25
23	CW	32	PSU	C4-N3-C2	6.58	120.93	115.25
23	CY	46	7MG	N3-C4-N9	6.79	136.95	126.75
23	CY	32	PSU	C4-N3-C2	6.92	121.23	115.25
24	AX	54	5MU	C4-N3-C2	6.95	121.25	115.25
23	AW	55	PSU	C4-N3-C2	7.03	121.33	115.25
23	AW	32	PSU	C4-N3-C2	7.05	121.34	115.25
23	AW	54	5MU	C4-N3-C2	7.08	121.37	115.25
23	AW	46	7MG	N3-C4-N9	7.18	137.53	126.75
23	CW	55	PSU	C4-N3-C2	7.26	121.52	115.25
23	CY	55	PSU	C4-N3-C2	7.56	121.78	115.25
23	AY	39	PSU	C4-N3-C2	7.67	121.88	115.25
23	CW	46	7MG	N3-C4-N9	7.79	138.44	126.75
23	AY	46	7MG	N3-C4-N9	7.97	138.72	126.75
23	AW	39	PSU	C4-N3-C2	8.23	122.36	115.25
23	CW	54	5MU	C4-N3-C2	8.64	122.72	115.25
23	AY	54	5MU	C4-N3-C2	8.98	123.01	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

24 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	AW	32	PSU	1	0
23	AW	39	PSU	1	0
23	AW	46	7MG	1	0
23	AW	54	5MU	2	0
23	AW	55	PSU	3	0
23	AW	8	4SU	1	0
24	AX	8	4SU	1	0
23	AY	37	MIA	2	0
23	AY	39	PSU	1	0
23	AY	54	5MU	3	0
23	AY	55	PSU	3	0
23	AY	8	4SU	4	0
23	CW	32	PSU	1	0
23	CW	39	PSU	3	0
23	CW	46	7MG	3	0
23	CW	8	4SU	2	0
24	CX	54	5MU	2	0
24	CX	55	PSU	1	0
24	CX	8	4SU	1	0
23	CY	37	MIA	1	0
23	CY	39	PSU	1	0
23	CY	46	7MG	5	0
23	CY	54	5MU	1	0
23	CY	55	PSU	5	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2048 ligands modelled in this entry, 2027 are monoatomic - leaving 21 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	NEG	AA	3216	56	11,16,16	8.67	1 (9%)	12,20,20	3.24	4 (33%)
57	NEG	AA	3217	-	11,16,16	7.85	1 (9%)	12,20,20	2.91	4 (33%)
57	NEG	AA	3218	56	11,16,16	8.40	1 (9%)	12,20,20	1.84	3 (25%)
57	NEG	AA	3219	-	11,16,16	8.06	1 (9%)	12,20,20	2.34	4 (33%)
57	NEG	AA	3220	-	11,16,16	7.84	1 (9%)	12,20,20	2.14	3 (25%)
57	NEG	AA	3221	-	11,16,16	8.87	1 (9%)	12,20,20	2.05	3 (25%)
57	NEG	AA	3222	-	11,16,16	8.22	1 (9%)	12,20,20	1.76	2 (16%)
58	SF4	AD	501	4	0,12,12	0.00	-	0,24,24	0.00	-
57	NEG	AW	3004	-	11,16,16	7.94	1 (9%)	12,20,20	2.74	4 (33%)
57	NEG	AX	3013	-	11,16,16	8.77	1 (9%)	12,20,20	2.98	5 (41%)
57	NEG	CA	3170	56	11,16,16	8.43	1 (9%)	12,20,20	1.41	2 (16%)
57	NEG	CA	3171	-	11,16,16	7.92	1 (9%)	12,20,20	3.33	5 (41%)
57	NEG	CA	3172	-	11,16,16	8.61	1 (9%)	12,20,20	2.29	3 (25%)
57	NEG	CA	3173	-	11,16,16	8.19	1 (9%)	12,20,20	1.82	3 (25%)
57	NEG	CA	3174	-	11,16,16	7.74	1 (9%)	12,20,20	3.98	3 (25%)
57	NEG	CA	3175	-	11,16,16	8.50	2 (18%)	12,20,20	3.10	7 (58%)
57	NEG	CA	3176	-	11,16,16	8.37	1 (9%)	12,20,20	1.64	2 (16%)
57	NEG	CA	3177	-	11,16,16	7.43	2 (18%)	12,20,20	3.75	6 (50%)
58	SF4	CD	302	4	0,12,12	0.00	-	0,24,24	0.00	-
57	NEG	CW	3002	-	11,16,16	7.97	1 (9%)	12,20,20	2.47	4 (33%)
57	NEG	CX	3004	-	11,16,16	8.31	1 (9%)	12,20,20	1.83	3 (25%)

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	NEG	AA	3216	56	-	0/15/18/18	0/0/0/0
57	NEG	AA	3217	-	-	0/15/18/18	0/0/0/0
57	NEG	AA	3218	56	-	0/15/18/18	0/0/0/0
57	NEG	AA	3219	-	-	0/15/18/18	0/0/0/0
57	NEG	AA	3220	-	-	0/15/18/18	0/0/0/0
57	NEG	AA	3221	-	-	0/15/18/18	0/0/0/0
57	NEG	AA	3222	-	-	0/15/18/18	0/0/0/0

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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	NEG	AW	3004	-	-	0/15/18/18	0/0/0/0
57	NEG	AX	3013	-	-	0/15/18/18	0/0/0/0
57	NEG	CA	3170	56	-	0/15/18/18	0/0/0/0
57	NEG	CA	3171	-	-	0/15/18/18	0/0/0/0
57	NEG	CA	3172	-	-	0/15/18/18	0/0/0/0
57	NEG	CA	3173	-	-	0/15/18/18	0/0/0/0
57	NEG	CA	3174	-	-	0/15/18/18	0/0/0/0
57	NEG	CA	3175	-	-	0/15/18/18	0/0/0/0
57	NEG	CA	3176	-	-	0/15/18/18	0/0/0/0
57	NEG	CA	3177	-	-	0/15/18/18	0/0/0/0
58	SF4	CD	302	4	-	0/0/48/48	0/6/5/5
57	NEG	CW	3002	-	-	0/15/18/18	0/0/0/0
57	NEG	CX	3004	-	-	0/15/18/18	0/0/0/0

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	AA	3221	NEG	N2-N3	-29.34	1.11	1.41
57	AX	3013	NEG	N2-N3	-28.98	1.11	1.41
57	AA	3216	NEG	N2-N3	-28.69	1.11	1.41
57	CA	3172	NEG	N2-N3	-28.49	1.12	1.41
57	CA	3175	NEG	N2-N3	-28.07	1.12	1.41
57	CA	3170	NEG	N2-N3	-27.90	1.12	1.41
57	AA	3218	NEG	N2-N3	-27.77	1.12	1.41
57	CA	3176	NEG	N2-N3	-27.69	1.12	1.41
57	CX	3004	NEG	N2-N3	-27.53	1.13	1.41
57	AA	3222	NEG	N2-N3	-27.24	1.13	1.41
57	CA	3173	NEG	N2-N3	-27.06	1.13	1.41
57	AA	3219	NEG	N2-N3	-26.64	1.14	1.41
57	CW	3002	NEG	N2-N3	-26.33	1.14	1.41
57	AW	3004	NEG	N2-N3	-26.28	1.14	1.41
57	CA	3171	NEG	N2-N3	-26.21	1.14	1.41
57	AA	3217	NEG	N2-N3	-25.95	1.14	1.41
57	AA	3220	NEG	N2-N3	-25.86	1.14	1.41
57	CA	3174	NEG	N2-N3	-25.55	1.15	1.41
57	CA	3177	NEG	N2-N3	-24.43	1.16	1.41
57	CA	3175	NEG	C5-C6	2.19	1.55	1.51
57	CA	3177	NEG	C6-N2	2.51	1.37	1.34

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	AA	3216	NEG	C4-C5-C6	-8.07	103.90	112.61
57	CA	3171	NEG	C4-C5-C6	-7.81	104.18	112.61
57	AW	3004	NEG	C4-C5-C6	-7.11	104.94	112.61
57	AA	3217	NEG	C4-C5-C6	-6.55	105.54	112.61
57	CA	3172	NEG	C6-N2-N3	-5.89	114.40	120.32
57	CW	3002	NEG	C4-C5-C6	-5.39	106.79	112.61
57	AX	3013	NEG	C7-N3-N2	-5.12	102.11	110.00
57	CW	3002	NEG	C9-N3-C7	-4.94	104.56	121.82
57	CX	3004	NEG	C4-C5-C6	-4.74	107.49	112.61
57	AA	3221	NEG	C7-N3-N2	-4.54	103.00	110.00
57	AW	3004	NEG	C9-N3-C7	-4.33	106.68	121.82
57	CA	3176	NEG	C6-N2-N3	-3.90	116.40	120.32
57	AX	3013	NEG	C6-N2-N3	-3.82	116.48	120.32
57	AA	3218	NEG	C9-N3-C7	-3.80	108.55	121.82
57	CA	3172	NEG	C4-C5-C6	-3.72	108.60	112.61
57	AA	3219	NEG	C9-N3-C7	-3.64	109.10	121.82
57	AA	3218	NEG	C6-N2-N3	-3.48	116.83	120.32
57	CA	3176	NEG	C9-N3-C7	-3.41	109.90	121.82
57	CA	3177	NEG	C9-N3-C7	-3.33	110.17	121.82
57	AA	3221	NEG	C9-N3-C7	-3.29	110.31	121.82
57	CA	3172	NEG	C9-N3-C7	-3.17	110.75	121.82
57	AA	3222	NEG	C4-C5-C6	-3.14	109.22	112.61
57	AA	3220	NEG	C9-N3-C7	-3.13	110.89	121.82
57	AA	3218	NEG	C4-C5-C6	-3.10	109.27	112.61
57	CA	3174	NEG	C4-C5-C6	-3.00	109.37	112.61
57	AA	3216	NEG	C7-N3-N2	-2.93	105.48	110.00
57	CX	3004	NEG	C9-N3-C7	-2.90	111.69	121.82
57	CA	3177	NEG	C4-C5-C6	-2.89	109.49	112.61
57	CA	3175	NEG	O4-C6-N2	-2.87	120.45	123.81
57	AW	3004	NEG	C6-N2-N3	-2.81	117.49	120.32
57	AA	3217	NEG	C9-N3-C7	-2.79	112.06	121.82
57	CA	3173	NEG	C9-N3-C7	-2.69	112.42	121.82
57	CA	3173	NEG	C4-C5-C6	-2.68	109.72	112.61
57	CA	3171	NEG	C9-N3-C7	-2.56	112.87	121.82
57	AX	3013	NEG	C9-N3-C7	-2.20	114.15	121.82
57	CW	3002	NEG	C6-N2-N3	-2.18	118.13	120.32
57	CA	3175	NEG	C9-N3-C7	-2.10	114.48	121.82
57	CA	3175	NEG	O4-C6-C5	-2.07	118.29	121.30
57	AA	3216	NEG	C9-N3-C7	-2.00	114.83	121.82
57	CA	3177	NEG	O4-C6-N2	2.01	126.16	123.81
57	CA	3171	NEG	O4-C6-N2	2.15	126.33	123.81
57	CX	3004	NEG	C9-N3-N2	2.28	111.42	109.17
57	AW	3004	NEG	C5-C6-N2	2.40	117.37	114.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	CW	3002	NEG	C5-C6-N2	2.62	117.63	114.57
57	CA	3170	NEG	C9-N3-N2	2.66	111.79	109.17
57	CA	3175	NEG	C9-N3-N2	2.85	111.99	109.17
57	AA	3217	NEG	C6-N2-N3	2.87	123.21	120.32
57	AA	3219	NEG	C7-N3-N2	3.02	114.66	110.00
57	CA	3170	NEG	C4-C5-C6	3.13	115.99	112.61
57	CA	3177	NEG	C7-N3-N2	3.22	114.96	110.00
57	AA	3220	NEG	C9-N3-N2	3.41	112.54	109.17
57	AA	3221	NEG	C5-C6-N2	3.51	118.67	114.57
57	CA	3175	NEG	C4-C5-C6	3.61	116.51	112.61
57	AA	3219	NEG	C9-N3-N2	4.19	113.31	109.17
57	AA	3220	NEG	C6-N2-N3	4.19	124.53	120.32
57	CA	3173	NEG	C9-N3-N2	4.22	113.33	109.17
57	AA	3222	NEG	C7-N3-N2	4.37	116.74	110.00
57	AA	3219	NEG	C6-N2-N3	4.47	124.81	120.32
57	CA	3171	NEG	C6-N2-N3	4.48	124.83	120.32
57	AX	3013	NEG	C9-N3-N2	5.02	114.13	109.17
57	AX	3013	NEG	C4-C5-C6	5.70	118.77	112.61
57	CA	3175	NEG	C5-C6-N2	5.72	121.26	114.57
57	AA	3217	NEG	C9-N3-N2	5.73	114.83	109.17
57	CA	3171	NEG	C9-N3-N2	6.13	115.23	109.17
57	CA	3175	NEG	C6-N2-N3	6.29	126.64	120.32
57	AA	3216	NEG	C9-N3-N2	6.51	115.60	109.17
57	CA	3177	NEG	C6-N2-N3	6.85	127.21	120.32
57	CA	3174	NEG	C6-N2-N3	8.06	128.42	120.32
57	CA	3177	NEG	C9-N3-N2	9.23	118.29	109.17
57	CA	3174	NEG	C9-N3-N2	10.29	119.34	109.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	AA	3216	NEG	7	0
57	AA	3217	NEG	1	0
57	AA	3218	NEG	1	0
57	AA	3219	NEG	1	0
57	AA	3220	NEG	4	0
57	AA	3221	NEG	4	0
57	AW	3004	NEG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	AX	3013	NEG	3	0
57	CA	3171	NEG	1	0
57	CA	3173	NEG	2	0
57	CA	3174	NEG	5	0
57	CA	3175	NEG	3	0
57	CA	3177	NEG	2	0
57	CW	3002	NEG	1	0
57	CX	3004	NEG	5	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	1496/1521 (98%)	0.58	34 (2%) 64 64	36, 68, 97, 112	0
1	CA	1503/1521 (98%)	0.43	33 (2%) 65 66	38, 71, 97, 111	0
2	AB	231/256 (90%)	0.59	15 (6%) 22 20	67, 83, 93, 99	0
2	CB	231/256 (90%)	1.07	45 (19%) 1 1	69, 85, 94, 100	0
3	AC	206/239 (86%)	0.87	32 (15%) 3 2	65, 78, 88, 96	0
3	CC	206/239 (86%)	1.14	41 (19%) 1 1	68, 80, 90, 96	0
4	AD	208/209 (99%)	0.92	30 (14%) 3 3	53, 68, 80, 87	0
4	CD	208/209 (99%)	0.90	17 (8%) 14 11	54, 67, 80, 90	0
5	AE	148/162 (91%)	0.82	10 (6%) 20 19	54, 70, 81, 86	0
5	CE	148/162 (91%)	0.95	17 (11%) 6 5	57, 72, 82, 88	0
6	AF	100/101 (99%)	0.55	2 (2%) 68 69	53, 67, 78, 87	0
6	CF	100/101 (99%)	0.20	0 100 100	54, 68, 80, 87	0
7	AG	155/156 (99%)	0.69	15 (9%) 10 7	62, 75, 86, 95	0
7	CG	155/156 (99%)	0.93	20 (12%) 5 4	63, 77, 86, 99	0
8	AH	137/138 (99%)	1.16	28 (20%) 1 1	57, 70, 78, 85	0
8	CH	137/138 (99%)	1.05	26 (18%) 2 1	60, 72, 81, 85	0
9	AI	127/128 (99%)	1.04	24 (18%) 2 1	57, 82, 90, 94	0
9	CI	127/128 (99%)	2.02	63 (49%) 0 0	65, 84, 91, 95	0
10	AJ	97/105 (92%)	1.31	33 (34%) 0 0	63, 85, 94, 98	0
10	CJ	96/105 (91%)	1.38	29 (30%) 1 0	65, 86, 94, 99	0
11	AK	114/129 (88%)	0.89	5 (4%) 38 37	47, 66, 78, 84	0
11	CK	114/129 (88%)	0.75	11 (9%) 10 8	49, 68, 79, 85	0
12	AL	122/132 (92%)	0.89	10 (8%) 14 11	48, 57, 69, 79	0
12	CL	122/132 (92%)	0.99	20 (16%) 2 2	50, 60, 71, 80	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AM	123/126 (97%)	0.59	5 (4%) 41 41	52, 70, 84, 96	0
13	CM	122/126 (96%)	1.19	24 (19%) 1 1	70, 83, 93, 99	0
14	AN	60/61 (98%)	1.52	18 (30%) 1 0	64, 77, 83, 89	0
14	CN	60/61 (98%)	2.74	35 (58%) 0 0	67, 80, 87, 90	0
15	AO	88/89 (98%)	0.60	4 (4%) 37 36	49, 66, 77, 84	0
15	CO	88/89 (98%)	0.79	11 (12%) 5 4	51, 67, 79, 85	0
16	AP	82/88 (93%)	1.10	10 (12%) 5 4	53, 67, 78, 82	0
16	CP	82/88 (93%)	0.85	2 (2%) 62 62	54, 66, 77, 82	0
17	AQ	99/105 (94%)	0.85	8 (8%) 15 12	53, 69, 81, 83	0
17	CQ	99/105 (94%)	1.69	33 (33%) 0 0	55, 70, 81, 85	0
18	AR	68/88 (77%)	0.62	3 (4%) 38 37	54, 67, 80, 82	0
18	CR	68/88 (77%)	0.40	2 (2%) 55 55	54, 69, 81, 85	0
19	AS	83/93 (89%)	0.66	3 (3%) 46 46	68, 80, 88, 97	0
19	CS	83/93 (89%)	1.25	21 (25%) 1 1	71, 82, 91, 97	0
20	AT	96/106 (90%)	0.72	7 (7%) 18 16	57, 69, 85, 90	0
20	CT	96/106 (90%)	0.98	15 (15%) 3 2	56, 69, 85, 90	0
21	AU	23/27 (85%)	1.38	7 (30%) 1 0	62, 71, 78, 81	0
21	CU	23/27 (85%)	2.04	11 (47%) 0 0	65, 74, 80, 83	0
22	AV	13/24 (54%)	1.90	6 (46%) 0 0	51, 61, 91, 97	0
22	CV	12/24 (50%)	1.69	4 (33%) 0 0	55, 65, 91, 92	0
23	AW	67/76 (88%)	1.44	21 (31%) 1 0	50, 93, 102, 108	0
23	AY	67/76 (88%)	1.34	19 (28%) 1 0	37, 101, 106, 107	0
23	CW	65/76 (85%)	1.27	17 (26%) 1 1	69, 100, 108, 110	0
23	CY	66/76 (86%)	1.30	14 (21%) 1 1	40, 101, 106, 107	0
24	AX	72/77 (93%)	0.78	4 (5%) 28 26	45, 69, 85, 96	0
24	CX	72/77 (93%)	0.63	5 (6%) 20 18	46, 72, 87, 98	0
25	BA	2822/2915 (96%)	0.99	82 (2%) 55 55	22, 42, 94, 110	0
25	DA	2800/2915 (96%)	0.48	78 (2%) 56 57	25, 47, 96, 113	0
26	BB	120/121 (99%)	0.64	0 100 100	41, 61, 72, 92	0
26	DB	120/121 (99%)	0.08	1 (0%) 87 88	48, 67, 78, 93	0
27	BD	275/276 (99%)	1.00	13 (4%) 35 34	21, 38, 55, 86	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
27	DD	275/276 (99%)	0.77	9 (3%)	50	50	23, 41, 57, 85	0
28	BE	204/206 (99%)	0.86	6 (2%)	55	55	19, 45, 67, 84	0
28	DE	204/206 (99%)	0.58	6 (2%)	55	55	22, 49, 69, 84	0
29	BF	203/210 (96%)	0.78	7 (3%)	49	49	23, 50, 74, 95	0
29	DF	203/210 (96%)	0.67	14 (6%)	20	18	25, 55, 77, 95	0
30	BG	181/182 (99%)	0.59	6 (3%)	50	50	52, 68, 82, 94	0
30	DG	181/182 (99%)	1.02	30 (16%)	2	2	57, 72, 84, 92	0
31	BH	174/180 (96%)	0.82	5 (2%)	55	55	51, 69, 80, 87	0
31	DH	174/180 (96%)	1.36	44 (25%)	1	1	57, 74, 84, 88	0
32	BI	146/148 (98%)	0.33	3 (2%)	67	68	45, 71, 84, 88	0
32	DI	146/148 (98%)	0.29	4 (2%)	58	58	46, 72, 84, 89	0
33	BN	140/140 (100%)	0.90	4 (2%)	55	55	32, 48, 69, 78	0
33	DN	140/140 (100%)	0.87	15 (10%)	8	6	37, 53, 72, 79	0
34	BO	122/122 (100%)	0.60	0	100	100	23, 39, 59, 65	0
34	DO	122/122 (100%)	1.06	14 (11%)	6	5	43, 58, 72, 84	0
35	BP	149/150 (99%)	0.82	4 (2%)	58	58	23, 53, 76, 82	0
35	DP	149/150 (99%)	0.95	20 (13%)	4	3	28, 57, 78, 83	0
36	BQ	141/141 (100%)	1.18	18 (12%)	5	4	32, 53, 69, 81	0
36	DQ	141/141 (100%)	1.14	27 (19%)	2	1	36, 58, 73, 82	0
37	BR	118/118 (100%)	0.79	3 (2%)	61	61	19, 33, 48, 59	0
37	DR	118/118 (100%)	0.74	3 (2%)	61	61	32, 51, 65, 78	0
38	BS	110/112 (98%)	0.73	1 (0%)	85	86	36, 50, 67, 72	0
38	DS	110/112 (98%)	0.54	7 (6%)	23	21	64, 77, 88, 94	0
39	BT	131/146 (89%)	0.50	2 (1%)	76	76	28, 41, 69, 88	0
39	DT	131/146 (89%)	0.83	10 (7%)	17	15	45, 60, 78, 88	0
40	BU	116/118 (98%)	0.84	2 (1%)	73	74	17, 29, 43, 67	0
40	DU	116/118 (98%)	1.23	27 (23%)	1	1	36, 64, 80, 89	0
41	BV	101/101 (100%)	0.46	0	100	100	18, 36, 55, 73	0
41	DV	101/101 (100%)	1.26	21 (20%)	1	1	42, 77, 87, 93	0
42	BW	112/113 (99%)	0.83	3 (2%)	58	58	17, 29, 52, 89	0
42	DW	112/113 (99%)	0.88	6 (5%)	29	28	35, 49, 71, 91	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
43	BX	95/96 (98%)	0.57	2 (2%) 67 68	15, 33, 65, 84	0
43	DX	95/96 (98%)	1.17	16 (16%) 2 2	38, 57, 76, 84	0
44	BY	107/110 (97%)	0.47	1 (0%) 85 86	33, 48, 75, 84	0
44	DY	107/110 (97%)	1.56	31 (28%) 1 0	54, 70, 86, 93	0
45	BZ	171/206 (83%)	1.32	30 (17%) 2 1	38, 69, 102, 108	0
45	DZ	174/206 (84%)	1.56	51 (29%) 1 0	71, 88, 101, 108	0
46	B0	83/85 (97%)	1.10	9 (10%) 8 6	25, 37, 67, 83	0
46	D0	83/85 (97%)	1.68	19 (22%) 1 1	46, 69, 81, 91	0
47	B1	97/98 (98%)	0.95	5 (5%) 31 30	19, 40, 69, 76	0
47	D1	97/98 (98%)	0.71	2 (2%) 67 68	33, 53, 77, 79	0
48	B2	70/72 (97%)	0.65	1 (1%) 78 77	32, 42, 62, 80	0
48	D2	70/72 (97%)	0.84	5 (7%) 19 17	54, 70, 81, 84	0
49	B3	59/60 (98%)	0.59	0 100 100	22, 36, 55, 80	0
49	D3	59/60 (98%)	1.97	24 (40%) 0 0	52, 67, 82, 85	0
50	B4	69/71 (97%)	0.37	3 (4%) 39 38	53, 73, 93, 94	0
50	D4	69/71 (97%)	0.87	12 (17%) 2 1	76, 87, 99, 107	0
51	B5	59/60 (98%)	0.84	2 (3%) 49 49	18, 31, 46, 68	0
51	D5	59/60 (98%)	0.66	1 (1%) 73 74	28, 50, 68, 77	0
52	B6	53/54 (98%)	0.63	0 100 100	29, 40, 59, 67	0
52	D6	53/54 (98%)	0.89	4 (7%) 17 15	47, 61, 75, 79	0
53	B7	48/49 (97%)	1.10	6 (12%) 5 4	16, 25, 55, 66	0
53	D7	48/49 (97%)	1.30	6 (12%) 5 4	28, 37, 62, 71	0
54	B8	64/65 (98%)	0.77	2 (3%) 52 52	23, 32, 43, 58	0
54	D8	64/65 (98%)	1.45	15 (23%) 1 1	43, 57, 65, 71	0
55	B9	37/37 (100%)	1.45	9 (24%) 1 1	31, 50, 69, 75	0
55	D9	37/37 (100%)	1.54	13 (35%) 0 0	49, 60, 73, 77	0
All	All	20900/21748 (96%)	0.81	1633 (7%) 16 14	15, 62, 92, 113	0

All (1633) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	CG	82	GLY	17.6
13	CM	124	PRO	15.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
13	AM	123	ALA	13.8
45	BZ	111	VAL	12.9
45	BZ	115	GLY	12.5
13	CM	123	ALA	11.5
13	AM	124	PRO	11.4
14	CN	38	GLY	10.5
45	DZ	115	GLY	10.5
7	CG	83	ALA	10.1
46	D0	2	ALA	10.1
45	DZ	144	LEU	10.0
45	DZ	116	VAL	9.8
45	BZ	108	PRO	9.5
45	DZ	114	GLY	9.3
45	BZ	147	GLY	9.2
46	B0	5	LYS	8.8
45	BZ	114	GLY	8.8
25	DA	2155	G	8.6
25	DA	2154	G	8.5
1	CA	1030(B)	C	8.5
27	BD	276	LYS	8.3
7	AG	83	ALA	8.0
23	CW	76	A	7.9
25	DA	888	C	7.8
46	B0	7	LEU	7.8
25	DA	229	A	7.7
46	D0	3	HIS	7.7
25	BA	2168	C	7.6
45	BZ	113	ALA	7.6
2	CB	123	ALA	7.5
7	CG	81	GLY	7.4
45	DZ	170	THR	7.4
7	CG	84	ASN	7.4
25	DA	885	C	7.4
46	D0	7	LEU	7.4
14	CN	39	LEU	7.3
25	DA	2138	C	7.3
19	CS	80	TYR	7.2
46	D0	4	LYS	7.2
25	BA	931	C	7.2
10	CJ	47	PHE	7.1
25	BA	942	A	7.0
14	CN	34	TYR	6.9

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Mol	Chain	Res	Type	RSRZ
27	BD	275	LYS	6.9
25	DA	883	G	6.9
25	DA	2139	C	6.8
10	CJ	63	PHE	6.7
25	DA	2140	C	6.7
13	CM	121	LYS	6.7
45	BZ	146	ILE	6.6
1	CA	1035	A	6.5
7	AG	82	GLY	6.4
14	CN	37	PHE	6.4
45	DZ	149	SER	6.4
1	CA	1030(A)	G	6.4
7	CG	154	TYR	6.3
25	BA	932	C	6.3
45	BZ	106	GLY	6.3
13	CM	120	LYS	6.2
43	DX	92	LEU	6.2
7	AG	79	ARG	6.1
1	CA	1036	G	6.1
45	DZ	108	PRO	6.1
21	CU	16	GLY	6.1
47	B1	2	SER	6.0
14	CN	51	GLY	6.0
25	DA	2146	C	6.0
47	D1	2	SER	5.9
3	CC	39	ILE	5.9
14	CN	36	PHE	5.9
42	BW	112	GLY	5.9
2	CB	165	VAL	5.9
45	BZ	144	LEU	5.8
23	AW	76	A	5.8
3	CC	190	ARG	5.7
46	B0	4	LYS	5.7
45	DZ	141	VAL	5.7
10	CJ	65	LEU	5.7
17	CQ	100	LYS	5.6
23	AY	24	G	5.6
7	CG	156	TRP	5.6
25	DA	2156	G	5.6
10	AJ	46	ARG	5.6
9	CI	36	TYR	5.5
25	BA	1555	C	5.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
9	CI	9	ARG	5.5
45	BZ	116	VAL	5.5
25	DA	2145	C	5.4
45	DZ	111	VAL	5.4
49	D3	47	VAL	5.4
44	DY	1	MET	5.4
15	CO	60	VAL	5.4
13	CM	78	ILE	5.3
45	BZ	141	VAL	5.3
25	DA	2802	G	5.3
14	CN	35	ARG	5.3
25	DA	896	A	5.3
14	CN	44	LEU	5.2
25	DA	884	C	5.2
8	AH	93	VAL	5.2
45	BZ	112	ARG	5.2
23	CW	4	C	5.2
23	CW	73	A	5.2
46	B0	2	ALA	5.2
49	D3	29	ARG	5.2
23	AY	47	U	5.1
43	DX	68	ARG	5.1
5	CE	12	LEU	5.1
31	BH	174	GLY	5.1
23	CW	75	C	5.1
7	CG	4	ARG	5.1
30	DG	2	PRO	5.1
23	CW	71	G	5.0
9	CI	110	GLU	5.0
9	CI	28	VAL	5.0
25	BA	943	C	5.0
9	CI	106	ALA	5.0
3	CC	197	GLY	5.0
44	DY	55	TYR	5.0
14	CN	42	ILE	5.0
20	CT	9	ASN	4.9
40	DU	48	ALA	4.9
9	CI	76	ALA	4.9
25	BA	2162	C	4.9
46	B0	3	HIS	4.9
25	BA	1072	U	4.9
53	D7	1	MET	4.9

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Mol	Chain	Res	Type	RSRZ
23	AY	35	A	4.9
25	DA	1026	U	4.9
44	DY	93	GLY	4.8
50	D4	49	PHE	4.8
17	CQ	88	TYR	4.8
46	D0	5	LYS	4.8
17	CQ	95	TYR	4.8
13	CM	122	LYS	4.8
1	AA	1036	G	4.8
14	CN	25	VAL	4.8
17	CQ	23	VAL	4.8
1	AA	1002	G	4.8
25	BA	934	A	4.8
36	DQ	22	LYS	4.7
7	CG	7	ALA	4.7
25	DA	2159	G	4.7
10	CJ	71	LEU	4.7
25	BA	2167	C	4.7
14	CN	53	LEU	4.6
31	DH	52	VAL	4.6
54	D8	64	TYR	4.6
25	DA	2160	G	4.6
1	AA	1531	A	4.6
23	AW	3	C	4.6
9	CI	7	THR	4.6
50	D4	51	ASP	4.6
23	AW	71	G	4.6
10	CJ	62	HIS	4.6
1	AA	1001(A)	G	4.6
10	CJ	66	ARG	4.6
25	BA	2806	G	4.5
9	CI	125	TYR	4.5
3	CC	198	VAL	4.5
14	AN	59	ALA	4.5
23	CW	74	C	4.5
12	CL	18	VAL	4.5
30	DG	51	ARG	4.4
25	DA	2144	U	4.4
55	D9	13	LYS	4.4
25	DA	2149	G	4.4
25	DA	887	A	4.4
5	CE	13	ILE	4.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
9	AI	126	SER	4.4
9	CI	79	LEU	4.4
25	BA	935	C	4.4
31	DH	51	ARG	4.4
14	CN	55	GLY	4.3
23	AW	20	U	4.3
27	DD	2	ALA	4.3
21	CU	15	ARG	4.3
1	AA	204	U	4.3
14	CN	61	TRP	4.3
31	BH	2	SER	4.3
45	BZ	107	THR	4.3
25	DA	2801(A)	A	4.3
53	D7	48	LYS	4.3
9	CI	81	ILE	4.3
13	CM	94	ARG	4.3
9	AI	15	ALA	4.3
2	CB	163	PHE	4.2
7	CG	85	TYR	4.2
54	D8	16	ILE	4.2
31	DH	71	LEU	4.2
9	CI	30	GLY	4.2
2	CB	101	MET	4.2
10	AJ	8	LEU	4.2
1	AA	1030(B)	C	4.2
13	AM	121	LYS	4.2
40	DU	45	TYR	4.2
9	CI	66	ARG	4.1
25	BA	2163	G	4.1
9	CI	78	LYS	4.1
17	CQ	98	LEU	4.1
25	DA	2137	C	4.1
45	DZ	107	THR	4.1
55	D9	16	VAL	4.1
4	AD	167	GLY	4.1
1	CA	1257	U	4.1
25	BA	2814	C	4.1
44	DY	106	LEU	4.1
49	D3	26	LEU	4.1
49	D3	53	LEU	4.1
19	CS	84	GLY	4.1
22	CV	13	A	4.1

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Mol	Chain	Res	Type	RSRZ
14	CN	58	LYS	4.1
14	CN	56	VAL	4.0
9	CI	13	ALA	4.0
1	CA	1030(C)	G	4.0
10	CJ	48	THR	4.0
23	AY	12	U	4.0
2	CB	227	GLY	4.0
55	D9	17	ILE	4.0
2	AB	133	LYS	4.0
10	CJ	44	VAL	4.0
54	D8	61	LEU	4.0
19	CS	79	THR	4.0
35	DP	79	ARG	4.0
17	CQ	22	LEU	4.0
1	CA	1531	A	4.0
25	BA	696	C	4.0
2	CB	139	LYS	4.0
47	B1	98	LEU	4.0
21	CU	14	TRP	4.0
1	CA	1034	G	3.9
34	DO	1	MET	3.9
2	CB	132	LYS	3.9
9	AI	17	VAL	3.9
9	CI	108	VAL	3.9
31	DH	169	VAL	3.9
10	CJ	46	ARG	3.9
2	CB	211	ILE	3.9
44	DY	61	ILE	3.9
4	CD	18	LYS	3.9
9	CI	15	ALA	3.9
7	CG	32	ARG	3.9
13	CM	92	HIS	3.9
31	DH	35	VAL	3.9
3	CC	201	TYR	3.9
35	DP	15	ARG	3.9
36	DQ	5	ARG	3.9
19	CS	83	HIS	3.9
9	CI	52	ALA	3.9
45	DZ	113	ALA	3.9
13	AM	122	LYS	3.9
45	DZ	79	ARG	3.9
43	DX	69	TYR	3.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
31	DH	44	VAL	3.9
45	DZ	147	GLY	3.9
2	CB	122	PHE	3.9
30	DG	136	ARG	3.9
14	AN	2	ALA	3.8
31	DH	24	VAL	3.8
23	CY	36	A	3.8
3	AC	206	GLU	3.8
2	AB	196	LEU	3.8
9	CI	61	ALA	3.8
48	D2	1	MET	3.8
1	CA	1116	C	3.8
3	CC	196	LEU	3.8
50	D4	52	THR	3.8
23	CY	65	G	3.8
35	DP	45	LEU	3.8
1	AA	1257	U	3.8
22	CV	14	A	3.8
23	AW	73	A	3.8
45	BZ	143	GLY	3.8
40	DU	2	PRO	3.8
2	CB	51	LEU	3.8
15	CO	57	LEU	3.8
31	DH	105	LEU	3.8
9	AI	114	TYR	3.8
23	AW	72	C	3.8
24	AX	67	C	3.8
9	CI	37	PHE	3.8
25	DA	886	C	3.8
10	AJ	10	GLY	3.7
20	AT	9	ASN	3.7
10	AJ	60	ARG	3.7
31	DH	6	ARG	3.7
2	CB	136	VAL	3.7
31	DH	53	GLU	3.7
35	DP	73	GLY	3.7
9	CI	27	THR	3.7
17	CQ	91	ARG	3.7
14	CN	59	ALA	3.7
9	CI	17	VAL	3.7
1	AA	1003	G	3.7
31	DH	72	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
51	B5	60	VAL	3.7
52	D6	5	VAL	3.7
10	AJ	65	LEU	3.7
1	CA	1149	C	3.7
7	CG	152	ALA	3.7
10	CJ	10	GLY	3.7
12	CL	7	ILE	3.7
45	DZ	21	ALA	3.7
8	AH	4	ASP	3.7
38	DS	20	ARG	3.7
49	D3	54	VAL	3.7
9	AI	19	LEU	3.7
20	CT	26	ASN	3.6
39	DT	104	ASN	3.6
3	CC	182	ILE	3.6
10	AJ	50	ILE	3.6
4	CD	49	ARG	3.6
14	CN	22	THR	3.6
29	DF	131	GLY	3.6
3	CC	189	ALA	3.6
45	DZ	50	GLN	3.6
2	CB	187	LEU	3.6
19	CS	45	VAL	3.6
3	CC	59	ARG	3.6
3	AC	12	LEU	3.6
17	CQ	42	TYR	3.6
44	DY	44	ILE	3.6
44	DY	26	LYS	3.6
41	DV	77	ALA	3.6
1	CA	1286	A	3.6
14	CN	29	ARG	3.6
19	CS	82	GLY	3.6
24	CX	70	G	3.6
8	CH	83	ILE	3.6
10	AJ	47	PHE	3.6
9	AI	121	ARG	3.6
14	CN	57	ARG	3.6
5	CE	100	VAL	3.6
41	DV	94	LEU	3.6
17	CQ	87	LYS	3.6
5	CE	16	THR	3.6
45	DZ	20	ARG	3.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
12	CL	93	LEU	3.6
23	AW	4	C	3.6
23	CW	3	C	3.6
7	AG	156	TRP	3.5
31	DH	123	PHE	3.5
44	DY	75	ILE	3.5
45	BZ	149	SER	3.5
5	CE	31	LEU	3.5
44	DY	45	VAL	3.5
19	CS	81	ARG	3.5
3	AC	39	ILE	3.5
49	D3	28	LEU	3.5
9	CI	115	GLY	3.5
53	D7	47	ARG	3.5
25	DA	2153	G	3.5
53	B7	46	VAL	3.5
23	AY	14	A	3.5
2	CB	97	TRP	3.5
40	DU	16	LYS	3.5
3	CC	37	GLN	3.5
2	CB	183	PRO	3.5
2	CB	133	LYS	3.5
36	DQ	6	ARG	3.5
25	DA	2148	G	3.5
23	CY	47	U	3.5
25	BA	2166	U	3.5
11	CK	126	ARG	3.5
35	DP	65	ARG	3.5
10	AJ	48	THR	3.5
21	CU	17	THR	3.5
36	BQ	1	MET	3.5
10	CJ	72	VAL	3.5
10	CJ	11	PHE	3.4
25	DA	2157	G	3.4
3	CC	124	ILE	3.4
7	CG	80	VAL	3.4
17	CQ	21	VAL	3.4
45	DZ	71	VAL	3.4
30	DG	140	ILE	3.4
9	AI	106	ALA	3.4
19	CS	50	ALA	3.4
23	CW	70	G	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
13	CM	102	ARG	3.4
53	B7	47	ARG	3.4
19	AS	71	LEU	3.4
23	CW	72	C	3.4
23	CW	5	G	3.4
23	CY	6	G	3.4
25	DA	881	G	3.4
10	AJ	40	LEU	3.4
33	DN	116	LEU	3.4
21	CU	13	ILE	3.4
13	CM	88	ARG	3.4
10	CJ	55	LYS	3.4
42	BW	111	HIS	3.4
17	AQ	35	VAL	3.4
41	DV	30	GLY	3.4
45	BZ	148	ASP	3.4
30	BG	51	ARG	3.4
49	D3	35	ARG	3.4
17	CQ	80	GLY	3.4
20	AT	74	LYS	3.4
2	CB	69	LEU	3.4
41	DV	71	LEU	3.4
45	DZ	51	ALA	3.4
50	D4	45	GLY	3.4
4	AD	166	LYS	3.4
33	DN	26	LEU	3.3
4	CD	158	ILE	3.3
8	CH	128	GLY	3.3
4	AD	133	VAL	3.3
41	DV	72	VAL	3.3
41	DV	73	SER	3.3
43	DX	43	VAL	3.3
46	D0	69	PHE	3.3
2	CB	177	ALA	3.3
9	CI	105	ASP	3.3
9	CI	128	ARG	3.3
12	CL	97	ARG	3.3
2	CB	164	VAL	3.3
25	DA	2803	C	3.3
22	AV	12	A	3.3
17	CQ	6	LEU	3.3
21	AU	6	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
25	DA	2132	U	3.3
31	DH	113	VAL	3.3
45	BZ	118	GLN	3.3
13	CM	119	GLY	3.3
20	CT	12	ALA	3.3
10	CJ	68	HIS	3.3
23	CY	5	G	3.3
10	AJ	72	VAL	3.3
49	D3	23	LEU	3.3
55	D9	37	GLY	3.3
25	DA	2804	C	3.3
30	DG	27	ASN	3.3
8	CH	59	LEU	3.3
55	B9	12	ASP	3.3
44	DY	48	ALA	3.3
44	DY	65	ALA	3.3
4	AD	158	ILE	3.3
3	CC	64	VAL	3.3
15	CO	64	ARG	3.3
17	CQ	92	ARG	3.3
23	CY	1	G	3.3
14	CN	49	HIS	3.3
23	AW	74	C	3.2
31	DH	7	LEU	3.2
1	CA	1532	U	3.2
5	AE	95	ALA	3.2
9	AI	81	ILE	3.2
37	DR	68	ARG	3.2
45	BZ	169	GLU	3.2
4	AD	104	VAL	3.2
12	AL	18	VAL	3.2
33	DN	95	PRO	3.2
50	D4	59	PHE	3.2
45	DZ	112	ARG	3.2
10	CJ	50	ILE	3.2
3	CC	91	LEU	3.2
5	AE	151	LEU	3.2
41	DV	75	PHE	3.2
50	D4	56	VAL	3.2
1	AA	1030(C)	G	3.2
25	DA	2112	G	3.2
25	DA	2142	C	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
8	CH	94	TYR	3.2
17	AQ	36	ILE	3.2
40	DU	43	GLY	3.2
2	AB	61	LEU	3.2
1	CA	1026	G	3.2
11	CK	89	ALA	3.2
40	DU	88	ILE	3.2
8	CH	133	LEU	3.2
17	CQ	74	LEU	3.2
2	AB	165	VAL	3.2
9	CI	49	PRO	3.2
45	DZ	42	VAL	3.2
25	DA	899	A	3.2
23	CY	52	G	3.2
30	BG	49	ASP	3.2
3	AC	195	VAL	3.2
21	CU	6	ARG	3.2
40	DU	41	ALA	3.2
1	CA	1202	G	3.2
31	DH	2	SER	3.2
9	CI	80	GLY	3.2
9	CI	127	LYS	3.2
2	CB	92	TYR	3.1
10	AJ	66	ARG	3.1
44	DY	90	LEU	3.1
45	DZ	53	ILE	3.1
10	AJ	44	VAL	3.1
27	DD	276	LYS	3.1
45	DZ	16	SER	3.1
53	B7	48	LYS	3.1
3	AC	56	ASP	3.1
33	DN	84	LYS	3.1
44	DY	4	LYS	3.1
44	DY	63	LYS	3.1
25	BA	2176	G	3.1
25	BA	2813	G	3.1
25	DA	2147	G	3.1
8	AH	90	GLY	3.1
13	CM	93	ARG	3.1
5	CE	11	ILE	3.1
46	B0	8	GLY	3.1
30	DG	19	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
14	CN	45	ARG	3.1
36	BQ	10	ARG	3.1
8	CH	124	ALA	3.1
31	DH	3	ARG	3.1
9	AI	4	TYR	3.1
10	CJ	64	GLU	3.1
53	B7	1	MET	3.1
7	CG	155	ARG	3.1
14	CN	50	LYS	3.1
25	DA	2131	G	3.1
45	DZ	80	ARG	3.1
2	CB	200	ILE	3.1
7	AG	80	VAL	3.1
7	AG	4	ARG	3.0
5	AE	80	ILE	3.0
24	AX	47	U	3.0
43	DX	28	PHE	3.0
25	DA	2793	G	3.0
9	AI	86	VAL	3.0
35	DP	76	LYS	3.0
7	CG	79	ARG	3.0
8	AH	18	ARG	3.0
25	DA	1509	C	3.0
25	BA	2803	A	3.0
33	DN	45	ASN	3.0
2	CB	131	PRO	3.0
11	CK	125	PHE	3.0
16	AP	19	ILE	3.0
33	DN	8	GLN	3.0
17	CQ	9	VAL	3.0
47	B1	70	VAL	3.0
9	AI	113	LYS	3.0
23	CY	35	A	3.0
35	DP	75	ILE	3.0
50	B4	46	GLN	3.0
9	CI	54	ASP	3.0
23	AW	1	G	3.0
35	DP	59	LEU	3.0
2	CB	124	SER	3.0
30	DG	26	GLN	3.0
12	AL	7	ILE	3.0
10	CJ	49	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
3	CC	6	HIS	3.0
25	DA	614(A)	U	3.0
2	CB	232	PRO	3.0
3	CC	134	ILE	3.0
49	D3	20	LYS	3.0
9	CI	5	TYR	3.0
3	CC	188	LEU	3.0
18	AR	79	LEU	3.0
18	CR	85	LEU	3.0
22	AV	24	A	3.0
17	CQ	38	ARG	3.0
28	BE	1	MET	3.0
14	CN	7	ILE	3.0
30	DG	152	LEU	3.0
10	AJ	5	ARG	3.0
20	CT	59	ALA	3.0
14	AN	16	PHE	3.0
17	AQ	27	PHE	3.0
52	D6	54	ILE	3.0
33	DN	98	VAL	3.0
45	DZ	139	VAL	3.0
12	CL	69	TYR	2.9
19	AS	15	LEU	2.9
20	CT	24	LEU	2.9
21	AU	14	TRP	2.9
30	DG	175	LEU	2.9
41	DV	12	TYR	2.9
3	AC	15	THR	2.9
7	CG	2	ALA	2.9
23	AW	15	G	2.9
23	AW	70	G	2.9
23	CY	34	G	2.9
40	DU	40	PHE	2.9
36	BQ	33	GLY	2.9
9	AI	112	LYS	2.9
40	DU	24	TYR	2.9
10	AJ	11	PHE	2.9
1	AA	1037	C	2.9
23	AY	5	G	2.9
3	AC	57	ILE	2.9
17	CQ	90	ILE	2.9
9	AI	93	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
9	CI	109	VAL	2.9
10	AJ	71	LEU	2.9
36	DQ	80	GLU	2.9
22	AV	14	A	2.9
3	CC	65	ALA	2.9
11	CK	25	TYR	2.9
12	AL	23	LYS	2.9
19	CS	68	GLY	2.9
33	DN	1	MET	2.9
23	AY	25	C	2.9
45	DZ	146	ILE	2.9
19	CS	69	HIS	2.9
17	AQ	98	LEU	2.9
2	CB	55	PHE	2.9
44	DY	88	LYS	2.9
4	AD	23	GLY	2.9
4	AD	76	ARG	2.9
20	CT	83	ARG	2.9
17	CQ	65	ILE	2.9
19	CS	49	ILE	2.9
40	DU	90	VAL	2.9
4	AD	137	SER	2.9
10	CJ	85	LEU	2.9
36	DQ	37	LEU	2.9
38	DS	58	LEU	2.9
45	DZ	76	LEU	2.9
45	DZ	117	LEU	2.9
9	AI	6	GLY	2.9
21	AU	11	GLY	2.9
23	AY	21	A	2.9
25	DA	2136	C	2.9
25	DA	2143	C	2.9
3	CC	194	GLY	2.9
23	AY	15	G	2.9
25	DA	652(U)	G	2.9
25	DA	2162	G	2.9
31	BH	4	ILE	2.9
55	D9	26	ILE	2.9
9	CI	111	ARG	2.9
15	CO	61	GLY	2.9
2	CB	33	TYR	2.9
25	BA	2165	C	2.9

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Mol	Chain	Res	Type	RSRZ
25	BA	2807	C	2.9
25	DA	882	G	2.8
28	DE	77	ILE	2.8
8	AH	112	LEU	2.8
5	CE	10	MET	2.8
17	CQ	93	GLN	2.8
3	CC	204	LEU	2.8
45	BZ	102	LEU	2.8
44	DY	59	GLY	2.8
49	D3	27	GLY	2.8
33	DN	44	PRO	2.8
2	CB	96	ARG	2.8
9	CI	83	ARG	2.8
8	AH	2	LEU	2.8
3	AC	207	VAL	2.8
14	AN	33	VAL	2.8
43	DX	91	ALA	2.8
1	CA	1033	G	2.8
34	DO	82	ASN	2.8
3	CC	193	TYR	2.8
36	DQ	130	LYS	2.8
8	AH	133	LEU	2.8
28	DE	134	ILE	2.8
31	DH	67	LEU	2.8
39	DT	99	LEU	2.8
40	DU	20	LEU	2.8
41	DV	70	ILE	2.8
49	D3	8	LEU	2.8
1	AA	1503	A	2.8
22	AV	13	A	2.8
25	DA	898	C	2.8
9	AI	18	PHE	2.8
10	CJ	54	PHE	2.8
9	CI	4	TYR	2.8
30	DG	3	LEU	2.8
9	AI	65	VAL	2.8
12	CL	39	VAL	2.8
15	CO	45	VAL	2.8
36	DQ	109	VAL	2.8
12	CL	94	PRO	2.8
21	AU	10	ARG	2.8
25	DA	897	C	2.8

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Mol	Chain	Res	Type	RSRZ
2	CB	66	GLY	2.8
31	DH	66	GLY	2.8
4	CD	17	VAL	2.8
3	CC	179	ARG	2.8
14	AN	15	LYS	2.8
25	BA	2175	G	2.8
30	DG	181	ARG	2.8
46	D0	45	PHE	2.8
20	AT	13	LEU	2.8
4	CD	209	ARG	2.8
30	DG	92	VAL	2.8
45	DZ	98	MET	2.8
16	AP	7	ALA	2.8
10	AJ	59	SER	2.7
2	CB	196	LEU	2.7
30	DG	137	GLU	2.7
23	AY	62	C	2.7
8	CH	95	VAL	2.7
34	DO	61	VAL	2.7
46	D0	79	VAL	2.7
8	CH	64	LYS	2.7
55	D9	15	LYS	2.7
30	DG	29	TRP	2.7
5	CE	18	ARG	2.7
8	CH	2	LEU	2.7
25	BA	2805	G	2.7
36	DQ	2	LEU	2.7
49	D3	3	ARG	2.7
14	AN	34	TYR	2.7
40	DU	47	TYR	2.7
2	CB	185	ILE	2.7
3	CC	157	ILE	2.7
13	CM	60	VAL	2.7
54	D8	4	MET	2.7
17	AQ	37	LYS	2.7
43	DX	42	ALA	2.7
49	D3	21	ALA	2.7
9	CI	12	GLU	2.7
11	CK	36	ASP	2.7
4	AD	120	LEU	2.7
13	CM	90	LEU	2.7
41	DV	20	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
3	AC	201	TYR	2.7
9	CI	62	TYR	2.7
9	CI	92	TYR	2.7
45	DZ	9	TYR	2.7
1	CA	1117	G	2.7
34	DO	62	VAL	2.7
13	CM	68	GLY	2.7
14	CN	27	CYS	2.7
15	CO	68	ARG	2.7
44	DY	50	ARG	2.7
9	CI	114	TYR	2.7
31	DH	9	ILE	2.7
35	BP	71	VAL	2.7
55	D9	1	MET	2.7
4	AD	117	ALA	2.7
8	AH	5	PRO	2.7
9	CI	68	GLY	2.7
31	DH	112	PRO	2.7
31	DH	128	PRO	2.7
14	AN	44	LEU	2.7
17	CQ	84	LEU	2.7
23	AW	14	A	2.7
2	CB	214	ILE	2.7
3	AC	152	ILE	2.7
36	BQ	81	VAL	2.7
41	DV	14	VAL	2.7
2	CB	226	ARG	2.7
9	CI	8	GLY	2.7
30	BG	80	PHE	2.7
27	BD	38	LYS	2.7
30	DG	78	SER	2.7
9	CI	102	LEU	2.7
25	DA	889	C	2.7
8	AH	91	ARG	2.7
23	CW	23	A	2.7
36	DQ	35	VAL	2.7
43	DX	2	LYS	2.7
31	DH	20	ALA	2.7
25	BA	12	U	2.7
4	AD	157	LEU	2.7
1	AA	1529	G	2.7
17	CQ	54	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	AA	815	A	2.7
7	CG	16	LEU	2.6
20	CT	13	LEU	2.6
25	BA	2518	U	2.6
54	D8	15	LYS	2.6
31	DH	82	GLY	2.6
44	DY	58	GLY	2.6
8	CH	26	VAL	2.6
19	CS	40	ILE	2.6
3	AC	193	TYR	2.6
24	CX	68	C	2.6
3	CC	186	PHE	2.6
25	DA	614(B)	G	2.6
29	DF	171	PRO	2.6
33	DN	111	PRO	2.6
46	D0	57	PHE	2.6
21	CU	21	TYR	2.6
4	CD	135	LEU	2.6
18	AR	76	LEU	2.6
42	DW	92	ARG	2.6
23	AY	34	G	2.6
23	CW	6	G	2.6
24	CX	4	G	2.6
9	CI	6	GLY	2.6
23	AY	36	A	2.6
25	DA	2135	A	2.6
13	CM	74	VAL	2.6
28	BE	77	ILE	2.6
30	DG	163	ALA	2.6
45	DZ	48	PHE	2.6
2	CB	31	TYR	2.6
3	AC	184	TYR	2.6
4	AD	168	ARG	2.6
10	AJ	43	ARG	2.6
50	D4	58	ARG	2.6
8	AH	10	LEU	2.6
10	AJ	36	GLY	2.6
44	DY	107	ASP	2.6
1	AA	1385	G	2.6
9	AI	111	ARG	2.6
9	CI	65	VAL	2.6
10	CJ	98	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
15	AO	87	ILE	2.6
10	AJ	54	PHE	2.6
11	CK	109	VAL	2.6
40	DU	17	ILE	2.6
40	DU	42	ALA	2.6
23	AW	21	A	2.6
48	D2	32	LEU	2.6
9	CI	69	GLY	2.6
3	AC	21	ARG	2.6
10	CJ	43	ARG	2.6
2	CB	70	PHE	2.6
2	CB	71	VAL	2.6
5	AE	89	ILE	2.6
14	CN	54	PRO	2.6
31	BH	169	VAL	2.6
30	DG	169	ALA	2.6
31	DH	102	ALA	2.6
45	BZ	163	LEU	2.6
7	AG	81	GLY	2.6
9	CI	67	GLY	2.6
12	AL	91	LYS	2.6
43	DX	67	GLY	2.6
1	CA	1357	A	2.6
17	CQ	24	GLU	2.6
30	BG	149	VAL	2.6
40	DU	32	PHE	2.6
2	AB	27	LYS	2.6
44	DY	47	LYS	2.6
45	DZ	14	LYS	2.6
9	AI	125	TYR	2.6
1	AA	927	G	2.6
20	CT	8	ARG	2.6
40	DU	89	GLU	2.6
1	CA	1030	C	2.6
24	CX	71	C	2.6
45	DZ	96	VAL	2.6
34	DO	30	ALA	2.5
35	DP	31	ALA	2.5
5	CE	130	ASN	2.5
13	CM	96	LEU	2.5
33	DN	112	LEU	2.5
41	DV	18	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
45	BZ	155	LEU	2.5
10	CJ	13	HIS	2.5
33	DN	75	TYR	2.5
21	CU	24	ARG	2.5
23	AY	22	G	2.5
29	BF	89	VAL	2.5
29	DF	81	PRO	2.5
8	AH	7	ALA	2.5
9	CI	82	ALA	2.5
14	CN	2	ALA	2.5
11	CK	117	ASN	2.5
40	DU	18	LEU	2.5
1	CA	1400	C	2.5
25	DA	34	C	2.5
27	BD	50	THR	2.5
40	DU	52	ARG	2.5
36	DQ	103	MET	2.5
54	D8	35	GLN	2.5
17	CQ	12	SER	2.5
3	AC	189	ALA	2.5
5	CE	105	VAL	2.5
25	DA	2127	G	2.5
10	CJ	58	ASP	2.5
11	CK	15	ALA	2.5
17	CQ	44	ALA	2.5
27	BD	153	ALA	2.5
46	B0	44	ARG	2.5
46	D0	44	ARG	2.5
19	CS	70	LYS	2.5
38	DS	33	LYS	2.5
23	AY	20	U	2.5
25	DA	9	U	2.5
25	DA	2584	U	2.5
1	AA	525	C	2.5
25	BA	933	C	2.5
25	BA	2815	C	2.5
36	DQ	61	GLY	2.5
3	AC	14	ILE	2.5
3	AC	179	ARG	2.5
8	AH	35	ILE	2.5
10	AJ	98	ILE	2.5
14	AN	57	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
8	CH	112	LEU	2.5
9	CI	85	LEU	2.5
14	AN	30	ALA	2.5
33	DN	46	VAL	2.5
45	DZ	120	ILE	2.5
31	DH	159	GLU	2.5
49	D3	51	ALA	2.5
23	AW	6	G	2.5
25	BA	930	G	2.5
15	CO	69	TYR	2.5
31	DH	94	TYR	2.5
36	BQ	83	MET	2.5
22	CV	15	A	2.5
25	BA	218	A	2.5
7	AG	78	ARG	2.5
14	CN	31	ARG	2.5
36	BQ	60	ARG	2.5
46	D0	6	GLY	2.5
11	AK	125	PHE	2.5
27	DD	127	VAL	2.5
36	DQ	47	ILE	2.5
44	DY	7	VAL	2.5
45	BZ	145	GLU	2.5
55	B9	7	VAL	2.5
25	BA	2169	G	2.5
4	AD	3	ARG	2.5
21	AU	15	ARG	2.5
40	DU	36	ARG	2.5
45	DZ	110	GLY	2.5
46	D0	76	GLY	2.5
10	AJ	64	GLU	2.5
35	DP	70	GLN	2.5
12	CL	32	PHE	2.5
14	AN	36	PHE	2.5
3	AC	200	ALA	2.5
5	CE	55	VAL	2.5
12	CL	55	VAL	2.5
22	AV	15	A	2.5
36	BQ	35	VAL	2.5
41	DV	35	LEU	2.5
9	CI	16	ARG	2.5
10	CJ	60	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
16	AP	37	GLY	2.5
44	DY	80	GLY	2.5
4	CD	37	PRO	2.5
29	DF	172	TRP	2.5
39	DT	101	PHE	2.5
34	DO	69	ILE	2.5
36	DQ	102	VAL	2.5
39	DT	52	ILE	2.5
45	DZ	155	LEU	2.5
3	CC	4	LYS	2.5
45	DZ	156	LYS	2.5
1	CA	250	A	2.5
23	AW	7	A	2.5
20	CT	25	ARG	2.5
21	CU	22	ARG	2.5
44	BY	91	GLU	2.5
27	BD	180	GLY	2.5
36	DQ	113	GLN	2.5
3	CC	184	TYR	2.5
6	AF	55	ASP	2.5
25	BA	2154	U	2.5
2	CB	215	LEU	2.4
29	BF	41	LEU	2.4
29	DF	170	LEU	2.4
30	DG	60	LEU	2.4
38	DS	32	LEU	2.4
41	DV	74	LYS	2.4
7	AG	46	ALA	2.4
13	CM	84	ILE	2.4
14	AN	7	ILE	2.4
45	DZ	17	ALA	2.4
55	B9	17	ILE	2.4
8	CH	22	GLU	2.4
10	AJ	45	ARG	2.4
25	DA	2141	G	2.4
26	DB	119	G	2.4
41	DV	66	ARG	2.4
1	AA	1527	C	2.4
23	CW	13	C	2.4
23	AY	23	A	2.4
3	AC	18	TRP	2.4
3	AC	32	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
5	AE	123	LEU	2.4
16	CP	48	TRP	2.4
45	BZ	104	PHE	2.4
45	DZ	95	PRO	2.4
44	DY	14	LEU	2.4
2	CB	49	GLU	2.4
4	AD	118	ARG	2.4
14	AN	35	ARG	2.4
30	DG	149	VAL	2.4
30	DG	151	ALA	2.4
45	BZ	80	ARG	2.4
53	D7	46	VAL	2.4
29	DF	51	THR	2.4
1	AA	1028	C	2.4
40	DU	56	ASP	2.4
43	DX	1	MET	2.4
19	CS	59	PRO	2.4
3	CC	21	ARG	2.4
4	CD	64	LEU	2.4
8	AH	119	LEU	2.4
25	BA	1793	A	2.4
43	DX	9	LEU	2.4
45	BZ	122	ARG	2.4
3	CC	5	ILE	2.4
8	AH	95	VAL	2.4
11	CK	14	VAL	2.4
25	BA	271	U	2.4
25	DA	2897	U	2.4
45	DZ	126	VAL	2.4
17	CQ	33	GLY	2.4
3	AC	172	ARG	2.4
8	AH	31	PHE	2.4
12	AL	64	TYR	2.4
12	AL	89	ARG	2.4
23	AW	62	C	2.4
23	AY	11	C	2.4
25	BA	2040	G	2.4
49	D3	30	ARG	2.4
55	D9	22	ARG	2.4
8	AH	86	ILE	2.4
23	CY	64	A	2.4
25	DA	2062	A	2.4

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Mol	Chain	Res	Type	RSRZ
27	BD	49	ILE	2.4
40	DU	62	ILE	2.4
55	D9	33	LYS	2.4
7	CG	24	THR	2.4
8	AH	84	ARG	2.4
14	CN	23	ARG	2.4
2	CB	102	LEU	2.4
3	CC	23	TYR	2.4
4	AD	4	TYR	2.4
9	CI	33	PHE	2.4
29	DF	41	LEU	2.4
36	DQ	79	LEU	2.4
47	B1	46	LEU	2.4
23	AY	13	C	2.4
23	CW	2	C	2.4
25	BA	837	C	2.4
25	DA	2128	C	2.4
25	DA	2123	G	2.4
27	DD	18	VAL	2.4
29	DF	80	ALA	2.4
45	DZ	174	VAL	2.4
46	D0	66	VAL	2.4
51	B5	2	ALA	2.4
4	CD	70	ILE	2.4
39	DT	102	ILE	2.4
20	CT	11	SER	2.4
50	D4	57	GLU	2.4
55	D9	12	ASP	2.4
4	CD	47	ARG	2.4
9	AI	128	ARG	2.4
21	CU	10	ARG	2.4
5	CE	20	GLN	2.4
14	AN	17	LYS	2.4
5	CE	45	PHE	2.4
7	AG	124	LEU	2.4
30	DG	34	LEU	2.4
52	D6	11	LEU	2.4
5	CE	109	ILE	2.4
42	DW	85	VAL	2.4
35	DP	35	HIS	2.4
1	CA	1028	C	2.4
9	CI	103	THR	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
23	AW	75	C	2.4
23	CY	13	C	2.4
25	DA	2108	C	2.4
1	CA	1150	U	2.4
25	DA	243	U	2.4
31	DH	132	ARG	2.4
50	D4	13	ARG	2.4
7	AG	62	PHE	2.4
23	AW	26	A	2.4
35	BP	99	LEU	2.4
45	DZ	83	PRO	2.4
54	D8	34	TRP	2.4
3	CC	8	ILE	2.4
45	BZ	166	SER	2.4
8	CH	68	ARG	2.4
45	BZ	170	THR	2.4
25	DA	2506	U	2.4
1	CA	1001(A)	G	2.3
2	AB	28	PHE	2.3
23	CW	44	G	2.3
25	BA	2134	G	2.3
46	D0	37	LEU	2.3
19	AS	68	GLY	2.3
1	AA	1001	A	2.3
2	CB	216	SER	2.3
16	AP	48	TRP	2.3
31	DH	157	TYR	2.3
8	AH	83	ILE	2.3
14	AN	56	VAL	2.3
20	AT	80	ARG	2.3
25	BA	1174	A	2.3
27	DD	38	LYS	2.3
30	DG	5	VAL	2.3
39	DT	111	ARG	2.3
54	D8	30	ARG	2.3
10	AJ	58	ASP	2.3
19	CS	62	ILE	2.3
3	AC	196	LEU	2.3
2	AB	101	MET	2.3
12	AL	48	PRO	2.3
31	DH	32	GLU	2.3
12	CL	64	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
25	DA	2125	G	2.3
55	B9	24	TYR	2.3
49	D3	52	HIS	2.3
8	AH	134	ILE	2.3
21	AU	13	ILE	2.3
4	AD	24	GLU	2.3
12	AL	16	GLU	2.3
12	CL	23	LYS	2.3
14	CN	46	GLU	2.3
46	B0	6	GLY	2.3
4	AD	115	ARG	2.3
8	CH	91	ARG	2.3
9	CI	124	GLN	2.3
31	DH	145	ALA	2.3
29	BF	36	VAL	2.3
31	DH	76	VAL	2.3
36	BQ	9	TYR	2.3
36	BQ	74	TYR	2.3
40	BU	117	GLN	2.3
55	B9	25	VAL	2.3
29	DF	64	ILE	2.3
25	BA	2174	G	2.3
25	DA	744	G	2.3
25	DA	2133	G	2.3
4	AD	73	ARG	2.3
4	AD	135	LEU	2.3
5	CE	14	ARG	2.3
8	AH	92	ARG	2.3
8	AH	96	GLY	2.3
22	CV	24	A	2.3
24	AX	76	A	2.3
31	DH	69	ARG	2.3
40	DU	59	ARG	2.3
44	DY	2	ARG	2.3
48	D2	60	LEU	2.3
53	D7	23	ARG	2.3
44	DY	60	PHE	2.3
1	AA	841	U	2.3
2	AB	29	ALA	2.3
16	AP	38	TYR	2.3
25	BA	2510	C	2.3
35	DP	101	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
44	DY	6	HIS	2.3
45	BZ	165	VAL	2.3
3	AC	182	ILE	2.3
12	CL	16	GLU	2.3
27	BD	259	THR	2.3
39	DT	48	ILE	2.3
41	DV	34	GLU	2.3
55	B9	26	ILE	2.3
33	BN	105	GLY	2.3
14	CN	6	LEU	2.3
3	CC	7	PRO	2.3
9	CI	123	PRO	2.3
10	AJ	63	PHE	2.3
25	BA	2555	G	2.3
4	AD	165	MET	2.3
23	CY	14	A	2.3
40	DU	49	HIS	2.3
31	DH	43	VAL	2.3
3	AC	171	GLY	2.3
5	AE	18	ARG	2.3
45	DZ	24	LEU	2.3
46	B0	75	LEU	2.3
31	DH	55	PRO	2.3
44	DY	77	PRO	2.3
2	AB	179	LYS	2.3
10	AJ	55	LYS	2.3
12	CL	13	LYS	2.3
17	CQ	58	GLU	2.3
1	AA	1024	G	2.3
4	AD	181	MET	2.3
4	CD	195	ALA	2.3
36	BQ	121	ALA	2.3
50	D4	40	HIS	2.3
8	AH	61	VAL	2.3
14	AN	61	TRP	2.3
17	AQ	5	VAL	2.3
15	AO	36	ILE	2.3
25	BA	990	A	2.3
25	BA	1790	A	2.3
25	DA	2134	A	2.3
29	DF	186	ILE	2.3
34	DO	87	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
39	BT	112	ARG	2.3
45	BZ	120	ILE	2.3
6	AF	61	LEU	2.3
13	CM	13	LYS	2.3
29	DF	12	LEU	2.3
9	CI	90	PRO	2.3
31	DH	8	PRO	2.3
35	DP	74	GLU	2.3
13	CM	110	ARG	2.3
30	DG	50	ALA	2.3
32	BI	1	MET	2.3
8	CH	137	VAL	2.3
1	AA	1530	G	2.3
8	AH	6	ILE	2.3
28	DE	115	GLY	2.3
25	BA	586	G	2.3
25	BA	638	U	2.3
25	BA	1023	G	2.3
25	BA	2131	U	2.3
25	DA	2894	G	2.3
31	DH	162	ILE	2.3
34	DO	2	ILE	2.3
4	AD	201	GLN	2.3
9	CI	116	LYS	2.3
41	DV	85	LYS	2.3
54	D8	3	LYS	2.3
32	DI	35	LEU	2.2
37	DR	65	LEU	2.2
8	CH	74	PRO	2.2
36	BQ	59	ARG	2.2
2	CB	48	MET	2.2
7	AG	134	ALA	2.2
8	CH	9	MET	2.2
8	CH	28	ALA	2.2
40	DU	44	ASN	2.2
4	AD	180	GLY	2.2
27	DD	205	VAL	2.2
34	DO	38	VAL	2.2
5	CE	131	ILE	2.2
10	AJ	96	ILE	2.2
15	CO	33	THR	2.2
30	DG	157	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
49	D3	33	GLN	2.2
25	DA	2585	U	2.2
5	AE	119	LEU	2.2
16	AP	6	LEU	2.2
54	D8	62	LEU	2.2
25	BA	1033	G	2.2
25	DA	2166	G	2.2
54	B8	2	PRO	2.2
14	CN	41	ARG	2.2
48	D2	55	ARG	2.2
1	CA	1225	A	2.2
1	CA	1252	A	2.2
11	AK	123	LYS	2.2
12	CL	28	LYS	2.2
44	DY	46	LYS	2.2
9	AI	109	VAL	2.2
9	CI	14	VAL	2.2
40	DU	25	TRP	2.2
45	BZ	100	VAL	2.2
4	AD	204	ILE	2.2
9	CI	63	ILE	2.2
13	CM	105	THR	2.2
28	DE	105	THR	2.2
45	DZ	124	ILE	2.2
11	CK	75	TYR	2.2
12	CL	84	LEU	2.2
15	CO	81	LEU	2.2
9	CI	42	ARG	2.2
14	AN	41	ARG	2.2
45	DZ	52	SER	2.2
46	D0	49	LYS	2.2
8	CH	131	GLY	2.2
25	BA	2816	G	2.2
44	DY	57	GLN	2.2
54	D8	65	GLU	2.2
3	AC	68	VAL	2.2
23	AW	56	C	2.2
23	CW	7	A	2.2
29	BF	173	VAL	2.2
36	DQ	96	VAL	2.2
29	BF	64	ILE	2.2
30	DG	39	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
7	CG	151	TYR	2.2
9	CI	120	ARG	2.2
27	DD	155	LEU	2.2
28	DE	195	LEU	2.2
35	DP	62	LEU	2.2
42	DW	86	LEU	2.2
46	D0	55	ARG	2.2
21	CU	23	PRO	2.2
25	BA	1985	U	2.2
35	DP	51	PHE	2.2
36	BQ	65	PHE	2.2
9	AI	115	GLY	2.2
42	DW	55	ALA	2.2
45	DZ	172	ALA	2.2
17	AQ	9	VAL	2.2
17	CQ	35	VAL	2.2
23	CW	24	G	2.2
25	BA	11	G	2.2
25	BA	1310	G	2.2
28	BE	196	VAL	2.2
31	DH	115	VAL	2.2
13	CM	104	ARG	2.2
20	CT	33	ILE	2.2
21	AU	3	LYS	2.2
31	DH	4	ILE	2.2
33	BN	71	ILE	2.2
7	AG	154	TYR	2.2
13	CM	87	TYR	2.2
25	DA	2602	A	2.2
3	CC	10	PHE	2.2
32	DI	34	GLY	2.2
14	CN	30	ALA	2.2
53	B7	45	ALA	2.2
54	D8	10	ALA	2.2
50	D4	50	VAL	2.2
8	CH	17	THR	2.2
9	AI	47	LEU	2.2
15	CO	36	ILE	2.2
41	DV	26	ASP	2.2
41	DV	92	THR	2.2
36	BQ	79	LEU	2.2
43	DX	95	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	CA	1187	G	2.2
2	CB	152	PHE	2.2
3	CC	206	GLU	2.2
4	AD	110	PHE	2.2
10	CJ	53	PRO	2.2
2	CB	228	GLY	2.2
25	BA	944	C	2.2
43	DX	94	GLY	2.2
25	BA	2465	A	2.2
25	BA	2584	A	2.2
25	DA	900	A	2.2
25	BA	1003	U	2.2
30	DG	47	LYS	2.2
55	D9	8	LYS	2.2
3	AC	65	ALA	2.2
9	CI	10	ARG	2.2
10	AJ	18	ALA	2.2
13	AM	102	ARG	2.2
32	BI	27	ARG	2.2
8	CH	93	VAL	2.2
36	DQ	55	VAL	2.2
44	DY	12	THR	2.2
8	AH	109	ILE	2.2
10	AJ	75	ILE	2.2
10	CJ	96	ILE	2.2
32	DI	4	ILE	2.2
38	BS	4	LEU	2.2
39	DT	50	ILE	2.2
2	AB	78	GLN	2.2
45	DZ	119	GLU	2.2
47	B1	17	SER	2.2
7	AG	85	TYR	2.2
12	CL	25	PRO	2.2
10	AJ	69	ASN	2.2
10	AJ	93	GLY	2.2
34	DO	101	PRO	2.2
35	DP	78	PRO	2.2
50	B4	45	GLY	2.2
19	CS	47	HIS	2.2
43	BX	60	ARG	2.2
55	B9	22	ARG	2.2
28	BE	157	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
34	DO	33	ALA	2.2
4	CD	140	VAL	2.2
10	CJ	42	THR	2.2
43	DX	7	VAL	2.2
40	DU	60	LEU	2.1
54	D8	60	LEU	2.1
10	CJ	59	SER	2.1
53	D7	32	LYS	2.1
3	AC	181	ASN	2.1
4	AD	138	TYR	2.1
4	AD	122	ARG	2.1
29	BF	44	ARG	2.1
25	DA	652(T)	C	2.1
25	BA	721	G	2.1
49	D3	18	ASP	2.1
20	CT	30	LYS	2.1
2	AB	11	LEU	2.1
31	DH	49	VAL	2.1
36	DQ	17	LEU	2.1
37	BR	10	LEU	2.1
54	D8	25	MET	2.1
20	AT	55	ILE	2.1
3	CC	155	GLY	2.1
25	BA	1036	A	2.1
39	BT	37	GLY	2.1
42	DW	112	GLY	2.1
43	BX	94	GLY	2.1
17	CQ	28	PRO	2.1
19	CS	53	ASN	2.1
11	AK	96	ARG	2.1
42	BW	92	ARG	2.1
4	CD	20	TYR	2.1
50	B4	63	TYR	2.1
17	CQ	86	GLU	2.1
20	CT	18	GLN	2.1
49	D3	24	LYS	2.1
54	B8	51	ALA	2.1
2	AB	215	LEU	2.1
4	CD	88	VAL	2.1
8	AH	118	VAL	2.1
8	CH	97	VAL	2.1
10	CJ	40	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
20	AT	24	LEU	2.1
27	BD	229	VAL	2.1
36	BQ	102	VAL	2.1
40	BU	8	VAL	2.1
46	D0	21	LEU	2.1
1	CA	1325	C	2.1
27	BD	223	GLY	2.1
2	AB	130	ARG	2.1
12	CL	8	ASN	2.1
25	BA	16	G	2.1
27	BD	262	ARG	2.1
29	BF	83	PHE	2.1
32	BI	103	ARG	2.1
47	D1	61	ARG	2.1
3	AC	161	GLU	2.1
19	CS	43	GLU	2.1
30	DG	25	TYR	2.1
34	DO	108	GLU	2.1
34	DO	18	LYS	2.1
36	DQ	18	LYS	2.1
36	DQ	63	LYS	2.1
46	D0	40	GLN	2.1
3	CC	41	GLY	2.1
8	CH	63	LEU	2.1
10	AJ	49	VAL	2.1
15	CO	56	LEU	2.1
17	AQ	33	GLY	2.1
17	CQ	73	VAL	2.1
31	DH	14	GLY	2.1
33	DN	5	VAL	2.1
36	DQ	43	THR	2.1
38	DS	46	VAL	2.1
49	D3	6	VAL	2.1
35	BP	15	ARG	2.1
55	B9	21	GLY	2.1
2	CB	68	ILE	2.1
3	CC	167	TRP	2.1
30	BG	77	ILE	2.1
33	BN	45	ASN	2.1
52	D6	42	TRP	2.1
1	AA	163	C	2.1
11	CK	92	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
25	BA	187	C	2.1
36	DQ	4	PRO	2.1
1	AA	1368	G	2.1
8	AH	94	TYR	2.1
25	DA	1667	G	2.1
2	CB	161	ALA	2.1
25	BA	2577	A	2.1
39	DT	126	ALA	2.1
5	CE	33	VAL	2.1
8	AH	87	SER	2.1
8	CH	96	GLY	2.1
14	AN	18	VAL	2.1
18	AR	44	LEU	2.1
33	BN	112	LEU	2.1
40	DU	9	VAL	2.1
41	DV	22	VAL	2.1
10	AJ	97	GLU	2.1
1	AA	1040	U	2.1
2	AB	97	TRP	2.1
4	CD	33	MET	2.1
13	CM	82	MET	2.1
16	AP	41	PRO	2.1
23	CY	66	U	2.1
36	DQ	104	PHE	2.1
2	AB	95	GLN	2.1
1	AA	526	C	2.1
17	CQ	29	HIS	2.1
25	BA	2628	C	2.1
3	CC	53	ALA	2.1
7	CG	3	ARG	2.1
3	AC	26	LYS	2.1
14	CN	47	LEU	2.1
25	BA	1011	G	2.1
30	DG	75	LYS	2.1
36	BQ	17	LEU	2.1
38	DS	57	LYS	2.1
1	AA	814	A	2.1
2	CB	197	VAL	2.1
4	CD	198	VAL	2.1
25	BA	594	A	2.1
12	CL	85	ILE	2.1
30	DG	112	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
7	CG	78	ARG	2.1
10	AJ	7	LYS	2.1
34	DO	32	TYR	2.1
23	CY	2	C	2.1
36	BQ	76	LYS	2.1
41	DV	21	ARG	2.1
45	DZ	4	ARG	2.1
14	AN	8	GLU	2.1
15	AO	23	GLY	2.1
27	BD	93	ALA	2.1
27	DD	144	ALA	2.1
55	B9	37	GLY	2.1
3	AC	178	LEU	2.1
19	CS	38	SER	2.1
45	DZ	70	LEU	2.1
11	AK	117	ASN	2.1
19	CS	48	THR	2.1
38	DS	14	VAL	2.1
1	AA	1504	G	2.1
12	AL	94	PRO	2.1
18	CR	43	PHE	2.1
25	BA	2331	G	2.1
37	BR	1	MET	2.1
1	AA	1306	A	2.1
1	CA	908	A	2.1
25	BA	116	A	2.1
25	BA	1833	A	2.1
25	BA	2614	A	2.1
17	CQ	75	ARG	2.1
29	DF	77	ASP	2.1
35	DP	77	ARG	2.1
36	BQ	5	ARG	2.1
46	D0	24	LYS	2.1
53	B7	41	ARG	2.1
16	AP	39	TYR	2.1
29	DF	180	GLY	2.1
36	DQ	114	ALA	2.1
9	CI	19	LEU	2.0
51	D5	58	LEU	2.0
1	AA	1501	C	2.0
12	CL	49	ASN	2.0
23	AY	56	C	2.0

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Mol	Chain	Res	Type	RSRZ
23	AY	61	C	2.0
25	BA	2591	C	2.0
25	DA	2507	C	2.0
45	DZ	118	GLN	2.0
20	CT	14	LYS	2.0
33	DN	85	ILE	2.0
39	DT	1	MET	2.0
3	CC	85	ARG	2.0
4	AD	139	ARG	2.0
17	CQ	25	ARG	2.0
55	D9	19	ARG	2.0
1	CA	1185	G	2.0
1	CA	1186	G	2.0
23	AW	69	G	2.0
25	BA	234	G	2.0
25	BA	2024	G	2.0
25	BA	2586	G	2.0
25	DA	1042	G	2.0
1	AA	1080	A	2.0
1	CA	60	A	2.0
2	CB	38	GLY	2.0
25	BA	553	A	2.0
25	BA	849	A	2.0
25	BA	1047	A	2.0
25	DA	652(B)	A	2.0
25	DA	1780	A	2.0
36	DQ	19	GLY	2.0
50	D4	54	GLY	2.0
11	AK	75	TYR	2.0
19	CS	52	TYR	2.0
20	AT	40	ALA	2.0
28	BE	114	ALA	2.0
49	D3	42	ALA	2.0
9	CI	31	GLN	2.0
32	DI	38	LEU	2.0
35	BP	112	LEU	2.0
37	BR	111	LEU	2.0
3	AC	66	VAL	2.0
3	CC	95	THR	2.0
15	AO	60	VAL	2.0
44	DY	3	VAL	2.0
54	D8	21	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
3	AC	8	ILE	2.0
3	AC	77	ILE	2.0
9	AI	37	PHE	2.0
12	AL	45	PRO	2.0
25	DA	678	C	2.0
35	DP	50	ARG	2.0
16	AP	13	HIS	2.0
16	CP	30	GLY	2.0
35	DP	66	GLY	2.0
7	AG	86	GLN	2.0
25	BA	9	U	2.0
1	AA	926	G	2.0
1	CA	887	G	2.0
3	CC	160	ALA	2.0
35	DP	68	GLN	2.0
25	BA	1236	G	2.0
25	BA	2288	G	2.0
27	BD	247	ALA	2.0
37	DR	14	SER	2.0
23	AW	65	G	2.0
42	DW	56	ALA	2.0
48	D2	8	LYS	2.0
49	D3	15	TYR	2.0
22	AV	23	A	2.0
24	AX	72	A	2.0
24	CX	72	A	2.0
25	BA	998	A	2.0
25	BA	2141	A	2.0
25	DA	821	A	2.0
4	AD	105	VAL	2.0
8	AH	3	THR	2.0
9	CI	20	ARG	2.0
9	CI	104	ARG	2.0
12	CL	96	VAL	2.0
14	CN	26	ARG	2.0
30	BG	109	VAL	2.0
36	BQ	132	VAL	2.0
45	DZ	145	GLU	2.0
28	BE	51	PHE	2.0
31	DH	29	PRO	2.0
20	CT	41	ILE	2.0
31	BH	148	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
31	DH	57	ASP	2.0
5	AE	10	MET	2.0
36	DQ	3	MET	2.0
1	AA	290	C	2.0
1	CA	1029	C	2.0
3	CC	80	GLY	2.0
9	AI	116	LYS	2.0
16	AP	50	LYS	2.0
29	DF	15	SER	2.0
3	CC	43	LEU	2.0
4	AD	101	LEU	2.0
5	AE	17	ALA	2.0
14	CN	10	ALA	2.0
27	DD	147	LEU	2.0
43	DX	4	ALA	2.0
4	CD	54	TYR	2.0
43	DX	66	LEU	2.0
49	D3	37	LEU	2.0
8	CH	122	ARG	2.0
9	CI	107	ARG	2.0
28	DE	136	ARG	2.0
31	DH	54	ARG	2.0
5	AE	98	THR	2.0
30	DG	161	THR	2.0
48	B2	19	VAL	2.0
55	D9	25	VAL	2.0
8	CH	101	PRO	2.0
25	BA	17	G	2.0
25	BA	1049	G	2.0
31	DH	36	PRO	2.0
36	DQ	99	PRO	2.0
45	DZ	88	PHE	2.0
49	D3	12	PRO	2.0
1	AA	969	A	2.0
25	BA	1723	A	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( $\text{\AA}^2$ )	Q<0.9
23	PSU	AY	32	20/21	0.92	0.17	-	83,93,99,105	0
24	4SU	AX	8	20/21	0.95	0.20	-	47,62,81,87	0
24	5MC	CX	32	21/22	0.95	0.22	-	63,72,77,80	0
23	PSU	AW	32	20/21	0.96	0.21	-	39,59,64,65	0
23	5MU	CY	54	21/22	0.80	0.30	-	88,99,111,135	0
24	PSU	CX	55	20/21	0.91	0.15	-	62,70,83,92	0
23	5MU	CW	54	21/22	0.92	0.14	-	72,81,90,93	0
23	4SU	CW	8	20/21	0.72	0.22	-	85,105,116,130	0
23	4SU	AW	8	20/21	0.89	0.16	-	81,89,100,121	0
24	5MU	CX	54	21/22	0.94	0.24	-	69,80,89,95	0
23	PSU	CW	39	20/21	0.95	0.26	-	62,79,88,94	0
23	MIA	CW	37	22/30	0.94	0.20	-	53,72,83,85	0
24	PSU	AX	55	20/21	0.94	0.18	-	60,68,83,92	0
23	5MU	AW	54	21/22	0.93	0.23	-	57,76,85,89	0
23	7MG	CY	46	24/25	0.72	0.24	-	91,105,113,139	0
23	4SU	AY	8	20/21	0.77	0.20	-	99,105,115,127	0
23	PSU	CY	39	20/21	0.84	0.22	-	79,92,100,112	0
23	7MG	CW	46	24/25	0.82	0.24	-	93,104,114,127	0
23	4SU	CY	8	20/21	0.69	0.25	-	95,103,122,140	0
23	PSU	AW	39	20/21	0.96	0.21	-	37,57,68,72	0
23	MIA	AY	37	22/30	0.83	0.22	-	82,91,103,118	0
23	MIA	CY	37	22/30	0.86	0.27	-	75,93,102,117	0
23	PSU	CY	55	20/21	0.73	0.36	-	91,104,118,129	0
23	7MG	AY	46	24/25	0.81	0.28	-	92,100,111,135	0
23	7MG	AW	46	24/25	0.82	0.15	-	74,94,116,138	0
24	5MU	AX	54	21/22	0.95	0.17	-	60,70,77,80	0
24	4SU	CX	8	20/21	0.92	0.20	-	73,82,90,90	0
23	PSU	CW	32	20/21	0.95	0.23	-	62,82,97,97	0
23	PSU	CY	32	20/21	0.85	0.20	-	83,95,100,107	0
23	PSU	AY	55	20/21	0.70	0.25	-	88,103,115,132	0
23	PSU	CW	55	20/21	0.79	0.20	-	76,95,105,108	0
23	PSU	AW	55	20/21	0.81	0.26	-	57,85,93,93	0
23	5MU	AY	54	21/22	0.76	0.29	-	85,97,115,141	0
24	5MC	AX	32	21/22	0.97	0.24	-	38,56,66,77	0
23	PSU	AY	39	20/21	0.92	0.22	-	76,89,100,102	0
23	MIA	AW	37	29/30	0.96	0.27	-	36,49,67,72	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
56	MG	BA	3182	1/1	0.90	0.92	83.37	50,50,50,50	0
56	MG	BA	3127	1/1	0.86	0.58	79.97	38,38,38,38	0
56	MG	DA	3086	1/1	0.83	0.90	66.41	42,42,42,42	0
56	MG	BA	3615	1/1	0.94	0.72	66.20	41,41,41,41	0
56	MG	BA	3160	1/1	0.92	0.64	58.15	58,58,58,58	0
56	MG	BA	3776	1/1	0.96	1.10	56.08	52,52,52,52	0
56	MG	BU	206	1/1	0.95	0.88	55.07	54,54,54,54	0
56	MG	BA	3164	1/1	0.96	0.54	35.67	33,33,33,33	0
56	MG	BA	3094	1/1	0.97	0.79	35.59	49,49,49,49	0
56	MG	DA	3023	1/1	0.90	1.12	29.37	44,44,44,44	0
56	MG	DA	3415	1/1	0.95	0.58	29.28	45,45,45,45	0
56	MG	BU	209	1/1	0.96	0.65	29.07	41,41,41,41	0
56	MG	BA	3238	1/1	0.98	0.63	28.01	35,35,35,35	0
56	MG	B5	103	1/1	0.77	0.68	26.65	51,51,51,51	0
56	MG	DF	306	1/1	0.94	1.20	24.96	55,55,55,55	0
56	MG	BA	3110	1/1	0.94	0.72	22.77	49,49,49,49	0
56	MG	BA	3089	1/1	0.95	0.59	22.36	46,46,46,46	0
56	MG	BV	205	1/1	0.94	0.71	21.81	37,37,37,37	0
56	MG	BQ	3001	1/1	0.94	0.98	20.30	52,52,52,52	0
56	MG	DA	3160	1/1	0.93	0.52	20.06	51,51,51,51	0
56	MG	BA	3188	1/1	0.98	0.53	19.76	41,41,41,41	0
56	MG	BF	308	1/1	0.96	0.72	19.13	40,40,40,40	0
56	MG	BA	3132	1/1	0.89	0.53	18.43	42,42,42,42	0
56	MG	BA	3026	1/1	0.98	0.39	16.16	41,41,41,41	0
56	MG	DR	3001	1/1	0.93	0.66	16.09	55,55,55,55	0
56	MG	BA	3131	1/1	0.91	0.46	15.84	35,35,35,35	0
56	MG	DA	3065	1/1	0.86	0.51	15.54	56,56,56,56	0
56	MG	BA	3116	1/1	0.91	0.42	15.53	68,68,68,68	0
56	MG	BA	3028	1/1	0.95	0.55	15.35	48,48,48,48	0
56	MG	AE	3002	1/1	0.89	0.50	15.02	67,67,67,67	0
56	MG	BA	3091	1/1	0.97	0.63	14.96	43,43,43,43	0
56	MG	BN	3004	1/1	0.93	0.78	14.93	60,60,60,60	0
56	MG	BA	3190	1/1	0.97	0.67	14.91	35,35,35,35	0
56	MG	BA	3027	1/1	0.97	0.44	14.73	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	BN	3006	1/1	0.94	0.62	14.56	54,54,54,54	0
56	MG	BA	3777	1/1	0.94	0.55	14.33	40,40,40,40	0
56	MG	BE	304	1/1	0.95	0.50	14.19	42,42,42,42	0
56	MG	DU	3001	1/1	0.88	0.98	13.85	61,61,61,61	0
56	MG	BA	3774	1/1	0.97	0.64	13.67	32,32,32,32	0
56	MG	BU	205	1/1	0.94	0.63	13.59	39,39,39,39	0
56	MG	BA	3022	1/1	0.95	0.50	13.54	41,41,41,41	0
56	MG	CA	3092	1/1	0.90	0.23	13.51	55,55,55,55	0
56	MG	BA	3562	1/1	0.92	0.42	13.18	37,37,37,37	0
56	MG	AA	3127	1/1	0.90	0.29	12.90	52,52,52,52	0
56	MG	BA	3136	1/1	0.84	0.60	12.74	49,49,49,49	0
56	MG	BV	202	1/1	0.94	0.40	12.68	34,34,34,34	0
56	MG	BN	3001	1/1	0.86	0.62	12.57	51,51,51,51	0
56	MG	BF	305	1/1	0.95	0.46	12.37	40,40,40,40	0
56	MG	B5	101	1/1	0.94	0.62	12.26	42,42,42,42	0
56	MG	DE	301	1/1	0.98	0.89	12.04	50,50,50,50	0
56	MG	BU	202	1/1	0.95	0.45	11.93	32,32,32,32	0
56	MG	B7	102	1/1	0.94	0.47	11.50	40,40,40,40	0
56	MG	BF	309	1/1	0.95	0.49	11.30	40,40,40,40	0
56	MG	B5	102	1/1	0.92	0.57	11.13	42,42,42,42	0
56	MG	AA	3172	1/1	0.96	0.32	10.68	44,44,44,44	0
56	MG	AX	3010	1/1	0.87	0.49	10.56	54,54,54,54	0
56	MG	BD	311	1/1	0.90	0.71	10.48	46,46,46,46	0
56	MG	DA	3024	1/1	0.97	0.53	10.32	43,43,43,43	0
56	MG	DA	3078	1/1	0.85	0.31	10.14	64,64,64,64	0
56	MG	BF	302	1/1	0.97	0.45	10.05	29,29,29,29	0
56	MG	BD	309	1/1	0.98	0.64	9.98	39,39,39,39	0
56	MG	BA	3672	1/1	0.97	0.34	9.49	37,37,37,37	0
56	MG	DD	308	1/1	0.97	0.55	9.27	45,45,45,45	0
56	MG	DA	3251	1/1	0.93	0.33	9.21	47,47,47,47	0
56	MG	BF	306	1/1	0.92	0.48	9.21	41,41,41,41	0
56	MG	BA	3327	1/1	0.61	0.37	9.13	74,74,74,74	0
56	MG	BA	3029	1/1	0.96	0.33	8.97	44,44,44,44	0
56	MG	DA	3361	1/1	0.94	0.35	8.82	45,45,45,45	0
56	MG	D7	101	1/1	0.94	0.48	8.81	33,33,33,33	0
56	MG	BA	3785	1/1	0.97	0.52	8.79	42,42,42,42	0
56	MG	BR	202	1/1	0.77	0.49	8.77	51,51,51,51	0
56	MG	BA	3460	1/1	0.93	0.43	8.57	45,45,45,45	0
56	MG	DA	3621	1/1	0.83	0.41	8.54	73,73,73,73	0
56	MG	B0	101	1/1	0.93	0.40	8.43	49,49,49,49	0
56	MG	CA	3035	1/1	0.94	0.29	8.08	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	DD	306	1/1	0.97	0.55	8.05	35,35,35,35	0
56	MG	BA	3773	1/1	0.85	0.39	8.02	43,43,43,43	0
56	MG	BA	3143	1/1	0.88	0.37	7.79	35,35,35,35	0
56	MG	BA	3018	1/1	0.99	0.47	7.73	36,36,36,36	0
56	MG	DA	3449	1/1	0.94	0.35	7.68	49,49,49,49	0
56	MG	BR	201	1/1	0.92	0.55	7.59	40,40,40,40	0
56	MG	BF	301	1/1	0.94	0.41	7.41	39,39,39,39	0
56	MG	BA	3495	1/1	0.95	0.32	7.16	44,44,44,44	0
56	MG	DA	3037	1/1	0.89	0.40	7.12	46,46,46,46	0
56	MG	DD	304	1/1	0.96	0.44	7.10	56,56,56,56	0
56	MG	BA	3472	1/1	0.97	0.40	6.80	43,43,43,43	0
56	MG	DQ	3003	1/1	0.95	0.58	6.79	64,64,64,64	0
56	MG	BA	3141	1/1	0.93	0.42	6.69	55,55,55,55	0
56	MG	BD	307	1/1	0.95	0.38	6.64	38,38,38,38	0
56	MG	DA	3006	1/1	0.87	0.36	6.62	42,42,42,42	0
56	MG	DA	3025	1/1	0.91	0.71	6.22	49,49,49,49	0
56	MG	DA	3316	1/1	0.95	0.38	6.20	48,48,48,48	0
56	MG	BP	201	1/1	0.96	0.42	6.14	36,36,36,36	0
56	MG	DV	3002	1/1	0.98	0.70	6.02	51,51,51,51	0
56	MG	BA	3244	1/1	0.89	0.34	5.99	53,53,53,53	0
56	MG	BF	304	1/1	0.96	0.47	5.96	37,37,37,37	0
56	MG	AA	3094	1/1	0.90	0.30	5.83	53,53,53,53	0
57	NEG	AA	3221	17/17	0.90	0.34	5.80	44,57,69,70	0
56	MG	DA	3071	1/1	0.97	0.32	5.67	43,43,43,43	0
56	MG	BA	3782	1/1	0.97	0.37	5.58	48,48,48,48	0
57	NEG	CA	3170	17/17	0.87	0.36	5.44	58,72,83,86	0
57	NEG	CA	3175	17/17	0.88	0.39	5.44	48,61,79,89	0
56	MG	DA	3186	1/1	0.94	0.47	5.39	41,41,41,41	0
56	MG	AA	3034	1/1	0.89	0.24	5.38	56,56,56,56	0
56	MG	BA	3642	1/1	0.97	0.28	5.24	38,38,38,38	0
56	MG	BD	304	1/1	0.97	0.41	5.01	50,50,50,50	0
56	MG	DA	3015	1/1	0.97	0.45	4.98	49,49,49,49	0
56	MG	CA	3048	1/1	0.93	0.25	4.93	54,54,54,54	0
56	MG	BA	3649	1/1	0.89	0.27	4.92	49,49,49,49	0
56	MG	BU	207	1/1	0.98	0.40	4.84	22,22,22,22	0
57	NEG	CA	3174	17/17	0.83	0.29	4.84	38,53,68,69	0
56	MG	BU	208	1/1	0.98	0.36	4.83	35,35,35,35	0
57	NEG	AA	3219	17/17	0.91	0.30	4.82	61,71,78,79	0
56	MG	BA	3769	1/1	0.97	0.34	4.75	52,52,52,52	0
57	NEG	CX	3004	17/17	0.86	0.26	4.74	32,64,79,84	0
56	MG	DF	305	1/1	0.93	0.46	4.74	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	3244	1/1	0.98	0.27	4.52	58,58,58,58	0
56	MG	BD	305	1/1	0.89	0.32	4.38	41,41,41,41	0
57	NEG	CA	3173	17/17	0.84	0.31	4.37	54,76,85,86	0
56	MG	BA	3237	1/1	0.98	0.38	4.36	43,43,43,43	0
56	MG	BV	207	1/1	0.93	0.30	4.30	42,42,42,42	0
56	MG	BA	3541	1/1	0.95	0.35	4.24	31,31,31,31	0
56	MG	BA	3106	1/1	0.98	0.43	4.21	42,42,42,42	0
56	MG	BQ	3005	1/1	0.95	0.49	4.10	49,49,49,49	0
56	MG	BX	102	1/1	0.92	0.29	4.03	40,40,40,40	0
56	MG	BA	3271	1/1	0.94	0.26	4.02	39,39,39,39	0
56	MG	BA	3440	1/1	0.93	0.33	4.01	41,41,41,41	0
57	NEG	CA	3177	17/17	0.90	0.24	3.89	36,63,74,81	0
56	MG	BA	3203	1/1	0.93	0.31	3.80	51,51,51,51	0
56	MG	BA	3354	1/1	0.95	0.27	3.68	39,39,39,39	0
56	MG	DD	307	1/1	0.97	0.33	3.66	56,56,56,56	0
56	MG	D3	3001	1/1	0.95	0.61	3.63	70,70,70,70	0
56	MG	DA	3125	1/1	0.88	0.51	3.63	56,56,56,56	0
56	MG	BA	3209	1/1	0.88	0.36	3.41	57,57,57,57	0
56	MG	BA	3025	1/1	0.94	0.33	3.39	37,37,37,37	0
57	NEG	AA	3216	17/17	0.94	0.31	3.37	34,56,70,74	0
56	MG	DA	3558	1/1	0.94	0.35	3.33	48,48,48,48	0
56	MG	BA	3757	1/1	0.87	0.28	3.30	47,47,47,47	0
56	MG	DA	3233	1/1	0.97	0.23	3.30	40,40,40,40	0
56	MG	BU	201	1/1	0.89	0.33	3.27	29,29,29,29	0
56	MG	AA	3052	1/1	0.88	0.30	3.27	52,52,52,52	0
56	MG	DA	3617	1/1	0.95	0.38	3.23	55,55,55,55	0
56	MG	BA	3668	1/1	0.95	0.29	3.14	42,42,42,42	0
56	MG	BA	3061	1/1	0.92	0.31	3.11	48,48,48,48	0
57	NEG	AW	3004	17/17	0.89	0.37	3.02	37,50,72,73	0
56	MG	DA	3284	1/1	0.93	0.26	2.81	40,40,40,40	0
56	MG	DA	3156	1/1	0.96	0.23	2.81	45,45,45,45	0
56	MG	BA	3105	1/1	0.94	0.30	2.78	43,43,43,43	0
56	MG	BD	308	1/1	0.90	0.26	2.70	42,42,42,42	0
56	MG	DA	3553	1/1	0.91	0.23	2.67	45,45,45,45	0
57	NEG	AA	3222	17/17	0.90	0.29	2.66	30,45,63,66	0
56	MG	BP	202	1/1	0.96	0.32	2.64	36,36,36,36	0
56	MG	BA	3399	1/1	0.92	0.25	2.64	62,62,62,62	0
56	MG	CA	3140	1/1	0.95	0.27	2.60	49,49,49,49	0
56	MG	DA	3168	1/1	0.97	0.27	2.59	41,41,41,41	0
56	MG	BA	3220	1/1	0.96	0.26	2.56	45,45,45,45	0
56	MG	CA	3032	1/1	0.95	0.24	2.46	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	3002	1/1	0.79	0.24	2.35	71,71,71,71	0
56	MG	DV	3001	1/1	0.98	0.34	2.26	75,75,75,75	0
56	MG	AA	3130	1/1	0.87	0.21	2.26	74,74,74,74	0
56	MG	CA	3055	1/1	0.80	0.19	2.25	63,63,63,63	0
56	MG	DA	3471	1/1	0.90	0.20	2.24	58,58,58,58	0
56	MG	BA	3194	1/1	0.95	0.27	2.23	40,40,40,40	0
56	MG	BA	3783	1/1	0.89	0.29	2.16	36,36,36,36	0
56	MG	DW	3002	1/1	0.98	0.40	2.13	32,32,32,32	0
56	MG	BA	3479	1/1	0.94	0.27	2.06	36,36,36,36	0
56	MG	BA	3007	1/1	0.88	0.34	2.05	39,39,39,39	0
59	ZN	B5	105	1/1	0.99	0.26	2.02	52,52,52,52	0
56	MG	DA	3216	1/1	0.87	0.28	1.99	52,52,52,52	0
56	MG	CA	3168	1/1	0.92	0.26	1.99	62,62,62,62	0
56	MG	DO	201	1/1	0.73	0.38	1.90	59,59,59,59	0
56	MG	DA	3142	1/1	0.84	0.27	1.86	55,55,55,55	0
56	MG	BD	303	1/1	0.89	0.34	1.83	45,45,45,45	0
59	ZN	D5	501	1/1	0.99	0.21	1.81	57,57,57,57	0
56	MG	AA	3059	1/1	0.88	0.22	1.73	53,53,53,53	0
59	ZN	B4	501	1/1	0.98	0.18	1.69	86,86,86,86	0
56	MG	DA	3360	1/1	0.95	0.20	1.63	47,47,47,47	0
56	MG	BA	3505	1/1	0.87	0.29	1.62	54,54,54,54	0
57	NEG	CA	3176	17/17	0.91	0.30	1.59	46,65,76,84	0
56	MG	BD	302	1/1	0.97	0.30	1.58	33,33,33,33	0
56	MG	BN	3002	1/1	0.67	0.31	1.57	53,53,53,53	0
56	MG	B3	3001	1/1	0.95	0.33	1.55	41,41,41,41	0
56	MG	DA	3556	1/1	0.96	0.41	1.54	48,48,48,48	0
56	MG	AA	3146	1/1	0.82	0.21	1.52	65,65,65,65	0
56	MG	DA	3465	1/1	0.92	0.23	1.51	52,52,52,52	0
56	MG	CA	3089	1/1	0.97	0.25	1.50	46,46,46,46	0
57	NEG	AA	3217	17/17	0.90	0.27	1.48	45,55,78,95	0
56	MG	BA	3079	1/1	0.96	0.25	1.33	40,40,40,40	0
56	MG	DA	3424	1/1	0.96	0.31	1.33	35,35,35,35	0
57	NEG	CW	3002	17/17	0.88	0.31	1.31	41,56,78,84	0
56	MG	DU	3003	1/1	0.91	0.32	1.29	50,50,50,50	0
56	MG	BU	203	1/1	0.97	0.28	1.28	34,34,34,34	0
56	MG	DQ	3004	1/1	0.84	0.28	1.25	65,65,65,65	0
59	ZN	BY	501	1/1	0.98	0.20	1.25	60,60,60,60	0
56	MG	CA	3094	1/1	0.96	0.22	1.22	48,48,48,48	0
57	NEG	AX	3013	17/17	0.90	0.26	1.22	29,49,69,70	0
56	MG	BV	203	1/1	0.99	0.28	1.18	31,31,31,31	0
56	MG	BD	310	1/1	0.95	0.29	1.18	45,45,45,45	0
56	MG	BA	3260	1/1	0.91	0.28	1.17	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	BA	3201	1/1	0.87	0.24	1.13	49,49,49,49	0
57	NEG	AA	3220	17/17	0.93	0.26	1.06	29,49,59,65	0
56	MG	BA	3198	1/1	0.93	0.28	1.05	35,35,35,35	0
56	MG	AA	3073	1/1	0.94	0.23	0.97	60,60,60,60	0
56	MG	BA	3637	1/1	0.67	0.27	0.97	34,34,34,34	0
56	MG	AA	3087	1/1	0.78	0.17	0.96	59,59,59,59	0
56	MG	AA	3215	1/1	0.87	0.24	0.91	56,56,56,56	0
56	MG	BA	3156	1/1	0.95	0.16	0.90	64,64,64,64	0
56	MG	BU	204	1/1	0.86	0.27	0.86	43,43,43,43	0
59	ZN	B6	102	1/1	0.99	0.23	0.84	43,43,43,43	0
56	MG	CA	3129	1/1	0.93	0.20	0.79	49,49,49,49	0
56	MG	BA	3423	1/1	0.98	0.23	0.76	43,43,43,43	0
56	MG	BA	3322	1/1	0.69	0.23	0.72	58,58,58,58	0
56	MG	AA	3211	1/1	0.94	0.23	0.71	41,41,41,41	0
56	MG	DA	3615	1/1	0.83	0.26	0.68	59,59,59,59	0
56	MG	AA	3012	1/1	0.98	0.22	0.67	43,43,43,43	0
56	MG	DF	302	1/1	0.91	0.22	0.66	60,60,60,60	0
56	MG	CA	3056	1/1	0.90	0.17	0.66	74,74,74,74	0
57	NEG	AA	3218	17/17	0.91	0.21	0.64	57,72,76,91	0
56	MG	DA	3292	1/1	0.90	0.23	0.62	36,36,36,36	0
56	MG	BA	3359	1/1	0.88	0.25	0.61	43,43,43,43	0
56	MG	AA	3145	1/1	0.92	0.23	0.55	36,36,36,36	0
56	MG	BR	203	1/1	0.97	0.25	0.41	36,36,36,36	0
57	NEG	CA	3171	17/17	0.90	0.24	0.40	53,72,80,85	0
56	MG	DA	3166	1/1	0.85	0.15	0.38	57,57,57,57	0
56	MG	CA	3019	1/1	0.95	0.25	0.37	45,45,45,45	0
56	MG	BW	203	1/1	0.98	0.22	0.35	42,42,42,42	0
56	MG	BA	3298	1/1	0.97	0.26	0.33	24,24,24,24	0
56	MG	DA	3271	1/1	0.99	0.23	0.32	51,51,51,51	0
56	MG	AA	3091	1/1	0.96	0.21	0.31	62,62,62,62	0
56	MG	CN	101	1/1	0.98	0.20	0.26	69,69,69,69	0
56	MG	DA	3600	1/1	0.94	0.24	0.18	55,55,55,55	0
56	MG	BA	3536	1/1	0.99	0.25	0.16	30,30,30,30	0
56	MG	DA	3012	1/1	0.91	0.21	0.16	43,43,43,43	0
56	MG	CA	3086	1/1	0.94	0.20	0.15	53,53,53,53	0
56	MG	BA	3003	1/1	0.92	0.27	0.15	43,43,43,43	0
56	MG	BA	3639	1/1	0.65	0.25	0.13	55,55,55,55	0
56	MG	CA	3028	1/1	0.88	0.20	0.12	53,53,53,53	0
56	MG	DA	3619	1/1	0.89	0.21	0.08	57,57,57,57	0
56	MG	BA	3226	1/1	0.95	0.25	0.06	32,32,32,32	0
56	MG	DA	3381	1/1	0.91	0.21	0.04	55,55,55,55	0
56	MG	DA	3270	1/1	0.96	0.23	0.03	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	BB	3001	1/1	0.73	0.21	-0.03	56,56,56,56	0
59	ZN	D6	501	1/1	0.93	0.20	-0.05	70,70,70,70	0
56	MG	AA	3131	1/1	0.98	0.22	-0.13	63,63,63,63	0
56	MG	DA	3096	1/1	0.98	0.21	-0.15	29,29,29,29	0
56	MG	DA	3191	1/1	0.97	0.20	-0.15	35,35,35,35	0
56	MG	DA	3428	1/1	0.98	0.20	-0.23	50,50,50,50	0
56	MG	DA	3128	1/1	0.94	0.22	-0.28	45,45,45,45	0
56	MG	DA	3386	1/1	0.91	0.14	-0.29	59,59,59,59	0
56	MG	CA	3103	1/1	0.94	0.20	-0.29	78,78,78,78	0
56	MG	DB	3006	1/1	0.91	0.19	-0.33	63,63,63,63	0
56	MG	BA	3055	1/1	0.94	0.22	-0.36	30,30,30,30	0
56	MG	DA	3140	1/1	0.92	0.21	-0.41	36,36,36,36	0
59	ZN	AN	501	1/1	0.98	0.20	-0.44	65,65,65,65	0
56	MG	DA	3406	1/1	0.93	0.20	-0.44	48,48,48,48	0
56	MG	BV	201	1/1	0.97	0.24	-0.46	26,26,26,26	0
56	MG	BA	3517	1/1	0.98	0.23	-0.47	26,26,26,26	0
56	MG	AA	3139	1/1	0.94	0.20	-0.47	50,50,50,50	0
56	MG	DA	3543	1/1	0.87	0.21	-0.47	63,63,63,63	0
56	MG	DA	3365	1/1	0.81	0.21	-0.48	54,54,54,54	0
56	MG	DA	3371	1/1	0.97	0.21	-0.49	68,68,68,68	0
56	MG	CA	3061	1/1	0.81	0.19	-0.50	61,61,61,61	0
56	MG	CA	3141	1/1	0.93	0.20	-0.50	61,61,61,61	0
56	MG	AA	3192	1/1	0.71	0.20	-0.53	71,71,71,71	0
56	MG	AA	3204	1/1	0.95	0.21	-0.55	44,44,44,44	0
56	MG	CA	3146	1/1	0.88	0.14	-0.57	80,80,80,80	0
56	MG	DB	3007	1/1	0.89	0.15	-0.58	67,67,67,67	0
56	MG	BA	3527	1/1	0.95	0.23	-0.59	58,58,58,58	0
58	SF4	AD	501	8/8	0.99	0.18	-0.62	52,60,68,71	0
56	MG	DA	3620	1/1	0.88	0.17	-0.63	71,71,71,71	0
59	ZN	B9	501	1/1	0.99	0.21	-0.63	47,47,47,47	0
56	MG	CA	3004	1/1	0.60	0.18	-0.64	69,69,69,69	0
56	MG	CE	3001	1/1	0.97	0.14	-0.66	73,73,73,73	0
56	MG	CK	3001	1/1	0.97	0.17	-0.67	47,47,47,47	0
56	MG	DA	3393	1/1	0.93	0.19	-0.68	53,53,53,53	0
56	MG	BA	3032	1/1	0.92	0.22	-0.69	32,32,32,32	0
56	MG	DA	3076	1/1	0.94	0.20	-0.70	34,34,34,34	0
59	ZN	D4	501	1/1	0.69	0.12	-0.71	137,137,137,137	0
56	MG	CA	3030	1/1	0.97	0.20	-0.72	51,51,51,51	0
56	MG	AA	3125	1/1	0.96	0.20	-0.76	53,53,53,53	0
56	MG	CA	3159	1/1	0.92	0.17	-0.76	60,60,60,60	0
56	MG	DA	3537	1/1	0.97	0.21	-0.77	53,53,53,53	0
59	ZN	DY	501	1/1	0.97	0.13	-0.78	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	AA	3150	1/1	0.92	0.20	-0.79	58,58,58,58	0
56	MG	BG	3001	1/1	0.93	0.19	-0.80	42,42,42,42	0
56	MG	CA	3027	1/1	0.93	0.15	-0.82	64,64,64,64	0
56	MG	CA	3132	1/1	0.95	0.20	-0.83	54,54,54,54	0
56	MG	BA	3383	1/1	0.94	0.21	-0.83	49,49,49,49	0
56	MG	DA	3477	1/1	0.95	0.18	-0.87	41,41,41,41	0
58	SF4	CD	302	8/8	0.99	0.17	-0.87	51,66,73,73	0
56	MG	AA	3114	1/1	0.96	0.19	-0.88	66,66,66,66	0
56	MG	BA	3308	1/1	0.96	0.21	-0.89	38,38,38,38	0
56	MG	CA	3049	1/1	0.89	0.19	-0.91	54,54,54,54	0
56	MG	BA	3122	1/1	0.98	0.25	-0.91	42,42,42,42	0
56	MG	DA	3378	1/1	0.87	0.20	-0.92	51,51,51,51	0
56	MG	BA	3178	1/1	0.89	0.23	-0.92	43,43,43,43	0
56	MG	BA	3459	1/1	0.93	0.21	-0.92	56,56,56,56	0
56	MG	BA	3342	1/1	0.95	0.16	-0.97	43,43,43,43	0
59	ZN	D9	501	1/1	0.94	0.09	-0.99	82,82,82,82	0
56	MG	AA	3072	1/1	0.96	0.20	-0.99	48,48,48,48	0
56	MG	DA	3515	1/1	0.80	0.12	-1.00	56,56,56,56	0
56	MG	BA	3052	1/1	0.94	0.20	-1.04	34,34,34,34	0
56	MG	BA	3638	1/1	0.80	0.22	-1.06	47,47,47,47	0
56	MG	DA	3472	1/1	0.74	0.16	-1.08	40,40,40,40	0
56	MG	CA	3110	1/1	0.93	0.19	-1.08	62,62,62,62	0
56	MG	DA	3043	1/1	0.94	0.16	-1.09	49,49,49,49	0
56	MG	DA	3274	1/1	0.96	0.20	-1.09	43,43,43,43	0
56	MG	DA	3257	1/1	0.86	0.20	-1.10	58,58,58,58	0
56	MG	B9	502	1/1	0.84	0.20	-1.11	61,61,61,61	0
56	MG	BA	3568	1/1	0.92	0.20	-1.13	39,39,39,39	0
56	MG	DA	3114	1/1	0.70	0.21	-1.14	53,53,53,53	0
56	MG	AA	3166	1/1	0.99	0.19	-1.15	43,43,43,43	0
56	MG	AA	3046	1/1	0.91	0.21	-1.16	50,50,50,50	0
56	MG	DA	3494	1/1	0.96	0.20	-1.17	55,55,55,55	0
56	MG	BA	3781	1/1	0.92	0.23	-1.19	42,42,42,42	0
56	MG	B7	101	1/1	0.98	0.21	-1.20	35,35,35,35	0
56	MG	DA	3429	1/1	0.93	0.14	-1.21	57,57,57,57	0
56	MG	DA	3243	1/1	0.96	0.22	-1.22	42,42,42,42	0
56	MG	AN	504	1/1	0.92	0.20	-1.26	56,56,56,56	0
56	MG	BA	3592	1/1	0.99	0.18	-1.26	61,61,61,61	0
56	MG	DA	3536	1/1	0.94	0.14	-1.28	39,39,39,39	0
56	MG	DA	3215	1/1	0.95	0.22	-1.29	53,53,53,53	0
56	MG	DA	3306	1/1	0.69	0.14	-1.29	57,57,57,57	0
56	MG	DA	3144	1/1	0.84	0.11	-1.30	60,60,60,60	0
56	MG	CA	3091	1/1	0.98	0.17	-1.32	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	3499	1/1	0.99	0.17	-1.32	60,60,60,60	0
56	MG	BA	3695	1/1	0.86	0.23	-1.33	39,39,39,39	0
56	MG	DA	3542	1/1	0.91	0.12	-1.33	65,65,65,65	0
56	MG	AA	3092	1/1	0.82	0.18	-1.33	59,59,59,59	0
56	MG	DE	303	1/1	0.86	0.18	-1.35	40,40,40,40	0
56	MG	BA	3050	1/1	0.96	0.18	-1.36	34,34,34,34	0
56	MG	AA	3054	1/1	0.94	0.17	-1.37	46,46,46,46	0
56	MG	BQ	3002	1/1	0.97	0.23	-1.38	41,41,41,41	0
56	MG	BA	3275	1/1	0.89	0.19	-1.40	45,45,45,45	0
56	MG	DA	3368	1/1	0.94	0.17	-1.40	48,48,48,48	0
56	MG	DE	302	1/1	0.93	0.20	-1.44	30,30,30,30	0
56	MG	CA	3169	1/1	0.99	0.19	-1.44	49,49,49,49	0
56	MG	DD	305	1/1	0.90	0.18	-1.45	32,32,32,32	0
56	MG	DA	3395	1/1	0.92	0.21	-1.45	40,40,40,40	0
56	MG	AA	3018	1/1	0.87	0.21	-1.46	58,58,58,58	0
56	MG	DA	3405	1/1	0.90	0.15	-1.47	76,76,76,76	0
56	MG	DA	3011	1/1	0.92	0.14	-1.47	46,46,46,46	0
56	MG	DA	3033	1/1	0.93	0.19	-1.47	43,43,43,43	0
59	ZN	CN	102	1/1	0.95	0.09	-1.49	82,82,82,82	0
56	MG	BA	3049	1/1	0.90	0.23	-1.50	54,54,54,54	0
56	MG	CA	3002	1/1	0.74	0.12	-1.54	65,65,65,65	0
56	MG	BA	3473	1/1	0.92	0.21	-1.56	31,31,31,31	0
56	MG	DA	3126	1/1	0.88	0.13	-1.57	51,51,51,51	0
56	MG	CA	3036	1/1	0.68	0.15	-1.61	69,69,69,69	0
56	MG	BN	3003	1/1	0.84	0.16	-1.61	62,62,62,62	0
56	MG	CA	3025	1/1	0.84	0.16	-1.65	64,64,64,64	0
56	MG	DA	3366	1/1	0.91	0.15	-1.66	36,36,36,36	0
56	MG	DA	3265	1/1	0.97	0.17	-1.67	47,47,47,47	0
56	MG	AA	3006	1/1	0.92	0.23	-1.68	57,57,57,57	0
56	MG	AA	3214	1/1	0.83	0.13	-1.69	69,69,69,69	0
56	MG	BA	3014	1/1	0.94	0.17	-1.69	46,46,46,46	0
56	MG	BP	203	1/1	0.93	0.18	-1.70	37,37,37,37	0
56	MG	CA	3107	1/1	0.96	0.14	-1.72	63,63,63,63	0
56	MG	BA	3348	1/1	0.95	0.24	-1.74	35,35,35,35	0
56	MG	DA	3147	1/1	0.78	0.12	-1.75	49,49,49,49	0
56	MG	BD	306	1/1	0.90	0.19	-1.76	22,22,22,22	0
56	MG	DA	3295	1/1	0.94	0.18	-1.78	34,34,34,34	0
56	MG	BA	3448	1/1	0.96	0.20	-1.78	60,60,60,60	0
56	MG	BA	3362	1/1	0.90	0.20	-1.80	25,25,25,25	0
56	MG	DA	3035	1/1	0.95	0.17	-1.82	39,39,39,39	0
56	MG	BA	3552	1/1	0.94	0.18	-1.82	32,32,32,32	0
56	MG	DA	3063	1/1	0.85	0.14	-1.83	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	AA	3041	1/1	0.75	0.14	-1.85	64,64,64,64	0
56	MG	DA	3034	1/1	0.97	0.20	-1.87	35,35,35,35	0
56	MG	DA	3290	1/1	0.94	0.20	-1.87	36,36,36,36	0
56	MG	BA	3652	1/1	0.91	0.21	-1.88	25,25,25,25	0
56	MG	DA	3403	1/1	0.85	0.17	-1.89	54,54,54,54	0
56	MG	CA	3051	1/1	0.77	0.15	-1.92	78,78,78,78	0
56	MG	BA	3037	1/1	0.97	0.22	-1.93	33,33,33,33	0
56	MG	BF	303	1/1	0.95	0.19	-1.93	36,36,36,36	0
56	MG	CA	3104	1/1	0.95	0.17	-1.94	51,51,51,51	0
56	MG	BA	3729	1/1	0.79	0.18	-1.96	55,55,55,55	0
56	MG	AA	3002	1/1	0.85	0.15	-1.97	59,59,59,59	0
56	MG	D0	101	1/1	0.96	0.17	-1.98	73,73,73,73	0
56	MG	BA	3607	1/1	0.95	0.21	-1.98	45,45,45,45	0
56	MG	AA	3212	1/1	0.94	0.15	-2.01	33,33,33,33	0
56	MG	BA	3441	1/1	0.94	0.12	-2.01	37,37,37,37	0
56	MG	DQ	3001	1/1	0.98	0.11	-2.03	57,57,57,57	0
56	MG	AA	3001	1/1	0.98	0.15	-2.06	37,37,37,37	0
56	MG	BA	3390	1/1	0.95	0.23	-2.06	26,26,26,26	0
56	MG	DA	3438	1/1	0.84	0.14	-2.07	55,55,55,55	0
56	MG	AX	3005	1/1	0.92	0.12	-2.07	66,66,66,66	0
56	MG	BA	3332	1/1	0.93	0.20	-2.08	48,48,48,48	0
56	MG	DA	3203	1/1	0.91	0.18	-2.09	46,46,46,46	0
56	MG	DA	3004	1/1	0.97	0.18	-2.11	18,18,18,18	0
56	MG	BV	204	1/1	0.89	0.19	-2.11	39,39,39,39	0
56	MG	BA	3295	1/1	0.88	0.13	-2.13	66,66,66,66	0
56	MG	DF	304	1/1	0.87	0.12	-2.14	48,48,48,48	0
56	MG	BV	206	1/1	0.96	0.17	-2.15	38,38,38,38	0
56	MG	CA	3063	1/1	0.94	0.18	-2.15	59,59,59,59	0
56	MG	CA	3152	1/1	0.97	0.18	-2.16	58,58,58,58	0
56	MG	BA	3174	1/1	0.89	0.18	-2.17	52,52,52,52	0
56	MG	BA	3338	1/1	0.84	0.20	-2.19	39,39,39,39	0
56	MG	DA	3111	1/1	0.94	0.11	-2.19	49,49,49,49	0
56	MG	CT	3001	1/1	0.84	0.13	-2.21	50,50,50,50	0
56	MG	BA	3312	1/1	0.91	0.22	-2.22	41,41,41,41	0
56	MG	BA	3378	1/1	0.94	0.21	-2.23	24,24,24,24	0
56	MG	AA	3213	1/1	0.87	0.12	-2.27	44,44,44,44	0
56	MG	CA	3167	1/1	0.89	0.10	-2.30	55,55,55,55	0
56	MG	DA	3018	1/1	0.94	0.15	-2.33	29,29,29,29	0
56	MG	DG	3001	1/1	0.86	0.12	-2.33	55,55,55,55	0
56	MG	BA	3516	1/1	0.98	0.20	-2.34	36,36,36,36	0
56	MG	DA	3409	1/1	0.83	0.15	-2.36	41,41,41,41	0
56	MG	AE	3001	1/1	0.91	0.09	-2.38	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3035	1/1	0.92	0.22	-2.38	25,25,25,25	0
56	MG	DA	3188	1/1	0.96	0.12	-2.38	61,61,61,61	0
56	MG	DA	3119	1/1	0.84	0.17	-2.41	50,50,50,50	0
56	MG	DA	3124	1/1	0.93	0.12	-2.43	43,43,43,43	0
56	MG	BA	3770	1/1	0.96	0.19	-2.44	20,20,20,20	0
56	MG	DA	3313	1/1	0.98	0.19	-2.46	46,46,46,46	0
56	MG	CA	3082	1/1	0.90	0.18	-2.47	41,41,41,41	0
56	MG	DA	3091	1/1	0.80	0.15	-2.48	57,57,57,57	0
56	MG	DA	3275	1/1	0.93	0.13	-2.49	51,51,51,51	0
56	MG	AA	3137	1/1	0.91	0.16	-2.49	49,49,49,49	0
56	MG	CA	3050	1/1	0.86	0.10	-2.49	55,55,55,55	0
56	MG	CA	3166	1/1	0.96	0.11	-2.50	42,42,42,42	0
56	MG	DA	3088	1/1	0.93	0.17	-2.50	39,39,39,39	0
56	MG	BA	3303	1/1	0.82	0.20	-2.50	27,27,27,27	0
56	MG	BA	3534	1/1	0.91	0.20	-2.53	54,54,54,54	0
56	MG	BA	3016	1/1	0.98	0.21	-2.54	22,22,22,22	0
56	MG	BA	3024	1/1	0.99	0.19	-2.57	19,19,19,19	0
56	MG	CA	3106	1/1	0.90	0.15	-2.61	55,55,55,55	0
56	MG	AA	3029	1/1	0.93	0.15	-2.63	60,60,60,60	0
56	MG	BA	3487	1/1	0.96	0.20	-2.64	37,37,37,37	0
56	MG	BA	3693	1/1	0.83	0.19	-2.65	38,38,38,38	0
56	MG	AN	503	1/1	0.94	0.14	-2.66	59,59,59,59	0
56	MG	DA	3087	1/1	0.68	0.10	-2.68	49,49,49,49	0
56	MG	BA	3343	1/1	0.91	0.18	-2.70	44,44,44,44	0
56	MG	DA	3616	1/1	0.87	0.13	-2.72	47,47,47,47	0
56	MG	BA	3344	1/1	0.93	0.19	-2.73	36,36,36,36	0
56	MG	BA	3076	1/1	0.90	0.13	-2.76	58,58,58,58	0
56	MG	AA	3099	1/1	0.78	0.11	-2.78	59,59,59,59	0
56	MG	BA	3231	1/1	0.91	0.17	-2.80	42,42,42,42	0
56	MG	DA	3234	1/1	0.98	0.13	-2.84	42,42,42,42	0
56	MG	AA	3187	1/1	0.98	0.15	-2.89	56,56,56,56	0
56	MG	BA	3537	1/1	0.85	0.17	-2.89	55,55,55,55	0
56	MG	DA	3504	1/1	0.89	0.12	-2.90	55,55,55,55	0
56	MG	BA	3523	1/1	0.90	0.18	-2.90	39,39,39,39	0
56	MG	DA	3583	1/1	0.73	0.13	-2.91	44,44,44,44	0
56	MG	CA	3007	1/1	0.60	0.16	-2.91	69,69,69,69	0
56	MG	DA	3250	1/1	0.93	0.15	-2.93	37,37,37,37	0
56	MG	DB	3003	1/1	0.96	0.12	-2.99	62,62,62,62	0
56	MG	BA	3250	1/1	0.97	0.19	-3.00	40,40,40,40	0
56	MG	DA	3473	1/1	0.95	0.10	-3.02	60,60,60,60	0
56	MG	BA	3763	1/1	0.99	0.19	-3.02	10,10,10,10	0
56	MG	BA	3083	1/1	0.95	0.20	-3.02	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	AA	3076	1/1	0.95	0.17	-3.04	45,45,45,45	0
56	MG	AM	201	1/1	0.82	0.10	-3.07	61,61,61,61	0
56	MG	BA	3628	1/1	0.83	0.18	-3.09	55,55,55,55	0
56	MG	DA	3487	1/1	0.96	0.14	-3.09	37,37,37,37	0
56	MG	BA	3778	1/1	0.96	0.14	-3.10	36,36,36,36	0
56	MG	DA	3372	1/1	0.91	0.11	-3.11	67,67,67,67	0
56	MG	CA	3071	1/1	0.90	0.08	-3.11	58,58,58,58	0
56	MG	BA	3291	1/1	0.96	0.20	-3.11	26,26,26,26	0
56	MG	DA	3414	1/1	0.85	0.17	-3.13	46,46,46,46	0
56	MG	BA	3480	1/1	0.69	0.20	-3.14	29,29,29,29	0
56	MG	BA	3571	1/1	0.91	0.14	-3.15	40,40,40,40	0
56	MG	BE	301	1/1	0.91	0.19	-3.16	36,36,36,36	0
56	MG	AA	3036	1/1	0.98	0.16	-3.17	24,24,24,24	0
56	MG	BA	3236	1/1	0.98	0.16	-3.17	34,34,34,34	0
56	MG	DA	3380	1/1	0.88	0.14	-3.17	43,43,43,43	0
56	MG	DA	3137	1/1	0.95	0.13	-3.19	57,57,57,57	0
56	MG	BA	3585	1/1	0.84	0.18	-3.21	61,61,61,61	0
56	MG	DA	3502	1/1	0.95	0.12	-3.26	47,47,47,47	0
56	MG	DA	3541	1/1	0.95	0.17	-3.30	46,46,46,46	0
56	MG	BA	3361	1/1	0.92	0.17	-3.31	29,29,29,29	0
56	MG	BA	3043	1/1	0.97	0.17	-3.36	34,34,34,34	0
56	MG	DA	3296	1/1	0.95	0.14	-3.37	38,38,38,38	0
56	MG	BA	3513	1/1	0.95	0.17	-3.39	42,42,42,42	0
56	MG	BA	3273	1/1	0.97	0.18	-3.39	36,36,36,36	0
56	MG	BA	3184	1/1	0.93	0.18	-3.42	33,33,33,33	0
56	MG	DA	3337	1/1	0.94	0.13	-3.42	42,42,42,42	0
56	MG	BA	3382	1/1	0.91	0.19	-3.42	30,30,30,30	0
56	MG	DA	3606	1/1	0.86	0.12	-3.44	54,54,54,54	0
56	MG	AA	3154	1/1	0.92	0.13	-3.45	67,67,67,67	0
56	MG	DA	3442	1/1	0.86	0.15	-3.45	46,46,46,46	0
56	MG	AA	3060	1/1	0.94	0.14	-3.46	42,42,42,42	0
56	MG	BA	3005	1/1	0.98	0.13	-3.47	41,41,41,41	0
56	MG	DA	3182	1/1	0.91	0.11	-3.49	52,52,52,52	0
56	MG	DA	3505	1/1	0.95	0.18	-3.49	41,41,41,41	0
56	MG	DA	3085	1/1	0.79	0.12	-3.51	65,65,65,65	0
56	MG	BA	3744	1/1	0.95	0.15	-3.54	27,27,27,27	0
56	MG	DA	3280	1/1	0.97	0.15	-3.56	26,26,26,26	0
56	MG	BB	3003	1/1	0.90	0.17	-3.57	37,37,37,37	0
56	MG	BA	3054	1/1	0.87	0.18	-3.59	51,51,51,51	0
56	MG	BA	3369	1/1	0.97	0.19	-3.59	23,23,23,23	0
56	MG	BA	3663	1/1	0.93	0.16	-3.59	26,26,26,26	0
56	MG	BA	3063	1/1	0.93	0.15	-3.62	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3278	1/1	0.87	0.12	-3.63	44,44,44,44	0
56	MG	DA	3315	1/1	0.93	0.09	-3.65	28,28,28,28	0
56	MG	BF	307	1/1	0.93	0.20	-3.68	46,46,46,46	0
56	MG	BA	3766	1/1	0.96	0.20	-3.69	43,43,43,43	0
56	MG	BA	3316	1/1	0.94	0.20	-3.73	58,58,58,58	0
56	MG	BA	3372	1/1	0.93	0.20	-3.73	33,33,33,33	0
56	MG	DA	3369	1/1	0.92	0.19	-3.75	47,47,47,47	0
56	MG	BA	3755	1/1	0.91	0.16	-3.77	42,42,42,42	0
56	MG	BA	3526	1/1	0.86	0.18	-3.79	38,38,38,38	0
56	MG	DA	3005	1/1	0.98	0.15	-3.81	39,39,39,39	0
56	MG	DA	3136	1/1	0.94	0.15	-3.84	35,35,35,35	0
56	MG	BA	3352	1/1	0.94	0.15	-3.85	22,22,22,22	0
56	MG	DA	3089	1/1	0.90	0.10	-3.85	57,57,57,57	0
56	MG	AA	3119	1/1	0.96	0.17	-3.87	36,36,36,36	0
56	MG	CA	3023	1/1	0.97	0.11	-3.87	54,54,54,54	0
56	MG	BA	3510	1/1	0.89	0.17	-3.88	43,43,43,43	0
56	MG	DA	3319	1/1	0.97	0.13	-3.89	21,21,21,21	0
56	MG	BA	3439	1/1	0.93	0.20	-3.93	15,15,15,15	0
56	MG	BA	3347	1/1	0.96	0.19	-3.96	26,26,26,26	0
56	MG	BA	3768	1/1	0.90	0.18	-3.97	48,48,48,48	0
56	MG	BA	3294	1/1	0.92	0.16	-3.99	45,45,45,45	0
56	MG	BA	3366	1/1	0.92	0.16	-3.99	23,23,23,23	0
56	MG	DA	3614	1/1	0.76	0.14	-3.99	34,34,34,34	0
56	MG	BA	3357	1/1	0.97	0.18	-4.03	29,29,29,29	0
56	MG	DA	3267	1/1	0.95	0.14	-4.04	42,42,42,42	0
56	MG	BA	3259	1/1	0.95	0.16	-4.04	32,32,32,32	0
56	MG	BA	3261	1/1	0.91	0.21	-4.05	49,49,49,49	0
56	MG	CA	3165	1/1	0.89	0.15	-4.06	57,57,57,57	0
56	MG	DA	3008	1/1	0.95	0.14	-4.07	38,38,38,38	0
56	MG	DA	3497	1/1	0.94	0.14	-4.07	27,27,27,27	0
56	MG	DA	3392	1/1	0.97	0.16	-4.09	34,34,34,34	0
56	MG	BA	3167	1/1	0.96	0.19	-4.09	28,28,28,28	0
56	MG	BA	3494	1/1	0.86	0.16	-4.10	41,41,41,41	0
56	MG	AA	3023	1/1	0.92	0.13	-4.11	51,51,51,51	0
56	MG	DA	3579	1/1	0.86	0.10	-4.12	69,69,69,69	0
56	MG	BA	3764	1/1	0.92	0.17	-4.12	26,26,26,26	0
56	MG	DA	3399	1/1	0.98	0.16	-4.14	35,35,35,35	0
56	MG	AA	3111	1/1	0.77	0.16	-4.17	65,65,65,65	0
56	MG	DA	3440	1/1	0.97	0.13	-4.19	49,49,49,49	0
56	MG	DA	3554	1/1	0.84	0.13	-4.21	45,45,45,45	0
56	MG	AA	3123	1/1	0.96	0.15	-4.25	25,25,25,25	0
56	MG	BA	3640	1/1	0.94	0.11	-4.26	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	DA	3416	1/1	0.97	0.13	-4.28	39,39,39,39	0
56	MG	BA	3572	1/1	0.91	0.13	-4.32	55,55,55,55	0
56	MG	DA	3236	1/1	0.95	0.14	-4.36	59,59,59,59	0
56	MG	AA	3143	1/1	0.89	0.12	-4.38	57,57,57,57	0
56	MG	AA	3031	1/1	0.86	0.15	-4.38	63,63,63,63	0
56	MG	AA	3013	1/1	0.94	0.12	-4.39	66,66,66,66	0
56	MG	DA	3566	1/1	0.88	0.12	-4.40	51,51,51,51	0
56	MG	DA	3408	1/1	0.96	0.10	-4.43	25,25,25,25	0
56	MG	BA	3619	1/1	0.94	0.11	-4.49	49,49,49,49	0
56	MG	BA	3570	1/1	0.92	0.18	-4.50	57,57,57,57	0
56	MG	BA	3462	1/1	0.84	0.16	-4.52	59,59,59,59	0
56	MG	BA	3317	1/1	0.98	0.13	-4.56	47,47,47,47	0
56	MG	DA	3056	1/1	0.94	0.08	-4.60	51,51,51,51	0
56	MG	BA	3629	1/1	0.97	0.17	-4.68	62,62,62,62	0
56	MG	BA	3654	1/1	0.98	0.17	-4.68	24,24,24,24	0
56	MG	B0	102	1/1	0.95	0.09	-4.68	54,54,54,54	0
56	MG	DA	3102	1/1	0.94	0.10	-4.69	50,50,50,50	0
56	MG	BA	3468	1/1	0.91	0.14	-4.72	31,31,31,31	0
56	MG	DA	3030	1/1	0.79	0.13	-4.75	54,54,54,54	0
56	MG	BA	3096	1/1	0.96	0.16	-4.77	29,29,29,29	0
56	MG	AA	3014	1/1	0.72	0.10	-4.78	64,64,64,64	0
56	MG	BA	3279	1/1	0.91	0.14	-4.78	52,52,52,52	0
56	MG	DA	3252	1/1	0.98	0.09	-4.80	43,43,43,43	0
56	MG	DA	3204	1/1	0.96	0.13	-4.86	47,47,47,47	0
56	MG	BB	3006	1/1	0.94	0.13	-4.86	46,46,46,46	0
56	MG	CA	3038	1/1	0.93	0.13	-4.90	31,31,31,31	0
56	MG	AA	3048	1/1	0.93	0.14	-4.90	55,55,55,55	0
56	MG	BA	3493	1/1	0.97	0.14	-4.91	29,29,29,29	0
56	MG	BA	3427	1/1	0.97	0.17	-4.93	22,22,22,22	0
56	MG	DA	3404	1/1	0.95	0.12	-4.94	36,36,36,36	0
56	MG	AV	102	1/1	0.83	0.18	-4.95	52,52,52,52	0
56	MG	DA	3354	1/1	0.94	0.10	-4.95	56,56,56,56	0
56	MG	AA	3064	1/1	0.96	0.13	-4.95	47,47,47,47	0
56	MG	BA	3596	1/1	0.94	0.14	-4.96	52,52,52,52	0
56	MG	DE	304	1/1	0.93	0.14	-4.97	45,45,45,45	0
56	MG	AA	3183	1/1	0.68	0.16	-4.97	63,63,63,63	0
56	MG	BA	3353	1/1	0.93	0.16	-4.98	27,27,27,27	0
56	MG	DA	3391	1/1	0.96	0.14	-4.99	40,40,40,40	0
56	MG	BA	3511	1/1	0.97	0.19	-5.07	31,31,31,31	0
56	MG	BA	3145	1/1	0.81	0.14	-5.09	41,41,41,41	0
56	MG	CA	3015	1/1	0.95	0.10	-5.13	45,45,45,45	0
56	MG	BA	3270	1/1	0.95	0.14	-5.13	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	DA	3538	1/1	0.95	0.07	-5.14	50,50,50,50	0
56	MG	BA	3213	1/1	0.84	0.14	-5.15	48,48,48,48	0
56	MG	BA	3469	1/1	0.94	0.18	-5.17	49,49,49,49	0
56	MG	DA	3346	1/1	0.86	0.14	-5.18	29,29,29,29	0
56	MG	BE	302	1/1	0.95	0.20	-5.19	28,28,28,28	0
56	MG	BA	3144	1/1	0.85	0.16	-5.20	37,37,37,37	0
56	MG	BA	3355	1/1	0.92	0.17	-5.20	26,26,26,26	0
56	MG	BA	3334	1/1	0.99	0.18	-5.20	23,23,23,23	0
56	MG	DA	3282	1/1	0.96	0.14	-5.22	43,43,43,43	0
56	MG	DA	3327	1/1	0.97	0.12	-5.22	32,32,32,32	0
56	MG	DA	3559	1/1	0.94	0.09	-5.24	49,49,49,49	0
56	MG	BA	3319	1/1	0.95	0.17	-5.28	38,38,38,38	0
56	MG	BA	3381	1/1	0.92	0.17	-5.30	33,33,33,33	0
56	MG	DA	3317	1/1	0.96	0.05	-5.34	47,47,47,47	0
56	MG	BA	3414	1/1	0.99	0.16	-5.35	26,26,26,26	0
56	MG	DA	3110	1/1	0.96	0.09	-5.35	30,30,30,30	0
56	MG	DA	3237	1/1	0.97	0.09	-5.38	42,42,42,42	0
56	MG	BA	3720	1/1	0.98	0.10	-5.39	28,28,28,28	0
56	MG	BB	3014	1/1	0.93	0.16	-5.43	39,39,39,39	0
56	MG	BA	3465	1/1	0.93	0.21	-5.45	20,20,20,20	0
56	MG	BA	3349	1/1	0.91	0.19	-5.45	25,25,25,25	0
56	MG	BA	3478	1/1	0.96	0.19	-5.49	36,36,36,36	0
56	MG	AA	3040	1/1	0.88	0.10	-5.49	41,41,41,41	0
56	MG	AA	3180	1/1	0.94	0.12	-5.50	67,67,67,67	0
56	MG	BA	3535	1/1	0.94	0.16	-5.53	46,46,46,46	0
56	MG	BA	3034	1/1	0.95	0.15	-5.53	34,34,34,34	0
56	MG	BA	3708	1/1	0.97	0.13	-5.58	7,7,7,7	0
56	MG	BA	3709	1/1	0.98	0.20	-5.59	42,42,42,42	0
56	MG	CA	3012	1/1	0.95	0.13	-5.64	56,56,56,56	0
56	MG	BA	3496	1/1	0.89	0.20	-5.66	53,53,53,53	0
56	MG	BA	3426	1/1	0.97	0.15	-5.67	29,29,29,29	0
56	MG	BA	3564	1/1	0.95	0.15	-5.67	49,49,49,49	0
56	MG	DA	3362	1/1	0.88	0.16	-5.71	22,22,22,22	0
56	MG	AA	3163	1/1	0.92	0.20	-5.71	53,53,53,53	0
56	MG	BA	3461	1/1	0.88	0.18	-5.74	21,21,21,21	0
56	MG	BA	3310	1/1	0.93	0.11	-5.82	41,41,41,41	0
56	MG	DA	3045	1/1	0.87	0.12	-5.82	44,44,44,44	0
56	MG	DA	3238	1/1	0.94	0.11	-5.84	40,40,40,40	0
56	MG	BA	3604	1/1	0.90	0.14	-5.89	46,46,46,46	0
56	MG	DA	3286	1/1	0.91	0.14	-5.90	39,39,39,39	0
56	MG	BA	3758	1/1	0.95	0.14	-5.90	38,38,38,38	0
56	MG	BA	3109	1/1	0.86	0.16	-5.90	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	DA	3115	1/1	0.96	0.08	-5.92	51,51,51,51	0
56	MG	DA	3277	1/1	0.95	0.14	-5.99	52,52,52,52	0
56	MG	BA	3038	1/1	0.99	0.17	-5.99	31,31,31,31	0
56	MG	DA	3329	1/1	0.92	0.09	-6.09	62,62,62,62	0
56	MG	DA	3235	1/1	0.97	0.09	-6.09	29,29,29,29	0
56	MG	DA	3299	1/1	0.95	0.12	-6.12	40,40,40,40	0
56	MG	BA	3664	1/1	0.93	0.17	-6.12	25,25,25,25	0
56	MG	CA	3022	1/1	0.94	0.11	-6.16	53,53,53,53	0
56	MG	BE	308	1/1	0.92	0.12	-6.16	34,34,34,34	0
56	MG	DA	3092	1/1	0.97	0.12	-6.22	43,43,43,43	0
56	MG	BA	3682	1/1	0.87	0.11	-6.24	73,73,73,73	0
56	MG	BA	3078	1/1	0.75	0.13	-6.27	48,48,48,48	0
56	MG	DA	3232	1/1	0.94	0.09	-6.27	57,57,57,57	0
56	MG	BA	3456	1/1	0.88	0.12	-6.29	63,63,63,63	0
56	MG	AA	3070	1/1	0.93	0.12	-6.30	31,31,31,31	0
56	MG	DA	3325	1/1	0.92	0.13	-6.31	32,32,32,32	0
56	MG	DO	202	1/1	0.97	0.10	-6.33	57,57,57,57	0
56	MG	DA	3249	1/1	0.87	0.10	-6.41	43,43,43,43	0
56	MG	DA	3258	1/1	0.94	0.10	-6.42	24,24,24,24	0
56	MG	AA	3010	1/1	0.93	0.14	-6.42	22,22,22,22	0
56	MG	DA	3026	1/1	0.96	0.11	-6.45	24,24,24,24	0
56	MG	BA	3765	1/1	0.92	0.15	-6.49	59,59,59,59	0
56	MG	BA	3274	1/1	0.91	0.15	-6.52	29,29,29,29	0
56	MG	AA	3077	1/1	0.94	0.06	-6.53	69,69,69,69	0
56	MG	CA	3014	1/1	0.91	0.09	-6.53	46,46,46,46	0
56	MG	BB	3015	1/1	0.84	0.12	-6.55	54,54,54,54	0
56	MG	BA	3500	1/1	0.96	0.11	-6.68	37,37,37,37	0
56	MG	BA	3006	1/1	0.99	0.15	-6.69	26,26,26,26	0
56	MG	BA	3397	1/1	0.95	0.15	-6.71	29,29,29,29	0
56	MG	DA	3019	1/1	0.93	0.11	-6.74	40,40,40,40	0
56	MG	BA	3180	1/1	0.86	0.14	-6.74	46,46,46,46	0
56	MG	DA	3510	1/1	0.89	0.13	-6.76	32,32,32,32	0
56	MG	BA	3340	1/1	0.88	0.18	-6.81	34,34,34,34	0
56	MG	BA	3711	1/1	0.95	0.13	-6.86	51,51,51,51	0
56	MG	DA	3531	1/1	0.96	0.11	-7.07	40,40,40,40	0
56	MG	BA	3492	1/1	0.91	0.14	-7.15	33,33,33,33	0
56	MG	BA	3004	1/1	0.95	0.09	-7.17	25,25,25,25	0
56	MG	BA	3723	1/1	0.87	0.12	-7.18	41,41,41,41	0
56	MG	BA	3165	1/1	0.82	0.13	-7.20	53,53,53,53	0
56	MG	DA	3506	1/1	0.98	0.14	-7.21	37,37,37,37	0
56	MG	BA	3417	1/1	0.87	0.14	-7.22	56,56,56,56	0
56	MG	BA	3442	1/1	0.93	0.14	-7.22	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	3032	1/1	0.90	0.15	-7.22	40,40,40,40	0
56	MG	BA	3759	1/1	0.98	0.17	-7.27	29,29,29,29	0
56	MG	BA	3566	1/1	0.94	0.15	-7.27	28,28,28,28	0
56	MG	BA	3346	1/1	0.97	0.17	-7.30	28,28,28,28	0
56	MG	CA	3158	1/1	0.93	0.13	-7.33	72,72,72,72	0
56	MG	AA	3129	1/1	0.95	0.06	-7.37	77,77,77,77	0
56	MG	DA	3304	1/1	0.93	0.12	-7.52	32,32,32,32	0
56	MG	BA	3613	1/1	0.85	0.13	-7.52	53,53,53,53	0
56	MG	BA	3304	1/1	0.93	0.19	-7.52	21,21,21,21	0
56	MG	DA	3518	1/1	0.97	0.06	-7.55	57,57,57,57	0
56	MG	BA	3292	1/1	0.97	0.15	-7.63	26,26,26,26	0
56	MG	BA	3337	1/1	0.93	0.16	-7.67	25,25,25,25	0
56	MG	BA	3680	1/1	0.82	0.15	-7.68	32,32,32,32	0
56	MG	AA	3085	1/1	0.94	0.12	-7.69	63,63,63,63	0
56	MG	BA	3447	1/1	0.92	0.13	-7.73	38,38,38,38	0
56	MG	DA	3281	1/1	0.97	0.12	-7.75	39,39,39,39	0
56	MG	DA	3187	1/1	0.93	0.16	-7.77	41,41,41,41	0
56	MG	DA	3014	1/1	0.95	0.11	-7.82	37,37,37,37	0
56	MG	BA	3452	1/1	0.98	0.10	-7.86	41,41,41,41	0
56	MG	BA	3722	1/1	0.92	0.12	-7.90	46,46,46,46	0
56	MG	AA	3202	1/1	0.89	0.08	-7.92	63,63,63,63	0
56	MG	BA	3688	1/1	0.94	0.12	-7.98	24,24,24,24	0
56	MG	BA	3706	1/1	0.82	0.18	-8.00	52,52,52,52	0
56	MG	BA	3409	1/1	0.92	0.15	-8.04	43,43,43,43	0
56	MG	CA	3084	1/1	0.92	0.12	-8.14	46,46,46,46	0
56	MG	BA	3703	1/1	0.82	0.15	-8.14	56,56,56,56	0
56	MG	BA	3196	1/1	0.90	0.15	-8.21	46,46,46,46	0
56	MG	DA	3338	1/1	0.92	0.10	-8.35	60,60,60,60	0
56	MG	BA	3671	1/1	0.92	0.17	-8.36	33,33,33,33	0
56	MG	DA	3377	1/1	0.86	0.11	-8.40	48,48,48,48	0
56	MG	DA	3246	1/1	0.97	0.09	-8.53	53,53,53,53	0
56	MG	DA	3294	1/1	0.92	0.08	-8.60	53,53,53,53	0
56	MG	DA	3452	1/1	0.92	0.15	-8.61	44,44,44,44	0
56	MG	BA	3115	1/1	0.97	0.17	-8.67	13,13,13,13	0
56	MG	DA	3020	1/1	0.97	0.13	-8.71	33,33,33,33	0
56	MG	BA	3046	1/1	0.83	0.15	-8.72	50,50,50,50	0
56	MG	DA	3132	1/1	0.96	0.09	-8.81	39,39,39,39	0
56	MG	DA	3227	1/1	0.93	0.10	-8.82	47,47,47,47	0
56	MG	DA	3309	1/1	0.97	0.10	-8.91	42,42,42,42	0
56	MG	BA	3471	1/1	0.85	0.12	-8.93	33,33,33,33	0
56	MG	DA	3307	1/1	0.96	0.10	-9.04	28,28,28,28	0
56	MG	BA	3017	1/1	0.98	0.13	-9.28	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	BA	3320	1/1	0.98	0.15	-9.38	28,28,28,28	0
56	MG	AA	3022	1/1	0.94	0.09	-9.38	58,58,58,58	0
56	MG	BA	3147	1/1	0.90	0.09	-9.46	60,60,60,60	0
56	MG	AA	3065	1/1	0.94	0.11	-9.46	40,40,40,40	0
56	MG	BA	3262	1/1	0.86	0.13	-9.88	51,51,51,51	0
56	MG	DA	3314	1/1	0.81	0.09	-10.14	46,46,46,46	0
56	MG	BA	3269	1/1	0.96	0.15	-10.45	40,40,40,40	0
56	MG	BA	3333	1/1	0.92	0.11	-10.64	39,39,39,39	0
56	MG	DA	3441	1/1	0.93	0.10	-10.66	39,39,39,39	0
56	MG	DA	3618	1/1	0.94	0.10	-10.70	57,57,57,57	0
56	MG	DA	3121	1/1	0.95	0.11	-10.83	33,33,33,33	0
56	MG	BA	3010	1/1	0.90	0.13	-11.11	58,58,58,58	0
56	MG	DA	3490	1/1	0.80	0.08	-11.12	49,49,49,49	0
56	MG	BA	3289	1/1	0.98	0.14	-11.21	24,24,24,24	0
56	MG	DA	3302	1/1	0.86	0.13	-11.54	38,38,38,38	0
56	MG	AA	3071	1/1	0.96	0.13	-11.73	52,52,52,52	0
56	MG	BA	3699	1/1	0.95	0.12	-11.77	39,39,39,39	0
56	MG	BA	3376	1/1	0.96	0.17	-11.84	23,23,23,23	0
56	MG	BA	3626	1/1	0.97	0.12	-12.59	40,40,40,40	0
56	MG	BA	3276	1/1	0.87	0.14	-12.68	40,40,40,40	0
56	MG	CA	3078	1/1	0.95	0.12	-12.99	41,41,41,41	0
56	MG	BA	3257	1/1	0.88	0.16	-13.30	48,48,48,48	0
56	MG	BA	3392	1/1	0.97	0.14	-13.75	17,17,17,17	0
56	MG	BA	3567	1/1	0.91	0.09	-14.59	35,35,35,35	0
56	MG	BA	3569	1/1	0.93	0.12	-14.61	44,44,44,44	0
56	MG	BA	3263	1/1	0.96	0.10	-14.66	47,47,47,47	0
56	MG	BA	3282	1/1	0.97	0.08	-14.82	59,59,59,59	0
56	MG	DA	3478	1/1	0.95	0.08	-15.31	54,54,54,54	0
56	MG	DA	3101	1/1	0.98	0.09	-15.71	28,28,28,28	0
56	MG	BA	3393	1/1	0.96	0.17	-17.14	48,48,48,48	0
56	MG	BA	3296	1/1	0.95	0.10	-18.15	47,47,47,47	0
56	MG	DA	3219	1/1	0.91	0.10	-19.23	35,35,35,35	0
56	MG	BA	3245	1/1	0.90	0.12	-19.41	47,47,47,47	0
56	MG	BA	3488	1/1	0.97	0.12	-22.38	28,28,28,28	0
56	MG	DA	3344	1/1	0.97	0.07	-	54,54,54,54	0
56	MG	BA	3750	1/1	0.95	0.19	-	52,52,52,52	0
56	MG	AA	3053	1/1	0.95	0.15	-	41,41,41,41	0
56	MG	DA	3573	1/1	0.73	0.11	-	69,69,69,69	0
56	MG	BA	3082	1/1	0.98	0.17	-	27,27,27,27	0
56	MG	BA	3692	1/1	0.86	0.24	-	73,73,73,73	0
56	MG	BA	3632	1/1	0.95	0.15	-	53,53,53,53	0
56	MG	BA	3307	1/1	0.72	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	BA	3721	1/1	0.88	0.18	-	74,74,74,74	0
56	MG	CA	3090	1/1	0.72	0.14	-	70,70,70,70	0
56	MG	DA	3532	1/1	0.96	0.16	-	53,53,53,53	0
56	MG	DA	3199	1/1	0.79	0.30	-	57,57,57,57	0
56	MG	AA	3015	1/1	0.59	0.16	-	56,56,56,56	0
56	MG	DA	3591	1/1	0.98	0.14	-	46,46,46,46	0
56	MG	DA	3217	1/1	0.94	0.12	-	43,43,43,43	0
56	MG	DA	3483	1/1	0.92	0.07	-	64,64,64,64	0
56	MG	BA	3272	1/1	0.98	0.20	-	41,41,41,41	0
56	MG	DA	3396	1/1	0.97	0.10	-	27,27,27,27	0
56	MG	DA	3151	1/1	0.85	0.12	-	52,52,52,52	0
56	MG	DA	3098	1/1	0.89	0.21	-	61,61,61,61	0
56	MG	DA	3268	1/1	0.97	0.19	-	53,53,53,53	0
56	MG	DA	3129	1/1	0.94	0.15	-	42,42,42,42	0
56	MG	AV	103	1/1	0.91	0.13	-	70,70,70,70	0
56	MG	DA	3401	1/1	0.97	0.12	-	50,50,50,50	0
56	MG	AA	3104	1/1	0.84	0.16	-	44,44,44,44	0
56	MG	DA	3522	1/1	0.87	0.12	-	57,57,57,57	0
56	MG	BA	3044	1/1	0.92	0.14	-	39,39,39,39	0
56	MG	AA	3081	1/1	0.96	0.19	-	52,52,52,52	0
56	MG	BA	3756	1/1	0.95	0.12	-	56,56,56,56	0
56	MG	DW	3001	1/1	0.92	0.52	-	45,45,45,45	0
56	MG	DA	3589	1/1	0.96	0.13	-	55,55,55,55	0
56	MG	BA	3559	1/1	0.85	0.11	-	66,66,66,66	0
56	MG	AA	3206	1/1	0.69	0.24	-	62,62,62,62	0
56	MG	AA	3074	1/1	0.83	0.29	-	59,59,59,59	0
56	MG	DA	3220	1/1	0.94	0.08	-	45,45,45,45	0
56	MG	BA	3530	1/1	0.84	0.10	-	56,56,56,56	0
56	MG	AA	3004	1/1	0.81	0.10	-	67,67,67,67	0
56	MG	CA	3008	1/1	0.95	0.11	-	45,45,45,45	0
56	MG	BA	3126	1/1	0.89	0.43	-	48,48,48,48	0
56	MG	DA	3017	1/1	0.93	0.26	-	46,46,46,46	0
56	MG	DA	3563	1/1	0.97	0.06	-	45,45,45,45	0
56	MG	DA	3422	1/1	0.94	0.18	-	52,52,52,52	0
56	MG	BA	3424	1/1	0.94	0.22	-	51,51,51,51	0
56	MG	DA	3491	1/1	0.56	0.12	-	69,69,69,69	0
56	MG	DA	3310	1/1	0.96	0.07	-	39,39,39,39	0
56	MG	CA	3005	1/1	0.72	0.12	-	62,62,62,62	0
56	MG	AA	3117	1/1	0.91	0.14	-	66,66,66,66	0
56	MG	AA	3191	1/1	0.93	0.18	-	49,49,49,49	0
56	MG	DA	3482	1/1	0.90	0.15	-	42,42,42,42	0
56	MG	BA	3386	1/1	0.97	0.20	-	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3458	1/1	0.90	0.12	-	56,56,56,56	0
56	MG	BA	3225	1/1	0.91	0.17	-	43,43,43,43	0
56	MG	AA	3090	1/1	0.91	0.28	-	50,50,50,50	0
56	MG	AA	3151	1/1	0.95	0.19	-	65,65,65,65	0
56	MG	DA	3324	1/1	0.93	0.19	-	46,46,46,46	0
56	MG	BA	3402	1/1	0.92	0.19	-	67,67,67,67	0
56	MG	BA	3092	1/1	0.94	0.12	-	27,27,27,27	0
56	MG	BA	3600	1/1	0.90	0.09	-	59,59,59,59	0
56	MG	BA	3540	1/1	0.93	0.11	-	28,28,28,28	0
56	MG	BA	3690	1/1	0.92	0.16	-	44,44,44,44	0
56	MG	DA	3150	1/1	0.92	0.17	-	49,49,49,49	0
56	MG	DA	3016	1/1	0.85	0.31	-	34,34,34,34	0
56	MG	BA	3379	1/1	0.95	0.18	-	22,22,22,22	0
56	MG	CA	3113	1/1	0.85	0.11	-	79,79,79,79	0
56	MG	BA	3578	1/1	0.95	0.15	-	49,49,49,49	0
56	MG	DA	3127	1/1	0.89	0.16	-	53,53,53,53	0
56	MG	B8	101	1/1	0.92	0.19	-	35,35,35,35	0
56	MG	CA	3043	1/1	0.95	0.14	-	56,56,56,56	0
56	MG	AA	3088	1/1	0.81	0.15	-	63,63,63,63	0
56	MG	DA	3108	1/1	0.83	0.17	-	48,48,48,48	0
56	MG	AA	3209	1/1	0.97	0.09	-	62,62,62,62	0
56	MG	CA	3040	1/1	0.90	0.15	-	70,70,70,70	0
56	MG	DA	3453	1/1	0.75	0.31	-	77,77,77,77	0
56	MG	BA	3177	1/1	0.82	0.19	-	58,58,58,58	0
56	MG	BA	3539	1/1	0.91	0.15	-	58,58,58,58	0
56	MG	BA	3712	1/1	0.92	0.13	-	35,35,35,35	0
56	MG	DA	3247	1/1	0.86	0.08	-	51,51,51,51	0
56	MG	BA	3205	1/1	0.88	0.22	-	45,45,45,45	0
56	MG	DA	3516	1/1	0.95	0.14	-	35,35,35,35	0
56	MG	BA	3189	1/1	0.90	0.43	-	55,55,55,55	0
56	MG	BA	3446	1/1	0.96	0.22	-	40,40,40,40	0
56	MG	DR	3002	1/1	0.91	0.10	-	55,55,55,55	0
56	MG	DA	3107	1/1	0.83	0.17	-	47,47,47,47	0
56	MG	DA	3131	1/1	0.80	0.16	-	63,63,63,63	0
56	MG	BA	3554	1/1	0.88	0.07	-	56,56,56,56	0
56	MG	BP	204	1/1	0.81	0.13	-	54,54,54,54	0
56	MG	AA	3116	1/1	0.92	0.14	-	57,57,57,57	0
56	MG	BA	3148	1/1	0.88	0.19	-	50,50,50,50	0
56	MG	BA	3515	1/1	0.91	0.11	-	57,57,57,57	0
56	MG	BA	3665	1/1	0.81	0.18	-	45,45,45,45	0
56	MG	BA	3104	1/1	0.97	0.95	-	44,44,44,44	0
56	MG	AA	3142	1/1	0.98	0.13	-	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	3445	1/1	0.89	0.24	-	53,53,53,53	0
56	MG	BA	3589	1/1	0.95	0.18	-	41,41,41,41	0
56	MG	AA	3203	1/1	0.83	0.23	-	62,62,62,62	0
56	MG	B6	101	1/1	0.90	0.11	-	49,49,49,49	0
56	MG	BA	3197	1/1	0.90	0.15	-	46,46,46,46	0
56	MG	DA	3427	1/1	0.97	0.09	-	61,61,61,61	0
56	MG	DA	3256	1/1	0.94	0.17	-	48,48,48,48	0
56	MG	AA	3027	1/1	0.86	0.12	-	58,58,58,58	0
56	MG	BA	3501	1/1	0.90	0.28	-	74,74,74,74	0
56	MG	D8	5001	1/1	0.92	0.16	-	52,52,52,52	0
56	MG	CA	3134	1/1	0.57	0.14	-	78,78,78,78	0
56	MG	BA	3158	1/1	0.93	0.19	-	47,47,47,47	0
56	MG	AA	3126	1/1	0.83	0.33	-	65,65,65,65	0
56	MG	AA	3141	1/1	0.92	0.18	-	67,67,67,67	0
56	MG	AA	3101	1/1	0.87	0.21	-	52,52,52,52	0
56	MG	AA	3045	1/1	0.78	0.29	-	68,68,68,68	0
56	MG	DA	3577	1/1	0.79	0.46	-	72,72,72,72	0
56	MG	AA	3068	1/1	0.63	0.18	-	70,70,70,70	0
56	MG	CA	3080	1/1	0.97	0.13	-	62,62,62,62	0
56	MG	BD	301	1/1	0.91	0.54	-	45,45,45,45	0
56	MG	DA	3495	1/1	0.36	0.10	-	57,57,57,57	0
56	MG	AA	3208	1/1	0.87	0.28	-	67,67,67,67	0
56	MG	AA	3188	1/1	0.69	0.12	-	69,69,69,69	0
56	MG	BA	3051	1/1	0.83	0.17	-	63,63,63,63	0
56	MG	AA	3195	1/1	0.91	0.19	-	58,58,58,58	0
56	MG	DA	3155	1/1	0.96	0.15	-	53,53,53,53	0
56	MG	BA	3406	1/1	0.86	0.13	-	50,50,50,50	0
56	MG	DA	3066	1/1	0.83	0.13	-	39,39,39,39	0
56	MG	BA	3586	1/1	0.88	0.25	-	58,58,58,58	0
56	MG	BA	3107	1/1	0.99	0.73	-	49,49,49,49	0
56	MG	DA	3099	1/1	0.98	0.20	-	39,39,39,39	0
56	MG	CA	3102	1/1	0.94	0.11	-	48,48,48,48	0
56	MG	CA	3099	1/1	0.84	0.13	-	82,82,82,82	0
56	MG	DA	3492	1/1	0.94	0.43	-	51,51,51,51	0
56	MG	DA	3529	1/1	0.94	0.11	-	55,55,55,55	0
56	MG	BA	3149	1/1	0.94	0.19	-	57,57,57,57	0
56	MG	BA	3728	1/1	0.90	0.10	-	65,65,65,65	0
56	MG	DA	3174	1/1	0.94	0.11	-	42,42,42,42	0
56	MG	BA	3072	1/1	0.98	0.16	-	42,42,42,42	0
56	MG	BA	3644	1/1	0.94	0.31	-	34,34,34,34	0
56	MG	BA	3293	1/1	0.96	0.18	-	40,40,40,40	0
56	MG	DA	3212	1/1	0.88	0.26	-	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	BA	3560	1/1	0.92	0.25	-	47,47,47,47	0
56	MG	BA	3179	1/1	0.84	0.25	-	61,61,61,61	0
56	MG	DA	3576	1/1	0.98	0.14	-	46,46,46,46	0
56	MG	BA	3609	1/1	0.85	0.15	-	62,62,62,62	0
56	MG	BA	3647	1/1	0.97	0.15	-	48,48,48,48	0
56	MG	AA	3147	1/1	0.94	0.09	-	47,47,47,47	0
56	MG	DA	3133	1/1	0.86	0.15	-	50,50,50,50	0
56	MG	AA	3135	1/1	0.99	0.11	-	34,34,34,34	0
56	MG	BA	3657	1/1	0.91	0.16	-	54,54,54,54	0
56	MG	BA	3129	1/1	0.96	0.36	-	49,49,49,49	0
56	MG	BA	3233	1/1	0.89	0.13	-	49,49,49,49	0
56	MG	BA	3222	1/1	0.85	0.20	-	60,60,60,60	0
56	MG	BA	3090	1/1	0.92	0.23	-	40,40,40,40	0
56	MG	BA	3557	1/1	0.92	0.12	-	58,58,58,58	0
56	MG	BA	3313	1/1	0.93	0.13	-	32,32,32,32	0
56	MG	DA	3498	1/1	0.93	0.15	-	66,66,66,66	0
56	MG	DA	3503	1/1	0.96	0.06	-	58,58,58,58	0
56	MG	AX	3006	1/1	0.87	0.14	-	80,80,80,80	0
56	MG	DA	3348	1/1	0.96	0.15	-	46,46,46,46	0
56	MG	BQ	3003	1/1	0.81	0.26	-	67,67,67,67	0
56	MG	CA	3029	1/1	0.93	0.15	-	37,37,37,37	0
56	MG	BA	3241	1/1	0.93	0.22	-	59,59,59,59	0
56	MG	DB	3004	1/1	0.92	0.14	-	54,54,54,54	0
56	MG	BA	3111	1/1	0.91	0.32	-	45,45,45,45	0
56	MG	AA	3095	1/1	0.89	0.12	-	63,63,63,63	0
56	MG	DA	3350	1/1	0.87	0.16	-	61,61,61,61	0
56	MG	CA	3041	1/1	0.95	0.16	-	63,63,63,63	0
56	MG	DA	3263	1/1	0.96	0.06	-	48,48,48,48	0
56	MG	BA	3704	1/1	0.86	0.14	-	75,75,75,75	0
56	MG	BA	3040	1/1	0.93	0.13	-	60,60,60,60	0
56	MG	BA	3324	1/1	0.98	0.16	-	44,44,44,44	0
56	MG	BA	3389	1/1	0.90	0.14	-	51,51,51,51	0
56	MG	BA	3166	1/1	0.96	0.15	-	47,47,47,47	0
56	MG	CA	3010	1/1	0.93	0.21	-	60,60,60,60	0
56	MG	CA	3067	1/1	0.93	0.20	-	57,57,57,57	0
56	MG	BA	3302	1/1	0.95	0.11	-	46,46,46,46	0
56	MG	DA	3116	1/1	0.92	0.08	-	58,58,58,58	0
56	MG	BA	3407	1/1	0.93	0.22	-	44,44,44,44	0
56	MG	BA	3713	1/1	0.93	0.21	-	68,68,68,68	0
56	MG	AW	3005	1/1	0.96	0.12	-	52,52,52,52	0
56	MG	BA	3678	1/1	0.97	0.14	-	41,41,41,41	0
56	MG	DA	3394	1/1	0.94	0.11	-	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	BA	3734	1/1	0.88	0.16	-	24,24,24,24	0
60	K	CX	3001	1/1	0.89	0.46	-	84,84,84,84	0
56	MG	CA	3034	1/1	0.95	0.22	-	46,46,46,46	0
56	MG	CA	3079	1/1	0.92	0.12	-	61,61,61,61	0
56	MG	AA	3199	1/1	0.86	0.20	-	68,68,68,68	0
56	MG	DA	3117	1/1	0.91	0.10	-	46,46,46,46	0
56	MG	DA	3159	1/1	0.83	0.14	-	60,60,60,60	0
56	MG	BA	3351	1/1	0.97	0.16	-	61,61,61,61	0
56	MG	DA	3240	1/1	0.96	0.15	-	36,36,36,36	0
56	MG	BA	3561	1/1	0.83	0.22	-	64,64,64,64	0
56	MG	DA	3622	1/1	0.92	0.37	-	61,61,61,61	0
56	MG	BA	3252	1/1	0.92	0.27	-	61,61,61,61	0
56	MG	DA	3050	1/1	0.85	0.27	-	60,60,60,60	0
56	MG	DA	3417	1/1	0.53	0.18	-	71,71,71,71	0
56	MG	CA	3072	1/1	0.94	0.17	-	57,57,57,57	0
56	MG	AA	3043	1/1	0.92	0.11	-	62,62,62,62	0
56	MG	DA	3134	1/1	0.92	0.26	-	60,60,60,60	0
56	MG	AA	3190	1/1	0.91	0.08	-	61,61,61,61	0
56	MG	BA	3400	1/1	0.87	0.15	-	53,53,53,53	0
56	MG	BA	3735	1/1	0.92	0.13	-	41,41,41,41	0
56	MG	BA	3155	1/1	0.85	0.35	-	63,63,63,63	0
56	MG	BA	3264	1/1	0.93	0.19	-	19,19,19,19	0
56	MG	DA	3100	1/1	0.93	0.16	-	45,45,45,45	0
56	MG	BA	3202	1/1	0.92	0.25	-	41,41,41,41	0
56	MG	BA	3130	1/1	0.97	0.30	-	44,44,44,44	0
56	MG	DA	3287	1/1	0.78	0.21	-	50,50,50,50	0
56	MG	AA	3179	1/1	0.74	0.12	-	85,85,85,85	0
56	MG	DA	3145	1/1	0.95	0.26	-	61,61,61,61	0
56	MG	BA	3590	1/1	0.94	0.18	-	38,38,38,38	0
56	MG	DA	3339	1/1	0.85	0.33	-	46,46,46,46	0
56	MG	AA	3120	1/1	0.99	0.12	-	72,72,72,72	0
56	MG	BA	3522	1/1	0.91	0.25	-	59,59,59,59	0
56	MG	BA	3387	1/1	0.93	0.29	-	43,43,43,43	0
56	MG	CA	3112	1/1	0.96	0.29	-	59,59,59,59	0
56	MG	BA	3506	1/1	0.91	0.05	-	43,43,43,43	0
56	MG	AA	3138	1/1	0.93	0.08	-	73,73,73,73	0
56	MG	DA	3407	1/1	0.94	0.24	-	41,41,41,41	0
56	MG	DA	3605	1/1	0.80	0.12	-	53,53,53,53	0
56	MG	BA	3717	1/1	0.90	0.15	-	34,34,34,34	0
56	MG	DA	3437	1/1	0.62	0.14	-	47,47,47,47	0
56	MG	DA	3221	1/1	0.89	0.12	-	56,56,56,56	0
56	MG	CA	3161	1/1	0.97	0.10	-	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	3358	1/1	0.95	0.12	-	51,51,51,51	0
56	MG	BA	3064	1/1	0.94	0.34	-	46,46,46,46	0
56	MG	DA	3430	1/1	0.93	0.10	-	51,51,51,51	0
56	MG	DA	3570	1/1	0.94	0.10	-	62,62,62,62	0
56	MG	BA	3345	1/1	0.96	0.19	-	20,20,20,20	0
56	MG	DA	3072	1/1	0.97	0.19	-	60,60,60,60	0
56	MG	BA	3073	1/1	0.94	0.17	-	25,25,25,25	0
56	MG	AA	3113	1/1	0.85	0.13	-	57,57,57,57	0
56	MG	DA	3613	1/1	0.92	0.10	-	57,57,57,57	0
56	MG	BA	3335	1/1	0.91	0.12	-	50,50,50,50	0
56	MG	DA	3002	1/1	0.92	0.12	-	51,51,51,51	0
56	MG	BA	3573	1/1	0.94	0.13	-	53,53,53,53	0
56	MG	DA	3311	1/1	0.80	0.13	-	54,54,54,54	0
56	MG	DA	3106	1/1	0.92	0.27	-	56,56,56,56	0
56	MG	CA	3151	1/1	0.96	0.14	-	59,59,59,59	0
56	MG	BA	3176	1/1	0.76	0.19	-	41,41,41,41	0
56	MG	DA	3172	1/1	0.92	0.18	-	56,56,56,56	0
56	MG	BA	3048	1/1	0.93	0.14	-	56,56,56,56	0
56	MG	DA	3183	1/1	0.79	0.18	-	57,57,57,57	0
56	MG	BA	3433	1/1	0.96	0.15	-	48,48,48,48	0
56	MG	DA	3211	1/1	0.91	0.18	-	49,49,49,49	0
56	MG	AD	502	1/1	0.96	0.26	-	58,58,58,58	0
56	MG	DA	3261	1/1	0.87	0.34	-	60,60,60,60	0
56	MG	BA	3548	1/1	0.81	0.15	-	50,50,50,50	0
56	MG	DA	3326	1/1	0.89	0.22	-	31,31,31,31	0
56	MG	DA	3500	1/1	0.89	0.12	-	56,56,56,56	0
56	MG	AA	3186	1/1	0.88	0.17	-	65,65,65,65	0
56	MG	BA	3674	1/1	0.95	0.15	-	42,42,42,42	0
56	MG	DA	3374	1/1	0.97	0.13	-	52,52,52,52	0
56	MG	BA	3702	1/1	0.93	0.18	-	60,60,60,60	0
56	MG	BA	3685	1/1	0.93	0.22	-	43,43,43,43	0
56	MG	DA	3347	1/1	0.94	0.15	-	53,53,53,53	0
56	MG	CA	3156	1/1	0.90	0.12	-	58,58,58,58	0
56	MG	DA	3513	1/1	0.71	0.09	-	58,58,58,58	0
56	MG	DA	3321	1/1	0.82	0.17	-	58,58,58,58	0
56	MG	BA	3616	1/1	0.78	0.11	-	43,43,43,43	0
56	MG	DA	3567	1/1	0.97	0.07	-	52,52,52,52	0
56	MG	BA	3737	1/1	0.79	0.12	-	68,68,68,68	0
56	MG	DA	3080	1/1	0.89	0.20	-	48,48,48,48	0
56	MG	BA	3491	1/1	0.93	0.16	-	52,52,52,52	0
56	MG	DA	3333	1/1	0.92	0.07	-	53,53,53,53	0
56	MG	DA	3242	1/1	0.77	0.13	-	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	DA	3139	1/1	0.96	0.24	-	59,59,59,59	0
56	MG	DA	3521	1/1	0.98	0.16	-	29,29,29,29	0
56	MG	BA	3084	1/1	0.82	0.40	-	46,46,46,46	0
56	MG	BA	3039	1/1	0.86	0.22	-	34,34,34,34	0
56	MG	BA	3726	1/1	0.74	0.18	-	61,61,61,61	0
56	MG	AA	3189	1/1	0.83	0.10	-	56,56,56,56	0
56	MG	BA	3062	1/1	0.93	0.32	-	35,35,35,35	0
56	MG	DA	3460	1/1	0.93	0.08	-	64,64,64,64	0
56	MG	DA	3201	1/1	0.95	0.17	-	56,56,56,56	0
56	MG	DA	3001	1/1	0.84	0.27	-	49,49,49,49	0
56	MG	CA	3017	1/1	0.92	0.27	-	53,53,53,53	0
56	MG	BA	3724	1/1	0.91	0.14	-	84,84,84,84	0
56	MG	BA	3204	1/1	0.96	0.30	-	35,35,35,35	0
56	MG	DA	3209	1/1	0.89	0.19	-	52,52,52,52	0
56	MG	BA	3673	1/1	0.99	0.28	-	22,22,22,22	0
56	MG	DA	3331	1/1	0.96	0.14	-	46,46,46,46	0
56	MG	BA	3464	1/1	0.95	0.21	-	53,53,53,53	0
56	MG	DA	3420	1/1	0.96	0.08	-	40,40,40,40	0
56	MG	DA	3269	1/1	0.98	0.11	-	46,46,46,46	0
56	MG	BA	3211	1/1	0.88	0.20	-	57,57,57,57	0
56	MG	AA	3084	1/1	0.91	0.12	-	53,53,53,53	0
56	MG	DA	3146	1/1	0.94	0.13	-	50,50,50,50	0
56	MG	AA	3067	1/1	0.94	0.31	-	53,53,53,53	0
56	MG	BA	3443	1/1	0.94	0.15	-	50,50,50,50	0
56	MG	DA	3623	1/1	0.94	0.66	-	48,48,48,48	0
56	MG	DA	3041	1/1	0.95	0.40	-	51,51,51,51	0
56	MG	DA	3042	1/1	0.81	0.14	-	71,71,71,71	0
56	MG	DA	3575	1/1	0.67	0.19	-	58,58,58,58	0
56	MG	DA	3485	1/1	0.91	0.38	-	60,60,60,60	0
56	MG	BA	3658	1/1	0.89	0.15	-	41,41,41,41	0
56	MG	CA	3042	1/1	0.85	0.15	-	61,61,61,61	0
56	MG	DA	3213	1/1	0.81	0.21	-	58,58,58,58	0
56	MG	DA	3432	1/1	0.93	0.11	-	43,43,43,43	0
56	MG	BA	3731	1/1	0.80	0.13	-	57,57,57,57	0
56	MG	BA	3747	1/1	0.97	0.23	-	50,50,50,50	0
56	MG	AA	3100	1/1	0.88	0.25	-	53,53,53,53	0
56	MG	DA	3083	1/1	0.95	0.50	-	46,46,46,46	0
56	MG	AA	3205	1/1	0.94	0.07	-	66,66,66,66	0
56	MG	AA	3083	1/1	0.94	0.17	-	57,57,57,57	0
56	MG	BA	3030	1/1	0.80	0.12	-	50,50,50,50	0
56	MG	BA	3574	1/1	0.97	0.26	-	60,60,60,60	0
56	MG	DA	3163	1/1	0.81	0.68	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3101	1/1	0.98	0.28	-	36,36,36,36	0
56	MG	BA	3200	1/1	0.84	0.16	-	50,50,50,50	0
56	MG	DA	3184	1/1	0.91	0.23	-	56,56,56,56	0
56	MG	BA	3520	1/1	0.96	0.23	-	25,25,25,25	0
56	MG	BA	3434	1/1	0.89	0.15	-	65,65,65,65	0
56	MG	CA	3066	1/1	0.84	0.16	-	58,58,58,58	0
56	MG	AA	3112	1/1	0.90	0.15	-	53,53,53,53	0
56	MG	AA	3155	1/1	0.91	0.14	-	60,60,60,60	0
56	MG	CA	3003	1/1	0.78	0.20	-	65,65,65,65	0
56	MG	BA	3183	1/1	0.82	0.73	-	47,47,47,47	0
56	MG	BA	3474	1/1	0.95	0.17	-	37,37,37,37	0
56	MG	BA	3364	1/1	0.89	0.12	-	50,50,50,50	0
56	MG	DA	3384	1/1	0.94	0.21	-	55,55,55,55	0
56	MG	DA	3512	1/1	0.90	0.12	-	52,52,52,52	0
56	MG	DA	3509	1/1	0.98	0.13	-	38,38,38,38	0
56	MG	BA	3477	1/1	0.91	0.20	-	35,35,35,35	0
56	MG	DA	3488	1/1	0.88	0.11	-	66,66,66,66	0
56	MG	BA	3772	1/1	0.94	0.15	-	52,52,52,52	0
56	MG	AA	3132	1/1	0.97	0.19	-	75,75,75,75	0
56	MG	DA	3210	1/1	0.96	0.21	-	35,35,35,35	0
56	MG	DA	3550	1/1	0.87	0.11	-	61,61,61,61	0
56	MG	BA	3725	1/1	0.87	0.09	-	63,63,63,63	0
56	MG	BA	3662	1/1	0.95	0.11	-	56,56,56,56	0
56	MG	DA	3095	1/1	0.96	0.08	-	54,54,54,54	0
56	MG	BA	3374	1/1	0.92	0.20	-	34,34,34,34	0
56	MG	AA	3224	1/1	0.93	0.19	-	61,61,61,61	0
56	MG	DA	3202	1/1	0.94	0.15	-	51,51,51,51	0
56	MG	DA	3149	1/1	0.91	0.18	-	48,48,48,48	0
56	MG	DA	3511	1/1	0.94	0.12	-	62,62,62,62	0
56	MG	BA	3542	1/1	0.89	0.15	-	66,66,66,66	0
56	MG	AX	3011	1/1	0.85	0.13	-	62,62,62,62	0
56	MG	DA	3514	1/1	0.80	0.13	-	67,67,67,67	0
56	MG	BA	3365	1/1	0.93	0.09	-	47,47,47,47	0
56	MG	DA	3434	1/1	0.94	0.31	-	46,46,46,46	0
56	MG	BB	3005	1/1	0.87	0.19	-	54,54,54,54	0
56	MG	BA	3251	1/1	0.98	0.13	-	51,51,51,51	0
56	MG	BA	3732	1/1	0.88	0.14	-	57,57,57,57	0
56	MG	BO	5001	1/1	0.96	0.22	-	70,70,70,70	0
56	MG	BA	3584	1/1	0.93	0.20	-	47,47,47,47	0
56	MG	DA	3198	1/1	0.98	0.22	-	32,32,32,32	0
56	MG	BA	3253	1/1	0.90	0.17	-	30,30,30,30	0
56	MG	CA	3018	1/1	0.89	0.15	-	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	BA	3216	1/1	0.95	0.14	-	53,53,53,53	0
56	MG	DA	3097	1/1	0.91	0.14	-	52,52,52,52	0
56	MG	BA	3377	1/1	0.94	0.20	-	39,39,39,39	0
56	MG	DA	3535	1/1	0.96	0.10	-	38,38,38,38	0
56	MG	DA	3254	1/1	0.97	0.12	-	53,53,53,53	0
56	MG	B2	3001	1/1	0.77	0.28	-	54,54,54,54	0
56	MG	CA	3077	1/1	0.96	0.17	-	36,36,36,36	0
56	MG	AA	3158	1/1	0.97	0.14	-	62,62,62,62	0
56	MG	DA	3467	1/1	0.84	0.25	-	69,69,69,69	0
56	MG	DA	3120	1/1	0.94	0.18	-	42,42,42,42	0
56	MG	BA	3013	1/1	0.87	0.19	-	46,46,46,46	0
56	MG	BA	3171	1/1	0.94	0.10	-	58,58,58,58	0
56	MG	BA	3208	1/1	0.81	0.21	-	47,47,47,47	0
56	MG	CA	3033	1/1	0.97	0.19	-	44,44,44,44	0
56	MG	DA	3462	1/1	0.86	0.12	-	36,36,36,36	0
56	MG	AA	3011	1/1	0.84	0.19	-	66,66,66,66	0
56	MG	DA	3192	1/1	0.76	0.16	-	49,49,49,49	0
56	MG	BA	3133	1/1	0.95	0.30	-	43,43,43,43	0
56	MG	CA	3045	1/1	0.87	0.19	-	68,68,68,68	0
56	MG	BA	3463	1/1	0.98	0.16	-	34,34,34,34	0
56	MG	DA	3153	1/1	0.86	0.13	-	40,40,40,40	0
56	MG	BA	3278	1/1	0.97	0.12	-	48,48,48,48	0
56	MG	DA	3013	1/1	0.92	0.14	-	49,49,49,49	0
56	MG	DA	3519	1/1	0.97	0.06	-	78,78,78,78	0
56	MG	DA	3517	1/1	0.91	0.29	-	60,60,60,60	0
56	MG	BA	3482	1/1	0.88	0.32	-	27,27,27,27	0
56	MG	DD	301	1/1	0.93	0.22	-	44,44,44,44	0
56	MG	BA	3733	1/1	0.62	0.07	-	78,78,78,78	0
56	MG	BA	3760	1/1	0.93	0.12	-	78,78,78,78	0
56	MG	BA	3305	1/1	0.95	0.26	-	61,61,61,61	0
56	MG	DA	3525	1/1	0.97	0.07	-	33,33,33,33	0
56	MG	BA	3314	1/1	0.94	0.14	-	41,41,41,41	0
56	MG	DB	3012	1/1	0.96	0.08	-	61,61,61,61	0
56	MG	DA	3093	1/1	0.83	0.11	-	59,59,59,59	0
56	MG	AA	3058	1/1	0.88	0.23	-	63,63,63,63	0
56	MG	DA	3446	1/1	0.94	0.18	-	52,52,52,52	0
56	MG	DA	3051	1/1	0.98	0.14	-	54,54,54,54	0
56	MG	AA	3032	1/1	0.74	0.18	-	62,62,62,62	0
56	MG	BA	3457	1/1	0.97	0.10	-	46,46,46,46	0
56	MG	CA	3096	1/1	0.96	0.16	-	51,51,51,51	0
56	MG	DA	3308	1/1	0.91	0.25	-	57,57,57,57	0
56	MG	AA	3181	1/1	0.95	0.10	-	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	AA	3160	1/1	0.94	0.23	-	70,70,70,70	0
56	MG	AA	3198	1/1	0.92	0.13	-	82,82,82,82	0
56	MG	DA	3584	1/1	0.91	0.16	-	45,45,45,45	0
56	MG	BA	3551	1/1	0.94	0.15	-	56,56,56,56	0
56	MG	CA	3024	1/1	0.97	0.07	-	53,53,53,53	0
56	MG	BB	3009	1/1	0.93	0.14	-	49,49,49,49	0
56	MG	CA	3163	1/1	0.94	0.16	-	49,49,49,49	0
56	MG	BA	3161	1/1	0.90	0.46	-	40,40,40,40	0
56	MG	CA	3137	1/1	0.99	0.08	-	52,52,52,52	0
56	MG	BA	3247	1/1	0.75	0.20	-	49,49,49,49	0
56	MG	AA	3164	1/1	0.93	0.12	-	71,71,71,71	0
56	MG	BA	3301	1/1	0.85	0.11	-	55,55,55,55	0
56	MG	CX	3003	1/1	0.95	0.19	-	64,64,64,64	0
56	MG	BA	3780	1/1	0.94	0.52	-	45,45,45,45	0
56	MG	BA	3512	1/1	0.89	0.14	-	65,65,65,65	0
56	MG	DA	3260	1/1	0.96	0.19	-	36,36,36,36	0
56	MG	BA	3367	1/1	0.93	0.12	-	58,58,58,58	0
56	MG	BA	3114	1/1	0.94	0.61	-	49,49,49,49	0
56	MG	DA	3486	1/1	0.81	0.12	-	47,47,47,47	0
56	MG	BA	3287	1/1	0.94	0.14	-	21,21,21,21	0
56	MG	BA	3606	1/1	0.95	0.16	-	62,62,62,62	0
56	MG	CA	3070	1/1	0.96	0.33	-	52,52,52,52	0
56	MG	BA	3467	1/1	0.87	0.21	-	48,48,48,48	0
56	MG	DA	3177	1/1	0.93	0.23	-	54,54,54,54	0
56	MG	B5	106	1/1	0.97	0.15	-	55,55,55,55	0
56	MG	B3	3002	1/1	0.93	0.13	-	65,65,65,65	0
56	MG	AA	3193	1/1	0.87	0.25	-	69,69,69,69	0
56	MG	DA	3431	1/1	0.90	0.16	-	44,44,44,44	0
56	MG	BA	3329	1/1	0.75	0.30	-	57,57,57,57	0
56	MG	BA	3591	1/1	0.83	0.13	-	58,58,58,58	0
56	MG	DA	3064	1/1	0.95	0.22	-	52,52,52,52	0
56	MG	AA	3055	1/1	0.95	0.10	-	40,40,40,40	0
56	MG	DA	3581	1/1	0.85	0.16	-	67,67,67,67	0
56	MG	DA	3544	1/1	0.95	0.12	-	49,49,49,49	0
56	MG	AX	3008	1/1	0.98	0.18	-	52,52,52,52	0
56	MG	DA	3539	1/1	0.93	0.19	-	64,64,64,64	0
56	MG	DA	3320	1/1	0.91	0.15	-	53,53,53,53	0
56	MG	BA	3221	1/1	0.96	0.19	-	47,47,47,47	0
56	MG	DA	3528	1/1	0.90	0.15	-	70,70,70,70	0
56	MG	DA	3228	1/1	0.94	0.15	-	29,29,29,29	0
56	MG	BA	3385	1/1	0.96	0.20	-	50,50,50,50	0
56	MG	DA	3185	1/1	0.93	0.24	-	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	DF	301	1/1	0.96	0.16	-	49,49,49,49	0
56	MG	B5	104	1/1	0.90	0.42	-	55,55,55,55	0
56	MG	CA	3122	1/1	0.89	0.19	-	70,70,70,70	0
56	MG	DA	3105	1/1	0.87	0.20	-	54,54,54,54	0
56	MG	DA	3508	1/1	0.89	0.06	-	68,68,68,68	0
56	MG	BA	3670	1/1	0.90	0.19	-	55,55,55,55	0
56	MG	BA	3075	1/1	0.83	0.32	-	48,48,48,48	0
56	MG	BA	3268	1/1	0.98	0.19	-	40,40,40,40	0
56	MG	CA	3125	1/1	0.87	0.08	-	76,76,76,76	0
56	MG	DA	3572	1/1	0.86	0.14	-	70,70,70,70	0
56	MG	BA	3743	1/1	0.97	0.15	-	18,18,18,18	0
56	MG	DA	3461	1/1	0.96	0.14	-	49,49,49,49	0
56	MG	BA	3603	1/1	0.93	0.24	-	28,28,28,28	0
56	MG	BA	3435	1/1	0.89	0.34	-	52,52,52,52	0
56	MG	CA	3160	1/1	0.98	0.22	-	53,53,53,53	0
56	MG	BA	3476	1/1	0.93	0.21	-	37,37,37,37	0
56	MG	BA	3384	1/1	0.98	0.14	-	43,43,43,43	0
56	MG	AA	3175	1/1	0.84	0.10	-	54,54,54,54	0
56	MG	DB	3005	1/1	0.81	0.35	-	77,77,77,77	0
56	MG	DA	3349	1/1	0.88	0.12	-	46,46,46,46	0
56	MG	DA	3169	1/1	0.90	0.12	-	61,61,61,61	0
56	MG	CA	3143	1/1	0.90	0.25	-	59,59,59,59	0
56	MG	DA	3300	1/1	0.91	0.13	-	27,27,27,27	0
56	MG	BA	3538	1/1	0.98	0.10	-	43,43,43,43	0
56	MG	DA	3421	1/1	0.93	0.14	-	55,55,55,55	0
56	MG	BA	3002	1/1	0.75	0.17	-	36,36,36,36	0
56	MG	BA	3715	1/1	0.86	0.14	-	48,48,48,48	0
56	MG	DA	3048	1/1	0.78	0.13	-	58,58,58,58	0
56	MG	CA	3044	1/1	0.90	0.16	-	62,62,62,62	0
56	MG	CA	3095	1/1	0.88	0.08	-	47,47,47,47	0
56	MG	AA	3168	1/1	0.71	0.18	-	76,76,76,76	0
56	MG	CA	3117	1/1	0.94	0.18	-	71,71,71,71	0
56	MG	BA	3656	1/1	0.71	0.19	-	34,34,34,34	0
56	MG	DA	3264	1/1	0.93	0.12	-	44,44,44,44	0
56	MG	BA	3283	1/1	0.89	0.17	-	39,39,39,39	0
56	MG	DA	3061	1/1	0.77	0.14	-	63,63,63,63	0
56	MG	CA	3097	1/1	0.82	0.13	-	66,66,66,66	0
56	MG	BA	3008	1/1	0.94	0.23	-	27,27,27,27	0
56	MG	CA	3098	1/1	0.94	0.14	-	59,59,59,59	0
56	MG	BA	3614	1/1	0.94	0.14	-	54,54,54,54	0
56	MG	AA	3106	1/1	0.77	0.14	-	62,62,62,62	0
56	MG	DA	3197	1/1	0.89	0.12	-	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	3480	1/1	0.94	0.19	-	48,48,48,48	0
56	MG	BA	3550	1/1	0.63	0.49	-	74,74,74,74	0
56	MG	BA	3074	1/1	0.74	0.17	-	58,58,58,58	0
56	MG	DF	303	1/1	0.85	0.36	-	46,46,46,46	0
56	MG	BA	3015	1/1	0.88	0.27	-	52,52,52,52	0
56	MG	DA	3022	1/1	0.87	0.24	-	50,50,50,50	0
56	MG	BA	3752	1/1	0.96	0.22	-	48,48,48,48	0
56	MG	DA	3245	1/1	0.94	0.13	-	28,28,28,28	0
56	MG	BA	3120	1/1	0.98	0.40	-	45,45,45,45	0
56	MG	BA	3428	1/1	0.94	0.22	-	42,42,42,42	0
56	MG	DA	3113	1/1	0.93	0.27	-	51,51,51,51	0
56	MG	BA	3719	1/1	0.90	0.19	-	49,49,49,49	0
56	MG	DA	3448	1/1	0.97	0.19	-	40,40,40,40	0
56	MG	AA	3144	1/1	0.83	0.08	-	62,62,62,62	0
56	MG	AA	3140	1/1	0.91	0.21	-	61,61,61,61	0
56	MG	CV	101	1/1	0.98	0.17	-	56,56,56,56	0
56	MG	BW	201	1/1	0.94	0.20	-	45,45,45,45	0
56	MG	BE	307	1/1	0.92	0.08	-	71,71,71,71	0
56	MG	DA	3459	1/1	0.94	0.11	-	63,63,63,63	0
56	MG	AA	3118	1/1	0.94	0.12	-	40,40,40,40	0
56	MG	DA	3293	1/1	0.94	0.13	-	59,59,59,59	0
56	MG	BA	3300	1/1	0.90	0.17	-	55,55,55,55	0
56	MG	BA	3444	1/1	0.89	0.16	-	37,37,37,37	0
56	MG	AF	3001	1/1	0.76	0.14	-	48,48,48,48	0
56	MG	DA	3103	1/1	0.78	0.12	-	60,60,60,60	0
56	MG	BA	3021	1/1	0.98	0.31	-	32,32,32,32	0
56	MG	AA	3110	1/1	0.95	0.15	-	53,53,53,53	0
56	MG	DA	3044	1/1	0.92	0.25	-	60,60,60,60	0
56	MG	DA	3413	1/1	0.97	0.25	-	40,40,40,40	0
56	MG	DA	3376	1/1	0.89	0.15	-	46,46,46,46	0
56	MG	BA	3235	1/1	0.80	0.16	-	65,65,65,65	0
56	MG	DB	3008	1/1	0.97	0.10	-	62,62,62,62	0
56	MG	BA	3748	1/1	0.95	0.19	-	63,63,63,63	0
56	MG	BA	3341	1/1	0.95	0.17	-	59,59,59,59	0
56	MG	BA	3646	1/1	0.78	0.42	-	48,48,48,48	0
56	MG	BA	3746	1/1	0.92	0.10	-	71,71,71,71	0
56	MG	AA	3173	1/1	0.95	0.11	-	55,55,55,55	0
56	MG	DA	3334	1/1	0.95	0.24	-	51,51,51,51	0
56	MG	BA	3232	1/1	0.99	0.28	-	44,44,44,44	0
56	MG	BA	3173	1/1	0.95	0.44	-	46,46,46,46	0
56	MG	DA	3586	1/1	0.90	0.19	-	49,49,49,49	0
56	MG	DA	3356	1/1	0.96	0.09	-	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	3594	1/1	0.98	0.15	-	37,37,37,37	0
56	MG	DA	3602	1/1	0.96	0.19	-	62,62,62,62	0
56	MG	CA	3060	1/1	0.93	0.15	-	58,58,58,58	0
56	MG	DA	3598	1/1	0.97	0.24	-	63,63,63,63	0
56	MG	BA	3169	1/1	0.95	0.18	-	28,28,28,28	0
56	MG	DA	3054	1/1	0.62	0.32	-	59,59,59,59	0
56	MG	DA	3322	1/1	0.77	0.09	-	46,46,46,46	0
56	MG	CA	3006	1/1	0.94	0.27	-	50,50,50,50	0
56	MG	BA	3419	1/1	0.93	0.20	-	50,50,50,50	0
56	MG	BA	3081	1/1	0.85	0.15	-	61,61,61,61	0
56	MG	BA	3620	1/1	0.91	0.21	-	42,42,42,42	0
56	MG	BA	3418	1/1	0.90	0.14	-	57,57,57,57	0
56	MG	AA	3177	1/1	0.92	0.21	-	66,66,66,66	0
56	MG	AA	3037	1/1	0.98	0.14	-	55,55,55,55	0
56	MG	DA	3077	1/1	0.88	0.17	-	40,40,40,40	0
56	MG	BA	3290	1/1	0.91	0.19	-	61,61,61,61	0
56	MG	BA	3255	1/1	0.98	0.22	-	56,56,56,56	0
56	MG	BA	3618	1/1	0.75	0.19	-	64,64,64,64	0
56	MG	BA	3519	1/1	0.67	0.15	-	56,56,56,56	0
56	MG	BA	3455	1/1	0.98	0.13	-	28,28,28,28	0
56	MG	BA	3580	1/1	0.80	0.15	-	61,61,61,61	0
56	MG	DA	3122	1/1	0.41	0.30	-	71,71,71,71	0
56	MG	BA	3532	1/1	0.75	0.14	-	73,73,73,73	0
56	MG	DA	3332	1/1	0.92	0.13	-	46,46,46,46	0
56	MG	BA	3019	1/1	0.91	0.31	-	38,38,38,38	0
56	MG	BA	3224	1/1	0.95	0.17	-	55,55,55,55	0
56	MG	BA	3151	1/1	0.94	0.36	-	51,51,51,51	0
56	MG	BA	3277	1/1	0.98	0.17	-	40,40,40,40	0
56	MG	CA	3108	1/1	0.97	0.10	-	56,56,56,56	0
56	MG	BA	3701	1/1	0.89	0.12	-	66,66,66,66	0
56	MG	DA	3564	1/1	0.88	0.14	-	64,64,64,64	0
56	MG	BA	3565	1/1	0.94	0.12	-	50,50,50,50	0
56	MG	DA	3027	1/1	0.85	0.15	-	43,43,43,43	0
56	MG	DA	3164	1/1	0.95	0.06	-	58,58,58,58	0
56	MG	DA	3253	1/1	0.96	0.20	-	57,57,57,57	0
56	MG	BA	3627	1/1	0.93	0.19	-	52,52,52,52	0
56	MG	CA	3120	1/1	0.91	0.12	-	70,70,70,70	0
56	MG	CA	3111	1/1	0.92	0.12	-	69,69,69,69	0
56	MG	DA	3560	1/1	0.95	0.49	-	59,59,59,59	0
56	MG	BA	3625	1/1	0.89	0.14	-	49,49,49,49	0
56	MG	DA	3171	1/1	0.93	0.16	-	41,41,41,41	0
56	MG	BA	3036	1/1	0.91	0.21	-	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	3003	1/1	0.81	0.23	-	79,79,79,79	0
56	MG	AO	3101	1/1	0.83	0.19	-	58,58,58,58	0
56	MG	AA	3079	1/1	0.85	0.25	-	66,66,66,66	0
56	MG	BA	3068	1/1	0.92	0.77	-	56,56,56,56	0
56	MG	BA	3098	1/1	0.87	0.11	-	51,51,51,51	0
56	MG	AA	3128	1/1	0.79	0.14	-	60,60,60,60	0
56	MG	BA	3700	1/1	0.86	0.13	-	73,73,73,73	0
56	MG	BA	3306	1/1	0.95	0.21	-	51,51,51,51	0
56	MG	DA	3549	1/1	0.90	0.23	-	53,53,53,53	0
56	MG	BA	3531	1/1	0.87	0.09	-	56,56,56,56	0
56	MG	DA	3218	1/1	0.80	0.11	-	53,53,53,53	0
56	MG	BA	3223	1/1	0.89	0.19	-	42,42,42,42	0
56	MG	BA	3370	1/1	0.84	0.23	-	51,51,51,51	0
56	MG	BA	3311	1/1	0.94	0.18	-	34,34,34,34	0
56	MG	AA	3194	1/1	0.91	0.07	-	66,66,66,66	0
56	MG	BA	3410	1/1	0.98	0.18	-	33,33,33,33	0
56	MG	DA	3370	1/1	0.96	0.14	-	49,49,49,49	0
56	MG	BB	3018	1/1	0.90	0.17	-	46,46,46,46	0
56	MG	CA	3100	1/1	0.88	0.10	-	52,52,52,52	0
56	MG	BA	3449	1/1	0.87	0.16	-	59,59,59,59	0
56	MG	BA	3309	1/1	0.92	0.15	-	41,41,41,41	0
56	MG	BT	201	1/1	0.98	0.19	-	49,49,49,49	0
56	MG	DB	3011	1/1	0.91	0.14	-	49,49,49,49	0
56	MG	CA	3149	1/1	0.96	0.10	-	61,61,61,61	0
56	MG	AX	3004	1/1	0.87	0.22	-	67,67,67,67	0
56	MG	BA	3775	1/1	0.86	0.24	-	47,47,47,47	0
56	MG	DA	3433	1/1	0.87	0.11	-	58,58,58,58	0
56	MG	BA	3634	1/1	0.86	0.12	-	50,50,50,50	0
56	MG	DA	3444	1/1	0.96	0.17	-	59,59,59,59	0
56	MG	DA	3526	1/1	0.65	0.21	-	64,64,64,64	0
56	MG	BA	3503	1/1	0.87	0.20	-	43,43,43,43	0
56	MG	BA	3041	1/1	0.93	0.26	-	51,51,51,51	0
56	MG	BA	3421	1/1	0.83	0.12	-	46,46,46,46	0
56	MG	BA	3045	1/1	0.83	0.21	-	41,41,41,41	0
56	MG	BA	3123	1/1	0.95	0.58	-	39,39,39,39	0
56	MG	AA	3062	1/1	0.91	0.30	-	58,58,58,58	0
56	MG	DA	3601	1/1	0.70	0.16	-	75,75,75,75	0
56	MG	BA	3121	1/1	0.91	0.35	-	64,64,64,64	0
56	MG	AW	3001	1/1	0.93	0.12	-	67,67,67,67	0
56	MG	BA	3258	1/1	0.89	0.18	-	57,57,57,57	0
56	MG	BA	3099	1/1	0.62	0.37	-	58,58,58,58	0
56	MG	BA	3163	1/1	0.95	0.19	-	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	3067	1/1	0.95	0.09	-	52,52,52,52	0
56	MG	BB	3012	1/1	0.93	0.10	-	42,42,42,42	0
56	MG	DA	3040	1/1	0.95	0.12	-	47,47,47,47	0
56	MG	BA	3714	1/1	0.82	0.17	-	73,73,73,73	0
56	MG	BA	3398	1/1	0.96	0.18	-	37,37,37,37	0
56	MG	DA	3208	1/1	0.89	0.15	-	61,61,61,61	0
56	MG	BB	3011	1/1	0.83	0.13	-	56,56,56,56	0
56	MG	AW	3002	1/1	0.94	0.20	-	54,54,54,54	0
56	MG	DA	3104	1/1	0.97	0.25	-	49,49,49,49	0
56	MG	BA	3080	1/1	0.90	0.30	-	49,49,49,49	0
56	MG	BA	3498	1/1	0.92	0.05	-	70,70,70,70	0
56	MG	BA	3001	1/1	0.93	0.17	-	23,23,23,23	0
56	MG	DA	3489	1/1	0.92	0.07	-	53,53,53,53	0
56	MG	DA	3055	1/1	0.93	0.12	-	44,44,44,44	0
56	MG	AA	3103	1/1	0.89	0.22	-	59,59,59,59	0
56	MG	AA	3149	1/1	0.92	0.08	-	71,71,71,71	0
56	MG	BA	3544	1/1	0.74	0.26	-	57,57,57,57	0
56	MG	DA	3196	1/1	0.94	0.14	-	49,49,49,49	0
56	MG	BA	3395	1/1	0.87	0.13	-	65,65,65,65	0
56	MG	DA	3205	1/1	0.85	0.14	-	45,45,45,45	0
56	MG	B4	502	1/1	0.83	0.22	-	73,73,73,73	0
56	MG	DA	3009	1/1	0.92	0.11	-	46,46,46,46	0
56	MG	BA	3404	1/1	0.87	0.12	-	59,59,59,59	0
56	MG	BA	3484	1/1	0.87	0.13	-	64,64,64,64	0
56	MG	BA	3321	1/1	0.97	0.18	-	43,43,43,43	0
56	MG	AA	3017	1/1	0.87	0.14	-	49,49,49,49	0
56	MG	AA	3056	1/1	0.96	0.10	-	56,56,56,56	0
56	MG	BA	3667	1/1	0.92	0.12	-	64,64,64,64	0
56	MG	DA	3457	1/1	0.97	0.23	-	46,46,46,46	0
56	MG	CA	3148	1/1	0.86	0.11	-	72,72,72,72	0
56	MG	BA	3415	1/1	0.87	0.12	-	62,62,62,62	0
56	MG	B1	101	1/1	0.97	0.71	-	45,45,45,45	0
56	MG	BA	3718	1/1	0.93	0.17	-	49,49,49,49	0
56	MG	BA	3413	1/1	0.95	0.19	-	53,53,53,53	0
56	MG	AA	3196	1/1	0.96	0.17	-	66,66,66,66	0
56	MG	BA	3643	1/1	0.93	0.47	-	38,38,38,38	0
56	MG	BA	3242	1/1	0.88	0.21	-	58,58,58,58	0
56	MG	DA	3328	1/1	0.92	0.17	-	49,49,49,49	0
56	MG	AA	3049	1/1	0.81	0.13	-	59,59,59,59	0
56	MG	DA	3557	1/1	0.87	0.10	-	67,67,67,67	0
56	MG	DA	3229	1/1	0.94	0.16	-	49,49,49,49	0
56	MG	AX	3003	1/1	0.80	0.13	-	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3336	1/1	0.98	0.12	-	30,30,30,30	0
56	MG	AA	3033	1/1	0.93	0.32	-	45,45,45,45	0
56	MG	DA	3190	1/1	0.95	0.10	-	58,58,58,58	0
56	MG	BA	3545	1/1	0.84	0.18	-	58,58,58,58	0
56	MG	DA	3597	1/1	0.92	0.24	-	56,56,56,56	0
56	MG	AA	3008	1/1	0.90	0.18	-	53,53,53,53	0
56	MG	BA	3288	1/1	0.91	0.17	-	36,36,36,36	0
56	MG	DA	3595	1/1	0.87	0.12	-	34,34,34,34	0
56	MG	BA	3762	1/1	0.91	0.23	-	58,58,58,58	0
56	MG	BA	3749	1/1	0.90	0.12	-	38,38,38,38	0
56	MG	DD	302	1/1	0.92	0.44	-	40,40,40,40	0
56	MG	BA	3266	1/1	0.93	0.13	-	38,38,38,38	0
56	MG	DA	3158	1/1	0.85	0.30	-	55,55,55,55	0
56	MG	CA	3053	1/1	0.89	0.22	-	63,63,63,63	0
56	MG	AA	3066	1/1	0.91	0.11	-	53,53,53,53	0
56	MG	DA	3400	1/1	0.93	0.13	-	61,61,61,61	0
56	MG	DA	3578	1/1	0.83	0.10	-	71,71,71,71	0
56	MG	BA	3140	1/1	0.92	0.52	-	41,41,41,41	0
56	MG	BA	3033	1/1	0.91	0.12	-	45,45,45,45	0
56	MG	DA	3359	1/1	0.95	0.15	-	54,54,54,54	0
56	MG	DA	3443	1/1	0.93	0.15	-	49,49,49,49	0
56	MG	AA	3109	1/1	0.91	0.21	-	51,51,51,51	0
56	MG	DA	3450	1/1	0.97	0.08	-	50,50,50,50	0
56	MG	DA	3343	1/1	0.94	0.11	-	57,57,57,57	0
56	MG	DA	3481	1/1	0.92	0.16	-	51,51,51,51	0
56	MG	DA	3175	1/1	0.82	0.18	-	43,43,43,43	0
56	MG	AA	3020	1/1	0.84	0.25	-	53,53,53,53	0
56	MG	BA	3218	1/1	0.94	0.10	-	52,52,52,52	0
56	MG	BA	3191	1/1	0.85	0.45	-	50,50,50,50	0
56	MG	DA	3082	1/1	0.92	0.08	-	48,48,48,48	0
56	MG	BA	3583	1/1	0.95	0.12	-	46,46,46,46	0
56	MG	BA	3113	1/1	0.92	0.94	-	44,44,44,44	0
56	MG	BA	3429	1/1	0.90	0.09	-	71,71,71,71	0
56	MG	AA	3035	1/1	0.69	0.16	-	69,69,69,69	0
56	MG	DA	3588	1/1	0.90	0.18	-	57,57,57,57	0
56	MG	CA	3179	1/1	0.98	0.16	-	53,53,53,53	0
56	MG	BA	3508	1/1	0.69	0.31	-	61,61,61,61	0
56	MG	DA	3484	1/1	0.96	0.06	-	59,59,59,59	0
56	MG	DA	3419	1/1	0.92	0.07	-	59,59,59,59	0
56	MG	BA	3767	1/1	0.98	0.14	-	31,31,31,31	0
56	MG	CA	3126	1/1	0.60	0.23	-	76,76,76,76	0
56	MG	AA	3165	1/1	0.93	0.14	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3389	1/1	0.88	0.14	-	63,63,63,63	0
56	MG	BA	3128	1/1	0.96	0.39	-	46,46,46,46	0
56	MG	BA	3142	1/1	0.92	0.32	-	47,47,47,47	0
56	MG	BA	3648	1/1	0.82	0.14	-	39,39,39,39	0
56	MG	AA	3080	1/1	0.92	0.26	-	58,58,58,58	0
56	MG	DA	3226	1/1	0.73	0.26	-	70,70,70,70	0
56	MG	CA	3081	1/1	0.92	0.11	-	51,51,51,51	0
56	MG	DA	3596	1/1	0.91	0.11	-	64,64,64,64	0
56	MG	BA	3088	1/1	0.92	0.40	-	46,46,46,46	0
56	MG	BA	3100	1/1	0.93	0.35	-	46,46,46,46	0
56	MG	DA	3412	1/1	0.91	0.35	-	52,52,52,52	0
56	MG	BA	3576	1/1	0.97	0.10	-	56,56,56,56	0
56	MG	CA	3105	1/1	0.84	0.11	-	76,76,76,76	0
56	MG	CA	3130	1/1	0.91	0.11	-	70,70,70,70	0
56	MG	AA	3050	1/1	0.88	0.13	-	65,65,65,65	0
56	MG	BA	3754	1/1	0.94	0.21	-	36,36,36,36	0
56	MG	BF	310	1/1	0.82	0.20	-	44,44,44,44	0
56	MG	CA	3083	1/1	0.89	0.08	-	58,58,58,58	0
56	MG	DA	3231	1/1	0.97	0.10	-	54,54,54,54	0
56	MG	CA	3154	1/1	0.93	0.14	-	62,62,62,62	0
56	MG	CA	3139	1/1	0.83	0.11	-	63,63,63,63	0
56	MG	DA	3207	1/1	0.89	0.13	-	58,58,58,58	0
56	MG	CA	3074	1/1	0.93	0.09	-	62,62,62,62	0
56	MG	DA	3276	1/1	0.78	0.15	-	57,57,57,57	0
56	MG	CA	3127	1/1	0.85	0.13	-	69,69,69,69	0
56	MG	BA	3284	1/1	0.97	0.20	-	35,35,35,35	0
56	MG	BA	3697	1/1	0.94	0.13	-	34,34,34,34	0
56	MG	BA	3684	1/1	0.98	0.08	-	39,39,39,39	0
56	MG	DA	3239	1/1	0.87	0.09	-	61,61,61,61	0
56	MG	DA	3574	1/1	0.92	0.13	-	68,68,68,68	0
56	MG	BA	3575	1/1	0.90	0.17	-	48,48,48,48	0
56	MG	BA	3707	1/1	0.86	0.21	-	62,62,62,62	0
56	MG	CA	3021	1/1	0.81	0.12	-	66,66,66,66	0
56	MG	CA	3016	1/1	0.84	0.09	-	56,56,56,56	0
56	MG	AA	3207	1/1	0.95	0.13	-	57,57,57,57	0
56	MG	BA	3193	1/1	0.94	0.14	-	24,24,24,24	0
56	MG	DA	3474	1/1	0.82	0.14	-	55,55,55,55	0
56	MG	BA	3602	1/1	0.94	0.11	-	61,61,61,61	0
56	MG	DA	3038	1/1	0.94	0.14	-	56,56,56,56	0
56	MG	BB	3002	1/1	0.96	0.28	-	51,51,51,51	0
56	MG	BA	3059	1/1	0.81	0.15	-	40,40,40,40	0
56	MG	BA	3219	1/1	0.85	0.16	-	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3502	1/1	0.90	0.14	-	62,62,62,62	0
56	MG	AA	3201	1/1	0.84	0.10	-	60,60,60,60	0
56	MG	BA	3563	1/1	0.94	0.20	-	43,43,43,43	0
56	MG	CA	3020	1/1	0.84	0.15	-	48,48,48,48	0
56	MG	DA	3418	1/1	0.94	0.11	-	55,55,55,55	0
56	MG	BA	3009	1/1	0.86	0.30	-	41,41,41,41	0
56	MG	DA	3561	1/1	0.92	0.18	-	65,65,65,65	0
56	MG	DA	3036	1/1	0.79	0.34	-	48,48,48,48	0
56	MG	AA	3170	1/1	0.91	0.07	-	66,66,66,66	0
56	MG	BA	3599	1/1	0.75	0.10	-	59,59,59,59	0
56	MG	BA	3254	1/1	0.93	0.11	-	56,56,56,56	0
56	MG	DA	3555	1/1	0.94	0.22	-	48,48,48,48	0
56	MG	BA	3103	1/1	0.94	0.16	-	45,45,45,45	0
56	MG	CA	3085	1/1	0.89	0.13	-	60,60,60,60	0
56	MG	DA	3262	1/1	0.91	0.16	-	41,41,41,41	0
56	MG	DA	3568	1/1	0.95	0.11	-	61,61,61,61	0
56	MG	CY	3001	1/1	0.94	0.15	-	63,63,63,63	0
56	MG	BA	3315	1/1	0.98	0.11	-	40,40,40,40	0
56	MG	DA	3148	1/1	0.74	0.14	-	53,53,53,53	0
56	MG	DA	3342	1/1	0.86	0.10	-	55,55,55,55	0
56	MG	CA	3121	1/1	0.82	0.14	-	88,88,88,88	0
56	MG	AA	3069	1/1	0.91	0.13	-	59,59,59,59	0
56	MG	BA	3543	1/1	0.90	0.12	-	62,62,62,62	0
56	MG	DA	3367	1/1	0.96	0.20	-	44,44,44,44	0
56	MG	BA	3753	1/1	0.95	0.12	-	76,76,76,76	0
56	MG	BA	3328	1/1	0.95	0.10	-	56,56,56,56	0
56	MG	DA	3266	1/1	0.97	0.24	-	61,61,61,61	0
56	MG	DA	3189	1/1	0.96	0.21	-	42,42,42,42	0
56	MG	AA	3171	1/1	0.92	0.15	-	56,56,56,56	0
56	MG	DA	3161	1/1	0.88	0.30	-	57,57,57,57	0
56	MG	CA	3039	1/1	0.84	0.14	-	70,70,70,70	0
56	MG	CA	3069	1/1	0.89	0.20	-	75,75,75,75	0
56	MG	BA	3153	1/1	0.88	0.22	-	56,56,56,56	0
56	MG	BA	3675	1/1	0.91	0.28	-	39,39,39,39	0
56	MG	BA	3420	1/1	0.90	0.17	-	61,61,61,61	0
56	MG	BA	3394	1/1	0.93	0.17	-	53,53,53,53	0
56	MG	DA	3540	1/1	0.74	0.11	-	65,65,65,65	0
56	MG	DA	3464	1/1	0.95	0.15	-	51,51,51,51	0
56	MG	BA	3533	1/1	0.86	0.12	-	27,27,27,27	0
56	MG	BA	3521	1/1	0.88	0.21	-	28,28,28,28	0
56	MG	AA	3009	1/1	0.92	0.23	-	64,64,64,64	0
56	MG	DA	3323	1/1	0.95	0.10	-	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	3047	1/1	0.93	0.28	-	56,56,56,56	0
56	MG	CA	3009	1/1	0.85	0.27	-	55,55,55,55	0
56	MG	DA	3388	1/1	0.99	0.15	-	49,49,49,49	0
56	MG	DU	3002	1/1	0.93	0.80	-	58,58,58,58	0
56	MG	DA	3173	1/1	0.87	0.25	-	49,49,49,49	0
56	MG	BA	3168	1/1	0.89	0.15	-	57,57,57,57	0
56	MG	DA	3425	1/1	0.89	0.14	-	69,69,69,69	0
56	MG	DA	3355	1/1	0.94	0.12	-	53,53,53,53	0
56	MG	BA	3581	1/1	0.93	0.14	-	47,47,47,47	0
56	MG	DA	3003	1/1	0.93	0.09	-	55,55,55,55	0
56	MG	DA	3353	1/1	0.87	0.06	-	65,65,65,65	0
60	K	AX	3001	1/1	0.93	0.28	-	73,73,73,73	0
56	MG	BA	3240	1/1	0.93	0.19	-	43,43,43,43	0
56	MG	BA	3186	1/1	0.81	0.24	-	59,59,59,59	0
56	MG	BA	3779	1/1	0.73	0.40	-	52,52,52,52	0
56	MG	DA	3318	1/1	0.91	0.08	-	60,60,60,60	0
56	MG	AA	3021	1/1	0.87	0.16	-	60,60,60,60	0
56	MG	AA	3005	1/1	0.94	0.36	-	55,55,55,55	0
56	MG	AA	3097	1/1	0.95	0.17	-	45,45,45,45	0
56	MG	DA	3301	1/1	0.95	0.09	-	60,60,60,60	0
56	MG	BA	3047	1/1	0.94	0.13	-	51,51,51,51	0
56	MG	DA	3112	1/1	0.90	0.12	-	49,49,49,49	0
56	MG	DA	3590	1/1	0.85	0.12	-	61,61,61,61	0
56	MG	BG	3002	1/1	0.91	0.12	-	52,52,52,52	0
56	MG	BA	3162	1/1	0.98	0.16	-	37,37,37,37	0
56	MG	DA	3248	1/1	0.92	0.10	-	39,39,39,39	0
56	MG	DA	3527	1/1	0.94	0.17	-	67,67,67,67	0
56	MG	CX	3002	1/1	0.88	0.17	-	67,67,67,67	0
56	MG	BA	3181	1/1	0.84	0.17	-	48,48,48,48	0
56	MG	BA	3416	1/1	0.93	0.16	-	53,53,53,53	0
56	MG	DA	3345	1/1	0.92	0.10	-	57,57,57,57	0
56	MG	BA	3060	1/1	0.81	0.32	-	61,61,61,61	0
56	MG	DA	3241	1/1	0.91	0.14	-	51,51,51,51	0
56	MG	BA	3633	1/1	0.72	0.09	-	58,58,58,58	0
56	MG	BA	3553	1/1	0.98	0.11	-	49,49,49,49	0
56	MG	DB	3009	1/1	0.92	0.12	-	70,70,70,70	0
56	MG	BA	3159	1/1	0.93	0.14	-	45,45,45,45	0
56	MG	AA	3225	1/1	0.81	0.16	-	55,55,55,55	0
56	MG	BA	3453	1/1	0.83	0.16	-	59,59,59,59	0
56	MG	BA	3612	1/1	0.86	0.16	-	65,65,65,65	0
56	MG	CJ	5001	1/1	0.75	0.10	-	75,75,75,75	0
56	MG	DA	3195	1/1	0.75	0.15	-	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	AA	3078	1/1	0.95	0.18	-	59,59,59,59	0
56	MG	CA	3157	1/1	0.95	0.13	-	57,57,57,57	0
56	MG	BA	3112	1/1	0.97	0.07	-	50,50,50,50	0
56	MG	BA	3071	1/1	0.90	0.12	-	48,48,48,48	0
56	MG	BA	3546	1/1	0.84	0.12	-	57,57,57,57	0
56	MG	BA	3396	1/1	0.96	0.17	-	24,24,24,24	0
56	MG	DA	3469	1/1	0.94	0.05	-	56,56,56,56	0
56	MG	AA	3162	1/1	0.95	0.08	-	70,70,70,70	0
56	MG	BA	3299	1/1	0.97	0.07	-	53,53,53,53	0
56	MG	BA	3281	1/1	0.86	0.09	-	55,55,55,55	0
56	MG	CF	3001	1/1	0.91	0.17	-	44,44,44,44	0
56	MG	DA	3436	1/1	0.90	0.14	-	63,63,63,63	0
56	MG	CA	3162	1/1	0.91	0.07	-	57,57,57,57	0
56	MG	DA	3021	1/1	0.95	0.35	-	44,44,44,44	0
56	MG	DN	5001	1/1	0.88	0.15	-	75,75,75,75	0
56	MG	AA	3075	1/1	0.71	0.24	-	81,81,81,81	0
56	MG	BA	3138	1/1	0.97	0.17	-	50,50,50,50	0
56	MG	DA	3060	1/1	0.90	0.30	-	50,50,50,50	0
56	MG	DA	3058	1/1	0.90	0.14	-	48,48,48,48	0
56	MG	DA	3547	1/1	0.95	0.51	-	41,41,41,41	0
56	MG	DA	3423	1/1	0.96	0.18	-	34,34,34,34	0
56	MG	DA	3385	1/1	0.91	0.27	-	55,55,55,55	0
56	MG	BA	3330	1/1	0.98	0.18	-	35,35,35,35	0
56	MG	BA	3660	1/1	0.95	0.17	-	44,44,44,44	0
56	MG	AA	3042	1/1	0.89	0.14	-	52,52,52,52	0
56	MG	BA	3326	1/1	0.94	0.09	-	50,50,50,50	0
56	MG	BA	3108	1/1	0.87	0.38	-	52,52,52,52	0
56	MG	BA	3339	1/1	0.92	0.16	-	31,31,31,31	0
56	MG	BA	3117	1/1	0.93	0.45	-	41,41,41,41	0
56	MG	BA	3528	1/1	0.93	0.16	-	29,29,29,29	0
56	MG	BA	3736	1/1	0.73	0.09	-	73,73,73,73	0
56	MG	BA	3212	1/1	0.88	0.26	-	47,47,47,47	0
56	MG	BA	3597	1/1	0.84	0.09	-	51,51,51,51	0
56	MG	DA	3138	1/1	0.80	0.20	-	46,46,46,46	0
56	MG	DA	3507	1/1	0.95	0.19	-	54,54,54,54	0
56	MG	BA	3152	1/1	0.94	0.19	-	48,48,48,48	0
56	MG	BA	3653	1/1	0.84	0.14	-	23,23,23,23	0
56	MG	BA	3689	1/1	0.90	0.19	-	68,68,68,68	0
56	MG	DA	3193	1/1	0.87	0.09	-	57,57,57,57	0
56	MG	DA	3551	1/1	0.95	0.18	-	66,66,66,66	0
56	MG	AA	3161	1/1	0.94	0.07	-	59,59,59,59	0
56	MG	BA	3558	1/1	0.87	0.16	-	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	3116	1/1	0.90	0.17	-	64,64,64,64	0
56	MG	BA	3624	1/1	0.94	0.11	-	50,50,50,50	0
56	MG	BA	3086	1/1	0.84	0.20	-	67,67,67,67	0
56	MG	AA	3167	1/1	0.91	0.19	-	71,71,71,71	0
56	MG	DA	3070	1/1	0.90	0.12	-	34,34,34,34	0
56	MG	CA	3114	1/1	0.93	0.09	-	52,52,52,52	0
56	MG	DA	3496	1/1	0.96	0.27	-	51,51,51,51	0
56	MG	BA	3601	1/1	0.86	0.56	-	72,72,72,72	0
56	MG	AY	3003	1/1	0.57	0.26	-	78,78,78,78	0
56	MG	DA	3289	1/1	0.92	0.17	-	23,23,23,23	0
56	MG	DA	3611	1/1	0.94	0.09	-	53,53,53,53	0
56	MG	AA	3016	1/1	0.98	0.11	-	48,48,48,48	0
56	MG	DA	3341	1/1	0.88	0.09	-	54,54,54,54	0
56	MG	BA	3631	1/1	0.87	0.17	-	63,63,63,63	0
56	MG	DA	3206	1/1	0.96	0.17	-	45,45,45,45	0
56	MG	BQ	3004	1/1	0.90	0.27	-	48,48,48,48	0
56	MG	BA	3368	1/1	0.98	0.12	-	56,56,56,56	0
56	MG	BA	3093	1/1	0.94	0.23	-	39,39,39,39	0
56	MG	CA	3123	1/1	0.84	0.26	-	77,77,77,77	0
56	MG	BA	3053	1/1	0.94	0.15	-	56,56,56,56	0
56	MG	DD	309	1/1	0.86	0.36	-	65,65,65,65	0
56	MG	BN	3005	1/1	0.91	0.15	-	46,46,46,46	0
56	MG	DA	3470	1/1	0.71	0.13	-	65,65,65,65	0
56	MG	BE	305	1/1	0.97	0.28	-	38,38,38,38	0
56	MG	DA	3170	1/1	0.90	0.25	-	39,39,39,39	0
56	MG	AA	3024	1/1	0.94	0.11	-	49,49,49,49	0
56	MG	BB	3016	1/1	0.79	0.14	-	63,63,63,63	0
56	MG	DA	3398	1/1	0.79	0.17	-	73,73,73,73	0
56	MG	CA	3101	1/1	0.97	0.19	-	64,64,64,64	0
56	MG	DA	3179	1/1	0.74	0.19	-	61,61,61,61	0
56	MG	CA	3135	1/1	0.94	0.43	-	75,75,75,75	0
56	MG	AA	3156	1/1	0.91	0.08	-	65,65,65,65	0
56	MG	BX	101	1/1	0.91	0.15	-	48,48,48,48	0
56	MG	BA	3408	1/1	0.89	0.10	-	71,71,71,71	0
56	MG	BA	3745	1/1	0.96	0.16	-	27,27,27,27	0
56	MG	DA	3520	1/1	0.87	0.11	-	61,61,61,61	0
56	MG	DA	3493	1/1	0.88	0.16	-	64,64,64,64	0
56	MG	DA	3352	1/1	0.86	0.18	-	45,45,45,45	0
56	MG	BA	3388	1/1	0.96	0.17	-	40,40,40,40	0
56	MG	BA	3065	1/1	0.95	0.23	-	33,33,33,33	0
56	MG	AA	3121	1/1	0.88	0.10	-	54,54,54,54	0
57	NEG	CA	3172	17/17	0.83	0.23	-	61,76,83,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3402	1/1	0.95	0.10	-	57,57,57,57	0
56	MG	AA	3152	1/1	0.92	0.09	-	63,63,63,63	0
56	MG	AA	3051	1/1	0.90	0.12	-	64,64,64,64	0
56	MG	BA	3239	1/1	0.98	0.30	-	30,30,30,30	0
56	MG	DA	3230	1/1	0.98	0.12	-	23,23,23,23	0
56	MG	BA	3470	1/1	0.94	0.24	-	46,46,46,46	0
56	MG	BA	3358	1/1	0.94	0.14	-	30,30,30,30	0
56	MG	BA	3617	1/1	0.97	0.06	-	46,46,46,46	0
56	MG	BA	3023	1/1	0.97	0.32	-	38,38,38,38	0
56	MG	DA	3176	1/1	0.84	0.15	-	49,49,49,49	0
56	MG	DA	3109	1/1	0.91	0.34	-	47,47,47,47	0
56	MG	DA	3007	1/1	0.93	0.18	-	53,53,53,53	0
56	MG	D5	502	1/1	0.93	0.54	-	50,50,50,50	0
56	MG	BA	3514	1/1	0.90	0.12	-	50,50,50,50	0
56	MG	DA	3123	1/1	0.97	0.39	-	40,40,40,40	0
56	MG	DA	3297	1/1	0.93	0.50	-	70,70,70,70	0
56	MG	CA	3068	1/1	0.68	0.15	-	77,77,77,77	0
56	MG	AA	3026	1/1	0.96	0.11	-	68,68,68,68	0
56	MG	BA	3451	1/1	0.98	0.21	-	53,53,53,53	0
56	MG	DA	3612	1/1	0.92	0.57	-	38,38,38,38	0
56	MG	BA	3119	1/1	0.97	0.34	-	44,44,44,44	0
56	MG	BA	3622	1/1	0.88	0.21	-	48,48,48,48	0
56	MG	CA	3136	1/1	0.78	0.20	-	73,73,73,73	0
56	MG	CA	3119	1/1	0.91	0.15	-	84,84,84,84	0
56	MG	DA	3439	1/1	0.96	0.10	-	58,58,58,58	0
56	MG	BA	3154	1/1	0.78	0.29	-	58,58,58,58	0
56	MG	BW	204	1/1	0.96	0.48	-	41,41,41,41	0
56	MG	DA	3379	1/1	0.97	0.18	-	38,38,38,38	0
56	MG	DB	3002	1/1	0.95	0.20	-	58,58,58,58	0
56	MG	DA	3610	1/1	0.84	0.10	-	65,65,65,65	0
56	MG	AA	3061	1/1	0.96	0.17	-	44,44,44,44	0
56	MG	DB	3001	1/1	0.88	0.25	-	56,56,56,56	0
56	MG	AA	3096	1/1	0.89	0.16	-	53,53,53,53	0
56	MG	BA	3556	1/1	0.97	0.20	-	50,50,50,50	0
56	MG	AA	3197	1/1	0.91	0.12	-	64,64,64,64	0
56	MG	BW	202	1/1	0.94	0.18	-	43,43,43,43	0
56	MG	AA	3028	1/1	0.97	0.23	-	46,46,46,46	0
56	MG	AA	3038	1/1	0.91	0.25	-	56,56,56,56	0
56	MG	BA	3234	1/1	0.90	0.14	-	52,52,52,52	0
56	MG	BA	3422	1/1	0.97	0.12	-	45,45,45,45	0
56	MG	AA	3124	1/1	0.90	0.16	-	63,63,63,63	0
56	MG	DA	3604	1/1	0.82	0.10	-	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	3621	1/1	0.91	0.26	-	48,48,48,48	0
56	MG	BA	3659	1/1	0.96	0.19	-	24,24,24,24	0
56	MG	DA	3157	1/1	0.84	0.22	-	58,58,58,58	0
56	MG	DA	3475	1/1	0.93	0.17	-	32,32,32,32	0
56	MG	BA	3412	1/1	0.92	0.15	-	50,50,50,50	0
56	MG	DA	3143	1/1	0.94	0.13	-	35,35,35,35	0
56	MG	BA	3582	1/1	0.80	0.13	-	63,63,63,63	0
56	MG	CA	3013	1/1	0.91	0.14	-	52,52,52,52	0
56	MG	DA	3594	1/1	0.93	0.14	-	52,52,52,52	0
56	MG	DA	3059	1/1	0.90	0.12	-	49,49,49,49	0
56	MG	AA	3148	1/1	0.99	0.18	-	50,50,50,50	0
56	MG	AA	3185	1/1	0.98	0.21	-	51,51,51,51	0
56	MG	BA	3608	1/1	0.90	0.12	-	68,68,68,68	0
56	MG	CW	3003	1/1	0.96	0.10	-	64,64,64,64	0
56	MG	DA	3463	1/1	0.63	0.20	-	53,53,53,53	0
56	MG	CA	3138	1/1	0.89	0.11	-	52,52,52,52	0
56	MG	BA	3199	1/1	0.66	0.28	-	55,55,55,55	0
56	MG	DA	3397	1/1	0.91	0.12	-	50,50,50,50	0
56	MG	DA	3225	1/1	0.92	0.15	-	56,56,56,56	0
56	MG	DA	3426	1/1	0.80	0.11	-	53,53,53,53	0
56	MG	DW	3004	1/1	0.88	0.21	-	50,50,50,50	0
56	MG	AA	3105	1/1	0.77	0.10	-	66,66,66,66	0
56	MG	BA	3215	1/1	0.92	0.15	-	47,47,47,47	0
56	MG	BA	3375	1/1	0.85	0.20	-	52,52,52,52	0
56	MG	BA	3630	1/1	0.89	0.14	-	44,44,44,44	0
56	MG	CA	3058	1/1	0.79	0.20	-	64,64,64,64	0
56	MG	DA	3582	1/1	0.92	0.15	-	65,65,65,65	0
56	MG	BA	3771	1/1	0.93	0.10	-	73,73,73,73	0
56	MG	BA	3431	1/1	0.94	0.15	-	54,54,54,54	0
56	MG	DA	3053	1/1	0.84	0.21	-	61,61,61,61	0
56	MG	BA	3331	1/1	0.81	0.15	-	51,51,51,51	0
56	MG	BA	3489	1/1	0.97	0.09	-	43,43,43,43	0
56	MG	CA	3011	1/1	0.96	0.25	-	71,71,71,71	0
56	MG	DA	3523	1/1	0.92	0.33	-	62,62,62,62	0
56	MG	BA	3323	1/1	0.87	0.16	-	60,60,60,60	0
56	MG	BA	3373	1/1	0.84	0.12	-	35,35,35,35	0
56	MG	DA	3062	1/1	0.95	0.32	-	49,49,49,49	0
56	MG	BA	3466	1/1	0.95	0.30	-	52,52,52,52	0
56	MG	BA	3610	1/1	0.72	0.20	-	64,64,64,64	0
56	MG	CA	3128	1/1	0.95	0.08	-	72,72,72,72	0
56	MG	AA	3102	1/1	0.97	0.17	-	50,50,50,50	0
56	MG	CA	3065	1/1	0.85	0.31	-	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3438	1/1	0.83	0.15	-	44,44,44,44	0
56	MG	AA	3082	1/1	0.75	0.16	-	70,70,70,70	0
56	MG	CA	3073	1/1	0.90	0.20	-	70,70,70,70	0
56	MG	BA	3579	1/1	0.89	0.25	-	57,57,57,57	0
56	MG	BA	3012	1/1	0.88	0.11	-	49,49,49,49	0
56	MG	BA	3325	1/1	0.95	0.14	-	42,42,42,42	0
56	MG	BA	3696	1/1	0.94	0.13	-	38,38,38,38	0
56	MG	DA	3562	1/1	0.86	0.10	-	67,67,67,67	0
56	MG	DA	3273	1/1	0.94	0.17	-	36,36,36,36	0
56	MG	BA	3371	1/1	0.95	0.19	-	50,50,50,50	0
56	MG	AA	3178	1/1	0.81	0.11	-	60,60,60,60	0
56	MG	CA	3131	1/1	0.88	0.09	-	62,62,62,62	0
56	MG	BA	3475	1/1	0.96	0.17	-	52,52,52,52	0
56	MG	DA	3455	1/1	0.95	0.29	-	50,50,50,50	0
56	MG	BE	303	1/1	0.80	0.26	-	61,61,61,61	0
56	MG	DA	3447	1/1	0.94	0.17	-	49,49,49,49	0
56	MG	BA	3739	1/1	0.90	0.29	-	75,75,75,75	0
56	MG	BA	3683	1/1	0.92	0.19	-	50,50,50,50	0
56	MG	BA	3524	1/1	0.96	0.17	-	44,44,44,44	0
56	MG	DA	3081	1/1	0.79	0.20	-	53,53,53,53	0
56	MG	DA	3608	1/1	0.96	0.09	-	47,47,47,47	0
56	MG	BA	3246	1/1	0.94	0.15	-	57,57,57,57	0
56	MG	AW	3003	1/1	0.97	0.21	-	44,44,44,44	0
56	MG	CA	3037	1/1	0.87	0.16	-	67,67,67,67	0
56	MG	BA	3730	1/1	0.76	0.28	-	45,45,45,45	0
56	MG	BA	3588	1/1	0.89	0.17	-	62,62,62,62	0
56	MG	CD	301	1/1	0.94	0.12	-	67,67,67,67	0
56	MG	BA	3118	1/1	0.82	0.31	-	46,46,46,46	0
56	MG	BA	3437	1/1	0.92	0.10	-	55,55,55,55	0
56	MG	DA	3524	1/1	0.94	0.09	-	58,58,58,58	0
56	MG	BA	3710	1/1	0.93	0.15	-	51,51,51,51	0
56	MG	BA	3097	1/1	0.73	0.40	-	33,33,33,33	0
56	MG	BA	3095	1/1	0.93	0.32	-	39,39,39,39	0
56	MG	DA	3162	1/1	0.94	0.39	-	45,45,45,45	0
56	MG	AX	3007	1/1	0.91	0.24	-	66,66,66,66	0
56	MG	BA	3336	1/1	0.89	0.21	-	31,31,31,31	0
56	MG	DA	3351	1/1	0.89	0.11	-	40,40,40,40	0
56	MG	DA	3305	1/1	0.94	0.16	-	42,42,42,42	0
56	MG	BA	3669	1/1	0.88	0.30	-	45,45,45,45	0
56	MG	AA	3108	1/1	0.95	0.08	-	59,59,59,59	0
56	MG	DA	3364	1/1	0.96	0.20	-	54,54,54,54	0
56	MG	DP	201	1/1	0.72	0.26	-	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	BA	3207	1/1	0.90	0.08	-	52,52,52,52	0
56	MG	BA	3077	1/1	0.76	0.17	-	59,59,59,59	0
56	MG	DA	3118	1/1	0.90	0.16	-	50,50,50,50	0
56	MG	DW	3003	1/1	0.94	0.58	-	71,71,71,71	0
56	MG	BA	3280	1/1	0.95	0.22	-	25,25,25,25	0
56	MG	CA	3142	1/1	0.90	0.17	-	69,69,69,69	0
56	MG	DA	3180	1/1	0.77	0.12	-	50,50,50,50	0
56	MG	DA	3135	1/1	0.97	0.27	-	44,44,44,44	0
56	MG	BA	3518	1/1	0.95	0.17	-	25,25,25,25	0
56	MG	DA	3194	1/1	0.97	0.13	-	52,52,52,52	0
56	MG	BA	3056	1/1	0.93	0.27	-	26,26,26,26	0
56	MG	BA	3485	1/1	0.93	0.15	-	25,25,25,25	0
56	MG	CA	3064	1/1	0.86	0.10	-	67,67,67,67	0
56	MG	DA	3049	1/1	0.88	0.16	-	48,48,48,48	0
56	MG	BA	3641	1/1	0.97	0.26	-	46,46,46,46	0
56	MG	DA	3373	1/1	0.95	0.22	-	51,51,51,51	0
56	MG	BA	3458	1/1	0.98	0.21	-	52,52,52,52	0
56	MG	BA	3486	1/1	0.95	0.21	-	30,30,30,30	0
56	MG	DA	3039	1/1	0.80	0.21	-	50,50,50,50	0
56	MG	BA	3411	1/1	0.97	0.24	-	49,49,49,49	0
56	MG	BA	3686	1/1	0.92	0.12	-	61,61,61,61	0
56	MG	DA	3454	1/1	0.93	0.12	-	47,47,47,47	0
56	MG	DA	3363	1/1	0.85	0.16	-	61,61,61,61	0
56	MG	CA	3153	1/1	0.94	0.24	-	62,62,62,62	0
56	MG	DA	3609	1/1	0.92	0.14	-	47,47,47,47	0
56	MG	AA	3107	1/1	0.96	0.18	-	66,66,66,66	0
56	MG	BA	3636	1/1	0.93	0.22	-	61,61,61,61	0
56	MG	DD	303	1/1	0.95	0.27	-	60,60,60,60	0
56	MG	BA	3430	1/1	0.96	0.17	-	48,48,48,48	0
56	MG	BA	3217	1/1	0.72	0.28	-	66,66,66,66	0
56	MG	CA	3124	1/1	0.56	0.19	-	90,90,90,90	0
56	MG	AA	3210	1/1	0.92	0.10	-	65,65,65,65	0
56	MG	BA	3784	1/1	0.87	0.09	-	62,62,62,62	0
56	MG	AA	3134	1/1	0.92	0.17	-	73,73,73,73	0
56	MG	BA	3170	1/1	0.90	0.20	-	30,30,30,30	0
56	MG	BA	3256	1/1	0.83	0.25	-	25,25,25,25	0
56	MG	BA	3187	1/1	0.86	0.21	-	42,42,42,42	0
56	MG	DA	3335	1/1	0.97	0.07	-	41,41,41,41	0
56	MG	AA	3025	1/1	0.97	0.25	-	54,54,54,54	0
56	MG	DA	3200	1/1	0.93	0.09	-	52,52,52,52	0
56	MG	DA	3178	1/1	0.93	0.09	-	45,45,45,45	0
56	MG	BA	3716	1/1	0.86	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	AV	101	1/1	0.96	0.10	-	47,47,47,47	0
56	MG	DA	3028	1/1	0.88	0.21	-	52,52,52,52	0
56	MG	BA	3403	1/1	0.91	0.19	-	53,53,53,53	0
56	MG	BE	306	1/1	0.98	0.21	-	15,15,15,15	0
56	MG	DA	3593	1/1	0.87	0.23	-	57,57,57,57	0
56	MG	AA	3223	1/1	0.96	0.12	-	52,52,52,52	0
56	MG	BA	3195	1/1	0.71	0.50	-	53,53,53,53	0
56	MG	AA	3174	1/1	0.88	0.09	-	59,59,59,59	0
56	MG	BA	3230	1/1	0.97	0.20	-	53,53,53,53	0
56	MG	CA	3076	1/1	0.93	0.15	-	54,54,54,54	0
56	MG	DA	3383	1/1	0.95	0.20	-	40,40,40,40	0
56	MG	BB	3007	1/1	0.85	0.23	-	84,84,84,84	0
56	MG	BA	3681	1/1	0.92	0.22	-	47,47,47,47	0
56	MG	DA	3084	1/1	0.83	0.20	-	53,53,53,53	0
56	MG	DA	3073	1/1	0.77	0.24	-	50,50,50,50	0
56	MG	DQ	3002	1/1	0.92	0.13	-	50,50,50,50	0
56	MG	BA	3087	1/1	0.93	0.13	-	63,63,63,63	0
56	MG	CA	3109	1/1	0.98	0.14	-	67,67,67,67	0
56	MG	BA	3635	1/1	0.96	0.19	-	56,56,56,56	0
56	MG	BA	3595	1/1	0.85	0.07	-	65,65,65,65	0
56	MG	BA	3206	1/1	0.95	0.31	-	49,49,49,49	0
56	MG	BA	3577	1/1	0.82	0.19	-	62,62,62,62	0
56	MG	DA	3167	1/1	0.92	0.77	-	51,51,51,51	0
56	MG	AY	3002	1/1	0.92	0.13	-	70,70,70,70	0
56	MG	BA	3229	1/1	0.89	0.09	-	38,38,38,38	0
56	MG	BA	3042	1/1	0.88	0.20	-	54,54,54,54	0
56	MG	AA	3115	1/1	0.86	0.14	-	61,61,61,61	0
56	MG	DA	3312	1/1	0.95	0.14	-	40,40,40,40	0
56	MG	CA	3150	1/1	0.93	0.08	-	80,80,80,80	0
56	MG	DA	3214	1/1	0.90	0.11	-	58,58,58,58	0
56	MG	CA	3178	1/1	0.93	0.09	-	54,54,54,54	0
56	MG	BA	3436	1/1	0.88	0.13	-	67,67,67,67	0
56	MG	DA	3291	1/1	0.87	0.14	-	41,41,41,41	0
56	MG	CA	3118	1/1	0.92	0.21	-	61,61,61,61	0
56	MG	BA	3751	1/1	0.77	0.14	-	51,51,51,51	0
56	MG	BB	3013	1/1	0.93	0.24	-	46,46,46,46	0
56	MG	DA	3052	1/1	0.90	0.09	-	44,44,44,44	0
56	MG	DA	3533	1/1	0.86	0.13	-	50,50,50,50	0
56	MG	CA	3180	1/1	0.92	0.12	-	61,61,61,61	0
56	MG	DA	3283	1/1	0.86	0.10	-	53,53,53,53	0
56	MG	DA	3476	1/1	0.89	0.09	-	62,62,62,62	0
56	MG	BA	3499	1/1	0.94	0.12	-	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	BA	3598	1/1	0.93	0.07	-	58,58,58,58	0
56	MG	DA	3222	1/1	0.96	0.10	-	46,46,46,46	0
56	MG	BA	3450	1/1	0.92	0.15	-	59,59,59,59	0
56	MG	BA	3137	1/1	0.89	0.21	-	41,41,41,41	0
56	MG	BA	3727	1/1	0.95	0.09	-	57,57,57,57	0
56	MG	BA	3391	1/1	0.93	0.13	-	36,36,36,36	0
56	MG	BA	3687	1/1	0.94	0.18	-	56,56,56,56	0
56	MG	BA	3067	1/1	0.91	0.44	-	35,35,35,35	0
56	MG	DA	3580	1/1	0.91	0.09	-	44,44,44,44	0
56	MG	BA	3125	1/1	0.97	0.37	-	34,34,34,34	0
56	MG	DA	3046	1/1	0.95	0.17	-	30,30,30,30	0
56	MG	CA	3145	1/1	0.70	0.14	-	62,62,62,62	0
56	MG	DA	3181	1/1	0.95	0.28	-	50,50,50,50	0
56	MG	DA	3224	1/1	0.77	0.22	-	27,27,27,27	0
56	MG	CA	3147	1/1	0.93	0.12	-	51,51,51,51	0
56	MG	B0	103	1/1	0.91	0.14	-	61,61,61,61	0
56	MG	CA	3087	1/1	0.93	0.17	-	65,65,65,65	0
56	MG	DA	3390	1/1	0.97	0.15	-	48,48,48,48	0
56	MG	AN	502	1/1	0.95	0.22	-	56,56,56,56	0
56	MG	BA	3360	1/1	0.87	0.21	-	41,41,41,41	0
56	MG	DA	3445	1/1	0.93	0.30	-	50,50,50,50	0
56	MG	DA	3069	1/1	0.91	0.13	-	49,49,49,49	0
56	MG	BA	3157	1/1	0.95	0.34	-	59,59,59,59	0
56	MG	BA	3228	1/1	0.95	0.32	-	51,51,51,51	0
56	MG	DA	3330	1/1	0.84	0.12	-	54,54,54,54	0
56	MG	BA	3102	1/1	0.92	0.35	-	47,47,47,47	0
56	MG	BA	3741	1/1	0.72	0.15	-	68,68,68,68	0
56	MG	BA	3676	1/1	0.95	0.14	-	55,55,55,55	0
56	MG	DA	3382	1/1	0.97	0.14	-	53,53,53,53	0
56	MG	AA	3157	1/1	0.94	0.16	-	46,46,46,46	0
56	MG	DA	3165	1/1	0.93	0.18	-	69,69,69,69	0
56	MG	DA	3152	1/1	0.93	0.27	-	53,53,53,53	0
56	MG	BZ	3001	1/1	0.85	0.17	-	52,52,52,52	0
56	MG	CA	3115	1/1	0.89	0.06	-	58,58,58,58	0
56	MG	B7	103	1/1	0.94	0.14	-	69,69,69,69	0
56	MG	BA	3401	1/1	0.93	0.59	-	67,67,67,67	0
56	MG	DA	3501	1/1	0.83	0.18	-	67,67,67,67	0
56	MG	DA	3592	1/1	0.96	0.10	-	57,57,57,57	0
56	MG	CA	3088	1/1	0.96	0.15	-	48,48,48,48	0
56	MG	DA	3599	1/1	0.95	0.10	-	72,72,72,72	0
56	MG	DA	3552	1/1	0.95	0.13	-	43,43,43,43	0
56	MG	AA	3030	1/1	0.90	0.20	-	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	3466	1/1	0.93	0.20	-	46,46,46,46	0
56	MG	BA	3265	1/1	0.94	0.25	-	55,55,55,55	0
56	MG	CA	3031	1/1	0.69	0.22	-	71,71,71,71	0
56	MG	BB	3008	1/1	0.89	0.11	-	71,71,71,71	0
56	MG	BA	3645	1/1	0.82	0.33	-	47,47,47,47	0
56	MG	CA	3155	1/1	0.91	0.18	-	61,61,61,61	0
56	MG	CW	3001	1/1	0.94	0.65	-	69,69,69,69	0
56	MG	AA	3047	1/1	0.93	0.25	-	68,68,68,68	0
56	MG	DA	3411	1/1	0.94	0.41	-	43,43,43,43	0
56	MG	BA	3175	1/1	0.89	0.18	-	44,44,44,44	0
56	MG	BA	3172	1/1	0.94	0.30	-	58,58,58,58	0
56	MG	BF	311	1/1	0.95	0.08	-	60,60,60,60	0
56	MG	BA	3139	1/1	0.88	0.16	-	52,52,52,52	0
56	MG	BA	3593	1/1	0.98	0.20	-	53,53,53,53	0
56	MG	BA	3031	1/1	0.79	0.21	-	49,49,49,49	0
56	MG	BA	3214	1/1	0.71	0.26	-	64,64,64,64	0
56	MG	BA	3249	1/1	0.92	0.20	-	33,33,33,33	0
56	MG	DA	3255	1/1	0.95	0.12	-	50,50,50,50	0
56	MG	BA	3070	1/1	0.90	0.25	-	48,48,48,48	0
56	MG	BA	3363	1/1	0.92	0.16	-	53,53,53,53	0
56	MG	BA	3150	1/1	0.95	0.18	-	47,47,47,47	0
56	MG	DA	3057	1/1	0.86	0.20	-	54,54,54,54	0
56	MG	BA	3192	1/1	0.92	0.32	-	56,56,56,56	0
56	MG	BA	3509	1/1	0.94	0.17	-	46,46,46,46	0
56	MG	DA	3279	1/1	0.89	0.09	-	51,51,51,51	0
56	MG	BA	3481	1/1	0.94	0.18	-	32,32,32,32	0
56	MG	BA	3651	1/1	0.91	0.13	-	38,38,38,38	0
56	MG	DA	3571	1/1	0.94	0.14	-	49,49,49,49	0
56	MG	AA	3136	1/1	0.85	0.12	-	59,59,59,59	0
56	MG	DA	3357	1/1	0.97	0.12	-	44,44,44,44	0
56	MG	BA	3243	1/1	0.87	0.18	-	57,57,57,57	0
56	MG	AA	3044	1/1	0.76	0.17	-	67,67,67,67	0
56	MG	DA	3534	1/1	0.97	0.18	-	59,59,59,59	0
56	MG	AA	3176	1/1	0.88	0.18	-	69,69,69,69	0
56	MG	DA	3031	1/1	0.94	0.21	-	51,51,51,51	0
56	MG	BA	3267	1/1	0.99	0.20	-	14,14,14,14	0
56	MG	BB	3004	1/1	0.93	0.13	-	64,64,64,64	0
56	MG	BA	3066	1/1	0.93	0.41	-	40,40,40,40	0
56	MG	BA	3135	1/1	0.83	0.14	-	51,51,51,51	0
56	MG	DA	3607	1/1	0.94	0.05	-	60,60,60,60	0
56	MG	DA	3272	1/1	0.96	0.18	-	43,43,43,43	0
56	MG	AA	3098	1/1	0.95	0.17	-	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	3761	1/1	0.70	0.17	-	65,65,65,65	0
56	MG	BA	3611	1/1	0.95	0.20	-	23,23,23,23	0
56	MG	BA	3655	1/1	0.97	0.15	-	29,29,29,29	0
56	MG	DA	3079	1/1	0.75	0.16	-	60,60,60,60	0
56	MG	DA	3223	1/1	0.92	0.14	-	63,63,63,63	0
56	MG	DA	3565	1/1	0.91	0.16	-	48,48,48,48	0
56	MG	DA	3029	1/1	0.80	0.16	-	52,52,52,52	0
56	MG	DA	3435	1/1	0.92	0.25	-	59,59,59,59	0
56	MG	BA	3405	1/1	0.94	0.15	-	47,47,47,47	0
56	MG	DA	3387	1/1	0.95	0.14	-	47,47,47,47	0
56	MG	BA	3020	1/1	0.97	0.45	-	32,32,32,32	0
56	MG	CA	3046	1/1	0.92	0.22	-	68,68,68,68	0
56	MG	AA	3089	1/1	0.91	0.17	-	54,54,54,54	0
56	MG	CA	3164	1/1	0.98	0.19	-	65,65,65,65	0
56	MG	BA	3185	1/1	0.92	0.30	-	38,38,38,38	0
56	MG	CA	3054	1/1	0.84	0.16	-	65,65,65,65	0
56	MG	DA	3154	1/1	0.96	0.12	-	43,43,43,43	0
56	MG	BA	3605	1/1	0.90	0.21	-	69,69,69,69	0
56	MG	AA	3133	1/1	0.97	0.12	-	35,35,35,35	0
56	MG	AA	3159	1/1	0.78	0.11	-	70,70,70,70	0
56	MG	DA	3047	1/1	0.93	0.16	-	46,46,46,46	0
56	MG	DA	3545	1/1	0.93	0.13	-	68,68,68,68	0
56	MG	DA	3569	1/1	0.91	0.11	-	75,75,75,75	0
56	MG	BA	3623	1/1	0.91	0.15	-	59,59,59,59	0
56	MG	AA	3007	1/1	0.92	0.23	-	49,49,49,49	0
56	MG	BA	3497	1/1	0.95	0.23	-	24,24,24,24	0
56	MG	AA	3057	1/1	0.95	0.19	-	58,58,58,58	0
56	MG	CA	3052	1/1	0.84	0.09	-	65,65,65,65	0
56	MG	BA	3248	1/1	0.89	0.13	-	27,27,27,27	0
56	MG	AA	3093	1/1	0.85	0.16	-	58,58,58,58	0
56	MG	BA	3454	1/1	0.88	0.15	-	43,43,43,43	0
56	MG	DA	3010	1/1	0.80	0.20	-	55,55,55,55	0
56	MG	DA	3456	1/1	0.95	0.11	-	50,50,50,50	0
56	MG	DA	3410	1/1	0.95	0.09	-	37,37,37,37	0
56	MG	BA	3318	1/1	0.95	0.08	-	36,36,36,36	0
56	MG	DA	3075	1/1	0.89	0.25	-	51,51,51,51	0
56	MG	AA	3122	1/1	0.89	0.13	-	74,74,74,74	0
56	MG	BA	3547	1/1	0.95	0.17	-	47,47,47,47	0
56	MG	DA	3259	1/1	0.97	0.12	-	50,50,50,50	0
56	MG	BA	3738	1/1	0.85	0.15	-	41,41,41,41	0
56	MG	BA	3356	1/1	0.88	0.21	-	24,24,24,24	0
56	MG	AA	3184	1/1	0.92	0.09	-	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3546	1/1	0.89	0.14	-	64,64,64,64	0
56	MG	DY	502	1/1	0.89	0.20	-	86,86,86,86	0
56	MG	BA	3380	1/1	0.97	0.18	-	59,59,59,59	0
56	MG	BA	3432	1/1	0.96	0.13	-	48,48,48,48	0
56	MG	BA	3227	1/1	0.78	0.19	-	38,38,38,38	0
56	MG	BA	3650	1/1	0.97	0.10	-	38,38,38,38	0
56	MG	DA	3303	1/1	0.95	0.12	-	44,44,44,44	0
56	MG	BA	3549	1/1	0.89	0.22	-	53,53,53,53	0
56	MG	BA	3297	1/1	0.92	0.16	-	45,45,45,45	0
56	MG	BA	3661	1/1	0.87	0.13	-	61,61,61,61	0
56	MG	DA	3530	1/1	0.92	0.21	-	69,69,69,69	0
56	MG	BA	3705	1/1	0.92	0.16	-	52,52,52,52	0
56	MG	CA	3057	1/1	0.89	0.20	-	73,73,73,73	0
56	MG	BA	3694	1/1	0.85	0.22	-	57,57,57,57	0
56	MG	BA	3555	1/1	0.81	0.19	-	49,49,49,49	0
56	MG	AA	3086	1/1	0.88	0.18	-	53,53,53,53	0
56	MG	BA	3507	1/1	0.94	0.15	-	53,53,53,53	0
56	MG	DA	3141	1/1	0.95	0.32	-	56,56,56,56	0
56	MG	BA	3124	1/1	0.93	0.26	-	33,33,33,33	0
56	MG	BA	3679	1/1	0.94	0.16	-	47,47,47,47	0
56	MG	BA	3134	1/1	0.64	0.18	-	57,57,57,57	0
56	MG	DA	3375	1/1	0.98	0.17	-	42,42,42,42	0
56	MG	BA	3210	1/1	0.96	0.42	-	34,34,34,34	0
56	MG	CA	3133	1/1	0.93	0.22	-	67,67,67,67	0
56	MG	DA	3548	1/1	0.93	0.13	-	67,67,67,67	0
56	MG	BA	3011	1/1	0.89	0.32	-	51,51,51,51	0
56	MG	DA	3090	1/1	0.97	0.21	-	67,67,67,67	0
56	MG	BA	3425	1/1	0.94	0.13	-	31,31,31,31	0
56	MG	BA	3740	1/1	0.89	0.12	-	49,49,49,49	0
56	MG	BA	3525	1/1	0.98	0.20	-	40,40,40,40	0
56	MG	DA	3094	1/1	0.84	0.11	-	55,55,55,55	0
56	MG	BA	3504	1/1	0.91	0.23	-	57,57,57,57	0
56	MG	DA	3479	1/1	0.93	0.12	-	52,52,52,52	0
56	MG	AA	3039	1/1	0.93	0.19	-	57,57,57,57	0
56	MG	CA	3093	1/1	0.92	0.09	-	57,57,57,57	0
56	MG	DB	3010	1/1	0.92	0.24	-	72,72,72,72	0
56	MG	AY	3001	1/1	0.39	0.25	-	92,92,92,92	0
56	MG	BA	3069	1/1	0.78	0.19	-	46,46,46,46	0
56	MG	BA	3057	1/1	0.95	0.57	-	48,48,48,48	0
56	MG	AA	3019	1/1	0.91	0.18	-	53,53,53,53	0
56	MG	CA	3144	1/1	0.97	0.12	-	54,54,54,54	0
56	MG	AA	3153	1/1	0.91	0.19	-	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	3742	1/1	0.90	0.35	-	44,44,44,44	0
56	MG	BA	3666	1/1	0.99	0.18	-	11,11,11,11	0
56	MG	BA	3285	1/1	0.94	0.20	-	55,55,55,55	0
56	MG	CA	3059	1/1	0.89	0.39	-	70,70,70,70	0
56	MG	BA	3085	1/1	0.96	0.19	-	50,50,50,50	0
56	MG	DA	3468	1/1	0.95	0.06	-	54,54,54,54	0
56	MG	AX	3009	1/1	0.79	0.19	-	72,72,72,72	0
56	MG	DV	3003	1/1	0.88	0.18	-	62,62,62,62	0
56	MG	DA	3451	1/1	0.94	0.23	-	56,56,56,56	0
56	MG	BA	3677	1/1	0.92	0.20	-	63,63,63,63	0
56	MG	BY	502	1/1	0.92	0.15	-	60,60,60,60	0
56	MG	BA	3483	1/1	0.92	0.19	-	50,50,50,50	0
56	MG	AA	3169	1/1	0.94	0.11	-	57,57,57,57	0
56	MG	DA	3130	1/1	0.92	0.23	-	52,52,52,52	0
56	MG	DA	3585	1/1	0.90	0.13	-	55,55,55,55	0
56	MG	B7	104	1/1	0.87	0.20	-	55,55,55,55	0
56	MG	BB	3010	1/1	0.98	0.19	-	51,51,51,51	0
56	MG	BA	3490	1/1	0.91	0.07	-	66,66,66,66	0
56	MG	DA	3068	1/1	0.92	0.34	-	52,52,52,52	0
56	MG	BA	3058	1/1	0.96	0.14	-	23,23,23,23	0
56	MG	DA	3298	1/1	0.89	0.10	-	57,57,57,57	0
56	MG	AA	3200	1/1	0.96	0.14	-	61,61,61,61	0
56	MG	DA	3603	1/1	0.89	0.21	-	45,45,45,45	0
56	MG	AX	3012	1/1	0.97	0.22	-	66,66,66,66	0
56	MG	BA	3350	1/1	0.94	0.11	-	43,43,43,43	0
56	MG	DA	3074	1/1	0.85	0.36	-	49,49,49,49	0
56	MG	BA	3286	1/1	0.95	0.08	-	48,48,48,48	0
56	MG	BA	3587	1/1	0.93	0.36	-	58,58,58,58	0
56	MG	DA	3288	1/1	0.96	0.15	-	43,43,43,43	0
56	MG	BB	3017	1/1	0.94	0.14	-	48,48,48,48	0
56	MG	AA	3182	1/1	0.94	0.20	-	76,76,76,76	0
56	MG	CA	3001	1/1	0.74	0.14	-	59,59,59,59	0
56	MG	BA	3691	1/1	0.94	0.09	-	60,60,60,60	0
56	MG	CA	3062	1/1	0.91	0.22	-	65,65,65,65	0
56	MG	DA	3285	1/1	0.94	0.12	-	43,43,43,43	0
56	MG	BA	3529	1/1	0.98	0.17	-	57,57,57,57	0
56	MG	CA	3026	1/1	0.87	0.19	-	61,61,61,61	0
56	MG	AA	3063	1/1	0.90	0.23	-	56,56,56,56	0
56	MG	CA	3075	1/1	0.83	0.20	-	53,53,53,53	0
56	MG	BA	3698	1/1	0.94	0.10	-	59,59,59,59	0
56	MG	DA	3587	1/1	0.93	0.16	-	45,45,45,45	0
56	MG	BA	3146	1/1	0.92	0.17	-	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3340	1/1	0.65	0.18	-	60,60,60,60	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.